

A Theoretical Analysis of Interactions Energies and Intermolecular Interactions between Amphotericin B and Potential Bioconjugates Used in the Modification of Nanocarriers for Drug Delivery

Jennifer Cuellar ^{1,†} Lorena Parada-Díaz ^{1,†} Jorge Garza ² and Sol M. Mejía ^{1,*}

¹ Línea de Investigación en Química Computacional, Grupo de Investigación GIFUJ, Departamento de Química, Facultad de Ciencias, Pontificia Universidad Javeriana, Bogotá 110231, Colombia

² Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa. San Rafael Atlixco 186. Col.

Vicentina, Iztapalapa, Ciudad de Mexico 09340, México

* Corresponding author email: sol.mejia@javeriana.edu.co

† These authors contributed equally to this work.

Electronic Supporting Information

Table S1. Thermodynamic parameters of the AmB-bioconjugates dimers. CAM-B3LYP-D3/6-31+G(d,p)

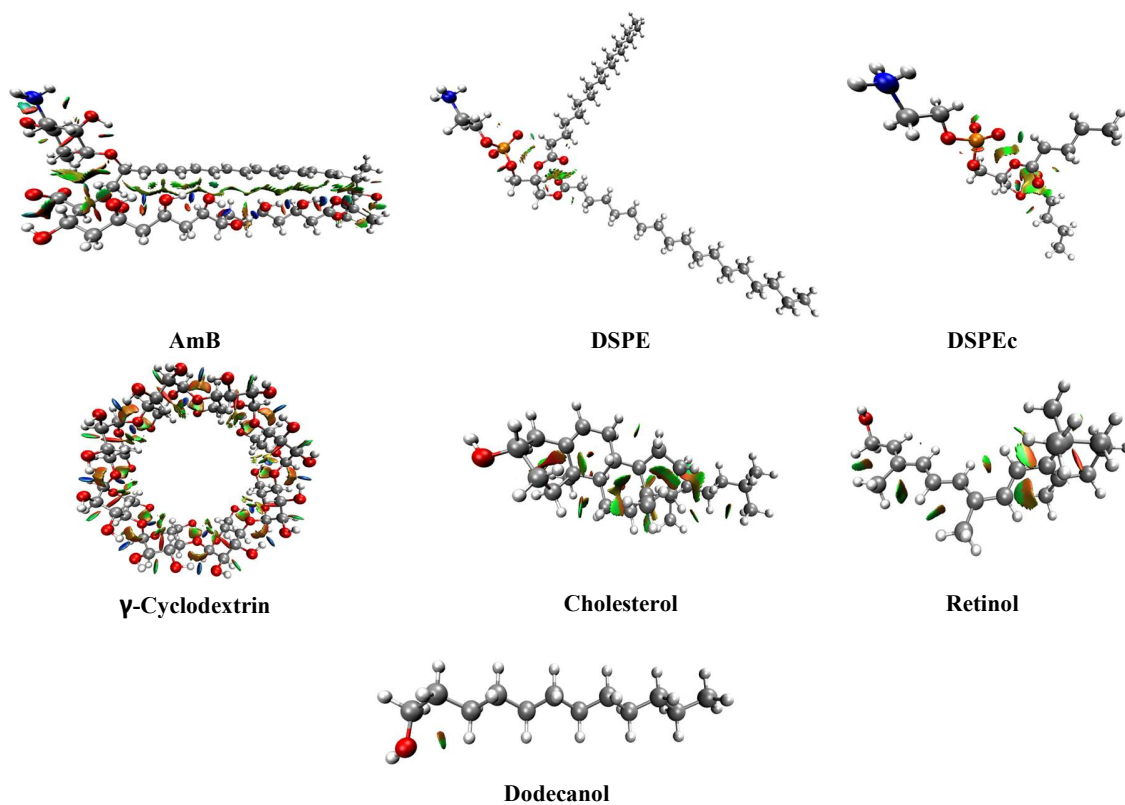
| Dimers | %X | $\Delta E^{a,b}$ | ΔH^b | ΔG^b | ΔS^c |
|------------------|--------|------------------|--------------|--------------|--------------|
| AmB-Cyc | | | | | |
| AmB-Cyc1 | 100.0 | -83.05 | -83.80 | -62.57 | -71.20 |
| AmB-Cyc2 | 0.0 | -75.15 | -75.71 | -54.95 | -69.64 |
| AmB-Cyc3 | 0.0 | -49.51 | -49.61 | -31.17 | -61.85 |
| AmB-Cyc4 | 0.0 | -27.79 | -27.63 | -13.75 | -46.55 |
| AmB-Cyc5 | 0.0 | -27.77 | -27.35 | -12.37 | -50.25 |
| AmB-Cyc6 | 0.0 | -25.66 | -25.87 | -12.24 | -50.33 |
| AmB-Cyc7 | 0.0 | -22.18 | -22.65 | -9.47 | -37.18 |
| AmB-DSPE | | | | | |
| AmB-DSPE1 | 100.00 | -81.72 | -84.30 | -47.02 | -125.04 |
| AmB-DSPE2 | 0.00 | -65.47 | -66.84 | -39.93 | -90.24 |
| AmB-DSPE3 | 0.00 | -65.45 | -66.90 | -37.35 | -99.10 |
| AmB-DSPE4 | 0.00 | -65.16 | -66.47 | -40.94 | -85.61 |
| AmB-DSPE5 | 0.00 | -55.15 | -55.96 | -33.60 | -75.00 |
| AmB-DSPE6 | 0.00 | -48.18 | -49.34 | -24.00 | -85.02 |
| AmB-DSPE7 | 0.00 | -29.15 | -29.07 | -15.63 | -45.06 |
| AmB-DSPE8 | 0.00 | -27.00 | -27.01 | -7.17 | -66.57 |
| AmB-DSPE9 | 0.00 | -16.61 | -18.87 | -3.52 | -75.09 |
| AmB-DSPE10 | 0.00 | -11.32 | -13.80 | -8.24 | -73.94 |
| AmB-DSPEc | | | | | |

| | | | | | |
|------------|-------|--------|--------|--------|--------|
| AmB-DSPE1c | 98.70 | -54.55 | -55.67 | -32.20 | -78.71 |
| AmB-DSPE2c | 1.23 | -51.95 | -52.85 | -30.17 | -76.06 |
| AmB-DSPE3c | 0.07 | -50.23 | -50.92 | -29.98 | -70.23 |
| AmB-DSPE4c | 0.00 | -47.70 | -48.40 | -27.99 | -68.44 |
| AmB-DSPE5c | 0.00 | -44.19 | -45.40 | -21.56 | -79.94 |
| AmB-DSPE6c | 0.00 | -43.59 | -44.53 | -23.77 | -69.61 |
| AmB-DSPE7c | 0.00 | -43.59 | -44.53 | -23.77 | -69.61 |
| AmB-Cho | | | | | |
| AmB-Chol1 | 99.91 | -39.27 | -39.37 | -20.76 | -62.43 |
| AmB-Chol2 | 0.08 | -35.08 | -34.95 | -17.59 | -58.23 |
| AmB-Chol3 | 0.00 | -32.05 | -31.64 | -15.62 | -53.73 |
| AmB-Chol4 | 0.00 | -31.28 | -30.75 | -16.25 | -48.65 |
| AmB-Chol5 | 0.00 | -28.40 | -29.23 | -8.78 | -68.61 |
| AmB-Chol6 | 0.00 | -26.91 | -27.55 | -8.58 | -63.62 |
| AmB-Chol7 | 0.00 | -22.86 | -22.44 | -7.88 | -48.83 |
| AmB-Chol8 | 0.00 | -20.76 | -21.21 | -3.59 | -59.09 |
| AmB-Chol9 | 0.00 | -19.51 | -18.85 | -6.90 | -40.08 |
| AmB-Chol10 | 0.00 | -15.79 | -16.81 | 2.58 | -65.04 |
| AmB-Chol11 | 0.00 | -11.27 | -10.65 | -0.30 | -34.71 |
| AmB-Chol12 | 0.00 | -6.77 | -9.44 | -2.56 | -37.83 |
| AmB-Chol13 | 0.00 | -4.44 | -7.95 | -1.30 | -32.37 |
| AmB-Chol14 | 0.00 | -4.00 | -6.84 | -0.92 | -30.40 |
| AmB-Chol15 | 0.00 | -2.99 | -3.94 | -0.45 | -28.90 |
| AmB-Chol16 | 0.00 | -1.93 | -2.07 | -0.98 | -26.76 |
| AmB-Ret | | | | | |
| AmB-Ret1 | 97.35 | -33.51 | -33.41 | -15.88 | -58.78 |
| AmB-Ret2 | 2.60 | -31.36 | -31.14 | -14.90 | -54.45 |
| AmB-Ret3 | 0.04 | -28.88 | -28.64 | -13.73 | -50.03 |
| AmB-Ret4 | 0.01 | -28.18 | -28.13 | -11.54 | -55.64 |
| AmB-Ret5 | 0.00 | -27.46 | -27.27 | -11.26 | -53.69 |
| AmB-Ret6 | 0.00 | -27.17 | -26.99 | -11.12 | -53.23 |
| AmB-Ret7 | 0.00 | -26.04 | -25.90 | -10.01 | -53.31 |
| AmB-Ret8 | 0.00 | -22.44 | -22.18 | -6.72 | -51.85 |
| AmB-Ret9 | 0.00 | -20.60 | -20.16 | -7.76 | -41.60 |
| AmB-Ret10 | 0.00 | -20.19 | -19.94 | -5.99 | -46.79 |
| AmB-Ret11 | 0.00 | -19.76 | -19.38 | -5.65 | -46.08 |
| AmB-Ret12 | 0.00 | -18.18 | -17.60 | -5.11 | -41.89 |
| AmB-Ret13 | 0.00 | -17.60 | -75.63 | -3.01 | -48.11 |
| AmB-Ret14 | 0.00 | -15.22 | -1453 | -1.89 | -42.41 |
| AmB-Dod | | | | | |
| AmB-Dod1 | 67.35 | -26.71 | -26.78 | -11.01 | -52.90 |

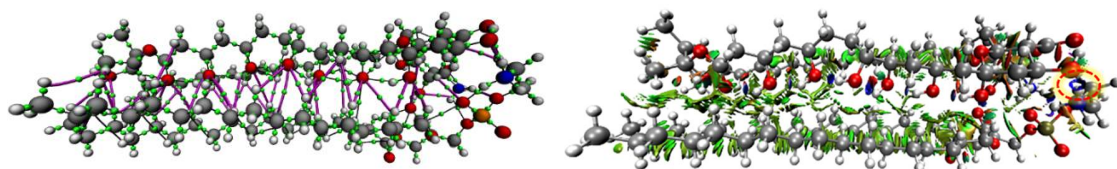
| | | | | | |
|------------------|-------|--------|--------|-------|--------|
| AmB-Dod2 | 13.86 | -25.77 | -25.99 | -8.65 | -58.17 |
| AmB-Dod3 | 10.88 | -25.63 | -25.56 | -9.43 | -54.10 |
| AmB-Dod4 | 4.90 | -25.15 | -25.27 | -9.10 | -54.22 |
| AmB-Dod5 | 3.00 | -24.86 | -24.87 | -8.39 | -55.29 |
| AmB-Dod6 | 0.02 | -21.76 | -22.85 | -3.51 | -64.88 |
| AmB-Dod7 | 0.00 | -19.92 | -19.96 | -3.87 | -53.96 |
| AmB-Dod8 | 0.00 | -18.36 | -18.20 | -3.39 | -49.68 |
| AmB-Dod9 | 0.00 | -17.88 | -19.63 | 3.89 | -78.91 |
| AmB-Dod10 | 0.00 | -17.26 | -17.40 | -1.82 | -52.26 |
| AmB-Dod11 | 0.00 | -15.80 | -15.53 | -1.71 | -46.38 |
| AmB-Dod12 | 0.00 | -12.32 | -13.68 | 6.63 | -68.14 |
| AmB-Dod13 | 0.00 | -9.62 | -10.70 | 9.19 | -66.73 |
| AmB-Dod14 | 0.00 | -7.14 | -10.32 | -7.99 | -22.36 |
| AmB-Dod15 | 0.00 | -4.55 | -6.31 | -3.30 | -13.76 |
| AmB-Dod16 | 0.00 | -4.14 | -5.96 | -1.01 | -13.96 |

^aDimerization energy including ZPE and Counterpoise correction, ^{a,b} in kcal/mol. ^c in cal/molK

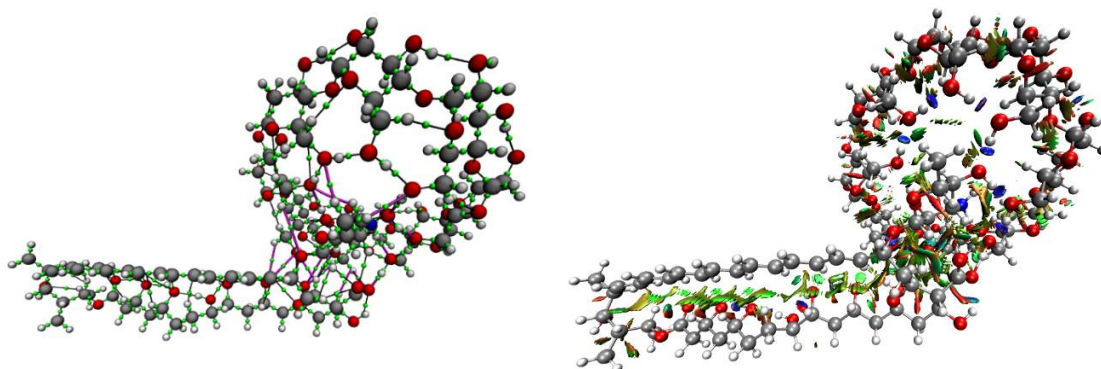
Monomers



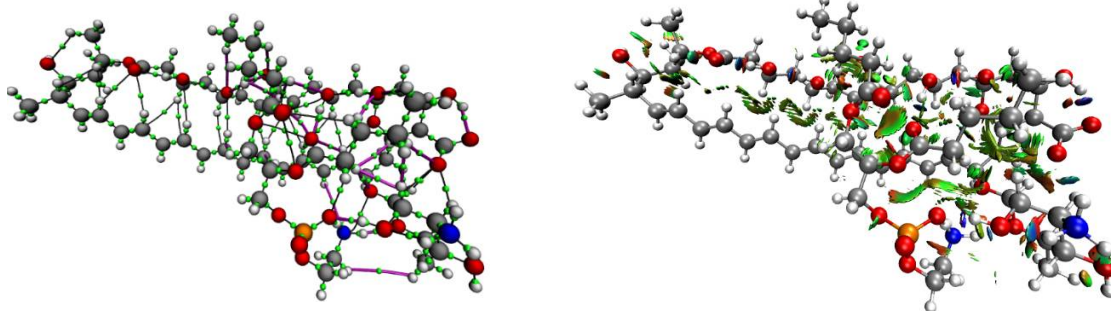
Dimers



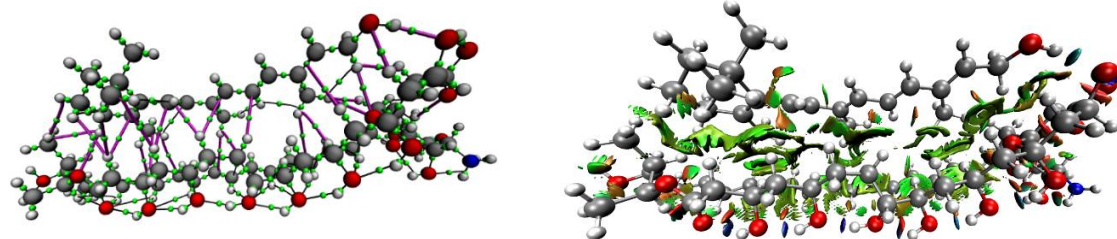
AmB-DSPE



AmB-Cyc



AmB-DSPEc



AmB-Ret

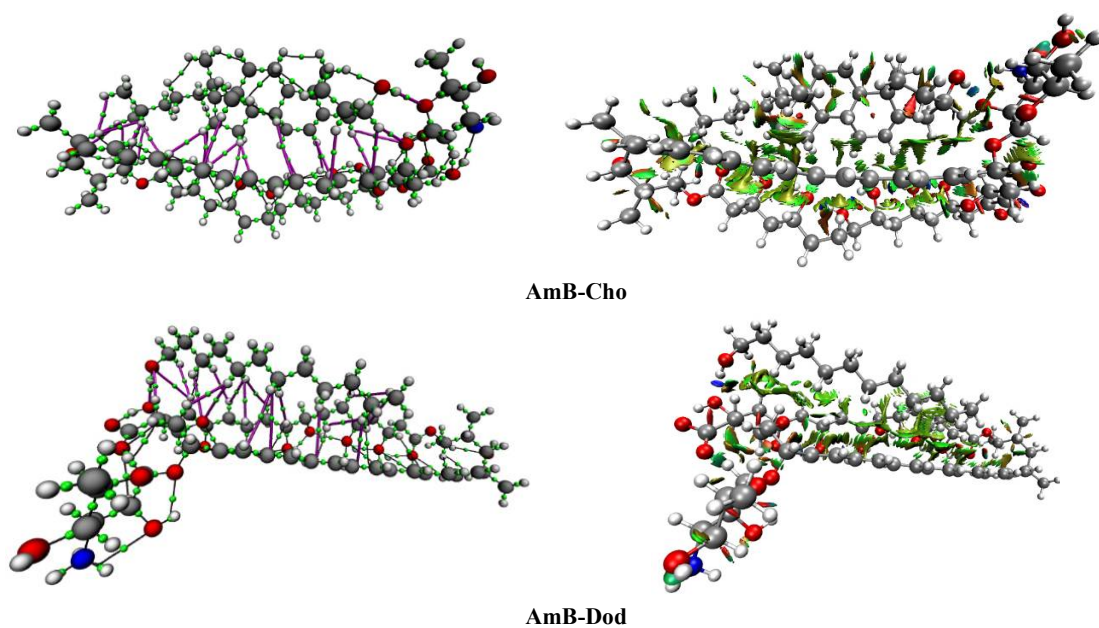


Figure S1. Plots revealing noncovalent interactions at the monomers and the most stable dimer of each type including the pH effect. Monomer: 3D-NCI plots. Dimers: molecular graphs (left) where purple lines: bond path associated with intermolecular interactions. Black lines: bond paths associated with intramolecular interactions. 3D-NCI plots (right)

Table S2. Length and topological parameters (ranges) evaluated at bond critical points (CP) for intermolecular interactions for the most stable dimer of each type including the pH effect. CAM-B3LYP-D3/6-31+G(d,p)

| Interaction type | Length ^a [Å] | $\rho(r_{CP})^b$ 10^{-2} | $\nabla^2\rho(r_{CP})^c$ 10^{-2} | $H(r_{CP})^e$ 10^{-4} | $IV(r_{CP})/G(r_{CP})^f$ | IE^g 10^{-2} [kcal/mol] |
|------------------|----------------------------|-------------------------------|---------------------------------------|----------------------------|--------------------------|-----------------------------------|
| AmB-DSPE | | | | | | |
| O-H...O | 1.58 - 1.81 | 3.28 - 6.47 | 10.40 - 16.30 | -87.00 - 3.00 | 0.99 - 1.18 | -1.26 - -2.91 |
| C-H...O | 2.21 - 3.32 | 0.14 - 1.65 | 0.65 - 5.32 | 3.00 - 17.00 | 0.55 - 0.98 | -0.01 - -0.63 |
| H...H | 2.14 - 2.97 | 0.16 - 0.86 | 0.49 - 2.96 | 3.00 - 15.00 | 0.63 - 0.78 | -0.03 - -0.24 |
| C-H...C | 2.95 - 3.10 | 0.38 - 0.52 | 1.34 - 1.82 | 8.00 - 10.00 | 0.70 - 0.71 | -0.09 - -0.13 |
| N-H...O | 1.69 - 2.24 | 1.73 - 5.11 | 7.15 - 12.90 | -38.00 - 17.00 | 0.89 - 1.11 | -0.72 - -2.00 |
| AmB-Cyc | | | | | | |
| O-H...O | 1.34 - 2.55 | 0.72 - 11.70 | 1.47 - 12.40 | -743.00 - 12.00 | 0.82 - 1.95 | -0.65 - -7.61 |
| C-H...O | 2.09 - 3.18 | 0.21 - 2.08 | 0.89 - 6.20 | -5.00 - 12.00 | 0.62 - 1.03 | -0.05 - -0.82 |
| H...H | 2.06 | 1.01 | 3.66 | 16.00 | 0.79 | -0.30 |
| N-H...O | 1.72 - 2.30 | 1.44 - 4.70 | 5.38 - 12.20 | -28.00 - 10.00 | 0.92 - 1.08 | -0.57 - -1.81 |
| C-H...N | 3.39 | 0.19 | 0.69 | 5.00 | 0.63 | -0.04 |
| AmB-DSPEc | | | | | | |
| O-H...O | 1.64 - 1.82 | 3.13 - 5.12 | 10.40 - 15.00 | -24.00 - 11.00 | 0.96 - 1.06 | -1.21 - -2.11 |
| C-H...O | 2.35 - 2.96 | 0.47 - 1.31 | 2.04 - 4.77 | 2.00 - 12.00 | 0.69 - 0.97 | -0.14 - -0.48 |

| | | | | | | |
|----------------|-------------|-------------|--------------|--------------|-------------|---------------|
| H---H | 2.03 - 3.31 | 0.08 - 1.04 | 0.27 - 3.48 | 2.00 - 18.00 | 0.64 - 0.82 | -0.06- -0.24 |
| C-H---C | 2.62 - 3.63 | 0.13 - 0.78 | 0.420 - 2.67 | 3.00 - 13.00 | 0.68 - 0.76 | -0.03- -0.21 |
| O---O | 3.10 | 0.66 | 2.74 | 9.00 | 0.86 | -0.26 |
| N-H---O | 1.88 | 3.01 | 8.66 | 8.00 | 1.03 | -1.17 |
| N---O | 2.77 | 1.47 | 6.04 | 18.00 | 0.86 | -0.57 |
| AmB-Ret | | | | | | |
| O-H---O | 1.98 | 2.55 | 6.21 | -18.00 | 1.10 | -0.95 |
| C-H---O | 2.24 - 2.62 | 0.78 - 1.68 | 2.62 - 5.19 | -1.00 - 7.00 | 0.88 - 1.01 | -0.25- -0.62 |
| H---H | 2.09 - 2.68 | 0.31 - 1.08 | 1.10 - 3.81 | 7.00 - 17.00 | 0.66 - 0.78 | -0.07- -0.31 |
| C-H---C | 2.67 - 3.37 | 0.24 - 0.80 | 0.75 - 2.57 | 4.00 - 14.00 | 0.69 - 0.79 | -0.05- -0.18 |
| AmB-Col | | | | | | |
| O-H---O | 1.96 | 2.52 | 7.11 | -10.00 | 1.05 | -0.98 |
| C-H---O | 2.56 - 3.16 | 0.24 - 0.94 | 1.00 - 3.19 | 7.00 - 13.00 | 0.63 - 0.89 | -0.05 - -0.33 |
| H---H | 2.04 - 2.61 | 0.41 - 0.94 | 1.38 - 3.53 | 8.00 - 16.00 | 0.67 - 0.79 | -0.09- -0.29 |
| C-H---C | 2.73 - 3.51 | 0.18 - 0.80 | 0.56 - 2.56 | 3.00 - 14.00 | 0.69 - 0.78 | -0.03- -0.20 |
| AmB-Dod | | | | | | |
| O-H---O | 1.75 | 4.23 | 11.43 | 18.00 | 1.06 | -1.61 |
| C-H---O | 2.31 - 3.03 | 0.34 - 1.39 | 1.40 - 4.46 | 4.00 - 11.00 | 0.69 - 0.96 | -0.09- -0.51 |
| H---H | 2.16 - 2.79 | 0.30 - 0.80 | 1.03 - 2.98 | 6.00 - 16.00 | 0.68 - 0.78 | -0.06- -0.21 |
| C-H---C | 2.73 - 3.47 | 0.24 - 0.81 | 0.77 - 2.55 | 4.00 - 14.00 | 0.70 - 0.78 | -0.05- -0.21 |

^a Euclidian distance between the attractors, ^b Electron density, ^c Electron density laplacian, ^d Bond ellipticity, ^e Total energy density, ^f Virial Field/ Kinetic energy density ^g Interaction energy.

Table S3. NBO Donor - acceptor second-order interaction energies $E_{i \rightarrow j}^{(2)}$ in kcal/mol for each interaction type of AmB-bioconjugate dimers including the pH effect. CAM-B3LYP-D3/6-31+G(d,p)

| Amb-Dod | | | | AmB-Ret | | | AmB-Cho | | | AmB_DSPEc | | | AmB-Cyc | | | AmB_DSPE | | | | | | | |
|--------------|------------------------|--|-----------------------------|--|--|-----------------------------|------------------------|---|---|---|---|-----------------------------|--|---|---|---|--|-----------------------------|--|--|--|--|--|
| Type | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | Donor | Acceptor | $E_{i \rightarrow j}^{(2)}$ | | | | | |
| C-H- --O | LP (O ₃₈) | H ₁₃₁ - C ₁₃₀) | 2.27 | LP (O ₅₀) | BD*(H ₁₃ 9- C ₁₃₇) | | LP (O ₂₈) | BD*(H ₇₈ -C ₇₇) | 2.40 | LP (O ₁₁₈) | BD*(H ₁₄₈ - C ₁₄₆) | 2.22 | LP (O ₇₄) | BD* (H ₁₇₈ -C ₁₇₇) | 4.85 | LP (O ₁₁₄) | BD*(H ₂₀₃ -C ₂₀₁) | 2.30 | | | | | |
| | | | | LP (O ₁₆₇) | BD* (H ₄₆ - C ₄₃) | 2.06 | | | | LP(O ₁₁₄) | BD*(H ₁₇₂ - C ₁₇₀) | 1.65 | BD* (O ₅₃ - H ₆₃) | BD* (C ₂₅₉ - C ₂₆₃) | 2.32 | LP (O ₁₁₇) | BD*(H ₂₆₃ -C ₂₆₂) | 1.99 | | | | | |
| | | | | LP (O ₁₆₇) | BD* (H ₄₉ - C ₄₇) | 1.73 | | | | LP (O ₁₁₄) | BD*(H ₁₆₆ - C ₁₆₄) | 1.47 | LP (O ₁₃₇) | BD* (H ₁₈₀ - C ₁₇₉) | 2.29 | LP (O ₁₂₂) | BD*(H ₂₂₀ -C ₂₁₉) | 1.85 | | | | | |
| | | | | LP (O ₁₂₂) | BD*(H ₁₄₂ - C ₁₄₀) | 1.17 | | | | LP (O ₁₂₂) | BD*(H ₁₄₂ - C ₁₄₀) | 1.17 | LP (O ₁₁) | BD* (H ₁₈₁ -C ₁₇₉) | 1.39 | LP (O ₁₀₈) | BD*(H ₁₉₅ -C ₁₉₄) | 1.79 | | | | | |
| | | | | | | | | | | | | | | | LP (O ₁₂₈) | BD*(H ₁₅₄ -C ₁₅₂) | 1.39 | | | | | | |
| | | | | | | | | | | | | | | | BD (C ₉₅ - O ₁₁₇) | BD*(H ₂₆₃ - C ₂₆₂) | 1.23 | | | | | | |
| | | | | | | | | | | | | | | | LP (O ₁₂₀) | BD*(H ₁₇₁ -C ₁₇₀) | 1.22 | | | | | | |
| | | | | | | | | | | | | | | | LP (O ₁₂₆) | BD*(H ₁₆₀ -C ₁₅₈) | 1.13 | | | | | | |
| | | | | | | | | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | | | | | | | |
| O-H- ---O | LP (O ₁₇₂) | BD*(H ₃₉ - O ₃₈) O- H—O | 27.18 | LP (O ₁₈₄) | BD* (H ₅₁ - O ₅₀) | 13.20 | LP (O ₁₈₂) | BD* (H ₇₄ - O ₂₈) | 11.30 | LP (O ₁₇₈) | BD* (H ₁₀₉ - O ₁₀₈) | 28.08 | LP (O ₂₇₈) | BD* (H ₂₁ - O ₁₁) | 25.70 | LP (O ₁₉₉) | BD*(H ₁₀₉ -O ₁₀₈) | 5.09 | | | | | |
| | | | | | | | | | | LP (O ₁₇₄) | BD* (H ₁₁₉ - O ₁₁₈) | 14.26 | LP (O ₃₂) | BD* (H ₂₇₉ - O ₂₇₈) | 23.38 | | | | | | | | |
| | | | | | | | | | | | | | LP (O ₁₁₆) | BD* (H ₂₇₇ - O ₂₇₆) | 22.93 | | | | | | | | |
| | | | | | | | | | | | | | LP (O ₂₈₆) | BD* (H ₆₃ -O ₅₃) | 15.15 | | | | | | | | |
| | | | | | | | | | | | | | LP (O ₂₈₁) | BD* (H ₁₀₅ - O ₉₅) | 12.46 | | | | | | | | |
| | | | | | | | | | | | | | BD (C ₂₆₃ - O ₂₈₆) | BD* (H ₆₃ - O ₅₃) | 4.98 | | | | | | | | |
| | | | | | | | | | | | | | LP (O ₉₅) | BD* (H ₂₈₃ -O ₂₈₂) | 3.92 | | | | | | | | |
| | | | | | | | | | | | | | BD* (O ₅₃ - H ₆₃) | BD* (C ₂₆₃ - O ₂₈₆) | 2.95 | | | | | | | | |
| C-H- --C | | | | BD (C ₈₀ - C ₈₂) | BD* (H ₃₃ - C ₃₂) | 1.34 | | | | BD (C ₁₆₇ - H ₁₆₉) | BD* (H ₁₀ - C ₉) | 1.45 | | | | | | | | | | | |
| N-H- -O | | | | | | | | | LP (O ₁₁₂) | BD*(H ₁₈₆ - N ₁₈₅) | 10.33 | LP (O ₃₂) | BD* (H ₃₀₄ -N ₃₀₃) | 1.09 | LP (O ₁₃₂) | BD*(H ₂₆₇ -N ₂₆₅) | 31.37 | | | | | | |
| | | | | | | | | | BD* (N ₁₈₅ - H ₁₉₂) | BD* (H ₁₀₉ - O ₁₀₈) | 1.66 | | | | LP (O ₂₅₆) | BD*(H ₁₃₅ -N ₁₃₄) | 30.55 | | | | | | |
| | | | | | | | | | | | | LP (O ₃₂) | BD* (H ₃₀₄ -N ₃₀₃) | 2.40 | BD (O ₁₃₂ - H ₁₃₃) | BD*(H ₂₆₇ -N ₂₆₅) | 3.43 | | | | | | |
| | | | | | | | | | | | | | | | LP (O ₂₅₅) | BD*(H ₂₇₁ -N ₁₃₄) | 1.21 | | | | | | |
| | | | | | | | | | | | | | LP (O ₅₃) | BD* (H ₃₀₆ - N ₃₀₃) | 25.10 | | | | | | | | |

Molecular structures with CAM-B3LYP/ 6-31G(d,p)

AmB-Cyc

AmB-Cyc1

0 1

| | | | |
|---|--------------|------------|-------------|
| C | -9.52017500 | 5.02018900 | -1.94736600 |
| C | -10.84501200 | 4.60196400 | -1.32282600 |
| C | -10.79224900 | 3.17137300 | -0.82275400 |
| C | -10.25495800 | 2.24911100 | -1.90911800 |
| C | -8.90360900 | 2.77187400 | -2.38776900 |
| C | -8.23503300 | 1.95601200 | -3.47468500 |
| O | -8.56396000 | 5.13078300 | -0.93767500 |
| O | -11.15466600 | 5.49821400 | -0.27231300 |
| O | -12.09986500 | 2.84825100 | -0.42410500 |
| O | -9.12149200 | 4.08532300 | -2.91645900 |
| O | -6.85982000 | 2.27808900 | -3.58097600 |
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| H | -10.08969700 | 3.12534200 | 0.02374800 |
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| H | -8.37016500 | 0.89088800 | -3.25986600 |
| H | -8.72123700 | 2.17575800 | -4.43089600 |
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| H | -12.14586400 | 1.89907500 | -0.20021400 |

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| H | -6.34285600 | 1.59498100 | -3.09557300 |
| C | -10.83479800 | -0.09911800 | -1.94013800 |
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| C | -10.73481100 | -1.51720400 | 0.11318400 |
| C | -9.78110000 | -2.41406100 | -0.65185300 |
| C | -9.00233800 | -1.61505200 | -1.69525000 |
| C | -8.07436300 | -2.47058700 | -2.55945600 |
| O | -10.14035500 | 0.95461800 | -1.33818800 |
| O | -12.51043600 | 0.08406000 | -0.22246300 |
| O | -11.56451400 | -2.23537600 | 0.99209000 |
| O | -9.95357400 | -0.99526400 | -2.57207100 |
| O | -6.71985200 | -2.17982100 | -2.25908000 |
| H | -10.37143400 | -3.17511200 | -1.17958300 |
| H | -11.49298500 | 0.27406100 | -2.73081400 |
| H | -12.24188600 | -1.60160500 | -1.38578200 |
| H | -10.14739000 | -0.75334500 | 0.64384500 |
| H | -8.39664500 | -0.84593700 | -1.20208800 |
| H | -8.26510500 | -3.53505800 | -2.39360900 |
| H | -8.28810000 | -2.23852200 | -3.60844400 |
| H | -12.82459400 | -0.37078600 | 0.57261400 |
| H | -11.01550300 | -2.78991400 | 1.57872000 |
| H | -6.20768900 | -2.99882500 | -2.10010800 |
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| C | -9.04308300 | -4.89409700 | 1.79056200 |
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| C | -6.58930900 | -5.18156400 | 1.80881000 |

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| O | -8.92262500 | -3.03289500 | 0.28924900 |
| O | -10.16328800 | -4.27099200 | 2.38969500 |
| O | -7.92992300 | -5.17814100 | 3.84035500 |
| O | -7.77424000 | -4.95793200 | -0.26248400 |
| O | -4.96328500 | -4.04807800 | -1.34345900 |
| H | -6.69700700 | -6.27199800 | 1.73713300 |
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| H | -9.18277600 | -5.98394900 | 1.77270400 |
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| H | -6.51083400 | -3.49619500 | 0.49138400 |
| H | -4.56211700 | -5.36120900 | 0.20807200 |
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| H | -10.08095400 | -4.42493300 | 3.34161000 |
| H | -7.08752100 | -5.09892100 | 4.32882600 |
| H | -4.68431300 | -3.23689000 | -0.80278700 |
| C | -4.59581900 | -5.88888300 | 2.96593500 |
| C | -4.20435300 | -5.61190700 | 4.41056500 |
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| O | -5.42246200 | -4.84282000 | 2.52713500 |
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| O | -2.88019900 | -4.30916500 | 5.83820400 |

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| O | -3.45714300 | -6.01679300 | 2.15901900 |
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| H | -5.12399400 | -6.84514400 | 2.89492300 |
| H | -3.64685100 | -6.48441800 | 4.77676100 |
| H | -3.85039100 | -3.51552100 | 4.18137700 |
| H | -3.22272900 | -3.98127900 | 1.78590200 |
| H | -0.59425100 | -5.37249400 | 1.51973100 |
| H | -1.88418600 | -5.90927000 | 0.43797500 |
| H | -5.09320100 | -5.05227800 | 6.02408200 |
| H | -2.08636600 | -3.74290700 | 5.89306700 |
| H | -0.48224600 | -3.55616300 | 0.35771400 |
| C | 0.04283900 | -3.54775800 | 3.78847500 |
| C | 0.46591900 | -2.72723600 | 5.00466100 |
| C | 0.25973700 | -1.25124700 | 4.74429500 |
| C | 0.94508900 | -0.85892000 | 3.45255800 |
| C | 0.50426000 | -1.74963500 | 2.29754200 |
| C | 1.29887600 | -1.49866100 | 1.03678300 |
| O | -1.34212900 | -3.41655300 | 3.62327600 |
| O | -0.27914100 | -3.15361100 | 6.13365900 |
| O | 0.77774200 | -0.54758400 | 5.85033700 |
| O | 0.73493100 | -3.12103300 | 2.65133400 |
| O | 0.76810800 | -2.25642100 | -0.02825700 |
| H | 2.03130300 | -0.94839900 | 3.59482900 |
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| H | 1.53709600 | -2.90266600 | 5.17060100 |

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| H | -0.81795200 | -1.06771600 | 4.62375400 |
| H | -0.55810600 | -1.58699700 | 2.08372100 |
| H | 1.27658900 | -0.43389600 | 0.79510200 |
| H | 2.33771300 | -1.81123700 | 1.19875600 |
| H | -0.11658400 | -2.49701700 | 6.82567800 |
| H | 0.96002600 | 0.36867300 | 5.57294200 |
| H | 0.32933800 | -1.65304400 | -0.65917100 |
| C | 1.53672800 | 1.35346800 | 2.67947300 |
| C | 1.70512700 | 2.54346400 | 3.62237500 |
| C | 0.46497000 | 3.41035100 | 3.60737200 |
| C | 0.09666500 | 3.73286300 | 2.16898100 |
| C | -0.13684300 | 2.44009600 | 1.39045100 |
| C | -0.59271900 | 2.61017600 | -0.05682900 |
| O | 0.58779500 | 0.49390300 | 3.23868000 |
| O | 1.97842900 | 2.05395400 | 4.92392300 |
| O | 0.76106300 | 4.56539900 | 4.35794400 |
| O | 1.13613700 | 1.77167500 | 1.39912100 |
| O | -1.99310900 | 2.35471800 | -0.10694400 |
| H | 0.93967000 | 4.24554600 | 1.68811400 |
| H | 2.49333000 | 0.83972300 | 2.54167100 |
| H | 2.54484600 | 3.15108400 | 3.25802100 |
| H | -0.36511100 | 2.84447100 | 4.05548000 |
| H | -0.88194100 | 1.81332700 | 1.89048300 |
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| H | -0.01739300 | 5.15201000 | 4.35775500 |
| H | -2.42992000 | 2.92740700 | -0.76765000 |
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| C | -1.59786700 | 6.85945500 | 2.62725700 |
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| C | -2.56369200 | 5.68132700 | 0.19472400 |
| C | -2.81742000 | 5.54346800 | -1.30178200 |
| O | -1.02627800 | 4.58980300 | 2.20987900 |
| O | -1.23914900 | 6.64411600 | 3.97894700 |
| O | -3.73558000 | 7.72572000 | 3.11339000 |
| O | -1.18184100 | 6.01276500 | 0.40202900 |
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| H | 0.25625300 | 6.14218500 | 1.79501600 |
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| H | -3.39154900 | 5.70480100 | 2.76685600 |
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| H | -3.46942100 | 6.34289200 | -1.66576400 |
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| H | -4.14546200 | 4.36868400 | -2.19565100 |
| C | -5.43929900 | 7.62412500 | 0.07143100 |
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| C | -7.76875400 | 6.30112300 | -0.88892700 |
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| C | -6.32865700 | 5.73090500 | -2.95718100 |
| O | -4.76525800 | 6.60708000 | 0.74813800 |
| O | -6.52860400 | 8.13171200 | 2.13377000 |
| O | -8.94739100 | 7.01340100 | 1.10836700 |
| O | -5.63771300 | 7.29377000 | -1.28065200 |
| O | -5.49241600 | 4.61739600 | -3.22701000 |
| H | -8.26131700 | 7.11932700 | -1.43164900 |
| H | -4.84923000 | 8.54608000 | 0.07032000 |
| H | -7.25000400 | 8.72841400 | 0.28442900 |
| H | -7.25015100 | 5.81278000 | 1.11892200 |
| H | -5.88887700 | 5.26355200 | -0.91436600 |
| H | -7.32965200 | 5.52664300 | -3.34118000 |
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| H | -7.38437700 | 8.08985000 | 2.58163300 |
| H | -9.60258700 | 6.36373500 | 0.79510800 |
| H | -6.04985500 | 3.81440300 | -3.33953800 |
| C | -3.78858500 | -1.14186800 | -1.49497000 |
| H | -3.96140700 | -1.85612900 | -2.31223200 |
| C | -4.16342300 | 0.23852800 | -2.03773100 |
| H | -3.99437400 | 1.01126300 | -1.27939900 |
| C | -3.26092900 | 0.53730700 | -3.25044800 |
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| C | -1.54197300 | -0.81794700 | -2.41698400 |
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| C | -2.29842900 | -1.20880500 | -1.16058800 |
| H | -2.05473900 | -2.23916300 | -0.89325200 |
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| H | 0.57025000 | -0.42409000 | -4.03699300 |
| C | 2.07350100 | -1.14513600 | -2.69673200 |
| H | 2.29177300 | -1.87194500 | -1.91918500 |
| C | 3.00698700 | -0.26034100 | -3.05861800 |
| H | 2.79803700 | 0.47317200 | -3.83694200 |
| C | 4.30940000 | -0.21976500 | -2.42444900 |
| H | 4.47610300 | -0.94060100 | -1.62755600 |
| C | 5.29805700 | 0.64298000 | -2.72463500 |
| H | 5.15483100 | 1.37673400 | -3.51735700 |
| C | 6.55816100 | 0.64340000 | -2.02042300 |
| H | 6.65840500 | -0.10447300 | -1.23596300 |
| C | 7.59169400 | 1.47285000 | -2.26753100 |
| H | 7.50838100 | 2.22240000 | -3.05391300 |
| C | 8.82734700 | 1.41900500 | -1.52625600 |
| H | 8.90330500 | 0.65417000 | -0.75345300 |
| C | 9.88591600 | 2.22926200 | -1.73147700 |
| H | 9.83458300 | 2.98792200 | -2.51174300 |
| C | 11.09816500 | 2.16292600 | -0.95426600 |
| H | 11.13307700 | 1.41818500 | -0.15924600 |

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| C | 12.17509000 | 2.95082600 | -1.14792900 |
| H | 12.16020600 | 3.68355100 | -1.95405000 |
| C | 13.36534400 | 2.88629900 | -0.33495900 |
| H | 13.34249700 | 2.20065100 | 0.51033200 |
| C | 14.49015400 | 3.59100000 | -0.55600400 |
| H | 14.54422500 | 4.26173000 | -1.41276300 |
| C | 0.33900400 | -2.56730200 | -3.88598200 |
| H | -0.62092300 | -2.50738500 | -4.39640200 |
| H | 1.09100400 | -2.79652300 | -4.64676700 |
| C | 15.67039300 | 3.46981600 | 0.27753000 |
| H | 15.54751500 | 2.88013000 | 1.18387200 |
| C | 16.87451600 | 3.97253500 | -0.01581600 |
| H | 17.00099100 | 4.54916700 | -0.93364900 |
| C | 18.11235400 | 3.76630900 | 0.80984500 |
| H | 17.83121800 | 3.30502400 | 1.76345800 |
| C | 19.09402900 | 2.80440800 | 0.11244100 |
| H | 19.48995200 | 3.32685600 | -0.77433900 |
| C | 18.46796000 | 1.49267100 | -0.39682900 |
| H | 17.67790000 | 1.79077700 | -1.09292800 |
| C | 17.75851500 | 0.69303500 | 0.70122400 |
| H | 17.13837200 | 1.35666100 | 1.29724800 |
| C | 15.58171100 | -0.26466800 | 0.37606400 |
| C | 14.77617500 | -1.23857700 | -0.44642200 |
| H | 15.26195600 | -1.38669000 | -1.41268000 |
| H | 14.78635200 | -2.19838500 | 0.08315200 |
| C | 13.32439900 | -0.78659800 | -0.62193500 |

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| H | 13.30863900 | 0.17989800 | -1.14572000 |
| C | 12.52662200 | -1.80645300 | -1.42145100 |
| H | 12.98986800 | -1.91896000 | -2.40754600 |
| H | 12.58293400 | -2.77748200 | -0.91497400 |
| C | 11.05465300 | -1.44538900 | -1.60625800 |
| H | 10.97561900 | -0.43609500 | -2.03284100 |
| C | 10.35830000 | -2.43126600 | -2.53861000 |
| H | 10.62000700 | -3.45175600 | -2.23260200 |
| H | 10.77800800 | -2.28780900 | -3.53900100 |
| C | 8.82896700 | -2.27721500 | -2.57739200 |
| H | 8.53695800 | -1.27953300 | -2.24096100 |
| H | 8.47176300 | -2.36617500 | -3.60795600 |
| C | 8.08377500 | -3.32941100 | -1.75823300 |
| H | 8.27100000 | -4.31260700 | -2.21235900 |
| C | 6.55491500 | -3.07672400 | -1.75244800 |
| H | 6.27430700 | -2.48433300 | -2.63121400 |
| C | 5.74159900 | -4.36595600 | -1.73820400 |
| H | 6.00459300 | -4.94955200 | -0.84757500 |
| H | 6.01612800 | -4.96166900 | -2.61665400 |
| C | 4.23545500 | -4.11563800 | -1.76202500 |
| H | 4.00023600 | -3.46531700 | -2.61643200 |
| C | 3.45206800 | -5.41163300 | -1.92812200 |
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| C | 1.16782200 | -6.45318700 | -2.37356100 |

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| H | 1.34548800 | -7.29666200 | -1.70257100 |
| H | 1.50701900 | -6.72875900 | -3.37639700 |
| C | -0.31540500 | -6.13991600 | -2.40082800 |
| H | -0.63024000 | -5.91106500 | -1.38028600 |
| C | -0.61205700 | -4.90235900 | -3.26434500 |
| H | -0.44814100 | -5.16611900 | -4.31619200 |
| C | 0.32341700 | -3.72498700 | -2.88616600 |
| H | 0.00927700 | -3.38037300 | -1.90005000 |
| C | -2.06192000 | -4.46421700 | -3.12237600 |
| C | 18.63682000 | -0.13658700 | 1.61518900 |
| H | 18.03026400 | -0.60498100 | 2.39366400 |
| H | 19.37958000 | 0.51361500 | 2.07942900 |
| H | 19.15187500 | -0.92350000 | 1.05999900 |
| C | 19.48275400 | 0.65395200 | -1.17204200 |
| H | 20.34052100 | 0.37390100 | -0.55304900 |
| H | 19.85741500 | 1.20531500 | -2.03931100 |
| H | 19.02495900 | -0.26989300 | -1.53262500 |
| C | 18.80752900 | 5.09648100 | 1.11354400 |
| H | 19.08123900 | 5.60940900 | 0.18482200 |
| H | 19.71713100 | 4.92741700 | 1.69140800 |
| H | 18.14547200 | 5.75763600 | 1.67725800 |
| O | -1.96683700 | -0.42412500 | -0.03631500 |
| H | -2.04743100 | 0.53246900 | -0.23934400 |
| O | -5.54969700 | 0.28198500 | -2.36754200 |
| H | -5.89520800 | -0.61672800 | -2.55264200 |
| O | -1.89807500 | 0.49222300 | -2.82091300 |

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| O | -0.17552400 | -0.86840500 | -2.16037100 |
| O | 1.47341400 | -4.93109300 | -0.61531700 |
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| O | 1.67243600 | -4.16388900 | -2.81235700 |
| O | -2.54199500 | -3.49442200 | -3.68032500 |
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| H | -3.64651300 | -4.74626800 | -2.11441100 |
| O | 3.80524300 | -3.47491500 | -0.56076200 |
| H | 4.52439500 | -2.87881300 | -0.28863600 |
| O | 6.24271300 | -2.27716500 | -0.61025400 |
| H | 6.94496900 | -2.52947100 | 0.02470100 |
| O | 8.50084900 | -3.39201500 | -0.40171900 |
| H | 9.21249000 | -2.73394500 | -0.25103100 |
| O | 10.36476000 | -1.45712900 | -0.35330700 |
| H | 10.97917800 | -1.12034900 | 0.32412100 |
| O | 12.68999800 | -0.64341700 | 0.64629900 |
| H | 13.29291400 | -0.12795900 | 1.21130600 |
| O | 15.10585100 | 0.38636400 | 1.29276000 |
| O | 16.85182500 | -0.21695600 | 0.00240200 |
| O | 20.14958900 | 2.57047300 | 1.03996800 |
| H | 20.90978400 | 2.22241600 | 0.56189900 |
| O | -0.99537700 | -7.27965300 | -2.89793500 |
| H | -1.92804100 | -7.14404600 | -2.68869500 |
| N | -4.54661100 | -1.59787000 | -0.32636400 |
| H | -5.49320300 | -1.22808400 | -0.35652500 |
| H | -4.07939300 | -1.24568100 | 0.50728000 |

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| C | -9.90649500 | -0.51710400 | -1.50897700 |
| C | -10.74213300 | -1.01477200 | -0.33525700 |
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| C | -8.46426500 | -2.40095900 | -1.43281200 |
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| O | -8.89940300 | 0.32466700 | -1.02037600 |
| O | -11.25887900 | 0.09586600 | 0.37619700 |
| O | -10.75933500 | -2.42159400 | 1.55062600 |
| O | -9.36271300 | -1.59690400 | -2.21616400 |
| O | -6.48008400 | -3.11757100 | -2.65373800 |
| H | -10.06428600 | -3.64376300 | -0.68319000 |
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| H | -11.56451800 | -1.61609000 | -0.74600400 |
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| H | -7.66459700 | -1.76817600 | -1.03425100 |
| H | -7.90213500 | -4.43395900 | -1.95681300 |
| H | -8.39368700 | -3.40356300 | -3.31674800 |
| H | -11.55602300 | -0.23741400 | 1.23391000 |
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| H | -5.90267400 | -3.61391800 | -2.03202500 |

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| C | -8.53913100 | -5.12549300 | 0.60536000 |
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| C | -7.34495000 | -5.40016700 | 2.77790500 |
| C | -6.16827900 | -5.95630800 | 1.98763000 |
| C | -6.16509400 | -5.32549600 | 0.58891000 |
| C | -5.07091500 | -5.75713300 | -0.37686100 |
| O | -8.45680300 | -3.73417600 | 0.61891200 |
| O | -9.72383900 | -4.96336000 | 2.67753500 |
| O | -7.45581500 | -6.01092400 | 4.04231900 |
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| H | -6.26700900 | -7.04665600 | 1.89747100 |
| H | -9.40563800 | -5.45710400 | 0.02403400 |
| H | -8.83325200 | -6.71047200 | 2.00457400 |
| H | -7.19200300 | -4.31479100 | 2.87510800 |
| H | -6.10534300 | -4.23659200 | 0.70020600 |
| H | -4.19261200 | -6.09771700 | 0.16904900 |
| H | -5.45067900 | -6.58799400 | -0.97665000 |
| H | -9.64639600 | -5.15999100 | 3.62140200 |
| H | -6.58258800 | -5.96655100 | 4.46818600 |
| H | -4.00665300 | -4.15929200 | -0.84853600 |
| C | -4.01586000 | -6.56409700 | 2.90335100 |
| C | -3.39309200 | -6.44930200 | 4.29566200 |
| C | -2.54292400 | -5.19480600 | 4.44994300 |
| C | -1.63152600 | -5.02034100 | 3.24571600 |
| C | -2.48996800 | -5.02919500 | 1.99166100 |

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| C | -1.82717500 | -4.67653000 | 0.67071700 |
| O | -5.04603100 | -5.62854900 | 2.78683700 |
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| O | -3.03814700 | -6.35802000 | 1.91803500 |
| O | -2.58062300 | -3.64568500 | 0.03985300 |
| H | -0.92114200 | -5.85632500 | 3.20675000 |
| H | -4.40109400 | -7.57788900 | 2.74822500 |
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| H | -3.21494100 | -4.32338400 | 4.48619900 |
| H | -3.30154900 | -4.30832600 | 2.12151200 |
| H | -0.80007000 | -4.34855600 | 0.79552800 |
| H | -1.81144200 | -5.56454600 | 0.02962300 |
| H | -4.02261400 | -6.33262000 | 6.11176800 |
| H | -1.07189700 | -4.69866900 | 5.62132200 |
| H | -2.01715700 | -2.85397600 | -0.09009500 |
| C | 0.39623300 | -3.74969100 | 3.03973700 |
| C | 1.22440400 | -3.18292100 | 4.18493000 |
| C | 0.94857600 | -1.70608800 | 4.37473200 |
| C | 1.07502900 | -0.96777200 | 3.04761100 |
| C | 0.13777800 | -1.60551900 | 2.02586500 |
| C | 0.16604600 | -0.97647600 | 0.64583900 |
| O | -0.94300500 | -3.80131200 | 3.44264700 |
| O | 0.93655300 | -3.91176900 | 5.36309000 |
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| O | 0.55725400 | -2.97040100 | 1.88376400 |

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| O | -1.00941200 | -1.28914200 | -0.08366000 |
| H | 2.10384400 | -1.05306100 | 2.67439100 |
| H | 0.75289000 | -4.74992600 | 2.77473600 |
| H | 2.28412200 | -3.29156700 | 3.91397000 |
| H | -0.08893300 | -1.58756300 | 4.72096700 |
| H | -0.89287500 | -1.57070400 | 2.39658300 |
| H | 0.27182600 | 0.10698700 | 0.75355000 |
| H | 1.04363900 | -1.34979900 | 0.10659000 |
| H | 1.34165900 | -3.40669700 | 6.08265800 |
| H | 1.65668900 | -0.33279100 | 5.57879300 |
| H | -1.50525100 | -0.45346900 | -0.21216600 |
| C | 1.80677700 | 1.30291100 | 3.28893000 |
| C | 1.66281200 | 2.22915500 | 4.49246000 |
| C | 0.44182800 | 3.10757500 | 4.33602800 |
| C | 0.52728400 | 3.83905500 | 3.00744200 |
| C | 0.66034100 | 2.83475600 | 1.86317200 |
| C | 0.82352300 | 3.45326900 | 0.47995900 |
| O | 0.74382100 | 0.39195000 | 3.27379200 |
| O | 1.59068200 | 1.47286600 | 5.68608700 |
| O | 0.43259300 | 3.98218500 | 5.43954000 |
| O | 1.84083400 | 2.05847700 | 2.10573800 |
| O | -0.43875000 | 3.55483400 | -0.15134800 |
| H | 1.42495800 | 4.47130200 | 3.00594400 |
| H | 2.76367300 | 0.77499100 | 3.33528800 |
| H | 2.54905600 | 2.87818400 | 4.51267700 |
| H | -0.45309500 | 2.46854800 | 4.32231000 |

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| H | -0.22138600 | 2.18261500 | 1.84138500 |
| H | 1.29228400 | 4.44122300 | 0.54936100 |
| H | 1.48718000 | 2.79808500 | -0.09692200 |
| H | 1.23305500 | 2.06905500 | 6.35957500 |
| H | -0.35105200 | 4.56206100 | 5.38523000 |
| H | -0.53612100 | 4.45945800 | -0.53339600 |
| C | -0.46418400 | 6.02776100 | 2.95704200 |
| C | -1.55342500 | 6.61388800 | 3.85253400 |
| C | -2.90971200 | 6.40931200 | 3.21514600 |
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| C | -1.76493500 | 6.35562500 | 1.00638000 |
| C | -1.62595100 | 6.88409100 | -0.40367600 |
| O | -0.63258900 | 4.64004600 | 2.88109400 |
| O | -1.50027000 | 6.00682300 | 5.13054600 |
| O | -3.86682000 | 7.02452900 | 4.04494300 |
| O | -0.53257400 | 6.61716300 | 1.68681400 |
| O | -0.85684300 | 6.00127500 | -1.20473200 |
| H | -2.84373300 | 8.05929300 | 1.82389600 |
| H | 0.52374900 | 6.27507800 | 3.35726700 |
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| H | -3.08781200 | 5.32682400 | 3.13937200 |
| H | -1.93353100 | 5.27989000 | 0.95059900 |
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| H | -1.13173700 | 7.86210800 | -0.36406300 |
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| H | -4.75224100 | 6.86477700 | 3.66710000 |

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| H | -1.44818500 | 5.65202400 | -1.91318800 |
| C | -5.10213500 | 7.48563500 | 0.83040800 |
| C | -6.45617500 | 6.98823100 | 1.32429900 |
| C | -6.73843500 | 5.61798900 | 0.72146300 |
| C | -6.64344300 | 5.70241300 | -0.79142800 |
| C | -5.31717800 | 6.33793800 | -1.21904900 |
| C | -5.25978800 | 6.60317800 | -2.71354200 |
| O | -4.15077900 | 6.55352200 | 1.23189700 |
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| O | -7.97974100 | 5.13399900 | 1.18885600 |
| O | -5.14457500 | 7.60123100 | -0.57481600 |
| O | -5.03054500 | 5.40394000 | -3.45349100 |
| H | -7.47782900 | 6.29844400 | -1.17808000 |
| H | -4.87696200 | 8.48527600 | 1.21557000 |
| H | -7.22409000 | 7.69823400 | 0.98703000 |
| H | -5.95950200 | 4.93518800 | 1.07524600 |
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| H | -6.17795100 | 7.09387700 | -3.06081100 |
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| H | -8.62994400 | 5.21255500 | 0.46744000 |
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| C | -7.60521500 | 4.06828700 | -2.34637300 |
| C | -9.05334500 | 3.90596300 | -1.88486600 |
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| C | -7.17710000 | 1.72894300 | -2.06354500 |
| C | -6.44364800 | 0.58277200 | -2.75219100 |
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| O | -9.50737700 | 5.05945300 | -1.18464600 |
| O | -10.62594100 | 2.55351000 | -0.82580000 |
| O | -7.13463900 | 2.88860000 | -2.93116500 |
| O | -5.91035500 | -0.23688200 | -1.73113900 |
| H | -9.14991700 | 1.39444500 | -2.76385200 |
| H | -7.55801700 | 4.83838700 | -3.12653000 |
| H | -9.65196100 | 3.77835900 | -2.79700700 |
| H | -8.69411800 | 2.79819200 | -0.09265500 |
| H | -6.64262700 | 1.94823400 | -1.13384100 |
| H | -7.13465000 | 0.02073200 | -3.39532100 |
| H | -5.64975400 | 1.00903200 | -3.38080700 |
| H | -10.40257100 | 4.82451300 | -0.89267300 |
| H | -10.80105600 | 1.78788200 | -0.24504500 |
| H | -5.50852100 | -1.03208500 | -2.12260000 |
| C | -3.41156400 | 2.86155400 | -1.64083400 |
| H | -4.41679000 | 2.87137800 | -2.07822700 |
| C | -2.44214900 | 3.40741600 | -2.69633400 |
| H | -1.41575500 | 3.18324500 | -2.39689700 |
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| C | -2.51268000 | 0.70321600 | -2.67489700 |
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| C | -3.04197400 | 1.37784800 | -1.38422600 |

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| H | -3.93839900 | 0.83700300 | -1.07467000 |
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| H | -0.71750300 | 2.69631600 | -4.71629100 |
| H | -1.70232900 | 4.02270900 | -5.33908400 |
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| H | -0.20705000 | 0.79883700 | -4.45951300 |
| C | 0.97559900 | -0.16689000 | -2.98087500 |
| H | 1.01291900 | -0.98026500 | -2.26397000 |
| C | 2.05019600 | 0.60332900 | -3.17711900 |
| H | 2.00092800 | 1.42846100 | -3.88774600 |
| C | 3.29938800 | 0.41080700 | -2.46854100 |
| H | 3.34135900 | -0.43686200 | -1.78858500 |
| C | 4.38400800 | 1.19986000 | -2.59093000 |
| H | 4.35199700 | 2.05704700 | -3.26298800 |
| C | 5.60936400 | 0.95333000 | -1.87001800 |
| H | 5.61816800 | 0.06542600 | -1.24126200 |
| C | 6.72603700 | 1.70477100 | -1.94795200 |
| H | 6.73820100 | 2.59529300 | -2.57551000 |
| C | 7.93485500 | 1.37319800 | -1.23542300 |
| H | 7.92171100 | 0.45237100 | -0.65234600 |
| C | 9.07222200 | 2.09762400 | -1.26077000 |
| H | 9.10911300 | 3.01438300 | -1.84821600 |
| C | 10.26057900 | 1.73065400 | -0.53222700 |
| H | 10.21466100 | 0.81116100 | 0.05127000 |
| C | 11.40890500 | 2.43722600 | -0.53255400 |

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| H | 11.47343400 | 3.34749900 | -1.12767600 |
| C | 12.57712300 | 2.05725300 | 0.22401300 |
| H | 12.48353100 | 1.17554100 | 0.85587000 |
| C | 13.76085100 | 2.69613600 | 0.18831200 |
| H | 13.88220300 | 3.56567400 | -0.45670600 |
| C | -1.00846200 | -1.15519500 | -4.24956700 |
| H | -2.00638400 | -0.87731300 | -4.59853500 |
| H | -0.43356900 | -1.42650900 | -5.14050000 |
| C | 14.91756700 | 2.25351300 | 0.94197000 |
| H | 14.73924700 | 1.44328500 | 1.64623400 |
| C | 16.16070800 | 2.72193300 | 0.78730400 |
| H | 16.34156100 | 3.52311400 | 0.06870700 |
| C | 17.37090200 | 2.19013200 | 1.50052200 |
| H | 17.04609100 | 1.48979300 | 2.27870500 |
| C | 18.28370900 | 1.40659900 | 0.53656600 |
| H | 18.73229900 | 2.13756500 | -0.15673500 |
| C | 17.56364200 | 0.36218300 | -0.33615100 |
| H | 16.80460100 | 0.91559700 | -0.89754100 |
| C | 16.78612300 | -0.67463200 | 0.48132400 |
| H | 16.21945400 | -0.17624400 | 1.26275400 |
| C | 14.54136300 | -1.31956900 | -0.06499200 |
| C | 13.65903300 | -1.94448400 | -1.11640700 |
| H | 14.12631000 | -1.83222000 | -2.09656800 |
| H | 13.60061800 | -3.01664100 | -0.89528300 |
| C | 12.24416600 | -1.36015100 | -1.10827400 |
| H | 12.29788900 | -0.28464300 | -1.32947200 |

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| C | 11.36138100 | -2.04361100 | -2.14294700 |
| H | 11.80369000 | -1.89614700 | -3.13411700 |
| H | 11.34766000 | -3.12163100 | -1.94209900 |
| C | 9.92068100 | -1.53884000 | -2.16460000 |
| H | 9.91732200 | -0.44625200 | -2.27853900 |
| C | 9.13043300 | -2.15629500 | -3.31392300 |
| H | 9.30483600 | -3.23927900 | -3.32184200 |
| H | 9.54609700 | -1.76542200 | -4.24763000 |
| C | 7.62126500 | -1.87071200 | -3.24146500 |
| H | 7.43034500 | -0.99968100 | -2.61043500 |
| H | 7.23878400 | -1.61591200 | -4.23458000 |
| C | 6.79142500 | -3.04862300 | -2.73324700 |
| H | 6.83703900 | -3.85558600 | -3.47750200 |
| C | 5.31128900 | -2.64656500 | -2.52785400 |
| H | 5.05685000 | -1.81199400 | -3.19047600 |
| C | 4.33503700 | -3.79476500 | -2.76271700 |
| H | 4.56484400 | -4.60712200 | -2.06250800 |
| H | 4.47949100 | -4.18304000 | -3.77732900 |
| C | 2.87751400 | -3.36900500 | -2.60562900 |
| H | 2.66579700 | -2.55240400 | -3.30819100 |
| C | 1.91250900 | -4.51379700 | -2.89734400 |
| H | 2.14247400 | -5.36476100 | -2.24850100 |
| H | 2.04798300 | -4.82828200 | -3.93628800 |
| C | 0.44590300 | -4.14136200 | -2.67983600 |
| C | -0.53314600 | -5.22107800 | -3.13259700 |
| H | -0.40395900 | -6.12168800 | -2.52780300 |

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| H | -0.34431700 | -5.47335000 | -4.18038900 |
| C | -1.95461600 | -4.71207800 | -2.97291000 |
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| C | -2.13358800 | -3.40104400 | -3.78271800 |
| H | -2.04802900 | -3.63897800 | -4.84728000 |
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| C | -3.52223300 | -2.89495300 | -3.49348300 |
| C | 17.58990500 | -1.80978700 | 1.08197900 |
| H | 16.94219500 | -2.44747300 | 1.68795100 |
| H | 18.37663600 | -1.39296900 | 1.71229300 |
| H | 18.04725100 | -2.42388000 | 0.30320800 |
| C | 18.51709800 | -0.27757500 | -1.34380700 |
| H | 19.34527600 | -0.79590100 | -0.85120200 |
| H | 18.94051800 | 0.47958100 | -2.01013400 |
| H | 17.99219600 | -1.01169900 | -1.95918000 |
| C | 18.16214000 | 3.31498100 | 2.17379900 |
| H | 18.48001400 | 4.05857300 | 1.43457400 |
| H | 19.05233800 | 2.91495600 | 2.66115500 |
| H | 17.54796000 | 3.82618100 | 2.91851400 |
| O | -2.11563100 | 1.24406400 | -0.31286300 |
| H | -1.34924600 | 1.81960400 | -0.49677400 |
| O | -2.48282000 | 4.80912800 | -2.89742900 |
| H | -3.39053600 | 5.06617900 | -3.16781700 |
| O | -3.02996400 | 1.31369200 | -3.83663500 |
| O | -1.11534600 | 0.73873200 | -2.61371200 |

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| O | 0.18127500 | -3.90079800 | -1.32572300 |
| H | 0.93977300 | -3.41303600 | -0.95817100 |
| O | 0.23549300 | -2.97901100 | -3.46871000 |
| O | -3.79225200 | -2.20688500 | -2.51646100 |
| O | -4.44223000 | -3.33903100 | -4.33311600 |
| H | -5.33345800 | -3.15343800 | -3.93799900 |
| O | 2.62819300 | -2.89579000 | -1.27623500 |
| H | 3.46977100 | -2.55148900 | -0.92195500 |
| O | 5.18072600 | -2.15589900 | -1.19011400 |
| H | 5.86404000 | -2.66829800 | -0.70992800 |
| O | 7.25359000 | -3.57374600 | -1.49591400 |
| H | 8.02399400 | -3.04780100 | -1.19046500 |
| O | 9.24744700 | -1.86432600 | -0.94502000 |
| H | 9.89458800 | -1.78053900 | -0.22084800 |
| O | 11.63517400 | -1.54730600 | 0.16650600 |
| H | 12.28254100 | -1.26404100 | 0.83696400 |
| O | 14.12124300 | -0.93754900 | 1.01592900 |
| O | 15.81039500 | -1.25599600 | -0.44020200 |
| O | 19.30439100 | 0.82254600 | 1.34065100 |
| H | 20.04269000 | 0.57712400 | 0.77291900 |
| O | -2.86146900 | -5.71554800 | -3.37027400 |
| H | -3.69199100 | -5.53069800 | -2.90548200 |
| N | -3.46441400 | 3.67211900 | -0.43536800 |
| H | -2.64252200 | 3.47541900 | 0.13055900 |
| H | -4.26634300 | 3.38346300 | 0.11780600 |

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| C | 1.66518900 | 9.98791900 | 0.03644500 |
| C | 2.88438400 | 9.83604700 | -0.86185800 |
| C | 3.56369900 | 8.50034100 | -0.64891500 |
| C | 3.89235700 | 8.32620100 | 0.82476600 |
| C | 2.62196800 | 8.47019400 | 1.66533400 |
| C | 2.83304300 | 8.47665300 | 3.17911700 |
| O | 0.65563100 | 9.10504000 | -0.35583300 |
| O | 2.50903500 | 9.99634900 | -2.21614700 |
| O | 4.70296200 | 8.52139600 | -1.47041900 |
| O | 2.04656000 | 9.76552500 | 1.37617600 |
| O | 3.22517100 | 7.23194600 | 3.68916200 |
| H | 4.60556000 | 9.10703700 | 1.12361500 |
| H | 1.30269000 | 11.02062300 | 0.00481100 |
| H | 3.59670600 | 10.62208100 | -0.57627600 |
| H | 2.86966400 | 7.69699000 | -0.93896300 |
| H | 1.90763300 | 7.68183100 | 1.40652300 |
| H | 3.54228300 | 9.28148500 | 3.42909800 |
| H | 1.87443700 | 8.72860300 | 3.63989400 |
| H | 3.25882400 | 9.66883800 | -2.73520700 |
| H | 5.29680500 | 7.77987800 | -1.23929400 |
| H | 4.15896600 | 7.07566900 | 3.48170000 |
| C | 5.75451400 | 6.94555300 | 1.54469800 |

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| C | 6.69503000 | 6.18408400 | 0.62361300 |
| C | 6.25698800 | 4.74355200 | 0.47383600 |
| C | 6.10832100 | 4.09788700 | 1.84267600 |
| C | 5.17978500 | 4.92685400 | 2.73250600 |
| C | 5.10521500 | 4.47831300 | 4.19177700 |
| O | 4.48814100 | 7.04419600 | 0.96091200 |
| O | 6.74961700 | 6.82044100 | -0.64005200 |
| O | 7.23517200 | 4.13218600 | -0.32741300 |
| O | 5.68780100 | 6.28007300 | 2.78595200 |
| O | 4.41665600 | 3.26990900 | 4.36512000 |
| H | 7.09861600 | 4.02791100 | 2.31382300 |
| H | 6.15670200 | 7.94056000 | 1.76241900 |
| H | 7.68902300 | 6.19149800 | 1.09060500 |
| H | 5.26849200 | 4.72600200 | -0.00934000 |
| H | 4.16937700 | 4.93016400 | 2.31176500 |
| H | 6.12636900 | 4.44913000 | 4.60401900 |
| H | 4.55132400 | 5.24508500 | 4.73951800 |
| H | 7.15798400 | 6.17328200 | -1.23511900 |
| H | 7.10689900 | 3.16175000 | -0.34146900 |
| H | 4.96541500 | 2.53075800 | 4.06064700 |
| C | 6.25881300 | 1.67719000 | 2.08714500 |
| C | 6.50097400 | 0.72080100 | 0.93544400 |
| C | 5.17334200 | 0.23490800 | 0.37955500 |
| C | 4.40413500 | -0.41469800 | 1.52258000 |
| C | 4.21271900 | 0.56592300 | 2.68324600 |
| C | 3.59567100 | -0.01922300 | 3.95289400 |

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| O | 5.57508100 | 2.80380900 | 1.61722800 |
| O | 7.30207200 | 1.37781000 | -0.02413600 |
| O | 5.42891900 | -0.67961600 | -0.66333800 |
| O | 5.51515300 | 1.03602600 | 3.09747100 |
| O | 2.21980900 | -0.26299200 | 3.84223100 |
| H | 4.98530500 | -1.27984500 | 1.87064700 |
| H | 7.21169500 | 1.96170200 | 2.54587200 |
| H | 7.03090100 | -0.15260100 | 1.32552000 |
| H | 4.59769000 | 1.08938700 | 0.00079000 |
| H | 3.60274700 | 1.41467100 | 2.35805500 |
| H | 4.16451900 | -0.91681200 | 4.24315500 |
| H | 3.73055400 | 0.72399600 | 4.74328200 |
| H | 7.70575700 | 0.66713100 | -0.55944300 |
| H | 4.67882900 | -1.30017900 | -0.78198700 |
| H | 2.07907800 | -1.07115700 | 3.32489100 |
| C | 2.78787200 | -2.17987000 | 1.20190800 |
| C | 2.53636800 | -2.87376100 | -0.13033500 |
| C | 1.25753500 | -2.38793100 | -0.78117800 |
| C | 0.10768300 | -2.45524400 | 0.21741000 |
| C | 0.44427400 | -1.66885200 | 1.48283100 |
| C | -0.55330600 | -1.80617500 | 2.63677000 |
| O | 3.15857600 | -0.84933400 | 0.98805900 |
| O | 3.66699300 | -2.67226900 | -0.94653400 |
| O | 0.99015200 | -3.23673300 | -1.89746100 |
| O | 1.64645200 | -2.25350300 | 2.01982200 |
| O | -1.87345600 | -1.46505700 | 2.30362800 |

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| H | -0.04115000 | -3.50186900 | 0.51087700 |
| H | 3.57239700 | -2.72097000 | 1.73609100 |
| H | 2.40654300 | -3.93523200 | 0.08160500 |
| H | 1.38421400 | -1.35246700 | -1.11790000 |
| H | 0.61451500 | -0.61428000 | 1.24117500 |
| H | -0.47600700 | -2.83294800 | 3.01211300 |
| H | -0.22786200 | -1.13196600 | 3.43334400 |
| H | 3.76206700 | -3.43740800 | -1.54287400 |
| H | 0.18504500 | -2.94119500 | -2.38106700 |
| H | -2.25212900 | -2.18600900 | 1.78230700 |
| C | -2.03860800 | -2.91049000 | -0.72949200 |
| C | -2.50347900 | -2.79831900 | -2.17497000 |
| C | -3.24853200 | -1.50641400 | -2.41893200 |
| C | -4.37860100 | -1.36581700 | -1.41521200 |
| C | -3.84227800 | -1.48448300 | 0.01063700 |
| C | -4.90863400 | -1.48929700 | 1.10482600 |
| O | -1.05073000 | -1.96777900 | -0.45051700 |
| O | -1.39064000 | -2.89405400 | -3.04567500 |
| O | -3.69975000 | -1.56403000 | -3.74985100 |
| O | -3.16037600 | -2.75425900 | 0.12262700 |
| O | -5.44811200 | -0.21915500 | 1.35055800 |
| H | -5.11590800 | -2.16091500 | -1.59460000 |
| H | -1.67266700 | -3.91978100 | -0.53951700 |
| H | -3.19170300 | -3.63314600 | -2.35895900 |
| H | -2.55532900 | -0.66601200 | -2.26398800 |
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| H | -5.68311900 | -2.22560800 | 0.84409300 |
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| H | -4.38659600 | -0.88532400 | -3.89360800 |
| H | -6.08979800 | -0.00112300 | 0.65825500 |
| C | -6.33574800 | 0.02544700 | -1.82430400 |
| C | -6.63158400 | 0.69591900 | -3.15682900 |
| C | -6.10972100 | 2.11713700 | -3.16151000 |
| C | -6.65034400 | 2.88476900 | -1.96503900 |
| C | -6.35652900 | 2.13568100 | -0.66345600 |
| C | -7.01669700 | 2.71026400 | 0.58868700 |
| O | -4.95685000 | -0.08977700 | -1.65716200 |
| O | -6.04385100 | -0.05218700 | -4.20531700 |
| O | -6.50981100 | 2.66755700 | -4.39123100 |
| O | -6.90146200 | 0.80314300 | -0.79059900 |
| O | -6.47124800 | 3.94036800 | 0.98427300 |
| H | -7.73789700 | 2.99436800 | -2.07748300 |
| H | -6.82236700 | -0.95401700 | -1.76275800 |
| H | -7.72222900 | 0.72885700 | -3.28095200 |
| H | -5.01409500 | 2.08586900 | -3.06933400 |
| H | -5.27592100 | 2.08009200 | -0.50096800 |
| H | -8.10423500 | 2.76204000 | 0.42216600 |
| H | -6.84120600 | 2.00213300 | 1.40261600 |
| H | -6.07548000 | 0.52447000 | -4.98345300 |
| H | -6.30921100 | 3.62373600 | -4.40501300 |
| H | -6.77818500 | 4.64086500 | 0.38951200 |

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| C | -6.82102400 | 5.30557100 | -2.03644700 |
| C | -6.40730400 | 6.18740400 | -3.20479300 |
| C | -5.01749300 | 6.74906200 | -2.99297100 |
| C | -4.95653300 | 7.47398500 | -1.65773000 |
| C | -5.38541700 | 6.53604900 | -0.52672500 |
| C | -5.53945200 | 7.19146500 | 0.84510300 |
| O | -6.02381200 | 4.16183900 | -1.99332100 |
| O | -6.46948300 | 5.45184900 | -4.41158600 |
| O | -4.78292300 | 7.59399800 | -4.09057400 |
| O | -6.70957200 | 6.04636600 | -0.84058300 |
| O | -4.32451500 | 7.63107700 | 1.38945800 |
| H | -5.64927200 | 8.32642200 | -1.68840600 |
| H | -7.87936200 | 5.03657600 | -2.11860700 |
| H | -7.10995400 | 7.03079500 | -3.24408200 |
| H | -4.29928400 | 5.91624000 | -2.96098100 |
| H | -4.68840100 | 5.69562700 | -0.44957700 |
| H | -6.28355000 | 7.99915600 | 0.76178900 |
| H | -5.94618700 | 6.43677200 | 1.52306600 |
| H | -5.98090500 | 5.97903400 | -5.06161100 |
| H | -3.95299700 | 8.09225600 | -3.95633500 |
| H | -4.04311700 | 8.43848000 | 0.93412700 |
| C | -3.41369600 | 9.31222400 | -1.35112500 |
| C | -2.38289200 | 9.80626100 | -2.35609000 |
| C | -1.00147900 | 9.27406900 | -2.03866100 |
| C | -0.64055500 | 9.63384000 | -0.60653700 |
| C | -1.69880800 | 9.08024300 | 0.35043500 |

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| C | -1.54851100 | 9.50204300 | 1.81178500 |
| O | -3.62137600 | 7.93928000 | -1.49751900 |
| O | -2.76952700 | 9.44256700 | -3.66669400 |
| O | -0.14877400 | 9.85983100 | -2.98882800 |
| O | -2.97753600 | 9.62757300 | -0.04682400 |
| O | -0.41563900 | 8.95918900 | 2.43299700 |
| H | -0.62223800 | 10.72848000 | -0.51193100 |
| H | -4.35452000 | 9.85695400 | -1.48152100 |
| H | -2.34530000 | 10.90078700 | -2.26890700 |
| H | -1.01165800 | 8.17696700 | -2.12422400 |
| H | -1.72849800 | 7.98737500 | 0.29044200 |
| H | -1.57198700 | 10.60219900 | 1.85834400 |
| H | -2.42471800 | 9.13103200 | 2.34966100 |
| H | -1.98224500 | 9.57247600 | -4.21643500 |
| H | 0.78440300 | 9.70411200 | -2.74370100 |
| H | 0.37281700 | 9.43361900 | 2.12982100 |
| C | 10.08825200 | -1.63550700 | -0.01713300 |
| H | 10.74943400 | -2.48421100 | 0.19512300 |
| C | 9.88392000 | -0.88355200 | 1.30059300 |
| H | 9.25923600 | 0.00146100 | 1.10382400 |
| C | 9.17152700 | -1.76818000 | 2.32146800 |
| H | 9.83962500 | -2.61883700 | 2.53646500 |
| C | 8.14281400 | -3.01446100 | 0.59137900 |
| H | 8.86280800 | -3.82138400 | 0.80779700 |
| C | 8.75712800 | -2.18394200 | -0.53431800 |
| H | 8.93650600 | -2.86255000 | -1.37593400 |

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| C | 8.83603000 | -1.04582000 | 3.60753300 |
| H | 8.09701500 | -0.26122300 | 3.42442000 |
| H | 9.74006400 | -0.59483500 | 4.01980200 |
| H | 8.41196800 | -1.73963800 | 4.33638300 |
| C | 6.62630500 | -4.81639600 | 0.81965600 |
| H | 6.99210200 | -4.80298900 | 1.85407100 |
| C | 5.15037800 | -5.03725500 | 0.83025900 |
| H | 4.67599400 | -5.01824800 | -0.14402900 |
| C | 4.43073800 | -5.33726600 | 1.91877000 |
| H | 4.89891700 | -5.33753800 | 2.90266500 |
| C | 3.00788100 | -5.60872800 | 1.82586200 |
| H | 2.63045500 | -5.76891000 | 0.81935500 |
| C | 2.09295400 | -5.58010000 | 2.81322200 |
| H | 2.38806900 | -5.41984900 | 3.84908400 |
| C | 0.68588300 | -5.62475700 | 2.48125500 |
| H | 0.47797400 | -5.70853900 | 1.41768100 |
| C | -0.35885100 | -5.45751200 | 3.31447200 |
| H | -0.20367800 | -5.36915700 | 4.38889900 |
| C | -1.70112900 | -5.26877900 | 2.81058700 |
| H | -1.82091100 | -5.25725900 | 1.72644000 |
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| C | -4.08017500 | -4.68486000 | 3.02461100 |
| H | -4.13539000 | -4.53096100 | 1.94779400 |
| C | -5.18717700 | -4.49466400 | 3.76985100 |
| H | -5.13448700 | -4.64662100 | 4.84719700 |

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| C | -6.45145200 | -4.06233100 | 3.22634800 |
| H | -6.46736000 | -3.81973800 | 2.16684000 |
| C | -7.59034500 | -3.92635600 | 3.92881600 |
| H | -7.60638800 | -4.18924600 | 4.98570500 |
| C | 7.35404700 | -5.93304900 | 0.04385200 |
| H | 8.41604200 | -5.88175000 | 0.28855500 |
| H | 6.98588900 | -6.90503200 | 0.38600000 |
| C | -8.82524000 | -3.45484100 | 3.33163900 |
| H | -8.73361400 | -3.04562800 | 2.32772700 |
| C | -10.03237500 | -3.52056800 | 3.90287900 |
| H | -10.12490600 | -3.94443000 | 4.90401900 |
| C | -11.31388200 | -3.08087100 | 3.25165700 |
| H | -11.07516500 | -2.47432500 | 2.37065700 |
| C | -12.13801600 | -4.28985100 | 2.76712800 |
| H | -12.45834800 | -4.84653500 | 3.66335000 |
| C | -11.36922500 | -5.28935400 | 1.88163500 |
| H | -10.51230100 | -5.61821900 | 2.47707100 |
| C | -10.77025900 | -4.64595600 | 0.62582800 |
| H | -10.26888900 | -3.71883200 | 0.88985500 |
| C | -8.51406000 | -5.10401000 | -0.05657400 |
| C | -7.56598600 | -6.16841400 | -0.55201100 |
| H | -7.94661900 | -7.15312400 | -0.27541800 |
| H | -7.55669100 | -6.10657600 | -1.64650800 |
| C | -6.13934800 | -5.96067200 | -0.03525900 |
| H | -6.14092000 | -6.04356800 | 1.06217200 |
| C | -5.18304900 | -6.99160800 | -0.61951100 |

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| H | -5.54389000 | -7.99439100 | -0.36619400 |
| H | -5.19500000 | -6.89678500 | -1.71166000 |
| C | -3.73913000 | -6.85102600 | -0.14048400 |
| H | -3.71174400 | -6.90902100 | 0.95843900 |
| C | -2.84758700 | -7.94562000 | -0.72193600 |
| H | -3.05649900 | -8.03031600 | -1.79523400 |
| H | -3.14825000 | -8.89512600 | -0.26891000 |
| C | -1.34233800 | -7.70082300 | -0.50786500 |
| H | -1.18545300 | -6.97730700 | 0.29636300 |
| H | -0.85636700 | -8.62808600 | -0.18923700 |
| C | -0.61106100 | -7.21212600 | -1.76076200 |
| H | -0.62339400 | -8.02784000 | -2.50165900 |
| C | 0.85099500 | -6.86521200 | -1.44876100 |
| H | 1.28274000 | -7.64860500 | -0.81347500 |
| C | 1.70338400 | -6.72499200 | -2.70822200 |
| H | 1.19278500 | -6.06779800 | -3.42182000 |
| H | 1.77703700 | -7.70543100 | -3.19065800 |
| C | 3.10830900 | -6.17566200 | -2.42462700 |
| H | 3.37649100 | -6.37807100 | -1.38248300 |
| C | 4.15281000 | -6.82578600 | -3.32179100 |
| H | 3.85916000 | -6.70905600 | -4.36994900 |
| H | 4.16523000 | -7.89555400 | -3.09434300 |
| C | 5.57682200 | -6.28485900 | -3.18525800 |
| C | 6.56250900 | -7.14197000 | -3.96631300 |
| H | 6.34081900 | -7.08694500 | -5.03395000 |
| H | 6.46556400 | -8.18345200 | -3.64686700 |

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| C | 7.99888700 | -6.71558800 | -3.73433600 |
| H | 8.14397100 | -5.70691700 | -4.14838100 |
| C | 8.28277800 | -6.65826300 | -2.21013300 |
| H | 8.28902000 | -7.69520000 | -1.85359000 |
| C | 7.19994400 | -5.85081600 | -1.47181900 |
| H | 7.26795500 | -4.80671600 | -1.78813800 |
| C | 9.65283800 | -6.07344000 | -1.97406900 |
| C | -11.71464700 | -4.40084900 | -0.53309200 |
| H | -11.18812300 | -3.89275400 | -1.34440400 |
| H | -12.54034400 | -3.77539800 | -0.19181600 |
| H | -12.11677700 | -5.33985000 | -0.91938000 |
| C | -12.21951900 | -6.51771500 | 1.56171600 |
| H | -13.13614600 | -6.25183100 | 1.02662000 |
| H | -12.50366800 | -7.03980400 | 2.47985300 |
| H | -11.66601300 | -7.21913900 | 0.93335600 |
| C | -12.14801600 | -2.22096700 | 4.20516000 |
| H | -12.39651500 | -2.78230400 | 5.11282900 |
| H | -13.07957900 | -1.91395700 | 3.72859600 |
| H | -11.59106400 | -1.33061300 | 4.50556000 |
| O | 7.97073800 | -1.08984100 | -0.95002000 |
| H | 7.00132600 | -1.26182100 | -0.89196800 |
| O | 11.13362000 | -0.50586700 | 1.83089500 |
| H | 11.63640000 | -0.19921900 | 1.05899100 |
| O | 7.94791900 | -2.25413000 | 1.76792800 |
| O | 6.91195600 | -3.54094800 | 0.21815000 |
| O | 5.68713200 | -4.97721700 | -3.67145600 |

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| H | 4.87599300 | -4.51065400 | -3.41338700 |
| O | 5.90567600 | -6.35311800 | -1.79876200 |
| O | 9.91730000 | -5.03407400 | -1.41592600 |
| O | 10.63542100 | -6.84260700 | -2.50215500 |
| H | 11.47160700 | -6.37775000 | -2.33403900 |
| O | 3.17226800 | -4.75118800 | -2.63106100 |
| H | 2.29888300 | -4.32041700 | -2.52891500 |
| O | 0.90114300 | -5.67898300 | -0.68076900 |
| H | 0.58859600 | -4.94257900 | -1.23863100 |
| O | -1.19675800 | -6.06718500 | -2.35211700 |
| H | -1.96470600 | -5.79430600 | -1.81826600 |
| O | -3.19079700 | -5.59667200 | -0.53677300 |
| H | -3.86706800 | -4.90238700 | -0.41459800 |
| O | -5.66090500 | -4.67112400 | -0.40736700 |
| H | -6.37229000 | -4.03723500 | -0.20309700 |
| O | -8.18061200 | -3.93827700 | 0.10239300 |
| O | -9.73302500 | -5.56883900 | 0.15911500 |
| O | -13.28027300 | -3.75901100 | 2.10107700 |
| H | -13.95565800 | -4.44378800 | 2.05192100 |
| O | 8.79979300 | -7.66721300 | -4.39851600 |
| H | 9.72420800 | -7.49850400 | -4.17745000 |
| N | 10.79606800 | -0.74531400 | -0.93081400 |
| H | 10.13007100 | -0.08636200 | -1.32655300 |
| H | 11.18539100 | -1.26909500 | -1.70809500 |

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| C | 0.63754700 | 3.28284400 | 0.29802600 |
| C | 0.65022400 | 4.32308800 | -0.81245000 |
| C | 2.05096100 | 4.85667900 | -1.02155100 |
| C | 2.59622300 | 5.40369800 | 0.28769700 |
| C | 2.52145200 | 4.34587700 | 1.39023600 |
| C | 2.82347600 | 4.85705000 | 2.79900600 |
| O | 1.38245300 | 2.16659100 | -0.08157000 |
| O | 0.14495300 | 3.76006400 | -2.00430500 |
| O | 1.94175000 | 5.84221900 | -2.01767100 |
| O | 1.15936100 | 3.86928300 | 1.47367900 |
| O | 4.15124200 | 5.27394500 | 2.96938400 |
| H | 1.99201100 | 6.27241300 | 0.58400100 |
| H | -0.39068400 | 2.99766500 | 0.54324400 |
| H | 0.01207600 | 5.15633700 | -0.48705100 |
| H | 2.69963300 | 4.02762000 | -1.33998100 |
| H | 3.19067000 | 3.51314000 | 1.15176600 |
| H | 2.09736600 | 5.64914100 | 3.03985000 |
| H | 2.65259300 | 4.03082700 | 3.49347100 |
| H | 0.41654900 | 4.36003900 | -2.71489400 |
| H | 2.81173700 | 6.26285500 | -2.16111000 |
| H | 4.28577900 | 6.11799500 | 2.51365500 |
| C | 4.27434500 | 7.14918800 | 0.19817700 |
| C | 4.99952100 | 7.65799000 | -1.03903600 |

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| C | 6.34971700 | 6.99028000 | -1.18738000 |
| C | 7.15749800 | 7.18480800 | 0.08578900 |
| C | 6.37738500 | 6.65796000 | 1.29212500 |
| C | 6.99836700 | 6.95370900 | 2.65672900 |
| O | 3.93889900 | 5.80454900 | 0.03982700 |
| O | 4.20583400 | 7.44077000 | -2.18907900 |
| O | 6.94474700 | 7.58499800 | -2.31282600 |
| O | 5.10147200 | 7.33732700 | 1.32699200 |
| O | 8.18825300 | 6.25006400 | 2.88899100 |
| H | 7.34367300 | 8.25883900 | 0.22473500 |
| H | 3.37960600 | 7.75134700 | 0.38690100 |
| H | 5.16880800 | 8.73427200 | -0.89850300 |
| H | 6.19709900 | 5.91043100 | -1.33228900 |
| H | 6.21933900 | 5.57912800 | 1.19581000 |
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| C | 10.44801800 | 7.01576000 | -1.21236800 |
| C | 10.95820000 | 5.59228900 | -1.30041700 |
| C | 11.66406700 | 5.22582500 | -0.00505900 |
| C | 10.71883200 | 5.43023200 | 1.18071200 |
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| O | 8.38999000 | 6.49877800 | -0.10126600 |

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| O | 11.80551100 | 5.56306600 | -2.42069500 |
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| O | 11.59987200 | 3.87241900 | 2.84521800 |
| H | 12.53534700 | 5.88321200 | 0.12089300 |
| H | 9.37255500 | 8.28328800 | 0.16566800 |
| H | 11.31975200 | 7.67590700 | -1.10822300 |
| H | 10.10100100 | 4.91342200 | -1.42393400 |
| H | 9.84353000 | 4.78011800 | 1.08409900 |
| H | 12.23076100 | 5.85656700 | 2.65228600 |
| H | 10.60893300 | 5.56969900 | 3.29973400 |
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| H | 12.36368100 | 4.76203700 | -2.39652600 |
| H | 12.40359200 | 3.59654700 | 2.37976200 |
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| C | 14.03994600 | 2.87257900 | -1.10472900 |
| C | 13.43851600 | 1.49792300 | -1.30755300 |
| C | 13.55367600 | 0.69277400 | -0.02296000 |
| C | 12.90076100 | 1.45305900 | 1.13313500 |
| C | 13.06130000 | 0.82134100 | 2.51500400 |
| O | 12.09079900 | 3.87610800 | -0.14072200 |
| O | 13.85975400 | 3.67370700 | -2.25656200 |
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| O | 13.56228900 | 2.73414500 | 1.23170700 |
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| H | 14.61757500 | 0.54529500 | 0.20833200 |

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| H | 11.83476500 | 1.60113800 | 0.93301300 |
| H | 14.13420300 | 0.67186000 | 2.71285200 |
| H | 12.68956500 | 1.54277400 | 3.24723700 |
| H | 14.08444100 | 3.10579800 | -3.00864900 |
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| C | 13.66030000 | -1.72944000 | -0.03671800 |
| C | 13.67535300 | -2.59410100 | -1.28786100 |
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| C | 11.71405900 | -3.82781000 | -0.39353900 |
| C | 11.74421300 | -2.92065300 | 0.83790200 |
| C | 11.38955000 | -3.60347400 | 2.15883000 |
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| O | 14.19261800 | -1.85414000 | -2.37659300 |
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| C | 9.39631500 | -5.91852200 | -2.07937600 |
| C | 8.05858500 | -5.22201000 | -2.19015100 |
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| O | 9.20674400 | -5.90887700 | 0.30275900 |
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| H | 6.97053900 | -6.65227100 | -1.02282600 |
| H | 10.96650700 | -6.17784900 | -0.61720500 |
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| H | 8.22566900 | -4.13520200 | -2.17848800 |
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| O | 2.62081700 | -3.19419800 | 2.29916600 |
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| C | 0.33689800 | -1.16511200 | -1.32192100 |
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| C | 0.79719300 | 0.87250500 | 0.02402100 |
| C | 1.53065700 | 0.02103500 | 1.05802500 |
| C | 1.33096900 | 0.44133600 | 2.51398300 |

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| O | 0.98468500 | -1.31074400 | 1.01235700 |
| O | 2.00751100 | 1.61818400 | 2.85596000 |
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| H | 0.54704100 | -2.91480300 | -0.06912900 |
| H | -0.73041800 | -1.12881200 | -1.07394400 |
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| H | 2.60100300 | -0.00307100 | 0.82578400 |
| H | 0.24859600 | 0.50030500 | 2.71143700 |
| H | 1.72194800 | -0.36379200 | 3.14282700 |
| H | -0.18503300 | -2.49168800 | -2.61469400 |
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| C | -10.20538600 | 0.57361600 | -1.81795500 |
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| H | -14.29712000 | 0.18683900 | -1.55128400 |
| C | -14.90488700 | 1.80393600 | -2.74498200 |
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| C | -2.67246700 | -1.85094500 | 1.12516400 |
| H | -1.60086500 | -1.83093200 | 0.92128800 |
| H | -2.94834300 | -0.84746400 | 1.46401200 |
| C | -18.69953300 | 2.07503400 | -2.95358900 |
| H | -18.93545800 | 1.10009000 | -2.53198300 |
| C | -19.69468300 | 2.92775600 | -3.21992800 |
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| C | -21.14787000 | 2.65563800 | -2.95335200 |
| H | -21.26885800 | 1.59929900 | -2.68700300 |
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| H | -19.79085600 | 3.77346800 | -0.80607100 |
| C | -20.56109200 | 1.99420900 | 0.01564600 |
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| C | -18.39453700 | 1.19668900 | 0.67100500 |
| C | -17.24922100 | 1.39204800 | 1.63241700 |
| H | -17.25634300 | 2.41918100 | 2.00195500 |
| H | -17.42536600 | 0.72845200 | 2.48701300 |
| C | -15.89882800 | 1.04052300 | 1.00350800 |
| H | -15.72048700 | 1.69978700 | 0.14197600 |
| C | -14.76677700 | 1.20533500 | 2.00701900 |
| H | -14.74536400 | 2.24734500 | 2.34377500 |

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| H | -13.19851100 | 1.39219900 | 0.53598400 |
| C | -12.29165900 | 1.16184100 | 2.47033700 |
| H | -12.58977200 | 0.78052700 | 3.45478700 |
| H | -12.24342400 | 2.25143700 | 2.55923800 |
| C | -10.91209500 | 0.59932100 | 2.09077800 |
| H | -10.86325800 | 0.40120000 | 1.01717000 |
| H | -10.13692400 | 1.34401200 | 2.29664800 |
| C | -10.52656200 | -0.66312600 | 2.86008500 |
| H | -10.43231700 | -0.40064900 | 3.92315200 |
| C | -9.16819800 | -1.23690300 | 2.37635300 |
| H | -8.59842200 | -0.45264200 | 1.86409400 |
| C | -8.32379800 | -1.80390300 | 3.51168100 |
| H | -8.88330600 | -2.59960300 | 4.01839100 |
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| C | -6.98135000 | -2.34676200 | 3.03004100 |
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| C | -6.08115700 | -2.75024600 | 4.18886500 |
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| C | -4.74600100 | -3.35742400 | 3.75257200 |
| C | -3.77346800 | -3.48536700 | 4.91950500 |
| H | -4.12934100 | -4.24579900 | 5.61766800 |
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| C | -2.35929400 | -3.82818900 | 4.47870200 |

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| C | -2.96115900 | -2.83747700 | 2.24785500 |
| H | -3.04035200 | -3.84918000 | 1.83900400 |
| C | -0.55339100 | -3.29796300 | 2.85072600 |
| C | -21.68532400 | 1.37980600 | 0.82425600 |
| H | -21.43928600 | 0.34705000 | 1.08181900 |
| H | -22.60018400 | 1.39427200 | 0.23030900 |
| H | -21.85461000 | 1.93405000 | 1.74995000 |
| C | -21.29547500 | 4.36397600 | 0.58893100 |
| H | -22.31362800 | 4.11095200 | 0.89950200 |
| H | -21.29775600 | 5.39855900 | 0.23376600 |
| H | -20.66117800 | 4.31424700 | 1.47679500 |
| C | -22.00375400 | 2.93359000 | -4.19229800 |
| H | -21.89025800 | 3.97485100 | -4.51399200 |
| H | -23.05770200 | 2.75629800 | -3.97416700 |
| H | -21.69947900 | 2.29264500 | -5.02283900 |
| O | -3.01233600 | -5.95751700 | 0.05543800 |
| H | -3.66660000 | -5.24631900 | 0.13470200 |
| O | -3.50516900 | -5.72663600 | -4.31228100 |
| H | -3.60108900 | -6.67423400 | -4.10856900 |
| O | -1.59927000 | -3.50024300 | -2.19513100 |
| O | -3.28796400 | -3.51159800 | -0.59291300 |
| O | -4.91274200 | -4.62534200 | 3.18491300 |
| H | -5.69899400 | -4.56524400 | 2.61370800 |

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| O | -0.36192900 | -3.86034700 | 1.78644600 |
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| H | 1.30681000 | -3.25744700 | 3.29848400 |
| O | -7.16234900 | -3.49022700 | 2.19054800 |
| H | -7.98868500 | -3.35315000 | 1.69234200 |
| O | -9.43136800 | -2.24837700 | 1.40336000 |
| H | -10.32920300 | -2.55606700 | 1.65086000 |
| O | -11.48333100 | -1.70690300 | 2.75550300 |
| H | -12.23509700 | -1.40408500 | 2.20172200 |
| O | -13.31640100 | -0.56327000 | 1.16755300 |
| H | -14.18643100 | -0.83766800 | 0.82379600 |
| O | -15.89031100 | -0.31603700 | 0.56619900 |
| H | -16.71265100 | -0.45973400 | 0.06422300 |
| O | -18.40607500 | 0.32273500 | -0.18173200 |
| O | -19.37845000 | 2.05992300 | 0.87368200 |
| O | -22.99064900 | 3.04518400 | -1.50899600 |
| H | -23.44501900 | 3.71413600 | -0.98585800 |
| O | -1.55196300 | -3.73265800 | 5.63093500 |
| H | -0.62469200 | -3.70883700 | 5.35839400 |
| N | -2.87219400 | -7.42090700 | -2.27155900 |
| H | -3.50817100 | -7.47859400 | -1.47837800 |
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| O | -10.40223000 | 0.29308000 | -6.19035100 |
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| O | -3.13250700 | 3.63932800 | -1.73453900 |
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| H | -5.53050500 | 7.32111100 | 1.66697300 |
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| C | 1.03586100 | 5.31624300 | 1.89017300 |
| H | 0.91125000 | 4.60473500 | 2.71407300 |
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| C | 5.52894900 | 2.61221400 | -0.56980900 |
| H | 5.32142900 | 2.93154700 | -1.59082300 |
| C | 6.89150000 | 2.22795800 | -0.25869500 |
| H | 7.07712800 | 1.88220300 | 0.75600600 |
| C | 7.91804700 | 2.27264400 | -1.12921500 |
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| C | 9.26278400 | 1.88823500 | -0.77396500 |
| H | 9.39942300 | 1.51932900 | 0.24057200 |
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| C | 14.06177300 | 1.19941800 | -1.52230600 |
| H | 14.14489500 | 0.85240200 | -0.49244200 |
| C | 15.17568600 | 1.23695700 | -2.28148300 |
| H | 15.10199400 | 1.56133300 | -3.31889300 |
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| C | 17.60240000 | 0.82350200 | -2.53897300 |
| H | 17.55012600 | 1.05399000 | -3.60241800 |
| C | 2.20183300 | 1.69307000 | 0.20612400 |
| H | 1.18657700 | 1.93142400 | -0.11349600 |
| H | 2.55286600 | 0.88119500 | -0.43615300 |
| C | 18.88920600 | 0.43109500 | -1.99826000 |
| H | 18.92667000 | 0.31054300 | -0.91738300 |
| C | 19.98200500 | 0.16355800 | -2.72151900 |
| H | 19.94060300 | 0.26740600 | -3.80705000 |
| C | 21.28464100 | -0.32347400 | -2.15336200 |
| H | 21.24330100 | -0.25377900 | -1.06023800 |
| C | 21.52885700 | -1.80416700 | -2.50422700 |
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| H | 19.50543200 | -2.34671300 | -2.81152400 |
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| H | 19.79745000 | -1.66961800 | -0.43290000 |
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| H | 16.06876800 | -3.82659900 | 0.60128900 |
| C | 15.05504400 | -2.18537100 | -0.35142700 |
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| C | 13.70237500 | -2.87889400 | -0.42479000 |
| H | 13.67373600 | -3.49680600 | -1.32874900 |
| H | 13.59651300 | -3.54724500 | 0.43825100 |

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| C | 12.51200100 | -1.92264500 | -0.44092900 |
| H | 12.64551100 | -1.18434500 | -1.24321400 |
| C | 11.20226400 | -2.66937100 | -0.67256100 |
| H | 11.17348600 | -3.54688500 | -0.01471600 |
| H | 11.21794700 | -3.04890000 | -1.69879800 |
| C | 9.95134700 | -1.80523800 | -0.44315100 |
| H | 10.20191900 | -0.74434000 | -0.51758900 |
| H | 9.21318700 | -1.99867000 | -1.22748200 |
| C | 9.25860800 | -2.06630000 | 0.89320000 |
| H | 8.84851300 | -3.08561800 | 0.87828500 |
| C | 8.09807700 | -1.07122300 | 1.13290200 |
| H | 7.71202300 | -0.71091200 | 0.17238000 |
| C | 6.95167300 | -1.66932800 | 1.94251700 |
| H | 7.33074800 | -1.99389300 | 2.91913200 |
| H | 6.57653900 | -2.55716200 | 1.42055600 |
| C | 5.80106800 | -0.68516900 | 2.12939200 |
| H | 5.46928200 | -0.33876800 | 1.14142900 |
| C | 4.60351900 | -1.30912200 | 2.83792300 |
| H | 4.90575600 | -1.67367100 | 3.82451700 |
| H | 4.25043800 | -2.16011800 | 2.24832600 |
| C | 3.44647800 | -0.32561500 | 3.02465500 |
| C | 2.16715600 | -0.97219500 | 3.55053500 |
| H | 2.32724100 | -1.34948500 | 4.56297000 |
| H | 1.88940500 | -1.81102600 | 2.90502600 |
| C | 1.04415300 | 0.05161500 | 3.56166700 |
| H | 1.33649300 | 0.86534400 | 4.23380100 |

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| C | 0.85674200 | 0.64066000 | 2.15567300 |
| H | 0.51798900 | -0.14423300 | 1.47211500 |
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| H | 2.49032000 | 2.01793600 | 2.31877300 |
| C | -0.18712900 | 1.73305300 | 2.13356800 |
| C | 20.66848100 | -3.50612200 | 0.23295500 |
| H | 20.27306900 | -3.35174400 | 1.23953700 |
| H | 21.70842600 | -3.17821600 | 0.20062900 |
| H | 20.62547000 | -4.57356400 | 0.00623000 |
| C | 20.62346700 | -4.16269600 | -2.71095200 |
| H | 21.49400400 | -4.59932000 | -2.21217000 |
| H | 20.81123000 | -4.17209700 | -3.78853600 |
| H | 19.77106000 | -4.81610800 | -2.51194300 |
| C | 22.45916800 | 0.53127600 | -2.63804500 |
| H | 22.52052400 | 0.51824100 | -3.73192800 |
| H | 23.39918500 | 0.14826300 | -2.23835400 |
| H | 22.33564400 | 1.56997900 | -2.32332600 |
| O | 1.96052800 | 6.30779100 | 2.29722900 |
| H | 2.51317500 | 6.50007400 | 1.52694800 |
| O | -1.42399100 | 7.32672500 | -0.09615100 |
| H | -1.87714400 | 7.47723500 | 0.75190500 |
| O | 1.71933000 | 5.50473100 | -0.40220200 |
| O | 2.73166900 | 3.96150000 | 0.93008900 |
| O | 3.78189700 | 0.70198300 | 3.91335800 |
| H | 4.70271900 | 0.95268700 | 3.71694800 |
| O | 3.19376100 | 0.18191700 | 1.71759700 |

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| O | -0.77401800 | 2.10706400 | 1.13509100 |
| O | -0.37503000 | 2.30601700 | 3.32157300 |
| H | -1.07306900 | 3.00590700 | 3.21982200 |
| O | 6.22303200 | 0.44825500 | 2.89374800 |
| H | 7.16250700 | 0.60670100 | 2.68801200 |
| O | 8.63709500 | 0.07085400 | 1.80360300 |
| H | 9.36921700 | -0.31579500 | 2.32653600 |
| O | 10.12935000 | -1.96683900 | 2.01180300 |
| H | 11.02584300 | -1.71843100 | 1.70028100 |
| O | 12.40648100 | -1.22088500 | 0.80095300 |
| H | 13.31169900 | -1.02999300 | 1.10731500 |
| O | 15.05655400 | -1.36666400 | 0.81522700 |
| H | 15.97027500 | -1.05562500 | 0.94435300 |
| O | 17.72459600 | -1.48469500 | 0.41060200 |
| O | 18.50323200 | -3.23047700 | -0.78134500 |
| O | 22.69941200 | -2.19480400 | -1.79237000 |
| H | 23.05079200 | -2.99765800 | -2.19191200 |
| O | -0.13690900 | -0.57236700 | 4.02151300 |
| H | -0.78218000 | 0.11843600 | 4.24137300 |
| N | -0.91352600 | 6.76219700 | 2.58738600 |
| H | -0.17990500 | 7.33317900 | 3.00295500 |
| H | -1.26790800 | 6.14138300 | 3.30868200 |

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| O | 11.38699700 | -0.72325300 | -5.88382100 |
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| H | 15.04527100 | -2.61449200 | -2.03628000 |
| H | 12.16675900 | -0.22572200 | -5.51492700 |
| C | 14.51776900 | -0.54560100 | -4.12873300 |
| C | 15.51357300 | 0.01715100 | -3.09142800 |
| C | 14.85539100 | 1.10474200 | -2.22058400 |
| C | 14.32185600 | 2.21491800 | -3.15530100 |

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| C | 13.31654500 | 1.62625100 | -4.16540100 |
| C | 12.96696800 | 2.57039100 | -5.33453300 |
| O | 13.44677900 | -1.22227100 | -3.46033600 |
| O | 15.97707300 | -1.07827900 | -2.29653200 |
| O | 15.92893200 | 1.58233100 | -1.41509400 |
| O | 13.93375900 | 0.51088000 | -4.87863200 |
| O | 11.85666700 | 3.38265900 | -4.98744400 |
| H | 15.16279000 | 2.73981900 | -3.66231600 |
| H | 14.99993600 | -1.17690800 | -4.90805000 |
| H | 16.41268600 | 0.43237200 | -3.61591500 |
| H | 14.05275900 | 0.70266000 | -1.56102400 |
| H | 12.39814700 | 1.25867000 | -3.65078100 |
| H | 13.82219800 | 3.19289800 | -5.64626100 |
| H | 12.60201500 | 1.98782200 | -6.20984600 |
| H | 16.41379500 | -0.71662500 | -1.47766800 |
| H | 15.63608500 | 2.40611200 | -0.91102100 |
| H | 12.10590300 | 4.00615300 | -4.25184400 |
| C | 14.03019100 | 4.49157500 | -2.35705500 |
| C | 14.38219400 | 5.00842400 | -0.94448200 |
| C | 13.13565100 | 5.06667400 | -0.03940600 |
| C | 12.07815800 | 5.95524900 | -0.73451000 |
| C | 11.72302800 | 5.36858300 | -2.11525800 |
| C | 10.88720000 | 6.30627800 | -3.01008200 |
| O | 13.60712100 | 3.12568700 | -2.28563300 |
| O | 15.37850000 | 4.13659700 | -0.40263300 |
| O | 13.61730500 | 5.67278400 | 1.15623900 |

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| O | 12.94517200 | 5.23088600 | -2.90336600 |
| O | 9.50393600 | 6.09206400 | -2.77665500 |
| H | 12.43590800 | 7.00700700 | -0.80993400 |
| H | 14.84430600 | 4.64736800 | -3.09971900 |
| H | 14.85265600 | 6.02280500 | -1.01903100 |
| H | 12.73101100 | 4.05748900 | 0.20247800 |
| H | 11.24238600 | 4.36723000 | -2.01771400 |
| H | 11.14600600 | 7.36886800 | -2.86880300 |
| H | 11.01628900 | 6.03890400 | -4.08295300 |
| H | 15.44427100 | 4.29609300 | 0.57797700 |
| H | 12.83863900 | 5.94428700 | 1.73931600 |
| H | 9.26329100 | 6.38344200 | -1.85485600 |
| C | 10.36881300 | 7.14266700 | 0.51867700 |
| C | 10.28250100 | 7.20828300 | 2.05846500 |
| C | 9.27747200 | 6.17736600 | 2.60762900 |
| C | 7.90334000 | 6.43514900 | 1.94664700 |
| C | 8.02223600 | 6.34001700 | 0.41187200 |
| C | 6.80127400 | 6.89159400 | -0.35387800 |
| O | 10.90727900 | 5.87875100 | 0.11281900 |
| O | 11.59757600 | 6.97698800 | 2.57275400 |
| O | 9.23949700 | 6.46934200 | 4.00164800 |
| O | 9.07288100 | 7.24087000 | -0.05502000 |
| O | 5.81861500 | 5.87839600 | -0.49820800 |
| H | 7.48965600 | 7.41662400 | 2.27169700 |
| H | 10.91417500 | 8.00218700 | 0.06880000 |
| H | 9.99003100 | 8.24132000 | 2.37921100 |

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| H | 9.61270500 | 5.12568200 | 2.45927400 |
| H | 8.27032900 | 5.30161500 | 0.09168500 |
| H | 6.37068800 | 7.78580000 | 0.12746500 |
| H | 7.07852700 | 7.13996600 | -1.40270400 |
| H | 11.52981500 | 6.79438900 | 3.54979500 |
| H | 8.52809200 | 5.91106500 | 4.44727000 |
| H | 5.45115500 | 5.63073000 | 0.39379200 |
| C | 5.86654600 | 5.76456300 | 3.08640700 |
| C | 5.77095800 | 5.05866100 | 4.45695700 |
| C | 5.54896500 | 3.54105800 | 4.29756200 |
| C | 4.26677100 | 3.33552200 | 3.45823300 |
| C | 4.44590800 | 3.99386100 | 2.07529600 |
| C | 3.15286200 | 4.07810800 | 1.23879600 |
| O | 7.05166700 | 5.35279100 | 2.39756300 |
| O | 6.97471700 | 5.33331300 | 5.17768900 |
| O | 5.38005900 | 3.08915000 | 5.63668900 |
| O | 4.76321500 | 5.40720700 | 2.26138100 |
| O | 2.97662300 | 2.88120600 | 0.49623600 |
| H | 3.37509700 | 3.73292100 | 3.99394800 |
| H | 5.78000700 | 6.87261300 | 3.15551300 |
| H | 4.93599300 | 5.50904300 | 5.05442200 |
| H | 6.42474600 | 3.02107600 | 3.84693800 |
| H | 5.26964600 | 3.51090600 | 1.50011100 |
| H | 2.26310800 | 4.28771100 | 1.85564700 |
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| H | 7.05518800 | 4.68481300 | 5.92886000 |

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| H | 5.02469200 | 2.14310000 | 5.63862400 |
| H | 2.81377400 | 2.11678100 | 1.11230600 |
| C | 2.90763300 | 1.33921600 | 3.71510000 |
| C | 3.16690500 | 0.22264500 | 4.74574800 |
| C | 3.95716100 | -0.93806800 | 4.11602900 |
| C | 3.14899900 | -1.47860800 | 2.91436600 |
| C | 2.86381700 | -0.35489600 | 1.89716500 |
| C | 1.75877600 | -0.69868700 | 0.87645000 |
| O | 4.14821500 | 1.90441600 | 3.27440600 |
| O | 3.86664700 | 0.79638700 | 5.85178100 |
| O | 4.02064000 | -1.90098700 | 5.16381400 |
| O | 2.27020300 | 0.79935100 | 2.56485000 |
| O | 2.30318800 | -1.39524000 | -0.23268000 |
| H | 2.20741400 | -1.97944600 | 3.26697900 |
| H | 2.18888700 | 2.11264900 | 4.06737900 |
| H | 2.17888500 | -0.15550500 | 5.15397700 |
| H | 4.98971300 | -0.64677000 | 3.81581500 |
| H | 3.80312600 | -0.02966700 | 1.39112800 |
| H | 0.93380700 | -1.27579900 | 1.32749000 |
| H | 1.34649800 | 0.23079900 | 0.42283300 |
| H | 4.24292300 | 0.05840800 | 6.40790300 |
| H | 4.45368900 | -2.74549900 | 4.82653300 |
| H | 2.70571000 | -2.25708800 | 0.06139400 |
| C | 3.51906900 | -3.76194800 | 2.15868600 |
| C | 4.52391500 | -4.77395400 | 2.75317500 |
| C | 5.83141200 | -4.81058200 | 1.93687600 |

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| C | 5.46357900 | -5.15697800 | 0.47510700 |
| C | 4.50712600 | -4.08755900 | -0.08998300 |
| C | 3.88239200 | -4.44769700 | -1.45255800 |
| O | 4.02987000 | -2.43246300 | 2.27090400 |
| O | 4.75882100 | -4.40269300 | 4.11352500 |
| O | 6.58332900 | -5.85298500 | 2.54801000 |
| O | 3.32635700 | -4.01312900 | 0.77033200 |
| O | 4.70498100 | -3.96514200 | -2.50323100 |
| H | 5.02509000 | -6.17882100 | 0.41163800 |
| H | 2.49438000 | -3.86107200 | 2.58030500 |
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| H | 6.41012800 | -3.86099300 | 2.00393800 |
| H | 4.99208900 | -3.08380100 | -0.12198800 |
| H | 3.70364000 | -5.52997400 | -1.56492200 |
| H | 2.92410500 | -3.90078900 | -1.59930800 |
| H | 5.59598300 | -4.84213100 | 4.42759900 |
| H | 7.33942500 | -6.13351300 | 1.93714900 |
| H | 5.57737900 | -4.44783000 | -2.50778000 |
| C | 6.99784300 | -6.25047400 | -1.05683300 |
| C | 8.34548800 | -6.87099700 | -0.63030500 |
| C | 9.52314500 | -5.92423700 | -0.93288400 |
| C | 9.49323800 | -5.58211800 | -2.44085100 |
| C | 8.14855100 | -4.92085300 | -2.80617000 |
| C | 7.89100600 | -4.80084700 | -4.32234200 |
| O | 6.71207300 | -5.09863900 | -0.25099900 |
| O | 8.25772800 | -7.16154100 | 0.76871900 |

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| O | 10.66661400 | -6.70653800 | -0.60332200 |
| O | 7.05404200 | -5.80091600 | -2.40201500 |
| O | 8.44132700 | -3.58786700 | -4.81084000 |
| H | 9.68747600 | -6.49149000 | -3.05394400 |
| H | 6.15881100 | -6.98150600 | -1.06494200 |
| H | 8.49561900 | -7.85095900 | -1.15259500 |
| H | 9.51262700 | -5.00579700 | -0.30306300 |
| H | 8.02839600 | -3.93846000 | -2.29408100 |
| H | 8.28386300 | -5.66281500 | -4.88732200 |
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| H | 9.17233200 | -7.36904100 | 1.10701600 |
| H | 11.50507800 | -6.22705800 | -0.89823300 |
| H | 9.43508700 | -3.61729000 | -4.75394200 |
| C | -20.57690100 | 5.41698400 | -0.83308700 |
| H | -21.43060400 | 5.26420500 | -1.54516600 |
| C | -19.61286700 | 6.46952200 | -1.43867700 |
| H | -18.88332200 | 6.83046800 | -0.68091300 |
| C | -18.89918000 | 5.92717100 | -2.70115900 |
| H | -19.63483500 | 5.68219100 | -3.49830800 |
| C | -19.03306100 | 3.64797900 | -1.85498100 |
| H | -19.63216600 | 3.25024900 | -2.70065700 |
| C | -19.85390900 | 4.06038300 | -0.61083700 |
| H | -20.58255600 | 3.25944900 | -0.34407900 |
| C | -17.80821600 | 6.85794800 | -3.19638200 |
| H | -16.96751100 | 6.90216600 | -2.49133900 |
| H | -18.20477700 | 7.87750900 | -3.31660200 |

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| H | -17.40486400 | 6.52640500 | -4.15976000 |
| C | -17.09601500 | 2.21540500 | -2.28276800 |
| H | -16.66822800 | 3.10830700 | -2.79588000 |
| C | -16.11743200 | 1.52815400 | -1.37104700 |
| H | -16.55448000 | 0.74372600 | -0.74579300 |
| C | -14.81707900 | 1.84680000 | -1.33408000 |
| H | -14.40688800 | 2.64793000 | -1.95484800 |
| C | -13.86570200 | 1.14567000 | -0.47348600 |
| H | -14.26704700 | 0.31304200 | 0.11840100 |
| C | -12.56524600 | 1.48128100 | -0.39254500 |
| H | -12.15445900 | 2.31941000 | -0.95901800 |
| C | -11.63196100 | 0.74200800 | 0.45296000 |
| H | -12.05302600 | -0.13141500 | 0.97543600 |
| C | -10.33754300 | 1.08095900 | 0.59405900 |
| H | -9.92139300 | 1.95829400 | 0.09441600 |
| C | -9.41742200 | 0.30438300 | 1.41926100 |
| H | -9.80840300 | -0.63991800 | 1.82649600 |
| C | -8.15341200 | 0.69088400 | 1.67409100 |
| H | -7.75370200 | 1.62749300 | 1.28068700 |
| C | -7.25107000 | -0.11113200 | 2.49434000 |
| H | -7.66999600 | -1.04338200 | 2.89229700 |
| C | -5.98218000 | 0.25131800 | 2.76058300 |
| H | -5.56583300 | 1.18495700 | 2.37606500 |
| C | -5.09170400 | -0.57371700 | 3.56947300 |
| H | -5.53545700 | -1.47399600 | 4.01296100 |
| C | -3.79328300 | -0.28708300 | 3.77701700 |

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| H | -3.32654700 | 0.60839700 | 3.36541500 |
| C | -17.72718800 | 1.25604300 | -3.30377600 |
| H | -18.37645700 | 1.83287900 | -3.99624200 |
| H | -16.92132100 | 0.81877400 | -3.93366500 |
| C | -2.93807600 | -1.18460900 | 4.55259700 |
| H | -3.46979300 | -1.97708300 | 5.09953400 |
| C | -1.60124700 | -1.10220200 | 4.58312900 |
| H | -1.05292600 | -0.31939000 | 4.06287000 |
| C | -0.75671300 | -2.09335200 | 5.33948900 |
| H | -1.40160700 | -2.73928400 | 5.99591000 |
| C | -0.01988700 | -3.03840400 | 4.35230400 |
| H | 0.82311600 | -2.50329400 | 3.84238300 |
| C | -0.94493100 | -3.68794300 | 3.29284300 |
| H | -1.50692600 | -2.85633600 | 2.78172000 |
| C | -2.00891000 | -4.58647700 | 3.95396700 |
| H | -2.48738800 | -4.06380100 | 4.81816800 |
| C | -4.29931300 | -4.29903200 | 3.12064700 |
| C | -5.18542200 | -4.62503300 | 1.95534900 |
| H | -4.60198200 | -4.64343200 | 1.01015300 |
| H | -5.56300700 | -5.66689600 | 2.08338700 |
| C | -6.37199200 | -3.64567100 | 1.85510200 |
| H | -6.01043600 | -2.59484000 | 1.75579400 |
| C | -7.33040900 | -4.04656900 | 0.73043900 |
| H | -6.76483900 | -4.24767400 | -0.19947800 |
| H | -7.82244000 | -5.00741300 | 1.00295700 |
| C | -8.41356700 | -2.98797300 | 0.46579800 |

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| H | -7.97615900 | -1.96965900 | 0.33520800 |
| C | -9.27356900 | -3.38860500 | -0.74635500 |
| H | -9.56964700 | -4.45504700 | -0.65618600 |
| H | -8.65351800 | -3.32520900 | -1.66146600 |
| C | -10.52328800 | -2.51447500 | -0.90395900 |
| H | -10.44503400 | -1.61194500 | -0.25521900 |
| H | -10.58927200 | -2.12555500 | -1.93784900 |
| C | -11.80304100 | -3.28352100 | -0.55724600 |
| H | -11.92532200 | -4.18202300 | -1.20364200 |
| C | -13.06989400 | -2.37516400 | -0.60377000 |
| H | -12.90579800 | -1.43972400 | -1.18510800 |
| C | -14.28848900 | -3.15514300 | -1.11424100 |
| H | -14.45279900 | -4.04521500 | -0.46875900 |
| H | -14.09236100 | -3.54561700 | -2.12964400 |
| C | -15.55884600 | -2.29277100 | -1.11055100 |
| H | -15.39088400 | -1.29845400 | -1.59060900 |
| C | -16.74900000 | -3.02083100 | -1.75216900 |
| H | -17.00797100 | -3.91440200 | -1.14465600 |
| H | -16.46692800 | -3.38344400 | -2.75874000 |
| C | -17.99185200 | -2.12745600 | -1.84887200 |
| C | -19.16307800 | -2.74888900 | -2.61486500 |
| H | -19.58973400 | -3.59879900 | -2.04242500 |
| H | -18.81732200 | -3.17849800 | -3.57786000 |
| C | -20.26292000 | -1.72013900 | -2.88388700 |
| H | -20.85367800 | -1.49503300 | -1.96818000 |
| C | -19.69625400 | -0.40980500 | -3.50383800 |

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| H | -19.30270200 | -0.67188200 | -4.52630900 |
| C | -18.51466800 | 0.12343400 | -2.64266600 |
| H | -18.87034200 | 0.39167800 | -1.61856300 |
| C | -20.75501600 | 0.63674800 | -3.67836400 |
| C | -1.59406600 | -5.99338000 | 4.32478600 |
| H | -2.41622400 | -6.53931700 | 4.80592700 |
| H | -0.75513700 | -5.96367800 | 5.03912700 |
| H | -1.28691800 | -6.58424200 | 3.45374100 |
| C | -0.13908700 | -4.41631100 | 2.21880300 |
| H | 0.50915700 | -5.19503800 | 2.63200600 |
| H | 0.47362100 | -3.72706700 | 1.62644600 |
| H | -0.82013600 | -4.91526700 | 1.51098200 |
| C | 0.25028400 | -1.38104800 | 6.24419000 |
| H | 0.92605100 | -0.71380600 | 5.68595000 |
| H | 0.87745500 | -2.11725400 | 6.77092700 |
| H | -0.26029500 | -0.77496900 | 7.00161400 |
| O | -19.03415000 | 4.19502300 | 0.55249000 |
| H | -18.07993700 | 4.04683200 | 0.31748300 |
| O | -20.36922600 | 7.58891300 | -1.92284700 |
| H | -20.99067800 | 7.89453000 | -1.21784000 |
| O | -18.18917400 | 4.71509300 | -2.33153300 |
| O | -18.11942300 | 2.68520300 | -1.34491100 |
| O | -18.50187000 | -1.73860600 | -0.59274700 |
| H | -17.76798500 | -1.54014600 | 0.06614800 |
| O | -17.53685200 | -0.93355400 | -2.52476600 |
| O | -20.65635600 | 1.83015500 | -3.85664400 |

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| O | -22.02340900 | 0.08919300 | -3.64131800 |
| H | -22.74082600 | 0.76474100 | -3.78119100 |
| O | -15.97612200 | -2.04639500 | 0.24866000 |
| H | -15.19633400 | -1.75249500 | 0.80327900 |
| O | -13.33763700 | -1.89058900 | 0.72235900 |
| H | -13.11219200 | -2.61856900 | 1.38669700 |
| O | -11.77670100 | -3.81333500 | 0.77713700 |
| H | -10.95591500 | -3.48783400 | 1.27375800 |
| O | -9.30480600 | -2.85699900 | 1.59600100 |
| H | -8.89604500 | -3.23136800 | 2.42571500 |
| O | -7.17271100 | -3.72967900 | 3.04793200 |
| H | -6.63111500 | -3.52406600 | 3.85845300 |
| O | -4.62008900 | -3.72142900 | 4.14312100 |
| O | -3.04218100 | -4.75992500 | 2.89364600 |
| O | 0.54883200 | -4.03926100 | 5.21775800 |
| H | 1.13870800 | -4.63475200 | 4.72017800 |
| O | -21.09758800 | -2.36501900 | -3.85457100 |
| H | -21.95429100 | -1.88662800 | -3.95474700 |
| N | -21.11661000 | 5.98303700 | 0.43042300 |
| H | -20.37913800 | 6.00443800 | 1.14074600 |
| H | -21.85289400 | 5.38733500 | 0.80132700 |

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| C | 4.39130700 | -7.17157100 | -1.49367800 |
| C | 4.40764100 | -6.07402100 | -2.61253600 |
| C | 2.97513300 | -5.75906800 | -3.11458600 |
| C | 2.25308900 | -7.08117400 | -3.50096100 |
| C | 2.37010200 | -8.14239500 | -2.35603700 |
| C | 1.82373600 | -9.55218600 | -2.76914600 |
| O | 3.76405300 | -6.67319700 | -0.29547100 |
| O | 5.03862900 | -4.89777400 | -2.09437000 |
| O | 3.10539300 | -4.85410600 | -4.21397700 |
| O | 3.74161100 | -8.36051200 | -1.96152400 |
| O | 0.41558400 | -9.70640300 | -2.60124400 |
| H | 2.70847300 | -7.47787100 | -4.41462600 |
| H | 5.42896500 | -7.47524100 | -1.29339000 |
| H | 4.98666400 | -6.47923100 | -3.45301200 |
| H | 2.41007200 | -5.30506000 | -2.28863500 |
| H | 1.76790400 | -7.78385700 | -1.51501700 |
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| H | 2.30589800 | -10.27891300 | -2.10846700 |
| H | 4.94385700 | -4.22340900 | -2.80820200 |
| H | 2.27284400 | -4.95722300 | -4.74508700 |
| H | -0.00520000 | -9.15056300 | -3.30539300 |
| C | 0.26398300 | -7.24301300 | -4.87242800 |
| C | -0.13810000 | -6.05201200 | -5.80131100 |
| C | -1.26181500 | -5.19913600 | -5.15228800 |
| C | -2.40446100 | -6.11399300 | -4.62206600 |
| C | -1.83959100 | -7.28386600 | -3.74870800 |

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| C | -2.94355000 | -8.29954100 | -3.29370100 |
| O | 0.88181800 | -6.70442800 | -3.70152200 |
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| O | -1.70951200 | -4.26511300 | -6.13712100 |
| O | -0.85794500 | -8.05102300 | -4.48655700 |
| O | -3.63766600 | -7.90554800 | -2.11163600 |
| H | -2.95097300 | -6.53127800 | -5.47476800 |
| H | 0.93600800 | -7.91477900 | -5.42600300 |
| H | -0.50602800 | -6.45680300 | -6.75273900 |
| H | -0.83472300 | -4.68474700 | -4.27985700 |
| H | -1.38135600 | -6.84993700 | -2.85210400 |
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| H | -2.62919400 | -4.00733600 | -5.86396400 |
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| C | -4.63416600 | -5.37134400 | -4.03795300 |
| C | -5.17147300 | -4.02120000 | -4.61564400 |
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| C | -5.06787900 | -4.71745800 | -1.79211300 |
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| O | -3.22495600 | -5.24228900 | -3.82862400 |
| O | -4.36168500 | -3.70628000 | -5.76008300 |
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| H | -6.81748700 | -3.58023800 | -2.40006200 |
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| H | -6.70175400 | -5.02166500 | -0.37295100 |
| H | -5.52354500 | -6.33798500 | -0.42094500 |
| H | -4.64267400 | -2.78921800 | -5.99805800 |
| H | -5.90069700 | -1.10079100 | -3.40234200 |
| H | -5.48867400 | -4.54924600 | 1.38012200 |
| C | -6.74363900 | -1.75680200 | -0.75222500 |
| C | -6.60588200 | -0.20320600 | -0.93555600 |
| C | -5.59183000 | 0.41064000 | 0.07848100 |
| C | -5.81950100 | -0.16649800 | 1.52118200 |
| C | -5.92037800 | -1.72426100 | 1.46496000 |
| C | -6.23396900 | -2.32542400 | 2.86922600 |
| O | -5.54454000 | -2.37712800 | -1.22909400 |
| O | -6.24179800 | 0.00361000 | -2.29982100 |
| O | -5.76368900 | 1.83308200 | 0.03524900 |
| O | -7.00010600 | -2.13340600 | 0.60468700 |
| O | -5.86960200 | -3.71294300 | 2.96876400 |
| H | -6.76005100 | 0.22948300 | 1.91814900 |
| H | -7.62593200 | -2.08779700 | -1.31855700 |
| H | -7.58806200 | 0.24195600 | -0.72148100 |
| H | -4.57693400 | 0.13076400 | -0.23078400 |

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| H | -7.31362900 | -2.25767200 | 3.03364600 |
| H | -5.79453300 | 0.89162900 | -2.40013300 |
| H | -4.94985800 | 2.20997200 | 0.46771400 |
| H | -4.92729200 | -3.69905500 | 3.26793800 |
| C | -4.89601000 | 1.36262900 | 3.13880600 |
| C | -3.75522700 | 2.38750200 | 2.81545200 |
| C | -2.37472500 | 1.90527900 | 3.34184300 |
| C | -2.50399200 | 1.46198300 | 4.82966600 |
| C | -3.69785300 | 0.46276900 | 4.99443600 |
| C | -3.95835700 | 0.05171400 | 6.48224400 |
| O | -4.70644700 | 0.16215700 | 2.37468700 |
| O | -3.70961800 | 2.57242100 | 1.39470200 |
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| O | -3.07343400 | -0.95311200 | 6.97614200 |
| H | -2.69380200 | 2.34719600 | 5.44552000 |
| H | -5.86369000 | 1.83986300 | 2.92229500 |
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| H | -3.46578800 | -0.44100200 | 4.41856000 |
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| H | -4.97043400 | -0.36238100 | 6.51958100 |
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| H | -0.71647900 | 2.83287500 | 3.78458000 |

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| H | -2.21146100 | -0.49229400 | 7.13330000 |
| C | -0.65632600 | 1.30536800 | 6.38178200 |
| C | 0.72494800 | 1.95416900 | 6.04774800 |
| C | 1.73403200 | 0.88826500 | 5.54488300 |
| C | 1.78426700 | -0.29743800 | 6.55424100 |
| C | 0.34111100 | -0.82906100 | 6.85406400 |
| C | 0.31525600 | -1.91150000 | 7.98711600 |
| O | -1.25555300 | 0.83138100 | 5.17343100 |
| O | 0.49429100 | 2.96057900 | 5.05189700 |
| O | 2.98297500 | 1.56182100 | 5.38401600 |
| O | -0.53423800 | 0.22435500 | 7.31957500 |
| O | 0.71573700 | -3.21273000 | 7.56362300 |
| H | 2.24130600 | 0.04987300 | 7.48674000 |
| H | -1.28350400 | 2.05422800 | 6.88712400 |
| H | 1.12498200 | 2.40458200 | 6.96540000 |
| H | 1.36793200 | 0.48693800 | 4.58950700 |
| H | -0.05450100 | -1.27346700 | 5.93260500 |
| H | 0.90760600 | -1.54589400 | 8.83510800 |
| H | -0.72158800 | -1.99048500 | 8.32700100 |
| H | 1.40248100 | 3.23057300 | 4.77111900 |
| H | 3.67825000 | 0.85361500 | 5.36856700 |
| H | 1.69854500 | -3.16757800 | 7.45436200 |
| C | 3.65928900 | -1.82505700 | 6.70260200 |
| C | 4.99242400 | -1.56478700 | 5.92977500 |
| C | 5.04623700 | -2.40450900 | 4.62638700 |
| C | 4.74769800 | -3.89683200 | 4.95522500 |

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| C | 3.42675900 | -4.03193700 | 5.78584100 |
| C | 3.16633900 | -5.49519900 | 6.28445300 |
| O | 2.56620300 | -1.32977900 | 5.92499900 |
| O | 5.05697200 | -0.15979200 | 5.64723900 |
| O | 6.33834300 | -2.19548900 | 4.05413100 |
| O | 3.46204100 | -3.21965800 | 6.98322000 |
| O | 2.59529900 | -6.35312600 | 5.29951600 |
| H | 5.58244200 | -4.30606600 | 5.53399000 |
| H | 3.72030400 | -1.33743100 | 7.68663500 |
| H | 5.82828000 | -1.86627600 | 6.57430000 |
| H | 4.24920000 | -2.05339700 | 3.95612200 |
| H | 2.59059200 | -3.72625200 | 5.14532000 |
| H | 4.09820500 | -5.89647800 | 6.70190600 |
| H | 2.44682200 | -5.42705600 | 7.10567200 |
| H | 5.82551000 | -0.07345800 | 5.03247700 |
| H | 6.48380500 | -2.95027900 | 3.42551700 |
| H | 3.32928100 | -6.56446400 | 4.66934600 |
| C | 5.38076200 | -5.74024500 | 3.51658800 |
| C | 6.34280100 | -5.54112100 | 2.30266800 |
| C | 5.57028600 | -5.45845000 | 0.95629200 |
| C | 4.63293800 | -6.70942300 | 0.85635300 |
| C | 3.71867700 | -6.72614300 | 2.12791500 |
| C | 2.69628300 | -7.90241900 | 2.09061600 |
| O | 4.60333600 | -4.55228500 | 3.68298800 |
| O | 7.08210000 | -4.33273100 | 2.53005800 |
| O | 6.58054000 | -5.35006000 | -0.04399700 |

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| O | 4.50534400 | -6.86411900 | 3.33187000 |
| O | 1.60403600 | -7.60835900 | 1.21730000 |
| H | 5.24377800 | -7.61942700 | 0.85101400 |
| H | 5.97711400 | -5.97406500 | 4.41052900 |
| H | 7.02088800 | -6.40308200 | 2.25624500 |
| H | 4.92817100 | -4.56814600 | 0.97765300 |
| H | 3.15253300 | -5.78752400 | 2.15736000 |
| H | 3.21790600 | -8.82453800 | 1.80445300 |
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| H | 7.52447000 | -4.16861400 | 1.66143600 |
| H | 6.09539900 | -5.08363600 | -0.86813300 |
| H | 2.06076100 | -7.30248800 | 0.39536500 |
| C | -9.36014300 | 4.03800600 | 2.48029400 |
| H | -10.09118700 | 4.75580100 | 2.10287700 |
| C | -8.66743500 | 4.65516200 | 3.72587600 |
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| C | -7.84145100 | 5.90896500 | 3.30472300 |
| H | -8.53118200 | 6.64373400 | 2.86732000 |
| C | -7.42025500 | 5.03269700 | 1.14717700 |
| H | -8.04790500 | 5.81035300 | 0.67510500 |
| C | -8.30755600 | 3.75288800 | 1.36794100 |
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| H | -6.59006500 | 7.44099400 | 4.20248700 |

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| C | -5.76993300 | 5.72644900 | -0.44539900 |
| H | -5.88437400 | 6.67295600 | 0.09390000 |
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| H | -4.05580500 | 4.51331900 | -1.14810400 |
| C | -3.30139800 | 6.13368000 | -0.08102300 |
| H | -3.50813200 | 7.03788200 | 0.47989500 |
| C | -1.87923100 | 5.73803000 | -0.21361100 |
| H | -1.70066400 | 4.83059200 | -0.77901600 |
| C | -0.84127600 | 6.37336900 | 0.30829900 |
| H | -0.97274100 | 7.28441000 | 0.88042000 |
| C | 0.53568300 | 5.85647800 | 0.15862100 |
| H | 0.61403000 | 4.92987600 | -0.40029100 |
| C | 1.63470000 | 6.41226700 | 0.64808400 |
| H | 1.58814900 | 7.34170000 | 1.20302200 |
| C | 2.96702000 | 5.79678800 | 0.47716200 |
| H | 2.96924600 | 4.83578800 | -0.02582300 |
| C | 4.11970100 | 6.30988200 | 0.88298800 |
| H | 4.15210800 | 7.27128000 | 1.38177600 |
| C | 5.40842800 | 5.61657100 | 0.67838300 |
| H | 5.33723700 | 4.62702700 | 0.24028100 |
| C | 6.60467500 | 6.10394000 | 0.97362000 |
| H | 6.70563700 | 7.09367600 | 1.40345800 |
| C | 7.85367800 | 5.35392900 | 0.72143200 |
| H | 7.72251400 | 4.33994000 | 0.36024800 |
| C | 9.07927700 | 5.82817400 | 0.88069900 |
| H | 9.23505900 | 6.84248800 | 1.22989000 |

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| C | -6.49520600 | 5.83221000 | -1.82408100 |
| H | -7.51144400 | 6.17789900 | -1.66011200 |
| H | -5.98741100 | 6.56111800 | -2.45115300 |
| C | 10.29291700 | 5.03688200 | 0.56536200 |
| H | 10.11319500 | 4.00155500 | 0.29897000 |
| C | 11.52294000 | 5.50867700 | 0.56014300 |
| H | 11.71000100 | 6.54331300 | 0.82653000 |
| C | 12.75561800 | 4.68340700 | 0.20113200 |
| H | 12.44021800 | 3.66897800 | -0.03661400 |
| C | 13.50495700 | 5.25951300 | -1.04688000 |
| H | 13.95049600 | 6.21828900 | -0.74961000 |
| C | 12.56579400 | 5.57759800 | -2.26290400 |
| H | 11.81834400 | 6.27806000 | -1.89228900 |
| C | 11.76630400 | 4.34336000 | -2.78503200 |
| H | 11.27297400 | 3.86132500 | -1.93777100 |
| C | 9.54027100 | 4.21707600 | -3.61287700 |
| C | 8.47066200 | 4.88412800 | -4.50854600 |
| H | 8.68919100 | 5.94498700 | -4.59844300 |
| H | 8.51719200 | 4.43981600 | -5.50179700 |
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| H | 7.05315200 | 5.15660000 | -2.90250800 |
| C | 5.92702800 | 5.26863700 | -4.74439000 |
| H | 6.05841200 | 6.34625700 | -4.79747100 |
| H | 5.97585800 | 4.86864400 | -5.75475800 |
| C | 4.53983800 | 4.93676100 | -4.12470400 |
| H | 4.55290500 | 5.26649400 | -3.07558400 |

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| C | 3.38768200 | 5.67944500 | -4.85007200 |
| H | 3.31384300 | 5.31072300 | -5.87140400 |
| H | 3.65182700 | 6.73322100 | -4.90233600 |
| C | 2.01450100 | 5.56062700 | -4.14303500 |
| H | 2.13670000 | 5.73216600 | -3.07502000 |
| H | 1.37673100 | 6.35534700 | -4.52338600 |
| C | 1.25558800 | 4.21748400 | -4.36479500 |
| H | 1.16155500 | 4.05762400 | -5.44716000 |
| C | -0.18581800 | 4.29354600 | -3.72754200 |
| H | -0.44736000 | 5.33810800 | -3.52713900 |
| C | -1.28735800 | 3.69353100 | -4.64787300 |
| H | -1.00450800 | 2.69078600 | -4.96129700 |
| H | -1.39315700 | 4.31079300 | -5.53645100 |
| C | -2.63273500 | 3.63733000 | -3.87445800 |
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| C | -3.82354500 | 3.16786800 | -4.74871300 |
| H | -3.61399500 | 2.18739200 | -5.17017400 |
| H | -3.97588900 | 3.86773600 | -5.56558900 |
| C | -5.13418800 | 3.07822100 | -3.90083000 |
| C | -6.33316000 | 2.64737200 | -4.79999200 |
| H | -6.20371000 | 1.61172400 | -5.10340500 |
| H | -6.33289700 | 3.26394600 | -5.69508600 |
| C | -7.69746000 | 2.80902200 | -4.08996800 |
| H | -7.76271300 | 2.06970300 | -3.28197800 |
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| H | -7.80317000 | 4.97969100 | -4.23686100 |

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| C | -6.52631200 | 4.46038600 | -2.55420900 |
| H | -6.50022300 | 3.66720800 | -1.79768700 |
| C | -9.11688400 | 4.39371400 | -2.65012100 |
| C | 12.60857600 | 3.27966700 | -3.52800300 |
| H | 11.99621900 | 2.41044800 | -3.74669500 |
| H | 13.44021500 | 2.97674000 | -2.90056000 |
| H | 12.99408700 | 3.67446500 | -4.46174400 |
| C | 13.33425200 | 6.29298100 | -3.39786500 |
| H | 14.13449500 | 5.67781900 | -3.79550400 |
| H | 13.76702900 | 7.21878400 | -3.03079300 |
| H | 12.65730300 | 6.53245100 | -4.21154900 |
| C | 13.73297200 | 4.60861400 | 1.40005100 |
| H | 14.04897800 | 5.60308600 | 1.70093200 |
| H | 14.61256800 | 4.03423700 | 1.12702400 |
| H | 13.25391200 | 4.12997700 | 2.24875600 |
| O | -7.55607400 | 2.60759200 | 1.75293700 |
| H | -6.93614600 | 2.41478800 | 0.99409100 |
| O | -9.63474800 | 5.04155100 | 4.70787400 |
| H | -10.23326700 | 4.25309800 | 4.74199700 |
| O | -6.82709700 | 5.54481900 | 2.35110400 |
| O | -6.34216700 | 4.62897100 | 0.30362900 |
| O | -4.97550500 | 2.15171200 | -2.82637900 |
| H | -4.02626600 | 2.25244200 | -2.54440300 |
| O | -5.34739600 | 4.40472000 | -3.37773800 |
| O | -9.46422600 | 5.34826600 | -1.97977800 |
| O | -9.96341500 | 3.29339100 | -2.79143900 |

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| H | -10.77752600 | 3.52850200 | -2.28200800 |
| O | -2.53468600 | 2.74225500 | -2.76023100 |
| H | -1.62704700 | 2.91834400 | -2.39002200 |
| O | -0.16257300 | 3.58984500 | -2.47543500 |
| H | 0.66972000 | 3.05292800 | -2.57617200 |
| O | 1.85031800 | 3.08990900 | -3.72873600 |
| H | 2.83681800 | 3.15965500 | -3.87590700 |
| O | 4.28862800 | 3.52825000 | -4.19167200 |
| H | 5.13526700 | 3.10732800 | -3.89355500 |
| O | 6.79007900 | 3.26186600 | -3.72128700 |
| H | 7.58042400 | 2.91206800 | -3.23820900 |
| O | 9.32077700 | 3.22960000 | -2.92405000 |
| O | 10.74692200 | 4.87924500 | -3.66841200 |
| O | 14.53934900 | 4.31378500 | -1.36250700 |
| H | 15.14357900 | 4.80124000 | -1.97568400 |
| O | -8.71427000 | 2.58288900 | -5.07262000 |
| H | -9.54545500 | 2.56936500 | -4.53731900 |
| N | -10.09655200 | 2.82619400 | 2.92990600 |
| H | -9.38532100 | 2.08302300 | 3.03156200 |
| H | -10.68767000 | 2.50932300 | 2.14409200 |

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| C | -10.55684100 | 3.77738100 | 0.23695300 |
| H | -11.02910500 | 3.57178400 | -0.74070500 |
| C | -10.08563500 | 5.22148500 | 0.20005100 |
| H | -9.57838100 | 5.43821400 | 1.14697200 |
| C | -9.10150100 | 5.41684300 | -0.96365700 |
| H | -9.66191800 | 5.22656300 | -1.89511300 |
| C | -8.41337700 | 3.15269800 | -0.84080200 |
| H | -8.93065900 | 2.90660300 | -1.78043700 |
| C | -9.33265300 | 2.87916100 | 0.33828500 |
| H | -9.64211700 | 1.82986300 | 0.27909900 |
| C | -8.51407000 | 6.81162400 | -1.00125300 |
| H | -7.96298400 | 7.00991700 | -0.07763900 |
| H | -9.30520900 | 7.55618600 | -1.11748500 |
| H | -7.82196100 | 6.90863000 | -1.83995000 |
| C | -6.38925300 | 2.29191400 | -1.77154600 |
| H | -6.31422300 | 3.28801100 | -2.22284400 |
| C | -5.05124500 | 1.88640000 | -1.23489000 |
| H | -4.99043700 | 0.90487300 | -0.77291900 |
| C | -3.96428300 | 2.65972300 | -1.31866900 |
| H | -4.04496000 | 3.65254700 | -1.76079400 |
| C | -2.65147200 | 2.24811300 | -0.86207600 |
| H | -2.56176600 | 1.22320700 | -0.50863200 |
| C | -1.55961600 | 3.03730200 | -0.87041900 |
| H | -1.64879400 | 4.06692200 | -1.21634900 |
| C | -0.25369600 | 2.57691900 | -0.46350900 |
| H | -0.18728500 | 1.53156300 | -0.17441600 |

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| C | 0.86900200 | 3.32459100 | -0.46376000 |
| H | 0.82034200 | 4.37356100 | -0.75476400 |
| C | 2.16651000 | 2.78521200 | -0.13540900 |
| H | 2.20420500 | 1.73091000 | 0.13153700 |
| C | 3.32308300 | 3.47855400 | -0.17079400 |
| H | 3.30066000 | 4.53659900 | -0.43054700 |
| C | 4.61444900 | 2.89346500 | 0.09621700 |
| H | 4.63300900 | 1.83111500 | 0.33143300 |
| C | 5.77805600 | 3.57302200 | 0.04653400 |
| H | 5.75792900 | 4.63581900 | -0.19371000 |
| C | 7.07354100 | 2.98087300 | 0.28125700 |
| H | 7.09081200 | 1.92238000 | 0.53304100 |
| C | 8.23747100 | 3.65137300 | 0.18980300 |
| H | 8.21949300 | 4.71051500 | -0.06629800 |
| C | -6.94003300 | 1.30666300 | -2.81157700 |
| H | -7.94828100 | 1.62144100 | -3.08408900 |
| H | -6.32507800 | 1.35929700 | -3.71514900 |
| C | 9.53795100 | 3.04190900 | 0.38490900 |
| H | 9.54063400 | 1.99121500 | 0.66514700 |
| C | 10.70419400 | 3.67463400 | 0.20845900 |
| H | 10.69825500 | 4.72724000 | -0.08064200 |
| C | 12.05441600 | 3.03488000 | 0.35239700 |
| H | 11.92140400 | 2.02251400 | 0.74141100 |
| C | 12.76683900 | 2.91113200 | -1.00773000 |
| H | 13.04078900 | 3.92852900 | -1.33211000 |
| C | 11.90654400 | 2.30055200 | -2.12860000 |

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| H | 10.99425700 | 2.90271100 | -2.16967600 |
| C | 11.44618400 | 0.87781600 | -1.79365700 |
| H | 11.16706500 | 0.82064500 | -0.74471100 |
| C | 9.16594700 | 0.16531500 | -1.93801700 |
| C | 7.97880600 | -0.04022700 | -2.84230500 |
| H | 8.12626900 | 0.50704500 | -3.77467900 |
| H | 7.93462700 | -1.11006400 | -3.07738000 |
| C | 6.66354000 | 0.37030200 | -2.17007900 |
| H | 6.70183300 | 1.44400400 | -1.93688200 |
| C | 5.47655300 | 0.08959700 | -3.07735300 |
| H | 5.61011700 | 0.64368300 | -4.01257600 |
| H | 5.46461700 | -0.97939000 | -3.32213400 |
| C | 4.12303000 | 0.46403400 | -2.47794200 |
| H | 4.14497600 | 1.51341900 | -2.15448800 |
| C | 3.01367100 | 0.28744700 | -3.50745300 |
| H | 3.10860100 | -0.70880900 | -3.95734900 |
| H | 3.19827100 | 1.00980300 | -4.30857200 |
| C | 1.59352400 | 0.47383200 | -2.95235200 |
| H | 1.61123400 | 1.06735800 | -2.03585000 |
| H | 0.98954400 | 1.04051200 | -3.66759000 |
| C | 0.85919700 | -0.83647000 | -2.69088800 |
| H | 0.77598500 | -1.37796400 | -3.64412500 |
| C | -0.57064900 | -0.59707800 | -2.14479800 |
| H | -0.90590000 | 0.40965200 | -2.41907800 |
| C | -1.57691400 | -1.61537600 | -2.66638400 |
| H | -1.27559000 | -2.61916000 | -2.34206300 |

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| H | -1.55337900 | -1.60180600 | -3.76213800 |
| C | -3.00156700 | -1.32366600 | -2.20839500 |
| H | -3.27378300 | -0.30671200 | -2.52277500 |
| C | -3.99901600 | -2.29450800 | -2.82870300 |
| H | -3.74584000 | -3.31780700 | -2.53521200 |
| H | -3.92611300 | -2.21963900 | -3.91799400 |
| C | -5.44413700 | -2.02915400 | -2.41531700 |
| C | -6.45865200 | -2.88544200 | -3.16000400 |
| H | -6.29366100 | -3.94418400 | -2.94570800 |
| H | -6.35095200 | -2.72660400 | -4.23643200 |
| C | -7.86081300 | -2.49916000 | -2.72837700 |
| H | -7.96286700 | -2.71341800 | -1.66185200 |
| C | -8.10385500 | -0.98630600 | -2.92381800 |
| H | -8.18794900 | -0.80328300 | -4.00416900 |
| C | -6.94736400 | -0.14652800 | -2.33794000 |
| H | -7.02802100 | -0.18723500 | -1.24784800 |
| C | -9.40085400 | -0.55313900 | -2.26268500 |
| C | 12.40894600 | -0.24328600 | -2.12388400 |
| H | 11.98726000 | -1.19772200 | -1.80868800 |
| H | 13.34712200 | -0.07802600 | -1.59284200 |
| H | 12.60779300 | -0.29194400 | -3.19646600 |
| C | 12.59756700 | 2.40046800 | -3.48684800 |
| H | 13.56212700 | 1.88364200 | -3.49425800 |
| H | 12.77369200 | 3.44648200 | -3.75301500 |
| H | 11.98144600 | 1.95369700 | -4.27089600 |
| C | 12.93581200 | 3.80232300 | 1.34125500 |

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| H | 13.06769800 | 4.84173000 | 1.02072000 |
| H | 13.92038700 | 3.33699300 | 1.41039200 |
| H | 12.47904700 | 3.81399600 | 2.33368100 |
| O | -8.64997600 | 3.15434900 | 1.54614600 |
| H | -7.71707400 | 2.92672500 | 1.41113000 |
| O | -11.23317200 | 6.04575900 | 0.02041700 |
| H | -11.04735900 | 6.90966100 | 0.40148400 |
| O | -8.01155800 | 4.51156900 | -0.86145500 |
| O | -7.28316300 | 2.37126700 | -0.65111800 |
| O | -5.64677400 | -2.27759800 | -1.05625800 |
| H | -4.98419600 | -1.77070400 | -0.55569200 |
| O | -5.68638400 | -0.67003300 | -2.74459700 |
| O | -9.57007500 | 0.46499600 | -1.64243800 |
| O | -3.11232800 | -1.40649000 | -0.78503900 |
| H | -2.25343100 | -1.14307700 | -0.40817700 |
| O | -0.52639400 | -0.63111700 | -0.71720800 |
| H | 0.23353400 | -1.21794900 | -0.52748900 |
| O | 1.52568000 | -1.67812400 | -1.76345100 |
| H | 2.39211500 | -1.28631500 | -1.52053200 |
| O | 3.81482700 | -0.35007000 | -1.34232000 |
| H | 4.64329200 | -0.52818400 | -0.86286900 |
| O | 6.45817900 | -0.36338500 | -0.96749000 |
| H | 7.30545500 | -0.39272200 | -0.48866900 |
| O | 9.13652100 | -0.10621800 | -0.74650200 |
| O | 10.22466200 | 0.64788800 | -2.56723700 |
| O | 13.94897900 | 2.14885700 | -0.77092700 |

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| H | 14.56826200 | 2.30084700 | -1.49273400 |
| O | -8.77056600 | -3.29748500 | -3.48596900 |
| H | -9.63341700 | -2.86710500 | -3.40694900 |
| N | -11.46677100 | 3.55511500 | 1.35158000 |
| H | -11.95571500 | 2.67516900 | 1.21485500 |
| H | -12.16782600 | 4.29022200 | 1.33646700 |
| C | 14.61552500 | -0.82078800 | 2.25902000 |
| H | 14.85946000 | -0.88702800 | 3.32645900 |
| H | 14.49603800 | -1.85373300 | 1.90909800 |
| C | 13.29614100 | -0.07805700 | 2.08050900 |
| H | 13.07494900 | -0.01611500 | 1.00690300 |
| H | 13.41742800 | 0.96122100 | 2.41288800 |
| C | 12.11048500 | -0.70808200 | 2.80633300 |
| H | 12.28118200 | -0.68058800 | 3.89012600 |
| H | 12.03576900 | -1.76841400 | 2.53504600 |
| C | 10.79737700 | -0.01199300 | 2.46629900 |
| H | 10.86591000 | 1.05066400 | 2.73605200 |
| H | 10.65647000 | -0.04051000 | 1.37828200 |
| C | 9.55810800 | -0.61531800 | 3.11996200 |
| H | 9.63623000 | -0.54617000 | 4.21250000 |
| H | 9.50572200 | -1.68510900 | 2.88008000 |
| C | 8.28284400 | 0.06991100 | 2.63962200 |
| H | 8.33707800 | 1.14373500 | 2.86301700 |
| H | 8.25193800 | -0.00421700 | 1.54656700 |
| C | 6.98991000 | -0.49784500 | 3.21333900 |
| H | 6.97190900 | -0.35514500 | 4.30136100 |

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| H | 6.95795300 | -1.58210000 | 3.04522000 |
| C | 5.75600300 | 0.14525100 | 2.58737700 |
| H | 5.81866000 | 1.23623800 | 2.69462800 |
| H | 5.76708300 | -0.04854200 | 1.50654900 |
| C | 4.43512100 | -0.33915300 | 3.17290200 |
| H | 4.40630200 | -0.10178700 | 4.24426300 |
| H | 4.37817400 | -1.43271900 | 3.10054200 |
| C | 3.22126800 | 0.27748700 | 2.48483400 |
| H | 3.32847000 | 1.36981300 | 2.46736100 |
| H | 3.20336900 | -0.03879100 | 1.43233500 |
| C | 1.89991000 | -0.08120200 | 3.15541200 |
| H | 1.93229900 | 0.25137200 | 4.20129500 |
| H | 1.78631900 | -1.17236300 | 3.18687600 |
| C | 0.68453900 | 0.53522600 | 2.47044500 |
| H | 0.58290600 | 0.11903000 | 1.46070500 |
| H | 0.84562100 | 1.61231400 | 2.33525900 |
| C | -0.60987800 | 0.31507700 | 3.24537900 |
| H | -0.49846900 | 0.74161300 | 4.25108900 |
| H | -0.77125900 | -0.76101900 | 3.39033000 |
| C | -1.84314700 | 0.91973900 | 2.57982600 |
| H | -2.00086100 | 0.43823900 | 1.60651300 |
| H | -1.66673300 | 1.98118700 | 2.36359800 |
| C | -3.09130800 | 0.75245100 | 3.43900800 |
| H | -2.91980100 | 1.19497900 | 4.42740700 |
| H | -3.26977100 | -0.31119600 | 3.61687700 |
| C | -4.34885600 | 1.35942000 | 2.82904500 |

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| H | -4.48222700 | 1.04225900 | 1.78743800 |
| H | -4.31972400 | 2.45267500 | 2.80780500 |
| C | -5.59750100 | 0.90533700 | 3.53560100 |
| O | -5.66918600 | -0.04726600 | 4.27663800 |
| C | 15.75983200 | -0.15059900 | 1.50441600 |
| H | 16.69496900 | -0.70836800 | 1.60554400 |
| H | 15.52465900 | -0.06592400 | 0.43872700 |
| H | 15.93101500 | 0.86486500 | 1.87535300 |
| C | -7.96036800 | 1.16974800 | 3.57553800 |
| H | -7.88592300 | 0.59100900 | 4.49733500 |
| H | -8.57515000 | 2.05773500 | 3.70843800 |
| C | -8.52142200 | 0.31996100 | 2.44694300 |
| H | -8.23882000 | 0.76158100 | 1.49462300 |
| C | -10.02599200 | 0.18194500 | 2.50639700 |
| H | -10.34433600 | -0.41751400 | 3.36368700 |
| H | -10.47786900 | 1.17480300 | 2.54614100 |
| O | -6.66342700 | 1.66110700 | 3.19886000 |
| C | -6.88351900 | -1.23256700 | 1.74285700 |
| C | -6.27970600 | -2.59415300 | 1.93395100 |
| H | -6.81880500 | -3.14110900 | 2.70779200 |
| H | -6.41246000 | -3.11042200 | 0.97969700 |
| C | -4.78326800 | -2.42796500 | 2.24673400 |
| H | -4.65096800 | -2.31892400 | 3.32729100 |
| H | -4.45949900 | -1.48024400 | 1.80769900 |
| C | -3.85202400 | -3.50010300 | 1.69114500 |
| H | -4.09132200 | -4.49044700 | 2.09795300 |

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| H | -3.98963000 | -3.55504200 | 0.60614800 |
| C | -2.40335500 | -3.12591700 | 2.00334600 |
| H | -2.19846400 | -3.29638900 | 3.06855900 |
| H | -2.29212800 | -2.04382300 | 1.85399200 |
| C | -1.34193400 | -3.81868900 | 1.15685100 |
| H | -1.55080600 | -3.61135100 | 0.09974700 |
| H | -1.39731200 | -4.90773500 | 1.28040100 |
| C | 0.05670500 | -3.31953200 | 1.50703900 |
| H | 0.05468200 | -2.22248300 | 1.45081200 |
| H | 0.27394400 | -3.55376900 | 2.55792300 |
| C | 1.17937000 | -3.85793300 | 0.62577200 |
| H | 0.96025500 | -3.64415300 | -0.42576400 |
| H | 1.23634800 | -4.94989700 | 0.72228900 |
| C | 2.52543700 | -3.23794700 | 0.98879800 |
| H | 2.43635400 | -2.14494000 | 0.94485000 |
| H | 2.76016000 | -3.47615700 | 2.03543000 |
| C | 3.68873500 | -3.67062200 | 0.10171500 |
| H | 3.53564100 | -3.28351300 | -0.91311100 |
| H | 3.70030000 | -4.76502800 | 0.01509100 |
| C | 5.03393300 | -3.19782700 | 0.64545700 |
| H | 5.00638300 | -2.11177300 | 0.79955200 |
| H | 5.18471300 | -3.63238100 | 1.64295800 |
| C | 6.22568000 | -3.54467600 | -0.23951800 |
| H | 6.19261200 | -4.61124900 | -0.49810600 |
| H | 6.14696300 | -2.98884500 | -1.18120900 |
| C | 7.56401700 | -3.23001000 | 0.42137400 |

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| H | 7.59037800 | -2.17413400 | 0.71588200 |
| H | 7.64690300 | -3.79894200 | 1.35695500 |
| C | 8.76970900 | -3.53743200 | -0.45889000 |
| H | 8.74146200 | -4.59397100 | -0.75657400 |
| H | 8.69572400 | -2.95664100 | -1.38853400 |
| C | 10.10231800 | -3.22866500 | 0.21530400 |
| H | 10.14512700 | -3.73420000 | 1.18921100 |
| H | 10.15114000 | -2.15357700 | 0.42287800 |
| C | 11.31292500 | -3.64074200 | -0.61665000 |
| H | 11.29733300 | -4.72603700 | -0.78104300 |
| H | 11.23583600 | -3.19046000 | -1.61611400 |
| C | 12.64122800 | -3.24079200 | 0.01953300 |
| H | 12.73370000 | -3.73104600 | 0.99644200 |
| H | 12.62996200 | -2.16499400 | 0.22562300 |
| C | 13.85213400 | -3.57674800 | -0.84328500 |
| H | 14.78517100 | -3.27796200 | -0.35699500 |
| H | 13.90852200 | -4.65068300 | -1.04658800 |
| H | 13.79995500 | -3.06122100 | -1.80797700 |
| O | -7.96546400 | -1.00507200 | 2.50566100 |
| O | -6.40982500 | -0.39129800 | 1.00594300 |
| O | -10.50684900 | -0.42256000 | 1.29053700 |
| O | -11.71346300 | -2.10302500 | -0.02778500 |
| O | -10.90033800 | -2.77781200 | 2.34667900 |
| O | -9.25463500 | -2.40844100 | 0.34389400 |
| C | -12.30402900 | -3.39747400 | -0.23744500 |
| H | -12.26762600 | -3.96060700 | 0.69989900 |

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| H | -13.35210600 | -3.22626200 | -0.49532100 |
| C | -11.61918600 | -4.15326000 | -1.36986200 |
| H | -11.67055600 | -3.54916900 | -2.27725100 |
| H | -12.19258600 | -5.06933900 | -1.56194300 |
| N | -10.20194100 | -4.43001800 | -1.08936300 |
| H | -10.09060800 | -5.30041900 | -0.57854500 |
| H | -9.66337500 | -4.48557100 | -1.95475400 |
| P | -10.56183700 | -2.00516000 | 1.13888100 |
| H | -9.49161500 | -3.22615600 | -0.22084200 |
| O | -10.40333000 | -1.45053100 | -2.41543900 |
| H | -11.07811900 | -1.27963200 | -1.72598900 |

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| C | 9.49754100 | 4.38392500 | -0.09686400 |
| H | 10.13517400 | 3.49159100 | -0.07163500 |
| C | 9.66943300 | 5.08796100 | 1.25048400 |
| H | 9.05627300 | 6.00407400 | 1.23952500 |
| C | 9.16495100 | 4.20582300 | 2.38593500 |
| H | 9.75500100 | 3.27785400 | 2.40461600 |
| C | 7.62230000 | 3.13073600 | 0.93808400 |
| H | 8.24201000 | 2.22412300 | 1.00848500 |
| C | 8.04552900 | 3.94634000 | -0.28321200 |
| H | 7.95538100 | 3.30677700 | -1.17305000 |

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| C | 9.22493900 | 4.88812200 | 3.73222800 |
| H | 8.60133300 | 5.78753300 | 3.72466400 |
| H | 10.25358900 | 5.18159300 | 3.94645200 |
| H | 8.86607600 | 4.21967000 | 4.51748200 |
| C | 5.58459400 | 2.27513400 | 1.93681600 |
| H | 5.58027400 | 3.03089900 | 2.72862500 |
| C | 4.18415400 | 2.03785500 | 1.46819300 |
| H | 4.04989500 | 1.25278000 | 0.73103700 |
| C | 3.13109500 | 2.75973200 | 1.86801100 |
| H | 3.27049800 | 3.57447500 | 2.57797700 |
| C | 1.79099300 | 2.52313700 | 1.37047800 |
| H | 1.67397500 | 1.67868800 | 0.69991900 |
| C | 0.69606700 | 3.26804300 | 1.61914100 |
| H | 0.75117800 | 4.14802600 | 2.25849400 |
| C | -0.57402800 | 2.89922500 | 1.03506600 |
| H | -0.54196200 | 2.00550900 | 0.41448900 |
| C | -1.76600700 | 3.50147800 | 1.21992500 |
| H | -1.84869300 | 4.39225300 | 1.84144200 |
| C | -2.97738300 | 2.94524500 | 0.66431300 |
| H | -2.85872100 | 2.03939400 | 0.06940600 |
| C | -4.22755200 | 3.41033700 | 0.86030800 |
| H | -4.37773800 | 4.31805300 | 1.44370700 |
| C | -5.40280600 | 2.73700800 | 0.36247200 |
| H | -5.23628500 | 1.79653900 | -0.16267100 |
| C | -6.66763800 | 3.16754300 | 0.54081500 |
| H | -6.83851600 | 4.10477300 | 1.06963100 |

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| C | -7.83390300 | 2.44538300 | 0.09073600 |
| H | -7.65313300 | 1.49594500 | -0.41199700 |
| C | -9.10357400 | 2.84655200 | 0.28842600 |
| H | -9.28822900 | 3.78980200 | 0.80187400 |
| C | 6.29874900 | 1.04232400 | 2.49279900 |
| H | 7.28128200 | 1.35014400 | 2.85167700 |
| H | 5.73953900 | 0.68421600 | 3.36223500 |
| C | -10.26021800 | 2.05932900 | -0.09046200 |
| H | -10.06006200 | 1.12791500 | -0.61374900 |
| C | -11.52460500 | 2.36079900 | 0.22442200 |
| H | -11.73480400 | 3.28830800 | 0.76048900 |
| C | -12.70896000 | 1.48330500 | -0.06350800 |
| H | -12.36187400 | 0.59222200 | -0.59798700 |
| C | -13.36405900 | 1.02689400 | 1.25387300 |
| H | -13.74522900 | 1.93398300 | 1.75112100 |
| C | -12.40557000 | 0.33736900 | 2.24134600 |
| H | -11.50955700 | 0.96336300 | 2.27724000 |
| C | -11.93348200 | -1.03769100 | 1.74122200 |
| H | -11.77510500 | -1.00443800 | 0.66496600 |
| C | -9.54743200 | -1.19863500 | 1.60954500 |
| C | -8.27587900 | -1.47725800 | 2.36823400 |
| H | -8.43243000 | -1.28019200 | 3.43045400 |
| H | -8.06203700 | -2.54660000 | 2.25504300 |
| C | -7.08698900 | -0.67683800 | 1.82561700 |
| H | -7.28911600 | 0.39730300 | 1.94884000 |
| C | -5.80537400 | -1.04775000 | 2.55485600 |

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| H | -5.93548900 | -0.84802200 | 3.62386800 |
| H | -5.63982400 | -2.12535400 | 2.43632500 |
| C | -4.55478200 | -0.31593800 | 2.07002800 |
| H | -4.71523400 | 0.76922000 | 2.13547600 |
| C | -3.35561900 | -0.69668000 | 2.93187900 |
| H | -3.34154500 | -1.78799200 | 3.04771400 |
| H | -3.53263200 | -0.28352900 | 3.93001700 |
| C | -1.99393500 | -0.22022000 | 2.40259900 |
| H | -2.11434300 | 0.63451400 | 1.73475000 |
| H | -1.38308100 | 0.13129200 | 3.23957300 |
| C | -1.19411500 | -1.30750800 | 1.68862900 |
| H | -1.05606800 | -2.14407600 | 2.39156700 |
| C | 0.19482800 | -0.80764100 | 1.25390500 |
| H | 0.57961800 | -0.11418800 | 2.01192500 |
| C | 1.19478000 | -1.94222300 | 1.07625200 |
| H | 0.85092500 | -2.61760000 | 0.28585800 |
| H | 1.23054800 | -2.51627400 | 2.01009800 |
| C | 2.60080600 | -1.44827400 | 0.74903700 |
| H | 2.82451500 | -0.57222500 | 1.36942100 |
| C | 3.65854400 | -2.50694400 | 1.05098300 |
| H | 3.48884900 | -3.38783200 | 0.42362700 |
| H | 3.56751400 | -2.81150500 | 2.09676800 |
| C | 5.08315400 | -2.01431900 | 0.80883000 |
| C | 6.15315600 | -3.00876600 | 1.24026500 |
| H | 6.09342600 | -3.91092000 | 0.62807700 |
| H | 6.00217400 | -3.28478700 | 2.28815300 |

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|---|--------------|-------------|-------------|
| C | 7.51863500 | -2.37650300 | 1.06639300 |
| H | 7.64314000 | -2.13320200 | 0.00911200 |
| C | 7.60904500 | -1.07698400 | 1.87553600 |
| H | 7.53719000 | -1.31900800 | 2.94180000 |
| C | 6.42923400 | -0.12977000 | 1.52420200 |
| H | 6.56273300 | 0.22881200 | 0.49475100 |
| C | 8.93523600 | -0.37318400 | 1.69309800 |
| C | -12.80799400 | -2.22317700 | 2.09258400 |
| H | -12.38459400 | -3.13771600 | 1.67283500 |
| H | -13.80001900 | -2.07156600 | 1.66721900 |
| H | -12.89261500 | -2.35184800 | 3.17326100 |
| C | -12.99274100 | 0.28458500 | 3.65104000 |
| H | -13.94891400 | -0.24800000 | 3.67982200 |
| H | -13.16149500 | 1.29465300 | 4.03381900 |
| H | -12.31407000 | -0.22607600 | 4.33859300 |
| C | -13.73577700 | 2.20031900 | -0.94558500 |
| H | -14.09415300 | 3.11341800 | -0.45739800 |
| H | -14.59504800 | 1.55611000 | -1.13661200 |
| H | -13.28572300 | 2.48546200 | -1.89893000 |
| O | 7.27257200 | 5.11532300 | -0.41884500 |
| H | 6.34579600 | 4.87732800 | -0.60567400 |
| O | 11.02772200 | 5.38367000 | 1.46488400 |
| H | 11.34146800 | 5.69772800 | 0.60094600 |
| O | 7.79393500 | 3.87869200 | 2.12804800 |
| O | 6.27489000 | 2.82563600 | 0.79492400 |
| O | 5.29827500 | -1.72917700 | -0.54221100 |

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| H | 4.43713600 | -1.41495600 | -0.89139600 |
| O | 5.20620000 | -0.84075800 | 1.61606600 |
| O | 9.35028600 | 0.54037600 | 2.36857600 |
| O | 2.73577000 | -1.09831900 | -0.63288600 |
| H | 2.43686500 | -0.18702700 | -0.79385800 |
| O | 0.06036900 | -0.06028900 | 0.05498200 |
| H | -0.65030600 | -0.52429000 | -0.42167500 |
| O | -1.82709600 | -1.78935500 | 0.51438600 |
| H | -2.75613400 | -1.48083100 | 0.49536300 |
| O | -4.25639800 | -0.64279300 | 0.71062100 |
| H | -5.09958700 | -0.77568000 | 0.24071400 |
| O | -6.88053900 | -0.96036600 | 0.44609300 |
| H | -7.74567100 | -0.90002200 | 0.00301200 |
| O | -9.56039500 | -0.94211100 | 0.41628200 |
| O | -10.63278300 | -1.29021200 | 2.36299900 |
| O | -14.45854800 | 0.18114400 | 0.90692400 |
| H | -15.04498600 | 0.09916100 | 1.66686800 |
| O | 8.49965500 | -3.31209000 | 1.48350300 |
| H | 9.34072100 | -3.02807100 | 1.10554200 |
| N | 10.00672700 | 5.27630400 | -1.13092000 |
| H | 9.28078300 | 5.95746500 | -1.34314000 |
| H | 10.19191900 | 4.76740900 | -1.98920300 |
| C | -18.53962500 | -2.26989800 | -0.30149600 |
| H | -18.34721200 | -1.36105600 | 0.28285200 |
| H | -18.82195400 | -1.92839800 | -1.30494300 |
| C | -17.25385200 | -3.08711500 | -0.39381300 |

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| H | -17.44288800 | -3.99525100 | -0.98159800 |
| H | -16.97253400 | -3.43277800 | 0.61058900 |
| C | -16.08967600 | -2.31516300 | -1.00654200 |
| H | -15.89899500 | -1.40663900 | -0.42187100 |
| H | -16.36872600 | -1.97415900 | -2.01236100 |
| C | -14.79929700 | -3.12588900 | -1.08991400 |
| H | -14.54278900 | -3.49999700 | -0.08985100 |
| H | -14.95897300 | -4.01625900 | -1.71220400 |
| C | -13.62853400 | -2.31549500 | -1.63686900 |
| H | -13.52733700 | -1.40468300 | -1.03456900 |
| H | -13.86181500 | -1.98016700 | -2.65598600 |
| C | -12.30273200 | -3.07054500 | -1.64239800 |
| H | -12.06099800 | -3.38071600 | -0.61691500 |
| H | -12.40489100 | -3.99840100 | -2.21999100 |
| C | -11.14809300 | -2.24229100 | -2.19668800 |
| H | -11.10933800 | -1.28235100 | -1.66709700 |
| H | -11.34232500 | -2.00334000 | -3.25035800 |
| C | -9.78447100 | -2.91288800 | -2.06265600 |
| H | -9.61069000 | -3.15019000 | -1.00589400 |
| H | -9.77909700 | -3.86886700 | -2.60219800 |
| C | -8.65075400 | -2.02449100 | -2.56159500 |
| H | -8.73908000 | -1.04731200 | -2.06840200 |
| H | -8.78161500 | -1.82640800 | -3.63328700 |
| C | -7.24874600 | -2.57926200 | -2.31652400 |
| H | -7.14429100 | -2.86094100 | -1.26173300 |
| H | -7.10180900 | -3.49646100 | -2.90074500 |

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| C | -6.17409000 | -1.55582000 | -2.66516400 |
| H | -6.33609700 | -0.65955400 | -2.05171000 |
| H | -6.30771300 | -1.23018000 | -3.70513000 |
| C | -4.73061100 | -2.01832400 | -2.47802000 |
| H | -4.50277700 | -2.81981000 | -3.19196300 |
| H | -4.59786100 | -2.44979100 | -1.47735900 |
| C | -3.76902000 | -0.84913000 | -2.67070600 |
| H | -3.88988500 | -0.15522300 | -1.82856600 |
| H | -4.07453400 | -0.29009800 | -3.56534600 |
| C | -2.28791900 | -1.19408200 | -2.80748900 |
| H | -2.13648700 | -1.83559100 | -3.68503000 |
| H | -1.94738200 | -1.76548900 | -1.93646000 |
| C | -1.48853200 | 0.09711900 | -2.95835900 |
| H | -1.61372200 | 0.70867100 | -2.05883200 |
| H | -1.93367600 | 0.68604600 | -3.76867200 |
| C | 0.00459400 | -0.06204500 | -3.23989600 |
| H | 0.19342600 | -0.73470100 | -4.08037900 |
| H | 0.53425000 | -0.47737300 | -2.37469700 |
| C | 0.67595100 | 1.24735300 | -3.57057000 |
| O | 1.65299000 | 1.38472500 | -4.26507300 |
| C | -19.69601800 | -3.04559600 | 0.32090700 |
| H | -20.60514100 | -2.44062200 | 0.37646900 |
| H | -19.92682100 | -3.94155100 | -0.26399500 |
| H | -19.44923000 | -3.37168800 | 1.33648800 |
| C | 0.52365100 | 3.59536000 | -3.18635400 |
| H | 1.07089700 | 3.65645900 | -4.12943400 |

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| H | -0.36313700 | 4.23270900 | -3.22957400 |
| C | 1.42251400 | 4.02850900 | -2.04096200 |
| H | 1.11358800 | 3.53644700 | -1.11774300 |
| C | 1.40269900 | 5.53706000 | -1.86519000 |
| H | 1.76619600 | 6.03052100 | -2.77175400 |
| H | 0.38426900 | 5.86612100 | -1.64871400 |
| O | 0.02633600 | 2.27719800 | -2.98405400 |
| C | 3.28100800 | 2.51629600 | -1.94936200 |
| C | 4.75357700 | 2.43643200 | -2.20719200 |
| H | 5.01475400 | 3.17086500 | -2.97252500 |
| H | 5.22084700 | 2.76704200 | -1.27337200 |
| C | 5.22368300 | 1.03260400 | -2.55878200 |
| H | 4.77840300 | 0.71910100 | -3.50970500 |
| H | 4.85646100 | 0.34242700 | -1.79841700 |
| C | 6.74453600 | 0.93727400 | -2.62331000 |
| H | 7.13633100 | 1.67659800 | -3.33582600 |
| H | 7.15181700 | 1.21331900 | -1.64073300 |
| C | 7.24065600 | -0.45701200 | -2.99159100 |
| H | 6.86893400 | -0.72481800 | -3.98948100 |
| H | 6.79604700 | -1.16960100 | -2.29174800 |
| C | 8.76367700 | -0.57687200 | -2.97191300 |
| H | 9.13050900 | -0.28369600 | -1.97817600 |
| H | 9.19047600 | 0.14157000 | -3.68326400 |
| C | 9.28087900 | -1.98208000 | -3.29384800 |
| H | 8.89804500 | -2.29735000 | -4.27327000 |
| H | 10.37394800 | -1.95436000 | -3.38840900 |

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| C | 8.90040400 | -3.01817900 | -2.23932300 |
| H | 7.80920200 | -3.09268100 | -2.16817900 |
| H | 9.24337200 | -2.65888100 | -1.26159700 |
| C | 9.47320300 | -4.41126000 | -2.47543500 |
| H | 9.22257500 | -4.75018200 | -3.48915900 |
| H | 10.57004600 | -4.36913900 | -2.43253000 |
| C | 8.95590300 | -5.42492300 | -1.45646900 |
| H | 7.87142900 | -5.53805500 | -1.58844700 |
| H | 9.08416100 | -5.02626700 | -0.44185100 |
| C | 9.62104900 | -6.79320500 | -1.56021100 |
| H | 9.49501700 | -7.18573700 | -2.57815300 |
| H | 10.70364500 | -6.68341700 | -1.41095700 |
| C | 9.07403400 | -7.80390500 | -0.55649200 |
| H | 9.19010200 | -7.40394100 | 0.45932100 |
| H | 7.99343800 | -7.92056000 | -0.71256100 |
| C | 9.74682200 | -9.17052200 | -0.64297900 |
| H | 9.63220600 | -9.56864900 | -1.65996500 |
| H | 10.82721100 | -9.05418800 | -0.48422500 |
| C | 9.19596200 | -10.18060500 | 0.35925200 |
| H | 9.30862700 | -9.78128400 | 1.37588200 |
| H | 8.11605300 | -10.29851100 | 0.19918700 |
| C | 9.87044900 | -11.54674200 | 0.27597000 |
| H | 10.95032000 | -11.42872400 | 0.43669500 |
| H | 9.75824700 | -11.94564800 | -0.74095100 |
| C | 9.31885700 | -12.55678000 | 1.27772500 |
| H | 9.43030500 | -12.15814100 | 2.29495400 |

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| H | 8.23903000 | -12.67593200 | 1.11694000 |
| C | 9.99372900 | -13.92333300 | 1.19586400 |
| H | 11.07224300 | -13.80282900 | 1.35691500 |
| H | 9.88163300 | -14.32029700 | 0.17926000 |
| C | 9.43379000 | -14.92404100 | 2.20167000 |
| H | 9.93142200 | -15.89468500 | 2.12531800 |
| H | 9.56167700 | -14.56309600 | 3.22721200 |
| H | 8.36287600 | -15.08444100 | 2.04111500 |
| O | 2.78849500 | 3.70017200 | -2.32553600 |
| O | 2.60138400 | 1.64886100 | -1.43529700 |
| O | 2.19618500 | 5.92941100 | -0.74814600 |
| O | 3.92742000 | 7.36177600 | 0.16188100 |
| O | 4.19349300 | 6.51319000 | -2.31150700 |
| O | 4.52351200 | 4.96741400 | -0.27537200 |
| C | 5.24499300 | 7.67749100 | 0.63341900 |
| H | 6.01617400 | 7.26324600 | -0.02430000 |
| H | 5.33609700 | 8.76606000 | 0.62358000 |
| C | 5.41117000 | 7.15167800 | 2.04809400 |
| H | 4.57155200 | 7.52058200 | 2.64260700 |
| H | 6.33279100 | 7.56699700 | 2.47659300 |
| N | 5.40011400 | 5.68182500 | 2.07508500 |
| H | 6.33688900 | 5.29650300 | 1.93845000 |
| H | 5.07422900 | 5.34197400 | 2.97304800 |
| P | 3.76698200 | 6.19707900 | -0.93961900 |
| H | 4.71419200 | 5.11169000 | 0.72786200 |
| O | 9.65875500 | -0.84290100 | 0.64990500 |

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| H | 10.47262400 | -0.31446400 | 0.61741200 |
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| C | -12.52622000 | 5.11758800 | 2.19728500 |
| H | -13.32048800 | 4.37979400 | 2.02332700 |
| C | -12.71920000 | 6.22529100 | 1.16088600 |
| H | -11.95374000 | 6.99748200 | 1.33566300 |
| C | -12.51030500 | 5.68233300 | -0.24743000 |
| H | -13.24816500 | 4.88657400 | -0.43680300 |
| C | -11.01179800 | 4.03984000 | 0.53891200 |
| H | -11.75264000 | 3.25805400 | 0.29648400 |
| C | -11.17657800 | 4.43064700 | 2.00641400 |
| H | -11.13278800 | 3.50745400 | 2.60768400 |
| C | -12.62264700 | 6.74669400 | -1.31341700 |
| H | -11.85309500 | 7.50826000 | -1.16103600 |
| H | -13.60368200 | 7.22055000 | -1.25461300 |
| H | -12.49010800 | 6.30719600 | -2.30407100 |
| C | -9.20119100 | 3.36192500 | -0.93038100 |
| H | -9.02262900 | 4.34217600 | -1.38394100 |
| C | -7.91076300 | 2.63131100 | -0.73192700 |
| H | -7.97405900 | 1.67921100 | -0.21420900 |
| C | -6.72109300 | 3.06903400 | -1.15223500 |
| H | -6.64810400 | 4.02332800 | -1.67387100 |

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| C | -5.48996100 | 2.33235000 | -0.93804600 |
| H | -5.57821100 | 1.37861300 | -0.42266600 |
| C | -4.27789200 | 2.76420400 | -1.33001700 |
| H | -4.19734200 | 3.71726700 | -1.85289200 |
| C | -3.04990100 | 2.04273800 | -1.09339400 |
| H | -3.12717800 | 1.09092600 | -0.56880100 |
| C | -1.84291100 | 2.48494800 | -1.49926000 |
| H | -1.78230200 | 3.43098900 | -2.03689000 |
| C | -0.60196200 | 1.79142300 | -1.26729900 |
| H | -0.64852100 | 0.85120700 | -0.71879300 |
| C | 0.59449400 | 2.23618800 | -1.70427500 |
| H | 0.63729900 | 3.15958900 | -2.28092200 |
| C | 1.84219900 | 1.57103400 | -1.43305700 |
| H | 1.80200200 | 0.68917700 | -0.79608400 |
| C | 3.04100700 | 1.96962700 | -1.90386200 |
| H | 3.09920700 | 2.83065800 | -2.56851200 |
| C | 4.27456100 | 1.31705200 | -1.54223600 |
| H | 4.20538500 | 0.53357300 | -0.79069300 |
| C | 5.48910800 | 1.59832200 | -2.04688600 |
| H | 5.59637600 | 2.35125000 | -2.82639200 |
| C | -10.20433100 | 2.60320300 | -1.80650200 |
| H | -11.10035400 | 3.21277200 | -1.92420900 |
| H | -9.76942800 | 2.47530300 | -2.80134700 |
| C | 6.67992800 | 0.90309700 | -1.59968600 |
| H | 6.55378700 | 0.30210300 | -0.70167200 |
| C | 7.86927100 | 0.91337900 | -2.20932900 |

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| H | 7.99833400 | 1.50069200 | -3.11947100 |
| C | 9.06318600 | 0.13059000 | -1.74228800 |
| H | 8.88532900 | -0.20137800 | -0.71377000 |
| C | 9.29274500 | -1.13446000 | -2.59209000 |
| H | 9.63389200 | -0.80203500 | -3.58644100 |
| C | 8.05125000 | -2.01295300 | -2.83792700 |
| H | 7.32219800 | -1.36245900 | -3.33143100 |
| C | 7.35587800 | -2.49964400 | -1.55971200 |
| H | 7.19158300 | -1.66448500 | -0.88399200 |
| C | 4.95362500 | -2.56050900 | -1.35307900 |
| C | 3.68184800 | -3.07605400 | -1.97662000 |
| H | 3.88004900 | -3.37615100 | -3.00712200 |
| H | 3.34716700 | -3.96093300 | -1.42285900 |
| C | 2.56663100 | -2.03062600 | -1.91460700 |
| H | 2.91525100 | -1.09748600 | -2.38092500 |
| C | 1.31695500 | -2.50851500 | -2.63857600 |
| H | 1.55524900 | -2.60398700 | -3.70335700 |
| H | 1.02989700 | -3.49613500 | -2.26233500 |
| C | 0.13089000 | -1.56493100 | -2.46295200 |
| H | 0.46760900 | -0.52438400 | -2.55986300 |
| C | -0.96583000 | -1.80822000 | -3.49347200 |
| H | -1.16732900 | -2.88306700 | -3.55367000 |
| H | -0.56976200 | -1.50147000 | -4.46598600 |
| C | -2.26206400 | -1.04673900 | -3.17027100 |
| H | -2.05698000 | -0.25516800 | -2.44560800 |
| H | -2.65535700 | -0.54736500 | -4.06094300 |

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| C | -3.36524200 | -1.95045300 | -2.62005300 |
| H | -3.78047300 | -2.54639700 | -3.44081300 |
| C | -4.51335500 | -1.14034400 | -1.96388400 |
| H | -4.50107200 | -0.11088800 | -2.33811300 |
| C | -5.88058800 | -1.76280200 | -2.21620300 |
| H | -5.90823500 | -2.77299300 | -1.79739000 |
| H | -6.03138000 | -1.85047700 | -3.29868400 |
| C | -7.04144100 | -0.95109900 | -1.64920500 |
| H | -7.08895000 | 0.02489800 | -2.14825600 |
| C | -8.36970500 | -1.68042600 | -1.84994500 |
| H | -8.28911300 | -2.68443000 | -1.42547000 |
| H | -8.56036200 | -1.77320600 | -2.92315800 |
| C | -9.55304800 | -0.96107900 | -1.21073200 |
| C | -10.89551800 | -1.62312400 | -1.50336900 |
| H | -10.94573200 | -2.59948500 | -1.01628700 |
| H | -10.99202100 | -1.77649600 | -2.58200500 |
| C | -12.04522100 | -0.75158100 | -1.02738500 |
| H | -11.98367900 | -0.65627900 | 0.06394400 |
| C | -11.91936800 | 0.65217800 | -1.63694500 |
| H | -11.96248100 | 0.58140900 | -2.72819300 |
| C | -10.53599900 | 1.22544800 | -1.25399800 |
| H | -10.46787700 | 1.24454700 | -0.15920200 |
| C | -13.04000700 | 1.57688200 | -1.23386400 |
| C | 8.02056300 | -3.63543200 | -0.80938700 |
| H | 7.45600100 | -3.86272100 | 0.09708600 |
| H | 9.03495100 | -3.34224100 | -0.53550800 |

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| H | 8.06638900 | -4.53814000 | -1.42210900 |
| C | 8.37525200 | -3.16228700 | -3.79259400 |
| H | 9.15192300 | -3.82025700 | -3.39099200 |
| H | 8.72283200 | -2.77819600 | -4.75594800 |
| H | 7.49022800 | -3.77562800 | -3.97304100 |
| C | 10.32180900 | 1.00215500 | -1.75292100 |
| H | 10.51546900 | 1.38356800 | -2.76175100 |
| H | 11.19193600 | 0.43107200 | -1.43083800 |
| H | 10.20100500 | 1.86077300 | -1.08942400 |
| O | -10.16723300 | 5.33193700 | 2.39863000 |
| H | -9.36372300 | 5.04929800 | 1.93802200 |
| O | -14.02170400 | 6.75025100 | 1.26786600 |
| H | -14.17007700 | 6.82988000 | 2.22377600 |
| O | -11.19330400 | 5.13290400 | -0.32125000 |
| O | -9.70982000 | 3.56727900 | 0.40656800 |
| O | -9.40837400 | -0.88729200 | 0.19403600 |
| H | -8.45052700 | -0.70254400 | 0.33157800 |
| O | -9.54447600 | 0.34636100 | -1.76229400 |
| O | -13.37192400 | 2.57622100 | -1.82429300 |
| O | -6.87455500 | -0.69563500 | -0.24433100 |
| H | -5.96179800 | -0.92984400 | 0.01114100 |
| O | -4.25836600 | -1.04281800 | -0.55671000 |
| H | -3.89023400 | -1.90645900 | -0.28664200 |
| O | -2.86568700 | -2.88689500 | -1.67506600 |
| H | -2.07309200 | -2.49682300 | -1.25531500 |
| O | -0.43322900 | -1.73154500 | -1.15301400 |

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| H | 0.31486300 | -1.74940100 | -0.53471100 |
| O | 2.21895300 | -1.75378200 | -0.55627000 |
| H | 3.05214700 | -1.59253100 | -0.08093600 |
| O | 4.96405500 | -1.84139000 | -0.36424000 |
| O | 6.03884900 | -2.96210100 | -1.99771300 |
| O | 10.34128300 | -1.85426000 | -1.94817100 |
| H | 10.71203600 | -2.49105100 | -2.56822000 |
| O | -13.25510400 | -1.38114000 | -1.40566000 |
| H | -13.96062000 | -0.96592500 | -0.89487400 |
| N | -12.73844700 | 5.70239300 | 3.51713600 |
| H | -11.89530100 | 6.20913800 | 3.77770500 |
| H | -12.87509500 | 4.97942500 | 4.21634200 |
| C | 18.84982900 | 2.95779000 | -0.35830500 |
| H | 18.74230600 | 3.49241400 | 0.59397200 |
| H | 19.52487600 | 2.11617000 | -0.15970900 |
| C | 17.48525900 | 2.42418600 | -0.78374500 |
| H | 17.58409000 | 1.87629900 | -1.73014600 |
| H | 16.82142700 | 3.27235700 | -0.99393900 |
| C | 16.82918500 | 1.52594000 | 0.26025500 |
| H | 16.80744500 | 2.05188900 | 1.22406400 |
| H | 17.44531800 | 0.63177000 | 0.42052700 |
| C | 15.40920000 | 1.11323300 | -0.11378100 |
| H | 14.81815100 | 2.01581400 | -0.32089600 |
| H | 15.42599100 | 0.54426900 | -1.05253500 |
| C | 14.70318900 | 0.29921500 | 0.96624600 |
| H | 14.73393200 | 0.85601600 | 1.91246500 |

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| H | 15.25090500 | -0.63510100 | 1.14554500 |
| C | 13.25121100 | -0.00773200 | 0.61900800 |
| H | 12.72533000 | 0.93929500 | 0.44023700 |
| H | 13.20469500 | -0.55757100 | -0.33032300 |
| C | 12.49933000 | -0.79241300 | 1.69098500 |
| H | 12.66062600 | -0.32316900 | 2.67053200 |
| H | 12.91217600 | -1.80684500 | 1.76661800 |
| C | 11.00441600 | -0.85482700 | 1.40063300 |
| H | 10.60743600 | 0.16861300 | 1.40766700 |
| H | 10.84698800 | -1.23217700 | 0.38387000 |
| C | 10.18810700 | -1.70068300 | 2.37327500 |
| H | 10.48725000 | -1.48942800 | 3.40793800 |
| H | 10.40268300 | -2.76424800 | 2.20458000 |
| C | 8.69349000 | -1.44031400 | 2.21067800 |
| H | 8.45615700 | -0.43987500 | 2.59458100 |
| H | 8.45384700 | -1.40888100 | 1.13951600 |
| C | 7.78150200 | -2.47282900 | 2.86060200 |
| H | 8.05422600 | -2.61256500 | 3.91367000 |
| H | 7.95589200 | -3.44288100 | 2.37700700 |
| C | 6.30272600 | -2.09308700 | 2.73700500 |
| H | 6.15825700 | -1.48199100 | 1.83863100 |
| H | 6.00502100 | -1.46147300 | 3.58320400 |
| C | 5.37008900 | -3.29300400 | 2.62187400 |
| H | 5.55581800 | -4.00673600 | 3.43426500 |
| H | 5.61307400 | -3.82268500 | 1.69138400 |
| C | 3.89472900 | -2.90074500 | 2.59681400 |

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| H | 3.79026500 | -1.94441300 | 2.07033300 |
| H | 3.53715600 | -2.72077700 | 3.61851500 |
| C | 3.01946900 | -3.93800500 | 1.90268800 |
| H | 3.18011300 | -4.92885500 | 2.34291000 |
| H | 3.32302000 | -4.01392500 | 0.85582400 |
| C | 1.54330900 | -3.57890900 | 1.95839900 |
| H | 1.41300900 | -2.51540500 | 1.73632300 |
| H | 1.11700600 | -3.73606900 | 2.95250100 |
| C | 0.69676800 | -4.30273800 | 0.94663500 |
| O | 1.08068300 | -4.79502700 | -0.09075900 |
| C | 19.47112400 | 3.88648200 | -1.39630800 |
| H | 20.44832900 | 4.25636800 | -1.07427800 |
| H | 19.60717500 | 3.37253900 | -2.35321000 |
| H | 18.82824200 | 4.75416000 | -1.57639600 |
| C | -1.54637400 | -4.87032000 | 0.43413200 |
| H | -1.48149100 | -4.39180200 | -0.54306700 |
| H | -1.34087800 | -5.93800100 | 0.31121700 |
| C | -2.89608400 | -4.65739800 | 1.09004900 |
| H | -2.89438800 | -5.09344600 | 2.09120600 |
| C | -4.03525800 | -5.25811600 | 0.29824200 |
| H | -4.23193900 | -4.66826000 | -0.59987300 |
| H | -3.78921300 | -6.28142500 | 0.00145300 |
| O | -0.58911700 | -4.29696300 | 1.32850900 |
| C | -3.20560300 | -2.73273200 | 2.48669000 |
| C | -2.90664900 | -1.25689800 | 2.47525500 |
| H | -3.47400000 | -0.75025500 | 1.69113500 |

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| H | -3.19024000 | -0.85130100 | 3.44788200 |
| C | -1.39765100 | -1.12095200 | 2.22817700 |
| H | -1.18470100 | -1.52753200 | 1.23601700 |
| H | -0.87710100 | -1.77174900 | 2.94105300 |
| C | -0.80309900 | 0.28076100 | 2.32972700 |
| H | -1.23857300 | 0.93886200 | 1.56831800 |
| H | -1.03844300 | 0.72781000 | 3.30321100 |
| C | 0.71031700 | 0.17759300 | 2.15124900 |
| H | 0.91188600 | -0.34778100 | 1.20851200 |
| H | 1.10305800 | -0.47617800 | 2.94194900 |
| C | 1.52498500 | 1.46601800 | 2.14617900 |
| H | 1.30686100 | 2.06179300 | 3.04102600 |
| H | 1.24405400 | 2.08130700 | 1.28361000 |
| C | 3.01588800 | 1.13064000 | 2.09309000 |
| H | 3.30267300 | 0.63045800 | 3.02790100 |
| H | 3.17691700 | 0.38336700 | 1.30390600 |
| C | 3.95526500 | 2.30166300 | 1.83489500 |
| H | 3.77538000 | 3.09805800 | 2.56830600 |
| H | 3.73061900 | 2.73015700 | 0.85113500 |
| C | 5.42190200 | 1.87566400 | 1.88847100 |
| H | 5.67852800 | 1.59038900 | 2.91751400 |
| H | 5.55318100 | 0.96534500 | 1.28914300 |
| C | 6.39419200 | 2.94016900 | 1.39254400 |
| H | 6.20022800 | 3.88666900 | 1.91432600 |
| H | 6.20080600 | 3.12987500 | 0.32963700 |
| C | 7.85863100 | 2.55486900 | 1.58438300 |

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| H | 8.06341200 | 2.44184400 | 2.65765700 |
| H | 8.03971100 | 1.56896100 | 1.13649200 |
| C | 8.83329400 | 3.56438200 | 0.98293800 |
| H | 8.74478900 | 3.53618400 | -0.11121100 |
| H | 8.54069900 | 4.57922600 | 1.28300800 |
| C | 10.28425200 | 3.32658400 | 1.39368800 |
| H | 10.37200800 | 3.44805700 | 2.48122800 |
| H | 10.56020200 | 2.28540000 | 1.18644400 |
| C | 11.27631700 | 4.25369600 | 0.69716900 |
| H | 11.26498800 | 4.05079600 | -0.38225600 |
| H | 10.94472800 | 5.29419900 | 0.81154900 |
| C | 12.70307300 | 4.12270400 | 1.22409200 |
| H | 13.02471500 | 3.07505200 | 1.15848300 |
| H | 12.71644800 | 4.37490500 | 2.29258000 |
| C | 13.70487600 | 5.00412400 | 0.48356100 |
| H | 13.72510000 | 4.71747300 | -0.57672900 |
| H | 13.36096500 | 6.04678200 | 0.50803800 |
| C | 15.11926100 | 4.92583300 | 1.05187800 |
| H | 15.45822800 | 3.88434800 | 1.02707100 |
| H | 15.09995100 | 5.21277700 | 2.11044600 |
| C | 16.11369000 | 5.80594900 | 0.30132800 |
| H | 17.12660000 | 5.70058100 | 0.70043100 |
| H | 16.14702500 | 5.54402300 | -0.76120800 |
| H | 15.83454500 | 6.86214100 | 0.36903800 |
| O | -3.10617900 | -3.24441200 | 1.22422400 |
| O | -3.38101300 | -3.40775700 | 3.46503200 |

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| O | -5.18162000 | -5.33263500 | 1.14728500 |
| O | -7.50966900 | -5.22833500 | 1.79676000 |
| O | -6.86281700 | -4.31327000 | -0.54316000 |
| O | -6.19382600 | -3.06087100 | 1.62857500 |
| C | -8.90180400 | -4.92098900 | 1.70152300 |
| H | -9.14191800 | -4.57897000 | 0.68805800 |
| H | -9.43944100 | -5.85407300 | 1.88406500 |
| C | -9.29593600 | -3.88705200 | 2.74181600 |
| H | -8.93667200 | -4.22988800 | 3.71555600 |
| H | -10.39285200 | -3.83658100 | 2.78561400 |
| N | -8.68688400 | -2.58433200 | 2.44605400 |
| H | -9.14797200 | -2.14788900 | 1.64325100 |
| H | -8.80144900 | -1.95264800 | 3.23289800 |
| P | -6.46225300 | -4.42725000 | 0.87812300 |
| H | -7.08412200 | -2.73344000 | 2.00841300 |
| O | -13.65613000 | 1.20635000 | -0.08354000 |
| H | -14.33859500 | 1.87731500 | 0.08208500 |

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| C | 10.15246400 | 3.66444200 | -1.90940900 |
| H | 10.96444000 | 3.05029800 | -1.50124500 |
| C | 10.03114400 | 4.89128500 | -1.00738800 |
| H | 9.23855400 | 5.54121300 | -1.41016100 |

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| C | 9.61384400 | 4.47234100 | 0.39680100 |
| H | 10.38013500 | 3.79426100 | 0.80435200 |
| C | 8.46999600 | 2.58213800 | -0.42849700 |
| H | 9.21749900 | 1.93357500 | 0.05035700 |
| C | 8.86507300 | 2.84650700 | -1.87983700 |
| H | 9.02580800 | 1.87904000 | -2.37536000 |
| C | 9.41410000 | 5.64614100 | 1.32679300 |
| H | 8.61819000 | 6.29119900 | 0.94472200 |
| H | 10.33693000 | 6.22509400 | 1.38826300 |
| H | 9.13435100 | 5.29969100 | 2.32396500 |
| C | 6.45477700 | 1.96489500 | 0.76290900 |
| H | 6.25679500 | 3.00600600 | 1.03336500 |
| C | 5.16216800 | 1.28714800 | 0.42359100 |
| H | 5.19258500 | 0.22005900 | 0.22090800 |
| C | 4.00300600 | 1.94992900 | 0.34951200 |
| H | 3.99077700 | 3.01903500 | 0.56261000 |
| C | 2.73102500 | 1.34508700 | 0.00315300 |
| H | 2.72913100 | 0.27947000 | -0.21190400 |
| C | 1.56872700 | 2.02369400 | -0.04598400 |
| H | 1.56996500 | 3.08917300 | 0.18427500 |
| C | 0.29131100 | 1.41643000 | -0.33835900 |
| H | 0.29957000 | 0.35599800 | -0.58212100 |
| C | -0.89037300 | 2.05800700 | -0.23116500 |
| H | -0.90197800 | 3.10967300 | 0.05474800 |
| C | -2.16492500 | 1.39883400 | -0.38635200 |
| H | -2.14509300 | 0.36566900 | -0.72748300 |

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| C | -3.35349000 | 1.96104500 | -0.08007200 |
| H | -3.38428300 | 2.99375000 | 0.26633900 |
| C | -4.61143700 | 1.25982400 | -0.16258900 |
| H | -4.56911900 | 0.22253400 | -0.49498700 |
| C | -5.81148900 | 1.80030900 | 0.13514500 |
| H | -5.85500800 | 2.83831300 | 0.46346800 |
| C | -7.06699000 | 1.10072400 | 0.00379500 |
| H | -7.02254800 | 0.05765900 | -0.30747900 |
| C | -8.27941000 | 1.64683700 | 0.22149800 |
| H | -8.35104600 | 2.68166500 | 0.55461600 |
| C | 7.24598600 | 1.33191300 | 1.91186200 |
| H | 8.15813300 | 1.90924500 | 2.05492700 |
| H | 6.65789300 | 1.42473600 | 2.82972600 |
| C | -9.51718500 | 0.91877200 | 0.02006300 |
| H | -9.40948800 | -0.08371800 | -0.38851100 |
| C | -10.74192300 | 1.36719900 | 0.32152900 |
| H | -10.85499200 | 2.36565800 | 0.74726800 |
| C | -12.00267000 | 0.56861800 | 0.14348000 |
| H | -11.76423800 | -0.34075800 | -0.41937800 |
| C | -12.59122200 | 0.11372500 | 1.49413500 |
| H | -13.02044600 | 1.00495300 | 1.98238600 |
| C | -11.57177600 | -0.48188000 | 2.47724500 |
| H | -10.80618100 | 0.28775400 | 2.61330600 |
| C | -10.82280100 | -1.69834900 | 1.91348700 |
| H | -10.59634700 | -1.53863000 | 0.86199600 |
| C | -8.43111300 | -1.81179000 | 1.89957000 |

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| C | -7.22932600 | -1.46616100 | 2.73700800 |
| H | -7.22757100 | -0.36964800 | 2.77328500 |
| H | -7.37144800 | -1.82597400 | 3.75812200 |
| C | -5.90448000 | -1.97572100 | 2.18300700 |
| H | -5.90546300 | -1.84323800 | 1.09254000 |
| C | -4.73686800 | -1.19764700 | 2.76797900 |
| H | -4.90222500 | -0.13320600 | 2.57383500 |
| H | -4.71218400 | -1.34504800 | 3.85425200 |
| C | -3.37993200 | -1.58177400 | 2.18555800 |
| H | -3.42974500 | -1.51214000 | 1.08723200 |
| C | -2.29901900 | -0.63724400 | 2.68747700 |
| H | -2.19095000 | -0.77968800 | 3.77037700 |
| H | -2.67170200 | 0.37991500 | 2.53456900 |
| C | -0.94540700 | -0.73588800 | 1.98410200 |
| H | -1.09628200 | -0.90256200 | 0.91644300 |
| H | -0.44910800 | 0.23380800 | 2.07660500 |
| C | 0.03563200 | -1.79030100 | 2.48429600 |
| H | 0.15153500 | -1.68979900 | 3.57672700 |
| C | 1.40544700 | -1.55015400 | 1.85572700 |
| H | 1.67400200 | -0.50195800 | 2.02687000 |
| C | 2.52305500 | -2.42978400 | 2.40844500 |
| H | 2.34277700 | -3.47350200 | 2.13022800 |
| H | 2.51347000 | -2.37258500 | 3.50237900 |
| C | 3.88475600 | -1.96668400 | 1.89907200 |
| H | 4.00532900 | -0.90187000 | 2.13839300 |
| C | 5.04971500 | -2.72060300 | 2.52097500 |

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| H | 4.96246600 | -3.78911100 | 2.30182600 |
| H | 5.01165000 | -2.58813400 | 3.60584300 |
| C | 6.41241300 | -2.24401000 | 2.01382000 |
| C | 7.57227400 | -2.83763500 | 2.79726700 |
| H | 7.62438100 | -3.91649500 | 2.63808200 |
| H | 7.41637000 | -2.65331000 | 3.86415000 |
| C | 8.88799300 | -2.20528100 | 2.38498000 |
| H | 9.09372900 | -2.47515000 | 1.34123000 |
| C | 8.80620200 | -0.66971300 | 2.47926400 |
| H | 8.68651100 | -0.39945400 | 3.53559500 |
| C | 7.56086300 | -0.14636900 | 1.71764800 |
| H | 7.69290200 | -0.36775700 | 0.65128100 |
| C | 10.08334600 | 0.00596000 | 2.02039600 |
| C | -11.49774600 | -3.04589100 | 2.06727500 |
| H | -10.89502900 | -3.81653300 | 1.58183500 |
| H | -12.48169800 | -3.00804700 | 1.59611300 |
| H | -11.61428100 | -3.31419200 | 3.11936600 |
| C | -12.19942100 | -0.75314400 | 3.84313400 |
| H | -13.01995700 | -1.47498700 | 3.78270900 |
| H | -12.59278100 | 0.16995000 | 4.27889500 |
| H | -11.45702000 | -1.16134700 | 4.53273200 |
| C | -13.05592000 | 1.35184800 | -0.64557300 |
| H | -13.31417800 | 2.28266200 | -0.12827400 |
| H | -13.96527700 | 0.75853300 | -0.75290800 |
| H | -12.68337500 | 1.61580400 | -1.63821100 |
| O | 7.85863100 | 3.58218100 | -2.54148300 |

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| H | 7.01839500 | 3.23738200 | -2.20558800 |
| O | 11.26983600 | 5.55988300 | -0.94645400 |
| H | 11.59573300 | 5.53961700 | -1.86057400 |
| O | 8.36918600 | 3.77844800 | 0.30273900 |
| O | 7.21504700 | 1.96359000 | -0.46603500 |
| O | 6.60191800 | -2.56726500 | 0.66348600 |
| H | 5.76237300 | -2.36245500 | 0.21379100 |
| O | 6.41332600 | -0.83439800 | 2.19869800 |
| O | 10.29669400 | 1.19646000 | 2.01108300 |
| O | 3.96990700 | -2.12296400 | 0.47665300 |
| H | 3.07592800 | -1.95215800 | 0.12253300 |
| O | 1.32780000 | -1.68530200 | 0.42917100 |
| H | 0.83404100 | -2.50049000 | 0.22664100 |
| O | -0.35036300 | -3.11400300 | 2.15223300 |
| H | -1.30142000 | -3.20626100 | 2.37429500 |
| O | -3.02115900 | -2.91655300 | 2.54910800 |
| H | -3.82560700 | -3.46268500 | 2.45476100 |
| O | -5.71964300 | -3.34690500 | 2.50286700 |
| H | -6.20020800 | -3.89793600 | 1.84919900 |
| O | -8.40413100 | -2.04829700 | 0.70920100 |
| O | -9.55353600 | -1.72711800 | 2.62002300 |
| O | -13.63138300 | -0.80620200 | 1.17519200 |
| H | -14.18414400 | -0.92636700 | 1.95497800 |
| O | 9.87944000 | -2.72704800 | 3.24877700 |
| H | 10.73393200 | -2.50466800 | 2.86047900 |
| N | 10.55931400 | 4.12095200 | -3.23516500 |

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| H | 9.73609900 | 4.48200100 | -3.71220600 |
| H | 10.90497500 | 3.34512200 | -3.79129900 |
| C | 19.06243600 | 3.13498500 | 1.65902000 |
| H | 19.13699300 | 2.34590600 | 2.41765300 |
| H | 19.63696100 | 2.77968900 | 0.79449300 |
| C | 17.60067400 | 3.30516600 | 1.25423500 |
| H | 17.52420400 | 4.09467400 | 0.49493700 |
| H | 17.02416600 | 3.66104700 | 2.11835400 |
| C | 16.96773900 | 2.02495400 | 0.71726700 |
| H | 17.04420100 | 1.23571300 | 1.47708000 |
| H | 17.54425000 | 1.66934200 | -0.14705800 |
| C | 15.50665900 | 2.19761200 | 0.31335700 |
| H | 14.92966200 | 2.55432400 | 1.17650600 |
| H | 15.42917800 | 2.98627100 | -0.44617000 |
| C | 14.87209500 | 0.91811500 | -0.22350800 |
| H | 14.94927600 | 0.12746200 | 0.53558400 |
| H | 15.44500700 | 0.56041300 | -1.08885900 |
| C | 13.41136300 | 1.09608300 | -0.62398300 |
| H | 12.83999900 | 1.47575000 | 0.23661400 |
| H | 13.33554500 | 1.88155500 | -1.38726800 |
| C | 12.75277200 | -0.17842900 | -1.14982800 |
| H | 12.81541400 | -0.97129400 | -0.39027800 |
| H | 13.31741700 | -0.56192800 | -2.00810800 |
| C | 11.29506700 | 0.04391600 | -1.54203400 |
| H | 10.80140300 | 0.62009100 | -0.74984200 |
| H | 11.25871600 | 0.68186600 | -2.43492200 |

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| C | 10.48819600 | -1.22752800 | -1.78465800 |
| H | 10.49746200 | -1.83129300 | -0.86853500 |
| H | 10.96578000 | -1.83661200 | -2.56257000 |
| C | 9.04596200 | -0.91678700 | -2.17261500 |
| H | 8.62310000 | -0.21185600 | -1.44549000 |
| H | 9.03448300 | -0.38905800 | -3.13606800 |
| C | 8.12555900 | -2.12901200 | -2.24719200 |
| H | 8.14942800 | -2.66185100 | -1.29014700 |
| H | 8.48234100 | -2.82901500 | -3.01402100 |
| C | 6.68525900 | -1.71898000 | -2.53800700 |
| H | 6.63262800 | -1.20385300 | -3.50645100 |
| H | 6.37805300 | -0.97713600 | -1.78901500 |
| C | 5.69635300 | -2.87932600 | -2.52117500 |
| H | 5.78836800 | -3.41729200 | -1.57063800 |
| H | 5.95626100 | -3.60542400 | -3.30201900 |
| C | 4.25231700 | -2.41986000 | -2.70428300 |
| H | 4.10200200 | -2.06208000 | -3.73088100 |
| H | 4.06611000 | -1.56104000 | -2.04856500 |
| C | 3.24263000 | -3.51349700 | -2.37994700 |
| H | 3.37018100 | -3.81045800 | -1.33360000 |
| H | 3.43141800 | -4.40121900 | -2.99387800 |
| C | 1.79511100 | -3.05310900 | -2.60165200 |
| H | 1.62948300 | -2.83601800 | -3.65944000 |
| H | 1.58942200 | -2.15295400 | -2.01713900 |
| C | 0.84598600 | -4.14645800 | -2.20659800 |
| O | 0.45629400 | -5.03285700 | -2.92155100 |

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| C | 19.68372300 | 4.42111400 | 2.19416100 |
| H | 20.72974300 | 4.27628900 | 2.47769200 |
| H | 19.64839400 | 5.21629600 | 1.44273000 |
| H | 19.14492700 | 4.77946500 | 3.07704400 |
| C | -0.39509800 | -5.01603000 | -0.35620500 |
| H | -0.33133900 | -5.93029600 | -0.94926700 |
| H | -0.08085900 | -5.18504400 | 0.67364800 |
| C | -1.80656500 | -4.44752600 | -0.36451800 |
| H | -1.86901200 | -3.59403800 | 0.30826400 |
| C | -2.80658400 | -5.50314000 | 0.04002200 |
| H | -2.97199400 | -6.20919700 | -0.77680900 |
| H | -2.44336400 | -6.04213300 | 0.91800800 |
| O | 0.51023200 | -4.04731300 | -0.88907300 |
| C | -2.05124700 | -2.72315000 | -1.98831700 |
| C | -2.10267800 | -2.50038500 | -3.47822400 |
| H | -1.13527800 | -2.84084200 | -3.86536500 |
| H | -2.84427700 | -3.18590600 | -3.89976600 |
| C | -2.39170200 | -1.04966600 | -3.84452400 |
| H | -2.15890700 | -0.88535900 | -4.90155100 |
| H | -1.73237000 | -0.39642800 | -3.26433000 |
| C | -3.84721300 | -0.69242400 | -3.56874300 |
| H | -4.48872700 | -1.29620300 | -4.22601100 |
| H | -4.08371900 | -0.99738500 | -2.54314600 |
| C | -4.20350100 | 0.78041000 | -3.73468100 |
| H | -3.86368000 | 1.14540400 | -4.71216100 |
| H | -3.66842300 | 1.36647500 | -2.97848300 |

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| C | -5.70668500 | 1.00102700 | -3.58966800 |
| H | -6.05582100 | 0.46101200 | -2.70003500 |
| H | -6.22734300 | 0.54579400 | -4.44343100 |
| C | -6.13883200 | 2.45392800 | -3.43421800 |
| H | -5.66250800 | 2.85757600 | -2.53319600 |
| H | -5.77295900 | 3.05528200 | -4.27575700 |
| C | -7.65710100 | 2.58040100 | -3.30608000 |
| H | -8.02635100 | 1.74687700 | -2.69653000 |
| H | -8.12636300 | 2.46869800 | -4.29215200 |
| C | -8.12402200 | 3.87491000 | -2.65018300 |
| H | -7.64030300 | 3.95711800 | -1.66798000 |
| H | -7.78688700 | 4.74305600 | -3.23117500 |
| C | -9.63777500 | 3.92149600 | -2.46324400 |
| H | -9.96372200 | 2.98184500 | -2.00043600 |
| H | -10.12992900 | 3.96648400 | -3.44367700 |
| C | -10.11694300 | 5.08135700 | -1.59644200 |
| H | -9.60819200 | 5.03388500 | -0.62345500 |
| H | -9.81750400 | 6.03666400 | -2.04695200 |
| C | -11.62564800 | 5.06671800 | -1.37150400 |
| H | -12.13991500 | 5.14942900 | -2.33802600 |
| H | -11.91362700 | 4.09023500 | -0.96179600 |
| C | -12.11999800 | 6.16650300 | -0.43766000 |
| H | -11.59262900 | 6.09045400 | 0.52283200 |
| H | -11.85278800 | 7.14753900 | -0.85176800 |
| C | -13.62480900 | 6.11197200 | -0.19082400 |
| H | -14.15343700 | 6.18896200 | -1.15001000 |

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| H | -13.88850500 | 5.12756400 | 0.21969000 |
| C | -14.12636700 | 7.20162700 | 0.75185700 |
| H | -13.86569500 | 8.18556500 | 0.34017500 |
| H | -13.59572900 | 7.12512100 | 1.71025400 |
| C | -15.63032900 | 7.14102300 | 1.00145000 |
| H | -16.16139700 | 7.21799700 | 0.04333600 |
| H | -15.89143300 | 6.15666400 | 1.41276900 |
| C | -16.13329800 | 8.23027700 | 1.94490800 |
| H | -15.87240900 | 9.21276600 | 1.53243000 |
| H | -15.60166700 | 8.15235800 | 2.90144800 |
| C | -17.63756700 | 8.15872700 | 2.18682400 |
| H | -17.97514300 | 8.94740400 | 2.86464900 |
| H | -18.19155600 | 8.26520800 | 1.24873000 |
| H | -17.91920800 | 7.19693600 | 2.62731900 |
| O | -2.12014900 | -4.03235600 | -1.69978000 |
| O | -1.91023200 | -1.85302300 | -1.15854800 |
| O | -4.04029100 | -4.90300800 | 0.43718400 |
| O | -5.12989400 | -3.31931200 | -1.19430500 |
| O | -6.58108000 | -4.75586100 | 0.35675500 |
| O | -5.21385900 | -5.83323500 | -1.58226800 |
| C | -6.29973700 | -2.64942800 | -1.70094200 |
| H | -7.10841200 | -2.72041600 | -0.96920900 |
| H | -6.02071000 | -1.60153900 | -1.80707000 |
| C | -6.70986600 | -3.18919000 | -3.05860300 |
| H | -5.85288700 | -3.14181300 | -3.73530000 |
| H | -7.49133500 | -2.52948700 | -3.45914700 |

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| N | -7.14369800 | -4.59367900 | -2.97268700 |
| H | -7.93726700 | -4.67732300 | -2.33962900 |
| H | -7.44471500 | -4.93119800 | -3.88187200 |
| P | -5.33780900 | -4.73822600 | -0.45256000 |
| H | -5.90159800 | -5.57000500 | -2.27515000 |
| O | 11.03221500 | -0.85983100 | 1.59452300 |
| H | 11.79397800 | -0.32552100 | 1.31620900 |

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| C | 5.97553500 | 1.78255100 | -3.06338400 |
| H | 6.79297800 | 1.10286200 | -2.79036600 |
| C | 6.25740100 | 3.10999200 | -2.36143700 |
| H | 5.45869000 | 3.82249200 | -2.62285300 |
| C | 6.22011500 | 2.91965000 | -0.84989900 |
| H | 6.96713900 | 2.15403000 | -0.57812200 |
| C | 4.62880600 | 1.19331600 | -1.04252500 |
| H | 5.37053900 | 0.46183500 | -0.67116700 |
| C | 4.66416500 | 1.17811100 | -2.57088300 |
| H | 4.59724900 | 0.12810800 | -2.88695100 |
| C | 6.50016700 | 4.19156800 | -0.08504200 |
| H | 5.78211300 | 4.96460800 | -0.36291600 |
| H | 7.50294200 | 4.54693500 | -0.32696000 |
| H | 6.42657200 | 4.01299300 | 0.98999400 |

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| C | 3.00618400 | 0.79459500 | 0.71260600 |
| H | 3.17803800 | 1.78818000 | 1.13895300 |
| C | 1.55017500 | 0.47156200 | 0.72759500 |
| H | 1.26080100 | -0.37817200 | 0.12064400 |
| C | 0.61718200 | 1.17885300 | 1.37148800 |
| H | 0.89930400 | 2.04821000 | 1.96493000 |
| C | -0.78933300 | 0.85121800 | 1.26640600 |
| H | -1.04195700 | 0.00639200 | 0.63177300 |
| C | -1.79886700 | 1.52611400 | 1.84796800 |
| H | -1.59238900 | 2.37719900 | 2.49647300 |
| C | -3.17466100 | 1.16060100 | 1.61296400 |
| H | -3.33363100 | 0.33930000 | 0.91645100 |
| C | -4.24564000 | 1.76589600 | 2.16590300 |
| H | -4.10595900 | 2.59341800 | 2.86072700 |
| C | -5.59380800 | 1.36910200 | 1.85443600 |
| H | -5.70149700 | 0.54081800 | 1.15410500 |
| C | -6.71098900 | 1.95194300 | 2.34193100 |
| H | -6.62807900 | 2.78092000 | 3.04360500 |
| C | -8.03013100 | 1.54569700 | 1.92959800 |
| H | -8.07308300 | 0.70004500 | 1.24580000 |
| C | -9.19383300 | 2.12522200 | 2.28978600 |
| H | -9.18792000 | 2.95185300 | 2.99903600 |
| C | -10.46721900 | 1.71218200 | 1.75013600 |
| H | -10.43618000 | 0.96249900 | 0.96092300 |
| C | -11.67104900 | 2.17228400 | 2.13624700 |
| H | -11.73905600 | 2.89636300 | 2.94709100 |

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| C | 3.88562000 | -0.21270600 | 1.46391900 |
| H | 4.88873300 | 0.20875900 | 1.56393000 |
| H | 3.49448700 | -0.32881100 | 2.47867100 |
| C | -12.90696800 | 1.71110300 | 1.53248700 |
| H | -12.79098100 | 1.11672400 | 0.62842200 |
| C | -14.13396900 | 1.91885900 | 2.02130900 |
| H | -14.25134200 | 2.49614700 | 2.93963900 |
| C | -15.39801700 | 1.37192900 | 1.41812800 |
| H | -15.19026000 | 1.04429200 | 0.39313500 |
| C | -15.90372600 | 0.14270700 | 2.19903900 |
| H | -16.18418400 | 0.49071900 | 3.20711400 |
| C | -14.86562600 | -0.97903100 | 2.39652600 |
| H | -14.01797300 | -0.51526200 | 2.90981600 |
| C | -14.29751700 | -1.52274400 | 1.07979900 |
| H | -14.00890700 | -0.69829200 | 0.43297500 |
| C | -11.93701100 | -1.90745300 | 0.83216900 |
| C | -10.76700200 | -2.73464900 | 1.29905900 |
| H | -11.00295000 | -3.19432600 | 2.26019200 |
| H | -10.62308600 | -3.53796100 | 0.56725800 |
| C | -9.47653000 | -1.91301700 | 1.38528000 |
| H | -9.62465300 | -1.09590100 | 2.10791900 |
| C | -8.31325700 | -2.77605800 | 1.84442800 |
| H | -8.54143500 | -3.15611900 | 2.84635400 |
| H | -8.21357200 | -3.63960500 | 1.17642400 |
| C | -6.96962800 | -2.05287700 | 1.88245700 |
| H | -7.09209200 | -1.07905200 | 2.37758600 |

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| C | -5.93577700 | -2.86441100 | 2.65961000 |
| H | -6.00633900 | -3.91301300 | 2.34665000 |
| H | -6.21866400 | -2.83128500 | 3.71617100 |
| C | -4.49340300 | -2.36907900 | 2.46920300 |
| H | -4.48764800 | -1.34297800 | 2.09338100 |
| H | -3.97043000 | -2.34790600 | 3.43008700 |
| C | -3.67741200 | -3.25442400 | 1.52829000 |
| H | -3.52845300 | -4.22652400 | 2.01941300 |
| C | -2.29250600 | -2.64445400 | 1.21962000 |
| H | -1.95750000 | -2.04477600 | 2.07644400 |
| C | -1.24476600 | -3.72105100 | 0.94814400 |
| H | -1.60094500 | -4.39762200 | 0.16382900 |
| H | -1.12995000 | -4.31259800 | 1.86499500 |
| C | 0.11148500 | -3.15954500 | 0.52114600 |
| H | 0.28622400 | -2.20271500 | 1.02737600 |
| C | 1.27073300 | -4.08841000 | 0.87296200 |
| H | 1.12539400 | -5.05589000 | 0.38120800 |
| H | 1.28123000 | -4.25471200 | 1.95345200 |
| C | 2.63738700 | -3.54595800 | 0.44924200 |
| C | 3.78944300 | -4.45484800 | 0.87435900 |
| H | 3.72556600 | -5.40141800 | 0.33375000 |
| H | 3.72263500 | -4.66096300 | 1.94688200 |
| C | 5.11648300 | -3.78532600 | 0.57336000 |
| H | 5.17638900 | -3.61165100 | -0.50477000 |
| C | 5.16890200 | -2.42899500 | 1.28474800 |
| H | 5.08179900 | -2.57587100 | 2.36487800 |

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| C | 3.96559700 | -1.58272600 | 0.80750000 |
| H | 4.04013600 | -1.46619300 | -0.27890000 |
| C | 6.46921800 | -1.70390900 | 1.06257100 |
| C | -15.16949400 | -2.49280400 | 0.30888600 |
| H | -14.68235600 | -2.77030300 | -0.62875200 |
| H | -16.12618100 | -2.01666600 | 0.09138400 |
| H | -15.34918600 | -3.40334600 | 0.88441000 |
| C | -15.41073400 | -2.08613500 | 3.29786700 |
| H | -16.30931200 | -2.54963400 | 2.87948300 |
| H | -15.66376300 | -1.68993800 | 4.28539400 |
| H | -14.66861000 | -2.87614700 | 3.43202800 |
| C | -16.48749600 | 2.44616600 | 1.36007300 |
| H | -16.72102100 | 2.81253900 | 2.36602600 |
| H | -17.40187300 | 2.04257200 | 0.92446000 |
| H | -16.15473100 | 3.29879800 | 0.76352300 |
| O | 3.60309200 | 1.92606600 | -3.12361600 |
| H | 2.81743900 | 1.74804100 | -2.58720400 |
| O | 7.52612300 | 3.58581800 | -2.74290300 |
| H | 7.57015000 | 3.40702900 | -3.69636900 |
| O | 4.91790700 | 2.45520000 | -0.49316200 |
| O | 3.33414100 | 0.83486600 | -0.69004100 |
| O | 2.72116500 | -3.39001800 | -0.93783400 |
| H | 1.81889300 | -3.12310900 | -1.22379400 |
| O | 2.76870300 | -2.28214300 | 1.11032900 |
| O | 7.03805300 | -1.00835800 | 1.86607600 |
| O | 0.14757900 | -2.96248500 | -0.89483800 |

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| H | -0.19149800 | -2.07285600 | -1.11908700 |
| O | -2.42373600 | -1.74613800 | 0.13036900 |
| H | -3.18419400 | -2.07676200 | -0.38291600 |
| O | -4.32022800 | -3.50198000 | 0.28777200 |
| H | -5.11179900 | -2.93161000 | 0.21098600 |
| O | -6.45156700 | -1.84010700 | 0.57254300 |
| H | -7.14883500 | -1.54641100 | -0.03641200 |
| O | -9.14422600 | -1.35770700 | 0.11659300 |
| H | -9.97766000 | -1.03615400 | -0.27245400 |
| O | -11.83330100 | -1.04336800 | -0.02642000 |
| O | -13.06805800 | -2.23155700 | 1.43779900 |
| O | -17.06371400 | -0.31969500 | 1.51387500 |
| H | -17.56569600 | -0.89022700 | 2.10558400 |
| O | 6.16353800 | -4.64403200 | 0.99588100 |
| H | 6.96761000 | -4.37155900 | 0.53767100 |
| N | 6.04394900 | 2.00796300 | -4.50286600 |
| H | 5.16411600 | 2.42325600 | -4.80107400 |
| H | 6.13786500 | 1.12868100 | -5.00125000 |
| C | 15.81067700 | -10.60556700 | 4.79520300 |
| H | 15.07217700 | -10.75086300 | 5.59339400 |
| H | 15.76622100 | -11.50820100 | 4.17316700 |
| C | 15.40862600 | -9.39688300 | 3.95431400 |
| H | 16.14717800 | -9.25001900 | 3.15489900 |
| H | 15.45266900 | -8.49254900 | 4.57582200 |
| C | 14.01728500 | -9.52094000 | 3.34056300 |
| H | 13.27948500 | -9.66838400 | 4.14034600 |

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| H | 13.97388700 | -10.42514000 | 2.71897100 |
| C | 13.61560500 | -8.31184300 | 2.50092200 |
| H | 13.65882000 | -7.40777400 | 3.12259100 |
| H | 14.35320500 | -8.16406900 | 1.70097800 |
| C | 12.22398200 | -8.43609600 | 1.88769000 |
| H | 11.48664900 | -8.58468700 | 2.68758400 |
| H | 12.18075600 | -9.33959600 | 1.26511200 |
| C | 11.82137200 | -7.22614700 | 1.04980700 |
| H | 11.86495700 | -6.32297800 | 1.67281100 |
| H | 12.55817500 | -7.07722100 | 0.24928400 |
| C | 10.42897800 | -7.35012100 | 0.43846200 |
| H | 9.69237500 | -7.49953400 | 1.23864400 |
| H | 10.38486400 | -8.25233000 | -0.18581300 |
| C | 10.02435000 | -6.13924100 | -0.39682500 |
| H | 10.07319500 | -5.23718500 | 0.22858700 |
| H | 10.75736600 | -5.98869000 | -1.20043500 |
| C | 8.62771400 | -6.26045700 | -0.99863700 |
| H | 7.89558700 | -6.41592000 | -0.19534800 |
| H | 8.57803500 | -7.15647900 | -1.63066600 |
| C | 8.21168100 | -5.04196000 | -1.81817500 |
| H | 8.26881100 | -4.14160000 | -1.18755700 |
| H | 8.93316400 | -4.87370700 | -2.62808800 |
| C | 6.80124300 | -5.15557200 | -2.39107200 |
| H | 6.11934900 | -5.44004100 | -1.58033500 |
| H | 6.76277700 | -5.97450900 | -3.12048800 |
| C | 6.30217700 | -3.85953700 | -3.02403300 |

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|---|-------------|--------------|-------------|
| H | 6.94046000 | -3.58699200 | -3.87463700 |
| H | 6.41981200 | -3.05255100 | -2.29114100 |
| C | 4.83779500 | -3.91372300 | -3.46126700 |
| H | 4.25375400 | -4.46449200 | -2.71547100 |
| H | 4.74211600 | -4.46216500 | -4.40696700 |
| C | 4.22083900 | -2.52471300 | -3.58107600 |
| H | 4.82173500 | -1.89549800 | -4.25274300 |
| H | 4.26368300 | -2.06202500 | -2.58895600 |
| C | 2.76845700 | -2.53818700 | -4.04384600 |
| H | 2.22208600 | -3.31511100 | -3.50369500 |
| H | 2.71526400 | -2.80314500 | -5.10650300 |
| C | 2.08275900 | -1.19255100 | -3.80463600 |
| H | 2.61813700 | -0.35959900 | -4.26749000 |
| H | 2.05126700 | -0.98563700 | -2.72676000 |
| C | 0.65984000 | -1.11481500 | -4.27887300 |
| O | 0.14691100 | -0.15078400 | -4.79670900 |
| C | 17.20293900 | -10.46990100 | 5.40327700 |
| H | 17.46955500 | -11.34594700 | 6.00080600 |
| H | 17.96236500 | -10.35410800 | 4.62339300 |
| H | 17.26334200 | -9.59137600 | 6.05356100 |
| C | -1.41145000 | -2.28356900 | -4.30266100 |
| H | -1.63233100 | -1.62996500 | -5.14944600 |
| H | -1.63676400 | -3.32120600 | -4.56032300 |
| C | -2.24380800 | -1.86422700 | -3.10295400 |
| H | -1.85158200 | -2.31582600 | -2.19269100 |
| C | -3.70367600 | -2.24600800 | -3.28737000 |

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| H | -4.07723500 | -1.88449000 | -4.24863500 |
| H | -3.81413800 | -3.32990600 | -3.22573600 |
| O | -0.01436100 | -2.25674700 | -4.01028300 |
| C | -1.27017300 | 0.13990200 | -2.26129000 |
| C | -1.34945700 | 1.63438000 | -2.22164600 |
| H | -1.97360500 | 1.98722900 | -3.04426000 |
| H | -1.86554800 | 1.87960100 | -1.28487000 |
| C | 0.05799100 | 2.23311500 | -2.22852600 |
| H | 0.48723600 | 2.11086400 | -3.23026300 |
| H | 0.67103100 | 1.64253800 | -1.54293300 |
| C | 0.12332200 | 3.68964500 | -1.78913400 |
| H | -0.41645800 | 4.33313000 | -2.49576300 |
| H | -0.38762200 | 3.79273800 | -0.82235500 |
| C | 1.56722300 | 4.16229400 | -1.64408000 |
| H | 2.09109800 | 4.05780100 | -2.60231300 |
| H | 2.09449000 | 3.49379500 | -0.95098700 |
| C | 1.70000100 | 5.59748500 | -1.14813400 |
| H | 1.11305900 | 5.72186700 | -0.22795600 |
| H | 1.26236400 | 6.28635200 | -1.88281100 |
| C | 3.14882600 | 5.98558700 | -0.87374600 |
| H | 3.55940300 | 5.29833700 | -0.12388700 |
| H | 3.74492100 | 5.82566800 | -1.78242500 |
| C | 3.32362800 | 7.42513200 | -0.40152500 |
| H | 2.70697300 | 7.59350100 | 0.49152200 |
| H | 2.93793500 | 8.10963600 | -1.16873200 |
| C | 4.77361800 | 7.78227500 | -0.08721500 |

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|---|-------------|-------------|-------------|
| H | 5.14902000 | 7.11383500 | 0.69870500 |
| H | 5.39571000 | 7.58682600 | -0.97082100 |
| C | 4.96320400 | 9.23073900 | 0.35242600 |
| H | 4.33982800 | 9.42745400 | 1.23487200 |
| H | 4.59300500 | 9.90088000 | -0.43476900 |
| C | 6.41416800 | 9.57904100 | 0.67106200 |
| H | 6.78372300 | 8.90845000 | 1.45809800 |
| H | 7.03675800 | 9.38029600 | -0.21120000 |
| C | 6.60783500 | 11.02742700 | 1.10991600 |
| H | 6.23778600 | 11.69788300 | 0.32289800 |
| H | 5.98580400 | 11.22581300 | 1.99289200 |
| C | 8.05938500 | 11.37476700 | 1.42696000 |
| H | 8.42958700 | 10.70416100 | 2.21369000 |
| H | 8.68108600 | 11.17634100 | 0.54392700 |
| C | 8.25375800 | 12.82312900 | 1.86580500 |
| H | 7.88296700 | 13.49366900 | 1.07923600 |
| H | 7.63254300 | 13.02135300 | 2.74934300 |
| C | 9.70559300 | 13.17050600 | 2.18166400 |
| H | 10.32655500 | 12.97233000 | 1.29799300 |
| H | 10.07643400 | 12.49973300 | 2.96799300 |
| C | 9.90032000 | 14.61870900 | 2.62064300 |
| H | 9.52947500 | 15.29007900 | 1.83461200 |
| H | 9.27988800 | 14.81742400 | 3.50478700 |
| C | 11.35247700 | 14.96700200 | 2.93620300 |
| H | 11.97096700 | 14.76826900 | 2.05214400 |
| H | 11.72162400 | 14.29561400 | 3.72142600 |

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|---|-------------|-------------|-------------|
| C | 11.53437500 | 16.41680400 | 3.37386800 |
| H | 12.58103600 | 16.64361200 | 3.59442900 |
| H | 11.20061400 | 17.10743200 | 2.59284000 |
| H | 10.94947700 | 16.63145300 | 4.27398000 |
| O | -2.23558300 | -0.43246300 | -2.97393500 |
| O | -0.39430000 | -0.48879100 | -1.69453900 |
| O | -4.48603000 | -1.69141100 | -2.22460500 |
| O | -6.75424800 | -0.66124900 | -2.07898500 |
| O | -5.11734500 | 0.25620800 | -3.84149300 |
| O | -4.72144800 | 0.59881300 | -1.26752100 |
| C | -7.78897600 | 0.18620500 | -2.59572100 |
| H | -7.47634900 | 0.58660400 | -3.56438800 |
| H | -8.66643200 | -0.44770800 | -2.74404900 |
| C | -8.12771500 | 1.28850700 | -1.60682400 |
| H | -8.46168100 | 0.81640300 | -0.68577100 |
| H | -8.97079600 | 1.86933400 | -2.00527900 |
| N | -6.96346400 | 2.12748700 | -1.28547100 |
| H | -6.79783600 | 2.81353400 | -2.01710200 |
| H | -7.12535500 | 2.63111000 | -0.41761300 |
| P | -5.22319300 | -0.28905700 | -2.47522600 |
| H | -5.45887300 | 1.26833200 | -1.10524100 |
| O | 6.95613700 | -1.87119100 | -0.19440500 |
| H | 7.77249800 | -1.34781400 | -0.24310400 |

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|---|-------------|-------------|-------------|
| C | 17.57677100 | -5.49773100 | -1.94692900 |
| H | 18.32922600 | -4.74540400 | -1.68862200 |
| C | 17.64645900 | -5.74773100 | -3.44816000 |
| H | 16.89508800 | -6.49986500 | -3.71999300 |
| C | 17.33846300 | -4.43657300 | -4.20293400 |
| H | 18.15895100 | -3.73928400 | -3.96226300 |
| C | 16.05938700 | -3.61269900 | -2.41696800 |
| H | 16.88051100 | -2.92901800 | -2.15291700 |
| C | 16.21441400 | -4.91447200 | -1.64906300 |
| H | 16.11566100 | -4.69926900 | -0.59105300 |
| C | 17.26089800 | -4.63662000 | -5.70154800 |
| H | 16.45983200 | -5.34008700 | -5.94482500 |
| H | 18.20838600 | -5.01916300 | -6.08969100 |
| H | 17.04578800 | -3.68836900 | -6.19703600 |
| C | 14.84161600 | -1.80021100 | -1.39938500 |
| H | 15.29220300 | -1.05521600 | -2.07041300 |
| C | 13.40721100 | -1.45075000 | -1.15531800 |
| H | 12.85789300 | -2.10255300 | -0.48100200 |
| C | 12.79738400 | -0.39396100 | -1.70014300 |
| H | 13.35028700 | 0.26012300 | -2.37411600 |
| C | 11.40696500 | -0.06773200 | -1.45286600 |
| H | 10.87334600 | -0.71574000 | -0.76190100 |
| C | 10.74683500 | 0.95644000 | -2.02587900 |
| H | 11.27039700 | 1.60894500 | -2.72436700 |

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|---|-------------|-------------|-------------|
| C | 9.35358100 | 1.23012100 | -1.76618900 |
| H | 8.86910100 | 0.57885600 | -1.04162300 |
| C | 8.63796800 | 2.22053100 | -2.33602600 |
| H | 9.11101700 | 2.88228400 | -3.06100700 |
| C | 7.24685500 | 2.44979200 | -2.03378700 |
| H | 6.79513500 | 1.80524000 | -1.27936300 |
| C | 6.48059700 | 3.40229200 | -2.60437500 |
| H | 6.91672500 | 4.06604700 | -3.34997700 |
| C | 5.08593300 | 3.58227600 | -2.28977900 |
| H | 4.66469900 | 2.90126100 | -1.55188600 |
| C | 4.28084600 | 4.51791600 | -2.83326000 |
| H | 4.69342000 | 5.21991900 | -3.55703200 |
| C | 2.88138700 | 4.64449600 | -2.50258700 |
| H | 2.47318300 | 3.89644900 | -1.82411200 |
| C | 2.06894100 | 5.62383600 | -2.94280200 |
| H | 2.46447500 | 6.40513500 | -3.59080800 |
| C | 15.67564900 | -1.83551500 | -0.10428500 |
| H | 16.71696100 | -2.05844200 | -0.33656000 |
| H | 15.66235000 | -0.83091500 | 0.32864200 |
| C | 0.67719600 | 5.71071900 | -2.54571000 |
| H | 0.29957200 | 4.85399400 | -1.99495900 |
| C | -0.13777200 | 6.75341200 | -2.73563800 |
| H | 0.22229400 | 7.63698000 | -3.26436800 |
| C | -1.55162300 | 6.79683300 | -2.23071200 |
| H | -1.79182000 | 5.81164200 | -1.81351400 |
| C | -1.74206100 | 7.82123300 | -1.09440800 |

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|---|-------------|------------|-------------|
| H | -1.69439300 | 8.82552800 | -1.54600300 |
| C | -0.68385100 | 7.78157800 | 0.02475000 |
| H | 0.28714400 | 7.83001000 | -0.47729900 |
| C | -0.68783700 | 6.44892300 | 0.78293600 |
| H | -0.82490300 | 5.65071200 | 0.06031700 |
| C | 1.31856900 | 5.17023600 | 1.01532900 |
| C | 2.59055700 | 5.04361200 | 1.80735100 |
| H | 2.95455600 | 6.04328000 | 2.05417300 |
| H | 2.31833200 | 4.55270800 | 2.74885400 |
| C | 3.68483500 | 4.23879600 | 1.10929700 |
| H | 3.86623300 | 4.66461900 | 0.11606900 |
| C | 4.98172300 | 4.28892300 | 1.91748300 |
| H | 5.28645500 | 5.33378000 | 2.04453200 |
| H | 4.79518900 | 3.87543100 | 2.91649800 |
| C | 6.13325300 | 3.52099900 | 1.27494200 |
| H | 6.30286500 | 3.90628300 | 0.25955400 |
| C | 7.42568200 | 3.66366500 | 2.07129800 |
| H | 7.21324300 | 3.46915300 | 3.12969800 |
| H | 7.74344600 | 4.70861200 | 2.00184500 |
| C | 8.54697700 | 2.73156800 | 1.58283700 |
| H | 8.35769800 | 2.41816600 | 0.55310100 |
| H | 9.50128600 | 3.26709500 | 1.56630600 |
| C | 8.74688700 | 1.49410600 | 2.45628700 |
| H | 9.12530600 | 1.81829900 | 3.43573400 |
| C | 9.77203900 | 0.51802900 | 1.82903300 |
| H | 10.45681800 | 1.06666800 | 1.17208500 |

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| C | 10.57896600 | -0.25184000 | 2.86877800 |
| H | 9.89203700 | -0.82553800 | 3.50265800 |
| H | 11.10244500 | 0.46450400 | 3.51223800 |
| C | 11.60682500 | -1.18589200 | 2.23680200 |
| H | 12.26443700 | -0.59970100 | 1.58073400 |
| C | 12.47208400 | -1.87986700 | 3.28174700 |
| H | 11.83658600 | -2.44377900 | 3.97154600 |
| H | 13.00823700 | -1.11782800 | 3.85464100 |
| C | 13.49020400 | -2.84845700 | 2.67909700 |
| C | 14.48021300 | -3.38895700 | 3.70628400 |
| H | 13.95951900 | -4.01909900 | 4.43027900 |
| H | 14.94210900 | -2.55336600 | 4.24079000 |
| C | 15.56235700 | -4.19630900 | 3.01361300 |
| H | 15.09124200 | -5.05545700 | 2.52320400 |
| C | 16.25007300 | -3.34851200 | 1.93554800 |
| H | 16.73611800 | -2.48820600 | 2.40732200 |
| C | 15.16786600 | -2.80120200 | 0.96213000 |
| H | 14.66606200 | -3.65450400 | 0.49090200 |
| C | 17.33240100 | -4.11772500 | 1.19580500 |
| C | -1.68802300 | 6.30104400 | 1.91442400 |
| H | -1.62154100 | 5.29286600 | 2.32850600 |
| H | -2.69791700 | 6.47609000 | 1.54133900 |
| H | -1.47961100 | 7.01288300 | 2.71585300 |
| C | -0.79709400 | 8.99165800 | 0.94975100 |
| H | -1.77766900 | 9.05014800 | 1.43345500 |
| H | -0.64040300 | 9.92080700 | 0.39485000 |

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|---|-------------|-------------|-------------|
| H | -0.04736100 | 8.94146000 | 1.74284300 |
| C | -2.54414200 | 7.08177400 | -3.36234800 |
| H | -2.31760000 | 8.04070500 | -3.84102600 |
| H | -3.56406700 | 7.12522000 | -2.97675500 |
| H | -2.48677200 | 6.30527800 | -4.12839900 |
| O | 15.22816300 | -5.85478200 | -2.03018800 |
| H | 14.38299200 | -5.38468500 | -2.02935900 |
| O | 18.96239700 | -6.19916800 | -3.73350700 |
| H | 18.95862200 | -6.63839400 | -4.59033400 |
| O | 16.09556300 | -3.86608000 | -3.80088100 |
| O | 14.81923600 | -3.06747200 | -2.08790900 |
| O | 12.86800400 | -3.94891300 | 2.07960300 |
| H | 12.07342500 | -3.60671800 | 1.63043800 |
| O | 14.20574800 | -2.07724100 | 1.71558500 |
| O | 18.16880400 | -3.58657100 | 0.49329300 |
| O | 17.23035900 | -5.44479600 | 1.32551400 |
| O | 10.96552200 | -2.19607900 | 1.45242600 |
| H | 10.13808300 | -1.81443300 | 1.10392800 |
| O | 9.05091400 | -0.39109500 | 0.99357500 |
| H | 8.17731300 | -0.43664500 | 1.43622700 |
| O | 7.55388200 | 0.75558400 | 2.67482100 |
| H | 6.81382000 | 1.18765200 | 2.19317600 |
| O | 5.81871000 | 2.12840100 | 1.17439300 |
| H | 4.84531700 | 2.07003400 | 1.08032600 |
| O | 3.30337500 | 2.87613600 | 0.90066700 |
| H | 2.54639200 | 2.64331700 | 1.48790300 |

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|---|--------------|-------------|-------------|
| O | 0.94406300 | 4.37327400 | 0.18322200 |
| O | 0.62975800 | 6.26404300 | 1.36601900 |
| O | -3.05894800 | 7.58620200 | -0.59202700 |
| H | -3.32337300 | 8.33368000 | -0.04442200 |
| O | 16.48879300 | -4.62874600 | 3.99361900 |
| H | 17.01428000 | -5.32566400 | 3.58041400 |
| N | 17.83096900 | -6.65407400 | -1.08569800 |
| H | 17.07070200 | -7.32185300 | -1.20029600 |
| H | 17.69783500 | -5.91529200 | 0.56650100 |
| H | 18.68926500 | -7.10652100 | -1.38916100 |
| C | -24.79356500 | -4.79234900 | -1.99114900 |
| H | -24.72163700 | -4.95442300 | -3.07364100 |
| H | -24.37540800 | -5.69049000 | -1.52136300 |
| C | -23.94252200 | -3.58502100 | -1.60741100 |
| H | -24.05184900 | -3.39188800 | -0.53166800 |
| H | -24.32902700 | -2.69048700 | -2.11337400 |
| C | -22.46402200 | -3.76044400 | -1.93860300 |
| H | -22.35046300 | -3.94985200 | -3.01401500 |
| H | -22.08555400 | -4.65788000 | -1.43219700 |
| C | -21.60721500 | -2.56228200 | -1.54238400 |
| H | -21.97341000 | -1.66469100 | -2.05764900 |
| H | -21.73346700 | -2.36577400 | -0.46916600 |
| C | -20.12511600 | -2.75418800 | -1.84771300 |
| H | -19.99591900 | -2.94403900 | -2.92125600 |
| H | -19.76430100 | -3.65559000 | -1.33572300 |
| C | -19.26377700 | -1.56415900 | -1.43723000 |

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| H | -19.62432400 | -0.66031600 | -1.94557400 |
| H | -19.39294500 | -1.37685500 | -0.36271300 |
| C | -17.78156400 | -1.75863200 | -1.74047600 |
| H | -17.65037700 | -1.93554700 | -2.81597400 |
| H | -17.42527200 | -2.66750800 | -1.23883700 |
| C | -16.91750900 | -0.57651100 | -1.31317400 |
| H | -17.27879400 | 0.33589600 | -1.80544500 |
| H | -17.04331900 | -0.40669900 | -0.23536200 |
| C | -15.43632300 | -0.76642400 | -1.62446000 |
| H | -15.30816100 | -0.91937800 | -2.70395900 |
| H | -15.07964200 | -1.68653800 | -1.14410800 |
| C | -14.57048500 | 0.40520500 | -1.17265000 |
| H | -14.93635500 | 1.32973300 | -1.63816600 |
| H | -14.68908900 | 0.54656200 | -0.08992300 |
| C | -13.09110200 | 0.22674300 | -1.49924500 |
| H | -12.96927000 | 0.11170400 | -2.58410100 |
| H | -12.73056300 | -0.70912100 | -1.05326900 |
| C | -12.22465500 | 1.38330200 | -1.01125100 |
| H | -12.33109000 | 1.48029300 | 0.07763800 |
| H | -12.60011700 | 2.32407400 | -1.43461400 |
| C | -10.74850200 | 1.22655100 | -1.36256000 |
| H | -10.63717200 | 1.16676000 | -2.45271800 |
| H | -10.37869000 | 0.27120000 | -0.96781600 |
| C | -9.88262400 | 2.36185600 | -0.82574800 |
| H | -9.97466300 | 2.39901300 | 0.26831700 |
| H | -10.27063900 | 3.32130500 | -1.19227800 |

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| C | -8.41333400 | 2.22939300 | -1.21066100 |
| H | -8.30258700 | 2.23843100 | -2.29913300 |
| H | -8.02811100 | 1.25706400 | -0.88209100 |
| C | -7.55543500 | 3.33601600 | -0.61287000 |
| H | -7.60027600 | 3.33675200 | 0.48111100 |
| H | -7.91785300 | 4.32353800 | -0.92365200 |
| C | -6.10986800 | 3.23856700 | -1.02534900 |
| O | -5.68336100 | 2.55166300 | -1.91835100 |
| C | -26.25615300 | -4.64215800 | -1.58692200 |
| H | -26.84691700 | -5.51420200 | -1.88006800 |
| H | -26.35144000 | -4.52418400 | -0.50260100 |
| H | -26.70625200 | -3.76066700 | -2.05456700 |
| C | -3.93310700 | 4.00356700 | -0.47089900 |
| H | -3.71946400 | 3.61502700 | -1.46946000 |
| H | -3.56774000 | 5.02938700 | -0.38160600 |
| C | -3.29747100 | 3.12518600 | 0.59432300 |
| H | -3.48687000 | 3.53094800 | 1.59078100 |
| C | -1.79810400 | 2.98002000 | 0.38270800 |
| H | -1.59590500 | 2.07214600 | -0.18782700 |
| H | -1.39040800 | 3.82649000 | -0.16975200 |
| O | -5.34224900 | 4.05090200 | -0.26004100 |
| C | -4.00777900 | 1.03860200 | 1.54150200 |
| C | -4.90278200 | -0.13665200 | 1.28153400 |
| H | -4.82175400 | -0.41576400 | 0.22820700 |
| H | -4.56538500 | -0.96819700 | 1.90319500 |
| C | -6.35923400 | 0.22339500 | 1.61179100 |

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| H | -6.63188300 | 1.13832100 | 1.07461700 |
| H | -6.44119100 | 0.44707500 | 2.68128500 |
| C | -7.32326400 | -0.89532000 | 1.23283400 |
| H | -7.25811200 | -1.07193100 | 0.15129300 |
| H | -7.00541000 | -1.82882400 | 1.71437900 |
| C | -8.77171400 | -0.60060400 | 1.61138200 |
| H | -9.08526100 | 0.34532700 | 1.15196900 |
| H | -8.84261700 | -0.45105400 | 2.69634300 |
| C | -9.72698000 | -1.71172600 | 1.18661100 |
| H | -9.39689900 | -2.66036900 | 1.62973800 |
| H | -9.66036100 | -1.84858800 | 0.09894900 |
| C | -11.18035300 | -1.45566900 | 1.57275500 |
| H | -11.25005300 | -1.31130700 | 2.65872000 |
| H | -11.51901900 | -0.51564600 | 1.11888500 |
| C | -12.11246700 | -2.58756600 | 1.15120700 |
| H | -11.77154500 | -3.52534400 | 1.60915500 |
| H | -12.03238200 | -2.73719400 | 0.06606600 |
| C | -13.57362100 | -2.34954800 | 1.51888900 |
| H | -13.65605300 | -2.18665000 | 2.60139700 |
| H | -13.92217100 | -1.42294600 | 1.04527800 |
| C | -14.48598700 | -3.50190400 | 1.10972400 |
| H | -14.13960900 | -4.42588100 | 1.59105600 |
| H | -14.39116400 | -3.67284000 | 0.02891500 |
| C | -15.95391600 | -3.27252800 | 1.45545700 |
| H | -16.05045700 | -3.08934400 | 2.53357900 |
| H | -16.30561400 | -2.35850800 | 0.96012400 |

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| C | -16.85193100 | -4.44046300 | 1.05888900 |
| H | -16.74607800 | -4.62988800 | -0.01780500 |
| H | -16.50225700 | -5.35261000 | 1.56001000 |
| C | -18.32451400 | -4.21628300 | 1.38804300 |
| H | -18.43118400 | -4.01495900 | 2.46198900 |
| H | -18.67819100 | -3.31329300 | 0.87413100 |
| C | -19.21246700 | -5.39641200 | 1.00502500 |
| H | -19.09924800 | -5.60233800 | -0.06788400 |
| H | -18.86046300 | -6.29822300 | 1.52294100 |
| C | -20.68808700 | -5.17457400 | 1.32219000 |
| H | -21.04233600 | -4.28114100 | 0.79218400 |
| H | -20.80169300 | -4.95666200 | 2.39221100 |
| C | -21.57023500 | -6.36338000 | 0.95295700 |
| H | -21.44827900 | -6.58850500 | -0.11530200 |
| H | -21.22219800 | -7.25578200 | 1.48980500 |
| C | -23.04940100 | -6.13722000 | 1.25243400 |
| H | -23.39502400 | -5.25267600 | 0.70481700 |
| H | -23.17117400 | -5.90168000 | 2.31684800 |
| C | -23.91973300 | -7.33603600 | 0.89007900 |
| H | -24.97752800 | -7.14022900 | 1.08603400 |
| H | -23.81923500 | -7.58872700 | -0.17041200 |
| H | -23.63011600 | -8.22077100 | 1.46577800 |
| O | -3.95882300 | 1.84921100 | 0.48452100 |
| O | -3.44605300 | 1.26780700 | 2.59547600 |
| O | -1.13801800 | 2.95010300 | 1.64493800 |
| O | -0.18886500 | 0.68365200 | 1.05877600 |

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| O | -0.88417200 | 1.25203600 | 3.44038500 |
| H | -1.85682600 | 1.22325200 | 3.30270300 |
| O | 1.23036100 | 2.30184800 | 2.49008100 |
| C | 1.00490800 | 0.31111000 | 0.32634400 |
| H | 1.86867200 | 0.38260400 | 0.99130900 |
| H | 0.87055600 | -0.73175600 | 0.04075500 |
| C | 1.19961200 | 1.20138400 | -0.89066800 |
| H | 1.06649700 | 2.24689900 | -0.58842600 |
| H | 0.43112100 | 0.96494300 | -1.63409000 |
| N | 2.51587500 | 0.91337400 | -1.44525900 |
| H | 2.60004400 | 1.28077900 | -2.38661100 |
| H | 3.20779800 | 1.39570100 | -0.87868800 |
| P | -0.13604400 | 1.82065500 | 2.17585900 |

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| C | 4.38343300 | 2.08353600 | -5.20660100 |
| H | 4.22594900 | 2.84317800 | -4.43660500 |
| C | 4.01121800 | 2.70030800 | -6.55753600 |
| H | 4.19488100 | 1.96666400 | -7.35174800 |
| C | 2.51774500 | 3.09149100 | -6.56218400 |
| H | 2.41133900 | 3.92039900 | -5.84179800 |
| C | 2.01099000 | 1.54288000 | -4.85290400 |
| H | 2.02337500 | 2.39447000 | -4.15806000 |

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| C | 3.40198800 | 0.94149300 | -4.96058500 |
| H | 3.64794800 | 0.41615800 | -4.04555000 |
| C | 2.04677300 | 3.53326500 | -7.93018500 |
| H | 2.12234700 | 2.70101300 | -8.63514500 |
| H | 2.66422600 | 4.35693400 | -8.29159600 |
| H | 1.00440300 | 3.85313700 | -7.88515400 |
| C | 0.38007500 | 0.82839000 | -3.23890300 |
| H | -0.21421500 | 1.74552700 | -3.35901100 |
| C | -0.53384500 | -0.34281200 | -3.06237400 |
| H | -0.05648900 | -1.31136500 | -2.93842400 |
| C | -1.86573400 | -0.24704600 | -3.01898400 |
| H | -2.34165800 | 0.72567700 | -3.14203100 |
| C | -2.73578900 | -1.38927800 | -2.82127100 |
| H | -2.24799600 | -2.35025100 | -2.67608500 |
| C | -4.08111600 | -1.33477200 | -2.81598100 |
| H | -4.58002900 | -0.37728600 | -2.96442400 |
| C | -4.90938400 | -2.50167500 | -2.62764400 |
| H | -4.37990600 | -3.43615700 | -2.45373900 |
| C | -6.25752100 | -2.50632200 | -2.63353100 |
| H | -6.80144200 | -1.57718900 | -2.80120800 |
| C | -7.03339700 | -3.70391300 | -2.42563800 |
| H | -6.47803800 | -4.61999800 | -2.22516100 |
| C | -8.38070000 | -3.76280200 | -2.44508300 |
| H | -8.95233100 | -2.85376400 | -2.62916200 |
| C | -9.12404800 | -4.98252700 | -2.25078800 |
| H | -8.54476100 | -5.88947600 | -2.07865000 |

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| C | -10.46946300 | -5.06957900 | -2.26557700 |
| H | -11.05947800 | -4.16617100 | -2.41617000 |
| C | -11.18859500 | -6.30906000 | -2.09740800 |
| H | -10.58866200 | -7.21318200 | -2.00871700 |
| C | -12.52766400 | -6.42109200 | -2.02648200 |
| H | -13.14550800 | -5.52583200 | -2.08677000 |
| C | 1.32292300 | 1.02269400 | -2.03597300 |
| H | 1.92207200 | 1.92145900 | -2.17554200 |
| H | 0.70923600 | 1.19261500 | -1.14678200 |
| C | -13.20099200 | -7.68958300 | -1.82717300 |
| H | -12.56556400 | -8.57175700 | -1.87269900 |
| C | -14.49957100 | -7.83512200 | -1.54227200 |
| H | -15.13305200 | -6.94870700 | -1.47965100 |
| C | -15.16845700 | -9.14666000 | -1.24427700 |
| H | -14.47152500 | -9.96127900 | -1.47220700 |
| C | -15.52720700 | -9.26085900 | 0.25030400 |
| H | -16.33705900 | -8.53907600 | 0.44851100 |
| C | -14.38394900 | -8.91284900 | 1.22164100 |
| H | -14.08890000 | -7.88737200 | 0.97895200 |
| C | -13.12514800 | -9.75896900 | 1.00166800 |
| H | -12.89869300 | -9.81316800 | -0.05954100 |
| C | -10.93257000 | -8.78701800 | 0.92674200 |
| C | -9.90365600 | -8.00654200 | 1.70548100 |
| H | -10.39962000 | -7.43757800 | 2.49408300 |
| H | -9.23882800 | -8.73381800 | 2.18594900 |
| C | -9.06869600 | -7.09188900 | 0.80602000 |

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| H | -9.73256200 | -6.36441000 | 0.31749700 |
| C | -8.01112200 | -6.34800800 | 1.60873200 |
| H | -8.51149800 | -5.74147200 | 2.37124300 |
| H | -7.37849400 | -7.07851600 | 2.12713500 |
| C | -7.11292700 | -5.44302700 | 0.76892600 |
| H | -7.73475500 | -4.76090900 | 0.17325400 |
| C | -6.17928500 | -4.61732200 | 1.64790200 |
| H | -5.71327900 | -5.27900000 | 2.38847500 |
| H | -6.79663600 | -3.90781600 | 2.20726500 |
| C | -5.09145800 | -3.86966300 | 0.85952800 |
| H | -5.38857500 | -3.75628600 | -0.18577400 |
| H | -4.97424100 | -2.85535000 | 1.25325700 |
| C | -3.71651100 | -4.53224900 | 0.92436600 |
| H | -3.35517000 | -4.47865400 | 1.96076100 |
| C | -2.69585800 | -3.81170500 | 0.00924500 |
| H | -3.00699400 | -2.77267000 | -0.14878700 |
| C | -1.27524100 | -3.83174700 | 0.56378500 |
| H | -0.95013000 | -4.87249400 | 0.68230900 |
| H | -1.27654800 | -3.36993400 | 1.55779800 |
| C | -0.29264000 | -3.07735600 | -0.32656900 |
| H | -0.65452100 | -2.04917800 | -0.46222400 |
| C | 1.10486000 | -3.01382700 | 0.27888600 |
| H | 1.48011100 | -4.02771200 | 0.44870100 |
| H | 1.04657600 | -2.50198800 | 1.24379100 |
| C | 2.11063500 | -2.27876900 | -0.60732300 |
| C | 3.45761700 | -2.04575100 | 0.07401400 |

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| H | 3.95905700 | -3.00084800 | 0.24275000 |
| H | 3.29976100 | -1.55771500 | 1.04055500 |
| C | 4.32542900 | -1.16179500 | -0.80250100 |
| H | 4.49199900 | -1.67922700 | -1.75280800 |
| C | 3.60543000 | 0.15916600 | -1.09784000 |
| H | 3.40700200 | 0.68888500 | -0.15976900 |
| C | 2.23243700 | -0.17080900 | -1.75436200 |
| H | 2.42302600 | -0.71979100 | -2.68433500 |
| C | 4.42328600 | 1.08825600 | -1.97247500 |
| C | -13.13101700 | -11.15476400 | 1.59057300 |
| H | -12.21165200 | -11.67894600 | 1.31967500 |
| H | -13.98757900 | -11.70311800 | 1.19615000 |
| H | -13.20099100 | -11.12302200 | 2.67998600 |
| C | -14.85978600 | -8.93293100 | 2.67321700 |
| H | -15.23687200 | -9.91746700 | 2.96600200 |
| H | -15.66123200 | -8.20459900 | 2.82721000 |
| H | -14.04153300 | -8.68149500 | 3.35173100 |
| C | -16.42220100 | -9.34140400 | -2.10161900 |
| H | -17.13719900 | -8.52910500 | -1.92986000 |
| H | -16.91040100 | -10.28472600 | -1.85309200 |
| H | -16.16677200 | -9.34202200 | -3.16366900 |
| O | 3.46844400 | -0.01383000 | -6.00314900 |
| H | 2.72458000 | 0.17039600 | -6.59482600 |
| O | 4.73597300 | 3.89473900 | -6.84617800 |
| H | 5.68627400 | 3.74362800 | -6.67639500 |
| O | 1.67166700 | 2.01525700 | -6.15110300 |

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| O | 1.09701900 | 0.58022800 | -4.46441800 |
| O | 2.36629300 | -2.97366000 | -1.79287000 |
| H | 1.51371000 | -3.33791100 | -2.09407100 |
| O | 1.50663400 | -1.01386300 | -0.87220100 |
| O | 4.10516400 | 2.25126200 | -2.16239900 |
| O | 5.45374000 | 0.51301000 | -2.57799400 |
| O | -0.18795600 | -3.69705800 | -1.61149700 |
| H | -1.04910900 | -4.10938100 | -1.81016200 |
| O | -2.73400200 | -4.44409200 | -1.27212200 |
| H | -2.98848100 | -5.36359700 | -1.04842600 |
| O | -3.72706100 | -5.89972700 | 0.53968400 |
| H | -4.64032600 | -6.15811200 | 0.29005300 |
| O | -6.30773200 | -6.21340000 | -0.12796400 |
| H | -6.84677500 | -6.96536100 | -0.43472500 |
| O | -8.39348700 | -7.85438600 | -0.19103100 |
| H | -9.05088300 | -8.45496300 | -0.58572400 |
| O | -10.74898700 | -9.17551000 | -0.21616300 |
| O | -12.03337400 | -9.01408000 | 1.62795100 |
| O | -16.01088000 | -10.58653900 | 0.44426100 |
| H | -16.50934800 | -10.61666900 | 1.26782300 |
| O | 5.56877300 | -0.94232500 | -0.14829300 |
| H | 6.19678100 | -0.70781400 | -0.84290900 |
| N | 5.74984200 | 1.59032800 | -5.02860500 |
| H | 5.92824800 | 0.82717700 | -5.67730000 |
| H | 5.72857600 | 1.03232600 | -3.41843500 |
| H | 6.43759000 | 2.33307400 | -5.15786000 |

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| C | -11.69090500 | 18.49119200 | 7.09516400 |
| H | -12.44018100 | 17.81571700 | 6.66393200 |
| H | -11.53059400 | 18.14828200 | 8.12489300 |
| C | -10.38670400 | 18.35770600 | 6.31357100 |
| H | -9.63561900 | 19.03334800 | 6.74417900 |
| H | -10.54557700 | 18.70080000 | 5.28250300 |
| C | -9.83479400 | 16.93540700 | 6.29357000 |
| H | -10.58624800 | 16.26042000 | 5.86283400 |
| H | -9.67664900 | 16.59280100 | 7.32479100 |
| C | -8.53076800 | 16.80246300 | 5.51249100 |
| H | -8.68853100 | 17.14532300 | 4.48133500 |
| H | -7.77901800 | 17.47688600 | 5.94345900 |
| C | -7.97982100 | 15.37971200 | 5.49239500 |
| H | -8.73147600 | 14.70547000 | 5.06089800 |
| H | -7.82277700 | 15.03664700 | 6.52360600 |
| C | -6.67531800 | 15.24613800 | 4.71228100 |
| H | -6.83191700 | 15.58980100 | 3.68121000 |
| H | -5.92328400 | 15.91957000 | 5.14431100 |
| C | -6.12585100 | 13.82282300 | 4.69181300 |
| H | -6.87777400 | 13.14971700 | 4.25901200 |
| H | -5.97038600 | 13.47888200 | 5.72296800 |
| C | -4.82059600 | 13.68818500 | 3.91314400 |
| H | -4.97544700 | 14.03298500 | 2.88218800 |
| H | -4.06812700 | 14.36013200 | 4.34672100 |
| C | -4.27330600 | 12.26404200 | 3.89215700 |
| H | -5.02562400 | 11.59253800 | 3.45757600 |

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| H | -4.11994400 | 11.91887300 | 4.92320300 |
| C | -2.96707900 | 12.12796900 | 3.11537500 |
| H | -3.11964500 | 12.47424100 | 2.08457000 |
| H | -2.21402000 | 12.79793600 | 3.55098000 |
| C | -2.42274500 | 10.70271400 | 3.09375300 |
| H | -3.17556600 | 10.03327200 | 2.65695000 |
| H | -2.27192100 | 10.35596200 | 4.12459700 |
| C | -1.11537400 | 10.56486800 | 2.31921800 |
| H | -0.36156200 | 11.23234300 | 2.75733600 |
| H | -1.26522600 | 10.91294600 | 1.28861100 |
| C | -0.57521200 | 9.13813500 | 2.29706900 |
| H | -1.32818200 | 8.47094900 | 1.85753700 |
| H | -0.42675200 | 8.78915100 | 3.32728300 |
| C | 0.73329200 | 8.99808600 | 1.52499300 |
| H | 1.48794900 | 9.66292700 | 1.96594600 |
| H | 0.58630600 | 9.34882700 | 0.49471300 |
| C | 1.26201000 | 7.56781800 | 1.50631500 |
| H | 0.51671800 | 6.89763200 | 1.06504100 |
| H | 1.41289000 | 7.20922400 | 2.52990200 |
| C | 2.56773900 | 7.43622200 | 0.73585900 |
| H | 3.35063500 | 8.07287900 | 1.16359200 |
| H | 2.45472700 | 7.76768600 | -0.30279900 |
| C | 3.08839200 | 6.02237900 | 0.71363300 |
| O | 2.56714300 | 5.07060900 | 1.24059200 |
| C | -12.23275600 | 19.91694000 | 7.10796300 |
| H | -13.16619200 | 19.98887600 | 7.67280400 |

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| H | -11.51375500 | 20.60608700 | 7.56230600 |
| H | -12.42981000 | 20.27114700 | 6.09109100 |
| C | 4.80979300 | 4.62867800 | -0.07448200 |
| H | 5.14105800 | 4.30122200 | 0.91258000 |
| H | 4.07724600 | 3.91675000 | -0.45996400 |
| C | 6.00118800 | 4.73265800 | -1.01518600 |
| H | 6.70894300 | 5.47904000 | -0.64646900 |
| C | 5.55378700 | 5.05936700 | -2.41676100 |
| H | 5.10946500 | 4.16248200 | -2.84925300 |
| H | 4.82020800 | 5.86672300 | -2.39290000 |
| O | 4.23797000 | 5.93927400 | 0.01575000 |
| C | 7.40777300 | 3.09148300 | -0.02267200 |
| C | 7.74215300 | 1.62973700 | -0.10644800 |
| H | 6.79259600 | 1.09975700 | 0.03047500 |
| H | 8.06199400 | 1.40488800 | -1.12955200 |
| C | 8.75058500 | 1.15994600 | 0.92957700 |
| H | 8.41233100 | 1.47713000 | 1.92122500 |
| H | 9.71410000 | 1.65557700 | 0.76544200 |
| C | 8.92237200 | -0.35645200 | 0.89414300 |
| H | 7.94268800 | -0.83438700 | 1.02417600 |
| H | 9.27973700 | -0.65958700 | -0.09990100 |
| C | 9.88810000 | -0.87703300 | 1.95368000 |
| H | 9.53130000 | -0.57462400 | 2.94689300 |
| H | 10.86723200 | -0.39706300 | 1.82415000 |
| C | 10.05778100 | -2.39287100 | 1.91800600 |
| H | 10.41800400 | -2.69486400 | 0.92557400 |

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| H | 9.07656700 | -2.86951400 | 2.04108900 |
| C | 11.01370900 | -2.92047900 | 2.98369600 |
| H | 11.99489200 | -2.44285700 | 2.86095000 |
| H | 10.65290300 | -2.61902000 | 3.97599400 |
| C | 11.18221200 | -4.43653600 | 2.94743600 |
| H | 11.54428200 | -4.73801700 | 1.95558200 |
| H | 10.20063800 | -4.91350000 | 3.06832400 |
| C | 12.13529900 | -4.96595900 | 4.01488100 |
| H | 13.11707200 | -4.48912800 | 3.89413100 |
| H | 11.77301800 | -4.66451300 | 5.00667500 |
| C | 12.30282800 | -6.48213000 | 3.97845200 |
| H | 12.66586500 | -6.78356200 | 2.98694500 |
| H | 11.32085800 | -6.95868000 | 4.09818700 |
| C | 13.25443200 | -7.01237100 | 5.04683400 |
| H | 14.23655400 | -6.53603000 | 4.92717000 |
| H | 12.89130100 | -6.71091700 | 6.03831600 |
| C | 13.42127100 | -8.52861700 | 5.01028600 |
| H | 12.43901300 | -9.00479400 | 5.12926900 |
| H | 13.78492300 | -8.83003900 | 4.01900400 |
| C | 14.37191700 | -9.05936400 | 6.07927200 |
| H | 15.35426600 | -8.58333000 | 5.96032900 |
| H | 14.00820500 | -8.75792600 | 7.07054300 |
| C | 14.53830000 | -10.57566100 | 6.04259800 |
| H | 13.55585500 | -11.05157000 | 6.16109300 |
| H | 14.90232500 | -10.87703500 | 5.05144400 |
| C | 15.48837100 | -11.10678500 | 7.11195100 |

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| H | 15.12422500 | -10.80529700 | 8.10307000 |
| H | 16.47082300 | -10.63082300 | 6.99340600 |
| C | 15.65463600 | -12.62301900 | 7.07533100 |
| H | 14.67234500 | -13.09960600 | 7.19379700 |
| H | 16.01913500 | -12.92514400 | 6.08441300 |
| C | 16.60459200 | -13.15523900 | 8.14489000 |
| H | 16.23918600 | -12.85282700 | 9.13416100 |
| H | 17.58539200 | -12.67842500 | 8.02529500 |
| C | 16.76254000 | -14.67162400 | 8.09812400 |
| H | 17.44657600 | -15.03025100 | 8.87210500 |
| H | 15.79983000 | -15.17133000 | 8.24587000 |
| H | 17.15550400 | -14.99566500 | 7.12915000 |
| O | 6.62869300 | 3.44723000 | -1.06771900 |
| O | 7.72185500 | 3.85054300 | 0.86197000 |
| O | 6.69222500 | 5.49837100 | -3.18285100 |
| O | 7.55322500 | 6.67963600 | -5.19114400 |
| O | 5.16977200 | 5.89120600 | -5.15095400 |
| H | 4.78685600 | 5.25752400 | -5.81560300 |
| O | 7.05224000 | 4.15913300 | -5.39329100 |
| C | 8.98733200 | 6.52821900 | -5.23586100 |
| H | 9.24649800 | 5.56531000 | -5.68160100 |
| H | 9.33901600 | 7.32577000 | -5.89393200 |
| C | 9.60036800 | 6.66418500 | -3.85037600 |
| H | 9.29504000 | 5.81031500 | -3.23963800 |
| H | 9.18303600 | 7.56123200 | -3.36879200 |
| N | 11.05068800 | 6.65234900 | -3.98810600 |

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| H | 11.38907100 | 7.55908100 | -4.29371900 |
| H | 11.49393200 | 6.45612500 | -3.09835900 |
| P | 6.64016000 | 5.45411100 | -4.77306700 |

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| C | 6.75694100 | -5.37116800 | -0.22825900 |
| H | 7.36381900 | -4.67942400 | 0.37341300 |
| C | 7.11355300 | -5.10016000 | -1.69012900 |
| H | 6.54794000 | -5.79753200 | -2.32221600 |
| C | 6.72764500 | -3.67221700 | -2.07576500 |
| H | 7.26725100 | -2.97011300 | -1.42116200 |
| C | 4.96078600 | -3.64807000 | -0.52386400 |
| H | 5.49588100 | -2.88416400 | 0.06426300 |
| C | 5.28927000 | -5.03913500 | 0.01783400 |
| H | 5.08901700 | -5.05081800 | 1.09887800 |
| C | 7.01426200 | -3.33663600 | -3.52233400 |
| H | 6.47321700 | -4.01840600 | -4.18511500 |
| H | 8.08559300 | -3.41042900 | -3.72506800 |
| H | 6.69570500 | -2.31568500 | -3.74019500 |
| C | 2.94364800 | -2.46763300 | -1.19183000 |
| H | 3.00098400 | -2.75574900 | -2.24653200 |
| C | 1.51668000 | -2.45886300 | -0.73927900 |
| H | 1.33896000 | -2.21002800 | 0.30379500 |

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|---|--------------|-------------|-------------|
| C | 0.48047300 | -2.71906900 | -1.54262600 |
| H | 0.65695200 | -2.96304300 | -2.59013300 |
| C | -0.89630700 | -2.70098700 | -1.08803300 |
| H | -1.05758700 | -2.45505600 | -0.04115000 |
| C | -1.96448400 | -2.97229200 | -1.86194200 |
| H | -1.81658200 | -3.22082200 | -2.91272300 |
| C | -3.31911700 | -2.95202300 | -1.36210900 |
| H | -3.43472000 | -2.68733700 | -0.31304700 |
| C | -4.41881000 | -3.21441600 | -2.09635200 |
| H | -4.31437900 | -3.47597000 | -3.14897800 |
| C | -5.75604000 | -3.16432400 | -1.55762100 |
| H | -5.85767100 | -2.87787200 | -0.51083100 |
| C | -6.87397500 | -3.43155500 | -2.26281700 |
| H | -6.78406600 | -3.70915500 | -3.31258300 |
| C | -8.20385100 | -3.39027400 | -1.70805500 |
| H | -8.29541300 | -3.11604300 | -0.65741800 |
| C | -9.32275600 | -3.66567700 | -2.40788000 |
| H | -9.23592500 | -3.92263600 | -3.46315600 |
| C | -10.65058600 | -3.64944700 | -1.84414400 |
| H | -10.72989600 | -3.44336500 | -0.77811400 |
| C | -11.77948500 | -3.85409800 | -2.54724200 |
| H | -11.71491800 | -4.03762300 | -3.61924300 |
| C | 3.64641500 | -1.11741100 | -1.03340400 |
| H | 4.66969500 | -1.21576000 | -1.39600800 |
| H | 3.14626500 | -0.39003200 | -1.67916900 |
| C | -13.10286300 | -3.80041300 | -1.95840400 |

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| H | -13.13571800 | -3.71027800 | -0.87441200 |
| C | -14.24656100 | -3.79591500 | -2.65182900 |
| H | -14.20682900 | -3.86986900 | -3.73995200 |
| C | -15.61496400 | -3.64211900 | -2.05287900 |
| H | -15.53661200 | -3.70954900 | -0.96180600 |
| C | -16.21004000 | -2.25890400 | -2.38191100 |
| H | -16.42755300 | -2.24467400 | -3.46294800 |
| C | -15.27229200 | -1.06769100 | -2.10924100 |
| H | -14.38188300 | -1.24426400 | -2.72058100 |
| C | -14.76894200 | -1.01647100 | -0.66318900 |
| H | -14.44575200 | -2.00503800 | -0.35014800 |
| C | -12.46827400 | -0.61833900 | -0.11336700 |
| C | -11.31580600 | 0.34494300 | -0.24049200 |
| H | -11.48437700 | 1.00238500 | -1.09527000 |
| H | -11.31092700 | 0.96538700 | 0.66239900 |
| C | -9.96913400 | -0.37350700 | -0.36039100 |
| H | -9.96845800 | -0.98655000 | -1.27284700 |
| C | -8.81935700 | 0.62204900 | -0.42299800 |
| H | -8.96017500 | 1.25949100 | -1.30238500 |
| H | -8.85251000 | 1.26615200 | 0.46286700 |
| C | -7.44080400 | -0.02859200 | -0.50293800 |
| H | -7.42237500 | -0.74103700 | -1.33941100 |
| C | -6.34263800 | 1.00514900 | -0.71706900 |
| H | -6.43979100 | 1.78783800 | 0.04620700 |
| H | -6.52896100 | 1.48483500 | -1.68274000 |
| C | -4.92236500 | 0.41492800 | -0.69227100 |

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| H | -4.94710000 | -0.65369700 | -0.92188600 |
| H | -4.31681500 | 0.87731100 | -1.47815300 |
| C | -4.17513600 | 0.63692200 | 0.61886800 |
| H | -4.05819200 | 1.71988500 | 0.76433300 |
| C | -2.76066500 | -0.01102100 | 0.60002100 |
| H | -2.47800400 | -0.25336400 | -0.43101700 |
| C | -1.70060100 | 0.89620000 | 1.20954500 |
| H | -1.97764800 | 1.12502600 | 2.24515400 |
| H | -1.68758800 | 1.84165800 | 0.65540000 |
| C | -0.30251000 | 0.29081100 | 1.18853600 |
| H | -0.04164300 | 0.01102500 | 0.15916800 |
| C | 0.73785200 | 1.28194500 | 1.69623600 |
| H | 0.45331300 | 1.64685600 | 2.68776300 |
| H | 0.76261100 | 2.13679700 | 1.01577700 |
| C | 2.14202300 | 0.69402700 | 1.79538400 |
| C | 3.21172000 | 1.74383500 | 2.08747400 |
| H | 3.04528400 | 2.18589700 | 3.07221000 |
| H | 3.15887100 | 2.53706400 | 1.33640300 |
| C | 4.57969100 | 1.09306800 | 2.04555300 |
| H | 4.62389100 | 0.34187000 | 2.83911600 |
| C | 4.79034200 | 0.39881900 | 0.69500700 |
| H | 4.82673900 | 1.15813300 | -0.09248900 |
| C | 3.62105900 | -0.56618100 | 0.38540600 |
| H | 3.64557600 | -1.38550700 | 1.11534000 |
| C | 6.09706100 | -0.34725600 | 0.63930800 |
| C | -15.71942900 | -0.44587800 | 0.36824200 |

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| H | -15.28707400 | -0.53582900 | 1.36612500 |
| H | -16.65749800 | -1.00150500 | 0.33135700 |
| H | -15.92453300 | 0.60944800 | 0.17476800 |
| C | -15.89808500 | 0.25062100 | -2.56083100 |
| H | -16.83286000 | 0.46070000 | -2.03252700 |
| H | -16.11263500 | 0.22962600 | -3.63326300 |
| H | -15.22023700 | 1.08548400 | -2.36945500 |
| C | -16.56059800 | -4.74808600 | -2.52982600 |
| H | -16.64458700 | -4.73969400 | -3.62224500 |
| H | -17.55672700 | -4.60389000 | -2.10928700 |
| H | -16.18714300 | -5.73022600 | -2.23131000 |
| O | 4.50731200 | -6.00649000 | -0.65050300 |
| H | 3.62538500 | -5.61611100 | -0.73606500 |
| O | 8.51601900 | -5.31102800 | -1.81252300 |
| H | 8.72888400 | -5.45842600 | -2.73970500 |
| O | 5.32502100 | -3.52499000 | -1.87764400 |
| O | 3.57834000 | -3.50178700 | -0.40901600 |
| O | 2.22911000 | -0.27781500 | 2.79696700 |
| H | 1.41505700 | -0.81046300 | 2.73355800 |
| O | 2.39555600 | 0.13412500 | 0.51005500 |
| O | 6.71236000 | -0.60589200 | -0.37209900 |
| O | -0.24648300 | -0.88023300 | 2.00810300 |
| H | -1.12531500 | -1.30093800 | 1.97588700 |
| O | -2.81448300 | -1.24910400 | 1.30862900 |
| H | -3.59791500 | -1.13877400 | 1.88804100 |
| O | -4.85419800 | 0.12435800 | 1.75620300 |

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| H | -5.72855100 | -0.23458700 | 1.48836800 |
| O | -7.14229800 | -0.74128100 | 0.70114600 |
| H | -7.96534600 | -1.15643600 | 1.01705600 |
| O | -9.74770200 | -1.22211100 | 0.76494100 |
| H | -10.57495600 | -1.71389200 | 0.92214900 |
| O | -12.38135300 | -1.68402400 | 0.47988500 |
| O | -13.57226100 | -0.17398100 | -0.69134300 |
| O | -17.42724200 | -2.16435400 | -1.64876500 |
| H | -17.96567500 | -1.46354400 | -2.03169000 |
| O | 5.56981700 | 2.09294000 | 2.25234400 |
| H | 6.37091500 | 1.64669900 | 2.55279700 |
| N | 7.03934700 | -6.72637800 | 0.21147600 |
| H | 6.32273500 | -7.34208900 | -0.16324200 |
| H | 7.92955200 | -7.01433100 | -0.18206400 |
| C | 10.11257600 | -14.68435400 | -0.77460800 |
| H | 9.56184200 | -14.51569000 | -1.70838800 |
| H | 11.17209900 | -14.74146700 | -1.05370500 |
| C | 9.90219800 | -13.49139100 | 0.15393100 |
| H | 10.45217300 | -13.65924700 | 1.08955200 |
| H | 8.84189900 | -13.43256800 | 0.43363700 |
| C | 10.33797600 | -12.16281900 | -0.45673600 |
| H | 9.78860100 | -11.99633300 | -1.39295800 |
| H | 11.39861500 | -12.22175500 | -0.73528800 |
| C | 10.12531900 | -10.97063500 | 0.47145800 |
| H | 9.06460700 | -10.91002600 | 0.74842000 |
| H | 10.67265600 | -11.13763400 | 1.40855300 |

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| C | 10.56292400 | -9.64198400 | -0.13760900 |
| H | 10.01938400 | -9.47835800 | -1.07814700 |
| H | 11.62538400 | -9.69848000 | -0.40982900 |
| C | 10.33833200 | -8.44927400 | 0.78673400 |
| H | 9.27539400 | -8.38976300 | 1.05513900 |
| H | 10.87584500 | -8.61306900 | 1.73001500 |
| C | 10.77763500 | -7.11976300 | 0.17849500 |
| H | 10.27748600 | -6.97370500 | -0.78769600 |
| H | 11.85470700 | -7.15107000 | -0.03420200 |
| C | 10.45784300 | -5.92403400 | 1.06929700 |
| H | 9.37543800 | -5.89990400 | 1.24499300 |
| H | 10.91802100 | -6.06381200 | 2.05658300 |
| C | 10.90342000 | -4.58620400 | 0.48306000 |
| H | 10.59750400 | -4.53684000 | -0.56786500 |
| H | 11.99874700 | -4.51361300 | 0.50418900 |
| C | 10.28209800 | -3.40620000 | 1.22010500 |
| H | 9.19410000 | -3.45736400 | 1.07265200 |
| H | 10.43987600 | -3.51303300 | 2.30146000 |
| C | 10.77219300 | -2.02818200 | 0.77507900 |
| H | 10.88226800 | -2.00564300 | -0.31621200 |
| H | 11.76719200 | -1.82952100 | 1.19180900 |
| C | 9.78479700 | -0.94606100 | 1.19966900 |
| H | 9.54129800 | -1.08924900 | 2.26398000 |
| H | 8.86864500 | -1.10848100 | 0.61909700 |
| C | 10.21353500 | 0.50225200 | 0.98877500 |
| H | 10.45667000 | 0.66147700 | -0.06896700 |

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| H | 11.13103700 | 0.70873100 | 1.55419400 |
| C | 9.11273100 | 1.47520500 | 1.40838000 |
| H | 8.87668800 | 1.30951100 | 2.46986100 |
| H | 8.20382100 | 1.24163600 | 0.84373500 |
| C | 9.44716800 | 2.94461700 | 1.18552400 |
| H | 9.63131700 | 3.11969800 | 0.12230000 |
| H | 10.37375900 | 3.20451500 | 1.71127200 |
| C | 8.30963000 | 3.84922000 | 1.65664400 |
| H | 8.14563700 | 3.76673000 | 2.73419300 |
| H | 7.36587600 | 3.55603200 | 1.17841300 |
| C | 8.46477700 | 5.31089900 | 1.35294700 |
| O | 8.02088900 | 6.21298300 | 2.02219900 |
| C | 9.67422400 | -16.00629600 | -0.15256300 |
| H | 9.83351800 | -16.84606000 | -0.83454400 |
| H | 10.23260200 | -16.21188600 | 0.76629300 |
| H | 8.61107200 | -15.98425300 | 0.10729100 |
| C | 9.15913900 | 6.84315400 | -0.31771700 |
| H | 9.17992300 | 7.55918100 | 0.50714000 |
| H | 10.08351700 | 6.91472500 | -0.89598400 |
| C | 7.96425100 | 7.11775200 | -1.21553900 |
| H | 7.77598600 | 6.25604500 | -1.85930500 |
| C | 8.17897200 | 8.37044700 | -2.05119900 |
| H | 8.39266200 | 9.22972600 | -1.40777000 |
| H | 9.02520800 | 8.21770700 | -2.72366700 |
| O | 9.12055900 | 5.51200000 | 0.18524700 |
| C | 5.94414500 | 6.30407500 | -0.18801200 |

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| C | 4.73156600 | 6.77267400 | 0.55426400 |
| H | 5.07790700 | 7.30592200 | 1.44694600 |
| H | 4.24572800 | 7.50700000 | -0.09955600 |
| C | 3.76901900 | 5.64884000 | 0.91313400 |
| H | 4.23995300 | 4.96657100 | 1.62964500 |
| H | 3.57132100 | 5.05571300 | 0.01398300 |
| C | 2.45687200 | 6.20124700 | 1.46416900 |
| H | 2.65474500 | 6.81277800 | 2.35428900 |
| H | 2.02088300 | 6.88105700 | 0.72024600 |
| C | 1.43720400 | 5.12083100 | 1.80739100 |
| H | 1.81222500 | 4.50779100 | 2.63672300 |
| H | 1.33804300 | 4.44086500 | 0.95095800 |
| C | 0.05746000 | 5.67670800 | 2.15398100 |
| H | -0.32807500 | 6.23186100 | 1.28860200 |
| H | 0.14327700 | 6.40725100 | 2.96865900 |
| C | -0.93955500 | 4.58847100 | 2.54067000 |
| H | -0.88553800 | 3.78061100 | 1.80115800 |
| H | -0.63750400 | 4.13711900 | 3.49512400 |
| C | -2.38904700 | 5.06010600 | 2.62952400 |
| H | -2.69886300 | 5.43722400 | 1.64567500 |
| H | -2.46981600 | 5.90995500 | 3.31918300 |
| C | -3.33332000 | 3.94159700 | 3.06473300 |
| H | -3.08919000 | 3.03542500 | 2.49919100 |
| H | -3.14551100 | 3.69273400 | 4.11719200 |
| C | -4.81596900 | 4.23905800 | 2.86390600 |
| H | -4.99272300 | 4.46135300 | 1.80223300 |

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| H | -5.09806700 | 5.14648800 | 3.41388600 |
| C | -5.70169300 | 3.07018000 | 3.28893200 |
| H | -5.34844600 | 2.14895400 | 2.81185300 |
| H | -5.58976400 | 2.90723300 | 4.36905300 |
| C | -7.18011400 | 3.26118100 | 2.96557000 |
| H | -7.56997100 | 4.13094400 | 3.51118400 |
| H | -7.29448700 | 3.50055700 | 1.89854500 |
| C | -8.02108600 | 2.03015300 | 3.29633500 |
| H | -7.71455400 | 1.19611700 | 2.65117900 |
| H | -7.80388600 | 1.70988800 | 4.32356400 |
| C | -9.52168300 | 2.27006600 | 3.16333200 |
| H | -9.81500400 | 3.08326700 | 3.84031100 |
| H | -9.74995100 | 2.63378400 | 2.15074500 |
| C | -10.36574900 | 1.03392000 | 3.46056400 |
| H | -10.06629600 | 0.61702700 | 4.43079800 |
| H | -10.14893700 | 0.25578100 | 2.71841200 |
| C | -11.86340300 | 1.32585600 | 3.49067800 |
| H | -12.07359400 | 2.04474000 | 4.29352200 |
| H | -12.16449300 | 1.83145600 | 2.56136000 |
| C | -12.72687100 | 0.08237100 | 3.68516000 |
| H | -12.38177200 | -0.46019300 | 4.57364500 |
| H | -12.58115600 | -0.59957000 | 2.83882500 |
| C | -14.20775100 | 0.41618600 | 3.83441400 |
| H | -14.81987500 | -0.48568400 | 3.92455600 |
| H | -14.38451900 | 1.02897200 | 4.72388100 |
| H | -14.57161500 | 0.98366900 | 2.97162900 |

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| O | 6.79103600 | 7.35410300 | -0.42168400 |
| O | 6.18608300 | 5.18508100 | -0.55670600 |
| O | 7.05558900 | 8.64191200 | -2.87900600 |
| O | 5.61273100 | 10.57563600 | -3.28112700 |
| O | 6.11351000 | 9.98614600 | -0.91712000 |
| H | 6.17207500 | 9.28855100 | -0.24269600 |
| O | 4.52608700 | 8.43705600 | -2.27922000 |
| C | 4.38008700 | 11.31793800 | -3.32525100 |
| H | 3.53105600 | 10.63312600 | -3.37628000 |
| H | 4.29583400 | 11.91813900 | -2.41155400 |
| C | 4.43140700 | 12.20667200 | -4.55188900 |
| H | 4.45166900 | 11.56646300 | -5.43832800 |
| H | 5.37830400 | 12.76810700 | -4.53945600 |
| N | 3.22888800 | 13.02845100 | -4.58932900 |
| H | 3.29138400 | 13.78176900 | -3.91171600 |
| H | 3.11965900 | 13.46038300 | -5.49955200 |
| P | 5.70885100 | 9.31447100 | -2.31984100 |
| O | 6.52261600 | -0.75133800 | 1.85278200 |
| H | 7.36694500 | -1.21470800 | 1.72693800 |

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|---|-------------|-------------|-------------|
| C | -1.19775900 | 11.21862100 | -5.49020100 |
| H | -0.21358400 | 11.39410400 | -5.00759800 |
| C | -2.26708200 | 12.23170100 | -4.97607600 |

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|---|-------------|-------------|-------------|
| H | -3.24084300 | 12.15648900 | -5.51910300 |
| C | -2.49083700 | 11.97788800 | -3.44514200 |
| H | -1.52099200 | 11.99561100 | -2.88905900 |
| C | -2.10777400 | 9.62038300 | -3.71736800 |
| H | -1.21051800 | 9.66642900 | -3.03384500 |
| C | -1.70221800 | 9.80124900 | -5.22531900 |
| H | -1.03484300 | 8.95539800 | -5.54643800 |
| C | -3.50600100 | 12.93322500 | -2.86089700 |
| H | -4.49950100 | 12.84921500 | -3.31433800 |
| H | -3.15832200 | 13.96943000 | -2.98248800 |
| H | -3.64016600 | 12.75442100 | -1.78499700 |
| C | -3.30864200 | 8.10900800 | -2.21327300 |
| H | -4.16481200 | 8.81082300 | -2.08294400 |
| C | -3.75441900 | 6.66905600 | -2.32817700 |
| H | -2.95093700 | 5.96374100 | -2.58507000 |
| C | -5.01149300 | 6.27190500 | -2.08277800 |
| H | -5.78616600 | 6.98840600 | -1.79879100 |
| C | -5.45638300 | 4.87666300 | -2.16640800 |
| H | -4.67717600 | 4.15583400 | -2.44971400 |
| C | -6.71408700 | 4.45500400 | -1.92502400 |
| H | -7.51329700 | 5.14406000 | -1.63731000 |
| C | -7.09776200 | 3.04612000 | -2.03949100 |
| H | -6.28422000 | 2.37699700 | -2.35019800 |
| C | -8.33263100 | 2.56047300 | -1.80408100 |
| H | -9.15594700 | 3.21795400 | -1.50883800 |
| C | -8.66372400 | 1.14010800 | -1.93296000 |

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|---|--------------|-------------|-------------|
| H | -7.84532600 | 0.49830300 | -2.28355000 |
| C | -9.87307700 | 0.61409600 | -1.65539500 |
| H | -10.70277800 | 1.24377900 | -1.32184400 |
| C | -10.16741900 | -0.81297500 | -1.78660300 |
| H | -9.34570600 | -1.42914900 | -2.17183800 |
| C | -11.35454900 | -1.36623700 | -1.47198700 |
| H | -12.18546900 | -0.75586200 | -1.10573200 |
| C | -11.62857900 | -2.79691800 | -1.60009600 |
| H | -10.81989000 | -3.39854900 | -2.03244700 |
| C | -12.78790600 | -3.37522000 | -1.23588200 |
| H | -13.62123500 | -2.78970300 | -0.83595800 |
| C | -2.25076000 | 8.33544000 | -1.13288700 |
| H | -1.99761000 | 9.42955700 | -1.03503400 |
| H | -2.67286300 | 8.09275000 | -0.13320400 |
| C | -13.01865700 | -4.81791900 | -1.34468200 |
| H | -12.20828900 | -5.38494300 | -1.82151600 |
| C | -14.11806400 | -5.43267700 | -0.89512000 |
| H | -14.95558500 | -4.89476200 | -0.44818400 |
| C | -14.32254600 | -6.92497900 | -0.94776500 |
| H | -13.47757700 | -7.42703900 | -1.48779100 |
| C | -14.36867900 | -7.49753700 | 0.49452000 |
| H | -15.33402600 | -7.25174300 | 0.98953500 |
| C | -13.19225600 | -7.04697000 | 1.39767300 |
| H | -13.23459800 | -5.92373200 | 1.48398700 |
| C | -11.82509000 | -7.36909400 | 0.75397300 |
| H | -11.81996500 | -7.09438600 | -0.33267400 |

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| C | -9.99418200 | -5.76874800 | 0.66529600 |
| C | -9.20488300 | -4.82770700 | 1.54949000 |
| H | -9.70513400 | -4.56374200 | 2.49571800 |
| H | -8.26908800 | -5.35717600 | 1.85391000 |
| C | -8.79925400 | -3.58770900 | 0.73065700 |
| H | -9.67345400 | -3.03302700 | 0.31125600 |
| C | -7.89471100 | -2.63607300 | 1.53155700 |
| H | -8.38207700 | -2.34528400 | 2.48402400 |
| H | -6.95237700 | -3.14894600 | 1.83402500 |
| C | -7.50011800 | -1.35790900 | 0.75507800 |
| H | -8.37834300 | -0.81974300 | 0.32731400 |
| C | -6.66177900 | -0.38204200 | 1.62789000 |
| H | -5.85157300 | -0.92166900 | 2.16468500 |
| H | -7.32320000 | 0.00235200 | 2.43667100 |
| C | -6.06191100 | 0.84472300 | 0.90257900 |
| H | -6.57614500 | 0.98061800 | -0.07201300 |
| H | -6.29737400 | 1.76049000 | 1.49521800 |
| C | -4.53329200 | 0.74768700 | 0.68797900 |
| H | -3.98633100 | 0.70641800 | 1.66179500 |
| C | -3.97720500 | 1.98271000 | -0.13386500 |
| H | -4.69549400 | 2.84096100 | -0.05053000 |
| C | -2.54449000 | 2.37943100 | 0.23168500 |
| H | -1.89504100 | 1.49878800 | 0.01437600 |
| H | -2.46858600 | 2.53897900 | 1.32921300 |
| C | -2.05727900 | 3.64030100 | -0.52754300 |
| H | -2.81059100 | 4.46576600 | -0.47868500 |

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| C | -0.67514800 | 4.06482400 | -0.02751600 |
| H | 0.06129000 | 3.24503900 | -0.16920900 |
| H | -0.71144900 | 4.27146500 | 1.06526300 |
| C | -0.16803100 | 5.30218400 | -0.77895900 |
| C | 1.12878200 | 5.83891900 | -0.18517300 |
| H | 1.97571500 | 5.14251600 | -0.31629100 |
| H | 1.04072300 | 5.94849400 | 0.92212000 |
| C | 1.45900000 | 7.19824600 | -0.79733400 |
| H | 1.71268500 | 7.10957300 | -1.88168000 |
| C | 0.28453800 | 8.18063600 | -0.62569700 |
| H | 0.09096100 | 8.35817100 | 0.45797600 |
| C | -0.94710500 | 7.54688200 | -1.30294700 |
| H | -0.72498300 | 7.34683100 | -2.37983200 |
| C | 0.57329900 | 9.56830900 | -1.27317400 |
| C | -11.24602600 | -8.75280900 | 0.95331500 |
| H | -10.26462000 | -8.84702300 | 0.46210400 |
| H | -11.91089400 | -9.51609300 | 0.51457300 |
| H | -11.08893600 | -9.01056900 | 2.00622900 |
| C | -13.34867500 | -7.60830300 | 2.80947000 |
| H | -13.30020200 | -8.70204100 | 2.83445700 |
| H | -14.29994500 | -7.30660700 | 3.26185800 |
| H | -12.54331400 | -7.23603400 | 3.45778600 |
| C | -15.61888500 | -7.27953700 | -1.68182900 |
| H | -16.50408200 | -6.84412100 | -1.20600100 |
| H | -15.75384800 | -8.37213600 | -1.69293100 |
| H | -15.59586800 | -6.93329100 | -2.72148800 |

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| O | -2.79818400 | 9.81585200 | -6.19886400 |
| H | -3.30862500 | 9.00709000 | -5.93696600 |
| O | -1.76849300 | 13.56191000 | -5.07157100 |
| H | -1.45672700 | 13.77862300 | -5.96766800 |
| O | -3.05599500 | 10.65596400 | -3.36418400 |
| O | -2.81752000 | 8.41497000 | -3.59261500 |
| O | 0.01793900 | 5.02992200 | -2.17854700 |
| H | -0.57263200 | 4.25823100 | -2.40274300 |
| O | -1.23030700 | 6.26357700 | -0.66839600 |
| O | -0.08280000 | 10.57972200 | -0.91241400 |
| O | -1.91522900 | 3.43853200 | -1.94863300 |
| H | -2.46493000 | 2.71672400 | -2.23990200 |
| O | -3.91133700 | 1.72169300 | -1.55357300 |
| H | -4.18389500 | 0.83763800 | -1.69964800 |
| O | -4.11591800 | -0.52306000 | 0.22921900 |
| H | -4.98256900 | -1.01219200 | -0.18866300 |
| O | -6.76478300 | -1.78084400 | -0.40021200 |
| H | -6.98591000 | -2.72020400 | -0.66815200 |
| O | -8.04996100 | -4.18969600 | -0.35082300 |
| H | -8.63076400 | -4.73685300 | -0.95491200 |
| O | -9.86329700 | -5.98047600 | -0.53698700 |
| O | -10.92318100 | -6.41711200 | 1.43076500 |
| O | -14.32717200 | -8.92502300 | 0.29066600 |
| H | -14.61412700 | -9.38712600 | 1.10125500 |
| O | 2.66529200 | 7.64002800 | -0.12377200 |
| H | 2.89568800 | 8.47585000 | -0.60820100 |

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| N | -1.08887300 | 11.35451000 | -7.02146000 |
| H | -1.95688300 | 10.96796800 | -7.48861600 |
| H | -1.00505700 | 12.34823800 | -7.26198000 |
| C | -10.02224400 | 3.31231600 | 8.58651500 |
| H | -10.74813200 | 2.81855900 | 7.91129600 |
| H | -9.96034400 | 2.64115500 | 9.46552400 |
| C | -8.65092800 | 3.40810200 | 7.90336400 |
| H | -7.91932300 | 3.89804900 | 8.57436500 |
| H | -8.70399500 | 4.07505300 | 7.02171100 |
| C | -8.14676200 | 2.02086500 | 7.49182000 |
| H | -8.87444400 | 1.53128700 | 6.81619500 |
| H | -8.09212400 | 1.35459400 | 8.37496000 |
| C | -6.77429800 | 2.10928100 | 6.81493900 |
| H | -6.81866200 | 2.76910300 | 5.92747900 |
| H | -6.04197400 | 2.59885200 | 7.48599200 |
| C | -6.28630300 | 0.71132400 | 6.42125600 |
| H | -7.01720400 | 0.22427800 | 5.74802900 |
| H | -6.24808200 | 0.05608900 | 7.31403500 |
| C | -4.90926000 | 0.77509500 | 5.75474200 |
| H | -4.93961000 | 1.42353500 | 4.85853800 |
| H | -4.17868100 | 1.26608600 | 6.42727800 |
| C | -4.42982300 | -0.63211400 | 5.38457400 |
| H | -5.15451900 | -1.12124700 | 4.70630400 |
| H | -4.40995300 | -1.27762400 | 6.28481300 |
| C | -3.04218100 | -0.58300000 | 4.73918300 |
| H | -3.05705700 | 0.05728900 | 3.83625800 |

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| H | -2.32012900 | -0.08977300 | 5.41915400 |
| C | -2.55753900 | -1.99303400 | 4.38362300 |
| H | -3.26988000 | -2.48042600 | 3.68993400 |
| H | -2.55287100 | -2.63643700 | 5.28449700 |
| C | -1.15941800 | -1.93911600 | 3.75860100 |
| H | -1.17473500 | -1.30647000 | 2.84901200 |
| H | -0.45389300 | -1.43009400 | 4.44372900 |
| C | -0.64786300 | -3.34421400 | 3.41672200 |
| H | -1.34134600 | -3.84104100 | 2.71084900 |
| H | -0.65482400 | -3.98587500 | 4.31852600 |
| C | 0.76318600 | -3.27012100 | 2.81969100 |
| H | 1.44160900 | -2.74327500 | 3.51901500 |
| H | 0.75351500 | -2.63722000 | 1.91030100 |
| C | 1.31564800 | -4.66396300 | 2.49076500 |
| H | 0.64286100 | -5.18227800 | 1.78098300 |
| H | 1.31351100 | -5.29846300 | 3.39750800 |
| C | 2.73242800 | -4.56069200 | 1.90910500 |
| H | 3.38909400 | -4.02027100 | 2.61982500 |
| H | 2.72122800 | -3.92312100 | 1.00323700 |
| C | 3.32563000 | -5.93917600 | 1.58219800 |
| H | 2.67991500 | -6.47749600 | 0.85901900 |
| H | 3.34128700 | -6.57446300 | 2.48857400 |
| C | 4.74349300 | -5.78598900 | 1.01478100 |
| H | 5.35947000 | -5.15699600 | 1.69597200 |
| H | 4.71593000 | -5.22906400 | 0.05131800 |
| C | 5.44563400 | -7.10312800 | 0.82691100 |

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| O | 6.18214800 | -7.68817800 | 1.57735300 |
| C | -10.53101800 | 4.69057100 | 9.00259100 |
| H | -11.50874100 | 4.63094400 | 9.49283600 |
| H | -9.84459900 | 5.18123200 | 9.70302900 |
| H | -10.63686300 | 5.36107700 | 8.14153000 |
| C | 5.90185500 | -8.78908100 | -0.84796500 |
| H | 6.47999400 | -9.21419300 | 0.00234200 |
| H | 5.10015300 | -9.49627000 | -1.15257500 |
| C | 6.81855900 | -8.37975800 | -2.01552700 |
| H | 6.37769900 | -7.52996900 | -2.59335800 |
| C | 7.14277900 | -9.60679500 | -2.90088300 |
| H | 7.68388300 | -10.38446100 | -2.33170200 |
| H | 6.20863100 | -10.03424400 | -3.33090600 |
| O | 5.14890700 | -7.62429700 | -0.42502900 |
| C | 8.34753700 | -6.58280900 | -1.45256600 |
| C | 9.81366100 | -6.33087100 | -1.23214400 |
| H | 10.36237500 | -7.27420700 | -1.03129600 |
| H | 10.24727100 | -5.97745600 | -2.19729600 |
| C | 10.02094700 | -5.31066700 | -0.10220300 |
| H | 9.98895300 | -5.82948000 | 0.87640300 |
| H | 9.17029200 | -4.59897700 | -0.07582900 |
| C | 11.33376400 | -4.53079900 | -0.24729400 |
| H | 12.20057600 | -5.21829800 | -0.24644700 |
| H | 11.37093800 | -4.02602200 | -1.23333100 |
| C | 11.47780700 | -3.49184500 | 0.87609300 |
| H | 11.45527900 | -3.98746500 | 1.86596900 |

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| H | 10.60146200 | -2.81316000 | 0.88536300 |
| C | 12.76974600 | -2.67995500 | 0.71949400 |
| H | 12.79833000 | -2.19672500 | -0.27705700 |
| H | 13.64860700 | -3.35347400 | 0.73204100 |
| C | 12.91003600 | -1.61696500 | 1.81782600 |
| H | 12.02959900 | -0.94557400 | 1.82343700 |
| H | 12.90698000 | -2.08855000 | 2.81895200 |
| C | 14.19574400 | -0.80638600 | 1.61434900 |
| H | 14.20479500 | -0.35171700 | 0.60429000 |
| H | 15.07727500 | -1.47620400 | 1.62751300 |
| C | 14.34750000 | 0.28328300 | 2.68109200 |
| H | 13.46285400 | 0.94895400 | 2.68484900 |
| H | 14.36547400 | -0.16272900 | 3.69362100 |
| C | 15.62370000 | 1.09439500 | 2.43200300 |
| H | 15.60795900 | 1.53047600 | 1.41396400 |
| H | 16.50892000 | 0.42941700 | 2.43726600 |
| C | 15.78723700 | 2.20135900 | 3.47769900 |
| H | 14.89765600 | 2.86042700 | 3.48614700 |
| H | 15.82461400 | 1.77043700 | 4.49643600 |
| C | 17.05289900 | 3.01706000 | 3.19559500 |
| H | 17.94261800 | 2.35797600 | 3.19301700 |
| H | 17.01656100 | 3.44073600 | 2.17302300 |
| C | 17.22337100 | 4.13601800 | 4.22735200 |
| H | 16.32899400 | 4.78842800 | 4.24009200 |
| H | 17.27542500 | 3.71452600 | 5.24954700 |
| C | 18.48007300 | 4.95734500 | 3.92216000 |

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| H | 19.37220900 | 4.30173000 | 3.90664200 |
| H | 18.42476900 | 5.37597100 | 2.89837400 |
| C | 18.66133200 | 6.08116100 | 4.94826900 |
| H | 18.72799000 | 5.66051600 | 5.97003600 |
| H | 17.76291500 | 6.72785300 | 4.97069900 |
| C | 19.91063700 | 6.90790700 | 4.62441800 |
| H | 20.80353700 | 6.25401600 | 4.59809500 |
| H | 19.83943200 | 7.31922300 | 3.59901700 |
| C | 20.11020400 | 8.04096100 | 5.63953900 |
| H | 20.18388300 | 7.62530900 | 6.66328900 |
| H | 19.21199400 | 8.68815900 | 5.66758700 |
| C | 21.35296400 | 8.86359400 | 5.30445500 |
| H | 21.50659500 | 9.67703700 | 6.02140600 |
| H | 22.25956800 | 8.24717100 | 5.30943700 |
| H | 21.28198300 | 9.31533900 | 4.30777500 |
| O | 8.10669400 | -7.95085600 | -1.49064700 |
| O | 7.45310000 | -5.78871200 | -1.59439100 |
| O | 7.84438400 | -9.17469900 | -4.08939400 |
| O | 9.57049300 | -10.03236500 | -5.67616100 |
| O | 9.98897900 | -10.43364200 | -3.11551600 |
| O | 10.08377900 | -7.97173300 | -4.18800500 |
| C | 10.78401500 | -10.74259400 | -5.98084000 |
| H | 11.16276600 | -11.34005300 | -5.12150600 |
| H | 10.43280400 | -11.43637100 | -6.77827200 |
| C | 11.84068900 | -9.77339500 | -6.54226300 |
| H | 11.37436600 | -9.13290600 | -7.33092300 |

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| H | 12.63704200 | -10.36420000 | -7.06179700 |
| N | 12.40174500 | -8.87909600 | -5.47482600 |
| H | 12.92330000 | -9.42558500 | -4.78378900 |
| H | 13.05142800 | -8.21236500 | -5.89213200 |
| P | 9.45719400 | -9.47739600 | -4.11014500 |
| H | 11.00387300 | -7.92535000 | -4.67513600 |
| O | 1.58385500 | 9.69241000 | -2.27730300 |
| H | 2.24190900 | 10.33073500 | -1.99251100 |

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| C | -1.08554300 | -5.63978400 | 2.11048600 |
| H | -0.94548900 | -5.95252000 | 3.17105500 |
| C | -0.17290300 | -4.42588400 | 1.75676000 |
| H | -0.20635400 | -4.16671100 | 0.66899500 |
| C | -0.63620800 | -3.19652800 | 2.61228900 |
| H | -0.66695400 | -3.46144100 | 3.69723600 |
| C | -2.92692300 | -3.92760100 | 2.52934400 |
| H | -2.95011000 | -4.04858900 | 3.65050100 |
| C | -2.54179600 | -5.27038600 | 1.81007800 |
| H | -3.30952500 | -6.05575200 | 2.02686200 |
| C | 0.20533800 | -1.97553100 | 2.33534300 |
| H | 0.15421300 | -1.63787500 | 1.29680100 |
| H | 1.25465100 | -2.18259600 | 2.58296100 |

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|---|--------------|-------------|-------------|
| H | -0.12251400 | -1.13220500 | 2.95669500 |
| C | -4.66000100 | -2.19634200 | 2.56949200 |
| H | -4.00136400 | -1.43813500 | 2.08486100 |
| C | -6.07742000 | -2.14310600 | 2.05738300 |
| H | -6.72088900 | -2.95546100 | 2.41874600 |
| C | -6.53512100 | -1.15329600 | 1.28024100 |
| H | -5.88343800 | -0.33848400 | 0.95753900 |
| C | -7.91883800 | -1.07012100 | 0.79588600 |
| H | -8.57688100 | -1.88911500 | 1.11818800 |
| C | -8.39928900 | -0.08660300 | 0.01140000 |
| H | -7.77708300 | 0.74583800 | -0.32613300 |
| C | -9.79161400 | -0.06703500 | -0.45110400 |
| H | -10.39401200 | -0.92316100 | -0.11622800 |
| C | -10.33430400 | 0.89017500 | -1.22661300 |
| H | -9.74439800 | 1.74093100 | -1.57805400 |
| C | -11.73466900 | 0.86058600 | -1.66054300 |
| H | -12.30359700 | -0.02428200 | -1.34750400 |
| C | -12.32157300 | 1.82618200 | -2.39235100 |
| H | -11.76425800 | 2.70590200 | -2.72453500 |
| C | -13.72728200 | 1.76897700 | -2.80173600 |
| H | -14.26545000 | 0.85968900 | -2.50762800 |
| C | -14.34546400 | 2.74264800 | -3.49424500 |
| H | -13.81162400 | 3.64453700 | -3.80614000 |
| C | -15.75457400 | 2.67328000 | -3.88671100 |
| H | -16.27213400 | 1.74120300 | -3.63285300 |
| C | -16.40378600 | 3.66125400 | -4.52759400 |

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| H | -15.89854800 | 4.58581000 | -4.81926400 |
| C | -4.54970100 | -2.11735400 | 4.09194700 |
| H | -3.47334400 | -2.09175300 | 4.42095700 |
| H | -4.93705800 | -1.13617000 | 4.44127400 |
| C | -17.82573900 | 3.57431700 | -4.87648100 |
| H | -18.30352300 | 2.61276500 | -4.64791100 |
| C | -18.52163400 | 4.57976900 | -5.41836000 |
| H | -18.06757200 | 5.53493100 | -5.68373600 |
| C | -19.99811500 | 4.51065900 | -5.71332000 |
| H | -20.40223000 | 3.48753900 | -5.49686900 |
| C | -20.76060200 | 5.51379100 | -4.80567500 |
| H | -20.60571900 | 6.55795400 | -5.15599200 |
| C | -20.40795000 | 5.41470500 | -3.29985000 |
| H | -19.30657300 | 5.63503400 | -3.19342600 |
| C | -20.61126800 | 3.98269900 | -2.77028400 |
| H | -20.18829200 | 3.22516100 | -3.48269100 |
| C | -18.96587200 | 2.85338200 | -1.36884400 |
| C | -18.13113600 | 3.06288900 | -0.12898600 |
| H | -18.00655900 | 4.11721700 | 0.16826100 |
| H | -18.66843600 | 2.57665500 | 0.72434400 |
| C | -16.78676800 | 2.33696300 | -0.29889100 |
| H | -16.19477900 | 2.69206600 | -1.17939600 |
| C | -15.92346300 | 2.40214100 | 0.97652800 |
| H | -15.77340700 | 3.45572800 | 1.28824700 |
| H | -16.44581500 | 1.91387000 | 1.83178600 |
| C | -14.54291500 | 1.71805000 | 0.82749900 |

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| H | -13.97051100 | 2.07558600 | -0.06282300 |
| C | -13.67126300 | 1.88238500 | 2.10367500 |
| H | -14.26008900 | 1.65625900 | 3.01718400 |
| H | -13.41127100 | 2.95955200 | 2.19430900 |
| C | -12.35884500 | 1.07485300 | 2.14652600 |
| H | -12.09017500 | 0.74594200 | 1.12130000 |
| H | -11.53271600 | 1.75849600 | 2.44357800 |
| C | -12.40034400 | -0.10358200 | 3.14202000 |
| H | -12.49268600 | 0.23339300 | 4.19884100 |
| C | -11.06688700 | -0.94732800 | 3.04014900 |
| H | -10.23116200 | -0.30555100 | 2.64718200 |
| C | -10.65213200 | -1.61392600 | 4.36080300 |
| H | -11.46375400 | -2.32395900 | 4.63428500 |
| H | -10.62327700 | -0.86203300 | 5.17601400 |
| C | -9.28377200 | -2.33800000 | 4.29684300 |
| H | -8.47945200 | -1.69688700 | 3.85083100 |
| C | -8.89117000 | -2.88508400 | 5.67778600 |
| H | -9.66293200 | -3.58303700 | 6.06173600 |
| H | -8.83141500 | -2.04942100 | 6.41058200 |
| C | -7.54882000 | -3.64204000 | 5.62578800 |
| C | -7.06584500 | -4.02862200 | 7.01943900 |
| H | -7.71665800 | -4.78225600 | 7.49415800 |
| H | -7.10579500 | -3.15731600 | 7.71130900 |
| C | -5.62920500 | -4.54059000 | 6.94514500 |
| H | -5.56654700 | -5.50394900 | 6.38538500 |
| C | -4.70753100 | -3.49876900 | 6.27503600 |

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| H | -4.68354600 | -2.56565500 | 6.88266100 |
| C | -5.27506300 | -3.21891700 | 4.86941300 |
| H | -5.32443200 | -4.16915600 | 4.28513100 |
| C | -3.23342900 | -4.01838000 | 6.14505300 |
| C | -21.98845900 | 3.56879200 | -2.30724900 |
| H | -21.98806700 | 2.53492400 | -1.93367100 |
| H | -22.69905800 | 3.62072800 | -3.14771600 |
| H | -22.37619800 | 4.19391300 | -1.49747900 |
| C | -21.15471000 | 6.47709900 | -2.49597500 |
| H | -22.23846100 | 6.33432200 | -2.52596000 |
| H | -20.93958600 | 7.48595500 | -2.86217600 |
| H | -20.85188300 | 6.43642400 | -1.44109800 |
| C | -20.28527000 | 4.82568700 | -7.18468500 |
| H | -19.93845200 | 5.82254000 | -7.47259200 |
| H | -21.36957100 | 4.78343900 | -7.36880400 |
| H | -19.80105800 | 4.09864600 | -7.84600000 |
| O | -2.40649200 | -5.23781000 | 0.36380600 |
| H | -3.27655200 | -4.76468300 | 0.09148800 |
| O | 1.16959800 | -4.68862000 | 2.15268100 |
| H | 1.51127000 | -5.51440700 | 1.78033300 |
| O | -1.97256000 | -2.90360800 | 2.15256200 |
| O | -4.16000100 | -3.50166800 | 2.01286400 |
| O | -7.62445500 | -4.81282800 | 4.78030000 |
| H | -8.38421800 | -4.63696200 | 4.17455200 |
| O | -6.64477700 | -2.71634700 | 5.00258000 |
| O | -2.29023700 | -3.20125200 | 5.98300000 |

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|---|--------------|-------------|-------------|
| O | -9.29551500 | -3.49558200 | 3.41839000 |
| H | -9.98305900 | -3.41091900 | 2.76443700 |
| O | -11.10433200 | -2.02507800 | 2.07735600 |
| H | -12.00884400 | -2.06935000 | 1.72253600 |
| O | -13.66624800 | -0.78254800 | 3.12748700 |
| H | -14.10315400 | -0.63997500 | 2.19075400 |
| O | -14.78798200 | 0.32878500 | 0.54879200 |
| H | -15.69423900 | 0.18638100 | 0.13921600 |
| O | -17.18944400 | 0.95192000 | -0.50094300 |
| H | -17.69798700 | 0.87209700 | -1.42100900 |
| O | -19.01025100 | 1.86373900 | -2.10955100 |
| O | -19.72084300 | 3.96153500 | -1.56836600 |
| O | -22.14721400 | 5.17492200 | -5.01985800 |
| H | -22.72016600 | 5.90409200 | -4.71106500 |
| O | -5.24869900 | -4.82835800 | 8.31607500 |
| H | -4.34772200 | -5.23052000 | 8.21181100 |
| N | -0.73957800 | -6.81372900 | 1.15590200 |
| H | -1.08242200 | -6.58872400 | 0.17858700 |
| H | 0.27837500 | -6.93283500 | 1.12590200 |
| C | 16.49283800 | 19.05592600 | 3.18104100 |
| H | 17.47038200 | 18.97466700 | 3.69744100 |
| H | 16.74836900 | 19.31326600 | 2.13352500 |
| C | 15.76445400 | 17.70505500 | 3.22497700 |
| H | 14.78739500 | 17.77827500 | 2.70815300 |
| H | 15.51146600 | 17.43863700 | 4.27001600 |
| C | 16.61821700 | 16.60241900 | 2.58915100 |

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| H | 17.59322900 | 16.52227200 | 3.10986900 |
| H | 16.87438700 | 16.86902200 | 1.54418800 |
| C | 15.89216600 | 15.25245600 | 2.62330300 |
| H | 15.64269800 | 14.97262600 | 3.66581300 |
| H | 14.91440400 | 15.32506300 | 2.10738400 |
| C | 16.75874800 | 14.16883000 | 1.97305600 |
| H | 17.73282300 | 14.09276300 | 2.49619200 |
| H | 17.01554100 | 14.45724300 | 0.93405100 |
| C | 16.04576600 | 12.81322600 | 1.98377400 |
| H | 15.79861100 | 12.51516500 | 3.02182300 |
| H | 15.06754000 | 12.88782100 | 1.46871900 |
| C | 16.91987100 | 11.74615200 | 1.31577400 |
| H | 17.89249200 | 11.66419000 | 1.84043100 |
| H | 17.17890900 | 12.05513800 | 0.28337100 |
| C | 16.20796300 | 10.39006900 | 1.30097600 |
| H | 15.95608700 | 10.07790900 | 2.33396400 |
| H | 15.23152000 | 10.47559200 | 0.78364300 |
| C | 17.07780000 | 9.32660000 | 0.62077900 |
| H | 18.04838700 | 9.23119900 | 1.14651400 |
| H | 17.34067700 | 9.64681000 | -0.40700900 |
| C | 16.35161200 | 7.97732800 | 0.59014700 |
| H | 16.10206400 | 7.65633400 | 1.62115300 |
| H | 15.37277200 | 8.08433900 | 0.08091500 |
| C | 17.19761800 | 6.90517000 | -0.10865000 |
| H | 18.16709900 | 6.78231800 | 0.41318700 |
| H | 17.46461100 | 7.23533400 | -1.13198800 |

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| C | 16.44031400 | 5.57159900 | -0.15559500 |
| H | 15.46065300 | 5.71332100 | -0.65535100 |
| H | 16.18987900 | 5.24509200 | 0.87387700 |
| C | 17.24970300 | 4.48299300 | -0.87486700 |
| H | 18.22329400 | 4.33528600 | -0.36780700 |
| H | 17.50733100 | 4.81626600 | -1.89959300 |
| C | 16.46276000 | 3.16588400 | -0.91976600 |
| H | 15.48339100 | 3.33422600 | -1.41197000 |
| H | 16.21039400 | 2.84421200 | 0.11059300 |
| C | 17.23571500 | 2.05621900 | -1.64764300 |
| H | 18.21048300 | 1.87363900 | -1.15160400 |
| H | 17.48421500 | 2.37565300 | -2.67886200 |
| C | 16.40668500 | 0.76494700 | -1.67683800 |
| H | 15.39069600 | 0.97306600 | -2.08207700 |
| H | 16.24024600 | 0.38895800 | -0.64208800 |
| C | 17.03190500 | -0.31297000 | -2.51296200 |
| O | 16.84414200 | -0.57916400 | -3.67882400 |
| C | 15.64816600 | 20.16205100 | 3.81050500 |
| H | 16.16352300 | 21.12853500 | 3.78059700 |
| H | 14.69051300 | 20.28326000 | 3.28939300 |
| H | 15.41726100 | 19.94457500 | 4.86050100 |
| C | 18.45711500 | -2.26837600 | -2.34780600 |
| H | 18.21870800 | -2.30392400 | -3.43760300 |
| H | 19.54969400 | -2.14491500 | -2.20115200 |
| C | 17.88257300 | -3.48487300 | -1.59946800 |
| H | 17.64458400 | -3.22310300 | -0.53453300 |

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| C | 18.83562400 | -4.69392100 | -1.72202800 |
| H | 18.96037300 | -5.00160700 | -2.77989900 |
| H | 19.82685900 | -4.45029700 | -1.28056600 |
| O | 17.91270800 | -1.05940400 | -1.74251600 |
| C | 15.45384700 | -3.57322700 | -1.62856500 |
| C | 14.32961200 | -4.37716200 | -2.21020700 |
| H | 14.66904600 | -4.97548000 | -3.08201800 |
| H | 14.03859500 | -5.14759000 | -1.45779400 |
| C | 13.15117900 | -3.46599500 | -2.58166000 |
| H | 13.32250100 | -3.02883200 | -3.58640300 |
| H | 13.11325000 | -2.59628600 | -1.89047200 |
| C | 11.80420400 | -4.20048200 | -2.54738200 |
| H | 11.80634200 | -5.05409400 | -3.25280000 |
| H | 11.64113800 | -4.65028300 | -1.54715100 |
| C | 10.65020600 | -3.24032200 | -2.88076100 |
| H | 10.79675300 | -2.79583700 | -3.88554500 |
| H | 10.65844600 | -2.37663100 | -2.18479300 |
| C | 9.29483800 | -3.95672300 | -2.81236500 |
| H | 9.15724800 | -4.41447700 | -1.81194500 |
| H | 9.27733700 | -4.80681700 | -3.52348700 |
| C | 8.13150300 | -3.00084600 | -3.11227300 |
| H | 8.14929600 | -2.13872200 | -2.41605800 |
| H | 8.24567100 | -2.55434800 | -4.11978800 |
| C | 6.79288700 | -3.74178600 | -3.00703300 |
| H | 6.69277100 | -4.20414700 | -2.00449900 |
| H | 6.77118500 | -4.59155800 | -3.71833700 |

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| C | 5.61004200 | -2.80417600 | -3.27280400 |
| H | 5.63512700 | -1.94181700 | -2.57734100 |
| H | 5.68893900 | -2.35641900 | -4.28306300 |
| C | 4.28831900 | -3.56656200 | -3.12914600 |
| H | 4.22023300 | -4.02206400 | -2.12144400 |
| H | 4.26257300 | -4.42083900 | -3.83471400 |
| C | 3.08997000 | -2.64443300 | -3.37361400 |
| H | 3.12180200 | -1.77692700 | -2.68466800 |
| H | 3.14342100 | -2.20113000 | -4.38789300 |
| C | 1.77910500 | -3.41793600 | -3.19804600 |
| H | 1.74747100 | -4.27611300 | -3.89873100 |
| H | 1.73351800 | -3.86480500 | -2.18605900 |
| C | 0.57063900 | -2.50553500 | -3.42776600 |
| H | 0.60829400 | -1.63330700 | -2.74508500 |
| H | 0.60715300 | -2.06696300 | -4.44524800 |
| C | -0.73394400 | -3.28395000 | -3.22963000 |
| H | -0.76816700 | -4.15104200 | -3.91894800 |
| H | -0.77227500 | -3.71725100 | -2.21102100 |
| C | -1.94950700 | -2.37907100 | -3.45996400 |
| H | -1.92151400 | -1.95017900 | -4.48139600 |
| H | -1.90848000 | -1.50285900 | -2.78208400 |
| C | -3.24850700 | -3.16316000 | -3.24155400 |
| H | -3.28359900 | -4.03828800 | -3.91995900 |
| H | -3.26610100 | -3.58807900 | -2.21904000 |
| C | -4.48069200 | -2.27549000 | -3.46346000 |
| H | -4.46115400 | -1.84744200 | -4.48574000 |

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| H | -4.44141600 | -1.39640200 | -2.78898900 |
| C | -5.77020300 | -3.06178700 | -3.23687500 |
| H | -6.65624400 | -2.43376600 | -3.38986400 |
| H | -5.84985100 | -3.91488300 | -3.92107200 |
| H | -5.82924800 | -3.45434100 | -2.21378100 |
| O | 16.64690900 | -3.91720000 | -2.25226500 |
| O | 15.41776100 | -2.74481900 | -0.74698400 |
| O | 18.37204000 | -5.76013600 | -0.86353400 |
| O | 18.38201000 | -8.25108100 | -0.79622800 |
| O | 17.80033500 | -7.12171100 | -3.08683500 |
| O | 16.14673000 | -6.96145900 | -0.99222300 |
| C | 18.27173700 | -9.55101100 | -1.40884600 |
| H | 18.28625200 | -9.50360200 | -2.52243900 |
| H | 19.20826100 | -10.04795400 | -1.05877700 |
| C | 17.03436000 | -10.29908000 | -0.86596100 |
| H | 17.02654600 | -10.21792900 | 0.25367200 |
| H | 17.13793400 | -11.39207800 | -1.10069300 |
| N | 15.75538800 | -9.71348100 | -1.39378500 |
| H | 15.69201600 | -9.85196500 | -2.41268900 |
| H | 14.95894500 | -10.19440000 | -0.95929100 |
| P | 17.64468800 | -7.01572100 | -1.62328500 |
| H | 15.68021700 | -7.90221400 | -0.94490000 |
| O | -2.96121200 | -5.42069600 | 6.21069000 |
| H | -2.34798900 | -5.59484100 | 6.92848600 |

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|---|-------------|-------------|-------------|
| C | 8.60280900 | -2.73830400 | 1.10801900 |
| H | 9.33703300 | -1.93782300 | 1.25877100 |
| C | 8.95540000 | -3.42848700 | -0.21053600 |
| H | 8.24009500 | -4.25177800 | -0.36924300 |
| C | 8.81549900 | -2.45972800 | -1.37819000 |
| H | 9.53328100 | -1.63801600 | -1.22847300 |
| C | 7.16300200 | -1.20452400 | -0.20831200 |
| H | 7.88136000 | -0.38251200 | -0.08578700 |
| C | 7.21056500 | -2.11796300 | 1.01577000 |
| H | 7.00669800 | -1.50832600 | 1.90674200 |
| C | 9.05293200 | -3.11837500 | -2.71755400 |
| H | 8.32003200 | -3.91567300 | -2.87542700 |
| H | 10.05149400 | -3.55728000 | -2.73703700 |
| H | 8.95709200 | -2.39235600 | -3.52771300 |
| C | 5.50325400 | -0.02459200 | -1.52815200 |
| H | 5.73823200 | -0.66542600 | -2.38427800 |
| C | 4.02318800 | 0.15667700 | -1.42897700 |
| H | 3.67362200 | 0.80816700 | -0.63471100 |
| C | 3.13266100 | -0.49557300 | -2.18300800 |
| H | 3.46924800 | -1.18243100 | -2.95823000 |
| C | 1.70889800 | -0.38054400 | -1.94553800 |

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| H | 1.40950900 | 0.38733600 | -1.23991700 |
| C | 0.74237000 | -1.19018900 | -2.41894200 |
| H | 0.97391800 | -2.01570400 | -3.08989900 |
| C | -0.61087400 | -1.01939600 | -1.94273800 |
| H | -0.75345400 | -0.14458200 | -1.31084600 |
| C | -1.67188900 | -1.82618100 | -2.14165800 |
| H | -1.59233300 | -2.71497100 | -2.76588600 |
| C | -2.93341900 | -1.54757200 | -1.49683900 |
| H | -2.96067000 | -0.65837500 | -0.86517300 |
| C | -4.05636700 | -2.28697900 | -1.60153500 |
| H | -4.06268700 | -3.17094600 | -2.23810500 |
| C | -5.26755000 | -1.97296000 | -0.88489500 |
| H | -5.23186200 | -1.10968700 | -0.21984500 |
| C | -6.42071000 | -2.66536900 | -0.97586700 |
| H | -6.47978100 | -3.51771600 | -1.65173700 |
| C | -7.60012800 | -2.34143700 | -0.21030900 |
| H | -7.50299300 | -1.53542700 | 0.51520800 |
| C | -8.79670900 | -2.94370600 | -0.33661900 |
| H | -8.92716700 | -3.73329400 | -1.07571500 |
| C | 6.30340800 | 1.26961600 | -1.68705900 |
| H | 7.36550000 | 1.01018600 | -1.67287200 |
| H | 6.09164400 | 1.68069300 | -2.67927400 |
| C | -9.95334600 | -2.55699700 | 0.44789300 |
| H | -9.75815600 | -1.85106300 | 1.25256300 |
| C | -11.20985700 | -2.95369200 | 0.21929000 |
| H | -11.40856300 | -3.64752200 | -0.59921200 |

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| C | -12.41027000 | -2.47345500 | 0.98510900 |
| H | -12.07035600 | -1.91325900 | 1.86352400 |
| C | -13.26471700 | -1.51173700 | 0.13638300 |
| H | -13.71993500 | -2.10643700 | -0.67306200 |
| C | -12.48050400 | -0.37405200 | -0.54456900 |
| H | -11.73186400 | -0.86470500 | -1.17416700 |
| C | -11.68047200 | 0.48440300 | 0.44090800 |
| H | -11.14581500 | -0.15566900 | 1.13683500 |
| C | -9.40485000 | 1.12505400 | 0.03003600 |
| C | -8.48828400 | 1.89073500 | -0.89045300 |
| H | -8.94155300 | 1.95746600 | -1.88126100 |
| H | -8.40713000 | 2.90875300 | -0.49170500 |
| C | -7.08821200 | 1.27690000 | -0.96422300 |
| H | -7.16243300 | 0.25611600 | -1.36625500 |
| C | -6.17606400 | 2.10746900 | -1.85617500 |
| H | -6.60332800 | 2.13778300 | -2.86433600 |
| H | -6.14993100 | 3.13559300 | -1.47555700 |
| C | -4.74090500 | 1.59460900 | -1.94581700 |
| H | -4.74460300 | 0.54210600 | -2.26208700 |
| C | -3.92445800 | 2.41116000 | -2.94687400 |
| H | -4.12566800 | 3.47599300 | -2.78117700 |
| H | -4.29846400 | 2.17083700 | -3.94675800 |
| C | -2.41148400 | 2.15115800 | -2.86126700 |
| H | -2.22620100 | 1.18984200 | -2.37773100 |
| H | -1.98120800 | 2.07827800 | -3.86471000 |
| C | -1.64093900 | 3.24256700 | -2.11245000 |

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| H | -1.58544500 | 4.13617500 | -2.74992200 |
| C | -0.21479000 | 2.78729200 | -1.76696700 |
| H | 0.21497900 | 2.23458200 | -2.61146500 |
| C | 0.69913600 | 3.95538200 | -1.41109000 |
| H | 0.20897300 | 4.59035700 | -0.66548000 |
| H | 0.85262700 | 4.56208300 | -2.31178000 |
| C | 2.04689800 | 3.50484400 | -0.85189600 |
| H | 2.41221400 | 2.64291900 | -1.42193500 |
| C | 3.10394300 | 4.60244200 | -0.93718300 |
| H | 2.76331700 | 5.48299700 | -0.38286200 |
| H | 3.23611800 | 4.89077600 | -1.98352100 |
| C | 4.45915500 | 4.18283200 | -0.36788000 |
| C | 5.53694500 | 5.23748900 | -0.55609600 |
| H | 5.25705000 | 6.16208400 | -0.04709700 |
| H | 5.65912000 | 5.44899600 | -1.62211200 |
| C | 6.85945800 | 4.74746800 | 0.00018500 |
| H | 6.76508400 | 4.64102800 | 1.08890700 |
| C | 7.21133100 | 3.36319900 | -0.60920700 |
| H | 7.56586000 | 3.57693400 | -1.62517200 |
| C | 6.02603300 | 2.37803200 | -0.67217200 |
| H | 5.86615000 | 1.95790200 | 0.32477500 |
| C | 8.35108700 | 2.74376400 | 0.15899600 |
| C | -12.45108200 | 1.53658900 | 1.21194300 |
| H | -11.78920300 | 2.03933400 | 1.92087700 |
| H | -13.26360400 | 1.05514500 | 1.75789700 |
| H | -12.87154100 | 2.28895800 | 0.54116300 |

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| C | -13.38423700 | 0.46057000 | -1.45052400 |
| H | -14.20040500 | 0.92872800 | -0.89211400 |
| H | -13.82441200 | -0.16094000 | -2.23569400 |
| H | -12.81697200 | 1.26020600 | -1.93203600 |
| C | -13.26561100 | -3.64618700 | 1.47265400 |
| H | -13.60503000 | -4.25407900 | 0.62650300 |
| H | -14.14466200 | -3.28101800 | 2.00527900 |
| H | -12.68929700 | -4.29282900 | 2.13820900 |
| O | 6.29588600 | -3.18470100 | 0.90577600 |
| H | 5.38211200 | -2.84813500 | 0.89438800 |
| O | 10.27903200 | -3.90282700 | -0.16506100 |
| H | 10.36679700 | -4.26936900 | 0.73043800 |
| O | 7.48815500 | -1.93031100 | -1.38706800 |
| O | 5.85930200 | -0.73699600 | -0.32530400 |
| O | 4.37917500 | 3.91263700 | 1.00016700 |
| H | 3.48228500 | 3.54134900 | 1.14734800 |
| O | 4.84153800 | 3.02433100 | -1.11270400 |
| O | 8.34486200 | 1.67904000 | 0.73199300 |
| O | 1.92143300 | 3.14036100 | 0.52809100 |
| H | 1.71542200 | 2.19052600 | 0.60303500 |
| O | -0.28782800 | 1.85490100 | -0.69912000 |
| H | -0.90856300 | 2.24316900 | -0.06401600 |
| O | -2.26154900 | 3.63058300 | -0.89608200 |
| H | -2.95921900 | 2.98169600 | -0.67544500 |
| O | -4.09215700 | 1.67324400 | -0.67162100 |
| H | -4.75224900 | 1.45307000 | 0.01172800 |

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| O | -6.49594900 | 1.22873500 | 0.33149300 |
| H | -7.16054600 | 0.85692500 | 0.93862400 |
| O | -9.01383800 | 0.55007200 | 1.03375500 |
| O | -10.66948400 | 1.17126900 | -0.36221800 |
| O | -14.28529400 | -1.01789200 | 0.99848000 |
| H | -14.99452600 | -0.65134300 | 0.45973200 |
| O | 7.82653000 | 5.71943200 | -0.33602500 |
| H | 8.68023800 | 5.41558900 | -0.00315700 |
| N | 8.77133100 | -3.71748400 | 2.17507300 |
| H | 7.93640700 | -4.29903900 | 2.20267000 |
| H | 8.84128700 | -3.25928500 | 3.07781700 |
| C | -4.19886900 | 4.16053300 | 1.92422100 |
| H | -4.48457600 | 3.63475600 | 1.00884000 |
| H | -4.82056700 | 3.76750200 | 2.73565800 |
| C | -2.71471200 | 3.97132100 | 2.22507100 |
| H | -2.44968900 | 4.51637900 | 3.13931900 |
| H | -2.12339500 | 4.40139500 | 1.41120200 |
| C | -2.34332900 | 2.50028800 | 2.38734100 |
| H | -2.58976500 | 1.95180400 | 1.47234300 |
| H | -2.95846900 | 2.05240100 | 3.17787600 |
| C | -0.86541400 | 2.29414000 | 2.72653500 |
| H | -0.58831200 | 2.83619200 | 3.63340300 |
| H | -0.21883400 | 2.67971200 | 1.92799200 |
| C | -0.48106900 | 0.85646000 | 2.95356500 |
| O | 0.27746700 | 0.46307400 | 3.80621000 |
| C | -0.83409100 | -1.36336600 | 2.18349300 |

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| H | -0.62465800 | -1.62401300 | 3.22303000 |
| H | -1.75599900 | -1.84786500 | 1.85336200 |
| C | 0.31496700 | -1.80478700 | 1.29450400 |
| H | 0.29977600 | -1.23573300 | 0.36763700 |
| C | 0.23699000 | -3.29040000 | 0.98873300 |
| H | 0.34494200 | -3.87693100 | 1.90608300 |
| H | -0.72050700 | -3.51229200 | 0.51348200 |
| O | -1.09495400 | 0.03725100 | 2.07117400 |
| C | 2.23517400 | -0.46393600 | 1.72764500 |
| C | 3.61870600 | -0.47767700 | 2.29755900 |
| H | 3.66036200 | -1.20608200 | 3.11044600 |
| H | 4.24502200 | -0.86398500 | 1.48634500 |
| C | 4.10990800 | 0.90304000 | 2.71263700 |
| H | 3.53207500 | 1.25837900 | 3.57374800 |
| H | 3.91747400 | 1.60555400 | 1.89900500 |
| C | 5.60314700 | 0.91278300 | 3.02887300 |
| H | 5.82374200 | 0.16133900 | 3.79856600 |
| H | 6.15356700 | 0.60917700 | 2.13129500 |
| C | 6.09792700 | 2.28336300 | 3.47966400 |
| H | 5.64266600 | 2.57245200 | 4.43227000 |
| H | 5.82865300 | 3.04450600 | 2.74224800 |
| O | 1.58126100 | -1.60645400 | 1.94379400 |
| O | 1.74864600 | 0.45348200 | 1.09300600 |
| O | 1.24047000 | -3.66799700 | 0.04933800 |
| O | 3.05807900 | -5.14688400 | -0.57065700 |
| O | 2.81947200 | -4.47097600 | 1.95662900 |

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| O | 3.65464800 | -2.82267700 | 0.15598200 |
| C | 4.42937000 | -5.52415300 | -0.75689700 |
| H | 5.05097700 | -5.20176200 | 0.08488900 |
| H | 4.45802200 | -6.61517200 | -0.80606900 |
| C | 4.94012500 | -4.92738200 | -2.05622000 |
| H | 4.24006300 | -5.20275100 | -2.84909800 |
| H | 5.91269800 | -5.37698700 | -2.29724700 |
| N | 5.01081000 | -3.46182800 | -1.97405500 |
| H | 5.91123500 | -3.15062300 | -1.60345300 |
| H | 4.91539600 | -3.04367600 | -2.89257000 |
| P | 2.71663300 | -4.04331500 | 0.55295300 |
| H | 4.06508000 | -2.92648400 | -0.78624700 |
| O | 9.44872700 | 3.53697300 | 0.18742900 |
| H | 10.10565400 | 3.08045400 | 0.73798200 |
| H | -4.44772000 | 5.21701700 | 1.79299600 |
| H | 7.18419100 | 2.29034800 | 3.60847700 |

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| C | 8.74089200 | -3.16060500 | 0.50865600 |
| H | 9.64236300 | -2.70717800 | 0.07807600 |
| C | 8.40046100 | -4.38154800 | -0.34522900 |
| H | 7.51010800 | -4.86717900 | 0.08283900 |
| C | 8.05592100 | -3.95838400 | -1.76834900 |

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| H | 8.94108300 | -3.46028000 | -2.19890700 |
| C | 7.24795400 | -1.86305700 | -1.00670200 |
| H | 8.08171400 | -1.32882700 | -1.48724800 |
| C | 7.60963900 | -2.14037700 | 0.44929900 |
| H | 7.92767900 | -1.18610300 | 0.89419900 |
| C | 7.64388100 | -5.12259100 | -2.64035100 |
| H | 6.75237700 | -5.59887000 | -2.22389600 |
| H | 8.45077500 | -5.85611600 | -2.67683300 |
| H | 7.41465500 | -4.78096400 | -3.65214100 |
| C | 5.61595300 | -0.57921100 | -2.22919200 |
| H | 5.72572000 | -1.35824200 | -2.99073300 |
| C | 4.17020100 | -0.30355100 | -1.98758500 |
| H | 3.96041200 | 0.34302100 | -1.14438500 |
| C | 3.16255300 | -0.85956100 | -2.66669200 |
| H | 3.36745700 | -1.53215600 | -3.49909200 |
| C | 1.78204300 | -0.64452100 | -2.28584600 |
| H | 1.61399500 | 0.00106700 | -1.42901900 |
| C | 0.70681500 | -1.21551400 | -2.86126300 |
| H | 0.82350100 | -1.87114100 | -3.72381000 |
| C | -0.61927000 | -1.00101100 | -2.33439400 |
| H | -0.67693500 | -0.38021700 | -1.44190900 |
| C | -1.75615400 | -1.52079200 | -2.84128700 |
| H | -1.72104800 | -2.15116200 | -3.72921900 |
| C | -3.03832200 | -1.28687800 | -2.23030400 |
| H | -3.03889500 | -0.65081200 | -1.34516100 |
| C | -4.21277200 | -1.80410300 | -2.65298400 |

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| H | -4.23844100 | -2.44370500 | -3.53424800 |
| C | -5.44752300 | -1.57737700 | -1.94658500 |
| H | -5.38565600 | -0.91199900 | -1.08743700 |
| C | -6.64619000 | -2.12500100 | -2.23580100 |
| H | -6.74808000 | -2.76952100 | -3.10792100 |
| C | -7.81511500 | -1.91479800 | -1.41571700 |
| H | -7.66265900 | -1.35584600 | -0.49371900 |
| C | -9.05872000 | -2.34726700 | -1.69252700 |
| H | -9.25201100 | -2.87987300 | -2.62277200 |
| C | 6.44264500 | 0.64669800 | -2.63595400 |
| H | 7.45440700 | 0.30756600 | -2.87410900 |
| H | 6.02130000 | 1.07856400 | -3.54903300 |
| C | -10.18010000 | -2.09984100 | -0.80611400 |
| H | -9.92135900 | -1.70421200 | 0.17402500 |
| C | -11.46888600 | -2.27272400 | -1.11724900 |
| H | -11.73301500 | -2.64853700 | -2.10687600 |
| C | -12.61886100 | -1.94149800 | -0.20711500 |
| H | -12.24178400 | -1.82703900 | 0.81549400 |
| C | -13.27847800 | -0.60622700 | -0.60491200 |
| H | -13.72306600 | -0.74850100 | -1.60395900 |
| C | -12.31378300 | 0.58990000 | -0.72130000 |
| H | -11.55295700 | 0.29139400 | -1.44856800 |
| C | -11.54810600 | 0.88233600 | 0.57524400 |
| H | -11.14062200 | -0.04029100 | 0.98072100 |
| C | -9.18661700 | 1.32982800 | 0.52095200 |
| C | -8.12494000 | 2.30066700 | 0.07192600 |

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| H | -8.52498900 | 2.94512400 | -0.71257100 |
| H | -7.87631300 | 2.93197000 | 0.93286400 |
| C | -6.85207600 | 1.58855700 | -0.39795700 |
| H | -7.10276100 | 0.94514500 | -1.25525200 |
| C | -5.79304400 | 2.59212000 | -0.82262500 |
| H | -6.18717200 | 3.17419800 | -1.66302800 |
| H | -5.59964300 | 3.28825000 | 0.00200800 |
| C | -4.46193200 | 1.96821600 | -1.23350900 |
| H | -4.64695100 | 1.13127100 | -1.92196200 |
| C | -3.57721100 | 2.99154800 | -1.94200500 |
| H | -3.61482300 | 3.93404200 | -1.38277800 |
| H | -4.02260000 | 3.18835100 | -2.92200600 |
| C | -2.11491000 | 2.54352700 | -2.09151600 |
| H | -2.03301100 | 1.46010500 | -1.97683800 |
| H | -1.74870500 | 2.77514000 | -3.09629800 |
| C | -1.17567200 | 3.22634900 | -1.09790000 |
| H | -1.11172500 | 4.29074600 | -1.36517300 |
| C | 0.24454200 | 2.62398700 | -1.14259600 |
| H | 0.46191600 | 2.27123200 | -2.15951700 |
| C | 1.30732800 | 3.64728800 | -0.75004700 |
| H | 1.05186100 | 4.09521700 | 0.21640800 |
| H | 1.29156700 | 4.44920900 | -1.49875000 |
| C | 2.71443100 | 3.06068000 | -0.65181500 |
| H | 2.84632700 | 2.29138500 | -1.42166000 |
| C | 3.80488200 | 4.10965500 | -0.85180900 |
| H | 3.68230800 | 4.91105800 | -0.11582900 |

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| H | 3.70418600 | 4.54693100 | -1.84897800 |
| C | 5.21965500 | 3.54660300 | -0.69949300 |
| C | 6.29963900 | 4.56568000 | -1.02622400 |
| H | 6.23738800 | 5.41645000 | -0.34428500 |
| H | 6.15995100 | 4.92799400 | -2.04859200 |
| C | 7.67802300 | 3.94272400 | -0.91531900 |
| H | 7.86236000 | 3.68502300 | 0.13608700 |
| C | 7.74700000 | 2.64019100 | -1.75804100 |
| H | 7.82407700 | 2.95994200 | -2.80398000 |
| C | 6.51746300 | 1.73339500 | -1.56881100 |
| H | 6.58547600 | 1.26342300 | -0.58593700 |
| C | 9.00160200 | 1.88846100 | -1.39399100 |
| C | -12.30070400 | 1.62635500 | 1.65973400 |
| H | -11.66914900 | 1.73776500 | 2.54415300 |
| H | -13.19548700 | 1.06205600 | 1.92468500 |
| H | -12.59581200 | 2.62193300 | 1.32154200 |
| C | -13.02600100 | 1.82546500 | -1.27013900 |
| H | -13.85509100 | 2.14048900 | -0.62900500 |
| H | -13.42785000 | 1.62736500 | -2.26784400 |
| H | -12.33527200 | 2.66808200 | -1.34671500 |
| C | -13.65904200 | -3.06496700 | -0.20513500 |
| H | -14.05943800 | -3.22071300 | -1.21318800 |
| H | -14.49010500 | -2.81833100 | 0.45616900 |
| H | -13.20875800 | -4.00449500 | 0.12370700 |
| O | 6.50959200 | -2.68039000 | 1.15603300 |
| H | 5.70865700 | -2.26301200 | 0.80850600 |

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| O | 9.50271900 | -5.25905300 | -0.37935500 |
| H | 9.83424000 | -5.25748400 | 0.53321800 |
| O | 6.96349700 | -3.04347500 | -1.72652700 |
| O | 6.09119500 | -1.09357700 | -0.97223200 |
| O | 5.45581400 | 3.08804600 | 0.59999600 |
| H | 4.60177200 | 2.70209800 | 0.89681800 |
| O | 5.31568700 | 2.48347000 | -1.65121600 |
| O | 9.06927200 | 0.80003900 | -0.87176600 |
| O | 2.92184300 | 2.48247100 | 0.63852500 |
| H | 2.67720800 | 1.53540900 | 0.63116200 |
| O | 0.27704900 | 1.47694000 | -0.30981700 |
| H | -0.38294600 | 1.64534500 | 0.38762000 |
| O | -1.62608800 | 3.15557300 | 0.24568600 |
| H | -2.38207600 | 2.53691800 | 0.30325900 |
| O | -3.73914700 | 1.48338400 | -0.10565700 |
| H | -4.32764800 | 1.02716100 | 0.51790600 |
| O | -6.30831800 | 0.78445700 | 0.64413200 |
| H | -7.06145600 | 0.34324400 | 1.07719600 |
| O | -8.92675000 | 0.30742000 | 1.13881200 |
| O | -10.40826500 | 1.71539400 | 0.18886800 |
| O | -14.31042700 | -0.36720700 | 0.34716100 |
| H | -14.91595600 | 0.29036100 | -0.01148000 |
| O | 8.59887100 | 4.91022800 | -1.37319100 |
| H | 9.47954300 | 4.51474000 | -1.35931800 |
| N | 9.07070800 | -3.63490900 | 1.84917100 |
| H | 8.20007100 | -3.83902900 | 2.33517600 |

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| H | 9.54127400 | -2.90961500 | 2.38102600 |
| C | 8.32679300 | 2.69882800 | 2.81983100 |
| H | 7.73633700 | 3.57601700 | 2.53871400 |
| H | 8.50386000 | 2.74595500 | 3.89924900 |
| C | 7.58818100 | 1.42407500 | 2.43046000 |
| H | 8.19804300 | 0.54436600 | 2.67315900 |
| H | 7.44344100 | 1.41044100 | 1.34693900 |
| C | 6.22904200 | 1.30752200 | 3.11361000 |
| H | 5.66726400 | 2.23198400 | 2.96172900 |
| H | 6.36910800 | 1.19654700 | 4.19618200 |
| C | 5.42273900 | 0.12747500 | 2.57166100 |
| H | 5.97147400 | -0.81295200 | 2.65130000 |
| H | 5.21136300 | 0.28817000 | 1.50698800 |
| C | 4.09369700 | -0.08680000 | 3.23621300 |
| O | 3.65906600 | -1.15193800 | 3.60715500 |
| C | 2.07201100 | 0.99081300 | 3.86921700 |
| H | 2.00054600 | 0.16601100 | 4.58163500 |
| H | 1.90459100 | 1.94264200 | 4.37886600 |
| C | 1.03209000 | 0.81460200 | 2.77541200 |
| H | 1.24716500 | 1.47682700 | 1.93888800 |
| C | -0.36929100 | 1.08540200 | 3.29763300 |
| H | -0.57366200 | 0.48221700 | 4.18572100 |
| H | -0.48231400 | 2.14568300 | 3.52959600 |
| O | 3.39630600 | 1.06919000 | 3.33994800 |
| C | 1.81802800 | -0.91913100 | 1.33479100 |
| C | 1.68971400 | -2.36269100 | 0.96205900 |

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| H | 1.16744200 | -2.89509200 | 1.75904800 |
| H | 1.05133500 | -2.39008000 | 0.07015600 |
| C | 3.06418800 | -2.95938700 | 0.65629000 |
| H | 3.66013200 | -2.94559800 | 1.57710100 |
| H | 3.56723300 | -2.31101700 | -0.06810200 |
| C | 2.99994800 | -4.37569100 | 0.09805800 |
| H | 2.47301700 | -5.02931200 | 0.80442100 |
| H | 2.40135000 | -4.36922100 | -0.82193700 |
| C | 4.39092300 | -4.93317200 | -0.19282700 |
| H | 4.99443600 | -4.96824500 | 0.71896600 |
| H | 4.93111300 | -4.29908200 | -0.90158700 |
| O | 1.00635700 | -0.54921500 | 2.32125100 |
| O | 2.60158900 | -0.16112900 | 0.79100000 |
| O | -1.32849500 | 0.78431100 | 2.27695400 |
| O | -3.58824000 | -0.27419700 | 2.22626400 |
| O | -1.69072700 | -1.52894800 | 3.43043200 |
| O | -1.70639400 | -1.20720600 | 0.82393500 |
| C | -4.52193200 | -1.26159700 | 2.68299300 |
| H | -4.05737800 | -1.85733800 | 3.47381900 |
| H | -5.37033700 | -0.71713300 | 3.10434800 |
| C | -5.00324200 | -2.12532400 | 1.52958000 |
| H | -5.48412100 | -1.47285800 | 0.80460800 |
| H | -5.76644500 | -2.81955300 | 1.90744900 |
| N | -3.89734400 | -2.81431900 | 0.84822900 |
| H | -3.60017500 | -3.63167200 | 1.37462600 |
| H | -4.19623400 | -3.12763800 | -0.07126900 |

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|---|-------------|-------------|-------------|
| P | -2.01229100 | -0.66634600 | 2.27802600 |
| H | -2.45009700 | -1.85808600 | 0.62438400 |
| O | 10.12488100 | 2.59402500 | -1.67301600 |
| H | 10.87170200 | 2.05693100 | -1.36149700 |
| H | 9.29793800 | 2.76908600 | 2.32018100 |
| H | 4.33821200 | -5.94495800 | -0.60613700 |

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|---|--------------|------------|-------------|
| C | -10.65989400 | 2.37919800 | 1.49046500 |
| H | -11.26441300 | 1.47944300 | 1.31517800 |
| C | -11.05971700 | 3.39338700 | 0.41885200 |
| H | -10.48767800 | 4.31922200 | 0.58973800 |
| C | -10.69143100 | 2.87852000 | -0.96733400 |
| H | -11.22192400 | 1.92964900 | -1.14914300 |
| C | -8.88070000 | 1.64487900 | -0.09351300 |
| H | -9.40308700 | 0.70564100 | -0.33866400 |
| C | -9.18694300 | 2.00149100 | 1.35868000 |
| H | -8.96944600 | 1.11310400 | 1.97244100 |
| C | -11.01249900 | 3.86231600 | -2.06779300 |
| H | -10.44631000 | 4.78549600 | -1.91753500 |
| H | -12.07802700 | 4.09618900 | -2.05004700 |
| H | -10.74775700 | 3.44329300 | -3.04064300 |
| C | -6.92123500 | 1.32223400 | -1.48195800 |

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|---|-------------|------------|-------------|
| H | -7.05232100 | 2.25115000 | -2.04599900 |
| C | -5.46847200 | 1.08056700 | -1.21906100 |
| H | -5.22513400 | 0.18336500 | -0.65507000 |
| C | -4.49535700 | 1.90818600 | -1.61641200 |
| H | -4.74563400 | 2.80079300 | -2.18958600 |
| C | -3.09784900 | 1.68809800 | -1.29926500 |
| H | -2.87385400 | 0.82294700 | -0.68210500 |
| C | -2.07029100 | 2.46042100 | -1.70119700 |
| H | -2.25640400 | 3.31942900 | -2.34537500 |
| C | -0.70454300 | 2.17959800 | -1.32125900 |
| H | -0.56725300 | 1.36452500 | -0.61431300 |
| C | 0.39126800 | 2.80423000 | -1.80002600 |
| H | 0.28788800 | 3.60468800 | -2.53190000 |
| C | 1.72311500 | 2.41625400 | -1.40021400 |
| H | 1.77824000 | 1.65658800 | -0.62376100 |
| C | 2.87579200 | 2.91116400 | -1.89708800 |
| H | 2.84985100 | 3.68549900 | -2.66274400 |
| C | 4.17080600 | 2.47697300 | -1.43101800 |
| H | 4.16936300 | 1.68131000 | -0.68582300 |
| C | 5.35830400 | 2.98659100 | -1.81837400 |
| H | 5.37908100 | 3.77758700 | -2.56701300 |
| C | 6.62131300 | 2.57172400 | -1.25436600 |
| H | 6.58565600 | 1.79308200 | -0.49387700 |
| C | 7.82587800 | 3.07939100 | -1.57830800 |
| H | 7.89986900 | 3.83817400 | -2.35646300 |
| C | -7.62897800 | 0.19581400 | -2.24293300 |

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| H | -8.63144000 | 0.53588000 | -2.50630400 |
| H | -7.09699400 | 0.01581400 | -3.18114500 |
| C | 9.05222800 | 2.65620700 | -0.92815000 |
| H | 8.92427900 | 1.97977700 | -0.08580200 |
| C | 10.29176600 | 2.99792200 | -1.29737300 |
| H | 10.43190100 | 3.65952500 | -2.15369700 |
| C | 11.54224200 | 2.50499200 | -0.62379000 |
| H | 11.26230900 | 1.98775100 | 0.30081500 |
| C | 12.30052400 | 1.48162400 | -1.49293300 |
| H | 12.74629600 | 2.03306300 | -2.33796700 |
| C | 11.42541800 | 0.37312000 | -2.09891300 |
| H | 10.64987000 | 0.88781800 | -2.67375900 |
| C | 10.66742600 | -0.44450500 | -1.04323200 |
| H | 10.31528200 | 0.21151300 | -0.25107600 |
| C | 8.29772700 | -0.76194100 | -1.15111400 |
| C | 7.18018400 | -1.05309000 | -2.11648100 |
| H | 7.12085200 | -0.16318300 | -2.75530100 |
| H | 7.45173000 | -1.89659800 | -2.75472000 |
| C | 5.83728400 | -1.31114400 | -1.44637300 |
| H | 5.69920000 | -0.57099400 | -0.64739400 |
| C | 4.69211000 | -1.16951400 | -2.43607800 |
| H | 4.74943000 | -0.17357000 | -2.88687800 |
| H | 4.80436700 | -1.91139900 | -3.23531800 |
| C | 3.31497700 | -1.33545400 | -1.79994900 |
| H | 3.24694000 | -0.66863600 | -0.92411900 |
| C | 2.21359600 | -0.96505800 | -2.78069200 |

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| H | 2.21693800 | -1.69730600 | -3.59785000 |
| H | 2.48493500 | 0.00199800 | -3.21472200 |
| C | 0.81613300 | -0.81610200 | -2.18029300 |
| H | 0.88597100 | -0.30995000 | -1.21601000 |
| H | 0.23765600 | -0.15325000 | -2.83087400 |
| C | -0.00850200 | -2.08274900 | -1.97026900 |
| H | -0.03851600 | -2.66435800 | -2.90660100 |
| C | -1.44082400 | -1.69737600 | -1.61208700 |
| H | -1.81137100 | -1.00358800 | -2.37513300 |
| C | -2.41199600 | -2.87018200 | -1.51266400 |
| H | -2.08416500 | -3.55583400 | -0.72478600 |
| H | -2.39802200 | -3.42075000 | -2.45997900 |
| C | -3.83053600 | -2.38234400 | -1.22966500 |
| H | -4.09197200 | -1.60791300 | -1.96314600 |
| C | -4.88276800 | -3.47805200 | -1.31628000 |
| H | -4.62894500 | -4.30046000 | -0.64057000 |
| H | -4.89880400 | -3.86676000 | -2.33837600 |
| C | -6.28165400 | -2.97947300 | -0.94516100 |
| C | -7.38508600 | -3.97720000 | -1.28248900 |
| H | -7.28165600 | -4.87135000 | -0.66465900 |
| H | -7.30252300 | -4.26919800 | -2.33357500 |
| C | -8.74790800 | -3.35112600 | -1.04804000 |
| H | -8.83887400 | -3.11186300 | 0.01758600 |
| C | -8.86552400 | -2.04736200 | -1.84984400 |
| H | -8.78213200 | -2.27151400 | -2.91799100 |
| C | -7.69186400 | -1.11341700 | -1.46726000 |

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|---|--------------|-------------|-------------|
| H | -7.75735800 | -0.90632600 | -0.39341500 |
| C | -10.19989900 | -1.36701200 | -1.66934400 |
| C | 11.40914800 | -1.60853300 | -0.41833600 |
| H | 10.78575900 | -2.07169200 | 0.34960500 |
| H | 12.32995300 | -1.24177500 | 0.03884200 |
| H | 11.65634600 | -2.36796400 | -1.16308400 |
| C | 12.21539300 | -0.50191400 | -3.07012000 |
| H | 13.04770200 | -1.01522300 | -2.57840400 |
| H | 12.62389800 | 0.09825600 | -3.88843100 |
| H | 11.57143900 | -1.27004900 | -3.50449900 |
| C | 12.46988400 | 3.66620700 | -0.25461800 |
| H | 12.74911300 | 4.23676100 | -1.14732800 |
| H | 13.38252700 | 3.28873500 | 0.20895500 |
| H | 11.97649200 | 4.35175800 | 0.43840100 |
| O | -8.40075200 | 3.09472600 | 1.78187800 |
| H | -7.57696400 | 3.04389400 | 1.27477000 |
| O | -12.44795600 | 3.62130700 | 0.47843300 |
| H | -12.64002400 | 3.68033800 | 1.42820600 |
| O | -9.28279100 | 2.64497400 | -0.99211100 |
| O | -7.49877800 | 1.50591900 | -0.17022700 |
| O | -6.37896800 | -2.70222000 | 0.42505100 |
| H | -5.55452100 | -2.23926900 | 0.66138500 |
| O | -6.47572500 | -1.79879300 | -1.72123400 |
| O | -10.68773700 | -0.56257100 | -2.42670400 |
| O | -3.90351400 | -1.80934800 | 0.08090300 |
| H | -3.07170300 | -1.31408100 | 0.20505200 |

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|---|--------------|-------------|-------------|
| O | -1.44149600 | -0.94209400 | -0.39394800 |
| H | -0.86410900 | -1.38481700 | 0.25108800 |
| O | 0.47369200 | -2.88784700 | -0.90601500 |
| H | 1.44400800 | -2.98521800 | -1.02775200 |
| O | 3.11039100 | -2.68284600 | -1.37477200 |
| H | 3.93289400 | -2.96318300 | -0.92833600 |
| O | 5.79293900 | -2.62051700 | -0.89825000 |
| H | 6.19152900 | -2.60303800 | -0.00161500 |
| O | 8.14573600 | -0.33017600 | -0.02641500 |
| O | 9.48897500 | -0.95648500 | -1.72306400 |
| O | 13.33391300 | 0.95570600 | -0.66459000 |
| H | 13.97480800 | 0.50370800 | -1.22399400 |
| O | -9.73702200 | -4.28668000 | -1.43901500 |
| H | -10.56400900 | -4.01099200 | -1.02582500 |
| N | -11.03950600 | 2.92827200 | 2.78777900 |
| H | -10.33700300 | 3.61266500 | 3.05933400 |
| H | -11.03731400 | 2.20595100 | 3.50091200 |
| C | -5.97893400 | 0.35859400 | 2.68645900 |
| H | -6.24719900 | -0.47147600 | 2.02619900 |
| H | -6.17732700 | 0.04633400 | 3.71710100 |
| C | -4.51789600 | 0.75850500 | 2.50946900 |
| H | -4.31216900 | 1.67036600 | 3.08394800 |
| H | -4.33563000 | 1.01230400 | 1.45934700 |
| C | -3.54374600 | -0.33146000 | 2.94986800 |
| H | -3.75085200 | -1.25824000 | 2.40576200 |
| H | -3.68665700 | -0.54962700 | 4.01425200 |

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| C | -2.08336800 | 0.08464200 | 2.71990200 |
| H | -1.86365500 | 0.98415400 | 3.30075000 |
| H | -1.90585300 | 0.30164300 | 1.66466100 |
| C | -1.12969600 | -0.97928100 | 3.18429000 |
| O | -0.72055700 | -1.11022100 | 4.31012700 |
| C | 0.21200100 | -2.81246300 | 2.42024200 |
| H | 0.20127100 | -3.08143000 | 3.47807900 |
| H | -0.05107200 | -3.66557500 | 1.79359600 |
| C | 1.56808000 | -2.26809600 | 2.00079300 |
| H | 1.53433400 | -1.97259600 | 0.95325000 |
| C | 2.66927700 | -3.27862400 | 2.21246800 |
| H | 2.84100900 | -3.45184900 | 3.27724000 |
| H | 2.41259800 | -4.22015800 | 1.72307700 |
| O | -0.78591500 | -1.81898800 | 2.16845700 |
| C | 1.64725200 | 0.09055800 | 2.31909100 |
| C | 1.83837800 | 1.13226700 | 3.38802900 |
| H | 1.07743700 | 0.91216500 | 4.14569100 |
| H | 2.80258100 | 0.94016600 | 3.86896200 |
| C | 1.72596900 | 2.55802200 | 2.86425100 |
| H | 1.59274700 | 3.24159300 | 3.70963700 |
| H | 0.82530900 | 2.63622200 | 2.24617000 |
| C | 2.93684100 | 2.98970200 | 2.04177200 |
| H | 3.83050400 | 2.96543500 | 2.67993600 |
| H | 3.09724700 | 2.25531800 | 1.24780200 |
| C | 2.77986900 | 4.37483700 | 1.42789800 |
| H | 2.65029900 | 5.13782300 | 2.20219000 |

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|---|--------------|-------------|-------------|
| H | 1.90719600 | 4.40660600 | 0.77017600 |
| O | 1.88127700 | -1.13409000 | 2.81559700 |
| O | 1.26711200 | 0.29895600 | 1.18749600 |
| O | 3.87396700 | -2.83050800 | 1.58612800 |
| O | 4.64303600 | -0.45890900 | 1.98456200 |
| O | 6.37162600 | -2.33201000 | 1.72028300 |
| O | 4.84668800 | -2.21140400 | 3.82395500 |
| C | 5.69557900 | 0.52399500 | 2.01101400 |
| H | 6.56236200 | 0.14482200 | 1.46285900 |
| H | 5.29821800 | 1.39515800 | 1.48956200 |
| C | 6.06874000 | 0.92424500 | 3.42736900 |
| H | 5.17947500 | 1.28690800 | 3.95030400 |
| H | 6.77769900 | 1.76029600 | 3.35563700 |
| N | 6.61087100 | -0.21383300 | 4.18661000 |
| H | 7.41908800 | -0.60366200 | 3.70375900 |
| H | 6.91846000 | 0.08411300 | 5.10715800 |
| P | 5.03427900 | -1.99977000 | 2.27091700 |
| H | 5.46128700 | -1.52959200 | 4.24225200 |
| O | -10.82833000 | -1.71256000 | -0.51872800 |
| H | -11.65645000 | -1.20534000 | -0.50423600 |
| H | -6.64264600 | 1.19331100 | 2.45368900 |
| H | 3.65312400 | 4.64142800 | 0.82703800 |

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|---|-------------|-------------|-------------|
| C | 9.32201500 | -4.66269900 | 0.59471600 |
| H | 9.80945800 | -3.74619500 | 0.95839600 |
| C | 9.55145700 | -4.70838000 | -0.91776200 |
| H | 9.09424700 | -5.62749400 | -1.30851200 |
| C | 8.88828800 | -3.50952200 | -1.59945400 |
| H | 9.33932600 | -2.58616600 | -1.20270300 |
| C | 7.24751800 | -3.38337200 | 0.08057000 |
| H | 7.70012100 | -2.44017700 | 0.43230300 |
| C | 7.83124800 | -4.54051000 | 0.88310100 |
| H | 7.68178000 | -4.33524300 | 1.95256700 |
| C | 9.01738400 | -3.52401300 | -3.10642000 |
| H | 8.56120200 | -4.42934900 | -3.51742200 |
| H | 10.06950700 | -3.48530700 | -3.39884800 |
| H | 8.51238700 | -2.65594300 | -3.53422100 |
| C | 5.07235900 | -2.55111000 | -0.54992900 |
| H | 5.07426800 | -2.97205800 | -1.56151100 |
| C | 3.68796000 | -2.59629200 | 0.01702500 |
| H | 3.58671000 | -2.36551500 | 1.07503800 |
| C | 2.60144900 | -2.84817000 | -0.72143700 |
| H | 2.71362100 | -3.06254600 | -1.78537100 |
| C | 1.25169600 | -2.84500000 | -0.19009900 |
| H | 1.14663000 | -2.72720900 | 0.88640500 |
| C | 0.14125700 | -2.95829700 | -0.94219300 |
| H | 0.23324700 | -3.05716100 | -2.02384600 |
| C | -1.19315700 | -2.91771400 | -0.39291300 |

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|---|--------------|-------------|-------------|
| H | -1.28243200 | -2.86163200 | 0.68767900 |
| C | -2.32134600 | -2.90911700 | -1.12932000 |
| H | -2.25038100 | -2.95757900 | -2.21575300 |
| C | -3.64238000 | -2.80189800 | -0.56035200 |
| H | -3.70345200 | -2.71334000 | 0.52270500 |
| C | -4.76674600 | -2.74899600 | -1.30376200 |
| H | -4.67705000 | -2.81345400 | -2.38841400 |
| C | -6.10097800 | -2.60650500 | -0.77768800 |
| H | -6.21650300 | -2.56074100 | 0.30519800 |
| C | -7.20104400 | -2.53475300 | -1.55745400 |
| H | -7.07821500 | -2.56837800 | -2.64013400 |
| C | -8.55171400 | -2.45383300 | -1.05746600 |
| H | -8.68061600 | -2.48588700 | 0.02244100 |
| C | -9.64326800 | -2.34091800 | -1.83664000 |
| H | -9.52371800 | -2.28089200 | -2.91809300 |
| C | 5.65033700 | -1.13536800 | -0.63693400 |
| H | 6.60271400 | -1.18072400 | -1.16446600 |
| H | 4.98136300 | -0.53117200 | -1.25169100 |
| C | -10.99073400 | -2.25786100 | -1.30838200 |
| H | -11.09055400 | -2.43712300 | -0.24027200 |
| C | -12.07355100 | -1.92917300 | -2.02138300 |
| H | -11.96706500 | -1.73203100 | -3.08951700 |
| C | -13.45262800 | -1.75291100 | -1.45281400 |
| H | -13.46308100 | -2.12657000 | -0.42259400 |
| C | -13.84535000 | -0.26308400 | -1.39969100 |
| H | -13.97405800 | 0.07910800 | -2.44017300 |

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|---|--------------|-------------|-------------|
| C | -12.79368700 | 0.66291200 | -0.76079800 |
| H | -11.88140400 | 0.52863700 | -1.34984400 |
| C | -12.41742100 | 0.25443700 | 0.66781500 |
| H | -12.25919900 | -0.81938700 | 0.71417700 |
| C | -10.13318000 | 0.13460800 | 1.39390800 |
| C | -8.87654900 | 0.92797400 | 1.63950700 |
| H | -8.88929300 | 1.83277600 | 1.02917700 |
| H | -8.89579500 | 1.23705300 | 2.69128200 |
| C | -7.60083000 | 0.11773100 | 1.39029500 |
| H | -7.56326400 | -0.17708100 | 0.33155000 |
| C | -6.37303200 | 0.95612200 | 1.71739900 |
| H | -6.32432500 | 1.77207000 | 0.99080600 |
| H | -6.48525000 | 1.38845400 | 2.71892700 |
| C | -5.04829100 | 0.19881300 | 1.67451400 |
| H | -4.95157300 | -0.29689900 | 0.69908000 |
| C | -3.87882100 | 1.15611100 | 1.87238800 |
| H | -3.91147300 | 1.51420700 | 2.90877500 |
| H | -4.06329200 | 2.02536900 | 1.23422300 |
| C | -2.48283200 | 0.62403100 | 1.54070300 |
| H | -2.48746800 | 0.14292600 | 0.55798800 |
| H | -1.81118900 | 1.48275600 | 1.45612400 |
| C | -1.87582200 | -0.37077600 | 2.51646300 |
| H | -1.90938300 | 0.03288200 | 3.54140500 |
| C | -0.41926400 | -0.68209000 | 2.15297900 |
| H | -0.36014500 | -0.81447900 | 1.06420000 |
| C | 0.58667900 | 0.38458300 | 2.56051200 |

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|---|--------------|-------------|-------------|
| H | 0.50946700 | 0.57368300 | 3.63774300 |
| H | 0.35570200 | 1.31211300 | 2.02666900 |
| C | 2.02309800 | -0.01733300 | 2.22605000 |
| H | 2.07845500 | -0.26217300 | 1.15778700 |
| C | 3.00997300 | 1.10589500 | 2.52239000 |
| H | 2.88985000 | 1.43722900 | 3.55863600 |
| H | 2.79687200 | 1.95532900 | 1.86950600 |
| C | 4.47103900 | 0.69266200 | 2.34576100 |
| C | 5.43978000 | 1.86790000 | 2.40942700 |
| H | 5.43024800 | 2.29683900 | 3.41354800 |
| H | 5.12385700 | 2.63218000 | 1.69878800 |
| C | 6.84426900 | 1.40506400 | 2.07252900 |
| H | 7.17716000 | 0.70140200 | 2.84224300 |
| C | 6.85623700 | 0.69404600 | 0.71440000 |
| H | 6.55328700 | 1.39578900 | -0.06590300 |
| C | 5.80836600 | -0.44427400 | 0.70853700 |
| H | 6.07333900 | -1.17576500 | 1.48002100 |
| C | 8.22700900 | 0.19952200 | 0.32956600 |
| C | -13.37056800 | 0.67282400 | 1.76877800 |
| H | -13.02990900 | 0.27751800 | 2.72850000 |
| H | -14.36312400 | 0.27718700 | 1.54901400 |
| H | -13.43057800 | 1.76049300 | 1.84675500 |
| C | -13.20550200 | 2.13039500 | -0.86385700 |
| H | -14.15286500 | 2.32647900 | -0.35271400 |
| H | -13.31872100 | 2.42735300 | -1.91053500 |
| H | -12.45021600 | 2.77628000 | -0.41050200 |

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|---|--------------|-------------|-------------|
| C | -14.49136800 | -2.54226000 | -2.25438900 |
| H | -14.49686400 | -2.22030500 | -3.30172300 |
| H | -15.48935600 | -2.38443100 | -1.84339000 |
| H | -14.26344200 | -3.61040300 | -2.23468200 |
| O | 7.21182400 | -5.75302200 | 0.50845600 |
| H | 6.26870800 | -5.55578800 | 0.42069300 |
| O | 10.95887700 | -4.69813200 | -1.11579100 |
| H | 11.14760600 | -5.05419300 | -1.99003000 |
| O | 7.49649500 | -3.52561700 | -1.29713600 |
| O | 5.87218100 | -3.40032500 | 0.29359600 |
| O | 4.87409900 | -0.23227700 | 3.31066200 |
| H | 4.13360200 | -0.86191900 | 3.40303900 |
| O | 4.54462900 | 0.11396200 | 1.03224100 |
| O | 8.58476400 | -0.07481900 | -0.79554500 |
| O | 2.43386100 | -1.16159100 | 2.98294800 |
| H | 1.65594300 | -1.73348900 | 3.10758500 |
| O | -0.05984700 | -1.91509400 | 2.78465000 |
| H | -0.89975900 | -2.38211100 | 2.93758100 |
| O | -2.53218800 | -1.63378900 | 2.48248800 |
| H | -3.47921900 | -1.49326000 | 2.70591900 |
| O | -5.00307400 | -0.78038900 | 2.71847800 |
| H | -5.86744600 | -1.22823500 | 2.73179600 |
| O | -7.58254300 | -1.05553100 | 2.19885700 |
| H | -8.46993800 | -1.45365000 | 2.15238100 |
| O | -10.22175000 | -1.06170100 | 1.62370700 |
| O | -11.12531000 | 0.88371200 | 0.93439000 |

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|---|--------------|-------------|-------------|
| O | -15.09535600 | -0.20443600 | -0.71958800 |
| H | -15.51004800 | 0.64438700 | -0.90737600 |
| O | 7.69200400 | 2.54839100 | 2.04748800 |
| H | 8.59455200 | 2.23390800 | 2.17880900 |
| N | 9.87711400 | -5.78796700 | 1.32198200 |
| H | 9.31941800 | -6.61221200 | 1.11582500 |
| H | 10.81869600 | -5.95803900 | 0.98181000 |
| C | 10.55471200 | 2.64222100 | -1.51719900 |
| H | 10.34669200 | 1.56831100 | -1.51299600 |
| H | 10.80316300 | 2.92787100 | -2.54435500 |
| C | 9.34855200 | 3.42425500 | -1.00725800 |
| H | 9.57642000 | 4.49711700 | -0.98951600 |
| H | 9.12560100 | 3.14473600 | 0.02862300 |
| C | 8.09822800 | 3.17886700 | -1.84716700 |
| H | 7.88178800 | 2.10721600 | -1.86149200 |
| H | 8.28493800 | 3.47363400 | -2.88718300 |
| C | 6.88607900 | 3.94652700 | -1.30719500 |
| H | 7.02225200 | 5.02530900 | -1.40313800 |
| H | 6.75713800 | 3.72111900 | -0.24142800 |
| C | 5.59956900 | 3.59918500 | -1.99957900 |
| O | 4.83390800 | 4.37243800 | -2.52271400 |
| C | 4.16817200 | 1.77033700 | -2.52630200 |
| H | 3.87026900 | 2.39098300 | -3.37456700 |
| H | 4.39605900 | 0.76090300 | -2.87476400 |
| C | 3.04986000 | 1.73225200 | -1.49886300 |
| H | 3.45473200 | 1.48489300 | -0.51551300 |

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| C | 1.97660400 | 0.72506000 | -1.89858800 |
| H | 1.68762800 | 0.85362800 | -2.94637000 |
| H | 2.36536500 | -0.28392600 | -1.75119800 |
| O | 5.38080000 | 2.26062600 | -1.96144400 |
| C | 2.78041100 | 3.89816000 | -0.46785200 |
| C | 1.93249300 | 5.13173100 | -0.50916700 |
| H | 1.93490500 | 5.50074200 | -1.54114600 |
| H | 0.90716300 | 4.81119000 | -0.28380400 |
| C | 2.41348800 | 6.20142700 | 0.46067700 |
| H | 3.44658400 | 6.47043800 | 0.21513000 |
| H | 2.44225000 | 5.78002700 | 1.47080600 |
| C | 1.52942100 | 7.44406600 | 0.43789300 |
| H | 1.50338100 | 7.85367200 | -0.57964500 |
| H | 0.49787700 | 7.15900100 | 0.67857600 |
| C | 2.00730600 | 8.51721700 | 1.41035600 |
| H | 3.02590900 | 8.83779300 | 1.17066600 |
| H | 2.01404700 | 8.13971200 | 2.43756200 |
| O | 2.41119900 | 3.02362500 | -1.44156700 |
| O | 3.66692100 | 3.66470700 | 0.31261300 |
| O | 0.82952800 | 0.83316500 | -1.05901300 |
| O | -1.54511500 | 1.05693500 | -1.70475700 |
| O | 0.03934700 | 2.69911500 | -2.64173800 |
| H | 0.83804800 | 3.24067200 | -2.51261800 |
| O | -0.50542400 | 2.81516300 | -0.09007600 |
| C | -2.85827300 | 1.65030600 | -1.72467600 |
| H | -3.06308500 | 2.12324400 | -0.76290200 |

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| H | -2.89587600 | 2.41407400 | -2.50968100 |
| C | -3.83351200 | 0.51888100 | -1.97855000 |
| H | -3.58999400 | -0.28367600 | -1.28391700 |
| H | -3.66188400 | 0.11703600 | -2.98867300 |
| N | -5.20597200 | 0.94419500 | -1.71892700 |
| H | -5.55179200 | 1.52700400 | -2.47540600 |
| H | -5.80520000 | 0.12442700 | -1.68241800 |
| P | -0.30305600 | 1.94753600 | -1.26828500 |
| O | 9.06769400 | 0.05620600 | 1.37694200 |
| H | 9.90368100 | -0.27895400 | 1.01366500 |
| H | 11.43971300 | 2.82424400 | -0.90049000 |
| H | 1.36341500 | 9.40027300 | 1.38271300 |

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|---|------------|-------------|-------------|
| C | 6.19543700 | -4.45567900 | 0.45056800 |
| H | 6.81860200 | -3.58265300 | 0.69283000 |
| C | 6.46781800 | -4.79998200 | -1.01297000 |
| H | 5.90188000 | -5.70290100 | -1.27482000 |
| C | 6.03467800 | -3.65747600 | -1.92899600 |
| H | 6.59961700 | -2.75221200 | -1.66594300 |
| C | 4.38117500 | -2.97218100 | -0.40434000 |
| H | 4.96556100 | -2.06125800 | -0.21615300 |
| C | 4.74345000 | -4.03015700 | 0.63295500 |

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|---|-------------|-------------|-------------|
| H | 4.61635000 | -3.59727800 | 1.63527000 |
| C | 6.20951500 | -3.95522700 | -3.40249900 |
| H | 5.64051600 | -4.84630700 | -3.68317700 |
| H | 7.26340200 | -4.10350000 | -3.65270900 |
| H | 5.84571300 | -3.11101200 | -3.99060900 |
| C | 2.35243300 | -2.01954500 | -1.33283200 |
| H | 2.26169600 | -2.69320300 | -2.19182900 |
| C | 0.99641000 | -1.69402000 | -0.79052000 |
| H | 0.96280800 | -1.02039900 | 0.06186700 |
| C | -0.14125100 | -2.17139400 | -1.30394700 |
| H | -0.10676900 | -2.84323400 | -2.16154500 |
| C | -1.44760700 | -1.84887300 | -0.76568100 |
| H | -1.46825800 | -1.16753200 | 0.08160200 |
| C | -2.61120600 | -2.34136700 | -1.23074300 |
| H | -2.60370300 | -3.02707200 | -2.07782500 |
| C | -3.88907500 | -2.00808500 | -0.64862100 |
| H | -3.86369300 | -1.30470200 | 0.18135400 |
| C | -5.07873700 | -2.48545800 | -1.06619800 |
| H | -5.11735700 | -3.18568900 | -1.90017000 |
| C | -6.32925800 | -2.11033700 | -0.45441900 |
| H | -6.28105200 | -1.38768900 | 0.35995900 |
| C | -7.53912500 | -2.57321000 | -0.82999100 |
| H | -7.60685200 | -3.28318900 | -1.65363600 |
| C | -8.77012400 | -2.19095700 | -0.18492300 |
| H | -8.69301200 | -1.49340800 | 0.64882000 |
| C | -9.99202600 | -2.63266600 | -0.54505200 |

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| H | -10.08398100 | -3.31357700 | -1.39053600 |
| C | -11.20638000 | -2.25620800 | 0.13684400 |
| H | -11.09592900 | -1.62599400 | 1.01763200 |
| C | -12.44751600 | -2.60979200 | -0.24416600 |
| H | -12.58241800 | -3.21783300 | -1.13801600 |
| C | 3.14052300 | -0.78741600 | -1.78178000 |
| H | 4.10203800 | -1.11211400 | -2.17924700 |
| H | 2.59593000 | -0.32005300 | -2.60726200 |
| C | -13.63856600 | -2.17906300 | 0.46147100 |
| H | -13.46625700 | -1.66256200 | 1.40348100 |
| C | -14.89111800 | -2.31973400 | 0.01447800 |
| H | -15.06258100 | -2.82190400 | -0.93910100 |
| C | -16.11196000 | -1.78573500 | 0.70773800 |
| H | -15.82987300 | -1.43844000 | 1.70832500 |
| C | -16.69303000 | -0.57475000 | -0.04836300 |
| H | -17.10198800 | -0.95018500 | -1.00128500 |
| C | -15.66891600 | 0.51664600 | -0.41204400 |
| H | -14.90378600 | 0.01798100 | -1.01473400 |
| C | -14.92334500 | 1.07851400 | 0.80390400 |
| H | -14.58994800 | 0.26354700 | 1.44064200 |
| C | -12.54168500 | 1.38549800 | 0.77612800 |
| C | -11.40320400 | 2.11351800 | 0.10667300 |
| H | -11.71031300 | 2.42689400 | -0.89286400 |
| H | -11.20256200 | 3.01734000 | 0.69357100 |
| C | -10.12939000 | 1.26663300 | 0.05342100 |
| H | -10.33066900 | 0.34973500 | -0.51887500 |

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| C | -8.98928100 | 2.02998800 | -0.60469600 |
| H | -9.28571700 | 2.28954500 | -1.62667200 |
| H | -8.82476200 | 2.96649300 | -0.05837300 |
| C | -7.66975400 | 1.26330000 | -0.65266400 |
| H | -7.83404900 | 0.27923800 | -1.11258400 |
| C | -6.62050900 | 2.01753000 | -1.46286800 |
| H | -6.61072800 | 3.06571000 | -1.13963100 |
| H | -6.94860700 | 2.01544600 | -2.50681800 |
| C | -5.20654800 | 1.42466600 | -1.34824900 |
| H | -5.25525500 | 0.38299700 | -1.02227200 |
| H | -4.72492500 | 1.41251600 | -2.33086100 |
| C | -4.28588900 | 2.20599400 | -0.41288300 |
| H | -4.11660500 | 3.20062000 | -0.84823800 |
| C | -2.91303500 | 1.50531900 | -0.24335100 |
| H | -2.72743800 | 0.84057300 | -1.09487600 |
| C | -1.75547800 | 2.48986600 | -0.11564600 |
| H | -1.92834800 | 3.13876000 | 0.75161500 |
| H | -1.73567900 | 3.12777600 | -1.00688900 |
| C | -0.40440500 | 1.79418300 | 0.02195500 |
| H | -0.26944000 | 1.10638100 | -0.82394700 |
| C | 0.75222200 | 2.78619000 | 0.01731700 |
| H | 0.61510800 | 3.52006800 | 0.81761200 |
| H | 0.75057100 | 3.31803500 | -0.93860900 |
| C | 2.11825100 | 2.12767200 | 0.21473200 |
| C | 3.27964700 | 3.07949100 | -0.03717600 |
| H | 3.27651900 | 3.88389600 | 0.70211500 |

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| H | 3.16997400 | 3.52337400 | -1.03133200 |
| C | 4.60756000 | 2.34456600 | 0.02378900 |
| H | 4.76156800 | 1.98647300 | 1.04768900 |
| C | 4.59987600 | 1.13006400 | -0.91384600 |
| H | 4.61290900 | 1.48462100 | -1.94877200 |
| C | 3.32883100 | 0.27175900 | -0.70263600 |
| H | 3.38942000 | -0.19205100 | 0.28986100 |
| C | 5.80916100 | 0.23788300 | -0.73338100 |
| C | -15.65977600 | 2.10692500 | 1.63738300 |
| H | -15.05611900 | 2.39013100 | 2.50270400 |
| H | -16.60177200 | 1.67678800 | 1.98005800 |
| H | -15.87128900 | 3.00702000 | 1.05618100 |
| C | -16.30063000 | 1.61112500 | -1.27035800 |
| H | -17.12830900 | 2.10914200 | -0.75618900 |
| H | -16.68610700 | 1.19450500 | -2.20541300 |
| H | -15.56410100 | 2.37760000 | -1.52147600 |
| C | -17.18224500 | -2.86936300 | 0.86579000 |
| H | -17.47561500 | -3.26731000 | -0.11201700 |
| H | -18.07063200 | -2.46002100 | 1.34853400 |
| H | -16.80312400 | -3.70080200 | 1.46428700 |
| O | 3.92924600 | -5.17171000 | 0.46715300 |
| H | 3.04176300 | -4.83429800 | 0.27636500 |
| O | 7.87625200 | -5.04815400 | -1.10549100 |
| H | 8.07773700 | -5.41878500 | -1.97144100 |
| O | 4.64636000 | -3.43526600 | -1.71048600 |
| O | 3.01598400 | -2.74388800 | -0.27182400 |

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| O | 2.26350700 | 1.61590700 | 1.50812700 |
| H | 1.41722800 | 1.18734900 | 1.72984700 |
| O | 2.17140000 | 1.08984700 | -0.75975700 |
| O | 6.30460900 | -0.42071700 | -1.62525700 |
| O | -0.34033300 | 1.04208000 | 1.23662300 |
| H | -1.24024400 | 0.71858900 | 1.42471000 |
| O | -2.98230300 | 0.66964900 | 0.91365200 |
| H | -3.65074200 | 1.12537300 | 1.46699200 |
| O | -4.82611800 | 2.39159700 | 0.88798500 |
| H | -5.70466400 | 1.95769000 | 0.93826600 |
| O | -7.15021300 | 1.06116200 | 0.66465800 |
| H | -7.90706700 | 0.89897100 | 1.25678300 |
| O | -9.70989900 | 0.91541700 | 1.36956800 |
| H | -10.49377500 | 0.57692000 | 1.83780500 |
| O | -12.37939800 | 0.59472500 | 1.69206900 |
| O | -13.72045200 | 1.71588200 | 0.26943300 |
| O | -17.75177500 | -0.06896600 | 0.75940400 |
| H | -18.31717000 | 0.48900900 | 0.21465600 |
| O | 5.60500000 | 3.27457400 | -0.34709500 |
| H | 6.47538300 | 2.84363100 | -0.36723900 |
| N | 6.51441300 | -5.53622900 | 1.37391700 |
| H | 5.72446200 | -6.17564400 | 1.40032600 |
| H | 7.30976800 | -6.05512500 | 1.01365900 |
| C | 4.44689700 | 7.04156100 | -1.66056200 |
| H | 3.94368300 | 6.56817700 | -0.81142200 |
| H | 4.71767600 | 8.05911700 | -1.36010000 |

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| C | 5.67703200 | 6.23840700 | -2.06838700 |
| H | 6.14616400 | 6.69480500 | -2.94956100 |
| H | 5.37137400 | 5.22647700 | -2.35703700 |
| C | 6.69182800 | 6.11527200 | -0.93626800 |
| H | 6.20811700 | 5.62444700 | -0.09109600 |
| H | 7.01383300 | 7.11058100 | -0.60527600 |
| C | 7.90530700 | 5.28709000 | -1.35302000 |
| H | 8.53269300 | 5.80210300 | -2.08440200 |
| H | 7.56020200 | 4.35953900 | -1.82649600 |
| C | 8.80730400 | 4.81500200 | -0.24632300 |
| O | 9.98844600 | 4.58767500 | -0.35362400 |
| C | 8.77430200 | 3.90485900 | 1.95180300 |
| H | 9.84868500 | 4.09855200 | 1.92320400 |
| H | 8.34515600 | 4.30031400 | 2.87531000 |
| C | 8.50831100 | 2.41261300 | 1.84957300 |
| H | 7.48188600 | 2.23847900 | 1.51777800 |
| C | 8.75518800 | 1.68081600 | 3.15748300 |
| H | 9.81512000 | 1.73106000 | 3.42262600 |
| H | 8.15071800 | 2.11177300 | 3.95704000 |
| O | 8.11296300 | 4.58994000 | 0.89420900 |
| C | 9.10219500 | 1.60620300 | -0.35063800 |
| C | 10.14641200 | 0.77990600 | -1.04517600 |
| H | 10.77257200 | 1.46900700 | -1.62383900 |
| H | 10.77473400 | 0.32725200 | -0.27497200 |
| C | 9.51418500 | -0.28289800 | -1.94545400 |
| H | 9.01892800 | 0.19510200 | -2.79569400 |

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|---|-------------|-------------|-------------|
| H | 8.71790300 | -0.78603300 | -1.39507200 |
| C | 10.52546000 | -1.31955700 | -2.42503400 |
| H | 11.25776700 | -0.85229100 | -3.09442900 |
| H | 11.09743900 | -1.68938600 | -1.56359900 |
| C | 9.85195200 | -2.49729800 | -3.12560400 |
| H | 9.23126600 | -2.15480300 | -3.95948500 |
| H | 9.19866700 | -3.03804900 | -2.43184400 |
| O | 9.42444300 | 1.80262000 | 0.93132300 |
| O | 8.08571000 | 2.02879100 | -0.86372600 |
| O | 8.34234600 | 0.31686000 | 3.04397800 |
| O | 8.97513600 | -2.04302500 | 3.36753800 |
| O | 10.73840800 | -0.48008100 | 2.31065100 |
| O | 8.55836200 | -1.16323900 | 1.04614700 |
| C | 9.83995100 | -3.18398000 | 3.28721300 |
| H | 10.87255800 | -2.84565700 | 3.14872600 |
| H | 9.76524000 | -3.68970900 | 4.25176600 |
| C | 9.41112100 | -4.14150900 | 2.18732600 |
| H | 8.36231000 | -4.41076700 | 2.33520300 |
| H | 10.00523300 | -5.06020600 | 2.28571100 |
| N | 9.54715500 | -3.54561800 | 0.84402800 |
| H | 10.52760900 | -3.42719900 | 0.59833700 |
| H | 9.11130900 | -4.13852200 | 0.13433000 |
| P | 9.29980700 | -0.78985600 | 2.41121400 |
| H | 8.88549900 | -2.13188700 | 0.80875300 |
| O | 6.21633400 | 0.16550900 | 0.53605200 |
| H | 7.01153500 | -0.41139500 | 0.61244800 |

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|---|-------------|-------------|-------------|
| H | 3.72460700 | 7.11642000 | -2.47847600 |
| H | 10.58589500 | -3.20569000 | -3.52160000 |

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|---|-------------|------------|-------------|
| C | -7.81454200 | 4.00076200 | -0.27901000 |
| H | -8.41722100 | 3.62544900 | -1.12551800 |
| C | -7.24719100 | 5.34391300 | -0.70747700 |
| H | -6.61312900 | 5.72017800 | 0.10336300 |
| C | -6.40142000 | 5.16882200 | -1.97898800 |
| H | -7.08536400 | 4.82987900 | -2.77600900 |
| C | -5.87556800 | 2.93536600 | -1.39435100 |
| H | -6.52434500 | 2.53698000 | -2.18866700 |
| C | -6.65513700 | 3.03269800 | -0.09381900 |
| H | -7.04265200 | 2.03414100 | 0.13405100 |
| C | -5.72099000 | 6.45198700 | -2.40617000 |
| H | -5.04795100 | 6.79861900 | -1.61692100 |
| H | -6.46255900 | 7.22667900 | -2.61547700 |
| H | -5.13124500 | 6.28512500 | -3.30959000 |
| C | -4.06505900 | 1.66167000 | -2.29919100 |
| H | -3.97994400 | 2.50298600 | -2.99676200 |
| C | -2.70366700 | 1.27447500 | -1.81455400 |
| H | -2.65499200 | 0.45075700 | -1.10624900 |
| C | -1.58359400 | 1.89203200 | -2.20262900 |

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|---|-------------|------------|-------------|
| H | -1.63934400 | 2.73182700 | -2.89467400 |
| C | -0.27337800 | 1.51382700 | -1.71582600 |
| H | -0.23749400 | 0.63122300 | -1.08364500 |
| C | 0.87039300 | 2.18081000 | -1.96146600 |
| H | 0.85044800 | 3.07175600 | -2.58845000 |
| C | 2.13451500 | 1.78258300 | -1.39076800 |
| H | 2.11539700 | 0.87996200 | -0.78510400 |
| C | 3.30577900 | 2.43248700 | -1.54257000 |
| H | 3.35351700 | 3.33653400 | -2.14867000 |
| C | 4.52106900 | 1.98355000 | -0.90996400 |
| H | 4.45324300 | 1.07215800 | -0.31566200 |
| C | 5.71835200 | 2.59738700 | -1.00207100 |
| H | 5.81293800 | 3.50059800 | -1.60384200 |
| C | 6.89765500 | 2.13010000 | -0.31751700 |
| H | 6.78417100 | 1.24255700 | 0.30511400 |
| C | 8.11188100 | 2.71119300 | -0.39387300 |
| H | 8.24558800 | 3.58616200 | -1.02898700 |
| C | 9.26335600 | 2.23840500 | 0.33552400 |
| H | 9.09866200 | 1.40796300 | 1.01997200 |
| C | 10.50969700 | 2.73240900 | 0.22089100 |
| H | 10.70455600 | 3.54543800 | -0.47752000 |
| C | -4.81579800 | 0.51204100 | -2.98176100 |
| H | -5.81417900 | 0.86292800 | -3.24669800 |
| H | -4.30190500 | 0.25070300 | -3.91190300 |
| C | 11.63479100 | 2.19775800 | 0.96294700 |
| H | 11.38601600 | 1.46471300 | 1.72769100 |

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| C | 12.91916700 | 2.49423200 | 0.73746600 |
| H | 13.17026500 | 3.21634000 | -0.04126900 |
| C | 14.08015600 | 1.86356900 | 1.45217200 |
| H | 13.70230100 | 1.28131500 | 2.30040200 |
| C | 14.83617400 | 0.88638300 | 0.53069500 |
| H | 15.33389400 | 1.48931700 | -0.24702700 |
| C | 13.94712100 | -0.13212800 | -0.20750400 |
| H | 13.23598600 | 0.46045400 | -0.79134000 |
| C | 13.08757900 | -0.98172900 | 0.73516100 |
| H | 12.62080100 | -0.34491400 | 1.48151100 |
| C | 10.75777800 | -1.38179300 | 0.31378500 |
| C | 9.76878800 | -1.98669100 | -0.65046400 |
| H | 10.21494400 | -2.03515300 | -1.64556300 |
| H | 9.57802100 | -3.01424700 | -0.31958300 |
| C | 8.44307700 | -1.22224300 | -0.67656300 |
| H | 8.63066500 | -0.18710300 | -0.99627000 |
| C | 7.45439600 | -1.87258800 | -1.63330500 |
| H | 7.88443000 | -1.86396500 | -2.64064000 |
| H | 7.31150400 | -2.92009400 | -1.34184500 |
| C | 6.08684900 | -1.19537300 | -1.67399500 |
| H | 6.21499600 | -0.12097100 | -1.86377200 |
| C | 5.20718100 | -1.78774400 | -2.77068600 |
| H | 5.25900800 | -2.88195300 | -2.71406100 |
| H | 5.64457900 | -1.50269400 | -3.73230800 |
| C | 3.74167900 | -1.33052800 | -2.69457300 |
| H | 3.66343600 | -0.40755600 | -2.11542800 |

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| H | 3.36833200 | -1.09390800 | -3.69563200 |
| C | 2.79907200 | -2.37738900 | -2.10232200 |
| H | 2.73289300 | -3.22241600 | -2.80141800 |
| C | 1.37925000 | -1.80003600 | -1.88872900 |
| H | 1.20555500 | -0.97161300 | -2.58510600 |
| C | 0.27395300 | -2.83814300 | -2.05812900 |
| H | 0.44764900 | -3.66703000 | -1.36127300 |
| H | 0.32645000 | -3.24334600 | -3.07546900 |
| C | -1.11820900 | -2.25559600 | -1.82255700 |
| H | -1.26265500 | -1.38913600 | -2.48303300 |
| C | -2.22281600 | -3.26531600 | -2.11865400 |
| H | -2.05497900 | -4.17802200 | -1.53865200 |
| H | -2.18522700 | -3.52150000 | -3.18199300 |
| C | -3.62045800 | -2.75035700 | -1.77437600 |
| C | -4.75356900 | -3.65006500 | -2.25094800 |
| H | -4.67636900 | -4.63954500 | -1.79339500 |
| H | -4.70268400 | -3.76186400 | -3.33732700 |
| C | -6.07742700 | -3.01882900 | -1.85774500 |
| H | -6.11509100 | -2.96416400 | -0.76855000 |
| C | -6.18931500 | -1.57725300 | -2.39994100 |
| H | -6.35955400 | -1.64776000 | -3.48338200 |
| C | -4.91042000 | -0.75206500 | -2.12862000 |
| H | -4.90152600 | -0.48974900 | -1.06601300 |
| C | -7.36784200 | -0.84860200 | -1.77755800 |
| C | 13.77493000 | -2.14511900 | 1.42007500 |
| H | 13.08409600 | -2.63441400 | 2.11049900 |

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| H | 14.63566900 | -1.77112700 | 1.97605000 |
| H | 14.11638000 | -2.88498400 | 0.69291500 |
| C | 14.76220800 | -0.97999800 | -1.18264800 |
| H | 15.54247200 | -1.55348700 | -0.67308500 |
| H | 15.24353200 | -0.34827600 | -1.93486700 |
| H | 14.12014400 | -1.69391800 | -1.70334000 |
| C | 15.04221500 | 2.92380500 | 1.99545100 |
| H | 15.42544800 | 3.54950800 | 1.18168700 |
| H | 15.89085900 | 2.45090600 | 2.49151000 |
| H | 14.53298400 | 3.57733500 | 2.70737300 |
| O | -5.80821000 | 3.51007500 | 0.93567400 |
| H | -4.91635800 | 3.17501700 | 0.75649600 |
| O | -8.34475100 | 6.21544700 | -0.96034300 |
| H | -8.04933400 | 7.12103900 | -0.82337900 |
| O | -5.37731000 | 4.20496700 | -1.77842900 |
| O | -4.79387100 | 2.10397400 | -1.14351900 |
| O | -3.79284300 | -2.61683100 | -0.39646500 |
| H | -3.08923200 | -2.03094400 | -0.06418800 |
| O | -3.74399800 | -1.50298800 | -2.44436900 |
| O | -7.38545500 | 0.31031400 | -1.44899900 |
| O | -1.25628000 | -1.82560100 | -0.46828400 |
| H | -0.39568300 | -1.46023000 | -0.19322600 |
| O | 1.33792100 | -1.23458400 | -0.57691700 |
| H | 1.96414300 | -1.79263700 | -0.07210600 |
| O | 3.23596400 | -2.88795600 | -0.85072900 |
| H | 4.05332200 | -2.41871300 | -0.57849400 |

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| O | 5.40264000 | -1.35161900 | -0.42696800 |
| H | 6.06761000 | -1.28584600 | 0.28237300 |
| O | 7.84662200 | -1.21273200 | 0.61764700 |
| H | 8.53962300 | -0.95318000 | 1.25053400 |
| O | 10.42598000 | -0.84157500 | 1.35707400 |
| O | 12.01081200 | -1.52316400 | -0.09295200 |
| O | 15.81836100 | 0.25037500 | 1.34332400 |
| H | 16.48682500 | -0.14115900 | 0.77101800 |
| O | -7.11976300 | -3.86299700 | -2.34730500 |
| H | -7.93039100 | -3.33701500 | -2.30764200 |
| N | -8.59537300 | 4.12884700 | 0.94348200 |
| H | -9.16705800 | 3.29759500 | 1.06333300 |
| H | -9.23125400 | 4.91304200 | 0.83005600 |
| C | 1.96631200 | -0.08458500 | 2.30678100 |
| H | 2.34751300 | 0.10910800 | 3.31425200 |
| H | 1.59396200 | -1.11484000 | 2.29106400 |
| C | 0.85701800 | 0.89254800 | 1.93277400 |
| H | 0.54649800 | 0.69605700 | 0.90433800 |
| H | 1.24400800 | 1.91891700 | 1.94077600 |
| C | -0.35847700 | 0.78456300 | 2.84643800 |
| H | -0.08704900 | 1.03939100 | 3.87685100 |
| H | -0.70238200 | -0.25374100 | 2.87755900 |
| C | -1.51714200 | 1.66138400 | 2.38988600 |
| H | -1.81779000 | 1.41966400 | 1.36404900 |
| H | -1.25360500 | 2.72471700 | 2.38711800 |
| C | -2.74557200 | 1.47016100 | 3.23506800 |

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| O | -2.85146900 | 0.68341500 | 4.14640700 |
| C | -5.04959500 | 2.04183200 | 3.38463400 |
| H | -4.95708000 | 1.68700700 | 4.41262700 |
| H | -5.55436300 | 3.00520500 | 3.33970200 |
| C | -5.80346500 | 1.03048500 | 2.53570100 |
| H | -5.55630100 | 1.18728500 | 1.48860500 |
| C | -7.30223200 | 1.12382900 | 2.72208700 |
| H | -7.60264400 | 0.79967500 | 3.72220700 |
| H | -7.62704400 | 2.14912600 | 2.53770300 |
| O | -3.74895600 | 2.27532600 | 2.82570800 |
| C | -4.42967300 | -0.86413800 | 2.17311200 |
| C | -4.10233100 | -2.25933600 | 2.61599200 |
| H | -4.56875100 | -2.45748500 | 3.58187600 |
| H | -4.57893900 | -2.90377900 | 1.87109700 |
| C | -2.58811200 | -2.49485500 | 2.62375000 |
| H | -2.17196700 | -2.14454100 | 3.57467900 |
| H | -2.13753300 | -1.87417200 | 1.84545500 |
| C | -2.18952700 | -3.94243300 | 2.35958400 |
| H | -2.57525400 | -4.59477100 | 3.15296200 |
| H | -2.66543600 | -4.26073000 | 1.42498700 |
| C | -0.67661200 | -4.09572500 | 2.23490200 |
| H | -0.16635700 | -3.75387200 | 3.14163800 |
| H | -0.31243400 | -3.49539300 | 1.39534500 |
| O | -5.41829500 | -0.30720300 | 2.89052100 |
| O | -3.86751600 | -0.28810100 | 1.26335200 |
| O | -7.97214600 | 0.31468000 | 1.73433300 |

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| O | -9.50963900 | -1.45959100 | 0.99585100 |
| O | -8.48983400 | -1.64787400 | 3.37704600 |
| O | -7.07101000 | -1.98659500 | 1.20072900 |
| C | -10.25692300 | -2.67421400 | 1.18525900 |
| H | -10.15978300 | -2.99257600 | 2.22741900 |
| H | -11.30553100 | -2.43075300 | 0.99670200 |
| C | -9.80973600 | -3.76914200 | 0.22339600 |
| H | -9.92389200 | -3.40896400 | -0.80021400 |
| H | -10.49163000 | -4.62128600 | 0.34072900 |
| N | -8.40158600 | -4.15035400 | 0.41491100 |
| H | -8.30973900 | -4.87843900 | 1.11667400 |
| H | -7.99151600 | -4.48584800 | -0.45721000 |
| P | -8.21959900 | -1.23608000 | 1.98860000 |
| H | -7.46186900 | -2.87278000 | 0.87952100 |
| O | -8.44985500 | -1.63934200 | -1.59037400 |
| H | -9.02439300 | -1.21358800 | -0.92057800 |
| H | -0.38452500 | -5.13513800 | 2.05926500 |
| H | 2.80854900 | -0.02112700 | 1.61078200 |

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|---|-------------|-------------|------------|
| C | 10.50039000 | -2.98146200 | 2.35016800 |
| H | 11.06849000 | -2.08715700 | 2.06241600 |
| C | 10.93953300 | -4.10386100 | 1.40922300 |

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| H | 10.40676300 | -5.02337500 | 1.69798700 |
| C | 10.55020900 | -3.77984600 | -0.02781900 |
| H | 11.04914300 | -2.84589100 | -0.33142800 |
| C | 8.70202700 | -2.50427300 | 0.69376700 |
| H | 9.20345400 | -1.58749200 | 0.33795600 |
| C | 9.01270000 | -2.68664800 | 2.17832900 |
| H | 8.74990300 | -1.74860100 | 2.69478700 |
| C | 10.89959200 | -4.88401700 | -0.99761100 |
| H | 10.35995700 | -5.79698000 | -0.73169700 |
| H | 11.97146100 | -5.08302900 | -0.95400200 |
| H | 10.62433300 | -4.59726100 | -2.01454700 |
| C | 6.72762100 | -2.47285900 | -0.72006700 |
| H | 6.80218800 | -3.50674300 | -1.07212100 |
| C | 5.29673500 | -2.09081400 | -0.50908400 |
| H | 5.12194700 | -1.09160900 | -0.12235100 |
| C | 4.25019500 | -2.88303400 | -0.75789600 |
| H | 4.40808000 | -3.89036300 | -1.14262100 |
| C | 2.88300100 | -2.46021800 | -0.52097100 |
| H | 2.75331900 | -1.44198800 | -0.16025700 |
| C | 1.79642800 | -3.23321900 | -0.70102100 |
| H | 1.91651700 | -4.25536700 | -1.05943000 |
| C | 0.45478200 | -2.77546100 | -0.42650900 |
| H | 0.35303700 | -1.74265800 | -0.09559600 |
| C | -0.65448900 | -3.52984400 | -0.56145900 |
| H | -0.56401900 | -4.56186600 | -0.89912200 |
| C | -1.97932200 | -3.04308100 | -0.26869400 |

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| H | -2.05905600 | -2.00602600 | 0.05560700 |
| C | -3.10599500 | -3.77765800 | -0.36989800 |
| H | -3.03998200 | -4.81110000 | -0.70845900 |
| C | -4.41205300 | -3.27642400 | -0.02247300 |
| H | -4.46501200 | -2.25175600 | 0.34392200 |
| C | -5.55871900 | -3.97900000 | -0.11925800 |
| H | -5.53484100 | -4.99441500 | -0.51320600 |
| C | -6.83794400 | -3.44906800 | 0.28655600 |
| H | -6.82627900 | -2.46997900 | 0.76043600 |
| C | -8.02723500 | -4.05391500 | 0.11448100 |
| H | -8.07553200 | -5.02167800 | -0.38330400 |
| C | 7.46181700 | -1.57013500 | -1.71819300 |
| H | 8.48240300 | -1.93456400 | -1.83611500 |
| H | 6.97451500 | -1.66018800 | -2.69272200 |
| C | -9.27571100 | -3.44306200 | 0.53009000 |
| H | -9.17838100 | -2.53937300 | 1.12767700 |
| C | -10.49662400 | -3.86704000 | 0.18787900 |
| H | -10.59837200 | -4.76062100 | -0.43019700 |
| C | -11.77551600 | -3.16924200 | 0.55555700 |
| H | -11.55832500 | -2.40140300 | 1.30692500 |
| C | -12.38853800 | -2.45566900 | -0.66490100 |
| H | -12.70114800 | -3.23894000 | -1.37578700 |
| C | -11.42516200 | -1.52970500 | -1.43167700 |
| H | -10.58073100 | -2.15897400 | -1.72953900 |
| C | -10.81819800 | -0.42196000 | -0.56136900 |
| H | -10.45482400 | -0.84514100 | 0.37183600 |

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| C | -8.46275000 | 0.03629000 | -0.70390400 |
| C | -7.36076800 | 0.57714500 | -1.57202000 |
| H | -7.67087600 | 0.54971600 | -2.61815300 |
| H | -7.19231600 | 1.62343600 | -1.28815800 |
| C | -6.05123900 | -0.18760300 | -1.36527900 |
| H | -6.21610800 | -1.25773300 | -1.55863400 |
| C | -4.96635100 | 0.32677100 | -2.29654400 |
| H | -5.27001100 | 0.11390300 | -3.32707300 |
| H | -4.88225100 | 1.41418200 | -2.18915200 |
| C | -3.59745600 | -0.29224600 | -2.03214900 |
| H | -3.70352000 | -1.37226200 | -1.86631900 |
| C | -2.64195500 | -0.07691800 | -3.20246900 |
| H | -2.71007900 | 0.96568900 | -3.53162000 |
| H | -3.00256100 | -0.69644900 | -4.02890000 |
| C | -1.18389100 | -0.42306300 | -2.86334400 |
| H | -1.14904600 | -1.05740100 | -1.97507600 |
| H | -0.72291000 | -1.00274600 | -3.66874100 |
| C | -0.31801800 | 0.81448300 | -2.62657400 |
| H | -0.09875500 | 1.28780500 | -3.59061000 |
| C | 1.01590900 | 0.46693300 | -1.92805600 |
| H | 1.29101700 | -0.57077400 | -2.14568500 |
| C | 2.14839300 | 1.40039600 | -2.33403700 |
| H | 1.89320900 | 2.42888500 | -2.06331000 |
| H | 2.25985900 | 1.36359400 | -3.42402000 |
| C | 3.49301400 | 1.02864100 | -1.71774400 |
| H | 3.80738400 | 0.04574900 | -2.09060900 |

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| C | 4.56570700 | 2.05864600 | -2.06453800 |
| H | 4.22567900 | 3.04661500 | -1.74173100 |
| H | 4.69664600 | 2.07919500 | -3.15032200 |
| C | 5.91523600 | 1.74982400 | -1.42288500 |
| C | 7.02706600 | 2.69995000 | -1.85377400 |
| H | 6.83440700 | 3.70287100 | -1.46664900 |
| H | 7.04785700 | 2.75547400 | -2.94591500 |
| C | 8.37864900 | 2.21069400 | -1.36158300 |
| H | 8.37626000 | 2.22139900 | -0.26454300 |
| C | 8.60874200 | 0.76463100 | -1.82524700 |
| H | 8.59887100 | 0.72673800 | -2.91898000 |
| C | 7.43797900 | -0.10377200 | -1.31163500 |
| H | 7.41240900 | -0.02761100 | -0.21743300 |
| C | 9.94530400 | 0.21034900 | -1.40095900 |
| C | -11.69986300 | 0.77621600 | -0.27354000 |
| H | -11.18099500 | 1.47600200 | 0.38524600 |
| H | -12.61587500 | 0.43631400 | 0.21098500 |
| H | -11.95895700 | 1.30277500 | -1.19446200 |
| C | -12.07287600 | -0.98419300 | -2.70367700 |
| H | -12.97275100 | -0.39993400 | -2.48822000 |
| H | -12.35345700 | -1.80092600 | -3.37490300 |
| H | -11.38094400 | -0.33030600 | -3.23898600 |
| C | -12.78738100 | -4.14948600 | 1.15588900 |
| H | -13.01698900 | -4.95000700 | 0.44379300 |
| H | -13.71727600 | -3.63614300 | 1.40309200 |
| H | -12.38451900 | -4.61238700 | 2.05966000 |

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| O | 8.28712300 | -3.77108300 | 2.71000100 |
| H | 7.42260400 | -3.75254500 | 2.27414400 |
| O | 12.33641100 | -4.26556500 | 1.48654700 |
| H | 12.53252500 | -4.20477200 | 2.43525200 |
| O | 9.13368200 | -3.59584300 | -0.07403800 |
| O | 7.31759200 | -2.39892100 | 0.59742200 |
| O | 5.83680600 | 1.79724000 | -0.01104300 |
| H | 4.98293000 | 1.35819500 | 0.20184300 |
| O | 6.23471100 | 0.43202700 | -1.84107800 |
| O | 10.50845400 | -0.72881100 | -1.90927300 |
| O | 3.41551300 | 0.93183900 | -0.28515400 |
| H | 2.47350800 | 0.90615800 | -0.02676500 |
| O | 0.80837400 | 0.51920100 | -0.50914100 |
| H | 0.26105400 | 1.31023600 | -0.34414700 |
| O | -0.99156100 | 1.79502600 | -1.85116300 |
| H | -1.63176400 | 1.33044800 | -1.27484000 |
| O | -3.01429100 | 0.28555300 | -0.85514100 |
| H | -3.70751100 | 0.32524600 | -0.17623800 |
| O | -5.59039600 | -0.03956800 | -0.02115800 |
| H | -6.35873700 | -0.21277500 | 0.55054600 |
| O | -8.26664800 | -0.36731300 | 0.43443200 |
| O | -9.64883200 | 0.06501900 | -1.29179100 |
| O | -13.53592900 | -1.75954200 | -0.18800100 |
| H | -14.08992000 | -1.52557500 | -0.94040700 |
| O | 9.36887900 | 3.08613900 | -1.86759600 |
| H | 10.17269300 | 2.92708900 | -1.35805600 |

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|---|-------------|-------------|-------------|
| N | 10.90247700 | -3.35267100 | 3.70274300 |
| H | 10.22957800 | -4.02811800 | 4.05843300 |
| H | 10.87041200 | -2.55040000 | 4.32368000 |
| C | -9.41215100 | 1.44096100 | 3.11711500 |
| H | -9.82809400 | 2.45355200 | 3.13465700 |
| H | -9.73062000 | 0.95695100 | 2.18993900 |
| C | -7.88994500 | 1.46621600 | 3.19594900 |
| H | -7.51248900 | 0.43761700 | 3.14340000 |
| H | -7.56840200 | 1.86432400 | 4.16615600 |
| C | -7.26082400 | 2.28243900 | 2.07151800 |
| H | -7.59871000 | 3.32335400 | 2.12503800 |
| H | -7.60891100 | 1.89922300 | 1.11183100 |
| C | -5.74099900 | 2.23871200 | 2.09797200 |
| H | -5.37618700 | 1.21026500 | 2.19463400 |
| H | -5.33239100 | 2.77687500 | 2.95907300 |
| C | -5.10221100 | 2.80217500 | 0.85607100 |
| O | -5.67110400 | 3.15290400 | -0.15348700 |
| C | -3.01824000 | 3.51434000 | -0.02322600 |
| H | -2.93653800 | 2.84819600 | -0.88149500 |
| H | -3.52601800 | 4.42987300 | -0.33839500 |
| C | -1.67454300 | 3.83034600 | 0.59718400 |
| H | -1.82692400 | 4.42114300 | 1.50241200 |
| C | -0.73821800 | 4.58160500 | -0.32335400 |
| H | -0.38800700 | 3.93789400 | -1.13259500 |
| H | -1.24687600 | 5.44946900 | -0.75186200 |
| O | -3.77257900 | 2.87802600 | 1.01449100 |

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|---|-------------|-------------|-------------|
| C | -0.79990700 | 2.40846700 | 2.30562400 |
| C | -0.35210800 | 1.00054200 | 2.57301000 |
| H | 0.37292600 | 0.68198900 | 1.82218200 |
| H | 0.12804100 | 0.99767400 | 3.55344800 |
| C | -1.56603100 | 0.06058100 | 2.57283900 |
| H | -2.02124700 | 0.06742100 | 1.57605200 |
| H | -2.31792100 | 0.45589600 | 3.26715600 |
| C | -1.20637700 | -1.36760700 | 2.97381600 |
| H | -0.56749100 | -1.81441300 | 2.20356500 |
| H | -0.60827200 | -1.34344700 | 3.89290500 |
| C | -2.43818700 | -2.23895800 | 3.19631500 |
| H | -3.06521500 | -2.27915300 | 2.30248100 |
| H | -3.04992200 | -1.84741300 | 4.01545700 |
| O | -1.04991800 | 2.59606100 | 0.97909300 |
| O | -1.00018500 | 3.24598700 | 3.14577900 |
| O | 0.34636200 | 5.07899700 | 0.46675000 |
| O | 2.60260200 | 5.65882900 | 1.11218800 |
| O | 2.28563800 | 4.35714900 | -1.10839300 |
| O | 1.90530700 | 3.21619700 | 1.18952600 |
| C | 4.02727600 | 5.73126900 | 1.03103800 |
| H | 4.36388000 | 5.38976100 | 0.04535100 |
| H | 4.29039900 | 6.78599500 | 1.13697600 |
| C | 4.67230400 | 4.92558200 | 2.14538000 |
| H | 4.21947600 | 5.23111200 | 3.09212600 |
| H | 5.74101800 | 5.17797800 | 2.18525900 |
| N | 4.44439300 | 3.48684300 | 1.95721300 |

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|---|-------------|-------------|-------------|
| H | 5.02621100 | 3.12981200 | 1.19529900 |
| H | 4.71634300 | 2.97582100 | 2.79186700 |
| P | 1.82440300 | 4.51884500 | 0.28959300 |
| H | 2.86027000 | 3.15891800 | 1.55023000 |
| O | 10.47923300 | 0.85192700 | -0.33197700 |
| H | 11.31937500 | 0.40283200 | -0.14260000 |
| H | -9.84906300 | 0.88613100 | 3.95163100 |
| H | -2.16138200 | -3.26668500 | 3.44482700 |

AmB-Chol

AmB-Chol1

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|---|-------------|------------|-------------|
| C | -4.60837300 | 2.60968700 | -0.67585700 |
| C | -3.36317100 | 2.86117000 | -1.50973000 |
| C | -2.24901800 | 3.64141600 | -0.79410000 |
| C | -4.22949000 | 1.89309600 | 0.64920100 |
| C | -2.74465300 | 1.91836900 | 0.91580600 |
| C | -2.08160100 | 0.80845500 | 1.23231000 |
| C | -0.59653000 | 0.73037000 | 1.41158300 |
| C | 0.12161700 | 1.92025100 | 0.77579700 |
| C | 1.58372600 | 1.97165600 | 1.21072600 |
| C | 2.45414600 | 0.75846800 | 0.90377200 |
| C | 3.89990700 | 1.28845300 | 1.01654000 |

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|---|-------------|------------|-------------|
| C | 3.83708500 | 2.84531600 | 1.14469000 |
| C | 4.23883800 | 3.39286900 | 2.53866000 |
| C | 5.44430600 | 2.66139200 | 3.16790600 |
| C | 6.69605600 | 2.58590000 | 2.29230300 |
| C | 7.87620200 | 1.93149100 | 3.00633600 |
| C | 9.12145900 | 1.74613000 | 2.13277500 |
| C | 9.66035600 | 3.07279100 | 1.59550200 |
| C | 10.21336500 | 0.99789400 | 2.89605300 |
| C | 4.55631000 | 4.89413400 | 2.47960300 |
| C | 2.38445900 | 3.15974700 | 0.64566800 |
| C | 2.43820000 | 3.14778800 | -0.89462500 |
| C | 1.68658100 | 4.43909100 | 1.12203700 |
| C | 0.20918600 | 4.46690100 | 0.70728900 |
| C | -0.58759600 | 3.23151700 | 1.16009400 |
| C | -2.07734000 | 3.26959100 | 0.71174200 |
| C | -2.81451500 | 4.31467700 | 1.57622200 |
| O | -5.26764300 | 3.85259400 | -0.44704300 |
| H | -0.60165600 | 3.24685200 | 2.26158400 |
| H | 0.07078100 | 1.79106800 | -0.31390600 |
| H | 1.57780600 | 2.10426200 | 2.30467500 |
| H | -5.28249500 | 1.96101800 | -1.24177500 |
| H | -3.64926300 | 3.37745600 | -2.43116900 |
| H | -2.97636600 | 1.87922700 | -1.79795500 |
| H | -2.43132600 | 4.71689000 | -0.87626900 |
| H | -1.31837800 | 3.44058500 | -1.33408500 |
| H | -4.57238900 | 0.85481000 | 0.61945400 |

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|---|-------------|-------------|-------------|
| H | -4.76370100 | 2.38970500 | 1.46804800 |
| H | -2.64581400 | -0.11246900 | 1.35282300 |
| H | -0.22586000 | -0.20293700 | 0.97290600 |
| H | -0.34480700 | 0.68147000 | 2.48221000 |
| H | 2.24229900 | 0.40440800 | -0.10644900 |
| H | 2.25873400 | -0.07723500 | 1.58140200 |
| H | 4.48070100 | 1.01548900 | 0.13343100 |
| H | 4.40696300 | 0.83182300 | 1.86565600 |
| H | 4.54878500 | 3.28209600 | 0.43458100 |
| H | 3.39564100 | 3.25115000 | 3.22823900 |
| H | 5.70048600 | 3.17962100 | 4.10066700 |
| H | 5.16104700 | 1.64822100 | 3.47201700 |
| H | 6.97599500 | 3.59331800 | 1.97052600 |
| H | 6.48143600 | 2.02179600 | 1.37679900 |
| H | 7.56362300 | 0.94686800 | 3.37790200 |
| H | 8.14373600 | 2.52394900 | 3.89275800 |
| H | 8.81691300 | 1.12439200 | 1.28200500 |
| H | 9.86855100 | 3.76411000 | 2.41996600 |
| H | 8.95377900 | 3.55953300 | 0.91921500 |
| H | 10.59476700 | 2.92606900 | 1.04580800 |
| H | 10.56213600 | 1.58833700 | 3.75044000 |
| H | 11.08033400 | 0.79342600 | 2.25915800 |
| H | 9.84368500 | 0.04290200 | 3.28131800 |
| H | 5.37617000 | 5.09149400 | 1.78227000 |
| H | 4.86385300 | 5.26265200 | 3.46308400 |
| H | 3.70831500 | 5.49290500 | 2.15508600 |

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|---|--------------|-------------|-------------|
| H | 2.97775800 | 2.28126700 | -1.28332000 |
| H | 2.96299400 | 4.04168800 | -1.24687500 |
| H | 1.44990700 | 3.14229800 | -1.35618400 |
| H | 2.18187800 | 5.33011400 | 0.72119800 |
| H | 1.74395500 | 4.50190600 | 2.21440500 |
| H | 0.14713700 | 4.57127600 | -0.37855800 |
| H | -0.24845000 | 5.37125600 | 1.11818800 |
| H | -2.29642100 | 5.27624600 | 1.53902500 |
| H | -2.85492500 | 3.99327100 | 2.62227300 |
| H | -3.82905900 | 4.47836400 | 1.21265200 |
| H | -6.09527800 | 3.62942200 | 0.00798300 |
| C | -9.44790800 | 3.39264400 | 0.01061200 |
| H | -10.40566500 | 3.06221800 | -0.41030400 |
| C | -8.74599200 | 4.19764600 | -1.08271900 |
| H | -7.80673100 | 4.60627600 | -0.68207400 |
| C | -8.39557900 | 3.31554400 | -2.27692000 |
| H | -9.34037700 | 2.98216800 | -2.73761600 |
| C | -8.28898800 | 1.37419400 | -0.88455700 |
| H | -9.20636800 | 0.93553900 | -1.31677100 |
| C | -8.64387300 | 2.15220100 | 0.37770200 |
| H | -9.22802600 | 1.48804400 | 1.02853100 |
| C | -7.53026500 | 4.04336400 | -3.28136900 |
| H | -6.58388800 | 4.30414700 | -2.79936100 |
| H | -8.03348600 | 4.95363600 | -3.61161200 |
| H | -7.32482300 | 3.40685800 | -4.14488000 |
| C | -7.08374500 | -0.61270600 | -1.48058000 |

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|---|-------------|-------------|-------------|
| H | -7.24607700 | -0.18764500 | -2.47643300 |
| C | -5.63284600 | -0.91728200 | -1.30082100 |
| H | -5.33559200 | -1.25292900 | -0.31139900 |
| C | -4.70509900 | -0.73819500 | -2.24552300 |
| H | -4.99237900 | -0.39774200 | -3.23965200 |
| C | -3.29530200 | -0.90926700 | -1.96951800 |
| H | -3.03851100 | -1.18619000 | -0.95112200 |
| C | -2.29168300 | -0.67228300 | -2.83457900 |
| H | -2.50970300 | -0.37272900 | -3.85884900 |
| C | -0.91359600 | -0.74603400 | -2.41821500 |
| H | -0.75704000 | -1.03539900 | -1.38064500 |
| C | 0.16426300 | -0.45923800 | -3.17580000 |
| H | 0.04331600 | -0.15239000 | -4.21360300 |
| C | 1.49288200 | -0.50291900 | -2.62222500 |
| H | 1.55912500 | -0.84323000 | -1.59011300 |
| C | 2.63373600 | -0.13544700 | -3.24105900 |
| H | 2.60891800 | 0.20384700 | -4.27549700 |
| C | 3.89895100 | -0.11256000 | -2.55041400 |
| H | 3.87788100 | -0.41449200 | -1.50430400 |
| C | 5.07921000 | 0.28455800 | -3.06805200 |
| H | 5.14036500 | 0.58091000 | -4.11417400 |
| C | 6.27974500 | 0.36274600 | -2.27161600 |
| H | 6.16437200 | 0.14759200 | -1.21063000 |
| C | 7.51131800 | 0.67653100 | -2.71325900 |
| H | 7.67956500 | 0.87588000 | -3.77058400 |
| C | -8.02651700 | -1.79721000 | -1.25720600 |

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| H | -9.04591500 | -1.45077100 | -1.44163200 |
| H | -7.80477300 | -2.59127900 | -1.97690900 |
| C | 8.64633600 | 0.73114900 | -1.81295300 |
| H | 8.39917700 | 0.64089800 | -0.75830000 |
| C | 9.93262200 | 0.83660600 | -2.16176300 |
| H | 10.20262700 | 0.91151400 | -3.21613400 |
| C | 11.06690200 | 0.82721600 | -1.17542600 |
| H | 10.65477200 | 0.96685900 | -0.17171500 |
| C | 11.80997900 | -0.52195800 | -1.17054700 |
| H | 12.31933500 | -0.62187200 | -2.14338400 |
| C | 10.90754000 | -1.75983500 | -1.01284500 |
| H | 10.15049300 | -1.68121700 | -1.79830200 |
| C | 10.12751400 | -1.77142900 | 0.30892900 |
| H | 9.72162100 | -0.78325700 | 0.51028300 |
| C | 7.76392000 | -2.22888500 | 0.32610600 |
| C | 6.72679200 | -3.30419500 | 0.11745200 |
| H | 7.12372100 | -4.06440600 | -0.55792300 |
| H | 6.55661100 | -3.77905600 | 1.09081900 |
| C | 5.39903900 | -2.74799600 | -0.39909500 |
| H | 5.56508500 | -2.27038000 | -1.37559800 |
| C | 4.36303500 | -3.85420300 | -0.55182600 |
| H | 4.73004500 | -4.58031900 | -1.28517100 |
| H | 4.25332200 | -4.37579700 | 0.40650800 |
| C | 2.98495800 | -3.36167700 | -0.98674300 |
| H | 3.08350500 | -2.74927100 | -1.89340500 |
| C | 2.03737100 | -4.52361600 | -1.28068600 |

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|---|-------------|-------------|-------------|
| H | 2.14300600 | -5.27831100 | -0.49226000 |
| H | 2.36911500 | -4.99274700 | -2.21162700 |
| C | 0.56519900 | -4.09182200 | -1.39068200 |
| H | 0.50334400 | -3.02563500 | -1.62066100 |
| H | 0.07809200 | -4.61154000 | -2.22135800 |
| C | -0.25631400 | -4.38776800 | -0.13324300 |
| H | -0.41812900 | -5.47169800 | -0.06740000 |
| C | -1.63272200 | -3.68005000 | -0.17422800 |
| H | -1.94264200 | -3.51624200 | -1.21251600 |
| C | -2.72455100 | -4.44562300 | 0.56931200 |
| H | -2.39429500 | -4.62912900 | 1.59890800 |
| H | -2.86118500 | -5.42066300 | 0.08746100 |
| C | -4.06245400 | -3.70687000 | 0.59150600 |
| H | -4.36452000 | -3.47247300 | -0.43850300 |
| C | -5.16626200 | -4.53713000 | 1.23871800 |
| H | -4.83985100 | -4.88173600 | 2.22489300 |
| H | -5.35273600 | -5.41598000 | 0.61465200 |
| C | -6.47759900 | -3.77196600 | 1.43035400 |
| C | -7.63046600 | -4.66632000 | 1.86298000 |
| H | -7.42567400 | -5.10760900 | 2.84066800 |
| H | -7.75101700 | -5.47415200 | 1.13580800 |
| C | -8.93460100 | -3.88856500 | 1.93466600 |
| H | -8.85668400 | -3.15198400 | 2.74704900 |
| C | -9.17924500 | -3.11981100 | 0.60693900 |
| H | -9.46622700 | -3.87063600 | -0.13922000 |
| C | -7.92226900 | -2.36510900 | 0.15196000 |

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|---|--------------|-------------|-------------|
| H | -7.75048600 | -1.54706700 | 0.85585900 |
| C | -10.32750500 | -2.15576000 | 0.77757900 |
| C | 10.86702000 | -2.27861400 | 1.53048900 |
| H | 10.22505700 | -2.20901000 | 2.41107300 |
| H | 11.75533600 | -1.66777100 | 1.69086100 |
| H | 11.16497100 | -3.32159400 | 1.40478800 |
| C | 11.68878700 | -3.05262900 | -1.24401300 |
| H | 12.52353000 | -3.15942200 | -0.54415300 |
| H | 12.09535100 | -3.08037500 | -2.25877700 |
| H | 11.04293300 | -3.92444800 | -1.11609000 |
| C | 12.04554200 | 1.97260400 | -1.44579300 |
| H | 12.47054300 | 1.88978100 | -2.45235400 |
| H | 12.86540000 | 1.95400700 | -0.72662300 |
| H | 11.53461800 | 2.93591500 | -1.37704500 |
| O | -7.45842100 | 2.57380100 | 1.03967600 |
| H | -6.89783600 | 1.78829500 | 1.12411300 |
| O | -9.59638300 | 5.23154700 | -1.52294200 |
| H | -9.96500700 | 5.60454800 | -0.70670200 |
| O | -7.64643300 | 2.18456300 | -1.83796000 |
| O | -7.38620000 | 0.39540300 | -0.49598000 |
| O | -6.35151500 | -2.76539400 | 2.39253700 |
| H | -5.49535600 | -2.33100200 | 2.22261200 |
| O | -6.79857900 | -3.23308900 | 0.15037500 |
| O | -10.28818300 | -0.95286200 | 0.66803400 |
| O | -11.48077000 | -2.78451800 | 1.11635100 |
| H | -12.14768700 | -2.08982900 | 1.24138200 |

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|---|--------------|-------------|-------------|
| O | -3.94291300 | -2.48279200 | 1.32235200 |
| H | -3.03940100 | -2.14827100 | 1.16740100 |
| O | -1.45573400 | -2.38224100 | 0.40135400 |
| H | -0.75348500 | -2.53532400 | 1.06657800 |
| O | 0.38518000 | -3.98574400 | 1.06988700 |
| H | 1.17678400 | -3.45008900 | 0.84246900 |
| O | 2.38830600 | -2.55632100 | 0.03485200 |
| H | 3.09248200 | -2.00919900 | 0.43060700 |
| O | 4.86945700 | -1.78769700 | 0.50979800 |
| H | 5.58201100 | -1.16477900 | 0.73728400 |
| O | 7.48696500 | -1.09532400 | 0.68703200 |
| O | 8.99145700 | -2.66941000 | 0.09898900 |
| O | 12.77916500 | -0.43589700 | -0.12859800 |
| H | 13.43681900 | -1.12766300 | -0.25830300 |
| O | -9.94871100 | -4.83486100 | 2.19343600 |
| H | -10.79778600 | -4.37542500 | 2.17835200 |
| N | -9.73369000 | 4.29903100 | 1.11764600 |
| H | -8.87914200 | 4.43570300 | 1.65240300 |
| H | -10.41602800 | 3.89401200 | 1.75040700 |

AmB-Chol2

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| C | 4.05152800 | -1.51997600 | -1.40991100 |
| C | 2.98183200 | -0.59413600 | -1.96720600 |

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|---|--------------|-------------|-------------|
| C | 1.91489600 | -1.33196300 | -2.78897200 |
| C | 3.40684000 | -2.60898800 | -0.51306900 |
| C | 1.90933900 | -2.66199100 | -0.69889100 |
| C | 1.08288400 | -2.57045800 | 0.34188500 |
| C | -0.40670500 | -2.44311200 | 0.22331100 |
| C | -0.82140000 | -1.98916200 | -1.17597700 |
| C | -2.33265600 | -2.03769200 | -1.36133200 |
| C | -3.15870200 | -1.15236200 | -0.43955900 |
| C | -4.51370800 | -1.00032500 | -1.15908100 |
| C | -4.36506600 | -1.57741200 | -2.60472900 |
| C | -5.20478400 | -2.85772200 | -2.84777300 |
| C | -6.63318300 | -2.75524800 | -2.25853200 |
| C | -7.39624800 | -1.48347800 | -2.63904000 |
| C | -8.81499100 | -1.43546700 | -2.07425300 |
| C | -9.52441900 | -0.09163300 | -2.28062100 |
| C | -9.83959700 | 0.17562800 | -3.75205500 |
| C | -10.79301500 | -0.01641400 | -1.43157400 |
| C | -5.31459600 | -3.19362700 | -4.34146600 |
| C | -2.80871500 | -1.66415700 | -2.77884800 |
| C | -2.35134700 | -0.25568700 | -3.20625000 |
| C | -2.19718900 | -2.69433200 | -3.73367800 |
| C | -0.66304600 | -2.69600800 | -3.64742800 |
| C | -0.10383000 | -2.86107700 | -2.22135800 |
| C | 1.43879800 | -2.67716800 | -2.14716500 |
| C | 2.10824400 | -3.85748400 | -2.87946700 |
| O | 4.76079100 | -2.05671800 | -2.52463000 |

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|---|-------------|-------------|-------------|
| H | -0.30496300 | -3.90190700 | -1.92337400 |
| H | -0.48894200 | -0.94775900 | -1.28547400 |
| H | -2.64592500 | -3.08202400 | -1.20197700 |
| H | 4.75183500 | -0.92898100 | -0.80554200 |
| H | 3.45500300 | 0.18140400 | -2.57746200 |
| H | 2.51249200 | -0.08991400 | -1.11638700 |
| H | 2.30163000 | -1.52671700 | -3.79273100 |
| H | 1.06647000 | -0.65188300 | -2.90807100 |
| H | 3.63305500 | -2.40628900 | 0.53687700 |
| H | 3.86972300 | -3.57386900 | -0.75405400 |
| H | 1.50264300 | -2.53465600 | 1.34500100 |
| H | -0.76700700 | -1.73216300 | 0.97437700 |
| H | -0.89451900 | -3.40088200 | 0.45849800 |
| H | -2.67035500 | -0.18424800 | -0.32447500 |
| H | -3.25937100 | -1.56422200 | 0.56839200 |
| H | -4.82207400 | 0.04604500 | -1.19333400 |
| H | -5.29007500 | -1.52274000 | -0.60800200 |
| H | -4.74144700 | -0.83767100 | -3.32086400 |
| H | -4.71589000 | -3.70158800 | -2.34153800 |
| H | -7.20368500 | -3.62632200 | -2.60651600 |
| H | -6.59826500 | -2.84378600 | -1.16865800 |
| H | -7.43072600 | -1.38537400 | -3.72910300 |
| H | -6.85525900 | -0.60515800 | -2.27133000 |
| H | -8.76891900 | -1.64036100 | -0.99831100 |
| H | -9.42499800 | -2.23740800 | -2.51408200 |
| H | -8.84103300 | 0.69312300 | -1.92997800 |

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| H | -10.50972000 | -0.59550500 | -4.14841300 |
| H | -8.93616700 | 0.18165200 | -4.36616000 |
| H | -10.33348300 | 1.14374700 | -3.88050300 |
| H | -11.48909200 | -0.82124400 | -1.69094400 |
| H | -11.32717900 | 0.92802800 | -1.59608500 |
| H | -10.55292400 | -0.10894800 | -0.36769700 |
| H | -5.77510100 | -2.36734100 | -4.89256400 |
| H | -5.94008000 | -4.07889400 | -4.49240400 |
| H | -4.35035700 | -3.39155100 | -4.80421800 |
| H | -2.81437700 | 0.52699300 | -2.60722100 |
| H | -2.64045200 | -0.08145200 | -4.24761700 |
| H | -1.27201800 | -0.11052500 | -3.13845900 |
| H | -2.48408000 | -2.49379400 | -4.77132600 |
| H | -2.57241000 | -3.69323600 | -3.48287500 |
| H | -0.28488300 | -1.77310500 | -4.09421400 |
| H | -0.28572000 | -3.50477200 | -4.27953900 |
| H | 1.73547600 | -3.93485700 | -3.90332700 |
| H | 1.89505700 | -4.80185100 | -2.36837100 |
| H | 3.18713600 | -3.72133800 | -2.94312800 |
| H | 5.40793400 | -2.68744600 | -2.18826500 |
| C | -8.44172800 | -2.58884800 | 2.12440300 |
| H | -9.29976200 | -1.91018000 | 2.21135100 |
| C | -8.11567900 | -3.08806500 | 3.53176700 |
| H | -7.26851300 | -3.78782300 | 3.46036400 |
| C | -7.68050200 | -1.92918200 | 4.42418800 |
| H | -8.52157000 | -1.21780400 | 4.48829800 |

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| C | -6.83242400 | -0.74264600 | 2.56741700 |
| H | -7.63024600 | 0.00889300 | 2.65581200 |
| C | -7.26152500 | -1.80569900 | 1.56564700 |
| H | -7.53909500 | -1.28360300 | 0.64207500 |
| C | -7.28155700 | -2.37997600 | 5.81090000 |
| H | -6.42594600 | -3.05741200 | 5.74586500 |
| H | -8.11383700 | -2.90760600 | 6.27930000 |
| H | -6.99926300 | -1.52292300 | 6.42628800 |
| C | -5.13388000 | 0.96482400 | 2.70745800 |
| H | -5.17902300 | 0.80924400 | 3.79096200 |
| C | -3.71197300 | 1.02324300 | 2.24846000 |
| H | -3.56564300 | 1.21071800 | 1.19008600 |
| C | -2.65008300 | 0.77801400 | 3.02095900 |
| H | -2.77582100 | 0.57791200 | 4.08432300 |
| C | -1.31317000 | 0.70016200 | 2.46783500 |
| H | -1.23038300 | 0.86940500 | 1.39702000 |
| C | -0.19651500 | 0.38398000 | 3.15031200 |
| H | -0.24722900 | 0.20353300 | 4.22346000 |
| C | 1.08069700 | 0.23900700 | 2.49500200 |
| H | 1.08047000 | 0.39976900 | 1.41847200 |
| C | 2.23932200 | -0.09053600 | 3.10042900 |
| H | 2.26171100 | -0.26624900 | 4.17525100 |
| C | 3.47173000 | -0.24292600 | 2.36871600 |
| H | 3.42971000 | -0.03562900 | 1.29978700 |
| C | 4.65233400 | -0.62018500 | 2.90211200 |
| H | 4.71779400 | -0.82529100 | 3.96994300 |

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| C | 5.84717400 | -0.79603900 | 2.11579800 |
| H | 5.76166900 | -0.59957500 | 1.04803200 |
| C | 7.04457800 | -1.18586000 | 2.59696500 |
| H | 7.16072500 | -1.36781200 | 3.66466600 |
| C | 8.19893800 | -1.38920500 | 1.75539300 |
| H | 8.04517500 | -1.26980800 | 0.68395600 |
| C | 9.43449200 | -1.69553800 | 2.19081800 |
| H | 9.62097200 | -1.79117500 | 3.25981300 |
| C | -5.96948900 | 2.19261400 | 2.32558100 |
| H | -6.99176000 | 2.03609900 | 2.67732400 |
| H | -5.57921700 | 3.07371800 | 2.84408700 |
| C | 10.55980400 | -1.86600900 | 1.29226700 |
| H | 10.31524300 | -1.88037500 | 0.23190600 |
| C | 11.84093400 | -1.94645100 | 1.66717000 |
| H | 12.08766600 | -1.91398200 | 2.72965800 |
| C | 13.00474100 | -2.02996000 | 0.72085100 |
| H | 12.62737200 | -2.21591900 | -0.29119300 |
| C | 13.78440200 | -0.70109900 | 0.67790800 |
| H | 14.28135600 | -0.58165000 | 1.65508000 |
| C | 12.91874700 | 0.55618700 | 0.47151100 |
| H | 12.20509000 | 0.56676200 | 1.30096400 |
| C | 12.06299500 | 0.50129100 | -0.79883100 |
| H | 11.57553600 | -0.46674900 | -0.87356800 |
| C | 9.74691300 | 1.13284300 | -0.81155000 |
| C | 8.77879500 | 2.26479400 | -0.57573300 |
| H | 9.23051500 | 2.99546400 | 0.09780700 |

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| H | 8.61371800 | 2.75766600 | -1.54095800 |
| C | 7.43387600 | 1.77414300 | -0.03506800 |
| H | 7.59483400 | 1.27409000 | 0.93082800 |
| C | 6.46397000 | 2.93309600 | 0.15467600 |
| H | 6.88654200 | 3.62765000 | 0.88860800 |
| H | 6.36167700 | 3.47356400 | -0.79406600 |
| C | 5.07295000 | 2.50778100 | 0.61603500 |
| H | 5.16134300 | 1.87979000 | 1.51304700 |
| C | 4.19130100 | 3.70915200 | 0.94173300 |
| H | 4.27234800 | 4.43966000 | 0.12753500 |
| H | 4.59977900 | 4.18844100 | 1.83647100 |
| C | 2.71630900 | 3.33371400 | 1.16274400 |
| H | 2.63082000 | 2.27441500 | 1.41572500 |
| H | 2.31238400 | 3.88356000 | 2.01836100 |
| C | 1.80901300 | 3.63916900 | -0.02917600 |
| H | 1.73958800 | 4.72953700 | -0.14396700 |
| C | 0.38429100 | 3.07215800 | 0.19085700 |
| H | 0.18126000 | 2.97483900 | 1.26317300 |
| C | -0.70676900 | 3.92505300 | -0.45541300 |
| H | -0.51074800 | 3.99760900 | -1.53207300 |
| H | -0.65515600 | 4.93837600 | -0.04111000 |
| C | -2.10776800 | 3.36441800 | -0.22488600 |
| H | -2.29351900 | 3.28702700 | 0.85500400 |
| C | -3.20168200 | 4.23433200 | -0.84003200 |
| H | -2.97110200 | 4.42994700 | -1.89185400 |
| H | -3.22886500 | 5.19196200 | -0.31194500 |

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| C | -4.59126000 | 3.59143500 | -0.78697100 |
| C | -5.71149400 | 4.52916500 | -1.20569500 |
| H | -5.57782300 | 4.85007500 | -2.24091300 |
| H | -5.70369300 | 5.41370100 | -0.56266900 |
| C | -7.05932100 | 3.84075900 | -1.07246300 |
| H | -7.10198200 | 3.01858500 | -1.80067600 |
| C | -7.22576400 | 3.24002300 | 0.35130400 |
| H | -7.43034400 | 4.08795700 | 1.01674100 |
| C | -5.97328200 | 2.48044700 | 0.82644200 |
| H | -5.92415900 | 1.53619900 | 0.27732200 |
| C | -8.42153500 | 2.31790000 | 0.37888100 |
| C | 12.76080800 | 0.81909800 | -2.10553200 |
| H | 12.06837300 | 0.69007900 | -2.94054500 |
| H | 13.60628800 | 0.14136400 | -2.23092200 |
| H | 13.12646800 | 1.84812200 | -2.11719000 |
| C | 13.75821200 | 1.82980000 | 0.55848400 |
| H | 14.54033300 | 1.85571000 | -0.20620400 |
| H | 14.23941100 | 1.90956200 | 1.53755000 |
| H | 13.13374200 | 2.71469300 | 0.41699200 |
| C | 13.94484900 | -3.17923500 | 1.09501300 |
| H | 14.32551800 | -3.05001600 | 2.11430600 |
| H | 14.79640800 | -3.21238200 | 0.41414100 |
| H | 13.41932300 | -4.13600800 | 1.05397100 |
| O | -6.20974300 | -2.72342700 | 1.32130300 |
| H | -5.38329500 | -2.22664000 | 1.40614600 |
| O | -9.25091600 | -3.70428000 | 4.09477900 |

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|---|--------------|-------------|-------------|
| H | -9.62836900 | -4.21879300 | 3.36307100 |
| O | -6.55065800 | -1.28820400 | 3.83713900 |
| O | -5.66086800 | -0.20157300 | 2.05220500 |
| O | -4.66695700 | 2.47109800 | -1.62327200 |
| H | -3.83503300 | 1.98204200 | -1.48538300 |
| O | -4.79924500 | 3.24151100 | 0.57682500 |
| O | -8.42657200 | 1.15834300 | 0.72274900 |
| O | -9.55185800 | 2.90714200 | -0.07537300 |
| H | -10.24303200 | 2.22380900 | -0.07733600 |
| O | -2.21274700 | 2.05796100 | -0.79389700 |
| H | -1.32299300 | 1.65353300 | -0.79644100 |
| O | 0.36717200 | 1.74372900 | -0.34448000 |
| H | 1.01706000 | 1.79891400 | -1.07686800 |
| O | 2.28076700 | 3.10588800 | -1.25795400 |
| H | 3.10192200 | 2.59231700 | -1.09272700 |
| O | 4.41071300 | 1.74981700 | -0.39960500 |
| H | 5.08111600 | 1.21145500 | -0.85877600 |
| O | 6.83356600 | 0.85533800 | -0.94368300 |
| H | 7.52025900 | 0.22216200 | -1.21863600 |
| O | 9.39530600 | 0.02024300 | -1.17145500 |
| O | 11.00476500 | 1.49220500 | -0.60456200 |
| O | 14.76663600 | -0.84829300 | -0.34283900 |
| H | 15.44713100 | -0.17850000 | -0.21635900 |
| O | -8.03734900 | 4.82013600 | -1.34521500 |
| H | -8.90346100 | 4.40172900 | -1.26191800 |
| N | -8.85662900 | -3.73722900 | 1.32390200 |

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| H | -8.02295100 | -4.24619500 | 1.03874000 |
| H | -9.32341600 | -3.43565400 | 0.47453800 |

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|---|--------------|-------------|------------|
| C | -10.46510100 | -2.67603900 | 1.31907400 |
| C | -9.56843900 | -3.15627200 | 2.44952800 |
| C | -8.28307100 | -3.84816800 | 1.96680800 |
| C | -9.68206600 | -1.70167300 | 0.39658300 |
| C | -8.19703200 | -1.75265300 | 0.66591700 |
| C | -7.51381300 | -0.64458300 | 0.94930600 |
| C | -6.07064300 | -0.61386900 | 1.34799800 |
| C | -5.57396900 | -1.97817600 | 1.83087100 |
| C | -4.04931900 | -1.98981900 | 1.90382100 |
| C | -3.36143500 | -0.96130900 | 2.79542000 |
| C | -1.92366600 | -1.51318300 | 2.95438800 |
| C | -1.89040200 | -2.95049800 | 2.33806900 |
| C | -1.15585800 | -3.08187900 | 0.97540500 |
| C | 0.05418200 | -2.15298000 | 0.78019500 |
| C | 1.20896800 | -2.27801400 | 1.77273000 |
| C | 2.32325400 | -1.27673500 | 1.46252300 |
| C | 3.49705300 | -1.27671900 | 2.44899300 |
| C | 4.31216800 | -2.56844600 | 2.36792800 |
| C | 4.40147900 | -0.06932700 | 2.20328600 |

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|---|--------------|-------------|-------------|
| C | -0.71457300 | -4.53154200 | 0.73498400 |
| C | -3.41185400 | -3.33091600 | 2.31026900 |
| C | -3.80268300 | -3.76200300 | 3.73529000 |
| C | -3.89164900 | -4.39075700 | 1.31054100 |
| C | -5.42280700 | -4.44324900 | 1.22769700 |
| C | -6.05444800 | -3.08712200 | 0.87405900 |
| C | -7.60287100 | -3.15008300 | 0.74442800 |
| C | -7.95704000 | -3.92117800 | -0.54623700 |
| O | -10.93396400 | -3.83456700 | 0.63720200 |
| H | -5.66982000 | -2.80596700 | -0.11595800 |
| H | -5.99147600 | -2.16051200 | 2.83164600 |
| H | -3.70585000 | -1.80756300 | 0.87916300 |
| H | -11.32618000 | -2.14404900 | 1.74987500 |
| H | -10.13720700 | -3.82892100 | 3.09763900 |
| H | -9.30312100 | -2.27713300 | 3.04623900 |
| H | -8.50011400 | -4.88883300 | 1.71141900 |
| H | -7.59228300 | -3.87144400 | 2.81428800 |
| H | -10.03865600 | -0.67801100 | 0.55571200 |
| H | -9.90128700 | -1.95984300 | -0.64715400 |
| H | -8.03203300 | 0.31047900 | 0.89686100 |
| H | -5.91642600 | 0.15098200 | 2.11692300 |
| H | -5.45899300 | -0.30417200 | 0.49117800 |
| H | -3.87163900 | -0.88982800 | 3.76180300 |
| H | -3.37747000 | 0.04191100 | 2.36067800 |
| H | -1.63943100 | -1.55283300 | 4.00921500 |
| H | -1.20246600 | -0.84974100 | 2.47931900 |

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| H | -1.36921100 | -3.61732400 | 3.03534300 |
| H | -1.85149600 | -2.80116700 | 0.17488300 |
| H | 0.44359200 | -2.34619600 | -0.22674800 |
| H | -0.28060700 | -1.11159800 | 0.77155600 |
| H | 1.60768100 | -3.29691100 | 1.75166400 |
| H | 0.84644000 | -2.10870500 | 2.79408000 |
| H | 1.88813200 | -0.26893900 | 1.43130800 |
| H | 2.72119900 | -1.46723200 | 0.45509500 |
| H | 3.08254900 | -1.19450100 | 3.46327400 |
| H | 4.74757500 | -2.68385100 | 1.36800400 |
| H | 3.70447000 | -3.45356100 | 2.57096800 |
| H | 5.13632200 | -2.55889900 | 3.08752600 |
| H | 4.82226800 | -0.11460800 | 1.19512000 |
| H | 5.23546000 | -0.04068600 | 2.91127000 |
| H | 3.85211700 | 0.87265000 | 2.29006300 |
| H | -0.00735300 | -4.85535800 | 1.50492500 |
| H | -0.21657900 | -4.63082600 | -0.23482800 |
| H | -1.54974700 | -5.23014100 | 0.75198300 |
| H | -3.43457100 | -3.06412100 | 4.49064400 |
| H | -3.36695200 | -4.74166000 | 3.95633700 |
| H | -4.88276600 | -3.84355800 | 3.86981600 |
| H | -3.51463400 | -5.38351000 | 1.58085800 |
| H | -3.50579200 | -4.15777700 | 0.31302300 |
| H | -5.82451400 | -4.81059400 | 2.17634600 |
| H | -5.70049000 | -5.18994100 | 0.47845600 |
| H | -7.44192100 | -4.88402800 | -0.56856100 |

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| H | -7.66846000 | -3.36707100 | -1.44428400 |
| H | -9.02497200 | -4.13198200 | -0.59462300 |
| H | -11.49962000 | -3.54964200 | -0.08961600 |
| C | -7.39270600 | 4.01385900 | 2.30623800 |
| H | -8.28247100 | 4.20751100 | 1.69385400 |
| C | -6.69770900 | 5.35697500 | 2.51968600 |
| H | -5.80583100 | 5.19053300 | 3.14406100 |
| C | -6.22418300 | 5.92210100 | 1.18558000 |
| H | -7.10860900 | 6.06019300 | 0.54024000 |
| C | -5.92178000 | 3.74321900 | 0.30228000 |
| H | -6.73083100 | 3.87402900 | -0.43420100 |
| C | -6.48152100 | 3.05717700 | 1.54654300 |
| H | -7.04691900 | 2.18201000 | 1.20401500 |
| C | -5.48673300 | 7.23345000 | 1.33387000 |
| H | -4.59162400 | 7.08551100 | 1.94379200 |
| H | -6.13123500 | 7.96427200 | 1.82476600 |
| H | -5.18107800 | 7.61363400 | 0.35664600 |
| C | -4.37374700 | 3.20457500 | -1.46434000 |
| H | -4.37249600 | 4.29129900 | -1.59830800 |
| C | -2.96673500 | 2.70160200 | -1.39467300 |
| H | -2.85337500 | 1.63962100 | -1.19311800 |
| C | -1.87811800 | 3.47296900 | -1.48167500 |
| H | -1.97514100 | 4.54076400 | -1.67365000 |
| C | -0.55067600 | 2.93790300 | -1.25731800 |
| H | -0.50524300 | 1.87573300 | -1.03500800 |
| C | 0.60371100 | 3.63144200 | -1.24056800 |

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| H | 0.60745800 | 4.69945500 | -1.45445500 |
| C | 1.85016700 | 2.99070600 | -0.89318000 |
| H | 1.77547600 | 1.92771200 | -0.67714400 |
| C | 3.06311800 | 3.57160200 | -0.80242100 |
| H | 3.18685200 | 4.63162700 | -1.01968900 |
| C | 4.22286300 | 2.82225700 | -0.38501900 |
| H | 4.05618100 | 1.76788700 | -0.16565400 |
| C | 5.46880900 | 3.31391400 | -0.22560700 |
| H | 5.66674200 | 4.36232200 | -0.44499600 |
| C | 6.56478300 | 2.51564300 | 0.26505300 |
| H | 6.33742100 | 1.48102900 | 0.51972400 |
| C | 7.82670400 | 2.95299000 | 0.44883600 |
| H | 8.08269300 | 3.97948300 | 0.18929300 |
| C | 8.87162000 | 2.12213800 | 0.99691100 |
| H | 8.58073900 | 1.11997500 | 1.30932200 |
| C | 10.15981900 | 2.48340500 | 1.13988500 |
| H | 10.48277400 | 3.47071800 | 0.81191500 |
| C | -5.24920300 | 2.54701200 | -2.54096000 |
| H | -6.23291100 | 3.01789500 | -2.50964700 |
| H | -4.81973800 | 2.73091300 | -3.53035600 |
| C | 11.16452800 | 1.59175000 | 1.68573200 |
| H | 10.78710600 | 0.65797500 | 2.09813800 |
| C | 12.48396900 | 1.80920000 | 1.66833100 |
| H | 12.86526100 | 2.73774000 | 1.24024600 |
| C | 13.51621100 | 0.83486100 | 2.16046300 |
| H | 13.01072400 | 0.01975500 | 2.69093900 |

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| C | 14.28977400 | 0.20085000 | 0.98795800 |
| H | 14.91840500 | 0.99109100 | 0.54468000 |
| C | 13.40973700 | -0.34765900 | -0.15031800 |
| H | 12.81720500 | 0.50171400 | -0.50389400 |
| C | 12.38626800 | -1.38593700 | 0.32240200 |
| H | 11.89611100 | -1.03544200 | 1.22634900 |
| C | 10.08857100 | -1.33947800 | -0.36867200 |
| C | 9.16143400 | -1.40201200 | -1.55660600 |
| H | 9.68616000 | -1.04197700 | -2.44384900 |
| H | 8.91439000 | -2.45711000 | -1.72254100 |
| C | 7.86820800 | -0.62035100 | -1.32242900 |
| H | 8.11349000 | 0.43528800 | -1.13951700 |
| C | 6.93907100 | -0.71492300 | -2.52483900 |
| H | 7.43881000 | -0.26411900 | -3.38885600 |
| H | 6.75714800 | -1.77064100 | -2.75962700 |
| C | 5.59079800 | -0.03211100 | -2.31279400 |
| H | 5.75252100 | 0.99579500 | -1.96118200 |
| C | 4.76653700 | 0.01407400 | -3.59421500 |
| H | 4.76327100 | -0.98315100 | -4.05157400 |
| H | 5.28116800 | 0.67855000 | -4.29477000 |
| C | 3.32373300 | 0.49537200 | -3.36741900 |
| H | 3.25781500 | 1.06149700 | -2.43487300 |
| H | 3.02984000 | 1.18543200 | -4.16416000 |
| C | 2.28332000 | -0.62483600 | -3.34381500 |
| H | 2.19787300 | -1.05031000 | -4.35366100 |
| C | 0.90685100 | -0.08714300 | -2.90908300 |

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| H | 0.76182900 | 0.93352800 | -3.28030100 |
| C | -0.25188300 | -0.97022400 | -3.36684600 |
| H | -0.07776300 | -1.99522100 | -3.01935500 |
| H | -0.26892100 | -0.98962000 | -4.46252100 |
| C | -1.60432300 | -0.48125900 | -2.85419400 |
| H | -1.75706700 | 0.56172400 | -3.16331700 |
| C | -2.76533300 | -1.31538800 | -3.38453900 |
| H | -2.58666100 | -2.37408700 | -3.17231600 |
| H | -2.82498400 | -1.18794100 | -4.46914000 |
| C | -4.10964100 | -0.93868700 | -2.76083300 |
| C | -5.29587600 | -1.63608700 | -3.40194700 |
| H | -5.22794600 | -2.71627500 | -3.25516600 |
| H | -5.30271400 | -1.43069000 | -4.47613400 |
| C | -6.59918400 | -1.14088200 | -2.80016000 |
| H | -6.63274800 | -1.42757200 | -1.74257600 |
| C | -6.68209700 | 0.40848500 | -2.86491500 |
| H | -6.84438100 | 0.68182900 | -3.91538800 |
| C | -5.38260900 | 1.04235300 | -2.33240500 |
| H | -5.34313800 | 0.83768900 | -1.26033100 |
| C | -7.86552400 | 0.90155000 | -2.06196000 |
| C | 12.89602500 | -2.79624900 | 0.53785000 |
| H | 12.09500500 | -3.42753500 | 0.92930900 |
| H | 13.71775300 | -2.77146900 | 1.25490700 |
| H | 13.25373800 | -3.23355500 | -0.39679200 |
| C | 14.25712200 | -0.84758800 | -1.31908200 |
| H | 14.92888100 | -1.65764500 | -1.01943600 |

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| H | 14.86675200 | -0.03707400 | -1.72890400 |
| H | 13.62194600 | -1.22979000 | -2.12133400 |
| C | 14.49236200 | 1.50043800 | 3.13457800 |
| H | 14.99956000 | 2.34539800 | 2.65565700 |
| H | 15.25039200 | 0.78694600 | 3.46063500 |
| H | 13.96295300 | 1.88211600 | 4.01050600 |
| O | -5.43806900 | 2.66429700 | 2.41872500 |
| H | -4.69020000 | 2.42064000 | 1.85408600 |
| O | -7.59116800 | 6.26512500 | 3.12106900 |
| H | -8.05907100 | 5.73255000 | 3.78451600 |
| O | -5.32846700 | 4.99008500 | 0.58792800 |
| O | -4.92555600 | 2.89909800 | -0.17088300 |
| O | -4.13973900 | -1.25627700 | -1.39593000 |
| H | -3.27780000 | -0.97491600 | -1.03322400 |
| O | -4.25125200 | 0.46112800 | -2.96749400 |
| O | -7.85947100 | 1.76979500 | -1.22154100 |
| O | -9.01476200 | 0.24538600 | -2.35668100 |
| H | -9.68789500 | 0.58443500 | -1.74475800 |
| O | -1.64038200 | -0.54020100 | -1.42493900 |
| H | -0.74162100 | -0.32888900 | -1.10682600 |
| O | 0.93112300 | 0.00496900 | -1.48138600 |
| H | 1.49591500 | -0.74646900 | -1.21520700 |
| O | 2.59606800 | -1.67945400 | -2.44400800 |
| H | 3.45775800 | -1.49644700 | -2.01215600 |
| O | 4.82319000 | -0.73219100 | -1.32855500 |
| H | 5.44259100 | -1.04265500 | -0.64285400 |

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| O | 7.16942900 | -1.14111700 | -0.19391600 |
| H | 7.80788400 | -1.19539900 | 0.53875400 |
| O | 9.69489100 | -1.23359400 | 0.78188200 |
| O | 11.36262800 | -1.43307800 | -0.72057300 |
| O | 15.12018000 | -0.80697400 | 1.55716800 |
| H | 15.81688800 | -1.02497200 | 0.92891500 |
| O | -7.63024000 | -1.77541900 | -3.52768300 |
| H | -8.47148400 | -1.48748100 | -3.15213800 |
| N | -7.84037300 | 3.52859600 | 3.60877100 |
| H | -7.03666000 | 3.12865900 | 4.08824500 |
| H | -8.51687100 | 2.77973200 | 3.49879200 |

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|---|-------------|------------|------------|
| C | 3.29838500 | 2.14111300 | 4.58458200 |
| C | 2.93272400 | 3.61669900 | 4.61838700 |
| C | 1.57593600 | 3.91013700 | 3.96857200 |
| C | 3.20787900 | 1.59556100 | 3.15577700 |
| C | 1.83080600 | 1.87262300 | 2.61011700 |
| C | 0.98447700 | 0.87185400 | 2.37173500 |
| C | -0.44910000 | 1.04676200 | 1.98772400 |
| C | -0.98547000 | 2.42516500 | 2.35689100 |
| C | -2.32145500 | 2.67801800 | 1.66539700 |
| C | -3.45301900 | 1.68755900 | 1.89656300 |

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|---|--------------|------------|-------------|
| C | -4.66047500 | 2.40927800 | 1.26992700 |
| C | -4.32711500 | 3.93577300 | 1.17329500 |
| C | -4.35864900 | 4.48965100 | -0.27200900 |
| C | -5.51706100 | 3.93662500 | -1.12893800 |
| C | -6.91133300 | 4.00082500 | -0.49640300 |
| C | -8.02660200 | 3.92421000 | -1.53957600 |
| C | -9.41447900 | 3.60576500 | -0.97400400 |
| C | -9.84733000 | 4.59645300 | 0.10639900 |
| C | -10.44342500 | 3.55359700 | -2.10221100 |
| C | -4.43865100 | 6.02197800 | -0.28722900 |
| C | -2.96355600 | 4.05081100 | 1.94596900 |
| C | -3.31601700 | 4.23630800 | 3.43382100 |
| C | -1.94961800 | 5.12530700 | 1.52920800 |
| C | -0.58815300 | 4.91320800 | 2.20473500 |
| C | 0.00977400 | 3.52268000 | 1.94522600 |
| C | 1.44317200 | 3.34616900 | 2.53079900 |
| C | 2.41334800 | 4.09398300 | 1.59295300 |
| O | 4.60789900 | 2.02605600 | 5.11664400 |
| H | 0.11954100 | 3.41867400 | 0.85360800 |
| H | -1.12124900 | 2.45578100 | 3.44618000 |
| H | -2.10895700 | 2.66406800 | 0.58226600 |
| H | 2.57711400 | 1.58350400 | 5.20466500 |
| H | 3.73200500 | 4.16632000 | 4.11001200 |
| H | 2.93628800 | 3.96066900 | 5.65676200 |
| H | 1.41873800 | 4.99252100 | 3.96294900 |
| H | 0.77941000 | 3.47745300 | 4.58570900 |

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|---|--------------|-------------|-------------|
| H | 3.40963800 | 0.51828300 | 3.14709000 |
| H | 3.99744600 | 2.07455200 | 2.56616600 |
| H | 1.34734300 | -0.14894500 | 2.45601600 |
| H | -1.05405700 | 0.26389100 | 2.45534200 |
| H | -0.57082400 | 0.88438900 | 0.90788200 |
| H | -3.58941800 | 1.50911500 | 2.96856000 |
| H | -3.27175500 | 0.71550000 | 1.43076100 |
| H | -5.57729300 | 2.23869300 | 1.84034400 |
| H | -4.82962700 | 1.99386800 | 0.27653600 |
| H | -5.08461500 | 4.50091800 | 1.72812600 |
| H | -3.42972200 | 4.18906900 | -0.77738700 |
| H | -5.53023800 | 4.50484400 | -2.06786700 |
| H | -5.31546400 | 2.90082700 | -1.41593300 |
| H | -7.02171000 | 4.92021300 | 0.08746500 |
| H | -7.02518900 | 3.17892000 | 0.22081700 |
| H | -7.78694100 | 3.16156300 | -2.28852700 |
| H | -8.07084800 | 4.87730700 | -2.08496400 |
| H | -9.36529800 | 2.60525600 | -0.52065500 |
| H | -9.85495600 | 5.61817700 | -0.29042800 |
| H | -9.17784700 | 4.57926100 | 0.97026400 |
| H | -10.85692000 | 4.37223300 | 0.46414700 |
| H | -10.57243500 | 4.54441500 | -2.55182900 |
| H | -11.42137000 | 3.22471200 | -1.73726100 |
| H | -10.12027200 | 2.87313800 | -2.89330300 |
| H | -5.39056300 | 6.36129800 | 0.13296900 |
| H | -4.37851700 | 6.40175600 | -1.31154300 |

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| H | -3.64663500 | 6.49676300 | 0.28806000 |
| H | -4.09038600 | 3.53644800 | 3.75609200 |
| H | -3.70655200 | 5.24637000 | 3.59291800 |
| H | -2.46036300 | 4.10414600 | 4.09844600 |
| H | -2.31149800 | 6.12667600 | 1.78323200 |
| H | -1.80843300 | 5.10123900 | 0.44307900 |
| H | -0.69766000 | 5.06562700 | 3.28203600 |
| H | 0.09909400 | 5.69176700 | 1.85945700 |
| H | 2.14616900 | 5.15162000 | 1.52656200 |
| H | 2.37114700 | 3.67601400 | 0.58363000 |
| H | 3.44962500 | 4.04663400 | 1.92899100 |
| H | 4.84149200 | 1.09063400 | 5.13095600 |
| C | -8.52090200 | -5.67432300 | 0.75055000 |
| H | -9.37957000 | -5.00547200 | 0.88946300 |
| C | -8.01541600 | -6.04976500 | 2.14292500 |
| H | -7.16251000 | -6.73653000 | 2.02697500 |
| C | -7.51108000 | -4.81223500 | 2.87545000 |
| H | -8.35435400 | -4.10733900 | 2.97429500 |
| C | -6.90166000 | -3.78153800 | 0.83403800 |
| H | -7.68726900 | -3.01913600 | 0.95066000 |
| C | -7.44097900 | -4.92397700 | -0.02204000 |
| H | -7.86295300 | -4.47731100 | -0.93481900 |
| C | -6.94449400 | -5.13003300 | 4.24048600 |
| H | -6.08720300 | -5.80039200 | 4.13649200 |
| H | -7.70513000 | -5.62235800 | 4.84839100 |
| H | -6.61223100 | -4.21715200 | 4.73979200 |

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| C | -5.18618700 | -2.10393300 | 0.70580300 |
| H | -5.15513000 | -2.20266500 | 1.79571800 |
| C | -3.79246100 | -2.08528800 | 0.16010100 |
| H | -3.69650100 | -2.02833700 | -0.92041800 |
| C | -2.69295700 | -2.16734500 | 0.91656700 |
| H | -2.78544600 | -2.23415600 | 2.00040200 |
| C | -1.35535600 | -2.19539700 | 0.35844700 |
| H | -1.28200400 | -2.11587400 | -0.72328300 |
| C | -0.22584400 | -2.32277200 | 1.07946300 |
| H | -0.28912700 | -2.40955400 | 2.16417300 |
| C | 1.08786600 | -2.33716500 | 0.48194700 |
| H | 1.12232500 | -2.22165400 | -0.59987800 |
| C | 2.24313900 | -2.44809500 | 1.16809700 |
| H | 2.21507200 | -2.56248000 | 2.25183500 |
| C | 3.54048400 | -2.41314600 | 0.54071200 |
| H | 3.56341900 | -2.27542900 | -0.54008200 |
| C | 4.71184500 | -2.51747200 | 1.20116200 |
| H | 4.70339200 | -2.63958100 | 2.28404600 |
| C | 5.99765300 | -2.50053500 | 0.54992800 |
| H | 5.99932800 | -2.39790600 | -0.53492900 |
| C | 7.17918300 | -2.60349100 | 1.19101200 |
| H | 7.18975000 | -2.68515100 | 2.27744700 |
| C | 8.45340000 | -2.62124000 | 0.51444300 |
| H | 8.42840600 | -2.60665700 | -0.57368900 |
| C | 9.65159200 | -2.63861700 | 1.12641400 |
| H | 9.69950300 | -2.62615700 | 2.21472400 |

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| C | -6.02734300 | -0.87835200 | 0.32786200 |
| H | -7.02106400 | -1.00142400 | 0.76319300 |
| H | -5.58826500 | 0.01515500 | 0.77350800 |
| C | 10.90556600 | -2.62989200 | 0.39851700 |
| H | 10.82405400 | -2.75010500 | -0.67982300 |
| C | 12.11044000 | -2.43164600 | 0.94392800 |
| H | 12.18958800 | -2.29321800 | 2.02349400 |
| C | 13.39377500 | -2.33153200 | 0.16969400 |
| H | 13.20685000 | -2.62835700 | -0.86865100 |
| C | 13.91444900 | -0.88110200 | 0.14066400 |
| H | 14.24002700 | -0.62971700 | 1.16383500 |
| C | 12.86924200 | 0.17731200 | -0.25795000 |
| H | 12.05588100 | 0.08075100 | 0.46777900 |
| C | 12.22724200 | -0.09071900 | -1.62369600 |
| H | 11.94994100 | -1.13832100 | -1.70136200 |
| C | 9.85693700 | 0.06283200 | -1.96695900 |
| C | 8.66347800 | 0.98344100 | -1.92467600 |
| H | 8.87159300 | 1.81790600 | -1.25244700 |
| H | 8.53192600 | 1.39190000 | -2.93345600 |
| C | 7.38220600 | 0.25247400 | -1.51622600 |
| H | 7.51179800 | -0.16359900 | -0.50688800 |
| C | 6.18799300 | 1.19518600 | -1.52223900 |
| H | 6.37726100 | 2.00589500 | -0.81050100 |
| H | 6.09284800 | 1.64302900 | -2.51873300 |
| C | 4.86186000 | 0.52829800 | -1.16641100 |
| H | 4.96362100 | -0.00275300 | -0.20993700 |

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| C | 3.74427600 | 1.55631600 | -1.03838500 |
| H | 3.78040900 | 2.23115600 | -1.90287100 |
| H | 3.96143000 | 2.16524500 | -0.15573100 |
| C | 2.34545100 | 0.93615100 | -0.91464900 |
| H | 2.41831100 | -0.09461700 | -0.55806800 |
| H | 1.77127800 | 1.46797300 | -0.15314200 |
| C | 1.52514200 | 0.96889600 | -2.19996100 |
| H | 1.31496800 | 2.01766300 | -2.45236900 |
| C | 0.17688200 | 0.22519800 | -2.01364200 |
| H | -0.06462100 | 0.16956100 | -0.94755600 |
| C | -0.98727900 | 0.87939100 | -2.75068400 |
| H | -0.77103500 | 0.89388300 | -3.82583400 |
| H | -1.07780100 | 1.91965400 | -2.41623900 |
| C | -2.31231300 | 0.16730800 | -2.49354300 |
| H | -2.51200000 | 0.17027100 | -1.41279800 |
| C | -3.48024400 | 0.84748800 | -3.19875500 |
| H | -3.28139800 | 0.89568500 | -4.27386700 |
| H | -3.57242800 | 1.87026300 | -2.82103400 |
| C | -4.81461700 | 0.12706700 | -2.99954700 |
| C | -5.99185100 | 0.89661700 | -3.58392200 |
| H | -5.91795900 | 0.91509900 | -4.67307000 |
| H | -5.97164300 | 1.92627100 | -3.22139300 |
| C | -7.32174000 | 0.27539300 | -3.18905900 |
| H | -7.40253500 | -0.71468900 | -3.66057300 |
| C | -7.38771500 | 0.06957800 | -1.64996400 |
| H | -7.43166300 | 1.05975300 | -1.18257200 |

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| C | -6.13846000 | -0.68627600 | -1.17911100 |
| H | -6.13507700 | -1.66810400 | -1.66152400 |
| C | -8.64635800 | -0.68072200 | -1.30563400 |
| C | 13.02848100 | 0.31322800 | -2.84435600 |
| H | 12.49811800 | 0.02072200 | -3.75350600 |
| H | 13.99698500 | -0.18788900 | -2.81558700 |
| H | 13.18837200 | 1.39322000 | -2.87153100 |
| C | 13.43549000 | 1.59148200 | -0.14210700 |
| H | 14.30127100 | 1.73961000 | -0.79454000 |
| H | 13.74692200 | 1.79998800 | 0.88550400 |
| H | 12.68410900 | 2.33286200 | -0.42294000 |
| C | 14.46524700 | -3.26285900 | 0.74364400 |
| H | 14.66326600 | -3.02222800 | 1.79408400 |
| H | 15.39776300 | -3.15827000 | 0.18746400 |
| H | 14.13731200 | -4.30371900 | 0.69582400 |
| O | -6.41587900 | -5.84422000 | -0.33431400 |
| H | -5.60937300 | -5.32251800 | -0.45196300 |
| O | -9.05855000 | -6.63775100 | 2.88543200 |
| H | -9.50529900 | -7.21680200 | 2.24673600 |
| O | -6.47174000 | -4.21808800 | 2.10430600 |
| O | -5.79353000 | -3.28542000 | 0.15466600 |
| O | -4.82208300 | -1.14087100 | -3.58416000 |
| H | -3.93605800 | -1.52333500 | -3.44263800 |
| O | -4.98543500 | 0.04409500 | -1.58212800 |
| O | -8.73108600 | -1.81841200 | -0.90919700 |
| O | -9.75915000 | 0.06262300 | -1.53587700 |

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| H | -10.52040300 | -0.50067200 | -1.31978400 |
| O | -2.25733200 | -1.19031600 | -2.94069700 |
| H | -1.32533500 | -1.48016300 | -2.90674000 |
| O | 0.35257300 | -1.12187100 | -2.45580900 |
| H | 1.07239500 | -1.03846000 | -3.11717700 |
| O | 2.18146800 | 0.37821400 | -3.31300300 |
| H | 3.06602900 | 0.05971800 | -3.03098100 |
| O | 4.48055400 | -0.42013000 | -2.16771500 |
| H | 5.29349100 | -0.85003600 | -2.49007600 |
| O | 7.09869300 | -0.80642800 | -2.42729800 |
| H | 7.92647600 | -1.30354400 | -2.55484700 |
| O | 9.78063200 | -1.11143200 | -2.29321500 |
| O | 10.98221400 | 0.67658200 | -1.63274100 |
| O | 15.03965200 | -0.87907600 | -0.73273700 |
| H | 15.56294400 | -0.08886600 | -0.56134400 |
| O | -8.32662400 | 1.14547200 | -3.66920500 |
| H | -9.17767200 | 0.85846000 | -3.31393900 |
| N | -9.00046700 | -6.89538600 | 0.10923000 |
| H | -8.19148900 | -7.40879300 | -0.23394900 |
| H | -9.57259300 | -6.67470800 | -0.69966200 |

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| C | 10.49545700 | 3.22320800 | 0.17215000 |
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| H | 11.34832000 | 2.75251300 | 0.67726600 |
| C | 9.86952600 | 4.19266100 | 1.17329400 |
| H | 9.03351000 | 4.71083600 | 0.68181300 |
| C | 9.31397100 | 3.43305900 | 2.37173900 |
| H | 10.15075600 | 2.90266000 | 2.85560000 |
| C | 8.88626100 | 1.52428000 | 1.04440200 |
| H | 9.66816700 | 0.95035800 | 1.57156000 |
| C | 9.48805900 | 2.14297200 | -0.21630000 |
| H | 9.98036900 | 1.33603700 | -0.77666600 |
| C | 8.63371700 | 4.34502000 | 3.36811000 |
| H | 7.77920300 | 4.83021700 | 2.89176300 |
| H | 9.33608200 | 5.10861900 | 3.70255300 |
| H | 8.27800900 | 3.77397900 | 4.22660600 |
| C | 7.35643100 | -0.20914100 | 1.63069400 |
| H | 7.42163300 | 0.27600600 | 2.60996400 |
| C | 5.91745900 | -0.46751900 | 1.30745200 |
| H | 5.69480100 | -0.77131100 | 0.28613900 |
| C | 4.92540500 | -0.35054000 | 2.19728600 |
| H | 5.14160100 | -0.04581600 | 3.21972800 |
| C | 3.53936500 | -0.57789500 | 1.83869400 |
| H | 3.35072100 | -0.85035800 | 0.80110600 |
| C | 2.47453600 | -0.41645400 | 2.64999400 |
| H | 2.61299700 | -0.12235800 | 3.68838100 |
| C | 1.13159600 | -0.55556500 | 2.13561900 |
| H | 1.06798800 | -0.85174700 | 1.09073000 |
| C | -0.01662400 | -0.29435900 | 2.79213600 |

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| H | -0.00222200 | 0.00943100 | 3.83691300 |
| C | -1.29394600 | -0.37624200 | 2.12409600 |
| H | -1.27616700 | -0.63560200 | 1.06374800 |
| C | -2.49179200 | -0.14987200 | 2.70138600 |
| H | -2.54183700 | 0.09742000 | 3.75995900 |
| C | -3.73324700 | -0.21973100 | 1.97129200 |
| H | -3.66470000 | -0.40798900 | 0.89834700 |
| C | -4.95452100 | -0.07672100 | 2.52576100 |
| H | -5.03830000 | 0.08737400 | 3.59852800 |
| C | -6.17463100 | -0.10752400 | 1.75627200 |
| H | -6.07370500 | -0.16016400 | 0.67263800 |
| C | -7.41260700 | -0.03886300 | 2.28116800 |
| H | -7.54027700 | 0.01874000 | 3.36086700 |
| C | 8.23087300 | -1.47408300 | 1.62099600 |
| H | 9.22920100 | -1.20435500 | 1.97246900 |
| H | 7.81760700 | -2.20741600 | 2.31897000 |
| C | -8.60413100 | -0.02212700 | 1.45579500 |
| H | -8.42779800 | 0.00752000 | 0.38171300 |
| C | -9.85781500 | -0.05290700 | 1.92401100 |
| H | -10.02187700 | -0.08288700 | 3.00240800 |
| C | -11.08712500 | -0.07886300 | 1.06218000 |
| H | -10.79418100 | 0.08594700 | 0.01938900 |
| C | -11.78792600 | -1.44946100 | 1.13296900 |
| H | -12.24502400 | -1.53585800 | 2.13157600 |
| C | -10.85167800 | -2.65992500 | 0.96809200 |
| H | -10.12562000 | -2.58966800 | 1.78347700 |

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| C | -10.02803500 | -2.59689600 | -0.32217200 |
| H | -9.68267200 | -1.58079500 | -0.48822100 |
| C | -7.67659000 | -2.92399900 | -0.50750400 |
| C | -6.51689900 | -3.85588000 | -0.24722600 |
| H | -6.78855300 | -4.56503100 | 0.53503700 |
| H | -6.34811500 | -4.41630700 | -1.17377100 |
| C | -5.23169100 | -3.10530500 | 0.12037900 |
| H | -5.39009500 | -2.57016200 | 1.06682900 |
| C | -4.06304600 | -4.07154800 | 0.27424200 |
| H | -4.29552500 | -4.78006000 | 1.07565700 |
| H | -3.94639500 | -4.63944200 | -0.65645400 |
| C | -2.73330200 | -3.38910200 | 0.59239700 |
| H | -2.86277300 | -2.72369000 | 1.45730200 |
| C | -1.64328500 | -4.40798200 | 0.91424400 |
| H | -1.64392500 | -5.17902000 | 0.13426100 |
| H | -1.90898000 | -4.90123400 | 1.85207200 |
| C | -0.24657900 | -3.76789000 | 1.01940000 |
| H | -0.34269100 | -2.68460600 | 1.12390900 |
| H | 0.26919800 | -4.12034500 | 1.91611600 |
| C | 0.65600800 | -4.06782900 | -0.17588000 |
| H | 0.88508600 | -5.14097800 | -0.18411600 |
| C | 1.98691600 | -3.28496600 | -0.09322300 |
| H | 2.24490400 | -3.10820500 | 0.95814100 |
| C | 3.13600400 | -4.01191500 | -0.78237400 |
| H | 2.88017900 | -4.17876500 | -1.83581900 |
| H | 3.25758500 | -4.99320100 | -0.31064200 |

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|---|--------------|-------------|-------------|
| C | 4.46452400 | -3.26390800 | -0.68905700 |
| H | 4.66865800 | -3.01777100 | 0.36261300 |
| C | 5.60799000 | -4.11973900 | -1.21705400 |
| H | 5.38792000 | -4.43491300 | -2.24185500 |
| H | 5.68422400 | -5.01260600 | -0.59112000 |
| C | 6.96446200 | -3.41578300 | -1.23050300 |
| C | 8.10058100 | -4.39243700 | -1.50454000 |
| H | 8.01690600 | -4.78884400 | -2.51798300 |
| H | 8.03773400 | -5.22389600 | -0.79762400 |
| C | 9.46160000 | -3.74098600 | -1.33411400 |
| H | 9.60146800 | -2.98765500 | -2.12214000 |
| C | 9.53822600 | -3.01667100 | 0.03860900 |
| H | 9.56260500 | -3.79571700 | 0.80957700 |
| C | 8.31940500 | -2.10612200 | 0.23697100 |
| H | 8.34613900 | -1.31677600 | -0.52026900 |
| C | 10.87146000 | -2.31147800 | 0.07247700 |
| C | -10.70095600 | -3.11004900 | -1.58121600 |
| H | -10.04501900 | -2.95329000 | -2.43949100 |
| H | -11.63119700 | -2.56342900 | -1.74054300 |
| H | -10.92115900 | -4.17588800 | -1.49969300 |
| C | -11.61032500 | -3.97685200 | 1.12253200 |
| H | -12.38485700 | -4.09259000 | 0.35943400 |
| H | -12.08616700 | -4.03332700 | 2.10475000 |
| H | -10.93053900 | -4.82611100 | 1.02934500 |
| C | -12.06629700 | 1.02951400 | 1.46091500 |
| H | -12.35762200 | 0.92483700 | 2.51045200 |

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|---|--------------|-------------|-------------|
| H | -12.96475100 | 0.98284800 | 0.84533200 |
| H | -11.60163900 | 2.01058300 | 1.34120200 |
| O | 8.49517100 | 2.75754200 | -1.00574600 |
| H | 7.71588100 | 2.18850500 | -0.99333800 |
| O | 10.84404400 | 5.10280100 | 1.62781600 |
| H | 11.32419800 | 5.36746600 | 0.83245800 |
| O | 8.34974100 | 2.49006600 | 1.91558600 |
| O | 7.84528600 | 0.70258200 | 0.63479200 |
| O | 7.02804100 | -2.40993200 | -2.20190600 |
| H | 6.19565200 | -1.91558000 | -2.15380600 |
| O | 7.13315100 | -2.87217000 | 0.07438500 |
| O | 11.93378600 | -2.87498600 | -0.00543700 |
| O | 10.80338600 | -0.96723500 | 0.12650300 |
| H | 11.71582000 | -0.64679800 | 0.08277900 |
| O | 4.44008900 | -2.05050100 | -1.44476200 |
| H | 3.56977300 | -1.64372300 | -1.32397400 |
| O | 1.79447900 | -1.99454300 | -0.67487300 |
| H | 1.16022300 | -2.14789400 | -1.39433200 |
| O | 0.05517400 | -3.74750900 | -1.42168100 |
| H | -0.81670800 | -3.34666800 | -1.25947100 |
| O | -2.27047200 | -2.61076900 | -0.51390000 |
| H | -3.03930500 | -2.17859300 | -0.91483500 |
| O | -4.87435900 | -2.16742600 | -0.88950500 |
| H | -5.67381900 | -1.69030700 | -1.16012900 |
| O | -7.55278800 | -1.85738700 | -1.07184500 |
| O | -8.83626000 | -3.40564600 | -0.08286600 |

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|---|--------------|-------------|-------------|
| O | -12.81085800 | -1.42176500 | 0.14362600 |
| H | -13.43894200 | -2.12335500 | 0.33077300 |
| O | 10.41697600 | -4.77013200 | -1.43718200 |
| H | 11.27200400 | -4.41749800 | -1.16477800 |
| N | 11.00963300 | 4.00994400 | -0.94683900 |
| H | 10.22674700 | 4.24152900 | -1.55379000 |
| H | 11.66104600 | 3.46672400 | -1.50245700 |
| C | -9.03738900 | 3.83489500 | -1.55185100 |
| C | -7.81973800 | 4.54918300 | -2.11946100 |
| C | -6.67437700 | 4.67549600 | -1.10223200 |
| C | -8.65255400 | 2.41185400 | -1.05871800 |
| C | -7.15257600 | 2.24512600 | -0.99082700 |
| C | -6.53829400 | 1.25816900 | -1.64631200 |
| C | -5.04566400 | 1.15114500 | -1.79056200 |
| C | -4.34853100 | 2.47653600 | -1.48251900 |
| C | -2.83670700 | 2.29499600 | -1.41982000 |
| C | -2.14250500 | 1.83240300 | -2.70087200 |
| C | -0.67030700 | 2.28287600 | -2.52838900 |
| C | -0.57792900 | 3.12351400 | -1.21310800 |
| C | 0.09618500 | 2.38448700 | -0.03095500 |
| C | 1.32870300 | 1.55406500 | -0.44161200 |
| C | 2.40728900 | 2.28279600 | -1.24490500 |
| C | 3.60989500 | 1.36878700 | -1.48280900 |
| C | 4.78802800 | 2.00579900 | -2.22533700 |
| C | 5.36415300 | 3.19227900 | -1.44997300 |
| C | 5.87564500 | 0.95757800 | -2.47203800 |

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| C | 0.52430700 | 3.35787800 | 1.07672000 |
| C | -2.06624400 | 3.56270600 | -1.00490400 |
| C | -2.31968800 | 4.73262200 | -1.97383700 |
| C | -2.55266900 | 3.94381200 | 0.39665800 |
| C | -4.07067400 | 4.18981900 | 0.42059900 |
| C | -4.90184600 | 3.02901000 | -0.15628200 |
| C | -6.41301400 | 3.36984500 | -0.27867800 |
| C | -6.99678600 | 3.54210500 | 1.13755500 |
| O | -9.54895200 | 4.65740700 | -0.50683700 |
| H | -4.83006600 | 2.19954200 | 0.56539900 |
| H | -4.58884500 | 3.17300900 | -2.29761400 |
| H | -2.63654200 | 1.54792100 | -0.63388000 |
| H | -9.79886500 | 3.74667100 | -2.33623500 |
| H | -8.11887700 | 5.53893700 | -2.47157200 |
| H | -7.47725200 | 3.97671500 | -2.98705100 |
| H | -6.89531600 | 5.49380200 | -0.41227000 |
| H | -5.77387800 | 4.95983900 | -1.65348900 |
| H | -9.06491600 | 1.65637100 | -1.73381400 |
| H | -9.10945100 | 2.25319000 | -0.07449700 |
| H | -7.14448700 | 0.50366900 | -2.14381700 |
| H | -4.80320000 | 0.82358800 | -2.80741500 |
| H | -4.64093300 | 0.37577600 | -1.12288700 |
| H | -2.60411900 | 2.31314300 | -3.56961400 |
| H | -2.22769000 | 0.75403800 | -2.85212300 |
| H | -0.35291700 | 2.88637500 | -3.38161000 |
| H | -0.00442400 | 1.42307000 | -2.50432900 |

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|---|-------------|------------|-------------|
| H | 0.03041700 | 4.01583600 | -1.40474400 |
| H | -0.62308000 | 1.67821300 | 0.40458700 |
| H | 1.80088600 | 1.20154800 | 0.47840200 |
| H | 1.02840200 | 0.64721600 | -0.97730800 |
| H | 2.72479500 | 3.17231100 | -0.69371100 |
| H | 2.01528500 | 2.63179200 | -2.20785200 |
| H | 3.27307700 | 0.48741500 | -2.04506700 |
| H | 3.97767100 | 1.00203500 | -0.51431000 |
| H | 4.42833300 | 2.36780900 | -3.19696700 |
| H | 5.67237400 | 2.87590900 | -0.44542700 |
| H | 4.63860000 | 3.99928400 | -1.33595800 |
| H | 6.23977600 | 3.60742400 | -1.95526200 |
| H | 6.24733700 | 0.56584000 | -1.51672400 |
| H | 6.72355200 | 1.38071500 | -3.01851800 |
| H | 5.48803100 | 0.11346400 | -3.04895600 |
| H | 1.23404000 | 4.09499200 | 0.69011300 |
| H | 1.01761300 | 2.81034500 | 1.88519400 |
| H | -0.31061300 | 3.90479600 | 1.50802600 |
| H | -1.94717800 | 4.51296400 | -2.97683400 |
| H | -1.79188600 | 5.62088600 | -1.61425300 |
| H | -3.37536600 | 4.99007500 | -2.06634400 |
| H | -2.04699200 | 4.84538100 | 0.75660700 |
| H | -2.31726500 | 3.13200700 | 1.09548300 |
| H | -4.29519900 | 5.11895200 | -0.11001800 |
| H | -4.36536300 | 4.35853000 | 1.45880500 |
| H | -6.46573300 | 4.33434600 | 1.66862500 |

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| H | -6.90281900 | 2.61511100 | 1.70871700 |
| H | -8.04445800 | 3.83665500 | 1.09631800 |
| H | -10.33772500 | 4.23791600 | -0.15495200 |

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|---|--------------|-------------|------------|
| C | -9.31002400 | -3.11908500 | 1.22658300 |
| H | -10.03539300 | -2.79499500 | 1.98270600 |
| C | -8.26191100 | -3.96135100 | 1.95273300 |
| H | -7.53773000 | -4.33658700 | 1.21451800 |
| C | -7.50596300 | -3.11238900 | 2.96825100 |
| H | -8.23389900 | -2.74961800 | 3.71259800 |
| C | -7.84736700 | -1.15813600 | 1.67818800 |
| H | -8.54276900 | -0.76346200 | 2.44518000 |
| C | -8.65366000 | -1.88749600 | 0.60604900 |
| H | -9.41960800 | -1.18832500 | 0.23841100 |
| C | -6.40337800 | -3.88755500 | 3.65451200 |
| H | -5.67390200 | -4.21456600 | 2.91029100 |
| H | -6.82639300 | -4.76325200 | 4.14704900 |
| H | -5.89686900 | -3.26120500 | 4.38978300 |
| C | -6.54156800 | 0.80244900 | 1.96194600 |
| H | -6.50964200 | 0.36169900 | 2.96360900 |
| C | -5.14028400 | 0.99920100 | 1.48000800 |
| H | -5.02815400 | 1.20646700 | 0.41964100 |

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|---|-------------|-------------|------------|
| C | -4.06070800 | 0.91161300 | 2.26114600 |
| H | -4.17144100 | 0.72567900 | 3.32804100 |
| C | -2.71314800 | 0.98771900 | 1.73230600 |
| H | -2.61561200 | 1.01719700 | 0.64652300 |
| C | -1.59409400 | 0.95777200 | 2.48069900 |
| H | -1.67592700 | 0.93328600 | 3.56594700 |
| C | -0.27085300 | 0.89825800 | 1.90707800 |
| H | -0.21978000 | 0.83447000 | 0.81990800 |
| C | 0.87016700 | 0.85597300 | 2.62667200 |
| H | 0.81844600 | 0.92729500 | 3.71192000 |
| C | 2.17188800 | 0.65889700 | 2.03603400 |
| H | 2.21843600 | 0.50112300 | 0.95861600 |
| C | 3.32351600 | 0.62579100 | 2.73904700 |
| H | 3.29889300 | 0.79361700 | 3.81444000 |
| C | 4.60921500 | 0.35126000 | 2.14418500 |
| H | 4.62300500 | 0.10892100 | 1.08068900 |
| C | 5.77093700 | 0.36000500 | 2.82970400 |
| H | 5.75896700 | 0.61891400 | 3.88715000 |
| C | 7.05245000 | 0.04167200 | 2.24476700 |
| H | 7.05194300 | -0.31182700 | 1.21417800 |
| C | 8.22927200 | 0.16887500 | 2.88742400 |
| H | 8.23980300 | 0.54548500 | 3.90882900 |
| C | -7.39770600 | 2.07158300 | 1.99081800 |
| H | -8.38274100 | 1.79674400 | 2.37585500 |
| H | -6.95326200 | 2.80119400 | 2.67444800 |
| C | 9.50719800 | -0.13866600 | 2.27228100 |

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| H | 9.45897500 | -0.63904000 | 1.30794100 |
| C | 10.69704400 | 0.18838000 | 2.78988800 |
| H | 10.73332800 | 0.70135200 | 3.75263500 |
| C | 12.02107700 | -0.06258500 | 2.12569300 |
| H | 11.86795600 | -0.70868100 | 1.25445000 |
| C | 12.64345100 | 1.25539300 | 1.62735900 |
| H | 12.91917900 | 1.84395200 | 2.51685700 |
| C | 11.70319200 | 2.13937900 | 0.78728900 |
| H | 10.85751700 | 2.38329400 | 1.43754100 |
| C | 11.09779600 | 1.40073300 | -0.41095800 |
| H | 10.75984000 | 0.41591200 | -0.10131200 |
| C | 8.77514100 | 1.48380400 | -0.96757400 |
| C | 7.62299600 | 2.37543800 | -1.36204800 |
| H | 7.84498800 | 3.40297500 | -1.07258700 |
| H | 7.54324100 | 2.33697500 | -2.45426200 |
| C | 6.29723100 | 1.90718700 | -0.75316300 |
| H | 6.37933200 | 1.92977600 | 0.34316300 |
| C | 5.15245700 | 2.81264200 | -1.19337000 |
| H | 5.38834300 | 3.83956000 | -0.89602100 |
| H | 5.08375900 | 2.78297500 | -2.28753700 |
| C | 3.79314500 | 2.42953500 | -0.60772900 |
| H | 3.87558100 | 2.39850000 | 0.49004300 |
| C | 2.71777200 | 3.44310600 | -0.99533700 |
| H | 2.72136300 | 3.48051300 | -2.09230300 |
| H | 2.99778100 | 4.43535800 | -0.62477900 |
| C | 1.34121900 | 3.03497400 | -0.47350200 |

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| H | 1.16673000 | 1.99435000 | -0.75116000 |
| H | 1.33003900 | 3.08643700 | 0.62081300 |
| C | 0.17979100 | 3.86221100 | -1.01649800 |
| H | 0.25071200 | 4.90448800 | -0.67592300 |
| C | -1.17303900 | 3.28907000 | -0.58089800 |
| H | -1.17265100 | 3.13961500 | 0.50391600 |
| C | -2.33887000 | 4.19089800 | -0.98504000 |
| H | -2.28368100 | 4.38679200 | -2.06083000 |
| H | -2.22705200 | 5.14920400 | -0.46574500 |
| C | -3.71592200 | 3.61169900 | -0.65649500 |
| H | -3.76687400 | 3.34352500 | 0.40772100 |
| C | -4.81538700 | 4.62363700 | -0.96253600 |
| H | -4.68418800 | 5.01296800 | -1.97696200 |
| H | -4.72383900 | 5.45652600 | -0.26018400 |
| C | -6.23499900 | 4.05941300 | -0.87299300 |
| C | -7.29054000 | 5.15453700 | -0.93172400 |
| H | -7.24747400 | 5.67122700 | -1.89235700 |
| H | -7.10816000 | 5.87923600 | -0.13391900 |
| C | -8.67978500 | 4.57310500 | -0.74188400 |
| H | -8.92040100 | 3.93926900 | -1.60532600 |
| C | -8.72393400 | 3.69211700 | 0.53600400 |
| H | -8.69383500 | 4.38469200 | 1.38650000 |
| C | -7.53853800 | 2.71721000 | 0.61791800 |
| H | -7.65749200 | 1.94098000 | -0.14348500 |
| C | -10.07973300 | 3.02456100 | 0.55754800 |
| C | 11.97454800 | 1.27240400 | -1.64239400 |

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| H | 11.45935700 | 0.68301600 | -2.40330300 |
| H | 12.90544700 | 0.77255800 | -1.37274500 |
| H | 12.20413800 | 2.25386900 | -2.06119300 |
| C | 12.38343000 | 3.44798300 | 0.38712900 |
| H | 13.27246800 | 3.27424000 | -0.22540500 |
| H | 12.68461900 | 4.01033500 | 1.27455200 |
| H | 11.70435800 | 4.07452500 | -0.19419500 |
| C | 12.98946900 | -0.76876800 | 3.08002900 |
| H | 13.14967300 | -0.16306100 | 3.97758700 |
| H | 13.95239700 | -0.92772200 | 2.59523700 |
| H | 12.58352500 | -1.73216700 | 3.39210900 |
| O | -7.83889600 | -2.33446300 | -0.44732100 |
| H | -7.37260100 | -1.58296100 | -0.85392000 |
| O | -8.89241100 | -5.02131600 | 2.63390600 |
| H | -9.54169500 | -5.36529100 | 2.00657800 |
| O | -6.90997100 | -2.00415800 | 2.30374000 |
| O | -7.15753400 | -0.13234000 | 1.06160300 |
| O | -6.51932600 | 3.16709300 | -1.91206100 |
| H | -5.77031800 | 2.55608300 | -1.97818900 |
| O | -6.32108900 | 3.41811500 | 0.39406900 |
| O | -11.12490700 | 3.62125700 | 0.47611600 |
| O | -10.05361100 | 1.68243000 | 0.62249300 |
| H | -10.97550200 | 1.39133700 | 0.58290700 |
| O | -3.97544100 | 2.44325100 | -1.43587400 |
| H | -3.16305600 | 1.91801500 | -1.45589500 |
| O | -1.31215900 | 1.98239200 | -1.15613100 |

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| H | -0.90260700 | 2.02866700 | -2.03224500 |
| O | 0.12558700 | 3.81846500 | -2.44193800 |
| H | 0.98708500 | 4.04389500 | -2.79757400 |
| O | 3.35276300 | 1.16689300 | -1.08632800 |
| H | 4.12989100 | 0.60153100 | -1.19497000 |
| O | 5.98293900 | 0.58269400 | -1.17157200 |
| H | 6.77071400 | 0.03201800 | -1.05308400 |
| O | 8.66845800 | 0.28194400 | -0.84375700 |
| O | 9.90500600 | 2.15331000 | -0.78765600 |
| O | 13.82062400 | 0.89717400 | 0.91282200 |
| H | 14.36952100 | 1.67843800 | 0.81383700 |
| O | -9.57082600 | 5.66060600 | -0.64626000 |
| H | -10.43689800 | 5.30778400 | -0.41108900 |
| N | -10.00282800 | -3.98956300 | 0.27895800 |
| H | -9.41934200 | -4.07651900 | -0.54963300 |
| H | -10.87847300 | -3.57402000 | -0.01863300 |
| C | -5.24881700 | -1.42747900 | -2.62650200 |
| C | -4.28283800 | -0.89024400 | -1.56306300 |
| C | -4.18905700 | -1.85747200 | -0.38615600 |
| C | -5.34361400 | -2.96752400 | -2.56898300 |
| C | -3.96889500 | -3.48582700 | -2.24364700 |
| C | -3.18743800 | -4.02919200 | -3.17592900 |
| C | -1.71694500 | -4.24723900 | -2.95912300 |
| C | -1.18921800 | -3.14955700 | -2.03367700 |
| C | 0.31134600 | -3.26841700 | -1.78654900 |
| C | 1.24666300 | -3.21734200 | -3.00190600 |

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| C | 2.59193500 | -2.67616400 | -2.44383900 |
| C | 2.39253700 | -2.40986700 | -0.91989200 |
| C | 2.93973400 | -3.50639300 | 0.03022000 |
| C | 4.24656800 | -4.15841500 | -0.45598700 |
| C | 5.40527900 | -3.18550000 | -0.70696100 |
| C | 6.55213200 | -3.85441800 | -1.46450500 |
| C | 7.80620400 | -2.98798700 | -1.62923800 |
| C | 8.55851200 | -2.82548000 | -0.30799300 |
| C | 8.73671200 | -3.58436600 | -2.68555400 |
| C | 3.16678700 | -2.93756900 | 1.43684400 |
| C | 0.85147300 | -2.17301200 | -0.84849800 |
| C | 0.59681500 | -0.76578500 | -1.42168700 |
| C | 0.13865800 | -2.31886500 | 0.50073700 |
| C | -1.38445900 | -2.21617300 | 0.33346600 |
| C | -1.94279800 | -3.21883000 | -0.68830900 |
| C | -3.51445100 | -3.19254100 | -0.81600300 |
| C | -4.07089300 | -4.30008400 | 0.10115600 |
| O | -6.52432300 | -0.81951000 | -2.37637700 |
| H | -1.69440300 | -4.21709700 | -0.29632600 |
| H | -1.39126900 | -2.18830700 | -2.52513800 |
| H | 0.47592400 | -4.23057600 | -1.27806100 |
| H | -4.90612000 | -1.12464200 | -3.62218600 |
| H | -4.65057800 | 0.08982000 | -1.25958600 |
| H | -3.29033600 | -0.74981300 | -2.00775100 |
| H | -5.20171400 | -2.06628600 | -0.02296500 |
| H | -3.67725500 | -1.40580900 | 0.46208100 |

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| H | -5.70267000 | -3.36744700 | -3.52112500 |
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| H | -1.19393300 | -4.22036000 | -3.91949800 |
| H | -1.50662700 | -5.23060300 | -2.51561100 |
| H | 0.84192900 | -2.54781700 | -3.76747200 |
| H | 1.36257200 | -4.19774000 | -3.46845500 |
| H | 2.85586700 | -1.73887500 | -2.93873300 |
| H | 3.41276100 | -3.36140700 | -2.64640200 |
| H | 2.90407600 | -1.47745300 | -0.64955700 |
| H | 2.19951200 | -4.31283300 | 0.10161500 |
| H | 4.56462400 | -4.88997900 | 0.29605000 |
| H | 4.05962800 | -4.73758000 | -1.36550700 |
| H | 5.76616700 | -2.79145200 | 0.24909900 |
| H | 5.05725500 | -2.32180700 | -1.28714400 |
| H | 6.18471700 | -4.14573000 | -2.45631100 |
| H | 6.83403800 | -4.78693900 | -0.95667200 |
| H | 7.49322000 | -1.99390000 | -1.97575100 |
| H | 8.89087000 | -3.80299100 | 0.05661800 |
| H | 7.94037900 | -2.37143800 | 0.47048200 |
| H | 9.43825700 | -2.19180700 | -0.44364300 |
| H | 9.05199600 | -4.58979100 | -2.38810600 |
| H | 9.63546800 | -2.97476800 | -2.80905300 |
| H | 8.24022100 | -3.66189000 | -3.65578900 |
| H | 3.93433400 | -2.15971600 | 1.41379600 |
| H | 3.50792900 | -3.71991000 | 2.12073300 |

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| H | 2.27081800 | -2.48681500 | 1.85989000 |
| H | 0.97210300 | -0.66570400 | -2.44289000 |
| H | 1.13935400 | -0.03412500 | -0.82207200 |
| H | -0.45601200 | -0.48498700 | -1.42752600 |
| H | 0.47090900 | -1.55589500 | 1.20915800 |
| H | 0.37964000 | -3.29496800 | 0.93769100 |
| H | -1.64690900 | -1.19566800 | 0.04146700 |
| H | -1.86124100 | -2.37518800 | 1.30674100 |
| H | -3.76842200 | -4.10686500 | 1.13572500 |
| H | -3.69222600 | -5.28096700 | -0.19605000 |
| H | -5.16387600 | -4.32271300 | 0.07225500 |
| H | -7.13273400 | -1.10748600 | -3.06352000 |

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|---|--------------|-------------|------------|
| C | -14.29847200 | -5.19284200 | 1.79104400 |
| C | -13.29441600 | -5.05134100 | 0.65846000 |
| C | -13.31051400 | -3.66205700 | 0.00254600 |
| C | -14.02137200 | -4.12837300 | 2.88621800 |
| C | -13.08969200 | -3.04767800 | 2.39155200 |
| C | -11.99467900 | -2.72041500 | 3.07516900 |
| C | -10.94415200 | -1.77210800 | 2.58111600 |
| C | -11.02224900 | -1.57702500 | 1.06776100 |
| C | -10.15769900 | -0.41335000 | 0.61027400 |

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| C | -8.68644200 | -0.33137000 | 0.98967200 |
| C | -8.28817700 | 0.94622900 | 0.24810800 |
| C | -8.99780200 | 0.86934100 | -1.12708400 |
| C | -9.33228100 | 2.23810200 | -1.75043300 |
| C | -8.20449600 | 3.27649100 | -1.58245100 |
| C | -6.84802400 | 2.92550100 | -2.19672000 |
| C | -5.86201700 | 4.08996000 | -2.10221300 |
| C | -4.40333200 | 3.75899300 | -2.44280300 |
| C | -4.25328900 | 3.03634600 | -3.78209100 |
| C | -3.55704300 | 5.03392400 | -2.43401200 |
| C | -9.68770400 | 2.10450500 | -3.23593500 |
| C | -10.17811900 | -0.16858900 | -0.91619800 |
| C | -9.81614000 | -1.42858900 | -1.72142700 |
| C | -11.61953700 | 0.25322100 | -1.23962900 |
| C | -12.63511600 | -0.81198600 | -0.78698700 |
| C | -12.48413700 | -1.29388900 | 0.66962400 |
| C | -13.42611800 | -2.48038500 | 1.01937100 |
| C | -14.87728500 | -1.95769600 | 1.03868400 |
| O | -15.59556700 | -5.07167000 | 1.21347200 |
| H | -12.79889100 | -0.45725500 | 1.31302000 |
| H | -10.68308300 | -2.50538100 | 0.59163800 |
| H | -10.61668600 | 0.48355300 | 1.06005600 |
| H | -14.19829100 | -6.19438600 | 2.23382100 |
| H | -13.48543400 | -5.82228900 | -0.09314400 |
| H | -12.30129200 | -5.24401200 | 1.07774500 |
| H | -14.13715200 | -3.60600200 | -0.71062100 |

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| H | -12.38864200 | -3.56725600 | -0.57843500 |
| H | -13.57940000 | -4.60656600 | 3.76504500 |
| H | -14.98066400 | -3.70467400 | 3.20743900 |
| H | -11.82125900 | -3.18866900 | 4.04295300 |
| H | -9.95328200 | -2.14762700 | 2.86046900 |
| H | -11.04411400 | -0.79686000 | 3.08136900 |
| H | -8.12759900 | -1.19812900 | 0.61739100 |
| H | -8.51536200 | -0.26586700 | 2.06763600 |
| H | -7.20936700 | 1.07740200 | 0.15435700 |
| H | -8.67892300 | 1.80245300 | 0.81702600 |
| H | -8.29668500 | 0.39186500 | -1.81912300 |
| H | -10.20483100 | 2.65025400 | -1.22671800 |
| H | -8.55144000 | 4.22162500 | -2.01950400 |
| H | -8.05776900 | 3.49151600 | -0.51638000 |
| H | -6.97582900 | 2.65422100 | -3.24973600 |
| H | -6.42411600 | 2.05373900 | -1.68988500 |
| H | -5.88904400 | 4.49726700 | -1.08134000 |
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| H | -4.02594000 | 3.09119800 | -1.65803800 |
| H | -4.70672700 | 3.62265700 | -4.58978900 |
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| H | -3.19642600 | 2.89532700 | -4.02541500 |
| H | -3.76808700 | 5.64024300 | -3.32191900 |
| H | -2.48948700 | 4.80234800 | -2.41292300 |
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| H | -8.86626800 | 1.64914700 | -3.79735600 |

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| H | -9.89035700 | 3.08385800 | -3.68018500 |
| H | -10.56521200 | 1.47984600 | -3.39672000 |
| H | -8.84764000 | -1.83958100 | -1.42816600 |
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| H | -10.54987000 | -2.22961300 | -1.62250000 |
| H | -11.76758800 | 0.41756400 | -2.30995500 |
| H | -11.84297400 | 1.20333900 | -0.74046900 |
| H | -12.56907300 | -1.66457600 | -1.46682200 |
| H | -13.63927600 | -0.40291300 | -0.92878300 |
| H | -15.12453600 | -1.47847700 | 0.08874100 |
| H | -15.01315000 | -1.21991300 | 1.83612400 |
| H | -15.58743900 | -2.77137900 | 1.17901700 |
| H | -16.24722600 | -5.16952000 | 1.91724500 |
| C | -5.70442600 | -0.93279800 | -2.18722800 |
| H | -6.39702800 | -0.61726600 | -1.39775000 |
| C | -5.55629400 | -2.44795300 | -2.07200300 |
| H | -4.87644400 | -2.79357400 | -2.86545000 |
| C | -4.92949200 | -2.82127600 | -0.73200300 |
| H | -5.60438300 | -2.46456500 | 0.06607900 |
| C | -3.77010800 | -0.77103900 | -0.63876500 |
| H | -4.40564000 | -0.44240400 | 0.19598700 |
| C | -4.36589100 | -0.25281100 | -1.94165000 |
| H | -4.50420700 | 0.82782000 | -1.82583500 |
| C | -4.70459100 | -4.30904500 | -0.58647200 |
| H | -4.01098000 | -4.65425000 | -1.35768500 |
| H | -5.65213200 | -4.83770300 | -0.70187500 |

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| H | -4.27595800 | -4.53703200 | 0.39184400 |
| C | -1.82844000 | -0.32755200 | 0.70863600 |
| H | -1.98260600 | -1.33577600 | 1.10954700 |
| C | -0.37827000 | -0.11643700 | 0.40763600 |
| H | -0.12118900 | 0.82277100 | -0.07535000 |
| C | 0.58029600 | -1.00810700 | 0.67495300 |
| H | 0.32537800 | -1.95157600 | 1.15678400 |
| C | 1.96919300 | -0.79170000 | 0.32282900 |
| H | 2.20018700 | 0.14847700 | -0.17185900 |
| C | 2.96823400 | -1.66827900 | 0.53776100 |
| H | 2.75641000 | -2.61832100 | 1.02760000 |
| C | 4.32790000 | -1.40790100 | 0.12915200 |
| H | 4.50137700 | -0.44571100 | -0.34886400 |
| C | 5.36906800 | -2.24629900 | 0.30378000 |
| H | 5.21251200 | -3.21169900 | 0.78397600 |
| C | 6.70748600 | -1.92387000 | -0.12511700 |
| H | 6.85381100 | -0.94505100 | -0.58162200 |
| C | 7.77812300 | -2.73263400 | 0.01168200 |
| H | 7.65439900 | -3.70857900 | 0.47982800 |
| C | 9.09823100 | -2.38367100 | -0.45047400 |
| H | 9.20945300 | -1.41276600 | -0.93298200 |
| C | 10.18683400 | -3.16916600 | -0.32446800 |
| H | 10.09298300 | -4.13312500 | 0.17440400 |
| C | 11.49050600 | -2.80693300 | -0.82543900 |
| H | 11.55798000 | -1.87121100 | -1.37777800 |
| C | 12.61421000 | -3.52520400 | -0.64643800 |

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| H | 12.57466200 | -4.45148200 | -0.07436800 |
| C | -2.41901300 | 0.70399800 | 1.68333500 |
| H | -3.46127700 | 0.44025300 | 1.87480700 |
| H | -1.88715300 | 0.64544500 | 2.63760400 |
| C | 13.90629300 | -3.09978900 | -1.14828000 |
| H | 13.89358800 | -2.22929800 | -1.80108400 |
| C | 15.07915500 | -3.65472800 | -0.82420100 |
| H | 15.09310700 | -4.51714100 | -0.15565100 |
| C | 16.41914200 | -3.14744000 | -1.27542500 |
| H | 16.26866500 | -2.37993200 | -2.04326600 |
| C | 17.18277600 | -2.48319900 | -0.11301400 |
| H | 17.46374500 | -3.28234500 | 0.59303600 |
| C | 16.37069000 | -1.45290100 | 0.69364600 |
| H | 15.49752600 | -1.99295700 | 1.07245000 |
| C | 15.80328900 | -0.32045800 | -0.16922000 |
| H | 15.35695100 | -0.73207000 | -1.07014800 |
| C | 13.53082600 | 0.42275900 | 0.03627300 |
| C | 12.51381900 | 1.03262500 | 0.96798400 |
| H | 12.80364700 | 0.83481100 | 2.00165800 |
| H | 12.54226200 | 2.11778500 | 0.81500500 |
| C | 11.09577300 | 0.53022500 | 0.68621400 |
| H | 11.06396900 | -0.55879900 | 0.83347000 |
| C | 10.08463300 | 1.19298000 | 1.61057400 |
| H | 10.35017100 | 0.95841200 | 2.64697600 |
| H | 10.15062900 | 2.28077900 | 1.48831700 |
| C | 8.63955200 | 0.76713900 | 1.36291700 |

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| H | 8.56991100 | -0.32875200 | 1.39545400 |
| C | 7.70153700 | 1.35196200 | 2.41368100 |
| H | 7.92083900 | 2.42076800 | 2.52776600 |
| H | 7.94447400 | 0.87915700 | 3.37016600 |
| C | 6.21149800 | 1.15752800 | 2.08828000 |
| H | 6.08009000 | 0.33285000 | 1.38369600 |
| H | 5.66541600 | 0.87262200 | 2.99291000 |
| C | 5.53143300 | 2.40919600 | 1.53659600 |
| H | 5.52683500 | 3.17443700 | 2.32535400 |
| C | 4.06503100 | 2.12527000 | 1.12014700 |
| H | 3.69358800 | 1.24090200 | 1.65061800 |
| C | 3.13112500 | 3.29976900 | 1.39026200 |
| H | 3.48739300 | 4.17820400 | 0.83855600 |
| H | 3.16890100 | 3.54206600 | 2.45865000 |
| C | 1.68577700 | 2.99913700 | 1.00493000 |
| H | 1.36120600 | 2.08627000 | 1.52271500 |
| C | 0.74334100 | 4.12966600 | 1.39604800 |
| H | 1.07083100 | 5.06290200 | 0.92756600 |
| H | 0.78473100 | 4.25808600 | 2.48146400 |
| C | -0.70828100 | 3.88247000 | 0.98548800 |
| C | -1.66398700 | 4.90748800 | 1.57880600 |
| H | -1.45722900 | 5.89876500 | 1.17001400 |
| H | -1.52299800 | 4.94330700 | 2.66273700 |
| C | -3.11299800 | 4.55059300 | 1.30063900 |
| H | -3.28965000 | 4.62768800 | 0.22104700 |
| C | -3.40135600 | 3.08445600 | 1.72246300 |

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| H | -3.40732000 | 3.05945800 | 2.81838900 |
| C | -2.32914700 | 2.13416400 | 1.16224600 |
| H | -2.42463600 | 2.12441900 | 0.07278200 |
| C | -4.76388900 | 2.68910500 | 1.21856200 |
| C | 16.75694800 | 0.79644400 | -0.54088700 |
| H | 16.25855300 | 1.50949200 | -1.20161900 |
| H | 17.61925300 | 0.37067800 | -1.05575800 |
| H | 17.10210100 | 1.33216000 | 0.34602400 |
| C | 17.16078300 | -0.93691400 | 1.89508600 |
| H | 18.08885100 | -0.44286700 | 1.59211600 |
| H | 17.41981300 | -1.75865000 | 2.56899100 |
| H | 16.57340300 | -0.21013900 | 2.46070200 |
| C | 17.26392200 | -4.26944100 | -1.88559900 |
| H | 17.41409800 | -5.07721900 | -1.16068800 |
| H | 18.24272500 | -3.89044700 | -2.18263700 |
| H | 16.76652600 | -4.69440200 | -2.76035300 |
| O | -3.52408700 | -0.53635700 | -3.04148000 |
| H | -2.61708800 | -0.40241100 | -2.73341800 |
| O | -6.82347000 | -3.06107400 | -2.17797900 |
| H | -7.26666200 | -2.57465800 | -2.89215300 |
| O | -3.66412500 | -2.17787200 | -0.61715700 |
| O | -2.49224300 | -0.23102900 | -0.56099900 |
| O | -0.86718100 | 3.90917800 | -0.40525400 |
| H | -0.10073300 | 3.43705400 | -0.77951100 |
| O | -1.03797700 | 2.60398000 | 1.51924900 |
| O | -4.99053600 | 1.83046700 | 0.39682900 |

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| O | -5.76574800 | 3.43291000 | 1.73790600 |
| H | -6.58991200 | 3.12439500 | 1.32284300 |
| O | 1.56430900 | 2.79315900 | -0.40502100 |
| H | 2.39553100 | 2.38601800 | -0.71212700 |
| O | 4.05505500 | 1.79738400 | -0.27027100 |
| H | 4.84077800 | 2.27636200 | -0.60868800 |
| O | 6.18825600 | 2.95995200 | 0.40427400 |
| H | 6.97254400 | 2.41131100 | 0.18633200 |
| O | 8.19097900 | 1.20623100 | 0.07751600 |
| H | 8.94475800 | 1.13725100 | -0.53677600 |
| O | 10.71589600 | 0.83402700 | -0.65348100 |
| H | 11.45139400 | 0.55738800 | -1.22901500 |
| O | 13.28143300 | 0.13085800 | -1.12279500 |
| O | 14.71334100 | 0.26389500 | 0.61178400 |
| O | 18.35786300 | -1.91334700 | -0.68170800 |
| H | 18.99443000 | -1.74980100 | 0.02232600 |
| O | -3.89718000 | 5.47942100 | 2.01694400 |
| H | -4.82616100 | 5.24098700 | 1.90614400 |
| N | -6.32587500 | -0.63084600 | -3.47316000 |
| H | -5.61445000 | -0.70669300 | -4.19691600 |
| H | -6.66064300 | 0.32730800 | -3.48780700 |

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|---|--------------|-------------|-------------|
| C | -9.85330200 | 1.92793000 | 1.90704000 |
| H | -10.70042200 | 1.23436400 | 1.84298400 |
| C | -9.96406000 | 2.87426700 | 0.71161300 |
| H | -9.15647800 | 3.61929600 | 0.77523300 |
| C | -9.79891400 | 2.10819400 | -0.59447800 |
| H | -10.60963600 | 1.36561300 | -0.66371500 |
| C | -8.42016500 | 0.47431800 | 0.45695300 |
| H | -9.17581800 | -0.31020000 | 0.31525800 |
| C | -8.55714600 | 1.12679400 | 1.83208200 |
| H | -8.54969800 | 0.33475900 | 2.59368700 |
| C | -9.80192500 | 3.01499200 | -1.80515700 |
| H | -8.93370100 | 3.67729600 | -1.76469100 |
| H | -10.71249100 | 3.61426800 | -1.80638000 |
| H | -9.74799000 | 2.42848900 | -2.72295900 |
| C | -6.59459400 | -0.44175300 | -0.85804700 |
| H | -6.54452100 | 0.44486700 | -1.49861300 |
| C | -5.20611800 | -0.88949000 | -0.51501900 |
| H | -5.12131500 | -1.56498800 | 0.33286500 |
| C | -4.10828000 | -0.44314100 | -1.13204200 |
| H | -4.19748200 | 0.23076500 | -1.98288900 |
| C | -2.77104500 | -0.75895800 | -0.66828300 |
| H | -2.69240400 | -1.31276500 | 0.26616800 |
| C | -1.63839100 | -0.36999800 | -1.28391400 |
| H | -1.70041700 | 0.17479000 | -2.22499900 |
| C | -0.32227100 | -0.62118400 | -0.74269900 |
| H | -0.27863700 | -1.05887800 | 0.25456600 |

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|---|-------------|-------------|-------------|
| C | 0.82438500 | -0.32956600 | -1.39063200 |
| H | 0.77274300 | 0.09132400 | -2.39349800 |
| C | 2.13482200 | -0.49561700 | -0.81035600 |
| H | 2.19339700 | -0.86502500 | 0.21365800 |
| C | 3.28017100 | -0.18586300 | -1.45527300 |
| H | 3.23433200 | 0.17084500 | -2.48336500 |
| C | 4.58297500 | -0.26357300 | -0.83964000 |
| H | 4.61564700 | -0.55304000 | 0.21097000 |
| C | 5.73818900 | 0.01295100 | -1.47936200 |
| H | 5.71173100 | 0.28302300 | -2.53372200 |
| C | 7.03184800 | -0.02941900 | -0.83869400 |
| H | 7.04256500 | -0.19556800 | 0.23801100 |
| C | 8.20519100 | 0.11948300 | -1.48211300 |
| H | 8.20996300 | 0.26731500 | -2.56067000 |
| C | -7.48345400 | -1.48257900 | -1.54965100 |
| H | -8.44933800 | -1.01406500 | -1.76088500 |
| H | -7.02212400 | -1.73434500 | -2.50917500 |
| C | 9.48792800 | 0.07793000 | -0.80412700 |
| H | 9.45188800 | 0.06297700 | 0.28397700 |
| C | 10.67132100 | 0.02513100 | -1.42733500 |
| H | 10.69318600 | 0.03534300 | -2.51862300 |
| C | 12.00213400 | -0.08025700 | -0.73992400 |
| H | 11.85754300 | 0.03279100 | 0.34015900 |
| C | 12.64126100 | -1.46182900 | -0.98039000 |
| H | 12.95456700 | -1.49905400 | -2.03589900 |
| C | 11.70082300 | -2.66034900 | -0.75609200 |

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|---|-------------|-------------|-------------|
| H | 10.87942300 | -2.53455400 | -1.46787800 |
| C | 11.05000000 | -2.65131900 | 0.63069500 |
| H | 10.73557700 | -1.64278300 | 0.88120400 |
| C | 8.72676800 | -2.96310300 | 1.05940400 |
| C | 7.54360300 | -3.89305500 | 0.92528700 |
| H | 7.71466000 | -4.57955500 | 0.09571900 |
| H | 7.49600600 | -4.48075500 | 1.84921500 |
| C | 6.22389600 | -3.13385500 | 0.74836500 |
| H | 6.26375200 | -2.57033300 | -0.19462000 |
| C | 5.03785000 | -4.09198900 | 0.71577100 |
| H | 5.19572000 | -4.82139500 | -0.08534100 |
| H | 5.00326200 | -4.63407900 | 1.66854200 |
| C | 3.69119400 | -3.39974600 | 0.49397400 |
| H | 3.74253400 | -2.82292300 | -0.44274300 |
| C | 2.55519400 | -4.41385600 | 0.38517500 |
| H | 2.58677500 | -5.00513800 | 1.30974700 |
| H | 2.74531600 | -5.09392300 | -0.45257000 |
| C | 1.19969100 | -3.72742800 | 0.22506100 |
| H | 1.09654300 | -2.97078700 | 1.00642700 |
| H | 1.16555800 | -3.20693900 | -0.73823000 |
| C | 0.00731100 | -4.67333700 | 0.30707000 |
| H | 0.05309700 | -5.41730100 | -0.50050200 |
| C | -1.32573500 | -3.92521600 | 0.21561400 |
| H | -1.30755300 | -3.25305800 | -0.64830100 |
| C | -2.51057100 | -4.88250900 | 0.10719900 |
| H | -2.47870000 | -5.58783100 | 0.94431400 |

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| H | -2.40260000 | -5.45867700 | -0.81836300 |
| C | -3.87260800 | -4.18827900 | 0.09422000 |
| H | -3.89639600 | -3.41888900 | -0.68953000 |
| C | -4.97867800 | -5.20027600 | -0.17822400 |
| H | -4.88447300 | -6.03963500 | 0.51813600 |
| H | -4.85194300 | -5.58243900 | -1.19424600 |
| C | -6.39884400 | -4.65195500 | -0.03410300 |
| C | -7.42660500 | -5.63874300 | -0.57171000 |
| H | -7.44077900 | -6.53598100 | 0.04965000 |
| H | -7.15550700 | -5.92350500 | -1.59162500 |
| C | -8.81975500 | -5.03839700 | -0.61695800 |
| H | -9.17422200 | -4.85887300 | 0.40797200 |
| C | -8.77584300 | -3.67370500 | -1.35662300 |
| H | -8.54760800 | -3.88854200 | -2.40634100 |
| C | -7.68468100 | -2.76925600 | -0.76187600 |
| H | -7.92893100 | -2.53992700 | 0.28135500 |
| C | -10.17935200 | -3.12961500 | -1.31427900 |
| C | 11.87581500 | -3.21883200 | 1.76952600 |
| H | 11.33872500 | -3.09775200 | 2.71201400 |
| H | 12.82280200 | -2.68135600 | 1.82887400 |
| H | 12.07551400 | -4.28068800 | 1.61621700 |
| C | 12.40140000 | -3.98151200 | -1.06941500 |
| H | 13.26036100 | -4.14863200 | -0.41408000 |
| H | 12.75171400 | -3.99478200 | -2.10458300 |
| H | 11.71786200 | -4.82203200 | -0.93434600 |
| C | 12.95406000 | 1.02324200 | -1.21329600 |

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|---|--------------|-------------|-------------|
| H | 13.09616900 | 0.96502900 | -2.29694300 |
| H | 13.92551400 | 0.91672300 | -0.73046500 |
| H | 12.54604800 | 2.00840200 | -0.98009300 |
| O | -7.48720400 | 2.02689300 | 2.03733700 |
| H | -6.67921200 | 1.55415100 | 1.79942700 |
| O | -11.22952500 | 3.49084500 | 0.70899500 |
| H | -11.37802200 | 3.75908700 | 1.62497100 |
| O | -8.54259200 | 1.42997900 | -0.57314800 |
| O | -7.12879500 | -0.04329900 | 0.41984100 |
| O | -6.72961800 | -4.38715400 | 1.29963600 |
| H | -5.96633800 | -3.93382500 | 1.68776100 |
| O | -6.44320500 | -3.46060700 | -0.81186800 |
| O | -11.10413300 | -3.61105000 | -1.91737600 |
| O | -10.36270900 | -2.09990000 | -0.46648000 |
| H | -11.30839700 | -1.89334300 | -0.48505900 |
| O | -4.14750100 | -3.57143300 | 1.35397700 |
| H | -3.33378400 | -3.13584900 | 1.64231400 |
| O | -1.45214500 | -3.08510300 | 1.36938200 |
| H | -1.07873000 | -3.59563500 | 2.10204300 |
| O | -0.05597600 | -5.33369800 | 1.57137300 |
| H | 0.80973000 | -5.68662800 | 1.78539800 |
| O | 3.35584200 | -2.53340700 | 1.56620700 |
| H | 4.17647600 | -2.15576200 | 1.90947900 |
| O | 6.00742800 | -2.23020000 | 1.82625100 |
| H | 6.83979000 | -1.76672700 | 1.99938100 |
| O | 8.66680300 | -1.89427900 | 1.63001100 |

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|---|--------------|-------------|-------------|
| O | 9.83269800 | -3.44983400 | 0.51495300 |
| O | 13.79023200 | -1.51768000 | -0.14243100 |
| H | 14.36919400 | -2.21499400 | -0.45877200 |
| O | -9.63712500 | -5.97310200 | -1.28211400 |
| H | -10.45736700 | -5.54047100 | -1.54486100 |
| N | -10.01272700 | 2.72649200 | 3.11941100 |
| H | -9.12770500 | 3.18717800 | 3.31681300 |
| H | -10.22398300 | 2.13684800 | 3.91669700 |
| C | -5.04657000 | 2.84943600 | -0.25268000 |
| C | -3.90362200 | 3.08432900 | -1.25425300 |
| C | -3.50160900 | 4.56061300 | -1.25914000 |
| C | -4.90423700 | 3.80484000 | 0.96138400 |
| C | -3.43641000 | 4.07586500 | 1.15518200 |
| C | -2.71470800 | 3.40459200 | 2.05189600 |
| C | -1.21250300 | 3.38009100 | 2.05637000 |
| C | -0.66084500 | 3.65812200 | 0.65568600 |
| C | 0.86072900 | 3.78676800 | 0.68648900 |
| C | 1.65935400 | 2.57018200 | 1.14227000 |
| C | 3.10300400 | 2.89780000 | 0.69873600 |
| C | 3.04272400 | 4.09537700 | -0.31103000 |
| C | 3.70331900 | 5.39674400 | 0.20825400 |
| C | 5.04414600 | 5.15645900 | 0.93867600 |
| C | 6.05041400 | 4.27791600 | 0.18942400 |
| C | 7.42234400 | 4.27220300 | 0.86450900 |
| C | 8.41603500 | 3.26623900 | 0.27241900 |
| C | 8.62352300 | 3.48609500 | -1.22678100 |

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|---|-------------|------------|-------------|
| C | 9.75336900 | 3.33032400 | 1.00959200 |
| C | 3.95667500 | 6.39373600 | -0.93241800 |
| C | 1.51494500 | 4.16635600 | -0.65778100 |
| C | 1.27430800 | 3.08833600 | -1.73251600 |
| C | 0.89846200 | 5.49230700 | -1.11886800 |
| C | -0.62920100 | 5.37403100 | -1.21431500 |
| C | -1.27591500 | 4.95963800 | 0.11448100 |
| C | -2.84132200 | 4.98780400 | 0.09045900 |
| C | -3.26501600 | 6.44014400 | 0.39367400 |
| O | -6.26268000 | 3.06215700 | -0.95054000 |
| H | -0.98231100 | 5.72705200 | 0.84808900 |
| H | -0.94354500 | 2.81324100 | 0.01239600 |
| H | 1.09129400 | 4.61376000 | 1.37807200 |
| H | -4.99639300 | 1.81282700 | 0.10359700 |
| H | -4.26080800 | 2.77161800 | -2.23822800 |
| H | -3.04508500 | 2.45803100 | -0.99083600 |
| H | -4.41629400 | 5.14528900 | -1.40269300 |
| H | -2.86278200 | 4.79711200 | -2.10876900 |
| H | -5.35550100 | 3.37863300 | 1.85891200 |
| H | -5.46057000 | 4.71396900 | 0.71807600 |
| H | -3.23438600 | 2.77705500 | 2.77267500 |
| H | -0.86990800 | 2.40153500 | 2.40638000 |
| H | -0.80204200 | 4.11874700 | 2.75967100 |
| H | 1.28174200 | 1.67171700 | 0.64358100 |
| H | 1.59079700 | 2.39833500 | 2.21816500 |
| H | 3.57740800 | 2.02924500 | 0.23819300 |

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|---|-------------|------------|-------------|
| H | 3.70577900 | 3.15320000 | 1.56917400 |
| H | 3.59155400 | 3.81944300 | -1.22006300 |
| H | 3.02791600 | 5.86987000 | 0.93372000 |
| H | 5.50391600 | 6.13608000 | 1.11711700 |
| H | 4.87451000 | 4.73074700 | 1.93156100 |
| H | 6.15748400 | 4.63355300 | -0.83966700 |
| H | 5.67735100 | 3.24824300 | 0.12299300 |
| H | 7.29572000 | 4.05616700 | 1.93263900 |
| H | 7.85847900 | 5.27876900 | 0.80333200 |
| H | 7.99490900 | 2.26327700 | 0.41198100 |
| H | 8.89220500 | 4.52987500 | -1.42477700 |
| H | 7.72210400 | 3.25215800 | -1.79792500 |
| H | 9.43056500 | 2.85193600 | -1.60274700 |
| H | 10.22159500 | 4.31041900 | 0.86997600 |
| H | 10.44382800 | 2.57114300 | 0.63012300 |
| H | 9.62525400 | 3.16992400 | 2.08337400 |
| H | 4.64381600 | 5.96828800 | -1.66892000 |
| H | 4.41212400 | 7.30869200 | -0.54469300 |
| H | 3.05059000 | 6.67663100 | -1.46136400 |
| H | 1.84621600 | 2.18642700 | -1.50998900 |
| H | 1.61217800 | 3.46326000 | -2.70412800 |
| H | 0.22668300 | 2.79632800 | -1.82721700 |
| H | 1.28998600 | 5.78517400 | -2.09787100 |
| H | 1.15160700 | 6.28872700 | -0.40967800 |
| H | -0.87170500 | 4.64534600 | -1.99200800 |
| H | -1.04555900 | 6.32925100 | -1.55028600 |

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| H | -2.86159800 | 7.11886600 | -0.36389200 |
| H | -2.89219500 | 6.75459800 | 1.37122400 |
| H | -4.35075500 | 6.55207200 | 0.38980000 |
| H | -6.98771000 | 2.62147800 | -0.48897500 |

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|---|-------------|-------------|-------------|
| C | -6.62724100 | -5.10271500 | -2.65398900 |
| C | -5.84058200 | -4.16981500 | -1.74763900 |
| C | -5.45729400 | -2.83585500 | -2.40575600 |
| C | -7.91409400 | -4.39989900 | -3.16127900 |
| C | -7.87939500 | -2.90832100 | -2.92331600 |
| C | -8.90111000 | -2.28157600 | -2.34228300 |
| C | -8.89509500 | -0.83451100 | -1.95493900 |
| C | -7.48000100 | -0.25820100 | -1.89469100 |
| C | -7.52190400 | 1.26330000 | -1.78648300 |
| C | -8.23336400 | 1.87029200 | -0.58105000 |
| C | -7.70304900 | 3.32151300 | -0.51777500 |
| C | -6.54901200 | 3.45440500 | -1.56480100 |
| C | -6.89853500 | 4.25861500 | -2.84671000 |
| C | -7.85699500 | 5.44397200 | -2.62416500 |
| C | -7.39895200 | 6.48921000 | -1.60635300 |
| C | -8.42769900 | 7.60201400 | -1.41787400 |
| C | -8.08271200 | 8.62668400 | -0.33134200 |

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| C | -6.79118500 | 9.38541200 | -0.63922200 |
| C | -9.24077500 | 9.60502100 | -0.13542700 |
| C | -5.62300300 | 4.76606600 | -3.53336100 |
| C | -6.14707300 | 1.95829200 | -1.79570600 |
| C | -5.27229300 | 1.53879500 | -0.59952200 |
| C | -5.44010900 | 1.56431000 | -3.09751200 |
| C | -5.33502600 | 0.04032200 | -3.23938600 |
| C | -6.69220000 | -0.67711000 | -3.14901200 |
| C | -6.57702900 | -2.22113100 | -3.30347800 |
| C | -6.27609700 | -2.52879000 | -4.78591000 |
| O | -5.74946800 | -5.49172700 | -3.70510100 |
| H | -7.29127500 | -0.33110300 | -4.00620000 |
| H | -6.98590300 | -0.67497400 | -1.00879200 |
| H | -8.04415900 | 1.62085300 | -2.68822100 |
| H | -6.91361200 | -5.99665000 | -2.08054200 |
| H | -4.93887100 | -4.68610900 | -1.40426600 |
| H | -6.46370100 | -3.97607900 | -0.86778400 |
| H | -4.54987900 | -2.96907900 | -3.00028400 |
| H | -5.20698700 | -2.14685000 | -1.59784400 |
| H | -8.78939100 | -4.82182700 | -2.65863100 |
| H | -8.02885900 | -4.62128700 | -4.22929400 |
| H | -9.79826500 | -2.85123200 | -2.10381000 |
| H | -9.39046900 | -0.71714300 | -0.98321400 |
| H | -9.49981800 | -0.25165400 | -2.66560400 |
| H | -7.96691000 | 1.32209800 | 0.32650500 |
| H | -9.32217400 | 1.82560800 | -0.66895200 |

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| H | -7.32822500 | 3.54734500 | 0.48402800 |
| H | -8.50512300 | 4.03376400 | -0.70220000 |
| H | -5.70820300 | 3.97691800 | -1.09421200 |
| H | -7.41223900 | 3.58754500 | -3.54761700 |
| H | -8.00570700 | 5.94063300 | -3.59147600 |
| H | -8.84744500 | 5.07520000 | -2.33648900 |
| H | -6.44565500 | 6.91879500 | -1.92832700 |
| H | -7.20720200 | 6.01187700 | -0.63782300 |
| H | -9.39704900 | 7.14742100 | -1.17398100 |
| H | -8.57333200 | 8.12989800 | -2.37101200 |
| H | -7.93824100 | 8.07750800 | 0.60992800 |
| H | -6.87286000 | 9.90857200 | -1.59885300 |
| H | -5.92594600 | 8.72046800 | -0.69380100 |
| H | -6.58408200 | 10.13464800 | 0.13059600 |
| H | -9.42082900 | 10.17747900 | -1.05224800 |
| H | -9.02799800 | 10.31971900 | 0.66508500 |
| H | -10.16798500 | 9.08173700 | 0.11703300 |
| H | -5.06788300 | 5.43945000 | -2.87356500 |
| H | -5.86610800 | 5.32139400 | -4.44450100 |
| H | -4.94660000 | 3.95862000 | -3.80928300 |
| H | -5.67200500 | 1.89817600 | 0.35004300 |
| H | -4.26963700 | 1.96485500 | -0.70694700 |
| H | -5.17024500 | 0.45646900 | -0.51262400 |
| H | -4.43417900 | 1.99513700 | -3.14366200 |
| H | -5.99660100 | 1.95557300 | -3.95585200 |
| H | -4.65755600 | -0.34390600 | -2.47227800 |

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|---|-------------|-------------|-------------|
| H | -4.85799000 | -0.18727800 | -4.19673200 |
| H | -5.40255200 | -1.96642400 | -5.12340700 |
| H | -7.12370300 | -2.24683900 | -5.41864300 |
| H | -6.05434200 | -3.58460800 | -4.93473800 |
| H | -6.22934700 | -6.08377900 | -4.29572000 |
| C | 12.22934300 | 4.09490000 | -0.66221100 |
| H | 13.15999700 | 3.56127800 | -0.43167900 |
| C | 11.88470400 | 4.94407700 | 0.56047400 |
| H | 10.96133600 | 5.50322100 | 0.34313700 |
| C | 11.60742100 | 4.05199000 | 1.76450100 |
| H | 12.52087900 | 3.46940800 | 1.97449500 |
| C | 10.82834200 | 2.30826100 | 0.36638900 |
| H | 11.69258300 | 1.67663700 | 0.62354500 |
| C | 11.13223100 | 3.06789300 | -0.92196300 |
| H | 11.46610200 | 2.32934900 | -1.66570900 |
| C | 11.20418400 | 4.83541500 | 2.99297100 |
| H | 10.27945300 | 5.38323500 | 2.79322900 |
| H | 11.98899100 | 5.54949000 | 3.24736800 |
| H | 11.03359600 | 4.16373700 | 3.83724600 |
| C | 9.27856000 | 0.64101100 | 1.13703300 |
| H | 9.39317000 | 1.13815500 | 2.10575100 |
| C | 7.82970700 | 0.37285300 | 0.87692300 |
| H | 7.58347800 | -0.06997800 | -0.08451200 |
| C | 6.85392600 | 0.66342000 | 1.74263100 |
| H | 7.09977500 | 1.11001300 | 2.70569000 |
| C | 5.45273200 | 0.43357300 | 1.45348200 |

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|---|-------------|-------------|------------|
| H | 5.22489000 | -0.00787700 | 0.48647600 |
| C | 4.43429800 | 0.74509700 | 2.27731200 |
| H | 4.64480200 | 1.19441800 | 3.24750200 |
| C | 3.05296200 | 0.51914100 | 1.92506300 |
| H | 2.88161300 | 0.05208700 | 0.95716100 |
| C | 1.99240900 | 0.82887900 | 2.69772500 |
| H | 2.14891700 | 1.29612900 | 3.66947600 |
| C | 0.63254100 | 0.57206500 | 2.29322700 |
| H | 0.49149100 | 0.07237100 | 1.33477200 |
| C | -0.46066900 | 0.89206300 | 3.01585700 |
| H | -0.33904200 | 1.38159900 | 3.98143900 |
| C | -1.80635800 | 0.63685500 | 2.56815600 |
| H | -1.91568900 | 0.15193000 | 1.59779000 |
| C | -2.92180000 | 0.95463200 | 3.25666000 |
| H | -2.83163700 | 1.42929100 | 4.23290700 |
| C | -4.24928400 | 0.69872000 | 2.75565300 |
| H | -4.31154900 | 0.26036500 | 1.76257000 |
| C | -5.40008600 | 0.94440200 | 3.40946700 |
| H | -5.37586500 | 1.37169500 | 4.41112900 |
| C | 10.16657400 | -0.60924300 | 1.09718900 |
| H | 11.19399600 | -0.30447200 | 1.30875000 |
| H | 9.86044000 | -1.29996100 | 1.88858000 |
| C | -6.69233000 | 0.61842100 | 2.83840300 |
| H | -6.66670100 | 0.26013200 | 1.81334600 |
| C | -7.86706200 | 0.66699100 | 3.47568800 |
| H | -7.90160300 | 1.00631100 | 4.51218200 |

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| C | -9.17539500 | 0.23266100 | 2.87624300 |
| H | -9.04829100 | 0.10839800 | 1.79563600 |
| C | -9.61803600 | -1.13072500 | 3.44018700 |
| H | -9.83374200 | -0.98815800 | 4.51227600 |
| C | -8.55566300 | -2.24353600 | 3.34981600 |
| H | -7.67706700 | -1.85987300 | 3.87686300 |
| C | -8.08538000 | -2.52001500 | 1.91591500 |
| H | -7.88283400 | -1.58274700 | 1.40356500 |
| C | -5.72813700 | -2.70686700 | 1.47147400 |
| C | -4.49449900 | -3.54131600 | 1.69924700 |
| H | -4.59062300 | -4.07649500 | 2.64615000 |
| H | -4.46122900 | -4.28741000 | 0.89760500 |
| C | -3.21296200 | -2.70670800 | 1.66340000 |
| H | -3.25022200 | -1.95690600 | 2.46648300 |
| C | -1.97856400 | -3.57675600 | 1.84594700 |
| H | -2.05662200 | -4.10225200 | 2.80370800 |
| H | -1.95626300 | -4.33270700 | 1.05192900 |
| C | -0.66386700 | -2.80064600 | 1.81431600 |
| H | -0.70526900 | -1.98221900 | 2.54654200 |
| C | 0.52127500 | -3.70033800 | 2.14875100 |
| H | 0.44306700 | -4.62191700 | 1.55893700 |
| H | 0.42647400 | -3.99199100 | 3.19916300 |
| C | 1.88632600 | -3.03735500 | 1.90162300 |
| H | 1.78463300 | -1.94947400 | 1.89090100 |
| H | 2.56976300 | -3.26946800 | 2.72424100 |
| C | 2.57040200 | -3.49510800 | 0.61461100 |

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| H | 2.82340800 | -4.55943000 | 0.71848700 |
| C | 3.87638700 | -2.70307300 | 0.35068400 |
| H | 4.25721200 | -2.29046200 | 1.29202000 |
| C | 4.96450300 | -3.54770700 | -0.30303700 |
| H | 4.59219900 | -3.93850600 | -1.25781800 |
| H | 5.18160600 | -4.40573000 | 0.34367600 |
| C | 6.25464200 | -2.76582500 | -0.53258200 |
| H | 6.58760600 | -2.33852000 | 0.42313600 |
| C | 7.37014500 | -3.65043300 | -1.07392000 |
| H | 7.04519900 | -4.12680800 | -2.00408900 |
| H | 7.57919200 | -4.43552500 | -0.34151400 |
| C | 8.66441100 | -2.88970100 | -1.36376700 |
| C | 9.82568200 | -3.81748200 | -1.69056300 |
| H | 9.63339100 | -4.35053800 | -2.62398900 |
| H | 9.93477700 | -4.55254800 | -0.88816200 |
| C | 11.13478400 | -3.05695700 | -1.81337500 |
| H | 11.07852500 | -2.39797200 | -2.69206400 |
| C | 11.35650100 | -2.16743000 | -0.55919800 |
| H | 11.58968100 | -2.84525000 | 0.27044900 |
| C | 10.10165600 | -1.34226200 | -0.23748200 |
| H | 9.95748500 | -0.61591900 | -1.04262600 |
| C | 12.54205600 | -1.26575900 | -0.78724100 |
| C | -8.98821400 | -3.38238600 | 1.05893900 |
| H | -8.59679200 | -3.44153700 | 0.04182800 |
| H | -9.98088900 | -2.93093600 | 1.02892200 |
| H | -9.06875900 | -4.39300200 | 1.46521700 |

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| C | -9.01565800 | -3.51171600 | 4.06719900 |
| H | -9.93803300 | -3.91387900 | 3.63716800 |
| H | -9.19652100 | -3.31141600 | 5.12710800 |
| H | -8.25578200 | -4.29327500 | 3.99687300 |
| C | -10.26339600 | 1.28544900 | 3.10049600 |
| H | -10.40994400 | 1.46950400 | 4.17067600 |
| H | -11.21185100 | 0.95180300 | 2.67822800 |
| H | -9.97960200 | 2.23170000 | 2.63360500 |
| O | 9.98911100 | 3.76374300 | -1.37476000 |
| H | 9.22884400 | 3.20512300 | -1.15915400 |
| O | 12.95740500 | 5.80818600 | 0.85759000 |
| H | 13.25433100 | 6.12243000 | -0.01183800 |
| O | 10.53543100 | 3.17191500 | 1.44263500 |
| O | 9.69163100 | 1.55110200 | 0.10332200 |
| O | 8.52082700 | -2.00385100 | -2.43544800 |
| H | 7.64784400 | -1.58310900 | -2.33146000 |
| O | 8.97190100 | -2.19880000 | -0.15667600 |
| O | 12.53270900 | -0.06055500 | -0.87030300 |
| O | 13.69595100 | -1.96281000 | -0.94192000 |
| H | 14.39004800 | -1.30828800 | -1.12387300 |
| O | 6.04778300 | -1.69959800 | -1.46275200 |
| H | 5.13098000 | -1.38754400 | -1.34885400 |
| O | 3.55377100 | -1.58587100 | -0.47965100 |
| H | 2.77546300 | -1.90949300 | -0.98019000 |
| O | 1.75700700 | -3.35591900 | -0.54132300 |
| H | 0.89274400 | -2.96813300 | -0.28436800 |

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| O | -0.43583200 | -2.23269500 | 0.52153400 |
| H | -1.30005300 | -1.95834800 | 0.16322300 |
| O | -3.08183100 | -2.04278800 | 0.40754700 |
| H | -3.91495000 | -1.56667200 | 0.25061000 |
| O | -5.72140200 | -1.68105400 | 0.80730000 |
| O | -6.80448700 | -3.22052300 | 2.04271700 |
| O | -10.81685800 | -1.47955100 | 2.75439600 |
| H | -11.26883100 | -2.16842800 | 3.25326600 |
| O | 12.14470000 | -4.03096200 | -1.96338000 |
| H | 13.00127600 | -3.58615700 | -1.93778100 |
| N | 12.49555500 | 5.00517200 | -1.77277600 |
| H | 11.60074100 | 5.32052100 | -2.14121200 |
| H | 12.96860000 | 4.51958500 | -2.52831200 |

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|---|-------------|-------------|-------------|
| C | -6.11272900 | 1.25219300 | 0.89937000 |
| H | -6.73826800 | 0.61707500 | 0.26249600 |
| C | -5.75724200 | 2.49396800 | 0.08180900 |
| H | -5.14451700 | 3.16251500 | 0.70234300 |
| C | -4.93982800 | 2.09869600 | -1.14267700 |
| H | -5.55903700 | 1.42789600 | -1.76103900 |
| C | -4.04825900 | 0.21603700 | -0.02479800 |
| H | -4.61837900 | -0.46238400 | -0.68203400 |

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| C | -4.84712100 | 0.47693500 | 1.25023400 |
| H | -5.10872500 | -0.49717400 | 1.69095600 |
| C | -4.50123700 | 3.29629700 | -1.95616600 |
| H | -3.85241000 | 3.92974700 | -1.34743800 |
| H | -5.37449900 | 3.87245000 | -2.26234500 |
| H | -3.94768600 | 2.97477200 | -2.83916500 |
| C | -1.91808100 | -0.65337700 | -0.68943400 |
| H | -1.89962500 | 0.19195700 | -1.38148000 |
| C | -0.57092800 | -0.78161400 | -0.04528200 |
| H | -0.46438700 | -1.51195200 | 0.75401200 |
| C | 0.47445400 | -0.04236400 | -0.42843600 |
| H | 0.34652300 | 0.67698400 | -1.23609600 |
| C | 1.79573000 | -0.11311200 | 0.16769400 |
| H | 1.93467000 | -0.78823700 | 1.00950100 |
| C | 2.83393800 | 0.62713800 | -0.26501200 |
| H | 2.67990800 | 1.29960200 | -1.10793400 |
| C | 4.15950700 | 0.60334700 | 0.31056200 |
| H | 4.31922300 | -0.04561900 | 1.17034300 |
| C | 5.17810700 | 1.33682100 | -0.18459700 |
| H | 4.98783700 | 1.97020300 | -1.05025200 |
| C | 6.52249000 | 1.35170800 | 0.33980400 |
| H | 6.74457400 | 0.74469600 | 1.21649700 |
| C | 7.51241800 | 2.07382100 | -0.22689400 |
| H | 7.28629600 | 2.66600400 | -1.11260700 |
| C | 8.87230300 | 2.12188400 | 0.25324300 |
| H | 9.10808200 | 1.56269000 | 1.15765700 |

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| C | 9.84882500 | 2.80856900 | -0.37513000 |
| H | 9.60573100 | 3.34580200 | -1.29048600 |
| C | 11.21966500 | 2.87853400 | 0.07530300 |
| H | 11.45461400 | 2.41363500 | 1.03139900 |
| C | 12.20662800 | 3.46257400 | -0.63055200 |
| H | 11.97385600 | 3.90744200 | -1.59677800 |
| C | -2.38898200 | -1.90261400 | -1.44264600 |
| H | -3.36701300 | -1.70494600 | -1.87744700 |
| H | -1.69728300 | -2.09912800 | -2.26629100 |
| C | 13.59281400 | 3.50057100 | -0.20224100 |
| H | 13.79463400 | 3.15007600 | 0.80775200 |
| C | 14.60798200 | 3.87928600 | -0.98777300 |
| H | 14.39032300 | 4.21654300 | -2.00295500 |
| C | 16.05962700 | 3.83847400 | -0.60647400 |
| H | 16.14658400 | 3.57550000 | 0.45315400 |
| C | 16.80591200 | 2.75968400 | -1.41534000 |
| H | 16.86685900 | 3.11439300 | -2.45668800 |
| C | 16.11210600 | 1.38610700 | -1.45499600 |
| H | 15.13417500 | 1.55515700 | -1.91606800 |
| C | 15.81576300 | 0.83077500 | -0.05797400 |
| H | 15.42677000 | 1.62157700 | 0.57672700 |
| C | 13.70764200 | -0.07243800 | 0.60533400 |
| C | 12.68646000 | -1.15726000 | 0.36056100 |
| H | 12.80687900 | -1.54707500 | -0.65042400 |
| H | 12.90419200 | -1.96627700 | 1.06706900 |
| C | 11.25273200 | -0.66919600 | 0.59377200 |

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| H | 11.02994400 | 0.13571700 | -0.12154100 |
| C | 10.25669100 | -1.80722100 | 0.40630300 |
| H | 10.39488600 | -2.23374200 | -0.59252000 |
| H | 10.48021700 | -2.58780000 | 1.14369100 |
| C | 8.79436600 | -1.38804400 | 0.56126000 |
| H | 8.58314000 | -0.57732300 | -0.15343500 |
| C | 7.85752900 | -2.55692100 | 0.27457100 |
| H | 8.14533100 | -3.35927000 | 0.96725700 |
| H | 8.02989400 | -2.92850600 | -0.74129500 |
| C | 6.38924400 | -2.17504100 | 0.45369800 |
| H | 6.26854600 | -1.65327500 | 1.40639700 |
| H | 6.09624000 | -1.47807900 | -0.33828200 |
| C | 5.44687000 | -3.37194900 | 0.43482500 |
| H | 5.59351600 | -3.95289500 | -0.48667700 |
| C | 3.97579300 | -2.96171600 | 0.52671800 |
| H | 3.76627900 | -2.18557200 | -0.21668700 |
| C | 3.04032300 | -4.15061100 | 0.32082500 |
| H | 3.26417300 | -4.91453800 | 1.07341900 |
| H | 3.24502400 | -4.58566200 | -0.66346500 |
| C | 1.55779400 | -3.78847900 | 0.38810100 |
| H | 1.33530700 | -3.00097600 | -0.34482100 |
| C | 0.69626100 | -5.00776700 | 0.08072100 |
| H | 0.96203300 | -5.82198100 | 0.76207400 |
| H | 0.90606700 | -5.33124800 | -0.94226100 |
| C | -0.80683900 | -4.76525100 | 0.21159500 |
| C | -1.62590100 | -5.93477000 | -0.31398500 |

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| H | -1.45070100 | -6.82243000 | 0.29624400 |
| H | -1.33161500 | -6.15152100 | -1.34478200 |
| C | -3.10039500 | -5.58899600 | -0.28239700 |
| H | -3.40759100 | -5.45529900 | 0.76059100 |
| C | -3.37597000 | -4.27162700 | -1.03238900 |
| H | -3.20523000 | -4.44389900 | -2.10359500 |
| C | -2.41881700 | -3.14837100 | -0.56157200 |
| H | -2.68100200 | -2.87691100 | 0.46831500 |
| C | -4.85101300 | -3.94532000 | -0.86539500 |
| C | 16.96153900 | 0.13075000 | 0.64901500 |
| H | 16.64982200 | -0.16670400 | 1.65194100 |
| H | 17.80866900 | 0.81289500 | 0.72731700 |
| H | 17.26907000 | -0.76213600 | 0.10199600 |
| C | 16.88361300 | 0.39925500 | -2.32989400 |
| H | 17.89070600 | 0.21702300 | -1.94526300 |
| H | 16.97125200 | 0.77975600 | -3.35063800 |
| H | 16.37000300 | -0.56319300 | -2.37170000 |
| C | 16.72684200 | 5.20140000 | -0.81877200 |
| H | 16.62924200 | 5.51559400 | -1.86250700 |
| H | 17.78706700 | 5.14539500 | -0.57204600 |
| H | 16.25455700 | 5.96004900 | -0.19304500 |
| O | -4.10465200 | 1.25234900 | 2.16259500 |
| H | -3.19028600 | 0.95105700 | 2.10360100 |
| O | -6.93138400 | 3.14224400 | -0.36088800 |
| H | -7.50621500 | 3.19407700 | 0.41387300 |
| O | -3.77066400 | 1.41114400 | -0.71698800 |

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| O | -2.84113200 | -0.34494700 | 0.37353200 |
| O | -1.19585900 | -4.54620400 | 1.53810400 |
| H | -0.51999200 | -3.98207700 | 1.94206200 |
| O | -1.07878600 | -3.62625000 | -0.59347900 |
| O | -5.63700000 | -4.66393700 | -0.29542600 |
| O | -5.24152800 | -2.79696100 | -1.42870200 |
| H | -6.20925700 | -2.70592600 | -1.31912000 |
| O | 1.19582600 | -3.31669200 | 1.68907500 |
| H | 1.93537200 | -2.79489200 | 2.02983700 |
| O | 3.75234400 | -2.35570000 | 1.80517200 |
| H | 4.26677300 | -2.88467900 | 2.43173500 |
| O | 5.64635100 | -4.21212500 | 1.57209800 |
| H | 6.58649800 | -4.27860500 | 1.75244100 |
| O | 8.50131400 | -0.94674100 | 1.87790100 |
| H | 9.29300000 | -0.51845300 | 2.22866500 |
| O | 11.09013800 | -0.17674000 | 1.91921400 |
| H | 11.85431300 | 0.38083800 | 2.12499100 |
| O | 13.59641900 | 0.75367300 | 1.48615200 |
| O | 14.73782300 | -0.13875100 | -0.22671100 |
| O | 18.11514700 | 2.68303500 | -0.86329800 |
| H | 18.68974800 | 2.24288600 | -1.49384000 |
| O | -3.80059900 | -6.66519100 | -0.87367700 |
| H | -4.72703300 | -6.53640000 | -0.64843900 |
| N | -6.91941000 | 1.66296300 | 2.04583500 |
| H | -6.29770800 | 2.04313800 | 2.75640400 |
| H | -7.38278500 | 0.85951100 | 2.46016700 |

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| C | -10.08636500 | -4.73920800 | -1.52168800 |
| C | -10.96012200 | -3.88723900 | -0.59431800 |
| C | -10.15441300 | -3.47644700 | 0.63678600 |
| C | -8.60326300 | -4.30852400 | -1.42590500 |
| C | -8.55668800 | -2.83324300 | -1.13379100 |
| C | -8.25979300 | -1.93860900 | -2.08250800 |
| C | -8.50007100 | -0.46532400 | -1.92086000 |
| C | -9.66912900 | -0.22415900 | -0.96357400 |
| C | -9.84840400 | 1.26148000 | -0.67019200 |
| C | -10.01093300 | 2.21564300 | -1.85055700 |
| C | -10.64955000 | 3.47965400 | -1.22211700 |
| C | -10.99016500 | 3.15316200 | 0.26852700 |
| C | -10.03895600 | 3.76533300 | 1.33281700 |
| C | -9.41513300 | 5.11988800 | 0.95075400 |
| C | -10.41290600 | 6.23849300 | 0.63887000 |
| C | -9.71715600 | 7.47783900 | 0.07792700 |
| C | -10.65789500 | 8.60590600 | -0.35758600 |
| C | -11.50359100 | 9.12958400 | 0.80415100 |
| C | -9.85804000 | 9.74720900 | -0.98578600 |
| C | -10.77263000 | 3.90536600 | 2.67345200 |
| C | -11.03202500 | 1.58762600 | 0.26091300 |
| C | -12.38130500 | 1.17164500 | -0.34993100 |
| C | -10.81518500 | 0.83605100 | 1.58162700 |
| C | -10.58919500 | -0.66651300 | 1.34851100 |
| C | -9.43539400 | -0.94793800 | 0.37455500 |
| C | -9.03170600 | -2.46245600 | 0.26851700 |

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| C | -7.85731100 | -2.68044200 | 1.24572800 |
| O | -10.24559400 | -6.08855300 | -1.10632900 |
| H | -8.55705000 | -0.44318000 | 0.80271500 |
| H | -10.57246500 | -0.62335500 | -1.44457800 |
| H | -8.94225800 | 1.57723100 | -0.13219900 |
| H | -10.42983400 | -4.62351800 | -2.55745900 |
| H | -11.83600900 | -4.48034500 | -0.32535500 |
| H | -11.30824400 | -2.99746000 | -1.12867800 |
| H | -9.69289700 | -4.38070000 | 1.04551400 |
| H | -10.79570200 | -3.08575600 | 1.42422400 |
| H | -8.06648300 | -4.54758600 | -2.34839700 |
| H | -8.13899400 | -4.87830200 | -0.61674400 |
| H | -7.92186900 | -2.30047200 | -3.05213200 |
| H | -8.72009300 | -0.02556800 | -2.89767800 |
| H | -7.60694100 | 0.05995200 | -1.55682400 |
| H | -10.66325000 | 1.77842200 | -2.61365100 |
| H | -9.05112100 | 2.43698200 | -2.32054300 |
| H | -11.56184200 | 3.75438500 | -1.75633300 |
| H | -9.97965300 | 4.33212000 | -1.31216000 |
| H | -11.99387300 | 3.53421600 | 0.48979200 |
| H | -9.20240300 | 3.07496200 | 1.49496000 |
| H | -8.77837100 | 5.44113600 | 1.78439200 |
| H | -8.73810600 | 4.99797100 | 0.09944000 |
| H | -10.96291600 | 6.50311800 | 1.54619000 |
| H | -11.15778800 | 5.88691900 | -0.08564500 |
| H | -9.10807400 | 7.17859800 | -0.78398900 |

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|---|--------------|-------------|-------------|
| H | -9.01539400 | 7.87120900 | 0.82610500 |
| H | -11.33594200 | 8.20095500 | -1.11984300 |
| H | -10.85749300 | 9.47046000 | 1.62024200 |
| H | -12.17359200 | 8.36501000 | 1.20162300 |
| H | -12.11709200 | 9.97700200 | 0.48822300 |
| H | -9.17618200 | 10.18344300 | -0.24858100 |
| H | -10.51552500 | 10.54262700 | -1.34496300 |
| H | -9.25841800 | 9.39562700 | -1.82899900 |
| H | -11.61065300 | 4.60130800 | 2.57988200 |
| H | -10.10056300 | 4.28952700 | 3.44569900 |
| H | -11.17703600 | 2.95560000 | 3.02279600 |
| H | -12.57722500 | 1.69427200 | -1.28869100 |
| H | -13.18797400 | 1.42672300 | 0.34338400 |
| H | -12.44566100 | 0.10162400 | -0.55255200 |
| H | -11.67176200 | 0.96702700 | 2.25075900 |
| H | -9.93546100 | 1.24028300 | 2.09352400 |
| H | -11.50949100 | -1.12415500 | 0.97191500 |
| H | -10.38323800 | -1.14191800 | 2.31319600 |
| H | -8.17867800 | -2.45296600 | 2.26779400 |
| H | -7.02087000 | -2.01750900 | 0.99745500 |
| H | -7.49023100 | -3.70774300 | 1.22102200 |
| H | -9.61971100 | -6.62924100 | -1.59474000 |

AmB-Chol11

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|---|--------------|-------------|-------------|
| C | -19.65446000 | -1.86274400 | -0.97030200 |
| C | -18.51415500 | -2.58636600 | -1.66761400 |
| C | -17.28559100 | -1.69570900 | -1.90939400 |
| C | -19.17400100 | -1.30358200 | 0.39539000 |
| C | -17.66759400 | -1.30956800 | 0.50567700 |
| C | -17.05830000 | -1.86396200 | 1.55166800 |
| C | -15.57418600 | -2.03480500 | 1.66817300 |
| C | -14.87676400 | -1.93234800 | 0.31188400 |
| C | -13.36360100 | -1.86086000 | 0.48284400 |
| C | -12.67272200 | -3.03682800 | 1.16758700 |
| C | -11.18623300 | -2.88625600 | 0.76672600 |
| C | -11.09067200 | -1.75215100 | -0.30687800 |
| C | -10.46952200 | -0.42370500 | 0.20005800 |
| C | -9.29422300 | -0.60615600 | 1.18109500 |
| C | -8.14343100 | -1.48582000 | 0.68846900 |
| C | -6.95468600 | -1.46443000 | 1.64591200 |
| C | -5.77692400 | -2.36157600 | 1.25032800 |
| C | -5.21284900 | -1.99112500 | -0.12292400 |
| C | -4.68182100 | -2.28287700 | 2.31410700 |
| C | -9.99993900 | 0.45664300 | -0.96750000 |
| C | -12.56797100 | -1.66673400 | -0.82152400 |
| C | -12.76625100 | -2.83244600 | -1.80896400 |
| C | -13.06163100 | -0.36781100 | -1.46884100 |
| C | -14.57670800 | -0.39489400 | -1.70800700 |
| C | -15.39556800 | -0.69410200 | -0.44108400 |

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|---|--------------|-------------|-------------|
| C | -16.92690600 | -0.76384200 | -0.70672800 |
| C | -17.43069400 | 0.66607500 | -0.99282600 |
| O | -20.10675200 | -0.84662200 | -1.86054700 |
| H | -15.24242100 | 0.15483800 | 0.24389300 |
| H | -15.13157100 | -2.83227700 | -0.26443900 |
| H | -13.16504400 | -0.96411900 | 1.09126100 |
| H | -20.47461900 | -2.57390400 | -0.79556900 |
| H | -18.87166200 | -2.99624000 | -2.61627200 |
| H | -18.23017900 | -3.43273400 | -1.03317800 |
| H | -17.44660500 | -1.08531500 | -2.80198700 |
| H | -16.44508700 | -2.35922600 | -2.13258800 |
| H | -19.59393300 | -1.90164000 | 1.20918400 |
| H | -19.57208200 | -0.28851600 | 0.51339000 |
| H | -17.66500900 | -2.24735000 | 2.37062100 |
| H | -15.35310300 | -3.00270300 | 2.13210900 |
| H | -15.15696300 | -1.27756900 | 2.34899100 |
| H | -13.08971500 | -3.98177900 | 0.80322400 |
| H | -12.81243400 | -3.02989300 | 2.25143600 |
| H | -10.79878300 | -3.82290400 | 0.35760700 |
| H | -10.57512900 | -2.67023700 | 1.64141000 |
| H | -10.44907800 | -2.09514800 | -1.12711400 |
| H | -11.24035500 | 0.13239900 | 0.74999200 |
| H | -8.89609300 | 0.39100600 | 1.40886700 |
| H | -9.65294800 | -0.99326400 | 2.14058500 |
| H | -7.82209700 | -1.14861800 | -0.30109900 |
| H | -8.48662500 | -2.51870200 | 0.55893000 |

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|---|--------------|-------------|-------------|
| H | -7.29943700 | -1.75206100 | 2.64768700 |
| H | -6.58369100 | -0.43469500 | 1.73814200 |
| H | -6.13759900 | -3.39843400 | 1.20513100 |
| H | -4.95539400 | -0.92734900 | -0.14917700 |
| H | -5.92793900 | -2.17875400 | -0.92728800 |
| H | -4.31022700 | -2.56850800 | -0.34634900 |
| H | -4.30164000 | -1.25807000 | 2.39296700 |
| H | -3.83804300 | -2.93555100 | 2.07063600 |
| H | -5.05888000 | -2.57261200 | 3.29936200 |
| H | -9.21291600 | -0.04125800 | -1.54155600 |
| H | -9.58649600 | 1.40070600 | -0.59895200 |
| H | -10.79940900 | 0.69875100 | -1.66428100 |
| H | -12.37343900 | -3.77330200 | -1.41775800 |
| H | -12.23179600 | -2.61840000 | -2.73984200 |
| H | -13.81381200 | -3.00146600 | -2.06262500 |
| H | -12.55641800 | -0.18616200 | -2.42366900 |
| H | -12.82939600 | 0.48005800 | -0.81535200 |
| H | -14.80396300 | -1.12997800 | -2.48381900 |
| H | -14.87762800 | 0.57215400 | -2.11983400 |
| H | -16.85678800 | 1.12117700 | -1.80329600 |
| H | -17.32332800 | 1.29865500 | -0.10579200 |
| H | -18.47412900 | 0.66087700 | -1.30450300 |
| H | -20.84350800 | -0.38658400 | -1.44197600 |
| C | 15.99011000 | 1.64809900 | -1.57950100 |
| H | 16.68860800 | 1.00206700 | -1.03290200 |
| C | 15.86938700 | 2.94916800 | -0.78806400 |

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|---|-------------|-------------|-------------|
| H | 15.18469800 | 3.62024600 | -1.32959200 |
| C | 15.25977300 | 2.68116900 | 0.58281900 |
| H | 15.92926700 | 1.99067200 | 1.12399100 |
| C | 14.04197700 | 0.83201800 | -0.25701200 |
| H | 14.64613300 | 0.12689200 | 0.33454900 |
| C | 14.63877200 | 0.94615700 | -1.65693900 |
| H | 14.75856800 | -0.07621000 | -2.04483600 |
| C | 15.06028200 | 3.94266200 | 1.39162800 |
| H | 14.36893100 | 4.60937300 | 0.86945700 |
| H | 16.01602800 | 4.45390500 | 1.51711900 |
| H | 14.64046300 | 3.70702000 | 2.37207700 |
| C | 12.00310200 | 0.07487000 | 0.76427500 |
| H | 12.22012000 | 0.84516200 | 1.51133400 |
| C | 10.55988900 | 0.14343600 | 0.37515700 |
| H | 10.23008300 | -0.55174100 | -0.39236200 |
| C | 9.68989700 | 1.01071300 | 0.90152700 |
| H | 10.02005200 | 1.71094400 | 1.66835900 |
| C | 8.30531000 | 1.08741600 | 0.48100200 |
| H | 7.99380600 | 0.38122200 | -0.28472500 |
| C | 7.40370600 | 1.97035100 | 0.95056500 |
| H | 7.70056400 | 2.68947700 | 1.71358200 |
| C | 6.04201600 | 2.01574600 | 0.47426400 |
| H | 5.77730600 | 1.26988200 | -0.27260700 |
| C | 5.09874300 | 2.88452200 | 0.89020600 |
| H | 5.34644700 | 3.63615700 | 1.63907900 |
| C | 3.74990200 | 2.86963900 | 0.38051300 |

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|---|-------------|-------------|-------------|
| H | 3.50710100 | 2.08973000 | -0.34116000 |
| C | 2.77848800 | 3.73262900 | 0.74223200 |
| H | 2.99948700 | 4.50995500 | 1.47288400 |
| C | 1.44546200 | 3.70028100 | 0.19446200 |
| H | 1.23554800 | 2.92501200 | -0.54244300 |
| C | 0.45764100 | 4.55406100 | 0.53145500 |
| H | 0.64949400 | 5.32033000 | 1.28173800 |
| C | -0.85948900 | 4.51765300 | -0.05645500 |
| H | -1.02035400 | 3.78773200 | -0.84800700 |
| C | -1.89282100 | 5.29711100 | 0.31173600 |
| H | -1.76298000 | 6.01597000 | 1.11993100 |
| C | 12.44571200 | -1.29332900 | 1.29804200 |
| H | 13.50677500 | -1.23377500 | 1.55064000 |
| H | 11.90213200 | -1.51939400 | 2.22029200 |
| C | -3.20737000 | 5.19303000 | -0.29147100 |
| H | -3.27460600 | 4.54168800 | -1.16060900 |
| C | -4.31786400 | 5.77537600 | 0.17380200 |
| H | -4.25383600 | 6.41429100 | 1.05620600 |
| C | -5.69299400 | 5.57471500 | -0.39730200 |
| H | -5.60876200 | 5.03052000 | -1.34495200 |
| C | -6.56258300 | 4.71802000 | 0.54370000 |
| H | -6.76745500 | 5.32465400 | 1.44149000 |
| C | -5.89968700 | 3.41816700 | 1.03660100 |
| H | -4.98367000 | 3.72635400 | 1.54997100 |
| C | -5.43638600 | 2.50765100 | -0.10502300 |
| H | -4.89486300 | 3.09355900 | -0.84185000 |

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|---|-------------|-------------|-------------|
| C | -3.28035200 | 1.45619900 | -0.09116100 |
| C | -2.37698800 | 0.49956800 | 0.64480000 |
| H | -2.66095300 | 0.47274800 | 1.69857000 |
| H | -2.55733000 | -0.49917600 | 0.23122800 |
| C | -0.89737300 | 0.85366200 | 0.48292900 |
| H | -0.71650500 | 1.84903200 | 0.91310300 |
| C | -0.00892400 | -0.16580900 | 1.18099600 |
| H | -0.27057900 | -0.19111700 | 2.24428900 |
| H | -0.21442100 | -1.15910500 | 0.76425700 |
| C | 1.48542200 | 0.11679300 | 1.04689100 |
| H | 1.69571400 | 1.13930800 | 1.38941600 |
| C | 2.31375400 | -0.85967300 | 1.87519700 |
| H | 1.96126000 | -1.87944000 | 1.67709200 |
| H | 2.10539200 | -0.65574700 | 2.92990600 |
| C | 3.82439300 | -0.76742000 | 1.60447300 |
| H | 4.07334600 | 0.20245900 | 1.16710300 |
| H | 4.37775900 | -0.82541900 | 2.54687100 |
| C | 4.36244300 | -1.88043600 | 0.70654200 |
| H | 4.26586700 | -2.83435700 | 1.24353700 |
| C | 5.85694200 | -1.65804900 | 0.36249500 |
| H | 6.32435600 | -1.02868800 | 1.12849700 |
| C | 6.64289500 | -2.95852000 | 0.23442600 |
| H | 6.19628800 | -3.57279100 | -0.55686100 |
| H | 6.55898400 | -3.51667400 | 1.17404000 |
| C | 8.12001700 | -2.72002700 | -0.06484800 |
| H | 8.53995000 | -2.06910400 | 0.71411500 |

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|---|-------------|-------------|-------------|
| C | 8.91862200 | -4.01707500 | -0.08330600 |
| H | 8.49432900 | -4.70133500 | -0.82458400 |
| H | 8.84343300 | -4.48806200 | 0.90105700 |
| C | 10.39644900 | -3.81515700 | -0.42078500 |
| C | 11.21821600 | -5.08136900 | -0.22772500 |
| H | 10.90303700 | -5.84920400 | -0.93730200 |
| H | 11.06081600 | -5.46075200 | 0.78586200 |
| C | 12.70357900 | -4.81908700 | -0.40716600 |
| H | 12.88952300 | -4.54957400 | -1.45708800 |
| C | 13.14759400 | -3.62444300 | 0.48128700 |
| H | 13.12441000 | -3.97798300 | 1.51888400 |
| C | 12.20506300 | -2.42456400 | 0.30515800 |
| H | 12.32705400 | -2.04461400 | -0.71346400 |
| C | 14.56442900 | -3.24298300 | 0.13820900 |
| C | -6.50017300 | 1.68453200 | -0.79911700 |
| H | -6.05218100 | 1.09736800 | -1.60433600 |
| H | -7.25321500 | 2.35388100 | -1.21663300 |
| H | -6.98885800 | 0.99883500 | -0.10666900 |
| C | -6.78464800 | 2.69733400 | 2.05138300 |
| H | -7.74888900 | 2.41065500 | 1.62143600 |
| H | -6.97819300 | 3.33702000 | 2.91744400 |
| H | -6.30334600 | 1.78491200 | 2.40936800 |
| C | -6.38332100 | 6.91235600 | -0.67776500 |
| H | -6.46247700 | 7.50573300 | 0.24000000 |
| H | -7.38947800 | 6.74728400 | -1.06557500 |
| H | -5.81326300 | 7.49583700 | -1.40424300 |

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| O | 13.80182100 | 1.71363100 | -2.49745400 |
| H | 12.89321000 | 1.50813300 | -2.23514400 |
| O | 17.14388200 | 3.52796200 | -0.62623400 |
| H | 17.57128800 | 3.40066900 | -1.48880700 |
| O | 13.98264500 | 2.07668100 | 0.40472800 |
| O | 12.73904700 | 0.37862400 | -0.43333000 |
| O | 10.57888800 | -3.39408200 | -1.74097500 |
| H | 9.87585900 | -2.74417300 | -1.92418500 |
| O | 10.86110500 | -2.83733800 | 0.50504400 |
| O | 14.93846600 | -2.20396600 | -0.35163900 |
| O | 15.44482400 | -4.24058600 | 0.40489900 |
| H | 16.31583600 | -3.92264700 | 0.11588100 |
| O | 8.28893300 | -2.08153700 | -1.33330800 |
| H | 7.50823700 | -1.51611800 | -1.48218000 |
| O | 5.92151600 | -0.92164400 | -0.86063100 |
| H | 5.09669100 | -1.19190600 | -1.31616300 |
| O | 3.66580000 | -2.00497400 | -0.52484400 |
| H | 2.95786200 | -1.32601600 | -0.56613200 |
| O | 1.90753000 | 0.00612100 | -0.31557600 |
| H | 1.18151300 | 0.33492300 | -0.87729200 |
| O | -0.53274300 | 0.86422200 | -0.89511600 |
| H | -1.20253400 | 1.39420300 | -1.36290000 |
| O | -2.95394400 | 2.02520000 | -1.12052300 |
| O | -4.46558000 | 1.58702800 | 0.49059000 |
| O | -7.78056000 | 4.46794000 | -0.15131900 |
| H | -8.45034900 | 4.19554200 | 0.48504500 |

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|---|-------------|-------------|-------------|
| O | 13.36081700 | -6.01813000 | -0.05861800 |
| H | 14.31237100 | -5.85445700 | -0.06189900 |
| N | 16.59120700 | 1.96983500 | -2.87116200 |
| H | 15.86463800 | 2.36293900 | -3.46573600 |
| H | 16.92220700 | 1.12779300 | -3.33139300 |

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|---|--------------|-------------|------------|
| C | -15.33356900 | -2.27637000 | 3.92845100 |
| H | -16.24316200 | -1.96158300 | 3.40141900 |
| C | -15.00863100 | -1.18073800 | 4.94314100 |
| H | -14.12662500 | -1.49039200 | 5.52213100 |
| C | -14.66721700 | 0.12176500 | 4.22973700 |
| H | -15.54643500 | 0.42640000 | 3.63868200 |
| C | -13.84478700 | -1.04133000 | 2.34831300 |
| H | -14.68317400 | -0.67144700 | 1.73589500 |
| C | -14.19633000 | -2.41364100 | 2.92014200 |
| H | -14.49655300 | -3.05653400 | 2.07972600 |
| C | -14.28354500 | 1.22320900 | 5.19226800 |
| H | -13.38262700 | 0.93274000 | 5.73693400 |
| H | -15.09307400 | 1.38258000 | 5.90462000 |
| H | -14.08271600 | 2.14974400 | 4.65304100 |
| C | -12.21159300 | -0.07065100 | 0.88570200 |
| H | -12.30761300 | 0.79970300 | 1.54081000 |

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| C | -10.75848500 | -0.33350800 | 0.62505600 |
| H | -10.51068300 | -1.26751200 | 0.12472600 |
| C | -9.79025000 | 0.51536100 | 0.98165600 |
| H | -10.05464700 | 1.45040000 | 1.47326400 |
| C | -8.37447400 | 0.26667300 | 0.77886100 |
| H | -8.08949500 | -0.69543700 | 0.35723700 |
| C | -7.41538500 | 1.15067900 | 1.11292200 |
| H | -7.71266000 | 2.11125100 | 1.53159100 |
| C | -5.99636400 | 0.91564100 | 0.96820700 |
| H | -5.68801700 | -0.05925300 | 0.59309500 |
| C | -5.06865300 | 1.84472900 | 1.27876400 |
| H | -5.40620400 | 2.81453600 | 1.64217100 |
| C | -3.64133900 | 1.65706900 | 1.17288500 |
| H | -3.26988800 | 0.68667100 | 0.84624200 |
| C | -2.75809400 | 2.63894800 | 1.45168000 |
| H | -3.13666400 | 3.61321500 | 1.75776300 |
| C | -1.32341700 | 2.49801600 | 1.37918000 |
| H | -0.92503700 | 1.51356000 | 1.13677100 |
| C | -0.47412600 | 3.52512900 | 1.58882600 |
| H | -0.88666900 | 4.50935500 | 1.80559800 |
| C | 0.96602800 | 3.42102200 | 1.54048000 |
| H | 1.39285900 | 2.42699400 | 1.41839500 |
| C | 1.79274800 | 4.48097000 | 1.62018100 |
| H | 1.36683000 | 5.47837400 | 1.71690300 |
| C | -13.04817600 | 0.14865000 | -0.38091700 |
| H | -14.08838900 | 0.31096900 | -0.08751800 |

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|---|--------------|-------------|-------------|
| H | -12.70408900 | 1.05609100 | -0.88498600 |
| C | 3.23886900 | 4.38133800 | 1.54479500 |
| H | 3.65557800 | 3.37694900 | 1.57618800 |
| C | 4.05451400 | 5.43177400 | 1.39487000 |
| H | 3.62363300 | 6.43399900 | 1.35536900 |
| C | 5.54535100 | 5.34569000 | 1.23257300 |
| H | 5.86664500 | 4.31127000 | 1.39081000 |
| C | 5.94380800 | 5.76481000 | -0.19532400 |
| H | 5.73067500 | 6.84029900 | -0.29601900 |
| C | 5.17329900 | 5.05199100 | -1.31976100 |
| H | 4.12745600 | 5.34293400 | -1.18149500 |
| C | 5.18210300 | 3.52218300 | -1.20513200 |
| H | 5.01307900 | 3.22640300 | -0.17345700 |
| C | 3.20909600 | 2.18940500 | -1.40733800 |
| C | 2.05848800 | 1.80139700 | -2.30509000 |
| H | 1.90809400 | 2.57761600 | -3.05597900 |
| H | 2.34838200 | 0.87932000 | -2.82144800 |
| C | 0.77212200 | 1.54329400 | -1.51386000 |
| H | 0.48386000 | 2.46624200 | -0.99024000 |
| C | -0.35839000 | 1.11118500 | -2.43944400 |
| H | -0.49812000 | 1.88188200 | -3.20440100 |
| H | -0.06120900 | 0.18269800 | -2.94191300 |
| C | -1.69128600 | 0.88036400 | -1.72588900 |
| H | -1.96403000 | 1.79887000 | -1.18296600 |
| C | -2.79698000 | 0.54910900 | -2.72313700 |
| H | -2.45470100 | -0.33750300 | -3.27316400 |

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| H | -2.90063100 | 1.36673100 | -3.44507000 |
| C | -4.13135300 | 0.27954200 | -2.03117600 |
| H | -3.97708000 | -0.45297000 | -1.23520500 |
| H | -4.48955900 | 1.20186700 | -1.56124800 |
| C | -5.21112700 | -0.24242900 | -2.97060900 |
| H | -5.38525300 | 0.47604700 | -3.78396100 |
| C | -6.53631800 | -0.49805100 | -2.25011300 |
| H | -6.81524000 | 0.38843400 | -1.67155900 |
| C | -7.65191400 | -0.86075700 | -3.22765100 |
| H | -7.34792400 | -1.74200000 | -3.80253600 |
| H | -7.77572100 | -0.03233500 | -3.93360100 |
| C | -8.99906400 | -1.13240800 | -2.56078900 |
| H | -9.30144200 | -0.26306400 | -1.96170700 |
| C | -10.06723900 | -1.40216700 | -3.61475500 |
| H | -9.73655500 | -2.21439700 | -4.26961800 |
| H | -10.19328600 | -0.50002900 | -4.21921100 |
| C | -11.42702500 | -1.79549700 | -3.04048700 |
| C | -12.511128200 | -1.83234000 | -4.10771200 |
| H | -12.29493000 | -2.61337900 | -4.83883800 |
| H | -12.54819000 | -0.86864500 | -4.62253600 |
| C | -13.87378500 | -2.09286500 | -3.49135600 |
| H | -13.88765500 | -3.10798300 | -3.07143300 |
| C | -14.13659200 | -1.08777800 | -2.33728200 |
| H | -14.30305300 | -0.11108200 | -2.80738500 |
| C | -12.94732600 | -1.00812100 | -1.36810900 |
| H | -12.86681000 | -1.95547000 | -0.82616600 |

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| C | -15.43844500 | -1.50056000 | -1.69500500 |
| C | 6.40669800 | 2.80073200 | -1.73299100 |
| H | 6.28663400 | 1.72546600 | -1.58475400 |
| H | 7.28075100 | 3.12158500 | -1.16582800 |
| H | 6.55959500 | 2.99332700 | -2.79625400 |
| C | 5.61677500 | 5.54203400 | -2.69776600 |
| H | 6.66974700 | 5.31965800 | -2.89256800 |
| H | 5.47150000 | 6.62160900 | -2.78827000 |
| H | 5.03436900 | 5.05685500 | -3.48311400 |
| C | 6.26220400 | 6.22578200 | 2.26232400 |
| H | 5.97438800 | 7.27465000 | 2.13942200 |
| H | 7.34410700 | 6.14982900 | 2.15166200 |
| H | 5.99367900 | 5.91516900 | 3.27274800 |
| O | -13.09240600 | -2.96800400 | 3.59948100 |
| H | -12.30440400 | -2.71518500 | 3.10434800 |
| O | -16.12110100 | -0.95959200 | 5.77878100 |
| H | -16.43843300 | -1.84266700 | 6.00742600 |
| O | -13.56228300 | -0.10510300 | 3.36114900 |
| O | -12.69671900 | -1.22655500 | 1.58933600 |
| O | -11.40201100 | -3.05594000 | -2.43269600 |
| H | -10.57404100 | -3.11227000 | -1.93252000 |
| O | -11.75061700 | -0.77948500 | -2.09916500 |
| O | -16.48642200 | -1.57877400 | -2.28520700 |
| O | -15.34564400 | -1.84920700 | -0.39819100 |
| H | -16.22849400 | -2.14301500 | -0.13148600 |
| O | -8.93312800 | -2.27635100 | -1.70480100 |

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| H | -8.06677400 | -2.27211700 | -1.27473700 |
| O | -6.33760900 | -1.54661800 | -1.29401300 |
| H | -5.75772400 | -2.18687500 | -1.73043200 |
| O | -4.86378800 | -1.51629500 | -3.51417400 |
| H | -3.95702800 | -1.48928400 | -3.82598800 |
| O | -1.62722500 | -0.20650700 | -0.81644200 |
| H | -0.73785900 | -0.22265000 | -0.43941900 |
| O | 0.96302600 | 0.50410700 | -0.56044200 |
| H | 1.79655700 | 0.67559400 | -0.09960200 |
| O | 3.36827300 | 1.72727300 | -0.29822400 |
| O | 4.02516200 | 3.06973700 | -1.97181400 |
| O | 7.35715700 | 5.57178300 | -0.30155300 |
| H | 7.67897400 | 5.98752500 | -1.10507600 |
| O | -14.82220600 | -1.95614900 | -4.52356600 |
| H | -15.70027300 | -1.96730100 | -4.12536500 |
| N | -15.64069200 | -3.49446700 | 4.67532300 |
| H | -14.76051600 | -3.91635800 | 4.96207700 |
| H | -16.11190600 | -4.17104300 | 4.08512200 |
| C | 9.45626400 | 2.93701800 | 1.29663000 |
| C | 9.49170100 | 1.42366900 | 1.53583300 |
| C | 9.46038700 | 0.69372200 | 0.19477200 |
| C | 10.22100200 | 3.30754000 | 0.00021300 |
| C | 11.30350700 | 2.28933400 | -0.23026300 |
| C | 12.58285100 | 2.56084100 | 0.02038600 |
| C | 13.64215100 | 1.49966400 | 0.08721000 |
| C | 13.02349500 | 0.17220600 | 0.52944300 |

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| C | 14.05974000 | -0.94735100 | 0.52862000 |
| C | 15.29530100 | -0.78103300 | 1.41294600 |
| C | 15.84586800 | -2.22216200 | 1.56435200 |
| C | 14.81065600 | -3.19834800 | 0.91501300 |
| C | 15.20645500 | -3.77632200 | -0.47007300 |
| C | 16.71424300 | -4.02267600 | -0.66056600 |
| C | 17.36619000 | -4.94480800 | 0.37227200 |
| C | 18.87633900 | -5.05519700 | 0.16537400 |
| C | 19.61709500 | -5.85502400 | 1.24233100 |
| C | 19.11334600 | -7.29599400 | 1.33479600 |
| C | 21.12184000 | -5.83617200 | 0.97333300 |
| C | 14.44561300 | -5.08242600 | -0.73683800 |
| C | 13.50706000 | -2.33259500 | 0.91840900 |
| C | 12.95951800 | -2.35185200 | 2.35804300 |
| C | 12.37599100 | -2.68386500 | -0.05635700 |
| C | 11.30113500 | -1.58705500 | -0.07642200 |
| C | 11.87270700 | -0.20436000 | -0.42106300 |
| C | 10.77899200 | 0.90769900 | -0.61053500 |
| C | 10.41388800 | 0.92365400 | -2.10968100 |
| O | 8.09208800 | 3.31937200 | 1.20456100 |
| H | 12.35641700 | -0.31260000 | -1.40389800 |
| H | 12.63343000 | 0.31142400 | 1.54638300 |
| H | 14.41220800 | -1.04095400 | -0.51081500 |
| H | 9.92821600 | 3.45073500 | 2.14352300 |
| H | 8.63065100 | 1.16467100 | 2.15503500 |
| H | 10.39693900 | 1.15624800 | 2.08962900 |

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| H | 8.62702400 | 1.11071700 | -0.38096800 |
| H | 9.23412600 | -0.36404600 | 0.31562800 |
| H | 10.63310700 | 4.31685700 | 0.07145800 |
| H | 9.50142500 | 3.30032700 | -0.82579800 |
| H | 12.86276500 | 3.58259300 | 0.26583400 |
| H | 14.42229400 | 1.80584700 | 0.79004900 |
| H | 14.13829300 | 1.36230100 | -0.88398400 |
| H | 15.01106500 | -0.36031600 | 2.38277500 |
| H | 16.03121500 | -0.10445800 | 0.97475800 |
| H | 15.98067200 | -2.47268800 | 2.61865000 |
| H | 16.83014100 | -2.30988700 | 1.10954600 |
| H | 14.66855600 | -4.05619300 | 1.58247900 |
| H | 14.92019300 | -3.05476700 | -1.24520400 |
| H | 16.85870700 | -4.45873300 | -1.65637900 |
| H | 17.24932900 | -3.06830200 | -0.68087800 |
| H | 16.91419200 | -5.93863700 | 0.30910500 |
| H | 17.16924700 | -4.57667600 | 1.38654900 |
| H | 19.30258000 | -4.04500100 | 0.12570700 |
| H | 19.07593400 | -5.51087300 | -0.81415700 |
| H | 19.43474400 | -5.36526500 | 2.20758700 |
| H | 19.21139500 | -7.79467200 | 0.36446200 |
| H | 18.06528300 | -7.34533700 | 1.63592400 |
| H | 19.69575900 | -7.86547900 | 2.06312300 |
| H | 21.34385100 | -6.33128900 | 0.02250100 |
| H | 21.67151100 | -6.35968300 | 1.75924600 |
| H | 21.50281600 | -4.81360400 | 0.91556400 |

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| H | 14.70725400 | -5.83711800 | 0.00961600 |
| H | 14.69782700 | -5.48427400 | -1.72185200 |
| H | 13.36580800 | -4.94934600 | -0.69612100 |
| H | 13.74839100 | -2.18554300 | 3.09391000 |
| H | 12.52124600 | -3.33284700 | 2.56402200 |
| H | 12.18807900 | -1.60102500 | 2.53292600 |
| H | 11.90932700 | -3.63548400 | 0.21764400 |
| H | 12.77633100 | -2.79651300 | -1.06961000 |
| H | 10.80680300 | -1.55007700 | 0.89815900 |
| H | 10.52782500 | -1.85884400 | -0.80242300 |
| H | 10.02777900 | -0.05518500 | -2.41200800 |
| H | 11.29058600 | 1.15337000 | -2.71960600 |
| H | 9.64017300 | 1.66495600 | -2.32573200 |
| H | 8.03554700 | 4.17543700 | 0.75813700 |

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| C | 4.25172700 | 3.33122500 | 3.03451400 |
| H | 4.49172200 | 4.30102700 | 2.55884900 |
| C | 4.99404100 | 2.24816300 | 2.23169400 |
| H | 4.79956500 | 1.26206200 | 2.70182800 |
| C | 4.46882200 | 2.19021600 | 0.79147300 |
| H | 4.62986000 | 3.18130100 | 0.31441500 |
| C | 2.32413100 | 2.94756800 | 1.48319700 |

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| H | 2.50705200 | 3.90597000 | 0.94551500 |
| C | 2.73053000 | 3.12815200 | 2.95561100 |
| H | 2.20930400 | 4.03267700 | 3.33546700 |
| C | 5.12230900 | 1.10469400 | -0.04278000 |
| H | 4.92562700 | 0.11623000 | 0.40068700 |
| H | 6.20869400 | 1.26708300 | -0.07406100 |
| H | 4.72592300 | 1.11856400 | -1.06843000 |
| C | 0.36076900 | 2.24962600 | 0.20573900 |
| H | 0.81196200 | 1.29901700 | -0.12592800 |
| C | -1.09083400 | 2.05455600 | 0.51177700 |
| H | -1.61397200 | 2.91133400 | 0.94962100 |
| C | -1.76801900 | 0.90149400 | 0.28496300 |
| H | -1.23736800 | 0.04539900 | -0.15289500 |
| C | -3.16059000 | 0.73196000 | 0.60021000 |
| H | -3.67117700 | 1.58911000 | 1.05537600 |
| C | -3.88763700 | -0.41232000 | 0.39333100 |
| H | -3.39666100 | -1.28203200 | -0.06323700 |
| C | -5.26597200 | -0.52727600 | 0.75037700 |
| H | -5.72552300 | 0.36194200 | 1.20011800 |
| C | -6.05209300 | -1.63719900 | 0.54755100 |
| H | -5.61077800 | -2.52495400 | 0.07561500 |
| C | -7.43072000 | -1.69326100 | 0.90700000 |
| H | -7.85510300 | -0.80473900 | 1.39354600 |
| C | -8.26605600 | -2.76267400 | 0.67586700 |
| H | -7.85588600 | -3.65084900 | 0.17742300 |
| C | -9.64433300 | -2.79009200 | 1.03863700 |

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| H | -10.04237000 | -1.90781800 | 1.55798900 |
| C | -10.50342900 | -3.83238600 | 0.77723500 |
| H | -10.11308100 | -4.71138100 | 0.24751100 |
| C | -11.88390400 | -3.84605000 | 1.14331300 |
| H | -12.26204500 | -2.97794000 | 1.69949300 |
| C | -12.76684700 | -4.85035900 | 0.83904300 |
| H | -12.40468000 | -5.71970300 | 0.27471500 |
| C | 0.64587100 | 3.31193000 | -0.87515500 |
| H | 1.72842200 | 3.32826000 | -1.07082900 |
| H | 0.16767600 | 2.98465900 | -1.81259800 |
| C | -14.16192800 | -4.81771200 | 1.18590500 |
| H | -14.49334100 | -3.95319100 | 1.77572900 |
| C | -15.08540300 | -5.73564700 | 0.80113600 |
| H | -14.75714500 | -6.59997500 | 0.20574800 |
| C | -16.55535900 | -5.65939200 | 1.10557700 |
| H | -16.74039300 | -4.79040400 | 1.76270500 |
| C | -17.38330100 | -5.44039300 | -0.18810600 |
| H | -17.33342400 | -6.38299500 | -0.77448100 |
| C | -16.85137200 | -4.32007200 | -1.11744200 |
| H | -15.81309200 | -4.61546200 | -1.35174700 |
| C | -16.73216600 | -2.95571500 | -0.41466900 |
| H | -16.28655900 | -3.08887100 | 0.57849800 |
| C | -14.80788700 | -1.49625500 | -0.53578000 |
| C | -13.85481400 | -0.76964700 | -1.46324500 |
| H | -13.83768900 | -1.27227100 | -2.44155500 |
| H | -14.25570500 | 0.24840100 | -1.61857400 |

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| C | -12.43875300 | -0.66607400 | -0.87100500 |
| H | -12.04599700 | -1.68972800 | -0.70532100 |
| C | -11.48648500 | 0.08929600 | -1.79839000 |
| H | -11.44120600 | -0.44651400 | -2.76208700 |
| H | -11.89063600 | 1.09875700 | -1.99523800 |
| C | -10.06139500 | 0.22441300 | -1.24518500 |
| H | -9.68287600 | -0.78090100 | -0.97127000 |
| C | -9.10623600 | 0.84413500 | -2.26894700 |
| H | -9.56482600 | 1.76284100 | -2.67893000 |
| H | -9.02270300 | 0.13417000 | -3.10813700 |
| C | -7.70017600 | 1.15949800 | -1.71056400 |
| H | -7.48394600 | 0.52509000 | -0.83577400 |
| H | -6.93920500 | 0.90180300 | -2.46599500 |
| C | -7.46721300 | 2.63192400 | -1.34639000 |
| H | -7.57159800 | 3.24041900 | -2.26674300 |
| C | -6.03636400 | 2.86165700 | -0.77060000 |
| H | -5.36001800 | 2.06957200 | -1.13818800 |
| C | -5.45157800 | 4.22873600 | -1.14549900 |
| H | -6.12192600 | 5.03274000 | -0.79193400 |
| H | -5.40513800 | 4.29374000 | -2.24745900 |
| C | -4.04185200 | 4.43775100 | -0.58298800 |
| H | -3.40568400 | 3.58398200 | -0.89005100 |
| C | -3.38930800 | 5.72391700 | -1.09171900 |
| H | -3.99903900 | 6.59404200 | -0.79709300 |
| H | -3.35207500 | 5.68662100 | -2.19206600 |
| C | -1.96027900 | 5.94422500 | -0.56727200 |

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| C | -1.27776400 | 7.15501300 | -1.21793600 |
| H | -1.77016600 | 8.07994200 | -0.88412200 |
| H | -1.37732600 | 7.08420900 | -2.31344800 |
| C | 0.20153600 | 7.20937300 | -0.85707700 |
| H | 0.29782000 | 7.34808500 | 0.23410400 |
| C | 0.88361400 | 5.88001900 | -1.24764500 |
| H | 0.78901100 | 5.72373200 | -2.33571500 |
| C | 0.13011100 | 4.71025700 | -0.53563700 |
| H | 0.18374500 | 4.88247100 | 0.55621300 |
| C | 2.36689000 | 5.85798900 | -0.95161400 |
| C | -17.99757600 | -2.12150600 | -0.29644400 |
| H | -17.78973600 | -1.19430100 | 0.25752200 |
| H | -18.75627200 | -2.69878500 | 0.25164900 |
| H | -18.40080100 | -1.85648900 | -1.28485500 |
| C | -17.63157500 | -4.26097000 | -2.43694100 |
| H | -18.69443700 | -4.01197500 | -2.28284000 |
| H | -17.58197000 | -5.23002600 | -2.95887900 |
| H | -17.21214700 | -3.49709200 | -3.10844800 |
| C | -17.04057900 | -6.92454800 | 1.83894400 |
| H | -16.84981900 | -7.82469900 | 1.23029200 |
| H | -18.11992900 | -6.86429600 | 2.03764100 |
| H | -16.50862900 | -7.04470900 | 2.79403800 |
| O | 2.38653100 | 1.98994500 | 3.74058900 |
| H | 1.52694000 | 1.67917700 | 3.39847700 |
| O | 6.39034300 | 2.53765100 | 2.21611800 |
| H | 6.57625800 | 2.83853700 | 3.13007800 |

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| O | 3.05135700 | 1.91224700 | 0.83588900 |
| O | 0.96224300 | 2.60982800 | 1.49272800 |
| O | -1.92481000 | 6.13857000 | 0.83255400 |
| H | -2.60879500 | 5.53930800 | 1.21173500 |
| O | -1.24277400 | 4.74125300 | -0.94486200 |
| O | 3.19886300 | 5.18946900 | -1.53689500 |
| O | 2.71485600 | 6.67698500 | 0.09820000 |
| H | 3.68258400 | 6.57129200 | 0.20484400 |
| O | -4.06478900 | 4.49960700 | 0.86290700 |
| H | -4.74908100 | 3.85387400 | 1.15666800 |
| O | -6.09292400 | 2.70498300 | 0.66531800 |
| H | -7.02396100 | 2.97509400 | 0.86904300 |
| O | -8.38836600 | 3.14744800 | -0.37340400 |
| H | -9.08073900 | 2.45884400 | -0.19432400 |
| O | -10.03860400 | 1.05140600 | -0.05987100 |
| H | -10.85529500 | 0.84872300 | 0.45086900 |
| O | -12.46756600 | 0.03428500 | 0.38925100 |
| H | -13.18157600 | -0.38686200 | 0.91971900 |
| O | -14.73260400 | -1.44566500 | 0.69127300 |
| O | -15.73932900 | -2.18920700 | -1.20989300 |
| O | -18.74280500 | -5.21589500 | 0.23398400 |
| H | -19.32332400 | -5.35684800 | -0.53108500 |
| O | 0.77524000 | 8.32792100 | -1.55125800 |
| H | 1.61506400 | 8.53564700 | -1.10781400 |
| N | 4.81781200 | 3.35210900 | 4.39037000 |
| H | 4.39960700 | 2.59059200 | 4.93494000 |

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| H | 4.58736900 | 4.22417400 | 4.87170600 |
| C | 7.49378000 | -0.66522000 | 0.67602300 |
| C | 8.08774200 | -1.99187300 | 0.13124800 |
| C | 9.01000800 | -1.84453400 | -1.11512000 |
| C | 8.31528200 | 0.57754500 | 0.30366500 |
| C | 9.73323600 | 0.09449800 | 0.23575400 |
| C | 10.44117700 | 0.02090800 | 1.38082400 |
| C | 11.57628500 | -0.93450000 | 1.59013600 |
| C | 11.80732300 | -1.93207900 | 0.42461800 |
| C | 13.22599800 | -2.47962200 | 0.53453700 |
| C | 13.52187200 | -3.51542800 | 1.61600600 |
| C | 14.94135800 | -3.99316600 | 1.25705200 |
| C | 15.27284400 | -3.40502700 | -0.16427700 |
| C | 16.31170800 | -2.22703500 | 0.00141600 |
| C | 17.68220500 | -2.73398300 | 0.53483200 |
| C | 18.30368300 | -3.77761200 | -0.38892100 |
| C | 19.76701500 | -4.06167600 | -0.07349000 |
| C | 20.35087100 | -5.10126500 | -1.04585800 |
| C | 20.36070200 | -4.59386500 | -2.49554100 |
| C | 21.76384500 | -5.48570300 | -0.61947800 |
| C | 16.58238600 | -1.39857700 | -1.26504700 |
| C | 13.83428800 | -3.12135800 | -0.71952300 |
| C | 13.19219700 | -4.48692100 | -1.12427400 |
| C | 13.64775400 | -2.18120800 | -1.90942100 |
| C | 12.16445200 | -1.85768700 | -2.14653500 |
| C | 11.57034200 | -1.16492700 | -0.90479400 |

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|---|-------------|-------------|-------------|
| C | 10.07339000 | -0.70110800 | -1.02315000 |
| C | 9.95610100 | 0.16442700 | -2.30495700 |
| O | 6.15404000 | -0.50367200 | 0.22202800 |
| H | 12.16515900 | -0.23848800 | -0.82011200 |
| H | 11.09418900 | -2.76328300 | 0.50117900 |
| H | 13.84034700 | -1.60137700 | 0.77093500 |
| H | 7.44909900 | -0.74960900 | 1.77076000 |
| H | 7.28392100 | -2.70163500 | -0.09654200 |
| H | 8.68616100 | -2.45181900 | 0.93072400 |
| H | 8.35054500 | -1.67588600 | -1.97280500 |
| H | 9.49516200 | -2.81030500 | -1.29981400 |
| H | 8.18279000 | 1.37053400 | 1.05246800 |
| H | 7.97624600 | 1.01352700 | -0.63445400 |
| H | 10.09491800 | 0.53931100 | 2.27086100 |
| H | 11.39042700 | -1.50690100 | 2.51020200 |
| H | 12.47257000 | -0.32988500 | 1.77886400 |
| H | 12.81342500 | -4.35386200 | 1.57793300 |
| H | 13.47308800 | -3.10021900 | 2.62645600 |
| H | 14.98610200 | -5.08867600 | 1.24172200 |
| H | 15.63200600 | -3.66258800 | 2.03542400 |
| H | 15.72883600 | -4.17982600 | -0.78943500 |
| H | 15.94180900 | -1.52565000 | 0.76016600 |
| H | 18.35950100 | -1.87564500 | 0.63955300 |
| H | 17.58728600 | -3.14766900 | 1.54431400 |
| H | 18.21808400 | -3.43079600 | -1.42079100 |
| H | 17.74596200 | -4.71693300 | -0.31178600 |

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| H | 19.84634800 | -4.43640400 | 0.95361200 |
| H | 20.34763300 | -3.13197700 | -0.11953600 |
| H | 19.72878300 | -6.00412900 | -1.01027500 |
| H | 20.83554300 | -3.60908000 | -2.56760600 |
| H | 19.34547300 | -4.51022400 | -2.89754000 |
| H | 20.90253500 | -5.28429400 | -3.14896300 |
| H | 22.43526100 | -4.62051800 | -0.64217100 |
| H | 22.17331600 | -6.25292400 | -1.28294800 |
| H | 21.76327600 | -5.89283100 | 0.39629500 |
| H | 16.49392000 | -1.99859400 | -2.17523200 |
| H | 17.58494500 | -0.95539700 | -1.25521000 |
| H | 15.90652900 | -0.54199500 | -1.32655000 |
| H | 13.37351300 | -5.29153000 | -0.40606600 |
| H | 13.61552000 | -4.83230500 | -2.07572100 |
| H | 12.10722000 | -4.42089500 | -1.24369600 |
| H | 14.09644300 | -2.59848500 | -2.81689300 |
| H | 14.12536100 | -1.22132200 | -1.72394400 |
| H | 11.58924700 | -2.74279800 | -2.42700900 |
| H | 12.13299900 | -1.17906800 | -3.00693100 |
| H | 10.12205900 | -0.44081000 | -3.20565100 |
| H | 10.68617200 | 0.98103000 | -2.30812500 |
| H | 8.96413200 | 0.60461900 | -2.43332900 |
| H | 5.78251600 | 0.25341900 | 0.71086000 |

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| C | 14.58539447 | 3.12973687 | 10.67721498 |
| H | 14.52731096 | 2.63959752 | 9.68688138 |
| C | 15.65820403 | 2.37551098 | 11.48269368 |
| H | 15.76479227 | 2.86191442 | 12.47430497 |
| C | 15.23076064 | 0.92136036 | 11.71973228 |
| H | 15.09113248 | 0.42688470 | 10.73395179 |
| C | 12.93290033 | 1.52843307 | 11.66437802 |
| H | 12.82649130 | 0.97481030 | 10.70350646 |
| C | 13.20802802 | 3.00823602 | 11.34773981 |
| H | 12.41644239 | 3.35079726 | 10.64761392 |
| C | 16.22118816 | 0.13301890 | 12.55576636 |
| H | 16.32740163 | 0.59276081 | 13.55063522 |
| H | 17.20264462 | 0.13182645 | 12.06147463 |
| H | 15.87832407 | -0.90451376 | 12.67922289 |
| C | 11.33470152 | 0.20689640 | 12.95786832 |
| H | 12.07246257 | -0.08863099 | 13.72311832 |
| C | 10.00673964 | 0.47202932 | 13.59432869 |
| H | 9.22614303 | 0.87357362 | 12.93943902 |
| C | 9.73301604 | 0.25082676 | 14.90418414 |
| H | 10.52053092 | -0.15051173 | 15.55607113 |
| C | 8.45275570 | 0.52641256 | 15.49778536 |
| H | 7.68331825 | 0.94564694 | 14.83839930 |
| C | 8.12822847 | 0.32337678 | 16.81468768 |
| H | 8.88303402 | -0.09757986 | 17.49216530 |
| C | 6.84287289 | 0.63991803 | 17.35149866 |

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| H | 6.11204324 | 1.05458204 | 16.64573324 |
| C | 6.45138241 | 0.43830472 | 18.65424250 |
| H | 7.16526156 | 0.00086135 | 19.36460208 |
| C | 5.14723914 | 0.75588387 | 19.13519276 |
| H | 4.44865294 | 1.20843518 | 18.41862172 |
| C | 4.69740688 | 0.52352268 | 20.41523679 |
| H | 5.38283229 | 0.05863129 | 21.13607630 |
| C | 3.38451494 | 0.84377228 | 20.86883803 |
| H | 2.71168259 | 1.33006892 | 20.14954696 |
| C | 2.90476174 | 0.57980201 | 22.13094416 |
| H | 3.56965097 | 0.08282711 | 22.84965754 |
| C | 1.58535956 | 0.90297284 | 22.57213433 |
| H | 0.93448804 | 1.42701416 | 21.85961135 |
| C | 1.07266641 | 0.59455143 | 23.80616351 |
| H | 1.70906210 | 0.06189976 | 24.52496255 |
| C | 11.31273603 | -0.88874214 | 11.87287973 |
| H | 12.34227987 | -1.05096640 | 11.52046688 |
| H | 10.99568976 | -1.83283602 | 12.34483742 |
| C | -0.27437814 | 0.89700188 | 24.20818921 |
| H | -0.88101331 | 1.45619764 | 23.48402347 |
| C | -0.84959892 | 0.50489492 | 25.37387841 |
| H | -0.24581411 | -0.05996438 | 26.09891745 |
| C | -2.27978943 | 0.76162372 | 25.75847577 |
| H | -2.75136456 | 1.39252509 | 24.98337908 |
| C | -3.08656180 | -0.56188334 | 25.82564444 |
| H | -2.72283918 | -1.12459752 | 26.71214375 |

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| C | -2.89797724 | -1.49973216 | 24.60637832 |
| H | -1.81152969 | -1.69476935 | 24.56429913 |
| C | -3.23741874 | -0.82514376 | 23.26500587 |
| H | -2.80933317 | 0.18420441 | 23.23978315 |
| C | -1.86311827 | -0.91985255 | 21.27757834 |
| C | -1.15174078 | -1.83367766 | 20.30015087 |
| H | -0.94232295 | -2.79916725 | 20.78387500 |
| H | -1.84495835 | -2.02476734 | 19.46098630 |
| C | 0.13809882 | -1.20020762 | 19.75084896 |
| H | 0.82496839 | -0.99889509 | 20.59776052 |
| C | 0.83971320 | -2.11463981 | 18.74636183 |
| H | 1.08569586 | -3.06388765 | 19.25259767 |
| H | 0.14761279 | -2.34712126 | 17.91687528 |
| C | 2.12969061 | -1.52062008 | 18.16475103 |
| H | 2.79333404 | -1.21202134 | 18.99740058 |
| C | 2.88001866 | -2.52814823 | 17.28932639 |
| H | 2.17246935 | -2.97321263 | 16.56565317 |
| H | 3.21220814 | -3.34778879 | 17.94743601 |
| C | 4.09536614 | -1.93368941 | 16.54246473 |
| H | 4.46688350 | -1.03824266 | 17.06652051 |
| H | 4.92597530 | -2.65895666 | 16.55780191 |
| C | 3.84253181 | -1.59639276 | 15.06691803 |
| H | 3.58694701 | -2.53329349 | 14.53296584 |
| C | 5.10755049 | -0.98180076 | 14.39338660 |
| H | 6.01074175 | -1.30986207 | 14.93798242 |
| C | 5.24874496 | -1.36965623 | 12.91654424 |

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| H | 4.34803376 | -1.05569481 | 12.35892017 |
| H | 5.31298084 | -2.47084074 | 12.85358810 |
| C | 6.50068367 | -0.76851432 | 12.26946676 |
| H | 7.38281177 | -1.03592767 | 12.88449418 |
| C | 6.73641422 | -1.28613336 | 10.84983727 |
| H | 5.87471971 | -1.03070116 | 10.21114360 |
| H | 6.82385218 | -2.38364024 | 10.88688560 |
| C | 8.00454025 | -0.72268560 | 10.18644686 |
| C | 8.29751071 | -1.37946545 | 8.83071557 |
| H | 7.52859130 | -1.08248534 | 8.10273766 |
| H | 8.26541720 | -2.47562781 | 8.94239378 |
| C | 9.67126715 | -0.97410537 | 8.31112199 |
| H | 9.67916706 | 0.11606557 | 8.13604232 |
| C | 10.74879571 | -1.31259826 | 9.36436016 |
| H | 10.74787366 | -2.39920430 | 9.55556485 |
| C | 10.37336340 | -0.59767189 | 10.70264187 |
| H | 10.33028078 | 0.49106985 | 10.50910787 |
| C | 12.15260190 | -0.97013707 | 8.91684010 |
| C | -4.70371052 | -0.76555376 | 22.86803842 |
| H | -4.81682397 | -0.22685276 | 21.91578230 |
| H | -5.26337042 | -0.22820196 | 23.64733988 |
| H | -5.13299041 | -1.77186251 | 22.75471362 |
| C | -3.60847683 | -2.84387491 | 24.81072658 |
| H | -4.70079706 | -2.72867996 | 24.90553338 |
| H | -3.23910620 | -3.34159993 | 25.72165181 |
| H | -3.42465195 | -3.51939191 | 23.96205971 |

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|---|-------------|-------------|-------------|
| C | -2.37153709 | 1.50843292 | 27.10299928 |
| H | -1.88656112 | 0.92686601 | 27.90530578 |
| H | -3.42210847 | 1.67201652 | 27.38165423 |
| H | -1.86416845 | 2.48212356 | 27.03883718 |
| O | 13.20870917 | 3.80809316 | 12.52683712 |
| H | 12.50263805 | 3.44663917 | 13.09545758 |
| O | 16.89347356 | 2.39673146 | 10.77039890 |
| H | 16.94222958 | 3.30887340 | 10.41537891 |
| O | 13.97074206 | 0.92803598 | 12.42737362 |
| O | 11.74560879 | 1.50335270 | 12.41177907 |
| O | 7.92597795 | 0.67272769 | 9.97386816 |
| H | 7.45030931 | 1.04412281 | 10.75267085 |
| O | 9.07568500 | -1.05001412 | 11.10842028 |
| O | 13.17284989 | -1.51372708 | 9.29796440 |
| O | 12.18811060 | 0.07088753 | 8.01742325 |
| H | 13.13573271 | 0.20998829 | 7.81320719 |
| O | 6.40643517 | 0.67416286 | 12.20043956 |
| H | 5.94814970 | 0.96126137 | 13.02449762 |
| O | 5.05010996 | 0.45488458 | 14.54252179 |
| H | 4.07447864 | 0.62328220 | 14.57536376 |
| O | 2.77125131 | -0.66464410 | 14.85433232 |
| H | 2.32291948 | -0.49140758 | 15.72301719 |
| O | 1.84909093 | -0.35449720 | 17.35801164 |
| H | 1.11859053 | 0.13511260 | 17.80024490 |
| O | -0.15462206 | 0.04210646 | 19.07962152 |
| H | -0.72005855 | 0.55964738 | 19.69687732 |

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| O | -1.85257991 | 0.30746073 | 21.19111280 |
| O | -2.50564077 | -1.60650703 | 22.23563055 |
| O | -4.46261341 | -0.18756538 | 26.03343976 |
| H | -4.94138794 | -0.96688130 | 26.35846487 |
| O | 9.89141400 | -1.67563402 | 7.07760449 |
| H | 10.60723041 | -1.21117059 | 6.61179754 |
| N | 15.06631791 | 4.50170877 | 10.46358147 |
| H | 14.88757832 | 5.05036813 | 11.31115735 |
| H | 14.55714067 | 4.95546667 | 9.70191917 |
| C | 16.00809282 | -3.67759620 | 9.57360951 |
| C | 17.03679432 | -4.54702051 | 10.34526584 |
| C | 17.31476572 | -5.95050220 | 9.72988967 |
| C | 15.86749971 | -4.05690477 | 8.09227899 |
| C | 17.22450153 | -4.55430121 | 7.69267679 |
| C | 18.15736212 | -3.65103740 | 7.32981794 |
| C | 19.63078672 | -3.88207021 | 7.47379082 |
| C | 20.01274121 | -5.20332667 | 8.19168078 |
| C | 21.45769522 | -5.54059538 | 7.84113716 |
| C | 22.57193568 | -4.73685886 | 8.50633444 |
| C | 23.84169433 | -5.51196802 | 8.10766040 |
| C | 23.36412835 | -6.86671512 | 7.46535449 |
| C | 23.58773419 | -6.79678916 | 5.90347438 |
| C | 25.09723211 | -6.71107090 | 5.53760988 |
| C | 25.88207171 | -7.90742414 | 6.06815780 |
| C | 27.27909123 | -8.02036587 | 5.47057080 |
| C | 28.01788241 | -9.25300903 | 6.02003551 |

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| C | 27.32322931 | -10.56512300 | 5.62640622 |
| C | 29.46259509 | -9.26209865 | 5.53135486 |
| C | 22.97709503 | -7.95225082 | 5.09380311 |
| C | 21.91629141 | -6.98929261 | 8.05438110 |
| C | 22.03624298 | -7.41649710 | 9.55237116 |
| C | 20.90815263 | -7.93870313 | 7.40877310 |
| C | 19.49698634 | -7.73996162 | 7.98339217 |
| C | 19.01813308 | -6.29903089 | 7.72029300 |
| C | 17.55477864 | -5.96241273 | 8.18427873 |
| C | 16.61464140 | -7.02838083 | 7.56315627 |
| O | 14.73413502 | -3.74675311 | 10.20555919 |
| H | 19.00600261 | -6.23115179 | 6.61824321 |
| H | 19.92747265 | -5.07284501 | 9.27843069 |
| H | 21.53174616 | -5.33989239 | 6.76463478 |
| H | 16.34074502 | -2.63271385 | 9.64524338 |
| H | 16.72469866 | -4.66620459 | 11.38937703 |
| H | 17.99234187 | -4.00377841 | 10.37044148 |
| H | 16.45272547 | -6.57729374 | 9.98083903 |
| H | 18.16737707 | -6.39435900 | 10.25737984 |
| H | 15.55184176 | -3.18941596 | 7.49653070 |
| H | 15.08802316 | -4.80214397 | 7.94352386 |
| H | 17.86475829 | -2.63519803 | 7.07830899 |
| H | 20.06684216 | -3.04099361 | 8.03160166 |
| H | 20.06128382 | -3.83939971 | 6.46515006 |
| H | 22.46058637 | -4.71818867 | 9.59884186 |
| H | 22.60461514 | -3.69696786 | 8.16966687 |

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| H | 24.46871609 | -5.70137503 | 8.98706317 |
| H | 24.43315008 | -4.89444009 | 7.42870658 |
| H | 23.96038604 | -7.69557610 | 7.86099617 |
| H | 23.13835093 | -5.87310542 | 5.51703906 |
| H | 25.19286419 | -6.65516626 | 4.44482867 |
| H | 25.54461666 | -5.78399612 | 5.91121537 |
| H | 25.32268628 | -8.81997462 | 5.85204688 |
| H | 25.97792726 | -7.83202555 | 7.15648346 |
| H | 27.84734688 | -7.11494180 | 5.71335762 |
| H | 27.21560180 | -8.07331220 | 4.37661307 |
| H | 28.03110747 | -9.19551674 | 7.11545532 |
| H | 27.13900042 | -10.60782678 | 4.54719095 |
| H | 26.36191623 | -10.67870805 | 6.13852485 |
| H | 27.93268826 | -11.43023085 | 5.90458462 |
| H | 29.51242608 | -9.32543232 | 4.43894230 |
| H | 30.00691664 | -10.11461237 | 5.94779380 |
| H | 29.98238475 | -8.35201998 | 5.84619529 |
| H | 22.96666690 | -8.88900258 | 5.65831227 |
| H | 23.52637916 | -8.13161725 | 4.16227487 |
| H | 21.96172598 | -7.71146058 | 4.76923508 |
| H | 22.82783556 | -6.89628337 | 10.09904557 |
| H | 22.27715067 | -8.48480455 | 9.61889277 |
| H | 21.11279103 | -7.24495329 | 10.11237572 |
| H | 21.22105313 | -8.98216060 | 7.51940042 |
| H | 20.81535967 | -7.73972207 | 6.34308726 |
| H | 19.44447035 | -7.99375837 | 9.04441847 |

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| H | 18.84992052 | -8.45293483 | 7.45920743 |
| H | 16.80973197 | -8.02151934 | 7.98826763 |
| H | 16.74274105 | -7.09521267 | 6.47734893 |
| H | 15.55794093 | -6.83323030 | 7.76202637 |
| H | 14.17380390 | -3.07227686 | 9.77978408 |

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| C | 7.61293000 | 7.96043500 | -1.10472500 |
| H | 8.40739500 | 7.20234600 | -1.24073300 |
| C | 7.76261000 | 8.50740900 | 0.32600500 |
| H | 6.99784400 | 9.29517700 | 0.48661800 |
| C | 7.51316100 | 7.39797500 | 1.35575300 |
| H | 8.25398600 | 6.58596400 | 1.18967600 |
| C | 6.04332600 | 6.26883700 | -0.13300400 |
| H | 6.79371400 | 5.45088400 | -0.22769700 |
| C | 6.25588000 | 7.26288400 | -1.28732700 |
| H | 6.25629900 | 6.67911300 | -2.23249500 |
| C | 7.59271400 | 7.88215000 | 2.79124200 |
| H | 6.82885500 | 8.65398100 | 2.97346000 |
| H | 8.58443700 | 8.31634200 | 2.97977500 |
| H | 7.42637400 | 7.04715900 | 3.48722500 |
| C | 4.23302500 | 4.91722400 | 0.79960900 |
| H | 4.14247800 | 5.52281900 | 1.71737300 |

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| C | 2.88001100 | 4.48478500 | 0.32928100 |
| H | 2.84431400 | 3.96443900 | -0.63374300 |
| C | 1.73025700 | 4.70407000 | 1.01452300 |
| H | 1.77254400 | 5.22781100 | 1.97894900 |
| C | 0.43852400 | 4.29170400 | 0.53623900 |
| H | 0.41081100 | 3.78806700 | -0.43749800 |
| C | -0.75075300 | 4.49245700 | 1.18899700 |
| H | -0.74585300 | 4.99291800 | 2.16645600 |
| C | -2.00748500 | 4.07959000 | 0.64985900 |
| H | -1.97480100 | 3.57906800 | -0.32613900 |
| C | -3.22769500 | 4.23188700 | 1.26544600 |
| H | -3.27134400 | 4.70872400 | 2.25353100 |
| C | -4.45319200 | 3.78449800 | 0.69015500 |
| H | -4.39731100 | 3.32470300 | -0.30571900 |
| C | -5.68798200 | 3.86988200 | 1.29253200 |
| H | -5.75365000 | 4.31499100 | 2.29408400 |
| C | -6.89820300 | 3.40726400 | 0.69810000 |
| H | -6.82882700 | 2.98465500 | -0.31341200 |
| C | -8.13344700 | 3.44562300 | 1.30263000 |
| H | -8.20585500 | 3.85600900 | 2.31848000 |
| C | -9.33855000 | 2.97553500 | 0.69711000 |
| H | -9.26590100 | 2.59410100 | -0.33010600 |
| C | -10.56655000 | 2.95253400 | 1.30726700 |
| H | -10.65186200 | 3.32163500 | 2.33774100 |
| C | 5.20586200 | 3.75689100 | 1.09171000 |
| H | 6.14017800 | 4.17781800 | 1.49214300 |

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| H | 4.77412000 | 3.14167600 | 1.89774000 |
| C | -11.75581700 | 2.43513100 | 0.68632600 |
| H | -11.65149100 | 2.10013200 | -0.35387300 |
| C | -12.95856600 | 2.28991000 | 1.29932300 |
| H | -13.06456200 | 2.61979600 | 2.34299100 |
| C | -14.17985500 | 1.68206700 | 0.66825200 |
| H | -13.96207400 | 1.45975700 | -0.39209900 |
| C | -14.55220000 | 0.33958500 | 1.35101500 |
| H | -14.93229000 | 0.58112900 | 2.36689400 |
| C | -13.36648900 | -0.63824900 | 1.55017500 |
| H | -12.63152300 | -0.07367900 | 2.15122800 |
| C | -12.63595000 | -0.97957000 | 0.23892300 |
| H | -12.48846900 | -0.06677700 | -0.35076800 |
| C | -10.23597600 | -0.96361800 | -0.05672400 |
| C | -8.91479400 | -1.48671700 | 0.46991100 |
| H | -9.02519500 | -1.76842700 | 1.52748700 |
| H | -8.67290500 | -2.40460500 | -0.09598100 |
| C | -7.77576500 | -0.46917700 | 0.28571400 |
| H | -8.02897500 | 0.45430000 | 0.84486700 |
| C | -6.43971200 | -1.01013800 | 0.79538800 |
| H | -6.54694800 | -1.24844000 | 1.86756600 |
| H | -6.19892100 | -1.94976300 | 0.26602600 |
| C | -5.27028700 | -0.03099500 | 0.62540000 |
| H | -5.54164400 | 0.94005100 | 1.08626300 |
| C | -3.99067800 | -0.54668500 | 1.28958100 |
| H | -3.81195100 | -1.58865100 | 0.96589100 |

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| H | -4.17912300 | -0.58368600 | 2.37511700 |
| C | -2.74034100 | 0.31626200 | 1.00632600 |
| H | -3.03589300 | 1.34536000 | 0.74538400 |
| H | -2.13615500 | 0.39935500 | 1.92513700 |
| C | -1.80629400 | -0.23938400 | -0.07706900 |
| H | -1.42532100 | -1.22364800 | 0.26100700 |
| C | -0.58434900 | 0.69887600 | -0.31823100 |
| H | -0.39743200 | 1.30053100 | 0.58898200 |
| C | 0.69512100 | -0.06433200 | -0.68141400 |
| H | 0.52172000 | -0.67873900 | -1.58320800 |
| H | 0.93443900 | -0.75191600 | 0.14964100 |
| C | 1.89037800 | 0.86770800 | -0.90523000 |
| H | 2.00159000 | 1.52337100 | -0.01885700 |
| C | 3.20232000 | 0.10660100 | -1.10111000 |
| H | 3.12370400 | -0.55316000 | -1.98101200 |
| H | 3.37847300 | -0.52242700 | -0.21407400 |
| C | 4.42538600 | 1.01837800 | -1.29726400 |
| C | 5.74273400 | 0.23186600 | -1.33174300 |
| H | 5.78496700 | -0.37773800 | -2.24606600 |
| H | 5.78681700 | -0.44334300 | -0.46155700 |
| C | 6.94230400 | 1.17046600 | -1.29219500 |
| H | 6.93287000 | 1.80004500 | -2.19923900 |
| C | 6.84697600 | 2.08796400 | -0.05362100 |
| H | 6.84783100 | 1.47182900 | 0.86161100 |
| C | 5.48382100 | 2.85082600 | -0.10761800 |
| H | 5.45709600 | 3.43875300 | -1.04479300 |

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| C | 8.01829000 | 3.03555700 | 0.08171100 |
| C | -13.25017500 | -2.05819000 | -0.63883300 |
| H | -12.66021400 | -2.17915300 | -1.55921300 |
| H | -14.27267900 | -1.75840300 | -0.91065900 |
| H | -13.29200700 | -3.02678600 | -0.11935900 |
| C | -13.78187600 | -1.87490600 | 2.35728100 |
| H | -14.55020700 | -2.47261900 | 1.83976000 |
| H | -14.18618500 | -1.57812800 | 3.33830400 |
| H | -12.92075600 | -2.53586700 | 2.53603800 |
| C | -15.37572600 | 2.65233000 | 0.71688700 |
| H | -15.61290400 | 2.92605900 | 1.75897000 |
| H | -16.26644700 | 2.18827100 | 0.27037400 |
| H | -15.14402500 | 3.57788800 | 0.16983000 |
| O | 5.23776600 | 8.25911900 | -1.31900800 |
| H | 4.40971400 | 7.80289100 | -1.07672800 |
| O | 9.07720700 | 9.03132300 | 0.50222900 |
| H | 9.25629000 | 9.49975200 | -0.33974700 |
| O | 6.18293600 | 6.87387500 | 1.14535200 |
| O | 4.73203900 | 5.78809000 | -0.26830200 |
| O | 4.34926800 | 1.77131400 | -2.49134700 |
| H | 3.40212500 | 2.01949400 | -2.60114300 |
| O | 4.42575100 | 1.88488400 | -0.13377900 |
| O | 8.43356500 | 3.50842700 | 1.12362900 |
| O | 8.59116300 | 3.35386100 | -1.12843100 |
| H | 9.31900100 | 3.97494800 | -0.91976000 |
| O | 1.68736400 | 1.69966200 | -2.07210700 |

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| H | 0.72769200 | 1.92390300 | -2.08848900 |
| O | -0.93183100 | 1.64064100 | -1.35839500 |
| H | -1.58709500 | 1.12731400 | -1.89544000 |
| O | -2.43640800 | -0.42817200 | -1.35312100 |
| H | -3.40869600 | -0.25184800 | -1.25725300 |
| O | -4.98262800 | 0.19978100 | -0.77224100 |
| H | -5.84501200 | 0.21938400 | -1.24640100 |
| O | -7.61054900 | -0.14188900 | -1.10897700 |
| H | -8.50901000 | 0.07485600 | -1.44715000 |
| O | -10.33086600 | -0.20827600 | -1.02333600 |
| O | -11.28017400 | -1.42614400 | 0.64890500 |
| O | -15.61962000 | -0.23063200 | 0.56853200 |
| H | -16.06126000 | -0.90616300 | 1.10780200 |
| O | 8.12626600 | 0.35826400 | -1.26510900 |
| H | 8.86701200 | 0.92890800 | -1.53111100 |
| N | 7.88885900 | 9.06176900 | -2.03754800 |
| H | 7.04911900 | 9.64454800 | -2.11858000 |
| H | 8.09715600 | 8.70736800 | -2.97365700 |
| C | -1.35058400 | -3.68796100 | -3.49857300 |
| C | -1.07995400 | -3.65341100 | -1.97045500 |
| C | -0.75395300 | -5.03150000 | -1.32214200 |
| C | -0.71768200 | -4.89248200 | -4.21029300 |
| C | 0.52757900 | -5.18925700 | -3.42940300 |
| C | 1.64412700 | -4.48843300 | -3.71215100 |
| C | 2.73188100 | -4.23002500 | -2.71460300 |
| C | 2.42562200 | -4.72857900 | -1.27772300 |

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| C | 3.74324700 | -4.85221300 | -0.52068800 |
| C | 4.42735200 | -3.57436400 | -0.04202900 |
| C | 5.55337600 | -4.10482000 | 0.86500400 |
| C | 5.28399600 | -5.64117600 | 1.07239800 |
| C | 6.33574100 | -6.46155400 | 0.22672000 |
| C | 7.78666800 | -6.25378000 | 0.74770900 |
| C | 7.93424600 | -6.67170600 | 2.20794000 |
| C | 9.38637200 | -6.78097900 | 2.65618100 |
| C | 9.47969700 | -7.22652400 | 4.12584500 |
| C | 8.90346500 | -8.63410600 | 4.33985000 |
| C | 10.92881300 | -7.17996000 | 4.59911000 |
| C | 6.08319600 | -7.97574600 | 0.14314900 |
| C | 3.75484400 | -5.73011800 | 0.73774600 |
| C | 2.95850100 | -5.14058100 | 1.94569900 |
| C | 3.12202500 | -7.08307400 | 0.41590200 |
| C | 1.68553700 | -6.92484800 | -0.10615300 |
| C | 1.68338300 | -6.08733300 | -1.39974000 |
| C | 0.28835500 | -5.90122300 | -2.09921100 |
| C | -0.32209000 | -7.31306200 | -2.29922900 |
| O | -2.75185000 | -3.66898900 | -3.74998000 |
| H | 2.28956600 | -6.69235300 | -2.09670500 |
| H | 1.78189900 | -4.00333400 | -0.76297900 |
| H | 4.42858900 | -5.31946100 | -1.23944100 |
| H | -0.93956600 | -2.76309400 | -3.92665400 |
| H | -1.92849500 | -3.19936000 | -1.44548500 |
| H | -0.21903500 | -2.99355200 | -1.79095100 |

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| H | -1.70403800 | -5.56939600 | -1.23869400 |
| H | -0.42101900 | -4.85667500 | -0.29219400 |
| H | -0.50146700 | -4.65444900 | -5.26085600 |
| H | -1.40109900 | -5.73910100 | -4.24596000 |
| H | 1.71565000 | -3.92649500 | -4.63946600 |
| H | 2.92611800 | -3.14856900 | -2.67676200 |
| H | 3.64484700 | -4.69366400 | -3.10961600 |
| H | 3.74007300 | -2.93785500 | 0.53140200 |
| H | 4.81595300 | -2.96711500 | -0.86423500 |
| H | 5.55195300 | -3.57912900 | 1.82730700 |
| H | 6.51518100 | -3.89253300 | 0.39383100 |
| H | 5.41382300 | -5.90157100 | 2.12805200 |
| H | 6.33724600 | -6.08786200 | -0.80518200 |
| H | 8.47393700 | -6.83686600 | 0.11992400 |
| H | 8.10588000 | -5.21289000 | 0.63001300 |
| H | 7.43943300 | -7.63456800 | 2.35084000 |
| H | 7.42853700 | -5.94477800 | 2.85226900 |
| H | 9.87259900 | -5.80564600 | 2.53801600 |
| H | 9.92549000 | -7.48629100 | 2.01161600 |
| H | 8.89940600 | -6.52880700 | 4.74218800 |
| H | 9.33740800 | -9.35151600 | 3.63452300 |
| H | 7.81628500 | -8.64605500 | 4.20875100 |
| H | 9.10235900 | -8.98896400 | 5.35560200 |
| H | 11.55807400 | -7.86538100 | 4.02110700 |
| H | 11.00068800 | -7.45854400 | 5.65443600 |
| H | 11.33663400 | -6.16979900 | 4.49515400 |

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| H | 5.60539500 | -8.36314400 | 1.04753400 |
| H | 7.01326800 | -8.53602200 | -0.00747500 |
| H | 5.47112200 | -8.22490700 | -0.72724200 |
| H | 3.39521300 | -4.22780300 | 2.36068500 |
| H | 2.93720100 | -5.86498100 | 2.76943100 |
| H | 1.92462200 | -4.89591400 | 1.68680300 |
| H | 3.13969400 | -7.74505800 | 1.28791900 |
| H | 3.66456800 | -7.58491500 | -0.38265400 |
| H | 1.01726600 | -6.50247900 | 0.64748200 |
| H | 1.32195200 | -7.93806600 | -0.31349800 |
| H | -0.56479900 | -7.77767600 | -1.33469300 |
| H | 0.36702000 | -7.97863000 | -2.83026600 |
| H | -1.26291400 | -7.29636200 | -2.85494600 |
| H | -2.86204100 | -3.53661300 | -4.70941100 |

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|---|-------------|-------------|------------|
| C | -8.24584100 | -3.66135400 | 3.27857800 |
| H | -8.64265500 | -4.47106000 | 2.63726300 |
| C | -8.85851400 | -2.34709600 | 2.76289600 |
| H | -8.50460200 | -1.51444300 | 3.40529600 |
| C | -8.39232000 | -2.06130400 | 1.32956600 |
| H | -8.71418300 | -2.90175800 | 0.67702700 |
| C | -6.35106100 | -3.22164100 | 1.70191600 |

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| H | -6.69245200 | -4.01495100 | 0.99820700 |
| C | -6.71601100 | -3.64864800 | 3.13378500 |
| H | -6.31433500 | -4.67294000 | 3.28745500 |
| C | -8.91815500 | -0.74984600 | 0.77733700 |
| H | -8.56286000 | 0.09034000 | 1.39399000 |
| H | -10.01693600 | -0.75756600 | 0.79163800 |
| H | -8.57197200 | -0.60271100 | -0.25599700 |
| C | -4.36411400 | -2.53882700 | 0.45306700 |
| H | -4.68787700 | -1.48909600 | 0.35070700 |
| C | -2.88782800 | -2.60458200 | 0.68783100 |
| H | -2.47493300 | -3.59487700 | 0.90756400 |
| C | -2.06240000 | -1.52909900 | 0.64808100 |
| H | -2.48282300 | -0.53847200 | 0.42873400 |
| C | -0.64775300 | -1.61373600 | 0.89094900 |
| H | -0.24658100 | -2.60633200 | 1.12842900 |
| C | 0.22656400 | -0.55747300 | 0.86538300 |
| H | -0.15347400 | 0.44500600 | 0.62764500 |
| C | 1.62108200 | -0.70181000 | 1.13922400 |
| H | 1.96695700 | -1.71763700 | 1.36863300 |
| C | 2.54904600 | 0.31252300 | 1.10656100 |
| H | 2.22004500 | 1.32913300 | 0.85387100 |
| C | 3.93550000 | 0.11056100 | 1.37097700 |
| H | 4.24827300 | -0.90759300 | 1.63899600 |
| C | 4.90510000 | 1.08501400 | 1.29906600 |
| H | 4.60582200 | 2.10342700 | 1.01833800 |
| C | 6.28723600 | 0.85464400 | 1.56103700 |

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| H | 6.57625800 | -0.16078800 | 1.86423900 |
| C | 7.27514400 | 1.80595900 | 1.45244200 |
| H | 6.99281300 | 2.81935200 | 1.13790300 |
| C | 8.65762000 | 1.56128200 | 1.71474500 |
| H | 8.93057400 | 0.55455900 | 2.05818000 |
| C | 9.66182400 | 2.48152900 | 1.55497900 |
| H | 9.40449500 | 3.48903300 | 1.20269100 |
| C | -4.84461900 | -3.30666400 | -0.79499100 |
| H | -5.92564800 | -3.13920000 | -0.91248100 |
| H | -4.36480700 | -2.85794300 | -1.67986800 |
| C | 11.05127300 | 2.19402400 | 1.78822300 |
| H | 11.27997600 | 1.18995800 | 2.16857800 |
| C | 12.07971700 | 3.04190900 | 1.52966700 |
| H | 11.85386900 | 4.04652700 | 1.14361000 |
| C | 13.53512600 | 2.71106800 | 1.70742400 |
| H | 13.62133000 | 1.70800100 | 2.16307700 |
| C | 14.26711600 | 2.65810400 | 0.34051200 |
| H | 14.32813200 | 3.70003000 | -0.04091900 |
| C | 13.54070200 | 1.83511600 | -0.75344800 |
| H | 12.54655400 | 2.30691500 | -0.84964000 |
| C | 13.25692000 | 0.38251000 | -0.33039300 |
| H | 12.87781200 | 0.36422900 | 0.69850000 |
| C | 11.13963700 | -0.75339500 | -0.60310500 |
| C | 10.05343800 | -1.13962900 | -1.58671800 |
| H | 10.06695200 | -0.44716800 | -2.44131100 |
| H | 10.29701400 | -2.14704700 | -1.97018000 |

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| C | 8.66373700 | -1.17626700 | -0.92786200 |
| H | 8.42945000 | -0.16663700 | -0.53374000 |
| C | 7.57420700 | -1.59050300 | -1.91719300 |
| H | 7.56527200 | -0.86519600 | -2.74888000 |
| H | 7.82046900 | -2.58141100 | -2.33975100 |
| C | 6.16938500 | -1.64842600 | -1.30213900 |
| H | 5.95115700 | -0.68090800 | -0.80691400 |
| C | 5.09236300 | -1.91079800 | -2.35838700 |
| H | 5.39639000 | -2.77668500 | -2.97500500 |
| H | 5.07591900 | -1.03747200 | -3.03092000 |
| C | 3.68069700 | -2.14701800 | -1.77559100 |
| H | 3.59529900 | -1.68509900 | -0.77868400 |
| H | 2.93309400 | -1.64017200 | -2.40832800 |
| C | 3.25448500 | -3.61912100 | -1.69692400 |
| H | 3.23107700 | -4.03172600 | -2.72523300 |
| C | 1.83134700 | -3.77268400 | -1.07826700 |
| H | 1.26067900 | -2.83948100 | -1.23135000 |
| C | 1.04088700 | -4.94293900 | -1.67585200 |
| H | 1.60331500 | -5.88399500 | -1.53842600 |
| H | 0.93864500 | -4.77116600 | -2.76246900 |
| C | -0.35895700 | -5.07644800 | -1.06754100 |
| H | -0.87846200 | -4.10130900 | -1.15202200 |
| C | -1.21050000 | -6.13157100 | -1.77495600 |
| H | -0.72001300 | -7.11649900 | -1.70401300 |
| H | -1.28888300 | -5.86218500 | -2.84023800 |
| C | -2.63267500 | -6.26558400 | -1.20472500 |

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| C | -3.50908200 | -7.21424000 | -2.03367800 |
| H | -3.14079700 | -8.24495700 | -1.92702800 |
| H | -3.44719500 | -6.93140900 | -3.09728000 |
| C | -4.96411000 | -7.14682600 | -1.58663400 |
| H | -5.03269000 | -7.49501500 | -0.54104800 |
| C | -5.46428500 | -5.68731700 | -1.65455900 |
| H | -5.39471100 | -5.32251600 | -2.69347800 |
| C | -4.52096600 | -4.80051400 | -0.77889000 |
| H | -4.55215900 | -5.18693700 | 0.25763000 |
| C | -6.91504200 | -5.53188200 | -1.25534600 |
| C | 14.39332500 | -0.61742500 | -0.47132000 |
| H | 14.07832800 | -1.60373200 | -0.10015900 |
| H | 15.24972000 | -0.27159500 | 0.12556000 |
| H | 14.71179900 | -0.72235900 | -1.51886100 |
| C | 14.24734800 | 1.94879100 | -2.11028900 |
| H | 15.26904200 | 1.53536500 | -2.08497200 |
| H | 14.31517900 | 3.00295300 | -2.42348500 |
| H | 13.69433900 | 1.40297800 | -2.88914700 |
| C | 14.22779600 | 3.72126700 | 2.64208600 |
| H | 14.14247200 | 4.74523700 | 2.24043400 |
| H | 15.29479400 | 3.47936500 | 2.74747600 |
| H | 13.75982900 | 3.70967100 | 3.63731700 |
| O | -6.17899600 | -2.75359700 | 4.10360000 |
| H | -5.29907100 | -2.49467800 | 3.77012100 |
| O | -10.28129400 | -2.44042200 | 2.78922800 |
| H | -10.46933700 | -2.89722000 | 3.63562900 |

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| O | -6.94903900 | -1.98791600 | 1.32761700 |
| O | -4.95563700 | -3.07575200 | 1.68175300 |
| O | -2.63595200 | -6.73976000 | 0.12707300 |
| H | -1.85747100 | -6.32772500 | 0.56857400 |
| O | -3.18546900 | -4.92660200 | -1.28266500 |
| O | -7.66660500 | -4.65276600 | -1.63476700 |
| O | -7.33190200 | -6.49772100 | -0.36803200 |
| H | -8.26899100 | -6.28984500 | -0.17388300 |
| O | -0.28349900 | -5.43945900 | 0.33156400 |
| H | 0.49831500 | -4.96469400 | 0.69883500 |
| O | 1.97100000 | -3.92623200 | 0.35230100 |
| H | 2.86144000 | -4.35304700 | 0.43128000 |
| O | 4.13272300 | -4.44214000 | -0.91441000 |
| H | 4.92379100 | -3.90308900 | -0.65123800 |
| O | 6.07866200 | -2.69299500 | -0.30712600 |
| H | 6.93702100 | -2.71016000 | 0.17437500 |
| O | 8.64541300 | -2.12044000 | 0.16199000 |
| H | 9.43445800 | -1.91640400 | 0.71366900 |
| O | 11.11026900 | -1.04712800 | 0.59135800 |
| O | 12.13131600 | -0.06459900 | -1.18989900 |
| O | 15.59705200 | 2.17371400 | 0.61152400 |
| H | 16.15863300 | 2.39257800 | -0.14934700 |
| O | -5.72154500 | -8.01138500 | -2.44745000 |
| H | -6.56280900 | -8.19405600 | -1.99578400 |
| N | -8.75071800 | -3.88832800 | 4.63976000 |
| H | -8.20467000 | -3.31830300 | 5.29417800 |

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|---|--------------|-------------|-------------|
| H | -8.62755500 | -4.86388600 | 4.91976700 |
| C | 1.44327300 | 3.47019000 | 1.01189900 |
| C | 0.83684200 | 4.80804800 | 0.50994700 |
| C | 0.04601200 | 4.71816200 | -0.82879400 |
| C | 0.72544100 | 2.22552700 | 0.47013200 |
| C | -0.70243700 | 2.64996900 | 0.29822100 |
| C | -1.51889100 | 2.60305500 | 1.37012700 |
| C | -2.71605900 | 3.48871400 | 1.53589800 |
| C | -2.88585300 | 4.56307000 | 0.42959600 |
| C | -4.33465200 | 5.03785300 | 0.43882400 |
| C | -4.78453400 | 5.97227100 | 1.55886000 |
| C | -6.18598700 | 6.41404700 | 1.09757500 |
| C | -6.35034100 | 5.92458400 | -0.38882300 |
| C | -7.33873900 | 4.69298900 | -0.41332500 |
| C | -8.77784100 | 5.09642900 | 0.01796400 |
| C | -9.36113600 | 6.18073800 | -0.88356600 |
| C | -10.86042000 | 6.37512400 | -0.69411800 |
| C | -11.40148300 | 7.46084300 | -1.64047800 |
| C | -11.24748800 | 7.06806400 | -3.11734600 |
| C | -12.86637900 | 7.74875200 | -1.32859100 |
| C | -7.44509500 | 3.95475200 | -1.75765900 |
| C | -4.85290200 | 5.74820500 | -0.81868200 |
| C | -4.24580500 | 7.16791900 | -1.05682700 |
| C | -4.50629600 | 4.91273500 | -2.05009900 |
| C | -2.99259100 | 4.67381800 | -2.16274800 |
| C | -2.48466100 | 3.91298600 | -0.92260800 |

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| C | -0.96151500 | 3.52567100 | -0.92634400 |
| C | -0.67881800 | 2.76865500 | -2.25033400 |
| O | 2.82660700 | 3.40323200 | 0.68172800 |
| H | -3.03674700 | 2.95765800 | -0.96522900 |
| H | -2.22661200 | 5.41614400 | 0.63692800 |
| H | -4.92304500 | 4.11784500 | 0.54837500 |
| H | 1.37927800 | 3.47084700 | 2.10892800 |
| H | 1.62138400 | 5.56785700 | 0.41528000 |
| H | 0.14240500 | 5.17767400 | 1.27803000 |
| H | 0.79179600 | 4.64587500 | -1.62725300 |
| H | -0.46806000 | 5.67326500 | -0.98913000 |
| H | 0.82644500 | 1.38312400 | 1.16816300 |
| H | 1.17397000 | 1.87924300 | -0.45938600 |
| H | -1.23282200 | 2.03247000 | 2.24955900 |
| H | -2.64801100 | 3.99521800 | 2.50931000 |
| H | -3.59418100 | 2.83263600 | 1.59038600 |
| H | -4.11941900 | 6.84127900 | 1.65249600 |
| H | -4.81092200 | 5.48208000 | 2.53600100 |
| H | -6.28495300 | 7.50441400 | 1.15830100 |
| H | -6.92973900 | 5.99392700 | 1.77762700 |
| H | -6.78378400 | 6.72509300 | -0.99741100 |
| H | -7.00733800 | 3.95142200 | 0.32472800 |
| H | -9.41730700 | 4.20376200 | -0.00791500 |
| H | -8.80059800 | 5.43390800 | 1.05949700 |
| H | -9.16020000 | 5.91949700 | -1.92459600 |
| H | -8.86197400 | 7.13466000 | -0.68307300 |

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|---|--------------|------------|-------------|
| H | -11.05609800 | 6.66481100 | 0.34484500 |
| H | -11.38579200 | 5.42736100 | -0.86531200 |
| H | -10.83251800 | 8.38450700 | -1.47754200 |
| H | -11.66241400 | 6.07208600 | -3.30796200 |
| H | -10.19569000 | 7.06046500 | -3.42223000 |
| H | -11.75927400 | 7.78299200 | -3.76864300 |
| H | -13.48753500 | 6.85945700 | -1.48083800 |
| H | -13.24954300 | 8.54673300 | -1.97116300 |
| H | -12.98320000 | 8.07508500 | -0.29060800 |
| H | -7.30123100 | 4.62719200 | -2.60819400 |
| H | -8.42010100 | 3.46876400 | -1.87935200 |
| H | -6.72359700 | 3.13592900 | -1.81482100 |
| H | -4.53544700 | 7.90539200 | -0.30294700 |
| H | -4.59381300 | 7.56759600 | -2.01749900 |
| H | -3.15243900 | 7.15888300 | -1.07310200 |
| H | -4.88737500 | 5.37948200 | -2.96436100 |
| H | -4.94973400 | 3.92135800 | -1.98357500 |
| H | -2.43927300 | 5.60239000 | -2.31940000 |
| H | -2.84484800 | 4.06636600 | -3.06328600 |
| H | -0.78906100 | 3.43443700 | -3.11617700 |
| H | -1.36262300 | 1.92366200 | -2.38542900 |
| H | 0.34204100 | 2.38358400 | -2.31211600 |
| H | 3.18813500 | 2.62729700 | 1.14798600 |

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| C | 6.55314500 | 3.65627800 | 1.14489100 |
| C | 7.96909900 | 4.18102800 | 0.90258300 |
| C | 9.00399300 | 3.35785800 | 1.71384300 |
| C | 8.76373500 | 1.85409300 | 1.56978900 |
| C | 7.37385600 | 1.48070400 | 2.09582600 |
| C | 6.29522600 | 2.43720900 | 1.65720900 |
| H | 10.02759800 | 3.61640400 | 1.38943800 |
| H | 8.85708600 | 1.55611500 | 0.50736400 |
| H | 9.54027500 | 1.28833800 | 2.11699700 |
| H | 7.12205100 | 0.44730700 | 1.77890300 |
| H | 7.38558200 | 1.45789900 | 3.20655000 |
| H | 8.94358100 | 3.64185400 | 2.78219600 |
| C | 4.90788600 | 1.91536500 | 1.87734500 |
| H | 4.14860700 | 2.46280100 | 1.30227000 |
| H | 4.81423900 | 0.85711900 | 1.59672000 |
| H | 4.62547800 | 1.99769400 | 2.93592300 |
| C | 8.28410900 | 4.07893700 | -0.60400300 |
| H | 7.60910700 | 4.70218600 | -1.19865100 |
| H | 9.30566700 | 4.40550100 | -0.82043100 |
| H | 8.17846500 | 3.04871300 | -0.95931500 |
| C | 8.07275300 | 5.65267900 | 1.35070700 |
| H | 9.09962400 | 6.02270600 | 1.27893000 |

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|---|-------------|------------|-------------|
| H | 7.44794600 | 6.30895300 | 0.73516000 |
| H | 7.74241400 | 5.77550700 | 2.38764000 |
| C | 5.48023500 | 4.57476900 | 0.72031300 |
| H | 5.49025700 | 4.82050900 | -0.34531000 |
| C | 4.57379700 | 5.09939600 | 1.55709200 |
| H | 4.59906400 | 4.87459700 | 2.62595500 |
| C | 3.49586100 | 6.01144900 | 1.13679700 |
| C | 2.82509500 | 5.82002700 | -0.01910200 |
| H | 3.09197800 | 4.97835700 | -0.66399500 |
| C | 3.20575200 | 7.11477200 | 2.10501900 |
| H | 2.71271100 | 6.72564200 | 3.00760100 |
| H | 4.12897800 | 7.61561400 | 2.42960900 |
| H | 2.54857700 | 7.88786500 | 1.68400900 |
| C | 1.72823900 | 6.65237600 | -0.49854100 |
| H | 1.43424500 | 7.48101400 | 0.15254900 |
| C | 1.10300100 | 6.41818800 | -1.66568500 |
| H | 1.41155400 | 5.57987900 | -2.29699400 |
| C | -0.02170400 | 7.20602300 | -2.19696200 |
| C | -0.76022400 | 6.70771500 | -3.20541200 |
| H | -0.54475200 | 5.72791100 | -3.63615900 |
| C | -0.29683000 | 8.53775600 | -1.56989200 |
| H | -0.77445700 | 8.41418900 | -0.58742700 |
| H | 0.62814200 | 9.11177900 | -1.42043300 |
| H | -0.96438400 | 9.16452300 | -2.17648300 |
| C | -1.94326400 | 7.37815700 | -3.82582600 |
| H | -1.85315600 | 8.48110300 | -3.85916400 |

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|---|--------------|-------------|-------------|
| H | -2.88833100 | 7.09992300 | -3.31495000 |
| O | -2.16171100 | 6.90094100 | -5.16521100 |
| H | -1.36067300 | 7.03567400 | -5.70807700 |
| C | -10.80747300 | -1.23948400 | 4.06600400 |
| H | -11.75664000 | -0.80460400 | 3.65488300 |
| C | -10.15017100 | -0.19476700 | 5.00423300 |
| H | -9.32748900 | -0.64890900 | 5.59941300 |
| C | -9.66558700 | 1.04429700 | 4.21240900 |
| H | -10.51743900 | 1.55337800 | 3.71132000 |
| C | -9.26189500 | -0.33208400 | 2.23293000 |
| H | -9.94692100 | 0.20605500 | 1.54528600 |
| C | -9.85892800 | -1.59843300 | 2.88961100 |
| H | -10.38692100 | -2.21712000 | 2.12642500 |
| C | -8.85199700 | 1.99851500 | 5.06724400 |
| H | -7.89965100 | 1.54785600 | 5.37693100 |
| H | -9.41237000 | 2.26680500 | 5.97542700 |
| H | -8.61051700 | 2.91827600 | 4.52242600 |
| C | -7.27071600 | 0.19251400 | 0.91392700 |
| H | -7.19504900 | 1.07127700 | 1.59534000 |
| C | -5.96544900 | -0.53069600 | 0.73161100 |
| H | -6.04118200 | -1.46494900 | 0.16646000 |
| C | -4.80612400 | -0.06834700 | 1.21699300 |
| H | -4.75581300 | 0.85876900 | 1.79388900 |
| C | -3.54051500 | -0.76817500 | 1.00414100 |
| H | -3.58667400 | -1.67830900 | 0.39198500 |
| C | -2.37105400 | -0.34643200 | 1.51845700 |

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| H | -2.30876800 | 0.54590800 | 2.14404700 |
| C | -1.12255700 | -1.06025700 | 1.26595400 |
| H | -1.19681600 | -1.91536600 | 0.57520900 |
| C | 0.05207600 | -0.71558700 | 1.82419200 |
| H | 0.12748200 | 0.11896500 | 2.52393000 |
| C | 1.28684900 | -1.43706300 | 1.53299000 |
| H | 1.22450500 | -2.20237100 | 0.74406000 |
| C | 2.44854100 | -1.19837800 | 2.16951600 |
| H | 2.52153600 | -0.44835900 | 2.95924900 |
| C | 3.66835800 | -1.93378300 | 1.85124600 |
| H | 3.58152400 | -2.68205300 | 1.05306600 |
| C | 4.83790100 | -1.72910600 | 2.48563700 |
| H | 4.92648600 | -0.99988600 | 3.29402000 |
| C | 6.04896800 | -2.46488900 | 2.13853300 |
| H | 5.93076700 | -3.27845400 | 1.41107900 |
| C | 7.26034100 | -2.18733400 | 2.65329000 |
| H | 7.40683900 | -1.39864700 | 3.39262400 |
| C | -7.91707100 | 0.59082300 | -0.42202600 |
| H | -8.82591700 | 1.19719700 | -0.22510800 |
| H | -7.22027700 | 1.25441900 | -0.98030300 |
| C | 8.45184800 | -2.92543200 | 2.23380100 |
| H | 8.25526500 | -3.88302000 | 1.73239200 |
| C | 9.69935000 | -2.46940300 | 2.40571200 |
| H | 9.90693500 | -1.52421000 | 2.90560800 |
| C | 10.91393400 | -3.22160400 | 1.92959000 |
| H | 10.64078000 | -4.26843200 | 1.63094200 |

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| C | 11.52576700 | -2.52582500 | 0.68513900 |
| H | 12.05280400 | -1.58940800 | 0.97715000 |
| C | 10.51089900 | -2.21165800 | -0.44290700 |
| H | 9.70630500 | -1.56378400 | 0.00289300 |
| C | 9.81289900 | -3.48433800 | -0.95790300 |
| H | 9.41162000 | -4.09091500 | -0.11044700 |
| C | 7.39672000 | -3.30837900 | -1.35111200 |
| C | 6.38223800 | -2.68697800 | -2.26647300 |
| H | 6.77837600 | -1.75288600 | -2.71838700 |
| H | 6.21607600 | -3.37751200 | -3.12643400 |
| C | 5.05059400 | -2.42976100 | -1.53386400 |
| H | 5.21124200 | -1.78690700 | -0.63621300 |
| C | 3.99212600 | -1.85460300 | -2.47975600 |
| H | 4.39846200 | -0.97364400 | -3.01270100 |
| H | 3.75737000 | -2.60630500 | -3.26606200 |
| C | 2.69166800 | -1.47613400 | -1.75169600 |
| H | 2.89264300 | -0.88667300 | -0.82602900 |
| C | 1.72932600 | -0.72878600 | -2.69226700 |
| H | 1.70246000 | -1.23480100 | -3.68021000 |
| H | 2.13076800 | 0.28496500 | -2.88425800 |
| C | 0.30802100 | -0.62643200 | -2.12469600 |
| H | 0.30658500 | -0.89742400 | -1.04368900 |
| H | -0.04452000 | 0.42187400 | -2.16292100 |
| C | -0.67459600 | -1.53090000 | -2.87776500 |
| H | -0.73829500 | -1.25648700 | -3.95480100 |
| C | -2.08464300 | -1.55315100 | -2.21248300 |

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| H | -2.27222800 | -0.66228500 | -1.57197200 |
| C | -3.18871300 | -1.74596800 | -3.26010400 |
| H | -2.98756700 | -2.67322800 | -3.83941700 |
| H | -3.16997100 | -0.91752900 | -3.99185700 |
| C | -4.57597800 | -1.85131800 | -2.61079500 |
| H | -4.75677700 | -1.02935000 | -1.87660500 |
| C | -5.70163200 | -1.91482800 | -3.65347400 |
| H | -5.59711300 | -2.84105000 | -4.25783100 |
| H | -5.61559800 | -1.06104900 | -4.35176000 |
| C | -7.08907900 | -1.91830800 | -2.99971900 |
| C | -8.26202700 | -1.81713600 | -3.97842500 |
| H | -8.33988200 | -2.74435300 | -4.58340900 |
| H | -8.09590500 | -0.99561600 | -4.70556800 |
| C | -9.58330700 | -1.58589500 | -3.24161300 |
| H | -9.94677100 | -2.51182200 | -2.74276200 |
| C | -9.48510500 | -0.41738000 | -2.21741600 |
| H | -9.33293000 | 0.52873900 | -2.80919800 |
| C | -8.25485200 | -0.62447900 | -1.28791600 |
| H | -8.37969000 | -1.55687800 | -0.68479100 |
| C | -10.74094400 | -0.25899200 | -1.41450400 |
| C | 10.57912000 | -4.34513500 | -1.93697600 |
| H | 10.02694100 | -5.25944400 | -2.18821100 |
| H | 11.54324500 | -4.64992200 | -1.49566800 |
| H | 10.78394500 | -3.82402700 | -2.87981200 |
| C | 11.17867100 | -1.41298600 | -1.56273700 |
| H | 12.05191800 | -1.92769300 | -1.97829700 |

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| H | 11.50307400 | -0.42535100 | -1.21689700 |
| H | 10.47363400 | -1.25460800 | -2.39155900 |
| C | 11.95924600 | -3.31120700 | 3.04573600 |
| H | 12.26981400 | -2.32727900 | 3.41039100 |
| H | 12.85866200 | -3.83074900 | 2.68475400 |
| H | 11.57114900 | -3.87379300 | 3.90255900 |
| O | -8.84490200 | -2.46537600 | 3.40287500 |
| H | -7.95184900 | -2.03618600 | 3.32183200 |
| O | -11.13497600 | 0.33105100 | 5.90552600 |
| H | -11.63020300 | -0.41634000 | 6.32195000 |
| O | -8.72940500 | 0.59769200 | 3.19764400 |
| O | -8.10419200 | -0.82142600 | 1.56762000 |
| O | -7.33293100 | -3.06166200 | -2.21040800 |
| H | -6.51614200 | -3.34542900 | -1.69555600 |
| O | -7.08332200 | -0.77163000 | -2.11943900 |
| O | -10.93466000 | 0.30916600 | -0.36286900 |
| O | -11.81913300 | -0.86293100 | -2.03357800 |
| H | -12.66867200 | -0.75030800 | -1.52840600 |
| O | -4.68256900 | -3.09862100 | -1.89198200 |
| H | -3.88299400 | -3.23028300 | -1.30417300 |
| O | -2.12442300 | -2.64251700 | -1.27433100 |
| H | -1.62260700 | -3.42623900 | -1.66781800 |
| O | -0.25384300 | -2.90422400 | -2.89011800 |
| H | 0.55176500 | -3.03640700 | -2.29108100 |
| O | 1.99377300 | -2.65799400 | -1.29780100 |
| H | 2.62322500 | -3.42037100 | -1.16531500 |

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| O | 4.49464100 | -3.67873700 | -1.08561800 |
| H | 5.14229100 | -4.17698500 | -0.51425800 |
| O | 7.16767000 | -4.03362200 | -0.40008000 |
| O | 8.64949900 | -2.95654300 | -1.73119700 |
| O | 12.51964600 | -3.46703800 | 0.22767400 |
| H | 13.02495700 | -3.08589400 | -0.51743500 |
| O | -10.49017900 | -1.20977400 | -4.28584300 |
| H | -11.42260200 | -1.23108400 | -3.96595800 |
| N | -11.15643000 | -2.42482300 | 4.89119000 |
| H | -10.30188300 | -2.91763800 | 5.16623600 |
| H | -11.70596900 | -3.08638700 | 4.34819400 |

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| C | 4.28779000 | 0.82998200 | 3.97177100 |
| C | 5.08065800 | -0.14318700 | 3.08750700 |
| C | 6.29297400 | -0.71271200 | 3.84388500 |
| C | 5.95585000 | -1.10483300 | 5.27434900 |
| C | 5.49929500 | 0.12643500 | 6.04499200 |
| C | 4.48522200 | 0.95859400 | 5.29393200 |
| H | 6.69805100 | -1.56352500 | 3.28622200 |
| H | 5.15796200 | -1.85576000 | 5.27847000 |
| H | 6.81995200 | -1.56468000 | 5.76465400 |
| H | 5.07465900 | -0.16154400 | 7.01441200 |

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| H | 6.36551200 | 0.76158300 | 6.28217000 |
| H | 7.07864400 | 0.05413800 | 3.87122000 |
| C | 3.72726900 | 1.91373500 | 6.17670900 |
| H | 2.98892100 | 2.50283300 | 5.63581200 |
| H | 3.21630900 | 1.36489900 | 6.97665900 |
| H | 4.41956800 | 2.60569700 | 6.67159500 |
| C | 4.16593800 | -1.28965000 | 2.61908800 |
| H | 3.27259100 | -0.91226400 | 2.11451900 |
| H | 4.69113300 | -1.92002600 | 1.89644100 |
| H | 3.83798700 | -1.91277700 | 3.45490700 |
| C | 5.59762700 | 0.60220500 | 1.84772000 |
| H | 6.22976100 | -0.05592900 | 1.24872900 |
| H | 4.77307800 | 0.92874200 | 1.21504400 |
| H | 6.17506200 | 1.48703700 | 2.13332000 |
| C | 3.26663900 | 1.62291200 | 3.24567700 |
| H | 2.44229100 | 1.06563700 | 2.80024100 |
| C | 3.33412500 | 2.94037800 | 3.03126200 |
| H | 4.21338000 | 3.47289700 | 3.39319500 |
| C | 2.35032500 | 3.74898600 | 2.29395800 |
| C | 1.03408400 | 3.47813500 | 2.38155100 |
| H | 0.73665100 | 2.65025900 | 3.02067800 |
| C | 2.94686900 | 4.83827100 | 1.44592700 |
| H | 3.62710000 | 5.46022500 | 2.03736400 |
| H | 3.54024600 | 4.38944300 | 0.64162800 |
| H | 2.20045000 | 5.49097600 | 0.99205100 |
| C | -0.05726100 | 4.18145900 | 1.73592900 |

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| H | 0.16205500 | 5.13134400 | 1.25621600 |
| C | -1.31539400 | 3.70818000 | 1.72787500 |
| H | -1.50005200 | 2.73001700 | 2.16731000 |
| C | -2.48755900 | 4.35645300 | 1.14174800 |
| C | -3.63651200 | 3.66173000 | 1.06737100 |
| H | -3.63062100 | 2.63373700 | 1.41207400 |
| C | -2.33741900 | 5.76624200 | 0.63289000 |
| H | -1.92922300 | 6.41651300 | 1.41196600 |
| H | -1.63443800 | 5.80144200 | -0.20665800 |
| H | -3.28312800 | 6.19530000 | 0.29691800 |
| C | -4.92467000 | 4.15053700 | 0.47092600 |
| H | -5.17468600 | 5.15154600 | 0.84905000 |
| H | -5.73957300 | 3.47854400 | 0.75018700 |
| O | -4.92093200 | 4.16231400 | -0.96139600 |
| H | -4.08210900 | 4.54457000 | -1.24389000 |
| C | 9.79447500 | -2.76227500 | 0.82693800 |
| H | 10.42664900 | -1.99833800 | 0.35743100 |
| C | 9.86623900 | -4.00650900 | -0.05690400 |
| H | 9.25210600 | -4.79491100 | 0.40601100 |
| C | 9.27639900 | -3.71292700 | -1.43090700 |
| H | 9.86296600 | -2.90084600 | -1.89132100 |
| C | 7.80915000 | -2.09250100 | -0.52702700 |
| H | 8.33339700 | -1.28309200 | -1.05124400 |
| C | 8.36342800 | -2.23747200 | 0.88881600 |
| H | 8.34347500 | -1.24537000 | 1.36553200 |
| C | 9.26732800 | -4.92316300 | -2.33614500 |

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| H | 8.65021800 | -5.71006000 | -1.89426000 |
| H | 10.28445400 | -5.29943200 | -2.45586100 |
| H | 8.85490100 | -4.66717500 | -3.31465200 |
| C | 5.60854900 | -1.87832100 | -1.53676500 |
| H | 5.63423600 | -2.90708500 | -1.91029100 |
| C | 4.23988400 | -1.56865500 | -1.01581100 |
| H | 4.11853500 | -0.60635000 | -0.52743900 |
| C | 3.21207700 | -2.42041700 | -1.08843600 |
| H | 3.34031800 | -3.37947900 | -1.59024000 |
| C | 1.90546800 | -2.13306100 | -0.52877000 |
| H | 1.81798600 | -1.22342200 | 0.06238700 |
| C | 0.80857100 | -2.89489400 | -0.70324700 |
| H | 0.87305400 | -3.80316800 | -1.30193500 |
| C | -0.48637900 | -2.53067000 | -0.17672900 |
| H | -0.52510900 | -1.64119300 | 0.44664700 |
| C | -1.64391500 | -3.17070100 | -0.43931600 |
| H | -1.63727400 | -4.06524500 | -1.06148000 |
| C | -2.91944600 | -2.69950300 | 0.04411600 |
| H | -2.90197100 | -1.77940800 | 0.62350100 |
| C | -4.10509900 | -3.29190700 | -0.20340100 |
| H | -4.13147400 | -4.20702200 | -0.79437000 |
| C | -5.36709500 | -2.78297500 | 0.27636200 |
| H | -5.33316200 | -1.86094100 | 0.85555700 |
| C | -6.55839300 | -3.36751700 | 0.03920900 |
| H | -6.58626300 | -4.27995200 | -0.55580500 |
| C | -7.82438400 | -2.86845400 | 0.52194900 |

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| H | -7.79924600 | -1.97717600 | 1.14819000 |
| C | -9.01439900 | -3.42596900 | 0.23064900 |
| H | -9.04141100 | -4.30692100 | -0.41013000 |
| C | 6.11029600 | -0.97496200 | -2.66984000 |
| H | 7.10409100 | -1.33018000 | -2.95344700 |
| H | 5.45476600 | -1.12555000 | -3.53358500 |
| C | -10.28773400 | -2.90750500 | 0.69058000 |
| H | -10.24410200 | -2.06576800 | 1.37899000 |
| C | -11.47843800 | -3.36515300 | 0.28652800 |
| H | -11.51220900 | -4.19923100 | -0.41672800 |
| C | -12.80821800 | -2.79998000 | 0.69538800 |
| H | -12.65144400 | -2.04852100 | 1.47729500 |
| C | -13.49922400 | -2.09295400 | -0.48677100 |
| H | -13.79328200 | -2.87337300 | -1.20830700 |
| C | -12.60956000 | -1.09727300 | -1.25308100 |
| H | -11.74460400 | -1.67354600 | -1.59542700 |
| C | -12.03455400 | 0.00185800 | -0.35354400 |
| H | -11.68793600 | -0.43175000 | 0.58040700 |
| C | -9.71734000 | 0.59497100 | -0.36368100 |
| C | -8.56888500 | 1.10291500 | -1.19901000 |
| H | -8.75819800 | 0.87985100 | -2.25063400 |
| H | -8.53341200 | 2.19295300 | -1.08944100 |
| C | -7.23442900 | 0.51559600 | -0.73685300 |
| H | -7.27485600 | -0.57856500 | -0.83296600 |
| C | -6.06619600 | 1.05560600 | -1.54642900 |
| H | -6.25327900 | 0.85216300 | -2.60624200 |

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| H | -6.00842900 | 2.14204000 | -1.42171300 |
| C | -4.71375400 | 0.44305600 | -1.17488600 |
| H | -4.72661900 | -0.63506600 | -1.39154000 |
| C | -3.59947300 | 1.10740000 | -1.97552700 |
| H | -3.64587500 | 2.18269000 | -1.77490100 |
| H | -3.84918300 | 0.97045400 | -3.03366900 |
| C | -2.17663800 | 0.58669800 | -1.74190500 |
| H | -2.16284900 | -0.50755400 | -1.68834800 |
| H | -1.57417900 | 0.86115000 | -2.61571100 |
| C | -1.45855800 | 1.13625500 | -0.51007400 |
| H | -1.61718600 | 2.22156800 | -0.45033400 |
| C | 0.05231300 | 0.85404400 | -0.58928600 |
| H | 0.19836100 | -0.09350400 | -1.12358100 |
| C | 0.83879300 | 1.94071400 | -1.30849000 |
| H | 0.69348700 | 2.89576800 | -0.79174400 |
| H | 0.45459800 | 2.04297900 | -2.32951200 |
| C | 2.33048100 | 1.62127100 | -1.36283300 |
| H | 2.46737500 | 0.60261200 | -1.74842700 |
| C | 3.10405100 | 2.57635500 | -2.25973400 |
| H | 2.90139100 | 3.61128800 | -1.96609100 |
| H | 2.76615200 | 2.44100500 | -3.29118600 |
| C | 4.61924700 | 2.36443300 | -2.20122700 |
| C | 5.35256700 | 3.15867400 | -3.26970700 |
| H | 5.23353700 | 4.22928700 | -3.09072900 |
| H | 4.93050000 | 2.92212800 | -4.25036100 |
| C | 6.83058200 | 2.81875800 | -3.29745800 |

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| H | 7.29023700 | 3.15138400 | -2.35576700 |
| C | 7.01403000 | 1.28048500 | -3.40975800 |
| H | 6.70072800 | 1.00535100 | -4.42367300 |
| C | 6.15687100 | 0.52105700 | -2.37937600 |
| H | 6.55877700 | 0.70580300 | -1.37763500 |
| C | 8.47445700 | 0.94525100 | -3.26094300 |
| C | -12.93704100 | 1.18166900 | -0.05644300 |
| H | -12.44211600 | 1.86473000 | 0.63766000 |
| H | -13.85980500 | 0.81650600 | 0.39668400 |
| H | -13.18063100 | 1.73241800 | -0.96744500 |
| C | -13.32162500 | -0.54194600 | -2.48482300 |
| H | -14.23796700 | -0.00620800 | -2.21905100 |
| H | -13.58889100 | -1.34842000 | -3.17377800 |
| H | -12.67754900 | 0.15878300 | -3.02113400 |
| C | -13.72354600 | -3.88910300 | 1.26281100 |
| H | -13.88053000 | -4.68464600 | 0.52592600 |
| H | -14.69563000 | -3.46901900 | 1.52484700 |
| H | -13.27957500 | -4.34124400 | 2.15252300 |
| O | 7.59236400 | -3.15663400 | 1.63739800 |
| H | 6.68633600 | -3.07997700 | 1.30376000 |
| O | 11.20725400 | -4.41155900 | -0.20280500 |
| H | 11.58624300 | -4.30114900 | 0.68428400 |
| O | 7.92507800 | -3.29030600 | -1.26182000 |
| O | 6.45049300 | -1.80423300 | -0.37205500 |
| O | 5.15640600 | 2.74333200 | -0.96542700 |
| H | 4.56281900 | 2.36792700 | -0.28913000 |

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| O | 4.81295200 | 0.97487100 | -2.44887900 |
| O | 8.99701600 | 0.35685700 | -2.34464400 |
| O | 9.21892200 | 1.43049400 | -4.28550400 |
| H | 10.14220300 | 1.20475600 | -4.08470900 |
| O | 2.90681100 | 1.70570800 | -0.05965800 |
| H | 2.24445900 | 1.41350900 | 0.58954700 |
| O | 0.58586700 | 0.70388900 | 0.72793000 |
| H | -0.18215200 | 0.55972200 | 1.30749500 |
| O | -1.89707000 | 0.53577300 | 0.69976600 |
| H | -2.88024400 | 0.55469600 | 0.70708100 |
| O | -4.45129600 | 0.60921400 | 0.22280900 |
| H | -5.30401700 | 0.65117100 | 0.69915000 |
| O | -7.00345200 | 0.85961300 | 0.63229000 |
| H | -7.81052300 | 0.61532200 | 1.12211500 |
| O | -9.60646200 | 0.30876500 | 0.81888600 |
| O | -10.84928400 | 0.50525300 | -1.04619200 |
| O | -14.66430700 | -1.47010600 | 0.04590100 |
| H | -15.26523400 | -1.26741100 | -0.67905600 |
| O | 7.37117000 | 3.50331500 | -4.40671000 |
| H | 8.28105700 | 3.20777600 | -4.53665100 |
| N | 10.38081700 | -3.10093600 | 2.12022000 |
| H | 9.68899200 | -3.62051700 | 2.65591700 |
| H | 10.59381700 | -2.26173400 | 2.64993100 |

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| C | -3.27957700 | 7.45177900 | -0.28796400 |
| C | -1.93559500 | 7.07854900 | -0.91563800 |
| C | -1.25538200 | 8.32958900 | -1.53095300 |
| C | -1.27760600 | 9.51288100 | -0.56189700 |
| C | -2.72052300 | 9.90096700 | -0.22247000 |
| C | -3.60936600 | 8.71376200 | 0.04818000 |
| H | -0.21675600 | 8.09012200 | -1.81978500 |
| H | -0.72877900 | 9.25399500 | 0.36491800 |
| H | -0.74609600 | 10.37750900 | -1.00036800 |
| H | -2.72395600 | 10.58801500 | 0.64727500 |
| H | -3.16171300 | 10.47931800 | -1.06218900 |
| H | -1.77626800 | 8.60809800 | -2.46719600 |
| C | -4.90517600 | 9.08245200 | 0.70457900 |
| H | -5.49057200 | 8.20943600 | 1.02520100 |
| H | -4.74205800 | 9.69578900 | 1.60071700 |
| H | -5.54260600 | 9.66014900 | 0.02171400 |
| C | -1.03329800 | 6.47541400 | 0.18037000 |
| H | -1.46381900 | 5.55980400 | 0.59733100 |
| H | -0.04265900 | 6.22583300 | -0.20938800 |
| H | -0.89934900 | 7.17918200 | 1.00945900 |
| C | -2.13969800 | 6.04449100 | -2.04134300 |
| H | -1.20402000 | 5.83584700 | -2.56757800 |
| H | -2.51485000 | 5.09158600 | -1.65233100 |
| H | -2.86909500 | 6.39944000 | -2.77712400 |

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| C | -4.16977400 | 6.30490800 | -0.02526700 |
| H | -3.77284300 | 5.57786500 | 0.68830600 |
| C | -5.35657900 | 6.13760500 | -0.62624000 |
| H | -5.71720200 | 6.86626600 | -1.35718600 |
| C | -6.25814700 | 4.99719400 | -0.39025500 |
| C | -6.37347500 | 4.41957000 | 0.82447300 |
| H | -5.77999800 | 4.79704100 | 1.66171400 |
| C | -7.04052900 | 4.57422000 | -1.59518200 |
| H | -7.78702000 | 5.33502700 | -1.86494100 |
| H | -6.38603300 | 4.43542800 | -2.46690700 |
| H | -7.58283000 | 3.63122600 | -1.44067000 |
| C | -7.26478200 | 3.30908600 | 1.14103600 |
| H | -7.84163100 | 2.90013100 | 0.30539100 |
| C | -7.39608800 | 2.81436200 | 2.38308200 |
| H | -6.82877500 | 3.22907500 | 3.21963800 |
| C | -8.31473500 | 1.71740200 | 2.74155300 |
| C | -8.99319200 | 1.77031700 | 3.90014900 |
| H | -8.88255600 | 2.61466200 | 4.58434400 |
| C | -8.43998300 | 0.59130700 | 1.76398500 |
| H | -9.18919700 | 0.81917000 | 0.99363200 |
| H | -7.48801900 | 0.38955800 | 1.25178400 |
| H | -8.74195100 | -0.35429700 | 2.24272700 |
| C | -9.98788500 | 0.75529500 | 4.36505500 |
| H | -9.67818500 | -0.28759300 | 4.16058300 |
| H | -10.99115000 | 0.93825000 | 3.92730400 |
| O | -10.23712700 | 0.89271300 | 5.77460200 |

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| H | -9.42483800 | 0.70182600 | 6.28231500 |
| C | -7.71444200 | -4.74590500 | 2.76451900 |
| H | -8.73949200 | -4.52948500 | 2.36295600 |
| C | -7.41244000 | -3.74775400 | 3.91128800 |
| H | -6.51731900 | -4.06153500 | 4.49227400 |
| C | -7.27221900 | -2.29926200 | 3.38626900 |
| H | -8.22436100 | -1.94501500 | 2.92453300 |
| C | -6.45269000 | -3.12223200 | 1.23122800 |
| H | -7.23895800 | -2.67677200 | 0.58752200 |
| C | -6.67951200 | -4.60299100 | 1.61592700 |
| H | -6.99493200 | -5.18959600 | 0.72109700 |
| C | -6.76460800 | -1.34134900 | 4.44870100 |
| H | -5.70136400 | -1.51501900 | 4.66506100 |
| H | -7.32826700 | -1.47218700 | 5.38364800 |
| H | -6.86094100 | -0.29527500 | 4.12834500 |
| C | -4.58744700 | -1.83590600 | 0.30019000 |
| H | -4.74371400 | -1.18269600 | 1.19090100 |
| C | -3.14340000 | -2.18481800 | 0.07086700 |
| H | -2.96468500 | -2.87360000 | -0.76026300 |
| C | -2.15694700 | -1.68336800 | 0.82475300 |
| H | -2.36433000 | -1.01251200 | 1.66342600 |
| C | -0.74916200 | -1.98621100 | 0.57376000 |
| H | -0.53528400 | -2.64752200 | -0.27520200 |
| C | 0.24574600 | -1.48685400 | 1.32885100 |
| H | 0.04029600 | -0.84684500 | 2.18977400 |
| C | 1.65024400 | -1.76271500 | 1.04134500 |

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| H | 1.84453400 | -2.37324500 | 0.14623900 |
| C | 2.65455200 | -1.29801800 | 1.80636900 |
| H | 2.45651000 | -0.70885500 | 2.70476000 |
| C | 4.05771000 | -1.54863200 | 1.49309100 |
| H | 4.26175700 | -2.05674300 | 0.53957600 |
| C | 5.06161900 | -1.17473100 | 2.30793000 |
| H | 4.86409100 | -0.67384800 | 3.25807100 |
| C | 6.46251100 | -1.42097300 | 1.98202600 |
| H | 6.64990700 | -1.95865500 | 1.04556800 |
| C | 7.47612900 | -1.02299900 | 2.77351600 |
| H | 7.28884800 | -0.49788300 | 3.71296000 |
| C | 8.87361600 | -1.26235300 | 2.43095400 |
| H | 9.05816400 | -1.86255400 | 1.53101100 |
| C | 9.90536600 | -0.78381200 | 3.14982700 |
| H | 9.75401500 | -0.19799000 | 4.05752700 |
| C | -5.25806400 | -1.22644100 | -0.93961100 |
| H | -6.29991300 | -0.93699100 | -0.68830100 |
| H | -4.73341000 | -0.28296500 | -1.20861800 |
| C | 11.28874400 | -1.00925900 | 2.73232300 |
| H | 11.42186700 | -1.75736000 | 1.93828800 |
| C | 12.33095200 | -0.33493000 | 3.23575900 |
| H | 12.21692600 | 0.40060800 | 4.03098000 |
| C | 13.73959800 | -0.53073300 | 2.74040500 |
| H | 13.81276500 | -1.45353400 | 2.10553900 |
| C | 14.16813600 | 0.67510500 | 1.86259500 |
| H | 14.38727500 | 1.56400400 | 2.49661000 |

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| C | 13.14911700 | 1.06966600 | 0.76350000 |
| H | 12.17230900 | 1.29056300 | 1.27669700 |
| C | 12.87859900 | -0.09172300 | -0.21123900 |
| H | 12.65366600 | -1.03526100 | 0.34242800 |
| C | 10.54709100 | -0.48374400 | -0.87343300 |
| C | 9.42349000 | 0.11249500 | -1.67070000 |
| H | 9.49144200 | 1.22101500 | -1.67729800 |
| H | 9.54975500 | -0.19295100 | -2.73583600 |
| C | 8.05111200 | -0.35644300 | -1.14798600 |
| H | 7.93198600 | -0.10229000 | -0.06787300 |
| C | 6.90663200 | 0.18991300 | -2.00672400 |
| H | 7.02507000 | 1.28087900 | -2.14908600 |
| H | 6.96947600 | -0.25984400 | -3.02283600 |
| C | 5.52189100 | -0.11609900 | -1.41163800 |
| H | 5.46926000 | 0.14797500 | -0.32880600 |
| C | 4.41370400 | 0.58780600 | -2.21536600 |
| H | 4.58205600 | 0.42631900 | -3.30099600 |
| H | 4.49496300 | 1.68029000 | -2.05691700 |
| C | 3.00775000 | 0.10994800 | -1.83159800 |
| H | 3.04796800 | -0.48215700 | -0.88821300 |
| H | 2.35890900 | 0.97689200 | -1.60412600 |
| C | 2.36961500 | -0.73686400 | -2.93912100 |
| H | 2.27716500 | -0.16240600 | -3.88827400 |
| C | 0.99848600 | -1.34016800 | -2.50625200 |
| H | 0.53921400 | -0.79073400 | -1.65373000 |
| C | 0.03716800 | -1.44855600 | -3.69781500 |

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| H | 0.50628500 | -2.06724800 | -4.49342900 |
| H | -0.13114000 | -0.45193800 | -4.14483100 |
| C | -1.30064200 | -2.08186900 | -3.29008800 |
| H | -1.72784400 | -1.60008600 | -2.37715700 |
| C | -2.32007800 | -2.08167000 | -4.43949200 |
| H | -1.95348400 | -2.73406800 | -5.26092500 |
| H | -2.41870900 | -1.06153100 | -4.85506300 |
| C | -3.69239200 | -2.59787200 | -3.98824200 |
| C | -4.80387900 | -2.47910800 | -5.03502600 |
| H | -4.61389600 | -3.17409900 | -5.87932600 |
| H | -4.81760700 | -1.46251700 | -5.47888900 |
| C | -6.17394900 | -2.78935900 | -4.42687800 |
| H | -6.30873100 | -3.87922600 | -4.24648800 |
| C | -6.42715200 | -1.98422500 | -3.11895400 |
| H | -6.48722900 | -0.89710100 | -3.40639500 |
| C | -5.23356200 | -2.17402400 | -2.13979800 |
| H | -5.14876900 | -3.24593700 | -1.83592800 |
| C | -7.72276000 | -2.35399000 | -2.46146200 |
| C | 13.89613800 | -0.32386200 | -1.30578900 |
| H | 13.64963700 | -1.20949100 | -1.90471400 |
| H | 14.89304700 | -0.48908200 | -0.86297700 |
| H | 13.96514100 | 0.52397700 | -1.99762700 |
| C | 13.59229100 | 2.34707600 | 0.04976900 |
| H | 14.58598800 | 2.25009100 | -0.40075600 |
| H | 13.61389300 | 3.20406300 | 0.73215700 |
| H | 12.89249200 | 2.59263400 | -0.76195400 |

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| C | 14.70782000 | -0.69434200 | 3.91592000 |
| H | 14.69046800 | 0.16246500 | 4.59655900 |
| H | 15.73832600 | -0.80586700 | 3.54825000 |
| H | 14.46527200 | -1.58789500 | 4.50280200 |
| O | -5.47181800 | -5.23311400 | 2.05022000 |
| H | -4.71651100 | -4.58484800 | 2.02224000 |
| O | -8.54012300 | -3.68026700 | 4.79619300 |
| H | -8.80272600 | -4.59506600 | 5.06385600 |
| O | -6.23608100 | -2.27139100 | 2.37250400 |
| O | -5.18644500 | -3.14466100 | 0.58086600 |
| O | -3.67595600 | -3.94868200 | -3.58288200 |
| H | -2.83314600 | -4.18328800 | -3.08539200 |
| O | -4.02265600 | -1.79706400 | -2.83084500 |
| O | -8.11273800 | -2.15735100 | -1.33182600 |
| O | -8.57306800 | -2.99709600 | -3.34014600 |
| H | -9.44784300 | -3.23487200 | -2.92990800 |
| O | -1.10751100 | -3.47881800 | -2.98414300 |
| H | -0.31056500 | -3.59920100 | -2.38964200 |
| O | 1.22785200 | -2.65083700 | -1.96239200 |
| H | 1.95673200 | -3.10127000 | -2.49801500 |
| O | 3.17495300 | -1.87233900 | -3.29177800 |
| H | 3.96651200 | -1.95712300 | -2.66587400 |
| O | 5.23691300 | -1.53181500 | -1.46096900 |
| H | 6.07746500 | -2.06738900 | -1.50922300 |
| O | 7.94514600 | -1.78533500 | -1.28108100 |
| H | 8.67985100 | -2.24525000 | -0.78883500 |

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|---|-------------|-------------|-------------|
| O | 10.52973700 | -1.54191300 | -0.27142600 |
| O | 11.63147400 | 0.32957400 | -0.91598100 |
| O | 15.40950900 | 0.23708300 | 1.27080100 |
| H | 15.81372400 | 0.96695100 | 0.76159700 |
| O | -7.09826600 | -2.34364700 | -5.42748700 |
| H | -8.00497600 | -2.68506400 | -5.24370900 |
| N | -7.72206400 | -6.10969200 | 3.35404200 |
| H | -6.76647800 | -6.38729800 | 3.59641900 |
| H | -8.05399600 | -6.78982600 | 2.67457800 |

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|---|------------|-------------|-------------|
| C | 3.65994700 | 7.44094100 | 1.19494400 |
| C | 4.18992000 | 8.49640600 | 2.16669600 |
| C | 4.42696200 | 9.84387900 | 1.43579100 |
| C | 3.24632300 | 10.21069600 | 0.53499400 |
| C | 3.04713500 | 9.14261100 | -0.54605100 |
| C | 3.12941300 | 7.73844300 | -0.00607400 |
| H | 4.60824800 | 10.64487700 | 2.17465400 |
| H | 2.32408100 | 10.31160100 | 1.14038200 |
| H | 3.41399300 | 11.19833900 | 0.06688800 |
| H | 2.07321800 | 9.30236200 | -1.05093800 |
| H | 3.81799600 | 9.25990100 | -1.33729100 |

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|---|------------|------------|-------------|
| H | 5.34970600 | 9.77740800 | 0.82782700 |
| C | 2.56399900 | 6.70544000 | -0.93391400 |
| H | 2.84941800 | 5.68061900 | -0.66255400 |
| H | 1.46550400 | 6.74438700 | -0.93107600 |
| H | 2.89509800 | 6.86404900 | -1.96849900 |
| C | 3.15703100 | 8.68862200 | 3.29576700 |
| H | 3.01619200 | 7.77171000 | 3.87610500 |
| H | 3.47103500 | 9.47096100 | 3.99349800 |
| H | 2.17953400 | 8.97526700 | 2.89251600 |
| C | 5.53238800 | 8.03778700 | 2.77092800 |
| H | 5.97299400 | 8.81688400 | 3.40019400 |
| H | 5.41152900 | 7.14600600 | 3.39541400 |
| H | 6.25531400 | 7.78858300 | 1.98731300 |
| C | 3.70646900 | 6.05755200 | 1.70723100 |
| H | 2.96181900 | 5.84032600 | 2.47891400 |
| C | 4.59194100 | 5.13975400 | 1.29421800 |
| H | 5.34985100 | 5.38814100 | 0.54801400 |
| C | 4.64033000 | 3.75964700 | 1.80575800 |
| C | 3.51117100 | 3.07515500 | 2.08682700 |
| H | 2.53988000 | 3.55806300 | 1.94311900 |
| C | 6.02093600 | 3.20150900 | 1.95726000 |
| H | 6.50856000 | 3.07417800 | 0.98160800 |
| H | 6.65417100 | 3.87976100 | 2.54908100 |
| H | 6.03404300 | 2.22748200 | 2.46496700 |
| C | 3.45932900 | 1.70647500 | 2.58392900 |
| H | 4.42263000 | 1.21156600 | 2.75011900 |

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|---|--------------|-------------|-------------|
| C | 2.30003100 | 1.07300100 | 2.83270800 |
| H | 1.34660800 | 1.58935000 | 2.68309400 |
| C | 2.17710900 | -0.31238100 | 3.31411600 |
| C | 0.99985500 | -0.73783500 | 3.80900000 |
| H | 0.13521400 | -0.07529500 | 3.87766900 |
| C | 3.36478300 | -1.21617700 | 3.19898300 |
| H | 3.27794800 | -1.85486300 | 2.30458200 |
| H | 4.31160500 | -0.66724900 | 3.11497900 |
| H | 3.46140900 | -1.88321100 | 4.06650900 |
| C | 0.72312700 | -2.13236300 | 4.26876700 |
| H | 1.54907400 | -2.57292900 | 4.85748800 |
| H | 0.48077900 | -2.79912100 | 3.40256700 |
| O | -0.48112800 | -2.19571400 | 5.04879300 |
| H | -0.41372800 | -1.61445100 | 5.83135300 |
| C | -11.10587100 | -3.64240000 | 0.92961200 |
| H | -11.98224800 | -2.94571600 | 1.00514800 |
| C | -10.60341100 | -3.95804300 | 2.36211000 |
| H | -9.88033000 | -4.80294400 | 2.36073400 |
| C | -10.00657300 | -2.69828500 | 3.03580800 |
| H | -10.77062900 | -1.89523300 | 3.12252000 |
| C | -9.29640400 | -1.82627000 | 0.86968100 |
| H | -9.86807100 | -0.87594300 | 0.91870000 |
| C | -9.99184600 | -2.96362900 | 0.08612800 |
| H | -10.40352700 | -2.57386500 | -0.87453400 |
| C | -9.34440500 | -3.00510800 | 4.36616500 |
| H | -8.42990100 | -3.59852600 | 4.23077200 |

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|---|--------------|-------------|-------------|
| H | -10.02889300 | -3.57865000 | 5.00931900 |
| H | -9.05892800 | -2.08759700 | 4.89313900 |
| C | -7.11600200 | -0.72386700 | 0.81123600 |
| H | -7.11779200 | -0.90183600 | 1.91196900 |
| C | -5.81081100 | -1.08075900 | 0.15617700 |
| H | -5.80922800 | -0.98930700 | -0.93428400 |
| C | -4.73470500 | -1.47196500 | 0.85126400 |
| H | -4.76265500 | -1.57844400 | 1.93938300 |
| C | -3.45708300 | -1.77091900 | 0.20574600 |
| H | -3.42234600 | -1.64286600 | -0.88351500 |
| C | -2.36902500 | -2.17812900 | 0.88429000 |
| H | -2.39000700 | -2.32818100 | 1.96715400 |
| C | -1.09657300 | -2.43292900 | 0.21323700 |
| H | -1.07488100 | -2.21769500 | -0.86665000 |
| C | -0.00642600 | -2.88912000 | 0.85527100 |
| H | -0.03174700 | -3.11499500 | 1.93168300 |
| C | 1.27209500 | -3.09098700 | 0.18181200 |
| H | 1.35082800 | -2.69300500 | -0.84140500 |
| C | 2.31930500 | -3.70291600 | 0.76563300 |
| H | 2.24418500 | -4.12169900 | 1.77110100 |
| C | 3.60662100 | -3.85193100 | 0.09410700 |
| H | 3.64208800 | -3.52598700 | -0.95205100 |
| C | 4.69604500 | -4.35184400 | 0.70671700 |
| H | 4.65766500 | -4.68693600 | 1.74545500 |
| C | 5.98339900 | -4.48167300 | 0.03287100 |
| H | 6.00029800 | -4.23718500 | -1.03642000 |

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| C | 7.10836800 | -4.87513700 | 0.65767600 |
| H | 7.11683200 | -5.13891600 | 1.71625400 |
| C | -7.56862000 | 0.71002700 | 0.49306000 |
| H | -8.49723000 | 0.93674300 | 1.05816100 |
| H | -6.80134200 | 1.42395700 | 0.86566800 |
| C | 8.38538600 | -4.95752700 | -0.05027300 |
| H | 8.32134400 | -4.87173100 | -1.14436400 |
| C | 9.56509000 | -5.09540000 | 0.56960500 |
| H | 9.64315400 | -5.18941300 | 1.65207000 |
| C | 10.87522000 | -5.13713400 | -0.17190500 |
| H | 10.70513300 | -5.30457600 | -1.26878500 |
| C | 11.62980400 | -3.78995000 | -0.01827000 |
| H | 12.08372300 | -3.70718600 | 0.99528600 |
| C | 10.77365900 | -2.52934500 | -0.29938300 |
| H | 9.89704700 | -2.55677500 | 0.40554500 |
| C | 10.18980200 | -2.54027900 | -1.72462500 |
| H | 9.70245600 | -3.52023100 | -1.94944500 |
| C | 7.84964400 | -1.85466400 | -1.99857900 |
| C | 6.93836000 | -0.66753400 | -1.88400200 |
| H | 7.31745000 | 0.04838600 | -1.12532100 |
| H | 6.96445800 | -0.11022100 | -2.84986300 |
| C | 5.49238800 | -1.10052100 | -1.56824500 |
| H | 5.45840300 | -1.71521000 | -0.63782100 |
| C | 4.54635800 | 0.10146000 | -1.51001300 |
| H | 4.96519800 | 0.88639900 | -0.85082700 |
| H | 4.47589800 | 0.55745800 | -2.52273600 |

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| C | 3.13344500 | -0.27774600 | -1.03501900 |
| H | 3.16043200 | -0.89022500 | -0.10274000 |
| C | 2.26228600 | 0.97665800 | -0.85389200 |
| H | 2.38922600 | 1.65222000 | -1.72485000 |
| H | 2.63359200 | 1.54438900 | 0.02492000 |
| C | 0.77774300 | 0.64215500 | -0.66495000 |
| H | 0.65159300 | -0.44644000 | -0.46198700 |
| H | 0.38401500 | 1.15028400 | 0.23550000 |
| C | -0.05327400 | 1.03389700 | -1.89157800 |
| H | 0.01641100 | 2.12527100 | -2.09881800 |
| C | -1.53741300 | 0.57250200 | -1.77305400 |
| H | -1.84876900 | 0.39115300 | -0.71968000 |
| C | -2.47816600 | 1.55211600 | -2.48750400 |
| H | -2.16940800 | 1.64668400 | -3.55115300 |
| H | -2.38216800 | 2.56226300 | -2.05006800 |
| C | -3.93796300 | 1.08262200 | -2.42719500 |
| H | -4.24631700 | 0.81733600 | -1.38663500 |
| C | -4.90405100 | 2.10499000 | -3.04455300 |
| H | -4.70229700 | 2.19483500 | -4.13333800 |
| H | -4.73347800 | 3.10268200 | -2.59922700 |
| C | -6.36877700 | 1.68992200 | -2.85651200 |
| C | -7.39736000 | 2.72953400 | -3.31021800 |
| H | -7.38174400 | 2.82693000 | -4.41575300 |
| H | -7.14145100 | 3.73397900 | -2.91515900 |
| C | -8.80932800 | 2.34929200 | -2.85865100 |
| H | -9.22774600 | 1.51607200 | -3.46639800 |

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| C | -8.86200100 | 1.99978500 | -1.34283000 |
| H | -8.62599200 | 2.94404500 | -0.77630200 |
| C | -7.77676200 | 0.93702200 | -1.00527800 |
| H | -7.97986000 | -0.01269400 | -1.55743500 |
| C | -10.22153500 | 1.53935700 | -0.91146400 |
| C | 11.10500300 | -2.11165500 | -2.84939600 |
| H | 10.62063400 | -2.22258100 | -3.82783600 |
| H | 12.01186300 | -2.74011200 | -2.85543500 |
| H | 11.41508400 | -1.06395300 | -2.76006800 |
| C | 11.56809600 | -1.25839100 | 0.00318000 |
| H | 12.49431700 | -1.19720500 | -0.57855100 |
| H | 11.83173600 | -1.18969700 | 1.06429000 |
| H | 10.97241800 | -0.36824200 | -0.24432300 |
| C | 11.74810000 | -6.28502900 | 0.34584900 |
| H | 11.95024800 | -6.20799100 | 1.41871200 |
| H | 12.71655100 | -6.29333500 | -0.17504400 |
| H | 11.26744200 | -7.25413700 | 0.16869700 |
| O | -9.07147200 | -3.98134800 | -0.31298500 |
| H | -8.17261500 | -3.80169100 | 0.07237800 |
| O | -11.71766900 | -4.30517600 | 3.19683400 |
| H | -12.26386200 | -4.99412800 | 2.74515900 |
| O | -8.91797800 | -2.21917000 | 2.20398900 |
| O | -8.05208900 | -1.67210400 | 0.19816800 |
| O | -6.70032000 | 0.49138700 | -3.52173200 |
| H | -5.95203700 | -0.18132900 | -3.48381200 |
| O | -6.49911700 | 1.45411200 | -1.43677900 |

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|---|--------------|-------------|-------------|
| O | -10.57038800 | 0.95543600 | 0.09008700 |
| O | -11.19201200 | 1.88397700 | -1.83345800 |
| H | -12.10599300 | 1.60616200 | -1.55517100 |
| O | -4.10608400 | -0.09922300 | -3.23796900 |
| H | -3.38055400 | -0.76246000 | -3.04287800 |
| O | -1.65944500 | -0.72703000 | -2.37607500 |
| H | -1.07026000 | -0.75958500 | -3.19653300 |
| O | 0.42664100 | 0.41550400 | -3.09639400 |
| H | 1.16640000 | -0.24469000 | -2.88691600 |
| O | 2.46626700 | -1.11594000 | -2.00700400 |
| H | 3.12280200 | -1.57738100 | -2.59879700 |
| O | 4.98598300 | -1.90500300 | -2.64862800 |
| H | 5.56067300 | -2.70538100 | -2.79722000 |
| O | 7.53831900 | -2.98036500 | -2.34158400 |
| O | 9.11699200 | -1.50401700 | -1.66449200 |
| O | 12.70402900 | -3.89801000 | -0.97643100 |
| H | 13.30089900 | -3.12791000 | -0.90034600 |
| O | -9.57007200 | 3.54339100 | -3.08295200 |
| H | -10.53725700 | 3.35851200 | -3.02637100 |
| N | -11.57288800 | -4.91812800 | 0.32779900 |
| H | -10.76874900 | -5.51963400 | 0.12694200 |
| H | -12.02951900 | -4.74404400 | -0.56433500 |

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| C | -1.83502200 | 0.02201500 | 3.93183800 |
| C | -1.16653100 | -1.14587600 | 3.18968600 |
| C | -0.28196800 | -1.97440400 | 4.13673400 |
| C | -0.93512100 | -2.21499200 | 5.48768700 |
| C | -1.17152400 | -0.87639400 | 6.17244300 |
| C | -1.82808600 | 0.14556900 | 5.27182600 |
| H | -0.02287000 | -2.91826500 | 3.64466300 |
| H | -1.89140900 | -2.73401400 | 5.35795800 |
| H | -0.30899400 | -2.85944700 | 6.11242700 |
| H | -1.78864900 | -1.00765400 | 7.06880400 |
| H | -0.21596000 | -0.46721400 | 6.53146500 |
| H | 0.66132200 | -1.43775800 | 4.29862300 |
| C | -2.47526200 | 1.27320600 | 6.03084800 |
| H | -3.04836600 | 1.94683900 | 5.39706100 |
| H | -3.14069400 | 0.87214700 | 6.80371600 |
| H | -1.71569400 | 1.86534500 | 6.55548500 |
| C | -2.23793400 | -2.04960000 | 2.55171600 |
| H | -2.89898000 | -1.48473600 | 1.88962500 |
| H | -1.76619800 | -2.83093300 | 1.94764200 |
| H | -2.86110600 | -2.53103500 | 3.30961400 |
| C | -0.26339100 | -0.59338100 | 2.07694700 |
| H | 0.28978600 | -1.40963400 | 1.60281400 |
| H | -0.83564700 | -0.07756200 | 1.30402700 |
| H | 0.46838400 | 0.10766700 | 2.49068500 |
| C | -2.53722100 | 0.98005600 | 3.05201000 |

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|---|--------------|------------|-------------|
| H | -3.27889000 | 0.54703900 | 2.38268000 |
| C | -2.32729000 | 2.30018500 | 2.97212600 |
| H | -1.52018400 | 2.73690100 | 3.55829300 |
| C | -3.08913700 | 3.22200900 | 2.11573700 |
| C | -4.39125700 | 2.98332300 | 1.85517500 |
| H | -4.85645300 | 2.13467700 | 2.34942700 |
| C | -2.31737700 | 4.40404700 | 1.59558300 |
| H | -1.83554400 | 4.92597200 | 2.42974000 |
| H | -1.52094300 | 4.07430200 | 0.92160100 |
| H | -2.94416500 | 5.12777700 | 1.07385000 |
| C | -5.25685500 | 3.71875200 | 0.95928100 |
| H | -4.82747500 | 4.53811100 | 0.39066600 |
| C | -6.55041100 | 3.39438400 | 0.78213100 |
| H | -6.95293500 | 2.56791300 | 1.36691600 |
| C | -7.46895200 | 3.98295900 | -0.19222100 |
| C | -8.71321900 | 3.48074500 | -0.28239000 |
| H | -9.00335900 | 2.70702400 | 0.42764900 |
| C | -6.93353600 | 5.07351700 | -1.08077500 |
| H | -6.61596100 | 5.93040500 | -0.47892600 |
| H | -6.05261000 | 4.72625700 | -1.63046200 |
| H | -7.66775900 | 5.43002200 | -1.80164500 |
| C | -9.77703900 | 3.78829700 | -1.28943100 |
| H | -9.38914300 | 4.40068400 | -2.11288300 |
| H | -10.59837500 | 4.35116200 | -0.83051400 |
| O | -10.35646100 | 2.58914800 | -1.79305600 |
| H | -9.66877800 | 1.90984100 | -1.82029400 |

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|---|-------------|-------------|-------------|
| C | 11.23683500 | -2.93923500 | 0.94586100 |
| H | 12.02512600 | -2.40380700 | 0.40190500 |
| C | 10.94913900 | -4.22354700 | 0.16962400 |
| H | 10.17118200 | -4.78615900 | 0.70886600 |
| C | 10.40092000 | -3.89534500 | -1.21413000 |
| H | 11.16560400 | -3.31010200 | -1.75320600 |
| C | 9.43793700 | -1.88521600 | -0.41870900 |
| H | 10.14197700 | -1.28083800 | -1.01107700 |
| C | 9.99408000 | -2.05701800 | 0.99193400 |
| H | 10.24869500 | -1.05477300 | 1.36682600 |
| C | 10.04363100 | -5.13000100 | -2.00996300 |
| H | 9.25995300 | -5.68850100 | -1.49126200 |
| H | 10.92282600 | -5.76807200 | -2.11174000 |
| H | 9.67518400 | -4.85461400 | -3.00064500 |
| C | 7.54854700 | -0.84538600 | -1.47957200 |
| H | 7.66812400 | -1.63781200 | -2.22578300 |
| C | 6.10305100 | -0.70892300 | -1.11792600 |
| H | 5.86467900 | 0.00957500 | -0.33804300 |
| C | 5.12612200 | -1.42762300 | -1.67928900 |
| H | 5.36514400 | -2.15091200 | -2.45840300 |
| C | 3.73836800 | -1.31483700 | -1.27814100 |
| H | 3.51850500 | -0.59328100 | -0.49510800 |
| C | 2.72700500 | -2.04904800 | -1.77938200 |
| H | 2.92814800 | -2.78340600 | -2.55886900 |
| C | 1.36908600 | -1.91756400 | -1.30833300 |
| H | 1.20739300 | -1.15881400 | -0.54596400 |

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|---|--------------|-------------|-------------|
| C | 0.31796900 | -2.64391500 | -1.73995600 |
| H | 0.46299200 | -3.40377900 | -2.50719100 |
| C | -1.01499100 | -2.46585700 | -1.21933400 |
| H | -1.14257700 | -1.69833200 | -0.45763300 |
| C | -2.10082400 | -3.16802300 | -1.60452600 |
| H | -2.00111300 | -3.93343100 | -2.37327100 |
| C | -3.40805400 | -2.96552300 | -1.03157600 |
| H | -3.48104500 | -2.21989500 | -0.24094900 |
| C | -4.52723900 | -3.62138700 | -1.39935800 |
| H | -4.47914600 | -4.35411700 | -2.20402500 |
| C | -5.80883500 | -3.40456800 | -0.77115800 |
| H | -5.82115600 | -2.73019900 | 0.08402900 |
| C | -6.97216600 | -3.95300400 | -1.16697600 |
| H | -6.99048400 | -4.60724300 | -2.03778200 |
| C | 8.19293900 | 0.44581700 | -1.99971300 |
| H | 9.23377700 | 0.22950900 | -2.25096300 |
| H | 7.69222500 | 0.75850600 | -2.92090700 |
| C | -8.23081600 | -3.68872400 | -0.49635300 |
| H | -8.15664400 | -3.12947100 | 0.43450900 |
| C | -9.44018100 | -4.03768000 | -0.94889200 |
| H | -9.51952300 | -4.58680300 | -1.88855700 |
| C | -10.73441200 | -3.71004100 | -0.26002900 |
| H | -10.51237100 | -3.26258500 | 0.71554900 |
| C | -11.56152100 | -2.67641000 | -1.04866200 |
| H | -11.94687000 | -3.18035800 | -1.95082800 |
| C | -10.77862400 | -1.44370500 | -1.54082600 |

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| H | -9.99214100 | -1.83516300 | -2.19436200 |
| C | -10.04339000 | -0.71563700 | -0.41158900 |
| H | -9.55534900 | -1.43986400 | 0.23265800 |
| C | -7.73284700 | -0.06128200 | -0.55607800 |
| C | -6.71020000 | 0.66064800 | -1.39095200 |
| H | -6.98683000 | 0.57049200 | -2.44419400 |
| H | -6.78297300 | 1.71846300 | -1.12508800 |
| C | -5.27836300 | 0.16864400 | -1.17400400 |
| H | -5.18219200 | -0.84353600 | -1.58839600 |
| C | -4.28746900 | 1.09510400 | -1.86469100 |
| H | -4.53842600 | 1.14849500 | -2.92959100 |
| H | -4.39686600 | 2.10028500 | -1.43995200 |
| C | -2.83509700 | 0.65625000 | -1.72004100 |
| H | -2.73644000 | -0.38834600 | -2.04533500 |
| C | -1.89103200 | 1.51761700 | -2.54904000 |
| H | -2.10004000 | 2.57394900 | -2.33911600 |
| H | -2.13051500 | 1.35282100 | -3.60398600 |
| C | -0.40732300 | 1.20938500 | -2.28806000 |
| H | -0.29911000 | 0.20842700 | -1.86306900 |
| H | 0.14350900 | 1.19734100 | -3.23359600 |
| C | 0.29575000 | 2.21854300 | -1.38264700 |
| H | 0.33092000 | 3.18563400 | -1.90313800 |
| C | 1.74398100 | 1.77661500 | -1.06351000 |
| H | 2.11480500 | 1.12278900 | -1.86113200 |
| C | 2.70563700 | 2.94674700 | -0.88976100 |
| H | 2.35293000 | 3.58723900 | -0.07228900 |

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| H | 2.70111900 | 3.54709200 | -1.80686200 |
| C | 4.13374900 | 2.48781900 | -0.60855500 |
| H | 4.44882800 | 1.79922700 | -1.40442900 |
| C | 5.11422300 | 3.65235900 | -0.57212400 |
| H | 4.79958100 | 4.37730000 | 0.18491200 |
| H | 5.10292800 | 4.14784300 | -1.54722700 |
| C | 6.54790200 | 3.22991700 | -0.25003000 |
| C | 7.54637000 | 4.36227300 | -0.44276400 |
| H | 7.35332300 | 5.16349000 | 0.27363500 |
| H | 7.43878200 | 4.76753000 | -1.45282000 |
| C | 8.97839900 | 3.88326700 | -0.27851800 |
| H | 9.13249800 | 3.58406500 | 0.76852000 |
| C | 9.23286300 | 2.64084600 | -1.17572400 |
| H | 9.25450000 | 2.99940500 | -2.21162400 |
| C | 8.12497200 | 1.59221600 | -0.99754900 |
| H | 8.19622800 | 1.19103800 | 0.01755200 |
| C | 10.58034000 | 2.05295100 | -0.84523000 |
| C | -10.85852000 | 0.24137000 | 0.43215900 |
| H | -10.25114700 | 0.61175800 | 1.26230800 |
| H | -11.71668800 | -0.29910200 | 0.83511100 |
| H | -11.20153500 | 1.09257800 | -0.15722500 |
| C | -11.67317600 | -0.52135300 | -2.36852100 |
| H | -12.51739200 | -0.14563000 | -1.78316800 |
| H | -12.07141300 | -1.05338900 | -3.23765800 |
| H | -11.13257400 | 0.35562900 | -2.72775700 |
| C | -11.56837000 | -4.97253000 | -0.02056700 |

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| H | -11.78362600 | -5.47872500 | -0.96810100 |
| H | -12.51672300 | -4.71554200 | 0.45351700 |
| H | -11.02986900 | -5.67568000 | 0.61881800 |
| O | 9.04827500 | -2.68793000 | 1.83080100 |
| H | 8.18001100 | -2.36373000 | 1.55254500 |
| O | 12.13413200 | -4.97419100 | 0.03553400 |
| H | 12.56301200 | -4.89478700 | 0.90304900 |
| O | 9.21577100 | -3.12036600 | -1.06328100 |
| O | 8.20842700 | -1.25236100 | -0.26893200 |
| O | 6.67524400 | 2.77798200 | 1.06674500 |
| H | 5.89110500 | 2.22822800 | 1.24713200 |
| O | 6.85493400 | 2.19947400 | -1.18427200 |
| O | 10.80016500 | 0.97124300 | -0.35417600 |
| O | 11.59632000 | 2.90778700 | -1.12423200 |
| H | 12.41357300 | 2.46511900 | -0.84235000 |
| O | 4.21474900 | 1.80648600 | 0.64597800 |
| H | 3.37378000 | 1.32957500 | 0.77183300 |
| O | 1.71291500 | 0.98264100 | 0.12384700 |
| H | 0.95439300 | 1.34999800 | 0.62115800 |
| O | -0.35764600 | 2.41690600 | -0.13662900 |
| H | -1.17455200 | 1.86934300 | -0.09976800 |
| O | -2.41336200 | 0.74323100 | -0.35594700 |
| H | -3.18402400 | 0.56525100 | 0.21237100 |
| O | -4.93662400 | 0.13881400 | 0.21143600 |
| H | -5.67921400 | -0.28101000 | 0.68159400 |
| O | -7.47813200 | -0.63814600 | 0.48826500 |

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| O | -8.95784900 | 0.03004600 | -1.06806000 |
| O | -12.64736500 | -2.31920000 | -0.19958200 |
| H | -13.32200900 | -1.88063100 | -0.72914000 |
| O | 9.80220400 | 4.97366500 | -0.62943700 |
| H | 10.71879900 | 4.67031000 | -0.63993900 |
| N | 11.76958100 | -3.32022500 | 2.25106900 |
| H | 10.98767600 | -3.59936900 | 2.83975100 |
| H | 12.20837000 | -2.52511700 | 2.70454300 |

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| C | -4.67506400 | 3.75755700 | -1.21679300 |
| C | -5.14080700 | 4.58564800 | -0.00909700 |
| C | -6.65939100 | 4.80903400 | -0.08054700 |
| C | -7.42612400 | 3.52359000 | -0.35075000 |
| C | -6.99991800 | 2.94256700 | -1.69396300 |
| C | -5.51202100 | 3.00527000 | -1.95580900 |
| H | -6.99495200 | 5.28090200 | 0.84940100 |
| H | -7.23384400 | 2.80099300 | 0.44700000 |
| H | -8.50493700 | 3.71094300 | -0.34761900 |
| H | -7.33358100 | 1.90160400 | -1.78210800 |
| H | -7.50450400 | 3.47712900 | -2.51238600 |
| H | -6.86945600 | 5.52475800 | -0.88583700 |
| C | -5.08164100 | 2.17898700 | -3.14047900 |

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| H | -4.00498600 | 2.02099600 | -3.17939100 |
| H | -5.57483300 | 1.20244900 | -3.12116700 |
| H | -5.38441700 | 2.65860900 | -4.07925200 |
| C | -4.75782200 | 3.87161000 | 1.30053100 |
| H | -3.68525000 | 3.65811100 | 1.33572800 |
| H | -4.99079300 | 4.50991700 | 2.15907900 |
| H | -5.29012500 | 2.92798100 | 1.43736100 |
| C | -4.46653900 | 5.96755500 | -0.02468300 |
| H | -4.88403000 | 6.59188700 | 0.77152200 |
| H | -3.38792700 | 5.90067300 | 0.13517400 |
| H | -4.63052700 | 6.47608100 | -0.97927200 |
| C | -3.23404800 | 3.87716600 | -1.52397200 |
| H | -2.53701900 | 3.73836800 | -0.69834100 |
| C | -2.74349600 | 4.26481700 | -2.70708900 |
| H | -3.45353700 | 4.52417000 | -3.49196500 |
| C | -1.32544300 | 4.46077600 | -3.03584000 |
| C | -0.37881000 | 3.59623100 | -2.61740800 |
| H | -0.70636700 | 2.70594900 | -2.08473800 |
| C | -1.05377200 | 5.68177600 | -3.87613900 |
| H | -1.71362100 | 5.68848400 | -4.75049800 |
| H | -1.27344500 | 6.59475100 | -3.31209400 |
| H | -0.02774900 | 5.74253600 | -4.23759700 |
| C | 1.04790800 | 3.71923200 | -2.84490300 |
| H | 1.39982200 | 4.64290000 | -3.29242500 |
| C | 1.94382900 | 2.76260700 | -2.54708800 |
| H | 1.59073500 | 1.83357200 | -2.10321400 |

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| C | 3.38484100 | 2.85054800 | -2.79301800 |
| C | 4.14825200 | 1.77201000 | -2.55421300 |
| H | 3.66344600 | 0.87896700 | -2.16652800 |
| C | 3.91933600 | 4.15024700 | -3.33523400 |
| H | 3.51958700 | 4.34422900 | -4.33576800 |
| H | 3.61229100 | 4.98656200 | -2.70002900 |
| H | 5.00615300 | 4.16182500 | -3.40754600 |
| C | 5.62030400 | 1.60985800 | -2.78477200 |
| H | 6.12646200 | 2.57848500 | -2.88408100 |
| H | 5.79356100 | 1.06854700 | -3.72293200 |
| O | 6.23959800 | 0.82016200 | -1.78047500 |
| H | 6.07144300 | 1.22753500 | -0.91809700 |
| C | -9.35024100 | -0.15696600 | 3.61354300 |
| H | -10.14173700 | -0.03275000 | 2.86383000 |
| C | -8.95167900 | 1.23749600 | 4.08699900 |
| H | -8.16562200 | 1.13070100 | 4.85043000 |
| C | -8.36833000 | 2.04904800 | 2.93616400 |
| H | -9.14941600 | 2.16090000 | 2.16530300 |
| C | -7.56289400 | 0.07022200 | 1.88667000 |
| H | -8.27374300 | 0.16455800 | 1.05017300 |
| C | -8.16116000 | -0.84290500 | 2.95533800 |
| H | -8.48126300 | -1.76457100 | 2.45010300 |
| C | -7.89098000 | 3.41021100 | 3.38950300 |
| H | -7.06982000 | 3.29141500 | 4.10143300 |
| H | -8.71101200 | 3.93728400 | 3.87967600 |
| H | -7.53244000 | 3.99946700 | 2.54567400 |

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| C | -5.79336000 | -0.10586200 | 0.25324900 |
| H | -5.90980900 | 0.97736500 | 0.15131300 |
| C | -4.34093200 | -0.43947100 | 0.37463500 |
| H | -4.10781900 | -1.46897600 | 0.63445200 |
| C | -3.35603200 | 0.45022900 | 0.21853200 |
| H | -3.59184800 | 1.47747000 | -0.05022800 |
| C | -1.96736900 | 0.10332300 | 0.43691500 |
| H | -1.76577800 | -0.93077000 | 0.70441300 |
| C | -0.93014800 | 0.96060400 | 0.38317100 |
| H | -1.10207700 | 2.00578100 | 0.13076300 |
| C | 0.42048200 | 0.55059300 | 0.68317100 |
| H | 0.54841700 | -0.49937700 | 0.94035100 |
| C | 1.50187800 | 1.35634900 | 0.67044800 |
| H | 1.39353400 | 2.40664100 | 0.40439100 |
| C | 2.82299400 | 0.88396300 | 0.99909000 |
| H | 2.92026600 | -0.17230600 | 1.25176300 |
| C | 3.93274600 | 1.65064800 | 1.00606400 |
| H | 3.85847600 | 2.70177600 | 0.73181700 |
| C | 5.23079800 | 1.14438200 | 1.37237200 |
| H | 5.28592100 | 0.09163500 | 1.65115200 |
| C | 6.37080900 | 1.86983700 | 1.39408700 |
| H | 6.34241900 | 2.92120100 | 1.10772600 |
| C | 7.64084700 | 1.32301700 | 1.80965600 |
| H | 7.62981700 | 0.29830800 | 2.17665800 |
| C | 8.81860700 | 1.97076600 | 1.76561800 |
| H | 8.86317000 | 2.98599200 | 1.37319100 |

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| C | -6.51256500 | -0.80002500 | -0.91043900 |
| H | -7.54352100 | -0.44047100 | -0.93653000 |
| H | -6.03699600 | -0.51383400 | -1.85247200 |
| C | 10.06123600 | 1.35428700 | 2.18890900 |
| H | 9.96064200 | 0.39169700 | 2.68594500 |
| C | 11.28326400 | 1.84916000 | 1.96686400 |
| H | 11.38595600 | 2.80435900 | 1.44941000 |
| C | 12.56437700 | 1.15923600 | 2.34130300 |
| H | 12.33386000 | 0.31839500 | 3.00543200 |
| C | 13.26917400 | 0.58014700 | 1.09912400 |
| H | 13.60009600 | 1.43342000 | 0.48360700 |
| C | 12.37993200 | -0.29290700 | 0.19405100 |
| H | 11.54147100 | 0.34376900 | -0.10473200 |
| C | 11.74503800 | -1.48158000 | 0.92561700 |
| H | 11.31594600 | -1.14871300 | 1.86699200 |
| C | 9.42475800 | -2.02356500 | 0.61815000 |
| C | 8.38807200 | -2.46584600 | -0.38185600 |
| H | 8.72603400 | -2.21807700 | -1.38957900 |
| H | 8.30634200 | -3.55680800 | -0.31194700 |
| C | 7.02021100 | -1.84350500 | -0.09670800 |
| H | 7.11740000 | -0.75223100 | -0.13071100 |
| C | 5.99387000 | -2.27437600 | -1.13126000 |
| H | 6.31390100 | -1.88671800 | -2.10188300 |
| H | 5.96568900 | -3.36965900 | -1.18609100 |
| C | 4.58377400 | -1.76776200 | -0.84926400 |
| H | 4.62238700 | -0.68895700 | -0.67301400 |

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| C | 3.65182200 | -2.03721100 | -2.02442200 |
| H | 3.77568600 | -3.07794800 | -2.34816800 |
| H | 3.98959500 | -1.40967900 | -2.85438300 |
| C | 2.17211500 | -1.76045300 | -1.71274200 |
| H | 2.08424000 | -1.08280900 | -0.85960200 |
| H | 1.69774300 | -1.25034900 | -2.55747700 |
| C | 1.35780700 | -3.02420700 | -1.44123200 |
| H | 1.30588000 | -3.60528000 | -2.37240400 |
| C | -0.08787300 | -2.69396400 | -0.98815400 |
| H | -0.36615100 | -1.68968700 | -1.32833900 |
| C | -1.11080900 | -3.70107100 | -1.50230600 |
| H | -0.82420700 | -4.70632600 | -1.17011600 |
| H | -1.08712200 | -3.69580600 | -2.59828500 |
| C | -2.53147300 | -3.39692400 | -1.03503400 |
| H | -2.78805400 | -2.36351400 | -1.30598900 |
| C | -3.55023000 | -4.32782400 | -1.68036600 |
| H | -3.27223800 | -5.36919500 | -1.49014900 |
| H | -3.53494400 | -4.16217800 | -2.76146800 |
| C | -4.97653100 | -4.12659300 | -1.16827800 |
| C | -6.00376600 | -4.89458400 | -1.98794100 |
| H | -5.84848600 | -5.96983400 | -1.87805600 |
| H | -5.88706700 | -4.63445100 | -3.04374900 |
| C | -7.42600400 | -4.55407900 | -1.57548800 |
| H | -7.59454400 | -4.92070300 | -0.55232100 |
| C | -7.62682200 | -3.01358600 | -1.57170900 |
| H | -7.62640800 | -2.69271600 | -2.62023900 |

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| C | -6.49516500 | -2.31806900 | -0.80097000 |
| H | -6.57382100 | -2.60492600 | 0.25125900 |
| C | -8.96791600 | -2.67607200 | -0.97273700 |
| C | 12.63363600 | -2.68448300 | 1.16978800 |
| H | 12.09049100 | -3.44038300 | 1.74163600 |
| H | 13.51385300 | -2.37016700 | 1.73201500 |
| H | 12.95594900 | -3.13312400 | 0.22763700 |
| C | 13.11989000 | -0.71383900 | -1.07489900 |
| H | 14.01497400 | -1.30294000 | -0.85270500 |
| H | 13.42779000 | 0.16352900 | -1.65104800 |
| H | 12.47653200 | -1.32562300 | -1.71096300 |
| C | 13.50586200 | 2.10870400 | 3.08762500 |
| H | 13.74931600 | 2.97779900 | 2.46626200 |
| H | 14.43663900 | 1.60094200 | 3.34299200 |
| H | 13.03671200 | 2.47435300 | 4.00392600 |
| O | -7.21247500 | -1.11903900 | 3.96585000 |
| H | -6.35920500 | -1.21811300 | 3.52094800 |
| O | -10.08108300 | 1.90954400 | 4.59619300 |
| H | -10.55227200 | 1.22746800 | 5.10175900 |
| O | -7.24774300 | 1.35464800 | 2.38827400 |
| O | -6.37688100 | -0.53435200 | 1.49453900 |
| O | -5.11321600 | -4.53219600 | 0.16257300 |
| H | -4.32168700 | -4.20748900 | 0.62964800 |
| O | -5.23925600 | -2.73430600 | -1.31535200 |
| O | -9.17519600 | -2.05161600 | 0.04115600 |
| O | -9.99708400 | -3.18963500 | -1.69136700 |

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| H | -10.81000200 | -2.95513900 | -1.21441000 |
| O | -2.63865400 | -3.53932100 | 0.38370900 |
| H | -1.79009700 | -3.24744400 | 0.76536500 |
| O | -0.10182200 | -2.65729500 | 0.44036800 |
| H | 0.63233100 | -3.26456700 | 0.67435600 |
| O | 1.92496400 | -3.86064100 | -0.44317600 |
| H | 2.74231200 | -3.44272500 | -0.09233400 |
| O | 4.03012600 | -2.39913600 | 0.31257400 |
| H | 4.74851000 | -2.47778200 | 0.96546700 |
| O | 6.54651600 | -2.24130500 | 1.19076300 |
| H | 7.27736500 | -2.10024500 | 1.81725400 |
| O | 9.16675800 | -1.80290500 | 1.79129400 |
| O | 10.63346600 | -1.91692600 | 0.08353500 |
| O | 14.40649700 | -0.12992100 | 1.57991900 |
| H | 15.01138900 | -0.27741200 | 0.84503500 |
| O | -8.26993700 | -5.20317500 | -2.50117300 |
| H | -9.17882200 | -4.92708800 | -2.32863100 |
| N | -9.91869900 | -0.86845200 | 4.75531000 |
| H | -9.14993900 | -1.19290200 | 5.33805200 |
| H | -10.42221800 | -1.69437300 | 4.44772500 |

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| C | -2.48965800 | 4.88238700 | 1.98145300 |
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| C | -2.24568900 | 5.84580700 | 3.15192900 |
| C | -1.61940200 | 7.15759200 | 2.65284600 |
| C | -2.32355500 | 7.70824200 | 1.42250400 |
| C | -2.22769300 | 6.70363300 | 0.28171300 |
| C | -2.51094800 | 5.27673500 | 0.69397300 |
| H | -1.62221300 | 7.88898900 | 3.46908900 |
| H | -3.37677800 | 7.90415900 | 1.65067400 |
| H | -1.88652400 | 8.66608700 | 1.12314200 |
| H | -2.90916500 | 6.98529900 | -0.52956600 |
| H | -1.22093500 | 6.73496400 | -0.16025600 |
| H | -0.56773700 | 6.97077800 | 2.40133500 |
| C | -2.79046900 | 4.36467400 | -0.47376200 |
| H | -3.24766200 | 3.42056400 | -0.17851600 |
| H | -3.45465100 | 4.86585200 | -1.18732600 |
| H | -1.86448300 | 4.12206700 | -1.00590700 |
| C | -3.57762400 | 6.13444600 | 3.86840200 |
| H | -4.04033600 | 5.21473500 | 4.23662000 |
| H | -3.41186200 | 6.78633600 | 4.73249900 |
| H | -4.29505400 | 6.62174100 | 3.20411200 |
| C | -1.27495300 | 5.21353100 | 4.16149500 |
| H | -1.04129000 | 5.92907900 | 4.95650100 |
| H | -1.69504200 | 4.31870300 | 4.62675500 |
| H | -0.33863800 | 4.92573800 | 3.67491500 |
| C | -2.73705200 | 3.48155400 | 2.37241600 |
| H | -3.49024000 | 3.31071800 | 3.14110300 |
| C | -2.07303800 | 2.42471200 | 1.88808700 |

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| H | -1.24107200 | 2.61258900 | 1.21230000 |
| C | -2.37485300 | 1.01460500 | 2.16919300 |
| C | -3.65209800 | 0.63171600 | 2.37539400 |
| H | -4.41261700 | 1.40518300 | 2.29805400 |
| C | -1.19673200 | 0.08097300 | 2.11363200 |
| H | -0.66242900 | 0.21901600 | 1.16784000 |
| H | -0.48641700 | 0.30113800 | 2.91736100 |
| H | -1.47407100 | -0.97100300 | 2.18547200 |
| C | -4.16790600 | -0.70211600 | 2.60093200 |
| H | -3.46387900 | -1.52566400 | 2.67467300 |
| C | -5.48929000 | -0.94677400 | 2.68217600 |
| H | -6.17385300 | -0.10256200 | 2.60247400 |
| C | -6.12450300 | -2.25217200 | 2.83632200 |
| C | -7.46333100 | -2.32757000 | 2.82142200 |
| H | -8.03791700 | -1.41173800 | 2.69117800 |
| C | -5.24120200 | -3.46556100 | 2.94194600 |
| H | -4.65703600 | -3.59055500 | 2.02419200 |
| H | -4.53232800 | -3.36176600 | 3.76915200 |
| H | -5.81078800 | -4.38168200 | 3.10069400 |
| C | -8.29048300 | -3.58230200 | 2.89369200 |
| H | -8.08933100 | -4.13507500 | 3.82430100 |
| H | -8.03841600 | -4.25100600 | 2.06536700 |
| O | -9.67751200 | -3.31498600 | 2.75456000 |
| H | -9.95964900 | -2.79407100 | 3.51539100 |
| C | 10.97721100 | -3.13296400 | 2.16567100 |
| H | 11.82062700 | -2.80691700 | 1.54412900 |

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| C | 10.64758100 | -4.56796400 | 1.75709900 |
| H | 9.81356000 | -4.92184300 | 2.38296800 |
| C | 10.18308900 | -4.61301100 | 0.30626700 |
| H | 11.00502700 | -4.23602500 | -0.32624000 |
| C | 9.30791200 | -2.41962400 | 0.45748100 |
| H | 10.07238300 | -2.03584600 | -0.23539700 |
| C | 9.78918200 | -2.21682300 | 1.89152100 |
| H | 10.08709500 | -1.16241500 | 1.99019400 |
| C | 9.78787500 | -6.00272900 | -0.13862300 |
| H | 8.94894700 | -6.35791700 | 0.46568200 |
| H | 10.63017200 | -6.68373000 | -0.00721900 |
| H | 9.48202100 | -5.99746100 | -1.18717400 |
| C | 7.51879600 | -1.64898300 | -0.95275900 |
| H | 7.60371300 | -2.63276700 | -1.42578300 |
| C | 6.07749100 | -1.32393000 | -0.71680400 |
| H | 5.87203700 | -0.40063000 | -0.18163800 |
| C | 5.06472300 | -2.10276300 | -1.10823900 |
| H | 5.26961900 | -3.02908900 | -1.64421500 |
| C | 3.67768200 | -1.78726000 | -0.83153800 |
| H | 3.49166000 | -0.86558400 | -0.28540400 |
| C | 2.62834000 | -2.55549100 | -1.17974700 |
| H | 2.79862400 | -3.48365000 | -1.72472800 |
| C | 1.26651500 | -2.20841900 | -0.85113400 |
| H | 1.13213000 | -1.27274000 | -0.31227600 |
| C | 0.17994300 | -2.94049300 | -1.16813900 |
| H | 0.29913800 | -3.87771300 | -1.71095500 |

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| C | -1.15958900 | -2.54037200 | -0.81589100 |
| H | -1.26853100 | -1.59100800 | -0.29379900 |
| C | -2.27442600 | -3.24434500 | -1.09762900 |
| H | -2.18967900 | -4.18769900 | -1.63614400 |
| C | -3.59590700 | -2.82073200 | -0.70863100 |
| H | -3.67058600 | -1.89257500 | -0.14145100 |
| C | -4.73026000 | -3.49061700 | -0.99977300 |
| H | -4.67307800 | -4.40957700 | -1.58234500 |
| C | -6.03390400 | -3.05251200 | -0.56770700 |
| H | -6.06283200 | -2.17015600 | 0.06756200 |
| C | -7.20165900 | -3.64527700 | -0.87996900 |
| H | -7.21238000 | -4.52417200 | -1.52374400 |
| C | 8.26587800 | -0.61030900 | -1.79920600 |
| H | 9.30006100 | -0.94308300 | -1.91295300 |
| H | 7.82369700 | -0.56838600 | -2.79909400 |
| C | -8.46744200 | -3.13653700 | -0.39183600 |
| H | -8.38915800 | -2.31949200 | 0.31962900 |
| C | -9.68361100 | -3.56383200 | -0.74534100 |
| H | -9.78144700 | -4.37862200 | -1.46487200 |
| C | -10.96098300 | -2.96464400 | -0.22797900 |
| H | -10.71661200 | -2.31374000 | 0.61654900 |
| C | -11.65176000 | -2.10902500 | -1.30535500 |
| H | -12.00431700 | -2.79171700 | -2.09661400 |
| C | -10.73755300 | -1.07521400 | -1.99149600 |
| H | -9.91344100 | -1.64894300 | -2.42593500 |
| C | -10.07854400 | -0.10452900 | -1.00484900 |

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| H | -9.69225800 | -0.65438800 | -0.15130500 |
| C | -7.74416500 | 0.44722100 | -1.10071900 |
| C | -6.65507300 | 1.03846900 | -1.96401900 |
| H | -6.93327200 | 0.93801600 | -3.01504100 |
| H | -6.59840600 | 2.10845700 | -1.73283700 |
| C | -5.29299900 | 0.40250600 | -1.68242900 |
| H | -5.35200300 | -0.67639800 | -1.88645900 |
| C | -4.18745600 | 1.01122700 | -2.53405600 |
| H | -4.42535600 | 0.85507600 | -3.59176800 |
| H | -4.15239700 | 2.09253000 | -2.35476500 |
| C | -2.80517900 | 0.42540900 | -2.24494300 |
| H | -2.84812800 | -0.66868600 | -2.33775200 |
| C | -1.75204600 | 0.95911400 | -3.21168900 |
| H | -1.85916700 | 2.04838300 | -3.28594200 |
| H | -1.97630100 | 0.55433200 | -4.20313700 |
| C | -0.31178900 | 0.60273000 | -2.80422000 |
| H | -0.30819600 | -0.26947300 | -2.14611800 |
| H | 0.26857400 | 0.31886000 | -3.68767800 |
| C | 0.44326300 | 1.74928900 | -2.13286900 |
| H | 0.58650500 | 2.54689800 | -2.87426600 |
| C | 1.83627400 | 1.30275500 | -1.61774100 |
| H | 2.15795900 | 0.39931100 | -2.14749400 |
| C | 2.89584000 | 2.38737200 | -1.77748700 |
| H | 2.58153700 | 3.28006300 | -1.22270300 |
| H | 2.95933000 | 2.66312800 | -2.83647000 |
| C | 4.27693100 | 1.94716700 | -1.30190000 |

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| H | 4.56465100 | 1.03002700 | -1.83364400 |
| C | 5.33150900 | 3.01196300 | -1.57517000 |
| H | 5.03751700 | 3.95238300 | -1.09872600 |
| H | 5.38719500 | 3.17777200 | -2.65490100 |
| C | 6.72314300 | 2.64314400 | -1.06188500 |
| C | 7.79335600 | 3.61783300 | -1.53166300 |
| H | 7.61972900 | 4.60690600 | -1.10269800 |
| H | 7.75023100 | 3.70046700 | -2.62134400 |
| C | 9.18642200 | 3.14857000 | -1.15019600 |
| H | 9.27980600 | 3.17491100 | -0.05467600 |
| C | 9.40357900 | 1.68234300 | -1.61575800 |
| H | 9.48901300 | 1.70820900 | -2.70851000 |
| C | 8.22859200 | 0.78765200 | -1.19369500 |
| H | 8.23521400 | 0.71058600 | -0.10258300 |
| C | 10.69874200 | 1.16323900 | -1.04690500 |
| C | -10.92649200 | 1.05239300 | -0.51765700 |
| H | -10.37154400 | 1.63772100 | 0.21936100 |
| H | -11.83292500 | 0.65777600 | -0.05666600 |
| H | -11.20559900 | 1.71280400 | -1.34157900 |
| C | -11.46077000 | -0.35684600 | -3.12909400 |
| H | -12.34558500 | 0.18075700 | -2.77497300 |
| H | -11.78301400 | -1.07067500 | -3.89273200 |
| H | -10.80321900 | 0.37346700 | -3.60622500 |
| C | -11.90435800 | -4.04886000 | 0.29611900 |
| H | -12.11486800 | -4.79542800 | -0.47839200 |
| H | -12.85108800 | -3.60704100 | 0.61115500 |

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| H | -11.44486000 | -4.55007100 | 1.15005400 |
| O | 8.77006300 | -2.54506100 | 2.81320400 |
| H | 7.93680900 | -2.27185400 | 2.40379500 |
| O | 11.78976700 | -5.37973200 | 1.90605600 |
| H | 12.18285200 | -5.08239700 | 2.74261100 |
| O | 9.04125500 | -3.77383600 | 0.16661100 |
| O | 8.11267200 | -1.71538200 | 0.35461900 |
| O | 6.77201100 | 2.60706600 | 0.33473600 |
| H | 5.94636800 | 2.18179800 | 0.62996700 |
| O | 7.00514000 | 1.36592500 | -1.62492800 |
| O | 10.83319300 | 0.27169100 | -0.24281800 |
| O | 11.77446200 | 1.84866000 | -1.50958200 |
| H | 12.55147400 | 1.47606700 | -1.06153900 |
| O | 4.27351000 | 1.67911200 | 0.10291300 |
| H | 3.38939700 | 1.34015800 | 0.33395200 |
| O | 1.70922400 | 0.93672800 | -0.24114700 |
| H | 0.97775600 | 1.50822100 | 0.06921900 |
| O | -0.25188600 | 2.31354800 | -1.02842900 |
| H | -1.09532900 | 1.82094600 | -0.89481200 |
| O | -2.37552100 | 0.74360900 | -0.91993300 |
| H | -3.14943700 | 0.70239100 | -0.32350000 |
| O | -4.92569900 | 0.60964500 | -0.32568900 |
| H | -5.63679700 | 0.26065200 | 0.23727800 |
| O | -7.55275600 | 0.02885300 | 0.02975700 |
| O | -8.92291100 | 0.45147500 | -1.70817900 |
| O | -12.77179800 | -1.49195400 | -0.67507400 |

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| H | -13.38343300 | -1.19524100 | -1.35729000 |
| O | 10.08681500 | 4.04370900 | -1.76583800 |
| H | 10.98371800 | 3.71251700 | -1.63117200 |
| N | 11.42549700 | -3.15998000 | 3.55517700 |
| H | 10.60199700 | -3.22915400 | 4.14926400 |
| H | 11.89025700 | -2.29101500 | 3.79864300 |

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| C | 1.20443000 | 4.76520900 | 1.96368400 |
| C | 2.46978100 | 4.17078200 | 1.33312800 |
| C | 3.68502600 | 5.08332000 | 1.57070600 |
| C | 3.74443300 | 5.62055500 | 2.99181300 |
| C | 2.50769600 | 6.46812800 | 3.25714900 |
| C | 1.22320800 | 5.80423200 | 2.81498900 |
| H | 4.59719300 | 4.53475100 | 1.31155400 |
| H | 3.78222000 | 4.79123000 | 3.70667700 |
| H | 4.65321100 | 6.21051400 | 3.14648400 |
| H | 2.43079900 | 6.71281100 | 4.32340300 |
| H | 2.59901400 | 7.43492500 | 2.74084200 |
| H | 3.62633500 | 5.93501300 | 0.88120600 |
| C | -0.00284800 | 6.41064600 | 3.44382000 |
| H | -0.93000000 | 5.94872700 | 3.11022400 |
| H | 0.05299900 | 6.32944300 | 4.53585700 |

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| H | -0.05366800 | 7.48234600 | 3.21686100 |
| C | 2.73810000 | 2.77573300 | 1.92776900 |
| H | 1.91672300 | 2.08476400 | 1.72057800 |
| H | 3.64497300 | 2.34612000 | 1.49275400 |
| H | 2.86880200 | 2.82155700 | 3.01173600 |
| C | 2.27470100 | 4.04182500 | -0.18537500 |
| H | 3.18347000 | 3.64417400 | -0.64383000 |
| H | 1.44944300 | 3.37231100 | -0.43205100 |
| H | 2.05256900 | 5.01759000 | -0.62859900 |
| C | -0.06334900 | 4.08328200 | 1.59930400 |
| H | -0.20835300 | 3.07133000 | 1.97915000 |
| C | -1.01058200 | 4.60680800 | 0.81700200 |
| H | -0.81956100 | 5.57817100 | 0.36050000 |
| C | -2.31578800 | 4.00081000 | 0.50892300 |
| C | -3.01497700 | 3.37447300 | 1.47644500 |
| H | -2.57410700 | 3.34018300 | 2.47041700 |
| C | -2.79397500 | 4.20062600 | -0.90333900 |
| H | -2.74596300 | 5.26116000 | -1.17361300 |
| H | -2.13464700 | 3.65722200 | -1.58598900 |
| H | -3.81597100 | 3.85717700 | -1.06523800 |
| C | -4.35572300 | 2.83402100 | 1.36710000 |
| H | -4.84059600 | 2.83937800 | 0.39554200 |
| C | -5.05209900 | 2.35287800 | 2.40881700 |
| H | -4.55884800 | 2.25564500 | 3.37628500 |
| C | -6.46414000 | 1.93913400 | 2.34807200 |
| C | -7.34417100 | 2.66574700 | 1.64515800 |

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| H | -6.97617600 | 3.57676700 | 1.17459000 |
| C | -6.80792900 | 0.70331700 | 3.13990900 |
| H | -7.82988200 | 0.36197000 | 2.97888400 |
| H | -6.13106800 | -0.11681500 | 2.87829200 |
| H | -6.67289900 | 0.88988300 | 4.21085400 |
| C | -8.80379800 | 2.41223000 | 1.43184200 |
| H | -9.40498300 | 3.14334800 | 1.99209000 |
| H | -9.09827200 | 1.41674800 | 1.75837300 |
| O | -9.14440300 | 2.47066100 | 0.04263900 |
| H | -9.03060600 | 3.38044200 | -0.25573600 |
| C | 10.52885000 | -2.46670600 | 2.68624400 |
| H | 11.31585200 | -2.51902900 | 1.92342200 |
| C | 10.13497000 | -3.90404100 | 3.02304800 |
| H | 9.35659000 | -3.87566900 | 3.80135200 |
| C | 9.53656300 | -4.58982600 | 1.80074900 |
| H | 10.30336300 | -4.60075800 | 1.00721800 |
| C | 8.72191000 | -2.52852800 | 0.97095500 |
| H | 9.42633400 | -2.55729900 | 0.12576600 |
| C | 9.33809400 | -1.71271800 | 2.10417600 |
| H | 9.66410000 | -0.75306300 | 1.67589500 |
| C | 9.07436500 | -6.00010900 | 2.08865400 |
| H | 8.28957400 | -5.98208200 | 2.84950900 |
| H | 9.91193800 | -6.59258100 | 2.46012100 |
| H | 8.67090900 | -6.46345300 | 1.18558300 |
| C | 6.82697500 | -2.39025600 | -0.50365500 |
| H | 6.84362000 | -3.48448700 | -0.46708500 |

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| C | 5.42183600 | -1.90091300 | -0.34813100 |
| H | 5.29376300 | -0.82767600 | -0.23533800 |
| C | 4.35241100 | -2.70187000 | -0.33476800 |
| H | 4.48102500 | -3.77750500 | -0.45411400 |
| C | 3.00108200 | -2.21245300 | -0.14691300 |
| H | 2.88814500 | -1.14389300 | 0.01579800 |
| C | 1.90065900 | -2.98745900 | -0.14163500 |
| H | 2.00143200 | -4.06063400 | -0.30320900 |
| C | 0.57015800 | -2.47100000 | 0.07823100 |
| H | 0.49270800 | -1.39879300 | 0.24830200 |
| C | -0.54727900 | -3.22446900 | 0.07986500 |
| H | -0.46507900 | -4.29760700 | -0.09157800 |
| C | -1.87096100 | -2.69870600 | 0.30544000 |
| H | -1.96321800 | -1.62372900 | 0.46066300 |
| C | -2.98617500 | -3.45673300 | 0.32720500 |
| H | -2.89666200 | -4.52979800 | 0.15948300 |
| C | -4.30817000 | -2.94492100 | 0.58464300 |
| H | -4.40324100 | -1.87472000 | 0.76598900 |
| C | -5.41944900 | -3.70821500 | 0.61250300 |
| H | -5.33626600 | -4.77547200 | 0.40896900 |
| C | -6.73302000 | -3.18988200 | 0.90411200 |
| H | -6.79419300 | -2.13638700 | 1.16693400 |
| C | -7.87420700 | -3.90078100 | 0.84850800 |
| H | -7.84309400 | -4.94953700 | 0.55488500 |
| C | 7.52073700 | -1.91602600 | -1.78790600 |
| H | 8.52676600 | -2.34131900 | -1.80994400 |

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| H | 6.98180800 | -2.30498400 | -2.65702100 |
| C | -9.17259400 | -3.31041300 | 1.10959600 |
| H | -9.15448900 | -2.29691900 | 1.50206000 |
| C | -10.35137900 | -3.87872200 | 0.83650500 |
| H | -10.37622500 | -4.88609900 | 0.41759700 |
| C | -11.68041600 | -3.19903500 | 1.00658400 |
| H | -11.53559300 | -2.27437900 | 1.57703500 |
| C | -12.27710500 | -2.80401900 | -0.35846600 |
| H | -12.52241500 | -3.74033700 | -0.88799600 |
| C | -11.32911700 | -2.01599700 | -1.28211100 |
| H | -10.43833600 | -2.64095800 | -1.39694100 |
| C | -10.82714700 | -0.70053100 | -0.67221000 |
| H | -10.48631500 | -0.87578200 | 0.34549200 |
| C | -8.49527700 | -0.15322300 | -0.83724900 |
| C | -7.40453000 | 0.30973300 | -1.76501900 |
| H | -7.66053900 | 0.05226000 | -2.79449300 |
| H | -7.38182900 | 1.40109300 | -1.67544600 |
| C | -6.03988400 | -0.25667600 | -1.37089000 |
| H | -6.09594300 | -1.35541400 | -1.34897100 |
| C | -4.95171300 | 0.16700300 | -2.34497500 |
| H | -5.18239100 | -0.24951300 | -3.33123100 |
| H | -4.94995500 | 1.25987900 | -2.43663100 |
| C | -3.55305700 | -0.28104700 | -1.92580400 |
| H | -3.57568600 | -1.34927700 | -1.66678900 |
| C | -2.54078600 | -0.07259600 | -3.04491600 |
| H | -2.61298500 | 0.96412500 | -3.39642900 |

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| H | -2.84326800 | -0.70924300 | -3.88176600 |
| C | -1.09401500 | -0.39276900 | -2.63738500 |
| H | -1.08062000 | -1.06058500 | -1.77135900 |
| H | -0.59062000 | -0.93649500 | -3.44327800 |
| C | -0.24223200 | 0.83716900 | -2.34279000 |
| H | -0.15792700 | 1.42749000 | -3.26508100 |
| C | 1.19401000 | 0.44228500 | -1.88169300 |
| H | 1.35062300 | -0.63114300 | -2.04049800 |
| C | 2.27385800 | 1.21617500 | -2.63023000 |
| H | 2.10083700 | 2.29088600 | -2.50673500 |
| H | 2.18162000 | 0.98945500 | -3.69917000 |
| C | 3.69150800 | 0.87490400 | -2.17991500 |
| H | 3.86249900 | -0.20380400 | -2.29253400 |
| C | 4.73218100 | 1.62025200 | -3.00694700 |
| H | 4.52092400 | 2.69414300 | -2.98731000 |
| H | 4.66111700 | 1.27820200 | -4.04357400 |
| C | 6.16606600 | 1.42073600 | -2.51664200 |
| C | 7.19796300 | 1.97917600 | -3.48560700 |
| H | 7.10183700 | 3.06454200 | -3.55794700 |
| H | 7.02901000 | 1.54946000 | -4.47695100 |
| C | 8.61297200 | 1.63269600 | -3.05569800 |
| H | 8.83362400 | 2.15747100 | -2.11483800 |
| C | 8.73428000 | 0.10612500 | -2.79452200 |
| H | 8.69666900 | -0.38450900 | -3.77428700 |
| C | 7.59206500 | -0.39852400 | -1.90024000 |
| H | 7.72507900 | 0.03185800 | -0.90356200 |

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| C | 10.07043600 | -0.18779600 | -2.16306400 |
| C | -11.78062400 | 0.47710500 | -0.69833700 |
| H | -11.29136700 | 1.34880400 | -0.26012800 |
| H | -12.68034600 | 0.22233100 | -0.13667300 |
| H | -12.06388200 | 0.72770000 | -1.72332100 |
| C | -11.94141400 | -1.82009800 | -2.66867100 |
| H | -12.88591700 | -1.26861000 | -2.62773000 |
| H | -12.13538200 | -2.78539000 | -3.14508500 |
| H | -11.26386700 | -1.25493700 | -3.31239400 |
| C | -12.66458700 | -4.08453400 | 1.77610200 |
| H | -12.81997100 | -5.03378800 | 1.25127000 |
| H | -13.63051200 | -3.58774000 | 1.87434200 |
| H | -12.27835700 | -4.31353700 | 2.77206500 |
| O | 8.40315900 | -1.51302800 | 3.14410000 |
| H | 7.53963800 | -1.41893300 | 2.71735300 |
| O | 11.27052000 | -4.62085500 | 3.45030300 |
| H | 11.74618200 | -3.99240500 | 4.01741800 |
| O | 8.40315200 | -3.84405900 | 1.36789100 |
| O | 7.53631000 | -1.88153100 | 0.63839500 |
| O | 6.38253200 | 2.03425000 | -1.27832900 |
| H | 5.60292900 | 1.82627300 | -0.73253000 |
| O | 6.34303300 | 0.01105600 | -2.43706900 |
| O | 10.26973200 | -0.60658700 | -1.04749600 |
| O | 11.10565400 | 0.11327100 | -2.98674500 |
| H | 11.91759800 | -0.06675200 | -2.48508000 |
| O | 3.88609900 | 1.22115000 | -0.80499800 |

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| H | 3.02799800 | 1.12340500 | -0.35094900 |
| O | 1.29701900 | 0.66567000 | -0.47610700 |
| H | 0.53722700 | 1.25663000 | -0.28239200 |
| O | -0.79722500 | 1.68728900 | -1.34894400 |
| H | -1.64669500 | 1.31606400 | -1.01971700 |
| O | -3.10026200 | 0.45330500 | -0.78626800 |
| H | -3.84115800 | 0.52947100 | -0.15811000 |
| O | -5.65921800 | 0.21350600 | -0.08337500 |
| H | -6.44220900 | 0.15444500 | 0.48999600 |
| O | -8.30380000 | -0.34951800 | 0.35338400 |
| O | -9.65391300 | -0.31774200 | -1.45343700 |
| O | -13.47484600 | -2.08714300 | -0.07745200 |
| H | -13.99082100 | -2.01978000 | -0.88807000 |
| O | 9.46035500 | 2.06474400 | -4.09806000 |
| H | 10.35709500 | 1.76333400 | -3.90483400 |
| N | 11.10619500 | -1.87195400 | 3.88858200 |
| H | 10.34188300 | -1.60715400 | 4.50631600 |
| H | 11.60754400 | -1.01923800 | 3.66077700 |

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| C | 12.12633200 | 5.44967400 | -0.55266600 |
| C | 13.20188400 | 6.09506000 | 0.33561600 |
| C | 13.52150900 | 7.51944300 | -0.14601000 |

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| C | 12.26975600 | 8.33246600 | -0.43432300 |
| C | 11.46588800 | 7.65887400 | -1.53836900 |
| C | 11.33154900 | 6.16138400 | -1.37443100 |
| H | 14.15089300 | 8.01595900 | 0.60135300 |
| H | 11.65744700 | 8.41108900 | 0.47018500 |
| H | 12.53041700 | 9.35534900 | -0.72390900 |
| H | 10.46570800 | 8.10253900 | -1.60509500 |
| H | 11.93623600 | 7.85460400 | -2.51343500 |
| H | 14.11744400 | 7.45395500 | -1.06536000 |
| C | 10.23200700 | 5.57318500 | -2.21978400 |
| H | 9.99690600 | 4.54252600 | -1.96041600 |
| H | 9.32066500 | 6.17212700 | -2.11684200 |
| H | 10.50111200 | 5.59996600 | -3.28291000 |
| C | 12.71284900 | 6.12973700 | 1.79523200 |
| H | 12.49030400 | 5.12632800 | 2.16770400 |
| H | 13.48432800 | 6.55694000 | 2.44444800 |
| H | 11.80516000 | 6.72787200 | 1.90113600 |
| C | 14.50116800 | 5.27659400 | 0.27332200 |
| H | 15.28946600 | 5.78169800 | 0.84094800 |
| H | 14.37552600 | 4.27520500 | 0.69151000 |
| H | 14.84285200 | 5.16450500 | -0.75971600 |
| C | 12.01303200 | 3.98632000 | -0.40259300 |
| H | 11.98745200 | 3.60598400 | 0.61755400 |
| C | 12.01602400 | 3.09446000 | -1.40151700 |
| H | 12.15872400 | 3.45898800 | -2.41789500 |
| C | 11.87856500 | 1.63941000 | -1.25304100 |

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| C | 11.12399900 | 1.11457400 | -0.26673500 |
| H | 10.59431000 | 1.80682600 | 0.38385700 |
| C | 12.60647500 | 0.82695100 | -2.29035500 |
| H | 12.30547300 | 1.14363300 | -3.29513900 |
| H | 13.68732500 | 0.98989900 | -2.22025900 |
| H | 12.41935500 | -0.24345500 | -2.20988500 |
| C | 10.89916900 | -0.28826000 | 0.01835600 |
| H | 11.44033600 | -1.03186100 | -0.56069700 |
| C | 10.04828000 | -0.69865600 | 0.97228400 |
| H | 9.53464300 | 0.05940100 | 1.55983100 |
| C | 9.70747000 | -2.09211300 | 1.28734300 |
| C | 9.68733200 | -3.04964800 | 0.34674900 |
| H | 9.91343200 | -2.77463200 | -0.67992600 |
| C | 9.33907000 | -2.34052200 | 2.72727800 |
| H | 10.18750800 | -2.11040000 | 3.38006400 |
| H | 8.52695900 | -1.66645700 | 3.02235200 |
| H | 9.00446500 | -3.35994700 | 2.90894400 |
| C | 9.30106900 | -4.48299100 | 0.59303300 |
| H | 9.94806500 | -4.95316400 | 1.33992700 |
| H | 9.39704700 | -5.06174400 | -0.33389200 |
| O | 7.97348700 | -4.59136600 | 1.11168700 |
| H | 7.37399700 | -4.03497300 | 0.57640100 |
| C | 6.85136100 | 0.00081900 | -0.52970500 |
| H | 7.49576400 | -0.74943900 | -0.05687800 |
| C | 6.69562400 | 1.16086300 | 0.45310000 |
| H | 6.02705700 | 1.90997800 | 0.00314400 |

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| C | 6.03040700 | 0.66842000 | 1.73143000 |
| H | 6.65301300 | -0.13810200 | 2.15808400 |
| C | 4.77893400 | -0.94017300 | 0.51007800 |
| H | 5.28354800 | -1.79134200 | 0.99505000 |
| C | 5.48887300 | -0.62633300 | -0.80777900 |
| H | 5.60534300 | -1.57922600 | -1.34524900 |
| C | 5.83622900 | 1.76293900 | 2.75559900 |
| H | 5.19172800 | 2.54327900 | 2.34261200 |
| H | 6.80166000 | 2.20311200 | 3.01052300 |
| H | 5.36588400 | 1.36546500 | 3.65770900 |
| C | 2.59942600 | -1.70394900 | 1.21148200 |
| H | 2.78161000 | -1.10148500 | 2.10729400 |
| C | 1.20836500 | -1.46769600 | 0.71367300 |
| H | 0.94342100 | -1.95163600 | -0.22270100 |
| C | 0.30678700 | -0.71183400 | 1.34732300 |
| H | 0.57100500 | -0.22482900 | 2.28562300 |
| C | -1.02841500 | -0.48595300 | 0.83122500 |
| H | -1.27217500 | -0.97786200 | -0.10742800 |
| C | -1.96133900 | 0.29008900 | 1.41453700 |
| H | -1.73244200 | 0.79469400 | 2.35284200 |
| C | -3.26899300 | 0.49580500 | 0.83922000 |
| H | -3.46643200 | -0.03733200 | -0.08861200 |
| C | -4.23946400 | 1.27011500 | 1.36459900 |
| H | -4.05943300 | 1.80853300 | 2.29455000 |
| C | -5.53100200 | 1.42710300 | 0.74270700 |
| H | -5.70828500 | 0.85917500 | -0.17048200 |

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| C | -6.52518600 | 2.20629700 | 1.21542500 |
| H | -6.37056700 | 2.77056300 | 2.13447100 |
| C | -7.79806900 | 2.35524100 | 0.55546800 |
| H | -7.94143600 | 1.79657100 | -0.36927500 |
| C | -8.80664800 | 3.12899100 | 1.00491400 |
| H | -8.68191300 | 3.67633300 | 1.93860000 |
| C | -10.06154500 | 3.28389300 | 0.31008200 |
| H | -10.15245600 | 2.78159300 | -0.65146500 |
| C | -11.11676600 | 3.98084200 | 0.76977300 |
| H | -11.05547400 | 4.46958800 | 1.74149300 |
| C | 2.90309300 | -3.17823900 | 1.51058200 |
| H | 3.91963500 | -3.24433200 | 1.90775900 |
| H | 2.22582500 | -3.54262200 | 2.28859300 |
| C | -12.36932500 | 4.07956100 | 0.04634000 |
| H | -12.36435000 | 3.66872700 | -0.96127600 |
| C | -13.50805900 | 4.57268200 | 0.54503400 |
| H | -13.51608900 | 4.96800000 | 1.56220900 |
| C | -14.82538300 | 4.58229100 | -0.17646200 |
| H | -14.66049500 | 4.29927800 | -1.22237600 |
| C | -15.79582700 | 3.54792700 | 0.42663600 |
| H | -16.07492900 | 3.90812200 | 1.43083200 |
| C | -15.20706600 | 2.13738100 | 0.61635600 |
| H | -14.33466400 | 2.26419400 | 1.26468400 |
| C | -14.66304700 | 1.52842400 | -0.68075300 |
| H | -14.06470600 | 2.26424900 | -1.21097200 |
| C | -12.52607000 | 0.43817300 | -0.76951100 |

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| C | -11.70917500 | -0.71427100 | -0.24109000 |
| H | -12.10946700 | -1.03031100 | 0.72405600 |
| H | -11.83148200 | -1.54799400 | -0.94236200 |
| C | -10.22136200 | -0.37034200 | -0.13585100 |
| H | -10.09427500 | 0.46763800 | 0.56435100 |
| C | -9.41515000 | -1.56386200 | 0.35573100 |
| H | -9.78879800 | -1.85754500 | 1.34258500 |
| H | -9.57756500 | -2.40735400 | -0.32599400 |
| C | -7.91354900 | -1.30538300 | 0.45371500 |
| H | -7.73506300 | -0.41105200 | 1.06627100 |
| C | -7.18733500 | -2.48813600 | 1.08590000 |
| H | -7.52934900 | -3.41196500 | 0.60317300 |
| H | -7.50305800 | -2.54640400 | 2.13201100 |
| C | -5.65545100 | -2.39053800 | 0.99802600 |
| H | -5.34779400 | -1.35326800 | 0.84527700 |
| H | -5.20607900 | -2.70289100 | 1.94576900 |
| C | -5.04148600 | -3.26630600 | -0.09290400 |
| H | -5.21270000 | -4.31899300 | 0.17224000 |
| C | -3.51499200 | -3.03231000 | -0.21640200 |
| H | -3.12247500 | -2.63882600 | 0.72842600 |
| C | -2.74307900 | -4.29279500 | -0.59263400 |
| H | -3.10936900 | -4.66617700 | -1.55664100 |
| H | -2.94095400 | -5.06573500 | 0.15901600 |
| C | -1.23827100 | -4.05170000 | -0.66566800 |
| H | -0.89926500 | -3.63560300 | 0.29273500 |
| C | -0.45832400 | -5.33420800 | -0.92868400 |

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| H | -0.79320500 | -5.78372400 | -1.86852700 |
| H | -0.66172600 | -6.03964500 | -0.11770700 |
| C | 1.05189400 | -5.11095600 | -1.02064600 |
| C | 1.84506300 | -6.41667500 | -1.08865700 |
| H | 1.63915900 | -6.92675200 | -2.03185000 |
| H | 1.53253000 | -7.06773200 | -0.26426000 |
| C | 3.34099000 | -6.14615500 | -0.97104600 |
| H | 3.65871600 | -5.54183000 | -1.82541500 |
| C | 3.60904500 | -5.34185400 | 0.31488400 |
| H | 3.30577700 | -5.94950400 | 1.17654900 |
| C | 2.76767000 | -4.06187400 | 0.27811700 |
| H | 3.06514700 | -3.48881900 | -0.60416500 |
| C | 5.07903800 | -5.05147800 | 0.43245000 |
| C | -15.67923600 | 0.92390600 | -1.62787800 |
| H | -15.18380700 | 0.57967400 | -2.53859000 |
| H | -16.41935500 | 1.68276100 | -1.88510800 |
| H | -16.18792700 | 0.07287000 | -1.16998100 |
| C | -16.19235100 | 1.21384900 | 1.33053700 |
| H | -17.12400500 | 1.09829800 | 0.76855200 |
| H | -16.44129500 | 1.60584800 | 2.32090300 |
| H | -15.76371300 | 0.21764400 | 1.46076100 |
| C | -15.46252400 | 5.97453700 | -0.15675100 |
| H | -15.61879000 | 6.31277400 | 0.87365100 |
| H | -16.42949400 | 5.95801200 | -0.66133700 |
| H | -14.81517200 | 6.70175200 | -0.65202900 |
| O | 4.74167300 | 0.29864300 | -1.57062100 |

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| H | 3.81021100 | 0.08534900 | -1.41682700 |
| O | 7.96026500 | 1.71622800 | 0.74179300 |
| H | 8.42300600 | 1.68463100 | -0.11441400 |
| O | 4.74459300 | 0.15832900 | 1.39502500 |
| O | 3.46590400 | -1.24306200 | 0.16163400 |
| O | 1.40243300 | -4.36732400 | -2.15063000 |
| H | 0.73109300 | -3.66703000 | -2.24400700 |
| O | 1.39576800 | -4.42228100 | 0.17900300 |
| O | 5.60295800 | -4.05510800 | -0.05051700 |
| O | 5.74243400 | -5.97644700 | 1.10641900 |
| H | 6.70250100 | -5.71779600 | 1.14575400 |
| O | -0.91879900 | -3.12382800 | -1.70575300 |
| H | -1.66595400 | -2.50184700 | -1.78268400 |
| O | -3.30397500 | -2.01406000 | -1.19627000 |
| H | -4.07711500 | -2.12332000 | -1.78860600 |
| O | -5.60168200 | -3.04718000 | -1.37949300 |
| H | -6.29152500 | -2.35168500 | -1.31792000 |
| O | -7.34769700 | -1.08169500 | -0.84091800 |
| H | -8.00351300 | -0.58948800 | -1.36808700 |
| O | -9.70357700 | 0.00077400 | -1.41081700 |
| H | -10.32436500 | 0.64557600 | -1.79492900 |
| O | -12.09802000 | 1.23904700 | -1.58569200 |
| O | -13.75078600 | 0.46315700 | -0.26519500 |
| O | -16.94538900 | 3.54093900 | -0.41454000 |
| H | -17.67885400 | 3.14355400 | 0.06690500 |
| O | 4.11167100 | -7.32901000 | -1.03288700 |

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| H | 4.03995200 | -7.78346300 | -0.18424400 |
| N | 7.54855400 | 0.50765000 | -1.70673900 |
| H | 6.86977200 | 0.95851200 | -2.31534000 |
| H | 7.97604500 | -0.24818500 | -2.23027500 |

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| C | 11.93393700 | -4.98030400 | -0.38820500 |
| C | 11.96225500 | -5.32280500 | 1.10739900 |
| C | 12.99526000 | -6.43153100 | 1.39061500 |
| C | 14.31951300 | -6.18406000 | 0.68003100 |
| C | 14.10166800 | -6.15613500 | -0.82939900 |
| C | 12.90213900 | -5.34110300 | -1.24613800 |
| H | 13.14781000 | -6.51339800 | 2.47478600 |
| H | 14.74862400 | -5.22923500 | 1.01161100 |
| H | 15.05120900 | -6.95815500 | 0.94406300 |
| H | 14.99983600 | -5.77005700 | -1.33256200 |
| H | 13.96840300 | -7.18298200 | -1.20708700 |
| H | 12.58614100 | -7.39773100 | 1.06189700 |
| C | 12.91031200 | -4.96686000 | -2.70314800 |
| H | 11.92674800 | -4.67670200 | -3.07633400 |
| H | 13.58871000 | -4.12188700 | -2.87725100 |
| H | 13.26834200 | -5.79852000 | -3.31988300 |
| C | 12.31643600 | -4.05492100 | 1.90742400 |

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| H | 11.55297300 | -3.28097800 | 1.78617800 |
| H | 12.38853400 | -4.27786700 | 2.97671600 |
| H | 13.27088600 | -3.63158000 | 1.58357200 |
| C | 10.58540200 | -5.82838500 | 1.56514100 |
| H | 10.62673800 | -6.15753600 | 2.60817800 |
| H | 9.82270800 | -5.04850100 | 1.49260500 |
| H | 10.25236600 | -6.67171300 | 0.95248600 |
| C | 10.78079000 | -4.14734000 | -0.80931300 |
| H | 10.78560000 | -3.11678800 | -0.45184800 |
| C | 9.75022700 | -4.58435400 | -1.53790100 |
| H | 9.71958500 | -5.62808500 | -1.85027400 |
| C | 8.59701900 | -3.75453400 | -1.93242800 |
| C | 8.76683900 | -2.47373500 | -2.31065700 |
| H | 9.78156700 | -2.07952800 | -2.34783300 |
| C | 7.27062400 | -4.45637300 | -1.85847200 |
| H | 7.25288300 | -5.32544300 | -2.52730500 |
| H | 7.09237100 | -4.83032100 | -0.84359200 |
| H | 6.42615700 | -3.81786400 | -2.12525400 |
| C | 7.71639500 | -1.52644200 | -2.65234000 |
| H | 6.71995400 | -1.92628400 | -2.82530400 |
| C | 7.92603800 | -0.20522400 | -2.73595100 |
| H | 8.92841300 | 0.18892200 | -2.56909800 |
| C | 6.88022600 | 0.79692600 | -3.01375100 |
| C | 7.18366300 | 1.90946200 | -3.70068100 |
| H | 8.19391900 | 2.03506400 | -4.08547000 |
| C | 5.51733900 | 0.51208800 | -2.45321000 |

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| H | 5.07319700 | -0.37345100 | -2.92189300 |
| H | 5.57790800 | 0.30861000 | -1.37684200 |
| H | 4.82993300 | 1.34841100 | -2.58250000 |
| C | 6.22929700 | 3.03658400 | -3.97929200 |
| H | 5.36363700 | 2.70733100 | -4.56895900 |
| H | 6.73290300 | 3.84337500 | -4.53011400 |
| O | 5.66705700 | 3.57969600 | -2.77529300 |
| H | 6.32464500 | 3.52502200 | -2.06429300 |
| C | 7.12105600 | 0.53704800 | 2.91719500 |
| H | 7.95044800 | 1.02081600 | 2.37594400 |
| C | 6.94224100 | -0.85757500 | 2.32477800 |
| H | 6.23272100 | -1.44204000 | 2.93261500 |
| C | 6.46010700 | -0.78215300 | 0.87940700 |
| H | 7.21277600 | -0.25764700 | 0.26912400 |
| C | 5.26671700 | 1.29122500 | 1.33700800 |
| H | 5.80920200 | 1.93297200 | 0.62944100 |
| C | 5.84099300 | 1.37646400 | 2.75715400 |
| H | 6.06131100 | 2.43203400 | 2.98972500 |
| C | 6.14132800 | -2.14473400 | 0.30263000 |
| H | 5.22079800 | -2.53010600 | 0.75004600 |
| H | 6.95858200 | -2.84076600 | 0.51467900 |
| H | 6.00735500 | -2.09496400 | -0.78083600 |
| C | 3.17493900 | 1.66384800 | 0.20937600 |
| H | 3.44492100 | 0.73412700 | -0.30646500 |
| C | 1.73091800 | 1.68619600 | 0.61447100 |
| H | 1.43380000 | 2.54632500 | 1.21192800 |

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| C | 0.83966900 | 0.75961000 | 0.25610000 |
| H | 1.15420100 | -0.10636100 | -0.32629300 |
| C | -0.57403100 | 0.84465000 | 0.58925800 |
| H | -0.90550500 | 1.75234100 | 1.09571400 |
| C | -1.46504200 | -0.11870500 | 0.30047400 |
| H | -1.13355500 | -1.03575800 | -0.18541100 |
| C | -2.87908700 | -0.01429400 | 0.60406200 |
| H | -3.21257200 | 0.93202900 | 1.03610600 |
| C | -3.76222300 | -1.00295300 | 0.37351000 |
| H | -3.41832200 | -1.95001000 | -0.04021000 |
| C | -5.17909300 | -0.89706700 | 0.65700900 |
| H | -5.54149700 | 0.07593500 | 0.99471800 |
| C | -6.04193600 | -1.92144800 | 0.52052000 |
| H | -5.67832700 | -2.89452200 | 0.19319600 |
| C | -7.45901500 | -1.82616700 | 0.80684100 |
| H | -7.81981800 | -0.86127400 | 1.16701600 |
| C | -8.31612700 | -2.85358400 | 0.66101600 |
| H | -7.94880100 | -3.81881800 | 0.31434700 |
| C | -9.73347400 | -2.76685600 | 0.95011100 |
| H | -10.08800100 | -1.82932100 | 1.38085400 |
| C | -10.61254500 | -3.75667300 | 0.71758200 |
| H | -10.27617400 | -4.70471100 | 0.29977800 |
| C | 3.50891800 | 2.87800300 | -0.64885700 |
| H | 4.53091200 | 2.83963300 | -1.03024600 |
| H | 2.86523200 | 2.85772600 | -1.53828900 |
| C | -12.03721300 | -3.61920000 | 0.98186900 |

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|---|--------------|-------------|-------------|
| H | -12.32857300 | -2.73380800 | 1.54897100 |
| C | -12.97277900 | -4.46681100 | 0.54303800 |
| H | -12.69243100 | -5.35799100 | -0.01909100 |
| C | -14.44548100 | -4.26730400 | 0.75890600 |
| H | -14.61127500 | -3.47165000 | 1.50235900 |
| C | -15.10858100 | -3.80633600 | -0.55023500 |
| H | -15.17947700 | -4.65737900 | -1.24996900 |
| C | -14.33212200 | -2.67316700 | -1.24280600 |
| H | -13.30451400 | -3.04572900 | -1.37870500 |
| C | -14.19723200 | -1.42593000 | -0.35836800 |
| H | -13.88038000 | -1.70942800 | 0.65073000 |
| C | -12.01301300 | -0.42074000 | -0.19154300 |
| C | -10.95217100 | 0.31978800 | -0.96000000 |
| H | -11.01459500 | 0.05450400 | -2.02212100 |
| H | -11.17697100 | 1.39507500 | -0.89693100 |
| C | -9.54561800 | 0.07288400 | -0.40345900 |
| H | -9.31794000 | -1.00642600 | -0.40805000 |
| C | -8.49681600 | 0.86133700 | -1.17682700 |
| H | -8.63171800 | 0.69918000 | -2.25468800 |
| H | -8.68172500 | 1.92919900 | -0.99072800 |
| C | -7.04294900 | 0.56051600 | -0.80275500 |
| H | -6.84139000 | -0.52422100 | -0.82172200 |
| C | -6.09413800 | 1.30024400 | -1.74228400 |
| H | -6.45923600 | 2.33196000 | -1.84586600 |
| H | -6.16668100 | 0.84677300 | -2.73929000 |
| C | -4.62824100 | 1.32135200 | -1.27581000 |

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| H | -4.45733200 | 0.58074900 | -0.48113700 |
| H | -3.95751300 | 1.03553200 | -2.09573900 |
| C | -4.23602200 | 2.69357600 | -0.74178100 |
| H | -4.34978000 | 3.46016200 | -1.52387300 |
| C | -2.79037300 | 2.74412900 | -0.18164200 |
| H | -2.14983100 | 1.96789800 | -0.62460100 |
| C | -2.18643700 | 4.13580100 | -0.37831100 |
| H | -2.83517100 | 4.87359000 | 0.11687100 |
| H | -2.18193400 | 4.38478900 | -1.44832500 |
| C | -0.77662600 | 4.26825200 | 0.18798100 |
| H | -0.13845000 | 3.44147500 | -0.16310000 |
| C | -0.12355100 | 5.60597400 | -0.15151700 |
| H | -0.66132600 | 6.41160800 | 0.36547700 |
| H | -0.18820500 | 5.80083300 | -1.22884800 |
| C | 1.33006900 | 5.63832000 | 0.30098900 |
| C | 2.12097200 | 6.86344800 | -0.13207800 |
| H | 1.73496200 | 7.75400400 | 0.37751800 |
| H | 2.00826600 | 7.03569600 | -1.20978700 |
| C | 3.59907400 | 6.70712400 | 0.19501200 |
| H | 3.74899000 | 6.76617800 | 1.28216600 |
| C | 4.16322100 | 5.36777500 | -0.33861000 |
| H | 4.16346700 | 5.41747400 | -1.44197200 |
| C | 3.24753700 | 4.18775800 | 0.07623200 |
| H | 3.27464700 | 4.06235700 | 1.16780300 |
| C | 5.59306900 | 5.12981700 | 0.08594500 |
| C | -15.36351700 | -0.46244500 | -0.30294100 |

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| H | -15.16126600 | 0.34065000 | 0.41147400 |
| H | -16.26500000 | -0.98844800 | 0.02114700 |
| H | -15.55089400 | -0.00455000 | -1.27730100 |
| C | -14.90194300 | -2.36918300 | -2.62983800 |
| H | -15.95822500 | -2.08416900 | -2.59612800 |
| H | -14.80878100 | -3.23640600 | -3.28990200 |
| H | -14.36071100 | -1.53923800 | -3.09357500 |
| C | -15.11589500 | -5.54491700 | 1.27544400 |
| H | -14.96172100 | -6.38238900 | 0.58694800 |
| H | -16.19286300 | -5.39318000 | 1.38765500 |
| H | -14.70799700 | -5.83189500 | 2.24876300 |
| O | 4.89407400 | 0.93181000 | 3.71813100 |
| H | 4.09384100 | 0.66331900 | 3.23290100 |
| O | 8.20143400 | -1.51808700 | 2.28979600 |
| H | 8.59370400 | -1.38534200 | 3.17007800 |
| O | 5.22557800 | -0.04169300 | 0.83106200 |
| O | 3.92488500 | 1.69711600 | 1.45200400 |
| O | 1.43123500 | 5.56035700 | 1.69899000 |
| H | 0.72760800 | 4.95239000 | 2.01353000 |
| O | 1.90132100 | 4.47884800 | -0.29680600 |
| O | 6.26698200 | 4.13061800 | -0.05724900 |
| O | 6.15381800 | 6.20516700 | 0.70538200 |
| H | 7.07122900 | 5.96916100 | 0.93617900 |
| O | -0.81667300 | 4.21517700 | 1.62438200 |
| H | -1.37992800 | 3.45032600 | 1.86331600 |
| O | -2.83220000 | 2.39790300 | 1.20725800 |

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| H | -3.66932000 | 2.80029700 | 1.53088400 |
| O | -5.10032500 | 3.10322000 | 0.32220000 |
| H | -5.70474000 | 2.35629000 | 0.55485900 |
| O | -6.75378900 | 1.00183500 | 0.53654900 |
| H | -7.58888200 | 0.99719600 | 1.04930000 |
| O | -9.47426500 | 0.54992000 | 0.94503700 |
| H | -10.16708800 | 0.09117300 | 1.45905400 |
| O | -11.92636100 | -0.73240200 | 0.98183300 |
| O | -13.07452100 | -0.68623500 | -0.96068100 |
| O | -16.44157900 | -3.42361300 | -0.18084200 |
| H | -16.94281800 | -3.22240400 | -0.98242100 |
| O | 4.24148500 | 7.80483900 | -0.44956500 |
| H | 5.13471000 | 7.87713700 | -0.08290800 |
| N | 7.53261100 | 0.37358500 | 4.31424600 |
| H | 6.71802200 | 0.06129300 | 4.84046200 |
| H | 7.80381400 | 1.26859800 | 4.71134700 |

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| C | 3.94517900 | -3.35679100 | 1.88188600 |
| C | 3.12127000 | -4.51781900 | 1.30036900 |
| C | 2.00082000 | -4.91171800 | 2.27575800 |
| C | 1.18286800 | -3.71847400 | 2.74229100 |
| C | 2.08261400 | -2.69890500 | 3.43326700 |

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|---|------------|-------------|-------------|
| C | 3.45425900 | -2.52373100 | 2.82167500 |
| H | 1.35688500 | -5.65699000 | 1.79502200 |
| H | 0.67408000 | -3.25760400 | 1.89281000 |
| H | 0.39613300 | -4.04359000 | 3.43050100 |
| H | 1.58619500 | -1.72121800 | 3.46729200 |
| H | 2.23236200 | -2.97948100 | 4.48643400 |
| H | 2.45638700 | -5.40216000 | 3.14561400 |
| C | 4.20121400 | -1.35542300 | 3.41164000 |
| H | 5.05047200 | -1.03504500 | 2.81214800 |
| H | 3.52791800 | -0.50071500 | 3.52742400 |
| H | 4.56996900 | -1.60198900 | 4.41475100 |
| C | 2.52578400 | -4.09736900 | -0.05550800 |
| H | 3.31096800 | -3.79007500 | -0.75440200 |
| H | 1.99152900 | -4.93634200 | -0.51406900 |
| H | 1.82362700 | -3.26850400 | 0.05335300 |
| C | 4.00712100 | -5.75683600 | 1.09087200 |
| H | 3.38984700 | -6.60517300 | 0.77908900 |
| H | 4.76686300 | -5.60226800 | 0.32091200 |
| H | 4.52149900 | -6.03270700 | 2.01577900 |
| C | 5.29494600 | -3.21961500 | 1.30667100 |
| H | 5.36458700 | -3.37380300 | 0.23018800 |
| C | 6.42878500 | -3.00897000 | 1.99388600 |
| H | 6.35480700 | -2.96199600 | 3.07763400 |
| C | 7.79058000 | -2.84613700 | 1.46634600 |
| C | 8.04384000 | -2.62828200 | 0.15825500 |
| H | 7.19890700 | -2.57320800 | -0.52355800 |

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|---|--------------|-------------|-------------|
| C | 8.86146600 | -2.90595900 | 2.52455400 |
| H | 8.67380400 | -2.14883800 | 3.29386100 |
| H | 8.84519800 | -3.87777900 | 3.02905600 |
| H | 9.86647400 | -2.74289800 | 2.13849100 |
| C | 9.33199700 | -2.41667400 | -0.46469700 |
| H | 10.21882600 | -2.52465400 | 0.15036400 |
| C | 9.46703200 | -2.06360300 | -1.75497200 |
| H | 8.56501800 | -1.95047800 | -2.35500200 |
| C | 10.72455900 | -1.77458000 | -2.44309900 |
| C | 10.67608800 | -1.35192500 | -3.71777900 |
| H | 9.70044800 | -1.25968900 | -4.19297700 |
| C | 11.99732100 | -1.93319800 | -1.65470500 |
| H | 12.02577000 | -1.21556500 | -0.82804600 |
| H | 12.05691900 | -2.93314700 | -1.21492600 |
| H | 12.88979300 | -1.77543700 | -2.25853200 |
| C | 11.80580000 | -0.97004000 | -4.62249200 |
| H | 12.78324100 | -1.21765800 | -4.18871300 |
| H | 11.79886800 | 0.11354400 | -4.78763100 |
| O | 11.65479600 | -1.54329200 | -5.91243800 |
| H | 11.61077900 | -2.50020900 | -5.79859700 |
| C | -12.31761100 | 2.70335700 | 1.17336600 |
| H | -13.04171600 | 2.15609100 | 0.55677800 |
| C | -12.06676300 | 4.04481600 | 0.48607600 |
| H | -11.35505700 | 4.61907400 | 1.09942500 |
| C | -11.42507400 | 3.82924700 | -0.87927000 |
| H | -12.12213200 | 3.23310800 | -1.49296100 |

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| C | -10.38589900 | 1.83517800 | -0.14108800 |
| H | -11.01776300 | 1.22596100 | -0.80556500 |
| C | -11.02779400 | 1.89258000 | 1.24236100 |
| H | -11.24104600 | 0.85723700 | 1.54676200 |
| C | -11.10012000 | 5.12625200 | -1.58472400 |
| H | -10.38220500 | 5.69850200 | -0.99120800 |
| H | -12.00940300 | 5.71743200 | -1.70407500 |
| H | -10.66067100 | 4.92980600 | -2.56520300 |
| C | -8.37279700 | 0.98952700 | -1.14547400 |
| H | -8.49876300 | 1.82489800 | -1.84187800 |
| C | -6.94562200 | 0.91545700 | -0.70182000 |
| H | -6.70571000 | 0.15243300 | 0.03404500 |
| C | -5.98806300 | 1.73775700 | -1.14136800 |
| H | -6.22911800 | 2.50496200 | -1.87663400 |
| C | -4.62135900 | 1.68008900 | -0.66303600 |
| H | -4.40017300 | 0.91283600 | 0.07491400 |
| C | -3.63287200 | 2.51072800 | -1.04541000 |
| H | -3.83726900 | 3.28945500 | -1.77968700 |
| C | -2.29530300 | 2.42202100 | -0.51011900 |
| H | -2.12724700 | 1.62252800 | 0.20882400 |
| C | -1.26465300 | 3.22643600 | -0.83996000 |
| H | -1.41209400 | 4.02978900 | -1.56096900 |
| C | 0.05154400 | 3.06903100 | -0.27209000 |
| H | 0.18481300 | 2.24193300 | 0.42522000 |
| C | 1.11941800 | 3.84486100 | -0.55064100 |
| H | 1.01634500 | 4.66731700 | -1.25759400 |

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| C | 2.41070200 | 3.64602800 | 0.05925500 |
| H | 2.49193700 | 2.83016000 | 0.77641500 |
| C | 3.51190000 | 4.38041100 | -0.19789700 |
| H | 3.46173500 | 5.18582800 | -0.92978000 |
| C | 4.77612200 | 4.15651600 | 0.46209900 |
| H | 4.78699700 | 3.39036200 | 1.23534600 |
| C | 5.92402100 | 4.80290200 | 0.18816000 |
| H | 5.94424800 | 5.55626700 | -0.59844400 |
| C | -8.90010400 | -0.29731200 | -1.79287400 |
| H | -9.93861000 | -0.12947100 | -2.08719600 |
| H | -8.33183100 | -0.50720400 | -2.70398800 |
| C | 7.16643400 | 4.51841500 | 0.88014500 |
| H | 7.08776200 | 3.83303800 | 1.72246300 |
| C | 8.36920900 | 4.99088300 | 0.53464500 |
| H | 8.44990900 | 5.66468900 | -0.31993200 |
| C | 9.65841100 | 4.63524500 | 1.21968800 |
| H | 9.43136800 | 4.08131300 | 2.13760700 |
| C | 10.52961700 | 3.71560700 | 0.34171400 |
| H | 10.89773800 | 4.32013600 | -0.50399200 |
| C | 9.79214000 | 2.51035000 | -0.26750600 |
| H | 8.97533100 | 2.93044400 | -0.86238700 |
| C | 9.11191500 | 1.62854700 | 0.78484600 |
| H | 8.60730700 | 2.25071700 | 1.51862900 |
| C | 6.87042100 | 0.81155700 | 0.61212100 |
| C | 5.90079900 | 0.03327700 | -0.23148800 |
| H | 6.29002700 | -0.06825400 | -1.24570200 |

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| H | 5.84087800 | -0.96175400 | 0.21762000 |
| C | 4.49448400 | 0.63365200 | -0.23911600 |
| H | 4.51476200 | 1.62772100 | -0.70706100 |
| C | 3.54592700 | -0.27635500 | -1.00686800 |
| H | 3.87304500 | -0.32236100 | -2.05119300 |
| H | 3.61070300 | -1.28798200 | -0.58926800 |
| C | 2.08587000 | 0.15817700 | -0.95761100 |
| H | 2.00114700 | 1.21607100 | -1.23823000 |
| C | 1.22800000 | -0.67300300 | -1.90649700 |
| H | 1.48948800 | -1.73180300 | -1.79220200 |
| H | 1.50887300 | -0.39148900 | -2.92591100 |
| C | -0.28268400 | -0.48152400 | -1.70374000 |
| H | -0.48323700 | 0.47969000 | -1.22428500 |
| H | -0.78915400 | -0.44768600 | -2.67333100 |
| C | -0.94618900 | -1.59741800 | -0.89921900 |
| H | -0.89514200 | -2.52572900 | -1.48360800 |
| C | -2.43206500 | -1.27796800 | -0.60353800 |
| H | -2.81435700 | -0.57525100 | -1.35252700 |
| C | -3.32013200 | -2.51693700 | -0.58070300 |
| H | -2.96168500 | -3.20499200 | 0.19464800 |
| H | -3.23383000 | -3.03085500 | -1.54502400 |
| C | -4.78709300 | -2.17619100 | -0.33435600 |
| H | -5.11254300 | -1.44441000 | -1.08627100 |
| C | -5.68699800 | -3.39990700 | -0.44101800 |
| H | -5.36032000 | -4.16253500 | 0.27267900 |
| H | -5.59649000 | -3.81274200 | -1.44988300 |

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| C | -7.15979900 | -3.09598200 | -0.16355100 |
| C | -8.06962300 | -4.27126500 | -0.49012100 |
| H | -7.85739400 | -5.11073800 | 0.17521100 |
| H | -7.88755600 | -4.59106400 | -1.51999500 |
| C | -9.53651500 | -3.89716100 | -0.36580900 |
| H | -9.75854200 | -3.68724700 | 0.69067700 |
| C | -9.83140000 | -2.60981800 | -1.18378000 |
| H | -9.77984700 | -2.89062700 | -2.24236400 |
| C | -8.80589400 | -1.50926700 | -0.87337100 |
| H | -8.95303300 | -1.19030600 | 0.16259100 |
| C | -11.22926600 | -2.13424800 | -0.88310700 |
| C | 9.98763400 | 0.62084500 | 1.50047500 |
| H | 9.40242700 | 0.08989600 | 2.25457700 |
| H | 10.81241300 | 1.14627200 | 1.98420400 |
| H | 10.38722800 | -0.11361200 | 0.79941400 |
| C | 10.69613700 | 1.71566400 | -1.20826000 |
| H | 11.57900900 | 1.32614400 | -0.69124900 |
| H | 11.04104900 | 2.34369100 | -2.03516300 |
| H | 10.16630200 | 0.86071300 | -1.63263900 |
| C | 10.44618300 | 5.88991500 | 1.60759200 |
| H | 10.66788100 | 6.49581800 | 0.72199800 |
| H | 11.39084700 | 5.61454000 | 2.07867000 |
| H | 9.87071800 | 6.50878000 | 2.29978900 |
| O | -10.16872300 | 2.52721300 | 2.16717100 |
| H | -9.26855400 | 2.27215200 | 1.91983800 |
| O | -13.28604300 | 4.73245300 | 0.32460600 |

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| H | -13.75536500 | 4.57941600 | 1.16073300 |
| O | -10.20507600 | 3.11652900 | -0.70255200 |
| O | -9.12966200 | 1.26765900 | 0.04508700 |
| O | -7.37997300 | -2.75422700 | 1.17390000 |
| H | -6.64253000 | -2.17381400 | 1.43649800 |
| O | -7.49054100 | -2.01959700 | -1.03560000 |
| O | -11.54379800 | -1.10654400 | -0.33145500 |
| O | -12.17162000 | -3.02984300 | -1.27164300 |
| H | -13.02890900 | -2.66106600 | -1.00265400 |
| O | -4.96961300 | -1.60934700 | 0.96566100 |
| H | -4.16621300 | -1.09931900 | 1.17651000 |
| O | -2.49914100 | -0.59963000 | 0.65289400 |
| H | -1.73521000 | -0.96701100 | 1.14146100 |
| O | -0.31134400 | -1.84453100 | 0.34948600 |
| H | 0.41982400 | -1.19594000 | 0.47603000 |
| O | 1.56719400 | 0.00782700 | 0.36985800 |
| H | 2.28404500 | 0.24192900 | 0.98832600 |
| O | 3.99373900 | 0.76186300 | 1.09001700 |
| H | 4.73322300 | 1.04553900 | 1.65957700 |
| O | 6.56708300 | 1.28785900 | 1.69767800 |
| O | 8.07145000 | 0.89945100 | 0.06656700 |
| O | 11.62805200 | 3.31476000 | 1.15637400 |
| H | 12.32699000 | 2.97851700 | 0.58534900 |
| O | -10.26833300 | -5.00841600 | -0.83538400 |
| H | -11.20182900 | -4.76423900 | -0.87034000 |
| N | -12.94205800 | 2.97731300 | 2.46477600 |

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|---|--------------|------------|------------|
| H | -12.21124500 | 3.26599000 | 3.11165200 |
| H | -13.35637300 | 2.13377600 | 2.84842100 |

AmB-Ret12

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|---|------------|-------------|-------------|
| C | 7.27275800 | 7.83226700 | 0.90265600 |
| C | 7.67641600 | 8.56244300 | 2.19418600 |
| C | 8.18879300 | 9.97767900 | 1.88225200 |
| C | 7.28928700 | 10.72188600 | 0.90844500 |
| C | 7.23408700 | 9.96770700 | -0.41311000 |
| C | 7.05166600 | 8.47416600 | -0.26047600 |
| H | 8.29908200 | 10.53283200 | 2.82081700 |
| H | 6.27959400 | 10.80923700 | 1.32348800 |
| H | 7.65068700 | 11.74278700 | 0.74933100 |
| H | 6.42922300 | 10.36393100 | -1.04329500 |
| H | 8.16016500 | 10.14314200 | -0.98050900 |
| H | 9.19189900 | 9.89946200 | 1.44380600 |
| C | 6.61009000 | 7.80253200 | -1.53470600 |
| H | 6.27918700 | 6.77662300 | -1.38347600 |
| H | 5.79109200 | 8.36858700 | -1.99203100 |
| H | 7.42365000 | 7.78745600 | -2.27041000 |
| C | 6.46702500 | 8.63800300 | 3.14416600 |
| H | 6.08841400 | 7.64233200 | 3.38985400 |
| H | 6.75138900 | 9.12162100 | 4.08463900 |

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|---|------------|-------------|-------------|
| H | 5.64312800 | 9.20376400 | 2.70320100 |
| C | 8.80807600 | 7.80022600 | 2.90179200 |
| H | 9.15060400 | 8.36513500 | 3.77492400 |
| H | 8.48706600 | 6.81398300 | 3.24428100 |
| H | 9.66046100 | 7.65739500 | 2.23141000 |
| C | 7.12275400 | 6.37188800 | 1.05412800 |
| H | 6.56349400 | 6.03084200 | 1.92416500 |
| C | 7.68207400 | 5.44092800 | 0.26984000 |
| H | 8.34202600 | 5.77337700 | -0.53065900 |
| C | 7.52904600 | 3.98756800 | 0.41603600 |
| C | 6.37873000 | 3.45186600 | 0.87299000 |
| H | 5.55249400 | 4.13296600 | 1.06755700 |
| C | 8.73281500 | 3.18109300 | 0.00390600 |
| H | 9.06060900 | 3.47923500 | -0.99808100 |
| H | 9.57617300 | 3.36589800 | 0.67862300 |
| H | 8.54330100 | 2.10819200 | -0.01750500 |
| C | 6.09992500 | 2.05215600 | 1.11487600 |
| H | 6.90262600 | 1.33893600 | 0.96155800 |
| C | 4.89617000 | 1.60281100 | 1.50601800 |
| H | 4.09296600 | 2.32526400 | 1.64511800 |
| C | 4.53923200 | 0.20125200 | 1.72174400 |
| C | 3.25709400 | -0.09630600 | 1.98010600 |
| H | 2.53574800 | 0.71579300 | 2.04771400 |
| C | 5.62642600 | -0.82916200 | 1.58908400 |
| H | 5.28948000 | -1.82755000 | 1.85894200 |
| H | 5.99136500 | -0.84049300 | 0.55773100 |

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|---|------------|-------------|-------------|
| H | 6.46961000 | -0.57827600 | 2.24081100 |
| C | 2.64334500 | -1.44743700 | 2.15494000 |
| H | 2.50461900 | -1.66532300 | 3.22558000 |
| H | 3.26435100 | -2.24339900 | 1.73066300 |
| O | 1.36447200 | -1.40050600 | 1.51141300 |
| H | 0.95994900 | -2.27473400 | 1.55297000 |
| C | 7.19173600 | -5.48986300 | 2.30843400 |
| H | 7.84406500 | -5.76990400 | 1.47188900 |
| C | 6.45674700 | -6.75397600 | 2.75349100 |
| H | 5.83426700 | -6.49682500 | 3.62780200 |
| C | 5.52028200 | -7.24881700 | 1.65723700 |
| H | 6.13332900 | -7.51701900 | 0.78144500 |
| C | 5.29949600 | -5.06315600 | 0.75946400 |
| H | 5.91426000 | -5.38363400 | -0.09447100 |
| C | 6.19170000 | -4.43846000 | 1.82155600 |
| H | 6.71489700 | -3.58377800 | 1.38414500 |
| C | 4.68707800 | -8.43411400 | 2.08721800 |
| H | 4.04964300 | -8.15335900 | 2.93014000 |
| H | 5.34262000 | -9.24865000 | 2.39936700 |
| H | 4.04877400 | -8.77237000 | 1.26834200 |
| C | 3.57371800 | -4.47076400 | -0.77792300 |
| H | 3.36088500 | -5.54575900 | -0.76403200 |
| C | 2.29510400 | -3.70875600 | -0.64691600 |
| H | 2.39149000 | -2.62923100 | -0.57962100 |
| C | 1.08893200 | -4.28309900 | -0.58021400 |
| H | 1.00287300 | -5.36823800 | -0.63303200 |

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| C | -0.12931000 | -3.51922000 | -0.39798600 |
| H | -0.02673200 | -2.43786100 | -0.36827400 |
| C | -1.36516300 | -4.02865100 | -0.23295400 |
| H | -1.52630200 | -5.10594500 | -0.26694900 |
| C | -2.50042200 | -3.17120500 | 0.01558100 |
| H | -2.27210900 | -2.10873400 | 0.07502900 |
| C | -3.77629700 | -3.57341200 | 0.17594400 |
| H | -4.02848300 | -4.63132000 | 0.10950300 |
| C | -4.84493000 | -2.64390200 | 0.44923800 |
| H | -4.56967200 | -1.59156800 | 0.52198300 |
| C | -6.14004300 | -2.98043000 | 0.61551700 |
| H | -6.43814700 | -4.02462600 | 0.52697100 |
| C | -7.16966700 | -2.02274400 | 0.93360900 |
| H | -6.85449000 | -0.98740600 | 1.06287600 |
| C | -8.47523700 | -2.32272400 | 1.08532200 |
| H | -8.80707700 | -3.34983400 | 0.93731000 |
| C | -9.47607800 | -1.34860700 | 1.44733900 |
| H | -9.12061200 | -0.34355500 | 1.66735000 |
| C | -10.79862700 | -1.58635900 | 1.51638800 |
| H | -11.18137900 | -2.57646900 | 1.27148200 |
| C | 4.38613100 | -4.12875100 | -2.03357500 |
| H | 5.23992700 | -4.80907300 | -2.08253600 |
| H | 3.77474800 | -4.30989800 | -2.92272100 |
| C | -11.76129200 | -0.55891600 | 1.86380500 |
| H | -11.33847300 | 0.37805800 | 2.22051900 |
| C | -13.08706600 | -0.66431500 | 1.72403100 |

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|---|--------------|-------------|-------------|
| H | -13.51033800 | -1.59750000 | 1.34872300 |
| C | -14.06648600 | 0.44100600 | 2.00018300 |
| H | -13.54683400 | 1.25582200 | 2.51718100 |
| C | -14.63324700 | 1.02197000 | 0.68998600 |
| H | -15.26569400 | 0.24247000 | 0.23325000 |
| C | -13.57714600 | 1.40119800 | -0.36552700 |
| H | -13.01838300 | 0.48314200 | -0.57163300 |
| C | -12.53623000 | 2.40178700 | 0.14841200 |
| H | -12.18037300 | 2.09276400 | 1.12735700 |
| C | -10.18927400 | 2.10566900 | -0.26488900 |
| C | -9.13052900 | 2.01855300 | -1.33472800 |
| H | -9.59088100 | 1.71896900 | -2.27802400 |
| H | -8.72005200 | 3.02619800 | -1.46853700 |
| C | -7.99195700 | 1.06963500 | -0.95139400 |
| H | -8.39856800 | 0.05770400 | -0.80979000 |
| C | -6.92333100 | 1.03641900 | -2.03434500 |
| H | -7.37997500 | 0.68539400 | -2.96597700 |
| H | -6.55976000 | 2.05664400 | -2.20643600 |
| C | -5.72311800 | 0.14998500 | -1.70965000 |
| H | -6.07366000 | -0.85679900 | -1.44157600 |
| C | -4.78240400 | 0.04532800 | -2.90566000 |
| H | -4.61472500 | 1.05175100 | -3.30853200 |
| H | -5.30408200 | -0.51999300 | -3.68418400 |
| C | -3.43063300 | -0.61256300 | -2.58315300 |
| H | -3.50053000 | -1.19946900 | -1.66420100 |
| H | -3.16169700 | -1.31739900 | -3.37581300 |

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| C | -2.27924700 | 0.38428200 | -2.46054700 |
| H | -2.13711000 | 0.86132900 | -3.44153700 |
| C | -0.96050000 | -0.31020400 | -2.05876100 |
| H | -0.95536800 | -1.33615900 | -2.44787200 |
| C | 0.27297100 | 0.41644000 | -2.58171000 |
| H | 0.26945800 | 1.45452800 | -2.23137100 |
| H | 0.22097400 | 0.43615200 | -3.67740100 |
| C | 1.57574200 | -0.25102300 | -2.14380200 |
| H | 1.46279100 | -1.34032500 | -2.22368600 |
| C | 2.75647100 | 0.15418600 | -3.01956400 |
| H | 2.89196000 | 1.23947500 | -2.97620600 |
| H | 2.54108500 | -0.12172500 | -4.05565400 |
| C | 4.07324400 | -0.49871900 | -2.59755400 |
| C | 5.19866500 | -0.25732200 | -3.59247600 |
| H | 5.42258700 | 0.80939200 | -3.65887800 |
| H | 4.89211900 | -0.61126400 | -4.58080400 |
| C | 6.45710100 | -1.00169200 | -3.18366600 |
| H | 6.83087700 | -0.56569300 | -2.24605000 |
| C | 6.13510000 | -2.50117500 | -2.93130100 |
| H | 5.98509700 | -2.95252200 | -3.91942100 |
| C | 4.87894900 | -2.68601300 | -2.06370300 |
| H | 5.11902700 | -2.36695300 | -1.04681600 |
| C | 7.31986000 | -3.16702200 | -2.28000400 |
| C | -12.95557000 | 3.85681100 | 0.19669900 |
| H | -12.15761400 | 4.46190200 | 0.63318300 |
| H | -13.85333700 | 3.94796400 | 0.80945500 |

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|---|--------------|-------------|-------------|
| H | -13.16873400 | 4.23914400 | -0.80388500 |
| C | -14.23148500 | 1.85416100 | -1.66985000 |
| H | -14.86441700 | 2.73520700 | -1.52608600 |
| H | -14.85239100 | 1.05662400 | -2.08809400 |
| H | -13.47339600 | 2.11508300 | -2.41163800 |
| C | -15.20855800 | -0.03961100 | 2.89981700 |
| H | -15.74055500 | -0.87640900 | 2.43358000 |
| H | -15.92362000 | 0.76579200 | 3.07249300 |
| H | -14.82197000 | -0.38455400 | 3.86151800 |
| O | 5.41166600 | -3.96262600 | 2.90863700 |
| H | 4.59920600 | -4.48819500 | 2.91554100 |
| O | 7.38068800 | -7.76560000 | 3.07243400 |
| H | 8.08003500 | -7.30343100 | 3.56234800 |
| O | 4.62700500 | -6.18949100 | 1.30914500 |
| O | 4.33922800 | -4.13851500 | 0.39424600 |
| O | 4.51263000 | -0.03987000 | -1.35802100 |
| H | 3.71812300 | 0.03329000 | -0.79016900 |
| O | 3.80937200 | -1.90522000 | -2.56869300 |
| O | 7.35860300 | -3.66644900 | -1.17892500 |
| O | 8.42724900 | -3.12996500 | -3.06083400 |
| H | 9.14168600 | -3.54059700 | -2.54695700 |
| O | 1.91939400 | 0.09979400 | -0.80712700 |
| H | 1.35406100 | -0.36298400 | -0.16322900 |
| O | -0.91978400 | -0.42577300 | -0.64451800 |
| H | -1.31444200 | 0.40926000 | -0.33459000 |
| O | -2.51826100 | 1.40826000 | -1.50697800 |

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| H | -3.39439600 | 1.26576000 | -1.09628600 |
| O | -4.98026600 | 0.67613200 | -0.60749000 |
| H | -5.61841100 | 1.05636500 | 0.02219000 |
| O | -7.36824200 | 1.49755800 | 0.25612100 |
| H | -8.07833800 | 1.69238100 | 0.89318700 |
| O | -9.93961100 | 2.02705800 | 0.92762200 |
| O | -11.40081000 | 2.29583100 | -0.76688600 |
| O | -15.44115100 | 2.13423800 | 1.06283500 |
| H | -16.02337300 | 2.35298900 | 0.32740300 |
| O | 7.38449500 | -0.83204800 | -4.23415900 |
| H | 8.17031900 | -1.35400500 | -4.02938800 |
| N | 8.03447300 | -5.06002300 | 3.41904500 |
| H | 7.44302500 | -4.56472200 | 4.08372900 |
| H | 8.73715400 | -4.39958200 | 3.10221800 |

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|---|--------------|------------|-------------|
| C | -13.05597700 | 0.50583100 | -0.52232800 |
| C | -13.47295000 | 0.86191300 | -1.95925200 |
| C | -14.33303600 | 2.13663700 | -1.98017100 |
| C | -13.77714400 | 3.22458700 | -1.07460600 |
| C | -13.80304100 | 2.72993600 | 0.36443600 |
| C | -13.23388800 | 1.33772700 | 0.52619800 |
| H | -14.42264300 | 2.48617700 | -3.01419500 |

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|---|--------------|-------------|-------------|
| H | -12.74527600 | 3.46284700 | -1.35311400 |
| H | -14.35791900 | 4.14675300 | -1.17061300 |
| H | -13.24478300 | 3.41444900 | 1.01413800 |
| H | -14.83313000 | 2.73331700 | 0.74860800 |
| H | -15.34786500 | 1.88739300 | -1.64454900 |
| C | -12.89542500 | 1.00625000 | 1.95742300 |
| H | -12.39582800 | 0.04757900 | 2.07697100 |
| H | -12.25875700 | 1.78719400 | 2.38905400 |
| H | -13.81006900 | 0.98883900 | 2.56144400 |
| C | -12.23617800 | 1.05572200 | -2.85667000 |
| H | -11.62711100 | 0.14904700 | -2.90175900 |
| H | -12.55430700 | 1.27829800 | -3.87997500 |
| H | -11.59916300 | 1.86978800 | -2.50695700 |
| C | -14.31281900 | -0.29135200 | -2.53215600 |
| H | -14.68722000 | -0.02229600 | -3.52481500 |
| H | -13.72833800 | -1.20946300 | -2.62719200 |
| H | -15.17276700 | -0.50689700 | -1.89102700 |
| C | -12.39806300 | -0.81165100 | -0.37912400 |
| H | -11.51872300 | -0.96415100 | -1.00231200 |
| C | -12.77653000 | -1.82740700 | 0.40587900 |
| H | -13.71824500 | -1.75700700 | 0.94997100 |
| C | -11.98017200 | -3.04959700 | 0.60619400 |
| C | -10.64398300 | -2.93030900 | 0.73218600 |
| H | -10.24881400 | -1.92088800 | 0.72320900 |
| C | -12.74104000 | -4.34186300 | 0.70191900 |
| H | -13.53130500 | -4.26225000 | 1.45655300 |

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|---|--------------|-------------|-------------|
| H | -13.23541900 | -4.57286500 | -0.24762000 |
| H | -12.10758200 | -5.18798900 | 0.97035700 |
| C | -9.63904400 | -3.95237700 | 0.94351400 |
| H | -9.93581000 | -4.99717600 | 0.94473000 |
| C | -8.35762100 | -3.60917000 | 1.16193000 |
| H | -8.10885300 | -2.54858700 | 1.15155400 |
| C | -7.23337700 | -4.50053000 | 1.43974500 |
| C | -6.07290100 | -3.93629900 | 1.81160100 |
| H | -6.04142600 | -2.85114600 | 1.88857000 |
| C | -7.46455900 | -5.98219500 | 1.32418000 |
| H | -8.17955300 | -6.31683300 | 2.08269100 |
| H | -7.89403900 | -6.22802700 | 0.34845400 |
| H | -6.55158100 | -6.56316100 | 1.45275000 |
| C | -4.77515300 | -4.58476800 | 2.17316100 |
| H | -4.74897000 | -5.64614300 | 1.89696000 |
| H | -4.61522900 | -4.53314400 | 3.25577000 |
| O | -3.67501000 | -3.88015300 | 1.60529300 |
| H | -3.76239100 | -3.92432100 | 0.64570600 |
| C | 13.53455400 | 3.12444100 | -0.68683600 |
| H | 14.29510100 | 2.46186200 | -0.25478200 |
| C | 13.21893500 | 4.18894900 | 0.36297200 |
| H | 12.46948800 | 4.87739000 | -0.05760400 |
| C | 12.60656700 | 3.54684600 | 1.60198200 |
| H | 13.34250800 | 2.83654400 | 2.01648500 |
| C | 11.67104900 | 1.80144800 | 0.30702500 |
| H | 12.34511000 | 1.06267700 | 0.76675200 |

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| C | 12.29107100 | 2.29778200 | -0.99618600 |
| H | 12.55801000 | 1.41064800 | -1.58950200 |
| C | 12.21996300 | 4.55939800 | 2.65586200 |
| H | 11.46551000 | 5.24054900 | 2.25335100 |
| H | 13.09721300 | 5.13853700 | 2.94848100 |
| H | 11.80289500 | 4.05968600 | 3.53301100 |
| C | 9.71903000 | 0.58609500 | 1.00963200 |
| H | 9.79456000 | 1.19423000 | 1.91692200 |
| C | 8.29714400 | 0.54648000 | 0.54559300 |
| H | 8.10460600 | 0.01250100 | -0.38114800 |
| C | 7.28775900 | 1.13758500 | 1.19199600 |
| H | 7.47973300 | 1.67598500 | 2.11971900 |
| C | 5.92418900 | 1.12010600 | 0.70168900 |
| H | 5.75204700 | 0.58085500 | -0.22647600 |
| C | 4.88244700 | 1.73347600 | 1.29454800 |
| H | 5.03806600 | 2.28507800 | 2.22138700 |
| C | 3.54890400 | 1.70390400 | 0.74291000 |
| H | 3.42865500 | 1.12556900 | -0.17112700 |
| C | 2.47165900 | 2.31785100 | 1.27231000 |
| H | 2.57517300 | 2.90141000 | 2.18660900 |
| C | 1.16313100 | 2.24492300 | 0.67080000 |
| H | 1.06653900 | 1.62329100 | -0.21916200 |
| C | 0.06335300 | 2.87428600 | 1.13305000 |
| H | 0.13592400 | 3.49076800 | 2.02841300 |
| C | -1.22165300 | 2.79764100 | 0.48433000 |
| H | -1.28303800 | 2.17887800 | -0.41081600 |

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|---|-------------|-------------|-------------|
| C | -2.33327700 | 3.43526300 | 0.90411900 |
| H | -2.28972800 | 4.04392700 | 1.80663100 |
| C | -3.59702500 | 3.36601100 | 0.21146500 |
| H | -3.61345900 | 2.79286900 | -0.71402100 |
| C | -4.74233000 | 3.93662200 | 0.62858500 |
| H | -4.75593100 | 4.49443800 | 1.56421700 |
| C | 10.33394700 | -0.79536400 | 1.26997900 |
| H | 11.36176200 | -0.65246900 | 1.61123800 |
| H | 9.78717100 | -1.29163600 | 2.07733100 |
| C | -5.99210300 | 3.80306600 | -0.09436400 |
| H | -5.92131200 | 3.31914700 | -1.06661700 |
| C | -7.19561400 | 4.16219300 | 0.36600300 |
| H | -7.27263700 | 4.63108200 | 1.34836700 |
| C | -8.49029700 | 3.90873100 | -0.35275500 |
| H | -8.26826400 | 3.56254400 | -1.36879200 |
| C | -9.30447000 | 2.79061900 | 0.33030200 |
| H | -9.68698800 | 3.19484200 | 1.28254300 |
| C | -8.49525500 | 1.52858500 | 0.68879600 |
| H | -7.66714000 | 1.87446600 | 1.31454600 |
| C | -7.83496300 | 0.87401400 | -0.52791500 |
| H | -7.37061200 | 1.63995900 | -1.14220700 |
| C | -5.56109300 | 0.12662000 | -0.59018500 |
| C | -4.56153200 | -0.85815300 | -0.03937300 |
| H | -4.85034700 | -1.16361900 | 0.96625900 |
| H | -4.61083500 | -1.74749800 | -0.67933700 |
| C | -3.13185400 | -0.31156300 | -0.04665200 |

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|---|-------------|-------------|-------------|
| H | -3.08408400 | 0.56029900 | 0.62170600 |
| C | -2.13689900 | -1.36201100 | 0.42111500 |
| H | -2.44127400 | -1.74529600 | 1.39855000 |
| H | -2.17043600 | -2.20591600 | -0.27984000 |
| C | -0.69824800 | -0.86174200 | 0.48911000 |
| H | -0.65455300 | 0.04760400 | 1.10460200 |
| C | 0.22531300 | -1.91188800 | 1.09607800 |
| H | 0.03403900 | -2.87552000 | 0.60829600 |
| H | -0.06261400 | -2.03352500 | 2.14442600 |
| C | 1.71699700 | -1.55661600 | 0.98968700 |
| H | 1.84279000 | -0.47979800 | 0.84992600 |
| H | 2.22820800 | -1.80160600 | 1.92595000 |
| C | 2.45269100 | -2.30136700 | -0.12275400 |
| H | 2.46610900 | -3.37096000 | 0.12876900 |
| C | 3.91756100 | -1.81046900 | -0.26326400 |
| H | 4.23882200 | -1.33293100 | 0.66961400 |
| C | 4.89336000 | -2.92844100 | -0.61373900 |
| H | 4.58982900 | -3.38763500 | -1.56241500 |
| H | 4.83790800 | -3.70153600 | 0.16137800 |
| C | 6.33398800 | -2.43601100 | -0.71607100 |
| H | 6.60685500 | -1.93533500 | 0.22291500 |
| C | 7.31421600 | -3.57811200 | -0.94963900 |
| H | 7.03461400 | -4.12556500 | -1.85515700 |
| H | 7.25681300 | -4.26647500 | -0.10148300 |
| C | 8.76238300 | -3.11475800 | -1.11097200 |
| C | 9.74766600 | -4.27447700 | -1.12484800 |

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|---|--------------|-------------|-------------|
| H | 9.58418100 | -4.89913900 | -2.00543400 |
| H | 9.59407500 | -4.88710000 | -0.23203800 |
| C | 11.18634800 | -3.78819900 | -1.12075800 |
| H | 11.38541700 | -3.26813200 | -2.06907000 |
| C | 11.40505000 | -2.77596600 | 0.03679200 |
| H | 11.37685900 | -3.35198000 | 0.96923500 |
| C | 10.31009100 | -1.69824600 | 0.04233800 |
| H | 10.42942500 | -1.08798400 | -0.85769900 |
| C | 12.76886200 | -2.14975800 | -0.09712500 |
| C | -8.70607400 | -0.00928500 | -1.39687600 |
| H | -8.13875800 | -0.34944200 | -2.26647500 |
| H | -9.56977800 | 0.56201900 | -1.73609900 |
| H | -9.04922700 | -0.88877200 | -0.84882500 |
| C | -9.33266900 | 0.55653200 | 1.51366600 |
| H | -10.22055500 | 0.22305100 | 0.97108100 |
| H | -9.67044700 | 1.02825300 | 2.44063000 |
| H | -8.75326400 | -0.32915400 | 1.78390400 |
| C | -9.33460200 | 5.18156800 | -0.45809000 |
| H | -9.55600100 | 5.58096400 | 0.53791600 |
| H | -10.28061500 | 4.97088300 | -0.95929900 |
| H | -8.80168300 | 5.95431300 | -1.01680300 |
| O | 11.38651400 | 3.12517200 | -1.69829700 |
| H | 10.50516500 | 2.75773100 | -1.54066700 |
| O | 14.40085900 | 4.86588400 | 0.72435100 |
| H | 14.86759700 | 4.99038100 | -0.11796400 |
| O | 11.42546000 | 2.85037600 | 1.21804100 |

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|---|--------------|-------------|-------------|
| O | 10.44710500 | 1.24132700 | -0.04318700 |
| O | 8.95059800 | -2.39055300 | -2.29155600 |
| H | 8.17396200 | -1.80895600 | -2.38541500 |
| O | 9.03091800 | -2.31510700 | 0.03713300 |
| O | 13.01635100 | -0.99099400 | -0.33270000 |
| O | 13.76744800 | -3.05875300 | 0.03694600 |
| H | 14.59844600 | -2.57656300 | -0.10529400 |
| O | 6.48028200 | -1.50361900 | -1.79035600 |
| H | 5.63660400 | -1.02142000 | -1.87465600 |
| O | 3.94911400 | -0.79679800 | -1.26958900 |
| H | 3.18591700 | -1.03618800 | -1.83721600 |
| O | 1.84043100 | -2.16589500 | -1.39727300 |
| H | 1.04684000 | -1.59288400 | -1.31491300 |
| O | -0.20585400 | -0.53651300 | -0.81670300 |
| H | -0.95418900 | -0.19011900 | -1.33662500 |
| O | -2.74176300 | 0.08178900 | -1.36078200 |
| H | -3.47690700 | 0.59639500 | -1.73964500 |
| O | -5.29858000 | 0.90108400 | -1.49721300 |
| O | -6.75047100 | 0.03584600 | -0.00989100 |
| O | -10.39250700 | 2.51252900 | -0.54176700 |
| H | -11.06634000 | 1.97578400 | -0.10027000 |
| O | 11.99178500 | -4.93899600 | -0.98481200 |
| H | 12.90765300 | -4.65669500 | -0.86761800 |
| N | 14.12691500 | 3.79991800 | -1.83825800 |
| H | 13.37300900 | 4.22433600 | -2.37432400 |
| H | 14.58082000 | 3.13016600 | -2.45132100 |

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|---|--------------|-------------|-------------|
| C | -11.19029900 | -0.96178300 | -1.10011200 |
| C | -9.90529800 | -1.73880600 | -0.76599100 |
| C | -10.05786200 | -3.23500700 | -1.08652900 |
| C | -10.73516100 | -3.48540800 | -2.42423000 |
| C | -12.13239900 | -2.88130800 | -2.40741800 |
| C | -12.17843300 | -1.47180300 | -1.86023600 |
| H | -9.06526900 | -3.70438600 | -1.07347200 |
| H | -10.15021600 | -3.03051300 | -3.23035900 |
| H | -10.78430000 | -4.55759800 | -2.63843900 |
| H | -12.55694100 | -2.88686300 | -3.41775600 |
| H | -12.80377200 | -3.51184500 | -1.80576000 |
| H | -10.65187700 | -3.71355200 | -0.29761400 |
| C | -13.42347100 | -0.71948700 | -2.24992900 |
| H | -13.32848200 | 0.35589200 | -2.10539400 |
| H | -13.66425100 | -0.90875700 | -3.30140000 |
| H | -14.28861700 | -1.05937900 | -1.66731000 |
| C | -8.73297200 | -1.15801900 | -1.57998800 |
| H | -8.64290100 | -0.07884700 | -1.44349700 |
| H | -7.78963800 | -1.61347900 | -1.26134800 |
| H | -8.86439700 | -1.33932900 | -2.64947700 |
| C | -9.59050900 | -1.60952800 | 0.73484300 |

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|---|--------------|-------------|-------------|
| H | -8.64767500 | -2.11433500 | 0.97055600 |
| H | -9.49193400 | -0.56707400 | 1.04376400 |
| H | -10.39033700 | -2.05097900 | 1.33699300 |
| C | -11.20034800 | 0.40483900 | -0.54827800 |
| H | -10.24985700 | 0.93353300 | -0.58913900 |
| C | -12.21307300 | 1.02175500 | 0.07820800 |
| H | -13.14130900 | 0.47747700 | 0.24264300 |
| C | -12.14226600 | 2.37330300 | 0.65248800 |
| C | -11.28908900 | 3.29240100 | 0.15546400 |
| H | -10.72177700 | 3.02223000 | -0.73142400 |
| C | -13.04687100 | 2.60903300 | 1.83263200 |
| H | -13.05756300 | 3.64711500 | 2.16434700 |
| H | -14.07584600 | 2.32765000 | 1.58324200 |
| H | -12.74682800 | 1.98546900 | 2.68209000 |
| C | -10.98465100 | 4.60199900 | 0.69521500 |
| H | -11.57993200 | 4.96788500 | 1.52610100 |
| C | -9.96718700 | 5.34701500 | 0.22644300 |
| H | -9.36365100 | 4.93598300 | -0.58025600 |
| C | -9.55237100 | 6.65528900 | 0.73132000 |
| C | -8.50378900 | 7.25970600 | 0.14759500 |
| H | -8.01044700 | 6.74645100 | -0.67656800 |
| C | -10.33632500 | 7.23938300 | 1.87666300 |
| H | -11.38016500 | 7.39410500 | 1.58572000 |
| H | -10.34063700 | 6.55151000 | 2.72805300 |
| H | -9.94148100 | 8.19595400 | 2.21617800 |
| C | -7.87355800 | 8.57491600 | 0.48287300 |

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| H | -8.29264900 | 9.01123600 | 1.39897800 |
| H | -8.05524200 | 9.29503700 | -0.32320100 |
| O | -6.45924700 | 8.46391400 | 0.56940900 |
| H | -6.26731400 | 7.76236800 | 1.20326700 |
| C | -7.01095300 | 1.12713300 | 1.00621200 |
| H | -7.58835600 | 0.32200200 | 0.54455900 |
| C | -6.94695100 | 2.26869900 | -0.00695000 |
| H | -6.42569900 | 3.11967800 | 0.45617700 |
| C | -6.16590400 | 1.86351400 | -1.25393300 |
| H | -6.72058600 | 1.05241300 | -1.75278700 |
| C | -4.95283600 | 0.25755700 | -0.03384300 |
| H | -5.53402800 | -0.52755900 | -0.53764300 |
| C | -5.62032100 | 0.58225300 | 1.29494100 |
| H | -5.69257800 | -0.35328400 | 1.86778500 |
| C | -5.97078600 | 3.01482300 | -2.21457700 |
| H | -5.39302500 | 3.80711000 | -1.73122500 |
| H | -6.94163400 | 3.41603500 | -2.51089300 |
| H | -5.42899100 | 2.68437700 | -3.10334400 |
| C | -2.92978300 | -0.73591300 | -0.83992000 |
| H | -3.06512500 | -0.09899100 | -1.72111300 |
| C | -1.49636300 | -0.71060800 | -0.41262000 |
| H | -1.25162600 | -1.26305100 | 0.49076400 |
| C | -0.53870100 | -0.03926200 | -1.05917900 |
| H | -0.78282900 | 0.51774100 | -1.96332400 |
| C | 0.83321700 | 0.01008700 | -0.59529500 |
| H | 1.05561000 | -0.54464300 | 0.31282800 |

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| C | 1.82508700 | 0.70194700 | -1.18721000 |
| H | 1.62011900 | 1.26864200 | -2.09508700 |
| C | 3.16771200 | 0.73712100 | -0.65848900 |
| H | 3.33662300 | 0.14896900 | 0.24137400 |
| C | 4.19984200 | 1.41791900 | -1.19568300 |
| H | 4.04806600 | 2.00863100 | -2.09851600 |
| C | 5.52288400 | 1.40401000 | -0.62238600 |
| H | 5.66711000 | 0.78657800 | 0.26416400 |
| C | 6.58294100 | 2.07952300 | -1.11116600 |
| H | 6.46147100 | 2.68978200 | -2.00545800 |
| C | 7.88804300 | 2.05567500 | -0.49956800 |
| H | 7.99762700 | 1.45388800 | 0.40255900 |
| C | 8.96507500 | 2.71806700 | -0.96762700 |
| H | 8.87295700 | 3.30631100 | -1.87998800 |
| C | 10.25402000 | 2.69923400 | -0.31964200 |
| H | 10.31826000 | 2.15908800 | 0.62343800 |
| C | 11.36864800 | 3.27877100 | -0.80166800 |
| H | 11.33176600 | 3.80227600 | -1.75635300 |
| C | -3.46942100 | -2.14170300 | -1.14681000 |
| H | -4.50771500 | -2.05029100 | -1.47378300 |
| H | -2.90455800 | -2.56980900 | -1.98017700 |
| C | 12.64909100 | 3.20398600 | -0.12569500 |
| H | 12.63083000 | 2.76374200 | 0.86934600 |
| C | 13.82034300 | 3.57466500 | -0.65424700 |
| H | 13.83939300 | 3.99948400 | -1.65929500 |
| C | 15.15425600 | 3.40577900 | 0.01525100 |

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| H | 14.99461800 | 3.10834400 | 1.05796800 |
| C | 15.97444900 | 2.28683100 | -0.65638500 |
| H | 16.26086600 | 2.64792300 | -1.65817100 |
| C | 15.21645900 | 0.96314600 | -0.86859800 |
| H | 14.34491600 | 1.21387200 | -1.48116100 |
| C | 14.64586400 | 0.37879600 | 0.42826700 |
| H | 14.15771100 | 1.16224200 | 1.00129900 |
| C | 12.39989100 | -0.45583600 | 0.56754800 |
| C | 11.43315600 | -1.48327100 | 0.03460400 |
| H | 11.75875700 | -1.80914400 | -0.95502400 |
| H | 11.47869100 | -2.35063600 | 0.70351000 |
| C | 9.99478200 | -0.96146600 | -0.00146000 |
| H | 9.94526200 | -0.08731100 | -0.66635900 |
| C | 9.03571100 | -2.03114000 | -0.50385000 |
| H | 9.33754900 | -2.32616900 | -1.51453200 |
| H | 9.12024100 | -2.91499000 | 0.13976300 |
| C | 7.57295100 | -1.59466000 | -0.53332100 |
| H | 7.48099500 | -0.65966000 | -1.10269600 |
| C | 6.69068300 | -2.65589200 | -1.18247700 |
| H | 6.93519600 | -3.63321100 | -0.74827700 |
| H | 6.96327600 | -2.70684800 | -2.24101700 |
| C | 5.18503000 | -2.38166600 | -1.03448800 |
| H | 5.00954000 | -1.32252400 | -0.83179200 |
| H | 4.67103500 | -2.59889100 | -1.97593100 |
| C | 4.50668700 | -3.22332800 | 0.04483600 |
| H | 4.54781500 | -4.27732600 | -0.26362300 |

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| C | 3.02001700 | -2.82363300 | 0.22899600 |
| H | 2.65255600 | -2.33313500 | -0.67965000 |
| C | 2.11968000 | -4.00953000 | 0.55676500 |
| H | 2.46954600 | -4.48219300 | 1.48254400 |
| H | 2.20519900 | -4.75062400 | -0.24636900 |
| C | 0.65425400 | -3.60962300 | 0.70265000 |
| H | 0.33384700 | -3.09109400 | -0.21137800 |
| C | -0.24895900 | -4.81848400 | 0.90694200 |
| H | 0.08080200 | -5.38157400 | 1.78558800 |
| H | -0.16380200 | -5.46894100 | 0.03162100 |
| C | -1.72026900 | -4.45546600 | 1.10918900 |
| C | -2.62737500 | -5.67674700 | 1.08592000 |
| H | -2.41122400 | -6.32490500 | 1.93766300 |
| H | -2.44597200 | -6.24090900 | 0.16680700 |
| C | -4.09538300 | -5.28917200 | 1.11728100 |
| H | -4.31796300 | -4.82699200 | 2.09020700 |
| C | -4.39870600 | -4.24210200 | 0.00892000 |
| H | -4.34756700 | -4.77286700 | -0.94888900 |
| C | -3.37531000 | -3.09445200 | 0.03955800 |
| H | -3.51959100 | -2.53375000 | 0.96788400 |
| C | -5.80082900 | -3.72233600 | 0.19384500 |
| C | 15.61281100 | -0.37361200 | 1.31936900 |
| H | 15.10953300 | -0.68767200 | 2.23668200 |
| H | 16.44647700 | 0.28292600 | 1.57225400 |
| H | 16.00089900 | -1.26270700 | 0.81771100 |
| C | 16.06148100 | -0.04482500 | -1.64564900 |

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| H | 16.98919100 | -0.29116900 | -1.12037200 |
| H | 16.32540900 | 0.35006400 | -2.63099200 |
| H | 15.51212700 | -0.97738200 | -1.79280500 |
| C | 15.94995800 | 4.71412800 | 0.01247800 |
| H | 16.10856500 | 5.06738800 | -1.01251100 |
| H | 16.92545200 | 4.56710300 | 0.47800800 |
| H | 15.41090200 | 5.49430900 | 0.55462600 |
| O | -4.89531700 | 1.56462500 | 2.00592100 |
| H | -3.95817200 | 1.37410200 | 1.86218200 |
| O | -8.26312300 | 2.62388400 | -0.38791700 |
| H | -8.75694000 | 2.67446900 | 0.44825200 |
| O | -4.87885900 | 1.39326600 | -0.86957900 |
| O | -3.66138500 | -0.16134800 | 0.25601600 |
| O | -1.93410000 | -3.79514500 | 2.32231700 |
| H | -1.19610900 | -3.16751400 | 2.42892000 |
| O | -2.05955800 | -3.62745000 | 0.00123500 |
| O | -6.11736600 | -2.59501900 | 0.49879300 |
| O | -6.73691700 | -4.68697000 | 0.02760800 |
| H | -7.60172800 | -4.28233400 | 0.21140600 |
| O | 0.47132900 | -2.73039700 | 1.81535800 |
| H | 1.28335000 | -2.19749700 | 1.90163200 |
| O | 2.94986600 | -1.84963600 | 1.27200200 |
| H | 3.72866200 | -2.07200400 | 1.82441300 |
| O | 5.12780900 | -3.12111000 | 1.31802700 |
| H | 5.89136800 | -2.50722500 | 1.25723800 |
| O | 7.08258000 | -1.36273100 | 0.79025000 |

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| H | 7.80900500 | -0.97112700 | 1.30900600 |
| O | 9.56882100 | -0.58226900 | 1.30467800 |
| H | 10.27436900 | -0.03011500 | 1.68664400 |
| O | 12.09994700 | 0.35873100 | 1.42623600 |
| O | 13.59961700 | -0.55557600 | 0.01465100 |
| O | 17.14223100 | 2.11388000 | 0.14094800 |
| H | 17.80741700 | 1.65233100 | -0.38074000 |
| O | -4.82140500 | -6.48527900 | 0.93627200 |
| H | -5.75681600 | -6.26423800 | 0.84534700 |
| N | -7.75687200 | 1.60101500 | 2.16607800 |
| H | -7.13419300 | 2.16397400 | 2.74105800 |
| H | -8.06157000 | 0.81893500 | 2.73698900 |

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|---|------------|-------------|-------------|
| C | 4.66938100 | 0.24751100 | -3.61237800 |
| H | 4.89758000 | -0.74195800 | -3.19970900 |
| H | 5.36887300 | 0.95979300 | -3.16501400 |
| H | 4.86736500 | 0.20668900 | -4.68812100 |
| C | 3.22281400 | 0.63249400 | -3.32173400 |
| H | 3.01795500 | 1.63484800 | -3.71882300 |
| H | 3.08351000 | 0.70579800 | -2.23975900 |

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| C | 2.20502700 | -0.35631100 | -3.88095700 |
| H | 2.46792600 | -1.36521300 | -3.53299800 |
| H | 2.27297700 | -0.39205400 | -4.97618600 |
| C | 0.77133300 | -0.05295300 | -3.45017300 |
| H | 0.45713300 | 0.91937900 | -3.85017000 |
| H | 0.74968100 | 0.06012000 | -2.36121300 |
| C | -0.22521500 | -1.13545400 | -3.86683700 |
| H | 0.25712200 | -2.11920700 | -3.78159600 |
| H | -0.48282600 | -1.02402700 | -4.92763000 |
| C | -1.49420200 | -1.15991800 | -3.01864900 |
| H | -1.95925300 | -0.16709800 | -2.99241700 |
| H | -1.21113500 | -1.37497800 | -1.98065500 |
| C | -2.50782100 | -2.20139200 | -3.48645400 |
| H | -1.97620700 | -3.11859300 | -3.77459100 |
| H | -3.00568600 | -1.84652100 | -4.39799800 |
| C | -3.55048300 | -2.55723500 | -2.43087600 |
| H | -4.02583800 | -1.64803100 | -2.04257700 |
| H | -3.03895400 | -3.00946100 | -1.57002100 |
| C | -4.61457400 | -3.52267600 | -2.94599900 |
| H | -4.12388400 | -4.36873400 | -3.44661900 |
| H | -5.21316300 | -3.02293600 | -3.71896900 |
| C | -5.53588400 | -4.04809000 | -1.85081100 |
| H | -5.99098600 | -3.20810900 | -1.31865700 |
| H | -4.93238900 | -4.58502500 | -1.10519500 |
| C | -6.62569700 | -4.98232400 | -2.36587600 |
| H | -6.17306100 | -5.86286500 | -2.83878300 |

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|---|-------------|-------------|-------------|
| H | -7.21620700 | -4.47543000 | -3.13836200 |
| C | -7.57645300 | -5.43829000 | -1.27126300 |
| H | -8.25123500 | -6.21651100 | -1.65773800 |
| H | -6.99858100 | -5.88932400 | -0.44987700 |
| O | -8.31590500 | -4.32065200 | -0.82036700 |
| H | -8.53461300 | -4.40527700 | 0.12390700 |
| C | -9.09290500 | 4.62270000 | 0.92127000 |
| H | -9.95814600 | 4.07391900 | 0.52856700 |
| C | -8.58056800 | 5.51698800 | -0.20678700 |
| H | -7.72096800 | 6.09184400 | 0.17162100 |
| C | -8.08608800 | 4.66838400 | -1.37195800 |
| H | -8.93467900 | 4.06760800 | -1.74153700 |
| C | -7.48632900 | 2.90467100 | 0.09026300 |
| H | -8.27276700 | 2.25261100 | -0.32048800 |
| C | -8.02223300 | 3.61590500 | 1.33004000 |
| H | -8.45022200 | 2.84584500 | 1.98897400 |
| C | -7.51443200 | 5.49734000 | -2.49951300 |
| H | -6.65233700 | 6.06491500 | -2.13917200 |
| H | -8.27005900 | 6.19615300 | -2.86181000 |
| H | -7.18789100 | 4.85476200 | -3.32020600 |
| C | -5.75489800 | 1.33112100 | -0.46368900 |
| H | -5.73050600 | 1.86384900 | -1.41961000 |
| C | -4.35995600 | 1.12282500 | 0.03662200 |
| H | -4.25877800 | 0.61488600 | 0.99159900 |
| C | -3.26420400 | 1.55901700 | -0.59199700 |
| H | -3.35407700 | 2.07947400 | -1.54503200 |

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| C | -1.93569000 | 1.40549700 | -0.03414000 |
| H | -1.86960200 | 0.86752100 | 0.90869300 |
| C | -0.80850700 | 1.90081800 | -0.57786400 |
| H | -0.85984300 | 2.45025100 | -1.51735700 |
| C | 0.48758200 | 1.73947000 | 0.03610700 |
| H | 0.51405700 | 1.14795300 | 0.94931600 |
| C | 1.63863800 | 2.23966100 | -0.45582000 |
| H | 1.62010800 | 2.82854500 | -1.37215000 |
| C | 2.92459400 | 2.00889100 | 0.15378700 |
| H | 2.94820400 | 1.37410200 | 1.03891700 |
| C | 4.08886700 | 2.48265000 | -0.33549700 |
| H | 4.07296900 | 3.09921400 | -1.23365100 |
| C | 5.37579500 | 2.21557600 | 0.25385300 |
| H | 5.39170900 | 1.59002900 | 1.14574500 |
| C | 6.54472600 | 2.67648100 | -0.23599600 |
| H | 6.53818500 | 3.28686300 | -1.13852500 |
| C | 7.82436800 | 2.41193400 | 0.37462400 |
| H | 7.81451700 | 1.84140100 | 1.30145600 |
| C | 9.01224600 | 2.79937400 | -0.12489200 |
| H | 9.04662200 | 3.34933000 | -1.06466800 |
| C | -6.57313000 | 0.04440600 | -0.61141400 |
| H | -7.58224700 | 0.31498300 | -0.92748000 |
| H | -6.14200300 | -0.57943800 | -1.40007900 |
| C | 10.27406200 | 2.47574700 | 0.51131100 |
| H | 10.20042500 | 2.00980500 | 1.49171100 |
| C | 11.48068100 | 2.64980700 | -0.03837900 |

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| H | 11.55469500 | 3.10115000 | -1.02918800 |
| C | 12.77450400 | 2.21405900 | 0.58781200 |
| H | 12.58160200 | 1.90043600 | 1.62022400 |
| C | 13.36604300 | 0.99888700 | -0.15299400 |
| H | 13.69577400 | 1.34939100 | -1.14527100 |
| C | 12.37648400 | -0.15389300 | -0.40420300 |
| H | 11.55202700 | 0.28173000 | -0.97681300 |
| C | 11.73619100 | -0.69344200 | 0.87963800 |
| H | 11.41332300 | 0.13316300 | 1.50668000 |
| C | 9.37616100 | -1.10154800 | 1.04098000 |
| C | 8.22735500 | -1.91185000 | 0.49516400 |
| H | 8.46281200 | -2.23671400 | -0.52008100 |
| H | 8.13934100 | -2.80870600 | 1.11958000 |
| C | 6.90154300 | -1.14776800 | 0.53558800 |
| H | 6.98169100 | -0.25302500 | -0.09800000 |
| C | 5.75618600 | -2.01808200 | 0.03924200 |
| H | 5.97014900 | -2.32586900 | -0.99003600 |
| H | 5.70917100 | -2.92448700 | 0.65481900 |
| C | 4.38910400 | -1.33979600 | 0.07170100 |
| H | 4.43645500 | -0.39819600 | -0.49283400 |
| C | 3.31919000 | -2.23392400 | -0.54559800 |
| H | 3.40485700 | -3.23843300 | -0.11327400 |
| H | 3.54839400 | -2.33003300 | -1.61141300 |
| C | 1.88883500 | -1.70533300 | -0.36281400 |
| H | 1.90440600 | -0.62684000 | -0.18305600 |
| H | 1.32158500 | -1.85194600 | -1.28625700 |

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| C | 1.09549100 | -2.39038000 | 0.74841000 |
| H | 0.92966700 | -3.43737100 | 0.45897500 |
| C | -0.28498500 | -1.70920800 | 0.94925800 |
| H | -0.55092800 | -1.14622800 | 0.04863000 |
| C | -1.40500900 | -2.69388000 | 1.26864900 |
| H | -1.16406300 | -3.22457900 | 2.19788400 |
| H | -1.45968200 | -3.43927700 | 0.46656600 |
| C | -2.76573200 | -2.01335800 | 1.39291700 |
| H | -2.98584300 | -1.48903800 | 0.45389400 |
| C | -3.88405300 | -3.01501300 | 1.65479800 |
| H | -3.66313300 | -3.58458000 | 2.56289200 |
| H | -3.93258400 | -3.71243300 | 0.81439100 |
| C | -5.25590500 | -2.36389900 | 1.83160500 |
| C | -6.38592300 | -3.38101200 | 1.89597400 |
| H | -6.27567600 | -4.01758300 | 2.77640600 |
| H | -6.35041500 | -4.00441600 | 1.00012900 |
| C | -7.73649700 | -2.69020600 | 1.94495500 |
| H | -7.82953700 | -2.16471700 | 2.90349600 |
| C | -7.87302100 | -1.66292500 | 0.79122100 |
| H | -8.00195500 | -2.24432700 | -0.12988900 |
| C | -6.62618500 | -0.77021200 | 0.67577700 |
| H | -6.60413700 | -0.09457300 | 1.53612800 |
| C | -9.10558400 | -0.81805500 | 0.98865200 |
| C | 12.56652300 | -1.65864300 | 1.70054900 |
| H | 12.03064500 | -1.93084800 | 2.61276600 |
| H | 13.50940600 | -1.17897700 | 1.96675900 |

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| H | 12.77861700 | -2.57187200 | 1.14048900 |
| C | 13.00596600 | -1.25487900 | -1.25571300 |
| H | 13.88673700 | -1.69185200 | -0.77551800 |
| H | 13.31248900 | -0.86193900 | -2.22940600 |
| H | 12.29303600 | -2.06416800 | -1.42867500 |
| C | 13.79335200 | 3.35657300 | 0.62082700 |
| H | 13.99372900 | 3.72443800 | -0.39161600 |
| H | 14.73481200 | 3.01463900 | 1.05292400 |
| H | 13.41442900 | 4.19393400 | 1.21111500 |
| O | -6.99053300 | 4.32612100 | 1.98364200 |
| H | -6.18718700 | 3.79771700 | 1.87282600 |
| O | -9.61610100 | 6.36286900 | -0.65097700 |
| H | -10.05874100 | 6.64233100 | 0.16684300 |
| O | -7.05276600 | 3.80905700 | -0.90159600 |
| O | -6.38048400 | 2.17765800 | 0.51804600 |
| O | -5.32315800 | -1.59153500 | 2.99459100 |
| H | -4.46820600 | -1.12850200 | 3.07095100 |
| O | -5.44985100 | -1.56848400 | 0.66682400 |
| O | -9.16896500 | 0.38743700 | 1.02037900 |
| O | -10.22505200 | -1.57006000 | 1.15746600 |
| H | -10.95809500 | -0.94873300 | 1.29594100 |
| O | -2.76904800 | -1.05795900 | 2.45832300 |
| H | -1.85537700 | -0.73448000 | 2.57131400 |
| O | -0.15655100 | -0.74904200 | 1.99883300 |
| H | 0.57808800 | -1.11379500 | 2.53636300 |
| O | 1.75318300 | -2.38916300 | 2.00663600 |

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| H | 2.61939700 | -1.93536100 | 1.91855800 |
| O | 3.99353400 | -1.03927400 | 1.41309800 |
| H | 4.79659300 | -0.80481800 | 1.91353200 |
| O | 6.59253900 | -0.75360300 | 1.87001500 |
| H | 7.39791400 | -0.35291200 | 2.24354700 |
| O | 9.24876500 | -0.28446600 | 1.93932800 |
| O | 10.52648300 | -1.39679000 | 0.45367100 |
| O | 14.49665100 | 0.58036000 | 0.60560200 |
| H | 15.05649000 | 0.02930400 | 0.04829800 |
| O | -8.71684700 | -3.72298900 | 1.86082200 |
| H | -9.58599400 | -3.29708300 | 1.84931900 |
| N | -9.56186100 | 5.49177900 | 1.99719800 |
| H | -8.74795300 | 5.81722400 | 2.51439000 |
| H | -10.13697900 | 4.97216900 | 2.65264400 |

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| C | 13.42888900 | 1.29187500 | 2.64365800 |
| H | 13.90765600 | 0.43509200 | 3.12925300 |
| H | 14.03654100 | 2.17615000 | 2.85649900 |
| H | 13.44535000 | 1.11886000 | 1.56336200 |
| C | 11.99476000 | 1.46584900 | 3.13352000 |
| H | 11.54819100 | 2.34241000 | 2.64858000 |
| H | 11.98491200 | 1.67903300 | 4.20943700 |

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| C | 11.12851400 | 0.24093900 | 2.85339800 |
| H | 11.52901400 | -0.62102400 | 3.40316200 |
| H | 11.21387500 | -0.01780300 | 1.79027000 |
| C | 9.65702400 | 0.43344000 | 3.20676200 |
| H | 9.25479100 | 1.27567800 | 2.62659300 |
| H | 9.56541600 | 0.72489900 | 4.26116100 |
| C | 8.80988500 | -0.80703700 | 2.94006100 |
| H | 9.17874700 | -1.64070500 | 3.55205000 |
| H | 8.93923900 | -1.10827800 | 1.89424000 |
| C | 7.32148300 | -0.59867900 | 3.19771400 |
| H | 6.98089600 | 0.26582700 | 2.61417200 |
| H | 7.15701700 | -0.34350900 | 4.25271200 |
| C | 6.47703000 | -1.81176100 | 2.82038800 |
| H | 6.80078600 | -2.68543500 | 3.40072000 |
| H | 6.66963500 | -2.05615200 | 1.76861600 |
| C | 4.97829000 | -1.59849200 | 3.01426000 |
| H | 4.67685400 | -0.66562700 | 2.51891900 |
| H | 4.75972700 | -1.45605300 | 4.08049300 |
| C | 4.13704600 | -2.74111200 | 2.45503400 |
| H | 4.42853800 | -3.68593800 | 2.93145700 |
| H | 4.35904300 | -2.84419400 | 1.38708400 |
| C | 2.63622200 | -2.52982400 | 2.62714200 |
| H | 2.37448200 | -1.53635200 | 2.23811700 |
| H | 2.38604200 | -2.52115500 | 3.69756900 |
| C | 1.80216500 | -3.58155700 | 1.90071400 |
| H | 2.12690900 | -4.58566500 | 2.20046100 |

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| H | 1.97750600 | -3.49865100 | 0.82402300 |
| C | 0.31025400 | -3.46906000 | 2.17864000 |
| H | -0.24601700 | -4.14090800 | 1.52420300 |
| H | 0.09353100 | -3.73783700 | 3.22194100 |
| O | -0.20818500 | -2.16900300 | 1.90350600 |
| H | 0.18479600 | -1.52874800 | 2.50590200 |
| C | -10.98699700 | 3.34238300 | 1.79677800 |
| H | -11.85535200 | 2.88017200 | 1.31054300 |
| C | -10.66738700 | 4.62044700 | 1.02308500 |
| H | -9.80804600 | 5.11076900 | 1.50640900 |
| C | -10.25913700 | 4.28616700 | -0.40672200 |
| H | -11.10624700 | 3.77105800 | -0.89145200 |
| C | -9.38713100 | 2.19189000 | 0.26977600 |
| H | -10.17794400 | 1.65384100 | -0.27516600 |
| C | -9.81494000 | 2.36968700 | 1.72400400 |
| H | -10.11344700 | 1.38006000 | 2.10001600 |
| C | -9.87639700 | 5.50997700 | -1.20750700 |
| H | -9.01447100 | 5.99811600 | -0.74494200 |
| H | -10.71121700 | 6.21228300 | -1.22621300 |
| H | -9.60987000 | 5.23164100 | -2.22953700 |
| C | -7.65345300 | 1.06924200 | -0.96052000 |
| H | -7.77220300 | 1.89739600 | -1.66665700 |
| C | -6.19872800 | 0.82499200 | -0.70955500 |
| H | -5.95236800 | 0.01028600 | -0.03393700 |
| C | -5.21762800 | 1.56249900 | -1.23916700 |
| H | -5.45828600 | 2.38630700 | -1.91043500 |

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| C | -3.82067700 | 1.33012500 | -0.93282500 |
| H | -3.60819800 | 0.48861200 | -0.27861000 |
| C | -2.78798000 | 2.07611500 | -1.36894700 |
| H | -2.97046500 | 2.93003200 | -2.02062000 |
| C | -1.42703900 | 1.78643000 | -0.98517400 |
| H | -1.29745000 | 0.90607900 | -0.35970900 |
| C | -0.33419400 | 2.48724400 | -1.34695400 |
| H | -0.43268200 | 3.36861600 | -1.97966000 |
| C | 0.99109000 | 2.11343700 | -0.91819400 |
| H | 1.07042300 | 1.20775000 | -0.31594800 |
| C | 2.12183100 | 2.78600000 | -1.21491400 |
| H | 2.06360300 | 3.68442800 | -1.82823200 |
| C | 3.42541100 | 2.38983700 | -0.74474200 |
| H | 3.47329300 | 1.49721400 | -0.12076000 |
| C | 4.57247100 | 3.04079200 | -1.02547600 |
| H | 4.54133800 | 3.92138800 | -1.66608500 |
| C | 5.86114700 | 2.63415400 | -0.52044500 |
| H | 5.87085400 | 1.79269900 | 0.16975800 |
| C | 7.03599300 | 3.19936300 | -0.85355600 |
| H | 7.05177900 | 4.02726300 | -1.56153500 |
| C | -8.41731200 | -0.15695900 | -1.47584200 |
| H | -9.45980600 | 0.13108600 | -1.62941200 |
| H | -8.01463100 | -0.45692500 | -2.44794400 |
| C | 8.30894600 | 2.72074800 | -0.35122200 |
| H | 8.25475000 | 1.95571200 | 0.42009200 |
| C | 9.50804800 | 3.09754400 | -0.80773300 |

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| H | 9.56743800 | 3.85030200 | -1.59559000 |
| C | 10.81283200 | 2.51626100 | -0.34432000 |
| H | 10.62413300 | 1.87816400 | 0.52547100 |
| C | 11.44637300 | 1.62638300 | -1.43121700 |
| H | 11.78228000 | 2.29062200 | -2.24433600 |
| C | 10.49530200 | 0.59786600 | -2.07128700 |
| H | 9.65084400 | 1.17562100 | -2.45886700 |
| C | 9.88933200 | -0.37894300 | -1.05655500 |
| H | 9.56228700 | 0.16390500 | -0.17299600 |
| C | 7.52996600 | -0.83610900 | -1.05705800 |
| C | 6.40216500 | -1.49343700 | -1.81043400 |
| H | 6.62720700 | -1.48771800 | -2.87874400 |
| H | 6.36877400 | -2.54043200 | -1.48597400 |
| C | 5.04546600 | -0.84262900 | -1.52941000 |
| H | 5.07391100 | 0.20591200 | -1.85831500 |
| C | 3.92652900 | -1.57131400 | -2.25826600 |
| H | 4.12502900 | -1.52529000 | -3.33450900 |
| H | 3.93454900 | -2.62777800 | -1.96416400 |
| C | 2.53212400 | -1.01030500 | -1.98709500 |
| H | 2.53892600 | 0.07616600 | -2.15312100 |
| C | 1.49485800 | -1.64018000 | -2.91076400 |
| H | 1.61521400 | -2.72876200 | -2.87856100 |
| H | 1.72679500 | -1.32034600 | -3.93124100 |
| C | 0.04980300 | -1.26812000 | -2.54382000 |
| H | 0.04234700 | -0.40507200 | -1.87443800 |
| H | -0.50894200 | -0.96633300 | -3.43480100 |

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| C | -0.71465500 | -2.41418300 | -1.87908500 |
| H | -0.93185800 | -3.17738900 | -2.63886400 |
| C | -2.04839800 | -1.93156200 | -1.29123200 |
| H | -2.49298900 | -1.19708500 | -1.97434500 |
| C | -3.05255600 | -3.05896700 | -1.06782000 |
| H | -2.64475900 | -3.76776900 | -0.33771200 |
| H | -3.19634100 | -3.60045500 | -2.00975800 |
| C | -4.40418300 | -2.53332900 | -0.59261600 |
| H | -4.76209800 | -1.78336700 | -1.31121500 |
| C | -5.45570800 | -3.62962700 | -0.49252500 |
| H | -5.11608400 | -4.40650300 | 0.19939800 |
| H | -5.58488700 | -4.08189400 | -1.48000700 |
| C | -6.81234300 | -3.12035200 | -0.00209800 |
| C | -7.90702000 | -4.17155800 | -0.11658600 |
| H | -7.70209200 | -5.00585300 | 0.55748500 |
| H | -7.93232600 | -4.55289700 | -1.14127200 |
| C | -9.27692900 | -3.59831900 | 0.20468000 |
| H | -9.30289100 | -3.32068400 | 1.26868900 |
| C | -9.52902600 | -2.31343100 | -0.63159000 |
| H | -9.67162000 | -2.63469500 | -1.67004900 |
| C | -8.33693100 | -1.35075500 | -0.53014900 |
| H | -8.27776900 | -0.99212100 | 0.50171600 |
| C | -10.79571400 | -1.64939000 | -0.15798400 |
| C | 10.75389000 | -1.55515900 | -0.64940300 |
| H | 10.25636100 | -2.13753500 | 0.12945400 |
| H | 11.70438200 | -1.18541600 | -0.26387500 |

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| H | 10.94584900 | -2.21228400 | -1.50016700 |
| C | 11.15719000 | -0.11542300 | -3.24920700 |
| H | 12.05979800 | -0.65440900 | -2.94562900 |
| H | 11.43741600 | 0.60132600 | -4.02631300 |
| H | 10.47518800 | -0.84404000 | -3.69329600 |
| C | 11.79316600 | 3.61530700 | 0.07469600 |
| H | 11.98996500 | 4.29574600 | -0.76119400 |
| H | 12.74182500 | 3.18414100 | 0.39673100 |
| H | 11.37852900 | 4.20641800 | 0.89454500 |
| O | -8.75922100 | 2.90785400 | 2.49349300 |
| H | -7.94379300 | 2.52933100 | 2.13488100 |
| O | -11.79941100 | 5.45937700 | 1.00135900 |
| H | -12.16094300 | 5.39009600 | 1.89988800 |
| O | -9.12684200 | 3.42390700 | -0.36737300 |
| O | -8.19931400 | 1.46992200 | 0.30903200 |
| O | -6.76358400 | -2.70620800 | 1.33202900 |
| H | -5.92005500 | -2.22978900 | 1.44268200 |
| O | -7.14128100 | -2.03782800 | -0.86870700 |
| O | -10.89364400 | -0.57600600 | 0.38757100 |
| O | -11.89105800 | -2.42223200 | -0.36986200 |
| H | -12.64577000 | -1.93639100 | 0.00116200 |
| O | -4.28963400 | -1.91772700 | 0.69303200 |
| H | -3.41160200 | -1.49117200 | 0.72442900 |
| O | -1.81791200 | -1.22373400 | -0.07346000 |
| H | -1.18539000 | -1.72571900 | 0.48578200 |
| O | 0.03872600 | -3.05404200 | -0.86491500 |

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| H | 0.70217200 | -2.42001800 | -0.53513300 |
| O | 2.13474200 | -1.25932300 | -0.63514700 |
| H | 2.91311900 | -1.10388200 | -0.07409600 |
| O | 4.74874500 | -0.88267400 | -0.13506200 |
| H | 5.53694400 | -0.55766700 | 0.33443600 |
| O | 7.38027600 | -0.30798800 | 0.03387700 |
| O | 8.68893400 | -0.92756700 | -1.69032000 |
| O | 12.57872500 | 1.00363600 | -0.82778200 |
| H | 13.17091700 | 0.69093300 | -1.51997700 |
| O | -10.20864200 | -4.61774700 | -0.08489500 |
| H | -11.09743400 | -4.24958800 | -0.00279000 |
| N | -11.38174300 | 3.73001600 | 3.14848700 |
| H | -10.53552900 | 3.93560500 | 3.67530800 |
| H | -11.84122600 | 2.95868600 | 3.62212700 |

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|---|-------------|-------------|-------------|
| C | 9.20164400 | 1.32075800 | -2.53807500 |
| H | 9.31053900 | 1.64732600 | -3.57703400 |
| H | 10.04061500 | 0.65837300 | -2.30965400 |
| H | 9.28927500 | 2.20515800 | -1.89912800 |
| C | 7.86305500 | 0.62340500 | -2.31980400 |
| H | 7.75899900 | 0.36828900 | -1.25847800 |
| H | 7.84724600 | -0.32403600 | -2.87430500 |

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| C | 6.67200800 | 1.47528900 | -2.75225400 |
| H | 6.81010600 | 1.78183600 | -3.79753000 |
| H | 6.65826700 | 2.40035400 | -2.16163600 |
| C | 5.33056200 | 0.76405100 | -2.60702000 |
| H | 5.17988700 | 0.50097800 | -1.55487200 |
| H | 5.36028600 | -0.18157500 | -3.16653400 |
| C | 4.14007100 | 1.59185200 | -3.08378600 |
| H | 4.30163600 | 1.89907500 | -4.12544600 |
| H | 4.08888400 | 2.51836500 | -2.49728300 |
| C | 2.81107100 | 0.85003900 | -2.97220800 |
| H | 2.64402700 | 0.56440500 | -1.92822100 |
| H | 2.87168200 | -0.08511600 | -3.54598000 |
| C | 1.61131000 | 1.65569300 | -3.46019200 |
| H | 1.76982200 | 1.95249300 | -4.50545600 |
| H | 1.54467700 | 2.58970000 | -2.88650300 |
| C | 0.29298700 | 0.89568500 | -3.33988200 |
| H | 0.11276900 | 0.65130000 | -2.28699600 |
| H | 0.38008600 | -0.06265800 | -3.87068900 |
| C | -0.90159300 | 1.66401700 | -3.89498900 |
| H | -0.71517400 | 1.91034300 | -4.94877100 |
| H | -0.99330200 | 2.62561100 | -3.37243000 |
| C | -2.22040100 | 0.90349200 | -3.78227500 |
| H | -2.44883600 | 0.74810000 | -2.72023800 |
| H | -2.10198300 | -0.09568300 | -4.22399700 |
| C | -3.37720800 | 1.62057600 | -4.47408300 |
| H | -3.13150600 | 1.75854200 | -5.53472500 |

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|---|--------------|-------------|-------------|
| H | -3.50690300 | 2.62134700 | -4.04551800 |
| C | -4.70645300 | 0.88492900 | -4.37663200 |
| H | -5.45717200 | 1.38770200 | -4.99257200 |
| H | -4.59783200 | -0.13886800 | -4.76748600 |
| O | -5.23754300 | 0.87399200 | -3.06356300 |
| H | -4.66832700 | 0.35279400 | -2.48406500 |
| C | -10.18474200 | 2.90538300 | 2.30165900 |
| H | -10.98843300 | 2.53928100 | 1.65044800 |
| C | -9.72508900 | 4.24764600 | 1.73475700 |
| H | -8.92935600 | 4.64255300 | 2.38543700 |
| C | -9.12901800 | 4.05941900 | 0.34477400 |
| H | -9.91339100 | 3.64053700 | -0.30872500 |
| C | -8.41791300 | 1.86658200 | 0.88283100 |
| H | -9.13961200 | 1.42706900 | 0.17678600 |
| C | -9.04106300 | 1.89697100 | 2.27565600 |
| H | -9.41645900 | 0.88496600 | 2.48758200 |
| C | -8.60247000 | 5.34743200 | -0.24630900 |
| H | -7.80152000 | 5.74158400 | 0.38481800 |
| H | -9.40601200 | 6.08384400 | -0.29737600 |
| H | -8.20110800 | 5.17298300 | -1.24697700 |
| C | -6.58100500 | 0.79433600 | -0.23434700 |
| H | -6.57108800 | 1.68401100 | -0.86914100 |
| C | -5.18251100 | 0.45601200 | 0.18456900 |
| H | -5.06975600 | -0.39374800 | 0.85284300 |
| C | -4.10161600 | 1.15688900 | -0.18000900 |
| H | -4.21300500 | 2.00761900 | -0.85042300 |

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| C | -2.76845500 | 0.84226600 | 0.29396900 |
| H | -2.68112700 | -0.00668400 | 0.96750400 |
| C | -1.65609600 | 1.53268500 | -0.02305300 |
| H | -1.72667100 | 2.38778600 | -0.69522100 |
| C | -0.35526800 | 1.19499300 | 0.50319700 |
| H | -0.31854200 | 0.32958500 | 1.16182000 |
| C | 0.78624800 | 1.85446300 | 0.22126300 |
| H | 0.75948700 | 2.71697900 | -0.44396500 |
| C | 2.06914400 | 1.47068800 | 0.75503300 |
| H | 2.09592100 | 0.59063100 | 1.39778500 |
| C | 3.22472000 | 2.11405200 | 0.49132100 |
| H | 3.20849300 | 2.98540000 | -0.16235900 |
| C | 4.50121900 | 1.72359500 | 1.03250400 |
| H | 4.51514700 | 0.85978400 | 1.69742700 |
| C | 5.66250800 | 2.35375600 | 0.76276800 |
| H | 5.65792300 | 3.20630200 | 0.08462000 |
| C | 6.92886500 | 1.96651600 | 1.33233300 |
| H | 6.91264700 | 1.14784900 | 2.04972700 |
| C | 8.11442600 | 2.53049600 | 1.03567600 |
| H | 8.16005900 | 3.33609900 | 0.30357500 |
| C | -7.31720900 | -0.33543000 | -0.96212400 |
| H | -8.32415400 | 0.01826600 | -1.19424700 |
| H | -6.82152900 | -0.53188600 | -1.91483400 |
| C | 9.35946600 | 2.08354300 | 1.62819400 |
| H | 9.26169700 | 1.34363900 | 2.41973100 |
| C | 10.58087300 | 2.46067600 | 1.23631900 |

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| H | 10.68126500 | 3.18758700 | 0.42860600 |
| C | 11.86163400 | 1.90100000 | 1.78651900 |
| H | 11.63565200 | 1.31174400 | 2.68273000 |
| C | 12.52356200 | 0.94929600 | 0.77029500 |
| H | 12.86732000 | 1.56604400 | -0.07693400 |
| C | 11.58486200 | -0.11738000 | 0.18013200 |
| H | 10.75097000 | 0.43559200 | -0.25877200 |
| C | 10.94955300 | -1.02775800 | 1.23674300 |
| H | 10.56816000 | -0.42912000 | 2.06017200 |
| C | 8.60376100 | -1.55333700 | 1.16288100 |
| C | 7.52784300 | -2.23650000 | 0.35784500 |
| H | 7.81479800 | -2.23910000 | -0.69547000 |
| H | 7.47793800 | -3.27867300 | 0.69389200 |
| C | 6.15887700 | -1.58313900 | 0.54868300 |
| H | 6.21863000 | -0.53541700 | 0.22547100 |
| C | 5.09308100 | -2.29618700 | -0.26793100 |
| H | 5.37666600 | -2.24707900 | -1.32438700 |
| H | 5.06301400 | -3.35290500 | 0.02305500 |
| C | 3.69446800 | -1.70813000 | -0.10973400 |
| H | 3.73211500 | -0.62853500 | -0.30113500 |
| C | 2.71332000 | -2.34237500 | -1.08649300 |
| H | 2.79437500 | -3.43366500 | -1.01048800 |
| H | 3.03681800 | -2.07122800 | -2.09529100 |
| C | 1.25718400 | -1.90527100 | -0.86663400 |
| H | 1.22249300 | -0.96455000 | -0.31103800 |
| H | 0.77977800 | -1.70285000 | -1.82984300 |

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| C | 0.39737500 | -2.94257900 | -0.15052800 |
| H | 0.31101900 | -3.82670500 | -0.79755700 |
| C | -1.02654000 | -2.39884500 | 0.13186600 |
| H | -1.25723600 | -1.58669700 | -0.56751300 |
| C | -2.10563500 | -3.47073300 | 0.02837700 |
| H | -1.88731000 | -4.27125100 | 0.74557000 |
| H | -2.07264600 | -3.90874200 | -0.97592600 |
| C | -3.50696300 | -2.92213400 | 0.28041300 |
| H | -3.69577500 | -2.09256100 | -0.41514800 |
| C | -4.58111700 | -3.98050100 | 0.06356400 |
| H | -4.37758000 | -4.84799500 | 0.69898900 |
| H | -4.54456100 | -4.30507600 | -0.98045000 |
| C | -5.99504800 | -3.49158000 | 0.38018700 |
| C | -7.06542200 | -4.48516300 | -0.04733300 |
| H | -6.97433500 | -5.41081400 | 0.52486100 |
| H | -6.93550600 | -4.71879800 | -1.10783600 |
| C | -8.46135400 | -3.91789200 | 0.14407800 |
| H | -8.64328800 | -3.78747100 | 1.22071100 |
| C | -8.56977700 | -2.52601300 | -0.53521500 |
| H | -8.57375800 | -2.70317400 | -1.61727200 |
| C | -7.39083400 | -1.62034700 | -0.15030600 |
| H | -7.48111100 | -1.37810500 | 0.91260400 |
| C | -9.87734800 | -1.88033300 | -0.15369800 |
| C | 11.81289800 | -2.14860800 | 1.77834400 |
| H | 11.27202200 | -2.69854700 | 2.55197300 |
| H | 12.72072300 | -1.72271000 | 2.20752200 |

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| H | 12.08882900 | -2.84974800 | 0.98775700 |
| C | 12.26353700 | -0.90236200 | -0.94070100 |
| H | 13.16296700 | -1.42037700 | -0.59392500 |
| H | 12.55310500 | -0.23476300 | -1.75760000 |
| H | 11.58728000 | -1.65772600 | -1.34747800 |
| C | 12.83679100 | 3.01339900 | 2.18022600 |
| H | 13.06871200 | 3.64653700 | 1.31655700 |
| H | 13.76987100 | 2.58785200 | 2.55171700 |
| H | 12.40333200 | 3.65055300 | 2.95444700 |
| O | -8.09006300 | 2.29777700 | 3.24122400 |
| H | -7.24197300 | 1.93229300 | 2.95183800 |
| O | -10.81990200 | 5.13189500 | 1.65846800 |
| H | -11.30575400 | 4.97644400 | 2.48464500 |
| O | -8.03818100 | 3.14962100 | 0.43677700 |
| O | -7.26705400 | 1.09535900 | 0.99560100 |
| O | -6.16834200 | -3.25458100 | 1.74730800 |
| H | -5.35727800 | -2.81194900 | 2.05638800 |
| O | -6.16276800 | -2.30019600 | -0.38101700 |
| O | -10.02928800 | -0.87245800 | 0.49449400 |
| O | -10.94775700 | -2.58992900 | -0.59354100 |
| H | -11.73658900 | -2.12548300 | -0.26919900 |
| O | -3.62946800 | -2.43149700 | 1.61739300 |
| H | -2.75283300 | -2.10245400 | 1.88995400 |
| O | -1.02618000 | -1.82144200 | 1.43869700 |
| H | -0.32130300 | -2.32802700 | 1.89528500 |
| O | 0.93471600 | -3.36440500 | 1.09456400 |

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|---|--------------|-------------|-------------|
| H | 1.79514600 | -2.91845300 | 1.24840200 |
| O | 3.19479400 | -1.90829600 | 1.21506700 |
| H | 3.94215300 | -1.80085400 | 1.83050800 |
| O | 5.76088100 | -1.62758800 | 1.91656200 |
| H | 6.50965200 | -1.29101900 | 2.43922600 |
| O | 8.39182800 | -1.00498300 | 2.23278900 |
| O | 9.79222300 | -1.63729800 | 0.58287700 |
| O | 13.64728500 | 0.37509700 | 1.43006000 |
| H | 14.23807100 | 0.00287000 | 0.76651600 |
| O | -9.35101500 | -4.85813100 | -0.41843800 |
| H | -10.23833100 | -4.47741600 | -0.40864500 |
| N | -10.75445700 | 3.15417100 | 3.62348200 |
| H | -9.98451600 | 3.26162300 | 4.28044000 |
| H | -11.29534600 | 2.35388700 | 3.93565800 |

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| C | -0.14024600 | -0.60891000 | -2.79545000 |
| H | 0.14960000 | 0.32365000 | -3.28902700 |
| H | 0.60393800 | -1.36621800 | -3.05893700 |
| H | -0.09232600 | -0.44156900 | -1.71578000 |
| C | -1.54168900 | -1.04201900 | -3.20908400 |
| H | -1.81050700 | -1.96209700 | -2.67526500 |
| H | -1.55458300 | -1.29456600 | -4.27619300 |

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| C | -2.59261600 | 0.02962000 | -2.93487600 |
| H | -2.32756300 | 0.94641500 | -3.47720500 |
| H | -2.56550200 | 0.29653900 | -1.86974900 |
| C | -4.00885100 | -0.39570100 | -3.30914800 |
| H | -4.25794900 | -1.31926000 | -2.77252200 |
| H | -4.04894300 | -0.64148800 | -4.37805800 |
| C | -5.05401400 | 0.66952000 | -2.99089200 |
| H | -4.85034500 | 1.57370800 | -3.57863500 |
| H | -4.94482000 | 0.97450800 | -1.94037700 |
| C | -6.49027000 | 0.21244200 | -3.22890500 |
| H | -6.68272100 | -0.69268200 | -2.64165600 |
| H | -6.61756400 | -0.07142600 | -4.28148300 |
| C | -7.52151800 | 1.27301600 | -2.85456200 |
| H | -7.44149300 | 2.12231000 | -3.54558000 |
| H | -7.28194300 | 1.66943200 | -1.85957200 |
| C | -8.95471300 | 0.75026600 | -2.84251700 |
| H | -9.03596500 | -0.01936800 | -2.06496800 |
| H | -9.17479400 | 0.24836300 | -3.79387500 |
| C | -9.98993600 | 1.84539200 | -2.60152200 |
| H | -9.95693600 | 2.56074700 | -3.43338900 |
| H | -9.71340700 | 2.42058400 | -1.70710700 |
| C | -11.41596200 | 1.32429500 | -2.44282500 |
| H | -11.47407000 | 0.69699500 | -1.54393900 |
| H | -11.66100400 | 0.66377400 | -3.28468600 |
| C | -12.45317500 | 2.44433800 | -2.36909500 |
| H | -12.47245600 | 2.97010500 | -3.33165200 |

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| H | -12.15817200 | 3.18283500 | -1.61411300 |
| C | -13.86245900 | 1.96486600 | -2.03642200 |
| H | -14.58384800 | 2.75836900 | -2.25303700 |
| H | -14.12086800 | 1.11135900 | -2.68529900 |
| O | -14.04662000 | 1.64238500 | -0.67307000 |
| H | -13.35749100 | 1.03112000 | -0.37164800 |
| C | 11.21311100 | 3.65894400 | -1.01941900 |
| H | 12.07157300 | 3.14832300 | -0.56529400 |
| C | 10.79647000 | 4.77434900 | -0.06164100 |
| H | 9.94519400 | 5.31166000 | -0.50774300 |
| C | 10.32475100 | 4.18688700 | 1.26326300 |
| H | 11.16636400 | 3.62733200 | 1.70639500 |
| C | 9.58610300 | 2.21061200 | 0.18992400 |
| H | 10.37240000 | 1.61631900 | 0.68046400 |
| C | 10.08048700 | 2.65134200 | -1.18461300 |
| H | 10.43965000 | 1.75198100 | -1.70625500 |
| C | 9.84198800 | 5.24216100 | 2.23220900 |
| H | 8.98549000 | 5.76999000 | 1.80453000 |
| H | 10.64082600 | 5.96105400 | 2.42095700 |
| H | 9.53200800 | 4.78468100 | 3.17437600 |
| C | 7.85533900 | 0.82061900 | 1.10925500 |
| H | 7.90157200 | 1.51300000 | 1.95613700 |
| C | 6.42605000 | 0.56836400 | 0.74421800 |
| H | 6.25062800 | -0.06220200 | -0.12348500 |
| C | 5.38914000 | 1.08892900 | 1.40757800 |
| H | 5.56643200 | 1.72184500 | 2.27673000 |

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| C | 4.01149900 | 0.87593900 | 1.01130200 |
| H | 3.84934300 | 0.25500100 | 0.13386900 |
| C | 2.94207800 | 1.40508900 | 1.63532100 |
| H | 3.08884400 | 2.03000200 | 2.51594600 |
| C | 1.58818600 | 1.19130200 | 1.18262900 |
| H | 1.47636400 | 0.56205200 | 0.30202300 |
| C | 0.48588500 | 1.69256000 | 1.77551900 |
| H | 0.58796700 | 2.31507400 | 2.66392400 |
| C | -0.84908900 | 1.44366700 | 1.29077800 |
| H | -0.94162600 | 0.81295200 | 0.40671700 |
| C | -1.97462000 | 1.91873000 | 1.86281800 |
| H | -1.89724500 | 2.53364100 | 2.75885500 |
| C | -3.29760400 | 1.67013100 | 1.34712700 |
| H | -3.36729600 | 1.08461100 | 0.43041700 |
| C | -4.43718500 | 2.10469000 | 1.92272400 |
| H | -4.38174700 | 2.66592900 | 2.85481800 |
| C | -5.74831100 | 1.87157200 | 1.36673600 |
| H | -5.78635800 | 1.39385900 | 0.38930200 |
| C | -6.91194900 | 2.18540900 | 1.96566600 |
| H | -6.90380000 | 2.63715900 | 2.95687600 |
| C | 8.65544900 | -0.44499500 | 1.44164700 |
| H | 9.67341200 | -0.14562900 | 1.70099000 |
| H | 8.22277200 | -0.93028000 | 2.32165800 |
| C | -8.20034700 | 1.91943900 | 1.35607100 |
| H | -8.16763800 | 1.58271000 | 0.32199100 |
| C | -9.38729400 | 2.01543400 | 1.96519600 |

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| H | -9.43195800 | 2.34013600 | 3.00575800 |
| C | -10.69898900 | 1.69445700 | 1.30522300 |
| H | -10.51095600 | 1.51987700 | 0.24135700 |
| C | -11.33145400 | 0.40442200 | 1.86178400 |
| H | -11.75584500 | 0.63907600 | 2.84935100 |
| C | -10.36784900 | -0.77686100 | 2.05785700 |
| H | -9.58156700 | -0.41010400 | 2.72509000 |
| C | -9.64660800 | -1.18049800 | 0.76728400 |
| H | -9.31612000 | -0.29030100 | 0.24005900 |
| C | -7.28997900 | -1.57274300 | 0.62356000 |
| C | -6.14275900 | -2.41209500 | 1.12551000 |
| H | -6.35825300 | -2.74844600 | 2.14172100 |
| H | -6.09081200 | -3.30159500 | 0.48658900 |
| C | -4.80579900 | -1.67154200 | 1.05861300 |
| H | -4.85799100 | -0.77833500 | 1.69655600 |
| C | -3.65691500 | -2.55413900 | 1.52226000 |
| H | -3.83856300 | -2.84980500 | 2.56110300 |
| H | -3.63743000 | -3.46718900 | 0.91512400 |
| C | -2.28761800 | -1.88473700 | 1.42891900 |
| H | -2.32291100 | -0.90907000 | 1.93223300 |
| C | -1.20488900 | -2.73582400 | 2.08168300 |
| H | -1.29611100 | -3.76560600 | 1.71464600 |
| H | -1.41282400 | -2.76667200 | 3.15552700 |
| C | 0.21900000 | -2.21384800 | 1.83019100 |
| H | 0.19196500 | -1.16041600 | 1.54112900 |
| H | 0.80331200 | -2.25986900 | 2.75427700 |

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| C | 0.99058000 | -3.00510200 | 0.77643500 |
| H | 1.15458500 | -4.02225900 | 1.15905000 |
| C | 2.36856200 | -2.36259200 | 0.48310800 |
| H | 2.69332800 | -1.77083700 | 1.34656200 |
| C | 3.44686300 | -3.38514500 | 0.14250300 |
| H | 3.13443800 | -3.96052700 | -0.73742800 |
| H | 3.54518100 | -4.08673000 | 0.97893900 |
| C | 4.80306100 | -2.73625600 | -0.11811000 |
| H | 5.07397200 | -2.11819800 | 0.74864800 |
| C | 5.90273200 | -3.76861800 | -0.32874500 |
| H | 5.63991300 | -4.42311400 | -1.16549200 |
| H | 5.98409000 | -4.38106500 | 0.57384500 |
| C | 7.26755200 | -3.14709200 | -0.62719200 |
| C | 8.39223900 | -4.17225500 | -0.61317500 |
| H | 8.26237000 | -4.88852700 | -1.42717200 |
| H | 8.36874700 | -4.71763300 | 0.33452300 |
| C | 9.75514000 | -3.51394100 | -0.74354600 |
| H | 9.83535300 | -3.06464000 | -1.74417800 |
| C | 9.90467700 | -2.37868500 | 0.30663100 |
| H | 10.00567700 | -2.86537000 | 1.28395300 |
| C | 8.68067900 | -1.45121200 | 0.29731500 |
| H | 8.66739100 | -0.91573600 | -0.65644700 |
| C | 11.16461800 | -1.60006300 | 0.02872100 |
| C | -10.39757300 | -2.08524800 | -0.18876000 |
| H | -9.80421900 | -2.24531000 | -1.09210900 |
| H | -11.34353300 | -1.61815700 | -0.46398900 |

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| H | -10.60198900 | -3.05634600 | 0.26683800 |
| C | -11.06079400 | -1.95444200 | 2.73997700 |
| H | -11.90570100 | -2.32109800 | 2.15016500 |
| H | -11.43511700 | -1.66561600 | 3.72633200 |
| H | -10.36630600 | -2.78672100 | 2.87496100 |
| C | -11.67716300 | 2.86765700 | 1.43175500 |
| H | -11.87514400 | 3.08943600 | 2.48639000 |
| H | -12.62428100 | 2.65221700 | 0.93521800 |
| H | -11.24825700 | 3.76580000 | 0.98032400 |
| O | 9.04576500 | 3.28124500 | -1.91170600 |
| H | 8.22859700 | 2.81965700 | -1.67580800 |
| O | 11.88815700 | 5.63395400 | 0.17229000 |
| H | 12.30122900 | 5.73279200 | -0.70089500 |
| O | 9.23666800 | 3.30380600 | 1.01030200 |
| O | 8.43611300 | 1.46256300 | -0.03892700 |
| O | 7.29231400 | -2.51312300 | -1.87269100 |
| H | 6.44284900 | -2.04334500 | -1.96079300 |
| O | 7.49533400 | -2.22126100 | 0.43087700 |
| O | 11.24386900 | -0.44190500 | -0.30579000 |
| O | 12.27935600 | -2.36336100 | 0.15503200 |
| H | 13.03030200 | -1.79434100 | -0.08075100 |
| O | 4.75668200 | -1.90247900 | -1.27898600 |
| H | 3.86139200 | -1.51897300 | -1.32471200 |
| O | 2.20370700 | -1.44203700 | -0.59687500 |
| H | 1.47265700 | -1.83845800 | -1.11258300 |
| O | 0.30737900 | -3.11335000 | -0.46430600 |

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|---|--------------|-------------|-------------|
| H | -0.55064900 | -2.64301800 | -0.40546300 |
| O | -1.91319600 | -1.67349200 | 0.06409600 |
| H | -2.71463500 | -1.41358100 | -0.42432200 |
| O | -4.52182600 | -1.27396000 | -0.27972400 |
| H | -5.30859000 | -0.81155200 | -0.61659000 |
| O | -7.16418800 | -0.71159700 | -0.23250000 |
| O | -8.44237000 | -1.89195700 | 1.19334100 |
| O | -12.39687900 | 0.05039200 | 0.96900100 |
| H | -13.08100200 | -0.42219900 | 1.45501900 |
| O | 10.70729000 | -4.53922600 | -0.56138600 |
| H | 11.58460000 | -4.13691500 | -0.53499300 |
| N | 11.66539400 | 4.28539600 | -2.25875400 |
| H | 10.84187800 | 4.55102600 | -2.79458900 |
| H | 12.18330400 | 3.62250000 | -2.82684700 |

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|---|-------------|-------------|------------|
| C | -9.29036600 | -2.24237200 | 3.28776000 |
| H | -9.94216500 | -1.39205400 | 3.51283700 |
| H | -9.64880500 | -3.10204200 | 3.86094500 |
| H | -9.41981800 | -2.47668700 | 2.22546800 |
| C | -7.83459800 | -1.91454000 | 3.60906100 |
| H | -7.19914500 | -2.78251700 | 3.39573500 |
| H | -7.73448500 | -1.71631500 | 4.68339400 |

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|---|-------------|-------------|-------------|
| C | -7.30597900 | -0.72214300 | 2.81860800 |
| H | -7.94826300 | 0.15246800 | 2.98965300 |
| H | -7.38646800 | -0.95612800 | 1.75067300 |
| C | -5.85725200 | -0.36570800 | 3.13785300 |
| H | -5.24285700 | -1.26516500 | 3.02631700 |
| H | -5.77424400 | -0.06900400 | 4.19202100 |
| C | -5.31574400 | 0.74834500 | 2.24689500 |
| H | -5.86309200 | 1.67677100 | 2.44961200 |
| H | -5.53324400 | 0.52119800 | 1.19756200 |
| C | -3.81492500 | 0.98915600 | 2.38829400 |
| H | -3.27382200 | 0.10188000 | 2.03082700 |
| H | -3.54876600 | 1.10455200 | 3.44803600 |
| C | -3.36446600 | 2.21754900 | 1.60425000 |
| H | -3.88156500 | 3.09737500 | 2.01014300 |
| H | -3.71011200 | 2.12677900 | 0.56870300 |
| C | -1.86041500 | 2.47434800 | 1.61907500 |
| H | -1.33189800 | 1.58953100 | 1.24134700 |
| H | -1.51511800 | 2.62294800 | 2.65120900 |
| C | -1.48453600 | 3.68255600 | 0.76634600 |
| H | -2.04559200 | 4.56040900 | 1.11257200 |
| H | -1.81777100 | 3.49705600 | -0.26228400 |
| C | 0.00339300 | 4.01669400 | 0.74943500 |
| H | 0.55946800 | 3.12717600 | 0.43411000 |
| H | 0.34214100 | 4.25971100 | 1.76590200 |
| C | 0.32230500 | 5.17903800 | -0.18876800 |
| H | -0.21869200 | 6.07503500 | 0.14172200 |

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| H | -0.04187000 | 4.94318900 | -1.19598200 |
| C | 1.80490500 | 5.51051100 | -0.28749400 |
| H | 1.94982500 | 6.39288300 | -0.91788200 |
| H | 2.20193100 | 5.75642600 | 0.71000300 |
| O | 2.56324800 | 4.47626500 | -0.89229700 |
| H | 2.57251700 | 3.71359700 | -0.30225200 |
| C | -8.37858900 | 3.96987200 | -0.40320300 |
| H | -8.62924900 | 4.34788100 | -1.40238900 |
| C | -7.11123400 | 4.70359700 | 0.03074900 |
| H | -6.82445400 | 4.35235100 | 1.03465200 |
| C | -5.96753700 | 4.36428800 | -0.91678600 |
| H | -6.27186600 | 4.65410800 | -1.93787800 |
| C | -6.84094100 | 2.19749600 | -1.29648200 |
| H | -7.03388800 | 2.42088900 | -2.36554700 |
| C | -8.12549200 | 2.46770200 | -0.50088500 |
| H | -8.94826200 | 1.97997800 | -1.04710300 |
| C | -4.67624000 | 5.05987700 | -0.55506600 |
| H | -4.37326600 | 4.77872900 | 0.45498700 |
| H | -4.81905700 | 6.14090000 | -0.59348300 |
| H | -3.87961600 | 4.76948100 | -1.24324900 |
| C | -5.71988400 | 0.19504400 | -2.06928000 |
| H | -5.70127100 | 0.77764600 | -3.00011800 |
| C | -4.32964100 | 0.06432600 | -1.52481300 |
| H | -4.21639900 | -0.56345200 | -0.64525100 |
| C | -3.25095400 | 0.66890500 | -2.03180500 |
| H | -3.34399300 | 1.31721400 | -2.90247100 |

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| C | -1.93408000 | 0.50396800 | -1.44968300 |
| H | -1.87406100 | -0.17590000 | -0.60251900 |
| C | -0.80777900 | 1.11833700 | -1.86004200 |
| H | -0.84226900 | 1.81815700 | -2.69427500 |
| C | 0.46502400 | 0.88075100 | -1.22105200 |
| H | 0.45911100 | 0.13720300 | -0.42663200 |
| C | 1.63039000 | 1.48481100 | -1.53014100 |
| H | 1.66608700 | 2.25700000 | -2.29596000 |
| C | 2.85976200 | 1.17351400 | -0.83824300 |
| H | 2.81701800 | 0.38116700 | -0.09061000 |
| C | 4.04493400 | 1.78192100 | -1.06090700 |
| H | 4.10119300 | 2.58157200 | -1.79739600 |
| C | 5.25227500 | 1.45562800 | -0.34264000 |
| H | 5.18656200 | 0.66795200 | 0.40767100 |
| C | 6.43944800 | 2.06043700 | -0.54824800 |
| H | 6.51189000 | 2.83742100 | -1.30822900 |
| C | 7.63895200 | 1.74271000 | 0.18800100 |
| H | 7.54491700 | 1.00815000 | 0.98605800 |
| C | 8.85119900 | 2.27247200 | -0.05824500 |
| H | 8.96659400 | 2.98955700 | -0.87021700 |
| C | -6.41852600 | -1.14408800 | -2.31549400 |
| H | -7.43519500 | -0.91553400 | -2.64562900 |
| H | -5.91502800 | -1.70542900 | -3.10761700 |
| C | 10.04188000 | 1.89916100 | 0.67990500 |
| H | 9.88006500 | 1.26129300 | 1.54654000 |
| C | 11.29165300 | 2.22930800 | 0.33644200 |

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| H | 11.45349900 | 2.85504400 | -0.54287200 |
| C | 12.52813300 | 1.75728800 | 1.04674600 |
| H | 12.23479200 | 1.25199000 | 1.97414000 |
| C | 13.30006700 | 0.73039600 | 0.19478700 |
| H | 13.72666800 | 1.27288100 | -0.66528100 |
| C | 12.44137100 | -0.40743400 | -0.38811400 |
| H | 11.67003900 | 0.08076100 | -0.99182300 |
| C | 11.67944100 | -1.19375700 | 0.68357500 |
| H | 11.22127700 | -0.50503900 | 1.38748500 |
| C | 9.35921300 | -1.75550800 | 0.47115800 |
| C | 8.33965300 | -2.51042800 | -0.34493500 |
| H | 8.70842500 | -2.63191900 | -1.36514200 |
| H | 8.24803100 | -3.50917900 | 0.09791400 |
| C | 6.96676800 | -1.83319300 | -0.33123200 |
| H | 7.05166700 | -0.83859200 | -0.79178400 |
| C | 5.93786400 | -2.65660400 | -1.09364200 |
| H | 6.28292200 | -2.78679700 | -2.12495500 |
| H | 5.87413300 | -3.65092500 | -0.63550000 |
| C | 4.54038400 | -2.04159400 | -1.11728800 |
| H | 4.59737500 | -1.02307400 | -1.52526700 |
| C | 3.58461800 | -2.86378600 | -1.97640800 |
| H | 3.68154200 | -3.92126600 | -1.70097200 |
| H | 3.91930900 | -2.77874500 | -3.01474600 |
| C | 2.11621600 | -2.42463500 | -1.85496300 |
| H | 2.05739500 | -1.39398300 | -1.49782300 |
| H | 1.64183400 | -2.43039500 | -2.84115300 |

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| C | 1.26874100 | -3.32067400 | -0.95164300 |
| H | 1.16738700 | -4.30362600 | -1.43253800 |
| C | -0.14146300 | -2.72525600 | -0.73843700 |
| H | -0.42379500 | -2.11444800 | -1.60363000 |
| C | -1.21345300 | -3.78141400 | -0.49117600 |
| H | -0.95179500 | -4.35106500 | 0.40855100 |
| H | -1.22625400 | -4.48159000 | -1.33416800 |
| C | -2.60426200 | -3.17246900 | -0.34144200 |
| H | -2.84149100 | -2.60305400 | -1.25011000 |
| C | -3.68291800 | -4.23312000 | -0.14769700 |
| H | -3.45407000 | -4.83456200 | 0.73732400 |
| H | -3.68997800 | -4.89268300 | -1.02032600 |
| C | -5.07865800 | -3.63704300 | 0.03134300 |
| C | -6.19001200 | -4.67456700 | 0.04131300 |
| H | -6.07002600 | -5.35803400 | 0.88462400 |
| H | -6.15210000 | -5.25377600 | -0.88546900 |
| C | -7.54893300 | -4.00259200 | 0.14117100 |
| H | -7.62470400 | -3.52199500 | 1.12527100 |
| C | -7.69997800 | -2.90341800 | -0.94918700 |
| H | -7.88465700 | -3.42947300 | -1.89321400 |
| C | -6.45225500 | -2.01417200 | -1.06009500 |
| H | -6.42424400 | -1.37728400 | -0.17360400 |
| C | -8.90578700 | -2.05590600 | -0.62354800 |
| C | 12.46008400 | -2.24705400 | 1.44264400 |
| H | 11.82968900 | -2.69476100 | 2.21440300 |
| H | 13.32552300 | -1.77818400 | 1.91306600 |

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| H | 12.80483200 | -3.04080300 | 0.77638300 |
| C | 13.25923900 | -1.30925000 | -1.31076900 |
| H | 14.09405300 | -1.78223600 | -0.78494900 |
| H | 13.66781500 | -0.73658100 | -2.14838200 |
| H | 12.63686400 | -2.10789700 | -1.72064500 |
| C | 13.44363900 | 2.92863800 | 1.41349600 |
| H | 13.73644800 | 3.48548300 | 0.51646600 |
| H | 14.34919200 | 2.56503200 | 1.90110300 |
| H | 12.93224000 | 3.62226100 | 2.08467300 |
| O | -8.04184000 | 1.95999900 | 0.80895700 |
| H | -7.89440000 | 1.00653700 | 0.73380700 |
| O | -7.34234700 | 6.09275100 | 0.01170800 |
| H | -8.23495500 | 6.18807000 | 0.38230400 |
| O | -5.74014100 | 2.95898900 | -0.86475600 |
| O | -6.55709900 | 0.85866800 | -1.11646500 |
| O | -5.18240000 | -2.91091300 | 1.22197200 |
| H | -4.34337100 | -2.42458600 | 1.33003000 |
| O | -5.27422100 | -2.80254500 | -1.10669000 |
| O | -8.91614300 | -0.87952900 | -0.34948200 |
| O | -10.05325200 | -2.78033100 | -0.60574600 |
| H | -10.75587700 | -2.17217600 | -0.32308200 |
| O | -2.65691900 | -2.28130000 | 0.77741700 |
| H | -1.76267000 | -1.91456400 | 0.91326900 |
| O | -0.06727700 | -1.83412900 | 0.37805200 |
| H | 0.62069300 | -2.25022600 | 0.93748400 |
| O | 1.82600900 | -3.52171000 | 0.33900700 |

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| H | 2.66970500 | -3.02391800 | 0.40707600 |
| O | 3.99114700 | -1.96302600 | 0.20158600 |
| H | 4.72660100 | -1.79436100 | 0.82010600 |
| O | 6.49231200 | -1.69365900 | 1.00564600 |
| H | 7.22605900 | -1.33156000 | 1.53498200 |
| O | 9.07403500 | -1.13316000 | 1.48249300 |
| O | 10.58533100 | -1.86653200 | -0.01726600 |
| O | 14.35202400 | 0.23878100 | 1.01970600 |
| H | 15.02129500 | -0.16726900 | 0.45867300 |
| O | -8.51455800 | -5.02075000 | -0.00679200 |
| H | -9.38754100 | -4.60956800 | 0.02714900 |
| N | -9.45624400 | 4.35129900 | 0.50421800 |
| H | -9.36599100 | 3.78779000 | 1.34689300 |
| H | -10.36056300 | 4.12938900 | 0.10029300 |

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| C | 9.44588900 | 3.54302300 | -0.77888300 |
| H | 10.21494500 | 2.87363500 | -1.18340500 |
| C | 9.89075500 | 3.93057500 | 0.63073900 |
| H | 9.16222700 | 4.64263100 | 1.04526900 |
| C | 9.91822800 | 2.70745900 | 1.53805000 |
| H | 10.63826300 | 1.98647400 | 1.11673800 |
| C | 8.21560500 | 1.65585200 | 0.29226500 |

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| H | 8.92795100 | 0.89738600 | -0.06169200 |
| C | 8.11933000 | 2.78843800 | -0.72947000 |
| H | 7.89772800 | 2.33977200 | -1.70809000 |
| C | 10.29867100 | 3.04970800 | 2.96087100 |
| H | 9.55835900 | 3.73368800 | 3.38143000 |
| H | 11.27447200 | 3.53536300 | 2.96966400 |
| H | 10.33221300 | 2.14880400 | 3.57484300 |
| C | 6.67829600 | 0.20191400 | 1.46750000 |
| H | 6.82513800 | 0.71765100 | 2.42068500 |
| C | 5.22919700 | -0.12515700 | 1.28637400 |
| H | 4.94442700 | -0.47678300 | 0.29702000 |
| C | 4.28624400 | 0.08380100 | 2.21070300 |
| H | 4.54917000 | 0.45448700 | 3.19930100 |
| C | 2.88550700 | -0.08055800 | 1.88230700 |
| H | 2.68080000 | -0.42181900 | 0.86936100 |
| C | 1.83030800 | 0.26319700 | 2.64483700 |
| H | 1.97063500 | 0.63215100 | 3.65841100 |
| C | 0.50054300 | 0.23011500 | 2.08444400 |
| H | 0.44985000 | -0.09612200 | 1.04678700 |
| C | -0.64252900 | 0.61321700 | 2.68812500 |
| H | -0.63581200 | 0.95555400 | 3.72081900 |
| C | -1.89878400 | 0.60534400 | 1.97918200 |
| H | -1.86684100 | 0.28569000 | 0.93655300 |
| C | -3.08978600 | 0.97330500 | 2.49525200 |
| H | -3.15008600 | 1.29969900 | 3.53179600 |
| C | -4.31008800 | 0.96506800 | 1.72628400 |

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| H | -4.23415000 | 0.66424000 | 0.68014000 |
| C | -5.51905000 | 1.30238500 | 2.22172600 |
| H | -5.60029800 | 1.59439700 | 3.26733700 |
| C | -6.73276400 | 1.30036200 | 1.43974900 |
| H | -6.63496300 | 1.07356000 | 0.37862400 |
| C | -7.95696900 | 1.54911500 | 1.94437100 |
| H | -8.06167700 | 1.76276500 | 3.00685300 |
| C | 7.64138100 | -0.99257000 | 1.43109200 |
| H | 8.64955000 | -0.61483200 | 1.62786800 |
| H | 7.37456800 | -1.66246400 | 2.25394200 |
| C | -9.16770700 | 1.51532700 | 1.14557200 |
| H | -9.02363100 | 1.39989700 | 0.07364200 |
| C | -10.40733200 | 1.57328100 | 1.64866700 |
| H | -10.53209700 | 1.68049700 | 2.72801600 |
| C | -11.67510000 | 1.47194200 | 0.84778300 |
| H | -11.43300300 | 1.50862300 | -0.21929100 |
| C | -12.38879900 | 0.13275200 | 1.11124300 |
| H | -12.76562100 | 0.15560600 | 2.14634200 |
| C | -11.48770600 | -1.11086000 | 0.99434200 |
| H | -10.72074300 | -0.99805900 | 1.76679900 |
| C | -10.72479800 | -1.16967100 | -0.33216000 |
| H | -10.31955000 | -0.18910100 | -0.56201000 |
| C | -8.39988600 | -1.65415500 | -0.55112900 |
| C | -7.29877700 | -2.64109400 | -0.24911400 |
| H | -7.60848600 | -3.28846100 | 0.57174600 |
| H | -7.16775600 | -3.26126600 | -1.14306000 |

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| C | -5.97026800 | -1.95018600 | 0.07383400 |
| H | -6.09977200 | -1.32031200 | 0.96527200 |
| C | -4.88011000 | -2.98146600 | 0.33609600 |
| H | -5.17961800 | -3.59508300 | 1.19178900 |
| H | -4.79395800 | -3.63911500 | -0.53713000 |
| C | -3.50784400 | -2.37710400 | 0.62423300 |
| H | -3.60052500 | -1.62480100 | 1.41912000 |
| C | -2.51305300 | -3.44499400 | 1.06855300 |
| H | -2.56679600 | -4.28589100 | 0.36654900 |
| H | -2.83776700 | -3.82076600 | 2.04156900 |
| C | -1.06958200 | -2.91777300 | 1.14950000 |
| H | -1.07172600 | -1.82558600 | 1.13299700 |
| H | -0.60558000 | -3.21238500 | 2.09399700 |
| C | -0.17201200 | -3.41715500 | 0.01956000 |
| H | -0.02885700 | -4.49973400 | 0.12796700 |
| C | 1.21202900 | -2.73111300 | 0.05993900 |
| H | 1.46457000 | -2.47940500 | 1.09666500 |
| C | 2.31939900 | -3.59445900 | -0.53571700 |
| H | 2.05794200 | -3.85867200 | -1.56765200 |
| H | 2.38179600 | -4.52392600 | 0.04058100 |
| C | 3.68747000 | -2.91244400 | -0.51544100 |
| H | 3.90295300 | -2.55962300 | 0.50317400 |
| C | 4.78718900 | -3.87762000 | -0.93596400 |
| H | 4.53125100 | -4.32961400 | -1.89949200 |
| H | 4.84917100 | -4.67338900 | -0.18912200 |
| C | 6.17002700 | -3.24114600 | -1.08717000 |

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|---|--------------|-------------|-------------|
| C | 7.24973800 | -4.30401900 | -1.24129100 |
| H | 7.11408600 | -4.83477400 | -2.18524200 |
| H | 7.17084700 | -5.02222500 | -0.42111200 |
| C | 8.64446200 | -3.70761700 | -1.19756900 |
| H | 8.80265300 | -3.07935500 | -2.08558500 |
| C | 8.78706700 | -2.80862600 | 0.05989900 |
| H | 8.75524100 | -3.47210500 | 0.93080000 |
| C | 7.63311000 | -1.79524100 | 0.13702500 |
| H | 7.67861000 | -1.12315800 | -0.72699000 |
| C | 10.17453300 | -2.22706100 | 0.00093100 |
| C | -11.48742000 | -1.69451300 | -1.53306600 |
| H | -10.86454000 | -1.62366000 | -2.42688500 |
| H | -12.38777000 | -1.09599200 | -1.67662000 |
| H | -11.77204800 | -2.73834100 | -1.38912800 |
| C | -12.26919800 | -2.39172300 | 1.28276800 |
| H | -13.07737000 | -2.54364700 | 0.56239600 |
| H | -12.70515300 | -2.35727100 | 2.28452700 |
| H | -11.61495200 | -3.26401200 | 1.23001500 |
| C | -12.61638200 | 2.63886100 | 1.16237500 |
| H | -12.85850200 | 2.65744800 | 2.22966900 |
| H | -13.54404900 | 2.54053900 | 0.59903400 |
| H | -12.14356900 | 3.58888100 | 0.90758400 |
| O | 7.10252700 | 3.70482500 | -0.37443900 |
| H | 6.43336200 | 3.22130500 | 0.13074800 |
| O | 11.18424400 | 4.48592000 | 0.58689900 |
| H | 11.17059500 | 5.08770300 | -0.16861200 |

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| O | 8.62033700 | 2.12094100 | 1.55797800 |
| O | 6.93186400 | 1.13487200 | 0.40338600 |
| O | 6.24603400 | -2.40169700 | -2.20386400 |
| H | 5.43845700 | -1.86643400 | -2.20431500 |
| O | 6.40246200 | -2.50744700 | 0.11195700 |
| O | 11.17903900 | -2.86622100 | 0.18152500 |
| O | 10.22804600 | -0.93418400 | -0.37120000 |
| H | 11.16572000 | -0.70297900 | -0.43882300 |
| O | 3.72000100 | -1.79361500 | -1.40419100 |
| H | 2.85816700 | -1.35618400 | -1.34440800 |
| O | 1.11881500 | -1.48760700 | -0.63969900 |
| H | 0.47465200 | -1.65810100 | -1.34683500 |
| O | -0.72190600 | -3.18198000 | -1.26884100 |
| H | -1.55996400 | -2.69745100 | -1.17369700 |
| O | -2.96356900 | -1.74587900 | -0.53800700 |
| H | -3.68476600 | -1.28449200 | -0.99134500 |
| O | -5.53639600 | -1.13521800 | -1.01123400 |
| H | -6.29316900 | -0.61326800 | -1.31626900 |
| O | -8.21304300 | -0.62152300 | -1.16004900 |
| O | -9.58115200 | -2.04632500 | -0.09821500 |
| O | -13.48765400 | 0.08481000 | 0.20792600 |
| H | -14.10258700 | -0.58907500 | 0.50678400 |
| O | 9.54452000 | -4.79133500 | -1.17397700 |
| H | 10.41113500 | -4.47326000 | -0.89689100 |
| N | 9.43455600 | 4.75866700 | -1.58867900 |
| H | 8.58737700 | 5.27844300 | -1.37289200 |

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| H | 9.40407900 | 4.53578800 | -2.57739500 |
| C | -9.83194400 | 2.71883600 | -2.28771200 |
| H | -9.86985600 | 1.62760700 | -2.19279300 |
| H | -10.64075400 | 3.02882100 | -2.95236600 |
| H | -10.02212400 | 3.14970000 | -1.29972100 |
| C | -8.46422000 | 3.15383600 | -2.80966000 |
| H | -8.43303000 | 4.24416900 | -2.90900300 |
| H | -8.30738900 | 2.74543200 | -3.81378800 |
| C | -7.32906200 | 2.69129200 | -1.89920300 |
| H | -7.39101000 | 1.60018700 | -1.79600700 |
| H | -7.47686500 | 3.10445800 | -0.89284400 |
| C | -5.94216900 | 3.07622100 | -2.40565900 |
| H | -5.86288400 | 4.16875000 | -2.45958900 |
| H | -5.81578700 | 2.70713900 | -3.43092300 |
| C | -4.81303900 | 2.52864100 | -1.53466800 |
| H | -4.87876700 | 1.43184200 | -1.50744300 |
| H | -4.94774800 | 2.86883200 | -0.50012100 |
| C | -3.42788000 | 2.93540000 | -2.03042800 |
| H | -3.34331800 | 4.02855100 | -2.00340200 |
| H | -3.32343300 | 2.64628300 | -3.08360000 |
| C | -2.28035500 | 2.32331500 | -1.22955200 |
| H | -2.34543200 | 1.22717800 | -1.28184800 |
| H | -2.38645000 | 2.58693100 | -0.16975000 |
| C | -0.91136300 | 2.77445600 | -1.73613700 |
| H | -0.83760100 | 3.86521000 | -1.64687100 |
| H | -0.83535500 | 2.55033100 | -2.80761600 |

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| C | 0.26728700 | 2.13176000 | -1.00873600 |
| H | 0.20507100 | 1.03898100 | -1.10510400 |
| H | 0.20055100 | 2.34549800 | 0.06541700 |
| C | 1.61733800 | 2.61097600 | -1.54267200 |
| H | 1.72702400 | 3.68597900 | -1.36962200 |
| H | 1.64709400 | 2.46343500 | -2.63002000 |
| C | 2.80312800 | 1.88722300 | -0.91130500 |
| H | 2.73318200 | 0.81343700 | -1.11916900 |
| H | 2.77539300 | 2.00259700 | 0.17743100 |
| C | 4.14550300 | 2.39249000 | -1.40652600 |
| H | 4.95012900 | 1.75378900 | -1.02006300 |
| H | 4.17268700 | 2.35262600 | -2.50514500 |
| O | 4.30490400 | 3.72882500 | -0.94861800 |
| H | 5.16342600 | 4.04757700 | -1.24298400 |

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| C | 5.01864500 | 3.26781400 | -0.59956400 |
| H | 5.02243200 | 2.20035600 | -0.84280100 |
| H | 5.88629000 | 3.45085900 | 0.03745200 |
| H | 5.15376700 | 3.82993800 | -1.52970800 |
| C | 3.70968700 | 3.64415500 | 0.08419900 |
| H | 3.70862800 | 4.71691400 | 0.31640900 |
| H | 3.63674300 | 3.12252100 | 1.04627400 |

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| C | 2.47892900 | 3.30641700 | -0.75195800 |
| H | 2.44871500 | 2.22196500 | -0.91887900 |
| H | 2.57467400 | 3.76674600 | -1.74468200 |
| C | 1.16906000 | 3.75456800 | -0.11208600 |
| H | 1.18778800 | 4.84421900 | 0.02514600 |
| H | 1.08951500 | 3.32025100 | 0.89252900 |
| C | -0.06582600 | 3.36671400 | -0.91922900 |
| H | -0.11740200 | 2.27285800 | -0.99143700 |
| H | 0.03842500 | 3.73795100 | -1.94759500 |
| C | -1.36703200 | 3.89365900 | -0.32276500 |
| H | -1.31928900 | 4.98920500 | -0.26120500 |
| H | -1.46460500 | 3.53169300 | 0.70842400 |
| C | -2.60655800 | 3.48540400 | -1.11236600 |
| H | -2.67876000 | 2.39030700 | -1.12553200 |
| H | -2.49292100 | 3.79855100 | -2.15882000 |
| C | -3.89960500 | 4.06592600 | -0.54875400 |
| H | -3.82866300 | 5.16176000 | -0.53194700 |
| H | -4.01186300 | 3.74791000 | 0.49531600 |
| C | -5.14114400 | 3.65095500 | -1.33128200 |
| H | -5.22064400 | 2.55653500 | -1.32338300 |
| H | -5.02721200 | 3.94331100 | -2.38332500 |
| C | -6.43170000 | 4.24710100 | -0.77834600 |
| H | -6.34582800 | 5.34206500 | -0.78605900 |
| H | -6.54605100 | 3.94464100 | 0.27077300 |
| C | -7.67431900 | 3.82663800 | -1.55789800 |
| H | -7.74009600 | 2.73250500 | -1.56830100 |

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| H | -7.58667400 | 4.15486700 | -2.60000500 |
| C | -8.96733300 | 4.38497800 | -0.97755100 |
| H | -9.82436700 | 4.02448900 | -1.55462200 |
| H | -9.09916500 | 4.01948400 | 0.05177800 |
| O | -9.03272000 | 5.80072000 | -1.03211600 |
| H | -8.36288800 | 6.14931800 | -0.43389100 |
| C | 10.08020400 | 3.13537500 | -0.77035100 |
| H | 10.93185100 | 2.65884800 | -0.26886300 |
| C | 9.57726800 | 4.24232800 | 0.15523200 |
| H | 8.73020100 | 4.74603800 | -0.33591700 |
| C | 9.06557900 | 3.64962800 | 1.46262800 |
| H | 9.90563300 | 3.12738900 | 1.95136600 |
| C | 8.44840600 | 1.63696600 | 0.36900600 |
| H | 9.23256300 | 1.07308600 | 0.89936100 |
| C | 8.99382900 | 2.08655600 | -0.98359200 |
| H | 9.41235500 | 1.19629400 | -1.47527700 |
| C | 8.49629000 | 4.69423500 | 2.39520600 |
| H | 7.64477700 | 5.18858200 | 1.91981000 |
| H | 9.25883500 | 5.44245100 | 2.61693300 |
| H | 8.15487400 | 4.23346400 | 3.32473500 |
| C | 6.76534600 | 0.15218200 | 1.21856400 |
| H | 6.80360200 | 0.80738100 | 2.09509800 |
| C | 5.33995900 | -0.09873700 | 0.84100300 |
| H | 5.17712900 | -0.64945000 | -0.08176000 |
| C | 4.29136700 | 0.33695100 | 1.54557800 |
| H | 4.44818900 | 0.89436300 | 2.46840300 |

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| C | 2.92570100 | 0.13744100 | 1.10718600 |
| H | 2.79523200 | -0.40248300 | 0.17270600 |
| C | 1.82964900 | 0.59666900 | 1.74044200 |
| H | 1.93383600 | 1.14867800 | 2.67392400 |
| C | 0.50233800 | 0.40460200 | 1.20931900 |
| H | 0.44477700 | -0.15581400 | 0.27810000 |
| C | -0.63985100 | 0.85452200 | 1.76693700 |
| H | -0.60648800 | 1.41658000 | 2.69947600 |
| C | -1.92906100 | 0.62750000 | 1.16456100 |
| H | -1.94095500 | 0.05005700 | 0.24027500 |
| C | -3.10633300 | 1.06368500 | 1.65783800 |
| H | -3.12284100 | 1.63121300 | 2.58744400 |
| C | -4.36468800 | 0.83331700 | 0.99523900 |
| H | -4.32861100 | 0.28619000 | 0.05334900 |
| C | -5.56477600 | 1.24618100 | 1.45084000 |
| H | -5.62351900 | 1.77924400 | 2.39899400 |
| C | -6.79480700 | 1.02963700 | 0.72981100 |
| H | -6.70678500 | 0.55247200 | -0.24482300 |
| C | -8.02295300 | 1.36553500 | 1.16528800 |
| H | -8.14114500 | 1.82498800 | 2.14591200 |
| C | 7.57896300 | -1.11945500 | 1.49052000 |
| H | 8.58759800 | -0.82068700 | 1.78405400 |
| H | 7.13864500 | -1.66487900 | 2.33065400 |
| C | -9.21989000 | 1.11669400 | 0.38666700 |
| H | -9.05280900 | 0.74668100 | -0.62286800 |
| C | -10.47459900 | 1.26609400 | 0.82457000 |

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| H | -10.64618700 | 1.62271400 | 1.84144800 |
| C | -11.69980200 | 0.93351700 | 0.02232200 |
| H | -11.40258800 | 0.74180500 | -1.01509500 |
| C | -12.37736100 | -0.34924700 | 0.54326400 |
| H | -12.81103200 | -0.11419600 | 1.52944300 |
| C | -11.42833600 | -1.54412900 | 0.75543300 |
| H | -10.66730300 | -1.19879700 | 1.46178200 |
| C | -10.65904300 | -1.93249600 | -0.51194100 |
| H | -10.28305600 | -1.03935900 | -1.00246700 |
| C | -8.29772000 | -2.34817100 | -0.52450600 |
| C | -7.19125400 | -3.21673700 | 0.02007300 |
| H | -7.50591100 | -3.65609600 | 0.96846500 |
| H | -7.04218400 | -4.03507300 | -0.69408600 |
| C | -5.87521100 | -2.44986800 | 0.17722500 |
| H | -6.01877400 | -1.63619400 | 0.90236300 |
| C | -4.75878200 | -3.36417900 | 0.66209500 |
| H | -5.04332800 | -3.78276000 | 1.63344100 |
| H | -4.65173800 | -4.19847100 | -0.04147400 |
| C | -3.40352300 | -2.67377600 | 0.79944400 |
| H | -3.50897900 | -1.78330300 | 1.43393000 |
| C | -2.36567900 | -3.60220100 | 1.42263400 |
| H | -2.41572800 | -4.57637300 | 0.92096100 |
| H | -2.65711700 | -3.77060200 | 2.46379100 |
| C | -0.93038800 | -3.05408500 | 1.35203100 |
| H | -0.94401600 | -1.97037300 | 1.21481800 |
| H | -0.41264500 | -3.23336000 | 2.29938200 |

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| C | -0.08158100 | -3.69327700 | 0.25413000 |
| H | 0.07458000 | -4.75025400 | 0.51054500 |
| C | 1.30359100 | -3.00836700 | 0.12895000 |
| H | 1.55922300 | -2.50987700 | 1.07112700 |
| C | 2.41597300 | -3.98277000 | -0.24254400 |
| H | 2.16505700 | -4.46969700 | -1.19278100 |
| H | 2.47112900 | -4.76377500 | 0.52465800 |
| C | 3.77964100 | -3.30712400 | -0.35676100 |
| H | 3.99791600 | -2.77785200 | 0.58086400 |
| C | 4.89399800 | -4.31569700 | -0.60623900 |
| H | 4.66747900 | -4.90312100 | -1.50144200 |
| H | 4.94260400 | -4.99799900 | 0.24734800 |
| C | 6.26695300 | -3.67295500 | -0.80468600 |
| C | 7.39384400 | -4.69578600 | -0.82431900 |
| H | 7.29355800 | -5.35432900 | -1.68960200 |
| H | 7.34114300 | -5.30496700 | 0.08243900 |
| C | 8.75789900 | -4.02784400 | -0.86442000 |
| H | 8.86794300 | -3.50967300 | -1.82819100 |
| C | 8.86929100 | -2.96864400 | 0.26640500 |
| H | 8.94483000 | -3.52232800 | 1.20987800 |
| C | 7.64095500 | -2.04724300 | 0.28386000 |
| H | 7.65488900 | -1.44782300 | -0.63063700 |
| C | 10.13148300 | -2.16495600 | 0.08305200 |
| C | -11.39508100 | -2.78922200 | -1.52121000 |
| H | -10.77081100 | -2.94706400 | -2.40365600 |
| H | -12.31225900 | -2.27803100 | -1.81688500 |

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| H | -11.65098800 | -3.76402700 | -1.10064500 |
| C | -12.15503100 | -2.72825700 | 1.39019100 |
| H | -12.97830800 | -3.08491700 | 0.76399400 |
| H | -12.56696700 | -2.45115800 | 2.36483800 |
| H | -11.47122300 | -3.56685500 | 1.54028000 |
| C | -12.69529900 | 2.09669900 | 0.02131000 |
| H | -12.99906200 | 2.34643200 | 1.04393900 |
| H | -13.58859500 | 1.83248100 | -0.54621500 |
| H | -12.24455500 | 2.98900900 | -0.41954000 |
| O | 7.98325900 | 2.67609300 | -1.77488000 |
| H | 7.17671400 | 2.16084800 | -1.63735100 |
| O | 10.62535700 | 5.14198300 | 0.43350100 |
| H | 11.07675600 | 5.24902000 | -0.41956300 |
| O | 8.02588400 | 2.72029800 | 1.17108700 |
| O | 7.33770600 | 0.84803500 | 0.09885500 |
| O | 6.33560500 | -2.95099700 | -1.99973600 |
| H | 5.49212700 | -2.46928000 | -2.07934600 |
| O | 6.45432500 | -2.82610900 | 0.32533400 |
| O | 10.21227400 | -0.98244800 | -0.15181500 |
| O | 11.24703400 | -2.93171600 | 0.17278300 |
| H | 12.00040000 | -2.34261600 | 0.00345100 |
| O | 3.79142700 | -2.36054500 | -1.42869500 |
| H | 2.89435700 | -1.98396800 | -1.49409200 |
| O | 1.19773200 | -1.97972200 | -0.85734300 |
| H | 0.48780200 | -2.31754600 | -1.44301000 |
| O | -0.68724200 | -3.64764600 | -1.02990000 |

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| H | -1.54514200 | -3.17462800 | -0.96544600 |
| O | -2.91084900 | -2.25670700 | -0.47751700 |
| H | -3.67674700 | -1.97133300 | -1.00928900 |
| O | -5.46456700 | -1.89830900 | -1.07109800 |
| H | -6.24678900 | -1.47798300 | -1.47265300 |
| O | -8.10150200 | -1.44978000 | -1.32863100 |
| O | -9.48904300 | -2.68400000 | -0.05450700 |
| O | -13.41997100 | -0.65145600 | -0.37853500 |
| H | -14.04906800 | -1.24305300 | 0.04792500 |
| O | 9.70768600 | -5.06165500 | -0.72379000 |
| H | 10.58263000 | -4.66038200 | -0.64842200 |
| N | 10.57264400 | 3.76796600 | -1.99067900 |
| H | 9.76900400 | 3.99802400 | -2.57123900 |
| H | 11.14408300 | 3.12065500 | -2.52429900 |

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|---|-------------|------------|------------|
| C | 0.68543200 | 2.90778700 | 3.03757800 |
| H | 0.94719900 | 3.23624500 | 2.02781100 |
| H | 1.42552900 | 2.16872300 | 3.35841200 |
| H | 0.77381800 | 3.77477600 | 3.69941100 |
| C | -0.73190200 | 2.34322900 | 3.06311900 |
| H | -0.99224900 | 2.03718700 | 4.08405900 |
| H | -0.78047600 | 1.43087000 | 2.45418700 |

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| C | -1.76952800 | 3.33410500 | 2.54148500 |
| H | -1.51138000 | 3.59559300 | 1.50909600 |
| H | -1.70971900 | 4.26549700 | 3.12001700 |
| C | -3.19690900 | 2.79660900 | 2.59014400 |
| H | -3.51343700 | 2.67596800 | 3.63446600 |
| H | -3.22604200 | 1.79493700 | 2.14608700 |
| C | -4.19597600 | 3.67520600 | 1.84398600 |
| H | -3.89902300 | 3.71676300 | 0.78664100 |
| H | -4.13814100 | 4.70741900 | 2.21352800 |
| C | -5.63298000 | 3.17063100 | 1.94185000 |
| H | -5.98332100 | 3.25068300 | 2.97881000 |
| H | -5.64555800 | 2.10157300 | 1.69629100 |
| C | -6.59330600 | 3.90922800 | 1.01391300 |
| H | -6.21900300 | 3.82690600 | -0.01691100 |
| H | -6.58976100 | 4.98228800 | 1.24381000 |
| C | -8.02064000 | 3.37219900 | 1.06457400 |
| H | -8.44682000 | 3.53809200 | 2.06146800 |
| H | -7.99477600 | 2.28245200 | 0.94246100 |
| C | -8.94735800 | 3.96209800 | -0.00006000 |
| H | -8.39521000 | 4.07723500 | -0.94243000 |
| H | -9.25905100 | 4.97301600 | 0.29114100 |
| C | -10.16405300 | 3.07742900 | -0.25016300 |
| H | -10.65287100 | 2.84591200 | 0.70187800 |
| H | -9.81840900 | 2.11275700 | -0.64137600 |
| C | -11.18928200 | 3.67348900 | -1.20965800 |
| H | -10.68740200 | 4.09534500 | -2.08969200 |

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| H | -11.70841200 | 4.51270800 | -0.72674200 |
| C | -12.20286400 | 2.64439100 | -1.69476100 |
| H | -12.96927400 | 3.12388800 | -2.32036100 |
| H | -11.69984400 | 1.89533200 | -2.31287700 |
| O | -12.80280200 | 1.90552200 | -0.63918000 |
| H | -13.23573800 | 2.52726800 | -0.04190500 |
| C | 11.41658800 | -2.78366200 | 1.56466800 |
| H | 12.19422200 | -2.27687800 | 0.97948900 |
| C | 11.15679300 | -4.13155900 | 0.89346200 |
| H | 10.38987400 | -4.66514500 | 1.47620600 |
| C | 10.60349900 | -3.92583200 | -0.51155000 |
| H | 11.35620800 | -3.36919700 | -1.09583400 |
| C | 9.59859400 | -1.87892700 | 0.12030300 |
| H | 10.29212800 | -1.31074700 | -0.51851900 |
| C | 10.15548500 | -1.92685800 | 1.54037000 |
| H | 10.38839000 | -0.89294600 | 1.83500100 |
| C | 10.27297000 | -5.22680100 | -1.20695800 |
| H | 9.50277400 | -5.76046400 | -0.64378600 |
| H | 11.16592000 | -5.85147900 | -1.26163600 |
| H | 9.89698400 | -5.03787500 | -2.21491600 |
| C | 7.68338300 | -0.98335400 | -1.02194300 |
| H | 7.81220600 | -1.84248500 | -1.68830600 |
| C | 6.23774600 | -0.83592100 | -0.66489600 |
| H | 5.99008400 | -0.04504900 | 0.03827900 |
| C | 5.27065300 | -1.62622200 | -1.14072400 |
| H | 5.51792500 | -2.42167900 | -1.84311900 |

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| C | 3.88397900 | -1.49760800 | -0.74015200 |
| H | 3.65764100 | -0.70216300 | -0.03428200 |
| C | 2.88244700 | -2.29740000 | -1.15321400 |
| H | 3.09103400 | -3.10296800 | -1.85669100 |
| C | 1.52643600 | -2.14498200 | -0.68298400 |
| H | 1.35673100 | -1.32182900 | 0.00792300 |
| C | 0.48244500 | -2.92125000 | -1.03677700 |
| H | 0.62974600 | -3.74656600 | -1.73253700 |
| C | -0.84654700 | -2.71226100 | -0.51775100 |
| H | -0.97646900 | -1.86881000 | 0.16043200 |
| C | -1.92458400 | -3.46657200 | -0.81507200 |
| H | -1.81979500 | -4.30214400 | -1.50614800 |
| C | -3.22744800 | -3.24064900 | -0.24057200 |
| H | -3.31032600 | -2.42312400 | 0.47589500 |
| C | -4.33195200 | -3.96198500 | -0.52044000 |
| H | -4.27244200 | -4.76846400 | -1.25036800 |
| C | -5.60809000 | -3.72892300 | 0.11220500 |
| H | -5.63071700 | -2.97170700 | 0.89440300 |
| C | -6.75786900 | -4.35685800 | -0.19572000 |
| H | -6.77232100 | -5.09704500 | -0.99482100 |
| C | 8.30323700 | 0.26141000 | -1.66934700 |
| H | 9.34960300 | 0.04290900 | -1.89420000 |
| H | 7.80054600 | 0.46823000 | -2.61886000 |
| C | -8.01003400 | -4.05899000 | 0.47329700 |
| H | -7.92878700 | -3.41167900 | 1.34454000 |
| C | -9.22134900 | -4.46488600 | 0.07706000 |

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| H | -9.30811900 | -5.10188500 | -0.80468200 |
| C | -10.51161200 | -4.06912000 | 0.73868800 |
| H | -10.28378900 | -3.54234600 | 1.67259800 |
| C | -11.32125100 | -3.09502500 | -0.14063900 |
| H | -11.68871600 | -3.66452100 | -1.01166200 |
| C | -10.51423500 | -1.91231300 | -0.70502500 |
| H | -9.71298900 | -2.36418800 | -1.29918400 |
| C | -9.80317600 | -1.09819800 | 0.37944100 |
| H | -9.26134400 | -1.76730500 | 1.04004000 |
| C | -7.54126600 | -0.34596800 | 0.12452900 |
| C | -6.57722400 | 0.39421400 | -0.77080000 |
| H | -6.92437400 | 0.32146300 | -1.80375800 |
| H | -6.60941600 | 1.45181600 | -0.49006600 |
| C | -5.14288800 | -0.12106200 | -0.64060800 |
| H | -5.10342300 | -1.16245100 | -0.98917200 |
| C | -4.17646100 | 0.72128500 | -1.46001300 |
| H | -4.48708400 | 0.69187800 | -2.51001700 |
| H | -4.23842900 | 1.76334800 | -1.12279200 |
| C | -2.72368200 | 0.26421300 | -1.35973100 |
| H | -2.66013000 | -0.80615600 | -1.59802600 |
| C | -1.82158500 | 1.03396000 | -2.31844800 |
| H | -2.03805900 | 2.10526400 | -2.22599900 |
| H | -2.09873300 | 0.74408700 | -3.33635500 |
| C | -0.32426700 | 0.77961000 | -2.07734000 |
| H | -0.18430100 | -0.14944800 | -1.51988800 |
| H | 0.19614500 | 0.64478000 | -3.03037700 |

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| C | 0.37777100 | 1.91853700 | -1.33996700 |
| H | 0.41686900 | 2.79273700 | -2.00393300 |
| C | 1.82149100 | 1.53759800 | -0.94063800 |
| H | 2.21702900 | 0.79273700 | -1.64053300 |
| C | 2.76310100 | 2.73607000 | -0.89487600 |
| H | 2.38122900 | 3.46985800 | -0.17487100 |
| H | 2.77138600 | 3.21431900 | -1.88109300 |
| C | 4.19101600 | 2.34511000 | -0.52736700 |
| H | 4.53910500 | 1.57308100 | -1.22701100 |
| C | 5.14742100 | 3.52752900 | -0.60883000 |
| H | 4.80630400 | 4.32447900 | 0.05913500 |
| H | 5.14180200 | 3.91154100 | -1.63297400 |
| C | 6.58428900 | 3.17216200 | -0.22512700 |
| C | 7.56307200 | 4.30015100 | -0.51799000 |
| H | 7.34574000 | 5.16342300 | 0.11441100 |
| H | 7.46002700 | 4.60254700 | -1.56396900 |
| C | 9.00222000 | 3.86910100 | -0.29280600 |
| H | 9.14906900 | 3.67669000 | 0.78003900 |
| C | 9.29258600 | 2.55049700 | -1.06116400 |
| H | 9.31760900 | 2.80570000 | -2.12713600 |
| C | 8.20424400 | 1.50159400 | -0.78902700 |
| H | 8.27265000 | 1.20580100 | 0.26201500 |
| C | 10.64827300 | 2.02695000 | -0.66307100 |
| C | -10.65831400 | -0.16608900 | 1.21135500 |
| H | -10.02814300 | 0.37971100 | 1.91818200 |
| H | -11.37939300 | -0.76854600 | 1.76650700 |

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| H | -11.20892400 | 0.54964000 | 0.60011300 |
| C | -11.35310200 | -1.04355800 | -1.64263000 |
| H | -12.16782000 | -0.52281600 | -1.13150700 |
| H | -11.77831500 | -1.64884800 | -2.44900900 |
| H | -10.72560000 | -0.27398700 | -2.09793500 |
| C | -11.36168200 | -5.29624400 | 1.08124100 |
| H | -11.58976400 | -5.87167700 | 0.17727400 |
| H | -12.30416900 | -4.99015500 | 1.53735800 |
| H | -10.82921100 | -5.95464100 | 1.77147200 |
| O | 9.22145700 | -2.50926800 | 2.42605500 |
| H | 8.34706400 | -2.22702800 | 2.12227200 |
| O | 12.35700400 | -4.86591800 | 0.81905500 |
| H | 12.78259200 | -4.70899700 | 1.67762700 |
| O | 9.40218600 | -3.16630200 | -0.42255000 |
| O | 8.35679600 | -1.26003400 | 0.21800400 |
| O | 6.70113600 | 2.85595300 | 1.13124300 |
| H | 5.91960900 | 2.32030600 | 1.35970200 |
| O | 6.92506200 | 2.06076600 | -1.04832800 |
| O | 10.88513400 | 1.00349100 | -0.06644800 |
| O | 11.64957000 | 2.87189800 | -1.01588500 |
| H | 12.47247400 | 2.47637500 | -0.68466300 |
| O | 4.25449400 | 1.82186600 | 0.80208700 |
| H | 3.41590600 | 1.35488600 | 0.97146100 |
| O | 1.77296600 | 0.89896100 | 0.33811900 |
| H | 1.01400200 | 1.33127100 | 0.77628300 |
| O | -0.29264100 | 2.31321700 | -0.15135800 |

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| H | -1.05519000 | 1.71597700 | 0.00787700 |
| O | -2.21983900 | 0.45682300 | -0.03325100 |
| H | -2.93455200 | 0.22318200 | 0.58698300 |
| O | -4.70589900 | -0.06972500 | 0.71715900 |
| H | -5.40499500 | -0.48706000 | 1.25408800 |
| O | -7.20474100 | -0.89553900 | 1.16217000 |
| O | -8.78413000 | -0.31808600 | -0.33261700 |
| O | -12.42280500 | -2.67315800 | 0.65360600 |
| H | -13.01136300 | -2.14210300 | 0.10519900 |
| O | 9.80845900 | 4.93730300 | -0.73993600 |
| H | 10.73102200 | 4.65390900 | -0.71124700 |
| N | 11.95553800 | -3.04819400 | 2.89600800 |
| H | 11.17864900 | -3.29483700 | 3.50546700 |
| H | 12.37772200 | -2.21063800 | 3.28415300 |

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| C | 10.01736600 | 4.14794700 | -0.98696100 |
| H | 10.82818100 | 3.67200200 | -0.42109700 |
| C | 9.38114100 | 5.18452200 | -0.06161400 |
| H | 8.59529200 | 5.71487100 | -0.61855100 |
| C | 8.72828100 | 4.50108200 | 1.13306300 |
| H | 9.51159800 | 3.95447700 | 1.68341200 |
| C | 8.30018500 | 2.54943700 | -0.12292800 |
| H | 9.02545900 | 1.98315200 | 0.48458700 |

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| C | 8.99064400 | 3.08585600 | -1.37619400 |
| H | 9.48095900 | 2.23796200 | -1.87681800 |
| C | 8.03692700 | 5.48159200 | 2.05366300 |
| H | 7.23922700 | 5.99225500 | 1.50986900 |
| H | 8.75629400 | 6.22101000 | 2.40588000 |
| H | 7.60037900 | 4.96123700 | 2.90709400 |
| C | 6.49269600 | 1.09021300 | 0.45721600 |
| H | 6.35070100 | 1.79346900 | 1.28156000 |
| C | 5.16190900 | 0.77848800 | -0.15734600 |
| H | 5.16678300 | 0.19246800 | -1.07414300 |
| C | 4.00602100 | 1.19981600 | 0.36469100 |
| H | 4.01390200 | 1.78017900 | 1.28574300 |
| C | 2.71333200 | 0.96672500 | -0.25097600 |
| H | 2.70001600 | 0.40374200 | -1.18271700 |
| C | 1.55744600 | 1.45112100 | 0.24165200 |
| H | 1.57648900 | 2.02070000 | 1.16976700 |
| C | 0.27549900 | 1.28808800 | -0.40450600 |
| H | 0.25816000 | 0.71258900 | -1.32893200 |
| C | -0.86857700 | 1.81800300 | 0.07643300 |
| H | -0.83487500 | 2.39226100 | 1.00167900 |
| C | -2.15653800 | 1.67981800 | -0.55975300 |
| H | -2.21625800 | 1.08902700 | -1.47297600 |
| C | -3.28531500 | 2.23032300 | -0.06347600 |
| H | -3.22912500 | 2.80993100 | 0.85751900 |
| C | -4.58936600 | 2.09237700 | -0.66717500 |
| H | -4.65547200 | 1.51978400 | -1.59131400 |

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| C | -5.71163800 | 2.60931500 | -0.12371500 |
| H | -5.63173800 | 3.16590500 | 0.80940000 |
| C | -7.03644900 | 2.45937100 | -0.68264100 |
| H | -7.11552200 | 1.98003800 | -1.65684500 |
| C | -8.16153400 | 2.84921000 | -0.05153300 |
| H | -8.08372300 | 3.30526200 | 0.93480300 |
| C | 7.25104100 | -0.14095900 | 0.96414700 |
| H | 8.21404300 | 0.18323200 | 1.36648700 |
| H | 6.67936800 | -0.58344500 | 1.78592700 |
| C | -9.49667100 | 2.65746400 | -0.58834200 |
| H | -9.55569600 | 2.30224300 | -1.61473200 |
| C | -10.62144800 | 2.84178300 | 0.11397400 |
| H | -10.54667300 | 3.18769400 | 1.14692700 |
| C | -12.01039500 | 2.58592400 | -0.39754500 |
| H | -11.95916000 | 2.33530500 | -1.46232600 |
| C | -12.66105100 | 1.39162900 | 0.32678600 |
| H | -12.88995000 | 1.71474900 | 1.35504800 |
| C | -11.76970900 | 0.14375900 | 0.44447400 |
| H | -10.88947700 | 0.45996900 | 1.00926800 |
| C | -11.23759000 | -0.33752700 | -0.90918100 |
| H | -10.92662800 | 0.51548800 | -1.50515200 |
| C | -8.94352800 | -0.84786500 | -1.33487000 |
| C | -7.77078000 | -1.72138000 | -0.95095200 |
| H | -7.90001500 | -2.06593800 | 0.07673900 |
| H | -7.80558200 | -2.59928300 | -1.60670300 |
| C | -6.41881700 | -1.01926300 | -1.12861600 |

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| H | -6.35564800 | -0.18020300 | -0.41902800 |
| C | -5.26907900 | -1.99294400 | -0.88078700 |
| H | -5.38953600 | -2.43996500 | 0.11196300 |
| H | -5.34165800 | -2.79609700 | -1.62447600 |
| C | -3.87671000 | -1.36373000 | -0.96652700 |
| H | -3.79980000 | -0.57357000 | -0.20075500 |
| C | -2.78364700 | -2.40346400 | -0.71840100 |
| H | -2.93510100 | -3.18628400 | -1.47351200 |
| H | -2.92051000 | -2.86823700 | 0.26392000 |
| C | -1.38782800 | -1.79113100 | -0.83545400 |
| H | -1.35065100 | -1.17917700 | -1.73982000 |
| H | -1.20913500 | -1.12468800 | 0.01442300 |
| C | -0.25673500 | -2.81123600 | -0.90417500 |
| H | -0.27259200 | -3.46376800 | -0.01938500 |
| C | 1.11472100 | -2.13747100 | -0.99948600 |
| H | 1.21933500 | -1.41130500 | -0.18658700 |
| C | 2.26604400 | -3.14132900 | -0.95164000 |
| H | 2.13799000 | -3.86946300 | -1.75971300 |
| H | 2.20983800 | -3.68487900 | -0.00099200 |
| C | 3.64987700 | -2.49767900 | -1.05151700 |
| H | 3.77712600 | -1.77691200 | -0.23274100 |
| C | 4.74709300 | -3.55168000 | -0.95353000 |
| H | 4.60437200 | -4.30104100 | -1.73821000 |
| H | 4.66709400 | -4.05009500 | 0.01742500 |
| C | 6.16306900 | -2.98812600 | -1.09544400 |
| C | 7.22656900 | -4.02105900 | -0.75409900 |

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| H | 7.20689800 | -4.83439400 | -1.48152300 |
| H | 7.02837100 | -4.43386900 | 0.23939300 |
| C | 8.61069600 | -3.39875300 | -0.73875200 |
| H | 8.86890700 | -3.07309500 | -1.75560400 |
| C | 8.61953200 | -2.15513600 | 0.18883900 |
| H | 8.53685200 | -2.53670700 | 1.21446000 |
| C | 7.45298600 | -1.20333900 | -0.11316900 |
| H | 7.62291400 | -0.72617000 | -1.08366200 |
| C | 9.98376400 | -1.51985700 | 0.05897700 |
| C | -12.16611100 | -1.21449800 | -1.72742300 |
| H | -11.71229200 | -1.43287000 | -2.69589200 |
| H | -13.10786900 | -0.68767600 | -1.88619300 |
| H | -12.36508800 | -2.15744900 | -1.21521200 |
| C | -12.45954200 | -0.96503800 | 1.23716500 |
| H | -13.38305700 | -1.29702300 | 0.75474100 |
| H | -12.70449900 | -0.62004400 | 2.24487900 |
| H | -11.80594600 | -1.83501000 | 1.32916400 |
| C | -12.89255100 | 3.82928300 | -0.24227800 |
| H | -12.93615000 | 4.13776700 | 0.80686900 |
| H | -13.90589800 | 3.61737400 | -0.58356500 |
| H | -12.48812000 | 4.66091700 | -0.82109900 |
| O | 8.05563000 | 3.69625200 | -2.23653200 |
| H | 7.24364700 | 3.17926400 | -2.17782600 |
| O | 10.36794400 | 6.07266900 | 0.40887800 |
| H | 10.89985800 | 6.28537600 | -0.36897000 |
| O | 7.75020000 | 3.58317100 | 0.65696500 |

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| O | 7.26277000 | 1.73998000 | -0.56919900 |
| O | 6.43283000 | -2.52205000 | -2.38517700 |
| H | 5.63772100 | -2.06019600 | -2.69092700 |
| O | 6.23320200 | -1.92878200 | -0.14953200 |
| O | 11.01953100 | -2.09742100 | 0.27299000 |
| O | 9.97505500 | -0.24863500 | -0.38079800 |
| H | 10.90146100 | 0.01623800 | -0.47242500 |
| O | 3.83114100 | -1.81052000 | -2.29218700 |
| H | 2.98321900 | -1.41415600 | -2.53755200 |
| O | 1.15839100 | -1.38140200 | -2.21728200 |
| H | 0.72400300 | -1.93737000 | -2.87994800 |
| O | -0.33812400 | -3.59993700 | -2.09207700 |
| H | -1.25130100 | -3.85661700 | -2.23627600 |
| O | -3.61474000 | -0.80931500 | -2.24675500 |
| H | -4.45723600 | -0.53776200 | -2.63426000 |
| O | -6.26964900 | -0.52495200 | -2.45543600 |
| H | -7.10172900 | -0.10192000 | -2.71209400 |
| O | -8.89735700 | -0.02075200 | -2.22093100 |
| O | -10.02957000 | -1.10588200 | -0.61929300 |
| O | -13.87503100 | 1.12177100 | -0.36629300 |
| H | -14.44379000 | 0.59808500 | 0.20287400 |
| O | 9.49739800 | -4.39186900 | -0.28010000 |
| H | 10.35486100 | -3.97880600 | -0.12439200 |
| N | 10.61130100 | 4.86497600 | -2.11307400 |
| H | 9.86657100 | 5.09727800 | -2.76592600 |
| H | 11.26718200 | 4.27495200 | -2.61279400 |

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| C | -8.60558800 | 0.40695100 | 2.34470000 |
| H | -8.62696400 | 0.11476300 | 1.28986800 |
| H | -9.28915700 | 1.25234800 | 2.46029200 |
| H | -8.99506500 | -0.42952500 | 2.93339600 |
| C | -7.18793100 | 0.77525000 | 2.76391000 |
| H | -7.18350000 | 1.16999300 | 3.78524600 |
| H | -6.82496900 | 1.57886500 | 2.11663600 |
| C | -6.21119300 | -0.39578800 | 2.67583400 |
| H | -6.38152800 | -0.94124300 | 1.73834600 |
| H | -6.40959100 | -1.10880100 | 3.48516100 |
| C | -4.75839300 | 0.06600000 | 2.72174800 |
| H | -4.61375100 | 0.72875400 | 3.58433200 |
| H | -4.55625400 | 0.67175600 | 1.82956000 |
| C | -3.74874100 | -1.07383200 | 2.79139100 |
| H | -3.95482400 | -1.79206900 | 1.98692000 |
| H | -3.87672000 | -1.62259600 | 3.73223800 |
| C | -2.30881700 | -0.58264100 | 2.67239500 |
| H | -2.11942500 | 0.16960500 | 3.44872000 |
| H | -2.18442600 | -0.06545000 | 1.71262800 |
| C | -1.27874000 | -1.69981300 | 2.79580000 |
| H | -1.46537200 | -2.45767800 | 2.02283300 |
| H | -1.41145300 | -2.21060500 | 3.75735400 |
| C | 0.16399800 | -1.21445200 | 2.68187500 |
| H | 0.36536500 | -0.48130400 | 3.47242600 |
| H | 0.30231800 | -0.67962500 | 1.73349300 |
| C | 1.16364400 | -2.36151400 | 2.79042800 |

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|---|------------|-------------|------------|
| H | 0.95289000 | -3.10055200 | 2.00449900 |
| H | 1.00155300 | -2.88345800 | 3.74173000 |
| C | 2.62531500 | -1.93489200 | 2.70127100 |
| H | 2.84100600 | -1.17194700 | 3.45514400 |
| H | 2.82126400 | -1.46675900 | 1.72730400 |
| C | 3.56574200 | -3.11894000 | 2.91366400 |
| H | 3.35351600 | -3.90095400 | 2.17326300 |
| H | 3.37873600 | -3.55570200 | 3.90080100 |
| C | 5.03260500 | -2.75242100 | 2.80985200 |
| H | 5.64864900 | -3.64427200 | 2.98745900 |
| H | 5.25360200 | -2.37637100 | 1.80544000 |
| O | 5.30974900 | -1.75187600 | 3.78634500 |
| H | 6.25969900 | -1.62992300 | 3.83192700 |

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|---|-------------|-------------|------------|
| C | 13.16893000 | 0.09147600 | 1.17749900 |
| H | 13.15554300 | 0.27019500 | 0.09740000 |
| H | 13.73608200 | -0.82602800 | 1.35382000 |
| H | 13.71499600 | 0.91914200 | 1.64096700 |
| C | 11.75213600 | -0.01178200 | 1.73289000 |
| H | 11.79184700 | -0.21326200 | 2.81052300 |
| H | 11.25532000 | -0.88306000 | 1.28815700 |
| C | 10.92811000 | 1.25272100 | 1.48947500 |

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|---|-------------|------------|------------|
| H | 10.84218800 | 1.43046800 | 0.40808100 |
| H | 11.47199800 | 2.12024300 | 1.88495700 |
| C | 9.53231100 | 1.20950800 | 2.10516600 |
| H | 9.61865400 | 1.10078500 | 3.19490900 |
| H | 9.00779800 | 0.31630100 | 1.74793000 |
| C | 8.66732100 | 2.42315200 | 1.77388600 |
| H | 8.63627000 | 2.51903000 | 0.68177100 |
| H | 9.13793400 | 3.33673900 | 2.15845200 |
| C | 7.24944000 | 2.29146300 | 2.32197700 |
| H | 7.29293600 | 2.14699600 | 3.40996600 |
| H | 6.79730800 | 1.37789500 | 1.91138100 |
| C | 6.32988100 | 3.46522900 | 1.99753100 |
| H | 6.27056600 | 3.57727900 | 0.90934500 |
| H | 6.75818800 | 4.39811200 | 2.38631800 |
| C | 4.91697900 | 3.26154600 | 2.54202800 |
| H | 4.92031500 | 3.34292100 | 3.63695700 |
| H | 4.61197400 | 2.23435900 | 2.31343300 |
| C | 3.88283700 | 4.21274300 | 1.94406600 |
| H | 4.00911200 | 4.20763700 | 0.85647500 |
| H | 4.06561500 | 5.24083100 | 2.28152500 |
| C | 2.44621500 | 3.80296300 | 2.26028400 |
| H | 2.27348600 | 3.87539200 | 3.34210000 |
| H | 2.31785300 | 2.74874700 | 1.98525500 |
| C | 1.39704900 | 4.62199200 | 1.51207000 |
| H | 1.64352100 | 4.62768700 | 0.44224700 |
| H | 1.41607300 | 5.66394400 | 1.85128500 |

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|---|-------------|-------------|-------------|
| C | -0.01287300 | 4.06678000 | 1.67012200 |
| H | -0.73049400 | 4.67586100 | 1.11298200 |
| H | -0.04920300 | 3.05443800 | 1.24085000 |
| O | -0.46415300 | 4.06768500 | 3.01426900 |
| H | 0.08447100 | 3.44734500 | 3.50684500 |
| C | 8.75149600 | -2.48380400 | 1.66647300 |
| H | 9.17373900 | -1.62034800 | 1.14157400 |
| C | 9.18745600 | -3.71333600 | 0.87344400 |
| H | 8.80961200 | -4.61401100 | 1.38073900 |
| C | 8.60002400 | -3.68019300 | -0.53423100 |
| H | 9.00477000 | -2.79954600 | -1.05771900 |
| C | 6.77792900 | -2.38159900 | 0.20235200 |
| H | 7.22673400 | -1.52083000 | -0.31615300 |
| C | 7.23811100 | -2.33154100 | 1.65339900 |
| H | 6.95519700 | -1.34670500 | 2.06093400 |
| C | 8.90680300 | -4.92779700 | -1.32880000 |
| H | 8.46045600 | -5.79873700 | -0.84139600 |
| H | 9.98749700 | -5.06882600 | -1.38394800 |
| H | 8.50015500 | -4.84476700 | -2.33867300 |
| C | 4.70629500 | -2.36336200 | -1.05334300 |
| H | 4.70232000 | -3.40346000 | -1.39707700 |
| C | 3.31518800 | -1.90724700 | -0.74249200 |
| H | 3.23081200 | -0.91373200 | -0.30984500 |
| C | 2.21073700 | -2.62965300 | -0.95222500 |
| H | 2.28585800 | -3.62795500 | -1.38236200 |
| C | 0.88917000 | -2.14594500 | -0.60353000 |

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|---|--------------|-------------|-------------|
| H | 0.84447600 | -1.15169500 | -0.16512800 |
| C | -0.25964300 | -2.83212300 | -0.75125900 |
| H | -0.24057000 | -3.83201400 | -1.18386700 |
| C | -1.53510400 | -2.29866600 | -0.33441300 |
| H | -1.51270800 | -1.29558500 | 0.08716100 |
| C | -2.71903100 | -2.93610100 | -0.42928900 |
| H | -2.76273500 | -3.93942600 | -0.85187200 |
| C | -3.95624200 | -2.34751500 | 0.02201400 |
| H | -3.90116400 | -1.33577400 | 0.42359300 |
| C | -5.16076300 | -2.95213700 | -0.02466200 |
| H | -5.23830600 | -3.95800900 | -0.43599800 |
| C | -6.37164300 | -2.34471100 | 0.46895000 |
| H | -6.28290900 | -1.34551300 | 0.89477600 |
| C | -7.58695100 | -2.92760300 | 0.43921600 |
| H | -7.69153900 | -3.91820400 | -0.00207200 |
| C | -8.77746800 | -2.31235100 | 0.97420900 |
| H | -8.64972000 | -1.35099400 | 1.46879200 |
| C | -10.01676200 | -2.82996900 | 0.89197500 |
| H | -10.16934700 | -3.77875200 | 0.37873800 |
| C | 5.40275000 | -1.50898500 | -2.12203700 |
| H | 6.37003400 | -1.95694100 | -2.35473900 |
| H | 4.80593800 | -1.54569600 | -3.03721700 |
| C | -11.18644400 | -2.15844300 | 1.42414100 |
| H | -10.98887400 | -1.26793200 | 2.01740600 |
| C | -12.45280900 | -2.51992700 | 1.19142700 |
| H | -12.65020300 | -3.40322600 | 0.58168900 |

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|---|--------------|-------------|-------------|
| C | -13.66014600 | -1.76576600 | 1.67093200 |
| H | -13.33960600 | -0.99408700 | 2.38004800 |
| C | -14.36512200 | -1.04649700 | 0.50464500 |
| H | -14.81347700 | -1.82413700 | -0.13585900 |
| C | -13.43871000 | -0.21430400 | -0.40133100 |
| H | -12.68929900 | -0.91380400 | -0.78433200 |
| C | -12.64487900 | 0.85254400 | 0.36110100 |
| H | -12.22738300 | 0.42459500 | 1.26831700 |
| C | -10.29320400 | 1.17876000 | 0.01215300 |
| C | -9.23644400 | 1.55011900 | -0.99762000 |
| H | -9.61149100 | 1.35745100 | -2.00445200 |
| H | -9.06339800 | 2.62869100 | -0.90564100 |
| C | -7.91719900 | 0.81447400 | -0.74951900 |
| H | -8.08832500 | -0.26822400 | -0.83456200 |
| C | -6.85487700 | 1.23586500 | -1.75461800 |
| H | -7.21155500 | 0.99903200 | -2.76272900 |
| H | -6.72018500 | 2.32259400 | -1.69571700 |
| C | -5.49775800 | 0.56980500 | -1.54158200 |
| H | -5.62664200 | -0.52065400 | -1.50746800 |
| C | -4.52601700 | 0.91531600 | -2.66493900 |
| H | -4.55729300 | 1.99776000 | -2.84009700 |
| H | -4.89588800 | 0.43950900 | -3.57819500 |
| C | -3.08051200 | 0.47424600 | -2.38358100 |
| H | -3.06439600 | -0.32123000 | -1.63458400 |
| H | -2.63618000 | 0.04753800 | -3.28818700 |
| C | -2.16317800 | 1.61080600 | -1.93530100 |

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|---|--------------|-------------|-------------|
| H | -2.04598700 | 2.31126000 | -2.77380800 |
| C | -0.76162900 | 1.08219700 | -1.53653100 |
| H | -0.57817300 | 0.11325700 | -2.01519200 |
| C | 0.36387200 | 2.04289300 | -1.90553200 |
| H | 0.18713900 | 3.01091700 | -1.42116100 |
| H | 0.34504500 | 2.20641700 | -2.98909700 |
| C | 1.73739500 | 1.51067300 | -1.51156200 |
| H | 1.88759700 | 0.52460400 | -1.97151400 |
| C | 2.86455500 | 2.42751300 | -1.96912800 |
| H | 2.71999800 | 3.42764500 | -1.54834600 |
| H | 2.83064300 | 2.50684200 | -3.05929200 |
| C | 4.25208000 | 1.93896100 | -1.55819600 |
| C | 5.37969700 | 2.78986700 | -2.13478300 |
| H | 5.34419000 | 3.79425700 | -1.70735100 |
| H | 5.26092900 | 2.86976100 | -3.21933800 |
| C | 6.72307800 | 2.15408300 | -1.82684600 |
| H | 6.84936900 | 2.12305500 | -0.73950900 |
| C | 6.74360300 | 0.71096300 | -2.34922100 |
| H | 6.59869200 | 0.70883700 | -3.43371200 |
| C | 5.55907900 | -0.05214900 | -1.70744100 |
| H | 5.66905000 | 0.00911900 | -0.61921400 |
| C | 8.06172200 | 0.02170700 | -2.10345200 |
| C | -13.37672800 | 2.13586300 | 0.69685600 |
| H | -12.73279600 | 2.78984600 | 1.28933500 |
| H | -14.27146100 | 1.89461800 | 1.27242600 |
| H | -13.67069700 | 2.67085700 | -0.20871000 |

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| C | -14.19732000 | 0.36082200 | -1.59626800 |
| H | -15.00959800 | 1.02388900 | -1.28374300 |
| H | -14.62925600 | -0.44084200 | -2.20229700 |
| H | -13.52867300 | 0.94244200 | -2.23486600 |
| C | -14.64558000 | -2.69053400 | 2.39092100 |
| H | -14.97142300 | -3.49951500 | 1.72762100 |
| H | -15.52765000 | -2.13297700 | 2.70864000 |
| H | -14.17766000 | -3.14544200 | 3.26688000 |
| O | 6.67403700 | -3.37472100 | 2.41411600 |
| H | 5.75748600 | -3.46450800 | 2.11805900 |
| O | 10.59586800 | -3.71953100 | 0.77927300 |
| H | 10.89395500 | -3.48605000 | 1.67367700 |
| O | 7.17761100 | -3.56389100 | -0.44180500 |
| O | 5.39286600 | -2.30635400 | 0.21465300 |
| O | 4.41019000 | 1.94225900 | -0.16668000 |
| H | 3.56836900 | 1.62939800 | 0.21361400 |
| O | 4.35826800 | 0.61403900 | -2.07177600 |
| O | 8.49771900 | -0.90497200 | -2.74168900 |
| O | 8.73511300 | 0.51937700 | -1.03493700 |
| H | 9.54701500 | -0.00650700 | -0.94428800 |
| O | 1.83315900 | 1.36782400 | -0.08966100 |
| H | 0.95205800 | 1.10115500 | 0.23673900 |
| O | -0.76855200 | 0.84186000 | -0.12717600 |
| H | -1.44959900 | 1.47083000 | 0.19594300 |
| O | -2.66034800 | 2.34455900 | -0.82625200 |
| H | -3.52109500 | 1.96462900 | -0.54405300 |

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|---|--------------|-------------|-------------|
| O | -4.91013800 | 0.98987400 | -0.30687700 |
| H | -5.63036400 | 1.09279700 | 0.34215700 |
| O | -7.41753400 | 1.10993200 | 0.55188100 |
| H | -8.15983500 | 1.00760200 | 1.17432100 |
| O | -10.03616900 | 0.91260700 | 1.17577700 |
| O | -11.51417200 | 1.19591900 | -0.50121300 |
| O | -15.39566600 | -0.25504800 | 1.08805000 |
| H | -16.03342600 | -0.02467400 | 0.40411200 |
| O | 7.73456600 | 2.94491700 | -2.42302100 |
| H | 8.55890800 | 2.74955500 | -1.96254500 |
| N | 9.36923000 | -2.54225500 | 2.98463800 |
| H | 8.81455600 | -3.15768400 | 3.57491200 |
| H | 9.36871100 | -1.62469100 | 3.41904000 |

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|---|-------------|------------|-------------|
| C | -7.00133500 | 4.08803400 | -3.08984900 |
| H | -7.39099200 | 4.92851500 | -2.50733300 |
| H | -7.78668700 | 3.32792400 | -3.13772900 |
| H | -6.82284100 | 4.44950700 | -4.10761700 |
| C | -5.72367900 | 3.53188300 | -2.46893300 |
| H | -5.36510000 | 2.68728100 | -3.07279100 |
| H | -5.94697700 | 3.13277600 | -1.47318700 |
| C | -4.60726100 | 4.56732000 | -2.34917300 |

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|---|-------------|------------|-------------|
| H | -4.92478700 | 5.36598800 | -1.66586800 |
| H | -4.44280800 | 5.04919100 | -3.32220300 |
| C | -3.29574500 | 3.96475300 | -1.85464900 |
| H | -2.94400800 | 3.23052700 | -2.59335900 |
| H | -3.47868200 | 3.40056500 | -0.93156700 |
| C | -2.19177100 | 4.98767600 | -1.60002500 |
| H | -2.49675500 | 5.65083200 | -0.78027000 |
| H | -2.06971500 | 5.62998000 | -2.48213300 |
| C | -0.85615700 | 4.33284400 | -1.25907500 |
| H | -0.51172800 | 3.75526300 | -2.12857900 |
| H | -1.00461300 | 3.60125300 | -0.45493200 |
| C | 0.23695500 | 5.31163300 | -0.84125600 |
| H | -0.07947600 | 5.83572500 | 0.07002400 |
| H | 0.35919100 | 6.08570600 | -1.61033700 |
| C | 1.57455700 | 4.62086000 | -0.59133600 |
| H | 1.93324400 | 4.18097800 | -1.53230400 |
| H | 1.42308700 | 3.77646800 | 0.09243700 |
| C | 2.65460500 | 5.53334000 | -0.01917900 |
| H | 2.30033200 | 5.95481900 | 0.93111600 |
| H | 2.81481500 | 6.38797800 | -0.68953700 |
| C | 3.97450100 | 4.80330800 | 0.20921600 |
| H | 4.37627000 | 4.45197600 | -0.74721700 |
| H | 3.78960300 | 3.90210000 | 0.80781900 |
| C | 5.03339600 | 5.65291800 | 0.90268300 |
| H | 4.65503600 | 6.00272000 | 1.87122900 |
| H | 5.25119800 | 6.54647600 | 0.30568400 |

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| C | 6.33035500 | 4.90090100 | 1.13512400 |
| H | 7.01587800 | 5.51214200 | 1.74138600 |
| H | 6.12164200 | 3.97842600 | 1.69819400 |
| O | 6.91019000 | 4.59736700 | -0.12385400 |
| H | 7.59224100 | 3.93240100 | 0.02602100 |
| C | -9.79427800 | 2.25057600 | 2.00791800 |
| H | -10.50221200 | 2.25237800 | 1.16949400 |
| C | -9.03027900 | 3.57046100 | 1.95676900 |
| H | -8.32266100 | 3.58983200 | 2.79994300 |
| C | -8.21591000 | 3.67296100 | 0.67197000 |
| H | -8.91635400 | 3.66321200 | -0.18027500 |
| C | -7.97471500 | 1.30217400 | 0.58760200 |
| H | -8.61005100 | 1.20857400 | -0.31150700 |
| C | -8.83166500 | 1.08312000 | 1.83272000 |
| H | -9.38330900 | 0.14461700 | 1.68491200 |
| C | -7.37399800 | 4.92935000 | 0.63999500 |
| H | -6.65220200 | 4.90539200 | 1.46068400 |
| H | -8.01753100 | 5.80214700 | 0.76149900 |
| H | -6.82555600 | 5.01014600 | -0.29882500 |
| C | -6.30377300 | 0.06479800 | -0.61522900 |
| H | -6.30803800 | 0.97336000 | -1.22528600 |
| C | -4.89517100 | -0.26777500 | -0.24021700 |
| H | -4.76629000 | -1.03825400 | 0.51543600 |
| C | -3.82773100 | 0.34056700 | -0.76494000 |
| H | -3.96154500 | 1.10586300 | -1.52724400 |
| C | -2.47392700 | 0.06055900 | -0.33412100 |

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| H | -2.35687900 | -0.67593100 | 0.45674700 |
| C | -1.37461500 | 0.67059900 | -0.81612500 |
| H | -1.47421400 | 1.41352700 | -1.60518800 |
| C | -0.05083700 | 0.40289700 | -0.30825700 |
| H | 0.01494400 | -0.34962000 | 0.47562100 |
| C | 1.07607800 | 1.00798300 | -0.73545800 |
| H | 1.01831500 | 1.76147500 | -1.51869300 |
| C | 2.37770400 | 0.71313200 | -0.19084400 |
| H | 2.42761700 | -0.06276000 | 0.57289700 |
| C | 3.52281400 | 1.31458500 | -0.57473900 |
| H | 3.48996400 | 2.08296100 | -1.34495000 |
| C | 4.81000300 | 1.01128200 | -0.00200900 |
| H | 4.83491300 | 0.25806600 | 0.78573300 |
| C | 5.96721400 | 1.58833700 | -0.38572100 |
| H | 5.95885800 | 2.34102200 | -1.17042300 |
| C | 7.23902800 | 1.27844700 | 0.22138300 |
| H | 7.21974000 | 0.63325300 | 1.09839900 |
| C | 8.43856100 | 1.70458000 | -0.22404200 |
| H | 8.49240200 | 2.29967200 | -1.13631500 |
| C | -7.05450000 | -1.04421600 | -1.36043500 |
| H | -8.05249800 | -0.66794800 | -1.59515300 |
| H | -6.54618200 | -1.26496800 | -2.30408200 |
| C | 9.68773500 | 1.34741200 | 0.42137100 |
| H | 9.59206500 | 0.81933300 | 1.36796900 |
| C | 10.90686100 | 1.57026200 | -0.08045300 |
| H | 11.00316900 | 2.08571700 | -1.03747900 |

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| C | 12.18829100 | 1.11916000 | 0.55994700 |
| H | 11.96871700 | 0.73658600 | 1.56332400 |
| C | 12.83187300 | -0.03399100 | -0.23415900 |
| H | 13.18991700 | 0.38575900 | -1.18891300 |
| C | 11.87686400 | -1.18716300 | -0.59463200 |
| H | 11.07091100 | -0.73392100 | -1.18014100 |
| C | 11.18851100 | -1.81090700 | 0.62451300 |
| H | 10.81188400 | -1.02705000 | 1.27574600 |
| C | 8.83329000 | -2.28368400 | 0.63289500 |
| C | 7.73809900 | -3.07204100 | -0.04021800 |
| H | 8.03867900 | -3.30745900 | -1.06300700 |
| H | 7.63552800 | -4.01905400 | 0.50236900 |
| C | 6.39590300 | -2.33843500 | -0.01309200 |
| H | 6.49845700 | -1.37748800 | -0.53771200 |
| C | 5.30690000 | -3.16283500 | -0.68379600 |
| H | 5.59456900 | -3.33944000 | -1.72573500 |
| H | 5.24070600 | -4.13844600 | -0.18747600 |
| C | 3.92565200 | -2.51367300 | -0.65500800 |
| H | 3.99185700 | -1.49244000 | -1.05482500 |
| C | 2.92325700 | -3.30496500 | -1.48855500 |
| H | 3.00259100 | -4.36631800 | -1.22283200 |
| H | 3.22907600 | -3.22046000 | -2.53578400 |
| C | 1.47070000 | -2.83076900 | -1.31919200 |
| H | 1.44791700 | -1.80708800 | -0.93789600 |
| H | 0.96984300 | -2.80193600 | -2.29190300 |
| C | 0.62862700 | -3.72801100 | -0.41468500 |

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| H | 0.52805200 | -4.70859900 | -0.90007000 |
| C | -0.79490300 | -3.14269500 | -0.19289900 |
| H | -1.00709700 | -2.38868000 | -0.95961200 |
| C | -1.88518800 | -4.20744100 | -0.22996000 |
| H | -1.68134900 | -4.96276400 | 0.53898800 |
| H | -1.85102500 | -4.70974700 | -1.20390400 |
| C | -3.28277800 | -3.63161200 | -0.01817400 |
| H | -3.45433500 | -2.82458300 | -0.74338400 |
| C | -4.36437900 | -4.68668200 | -0.21166600 |
| H | -4.17729600 | -5.53406000 | 0.45532000 |
| H | -4.31643200 | -5.04683400 | -1.24336700 |
| C | -5.77889500 | -4.17858400 | 0.06838500 |
| C | -6.84679300 | -5.18081200 | -0.34596900 |
| H | -6.77760400 | -6.08240700 | 0.26617600 |
| H | -6.68912900 | -5.46006500 | -1.39157900 |
| C | -8.24616400 | -4.60297000 | -0.22164800 |
| H | -8.46295500 | -4.42904300 | 0.84258800 |
| C | -8.32782400 | -3.23739700 | -0.95749700 |
| H | -8.28282300 | -3.45436900 | -2.03161100 |
| C | -7.16065700 | -2.32704900 | -0.54780100 |
| H | -7.28592300 | -2.07343800 | 0.50863600 |
| C | -9.64975700 | -2.57375300 | -0.66449000 |
| C | 12.00381200 | -2.79750800 | 1.43460100 |
| H | 11.43414500 | -3.12799100 | 2.30611700 |
| H | 12.92181600 | -2.31081600 | 1.76683800 |
| H | 12.26400200 | -3.67572200 | 0.83982500 |

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| C | 12.56668000 | -2.22714700 | -1.47601000 |
| H | 13.43271800 | -2.67459800 | -0.97910000 |
| H | 12.90996300 | -1.77463600 | -2.41082600 |
| H | 11.87908700 | -3.03782300 | -1.72704400 |
| C | 13.17956200 | 2.27794500 | 0.70023700 |
| H | 13.40661500 | 2.71238800 | -0.27961300 |
| H | 14.11277400 | 1.92804700 | 1.14364100 |
| H | 12.76247700 | 3.06899600 | 1.32751800 |
| O | -8.02363800 | 1.01931000 | 2.99096600 |
| H | -7.22307400 | 0.53719700 | 2.74161900 |
| O | -9.93560100 | 4.64897400 | 2.01437400 |
| H | -10.58969500 | 4.37205400 | 2.67636300 |
| O | -7.33005800 | 2.55854400 | 0.58446500 |
| O | -6.98880600 | 0.32721700 | 0.62035100 |
| O | -5.97012300 | -3.89527600 | 1.42421200 |
| H | -5.15892500 | -3.44881400 | 1.72837700 |
| O | -5.92934200 | -3.01012200 | -0.73180800 |
| O | -9.82567900 | -1.51737300 | -0.10574000 |
| O | -10.70403200 | -3.31968500 | -1.08195700 |
| H | -11.50384200 | -2.83436500 | -0.82144100 |
| O | -3.41519300 | -3.09859800 | 1.30217500 |
| H | -2.54925600 | -2.72611400 | 1.55079400 |
| O | -0.80984800 | -2.46064700 | 1.06123600 |
| H | -0.08299900 | -2.89745100 | 1.55418700 |
| O | 1.20719600 | -3.94391600 | 0.86448100 |
| H | 2.04574500 | -3.43860800 | 0.93058200 |

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| O | 3.42662700 | -2.43943700 | 0.68353500 |
| H | 4.18018700 | -2.23804100 | 1.26734500 |
| O | 5.98860400 | -2.09686900 | 1.33153000 |
| H | 6.74891700 | -1.69777600 | 1.79005200 |
| O | 8.63327700 | -1.53146800 | 1.57344200 |
| O | 10.02240900 | -2.51808900 | 0.09753900 |
| O | 13.94251600 | -0.47801600 | 0.53916100 |
| H | 14.53652000 | -0.97804200 | -0.03070900 |
| O | -9.11802800 | -5.56454200 | -0.77461000 |
| H | -10.00669000 | -5.18795300 | -0.79849900 |
| N | -10.56541800 | 2.23148300 | 3.24809000 |
| H | -9.93162300 | 1.99336400 | 4.00797400 |
| H | -11.27350800 | 1.50484000 | 3.21823600 |

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| C | 10.91969000 | -3.89000600 | 0.91734500 |
| H | 11.63828500 | -3.43745700 | 0.22254100 |
| C | 10.39414100 | -5.15816100 | 0.24662600 |
| H | 9.70334600 | -5.65915500 | 0.94010400 |
| C | 9.61921700 | -4.80753300 | -1.01721900 |
| H | 10.30821700 | -4.29232500 | -1.70660300 |
| C | 8.98029700 | -2.71258400 | -0.13032700 |
| H | 9.60552100 | -2.18777200 | -0.87116900 |

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|---|-------------|-------------|-------------|
| C | 9.77411600 | -2.91132600 | 1.16019200 |
| H | 10.16164200 | -1.92923700 | 1.46887400 |
| C | 9.02958700 | -6.02762900 | -1.68903000 |
| H | 8.31312800 | -6.50183900 | -1.01487000 |
| H | 9.82486900 | -6.73670500 | -1.91921300 |
| H | 8.51267300 | -5.74640600 | -2.60731000 |
| C | 6.98782400 | -1.60737900 | -0.86800300 |
| H | 6.91240900 | -2.45971400 | -1.54860600 |
| C | 5.64559200 | -1.35270900 | -0.25065700 |
| H | 5.60596000 | -0.63540000 | 0.56669800 |
| C | 4.53305600 | -1.96848200 | -0.66196600 |
| H | 4.59091200 | -2.67547600 | -1.48828100 |
| C | 3.22550400 | -1.77951100 | -0.06085800 |
| H | 3.16242800 | -1.12923500 | 0.80977700 |
| C | 2.11231900 | -2.38879700 | -0.51159400 |
| H | 2.18602200 | -3.03500800 | -1.38527500 |
| C | 0.80481900 | -2.25886200 | 0.09125400 |
| H | 0.73047700 | -1.64810400 | 0.99006300 |
| C | -0.29454000 | -2.85516500 | -0.41547300 |
| H | -0.19240500 | -3.44955300 | -1.32261200 |
| C | -1.61905200 | -2.77052000 | 0.15264900 |
| H | -1.74969200 | -2.21191200 | 1.07882400 |
| C | -2.69626200 | -3.34078100 | -0.42815700 |
| H | -2.56363400 | -3.87727800 | -1.36661600 |
| C | -4.03744100 | -3.29196700 | 0.10429900 |
| H | -4.17728600 | -2.81081000 | 1.07175400 |

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| C | -5.10591500 | -3.79728400 | -0.54707500 |
| H | -4.95623600 | -4.24969700 | -1.52629300 |
| C | -6.46029700 | -3.77528500 | -0.04233700 |
| H | -6.60699800 | -3.42597600 | 0.97825600 |
| C | -7.53412600 | -4.14017200 | -0.76870900 |
| H | -7.39047000 | -4.46297700 | -1.79855300 |
| C | 7.57580100 | -0.40800700 | -1.62129600 |
| H | 8.55352900 | -0.69340500 | -2.01740100 |
| H | 6.93317500 | -0.16797000 | -2.47305100 |
| C | -8.89863700 | -4.09322800 | -0.27341300 |
| H | -9.01802200 | -3.89827800 | 0.79029300 |
| C | -9.98456800 | -4.22725200 | -1.04467700 |
| H | -9.85305700 | -4.41432000 | -2.11203800 |
| C | -11.40357900 | -4.11482800 | -0.56458300 |
| H | -11.40617400 | -4.01031000 | 0.52564100 |
| C | -12.09232700 | -2.86708900 | -1.15046300 |
| H | -12.25153100 | -3.05326400 | -2.22438700 |
| C | -11.27535100 | -1.56671700 | -1.04221600 |
| H | -10.35094500 | -1.74527700 | -1.60025200 |
| C | -10.83662300 | -1.26067800 | 0.39328100 |
| H | -10.47440300 | -2.16772300 | 0.86829200 |
| C | -8.57971300 | -0.67644400 | 0.97044400 |
| C | -7.46584700 | 0.31248400 | 0.74917800 |
| H | -7.60185800 | 0.80072800 | -0.21647500 |
| H | -7.56614400 | 1.08870200 | 1.51593300 |
| C | -6.08482000 | -0.33632600 | 0.83905600 |

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| H | -5.99315500 | -1.09458600 | 0.04862200 |
| C | -4.99475700 | 0.71196100 | 0.66378000 |
| H | -5.15627000 | 1.22725100 | -0.28883100 |
| H | -5.09212200 | 1.45468600 | 1.46537900 |
| C | -3.57682000 | 0.14443500 | 0.68200700 |
| H | -3.49592200 | -0.63357100 | -0.09322500 |
| C | -2.55165300 | 1.23518500 | 0.39304500 |
| H | -2.71937900 | 2.02311600 | 1.13983400 |
| H | -2.75011700 | 1.67386500 | -0.59138600 |
| C | -1.12027800 | 0.70919800 | 0.45797400 |
| H | -0.99034000 | 0.14275800 | 1.38355100 |
| H | -0.94791100 | 0.01863500 | -0.37445500 |
| C | -0.06847400 | 1.80947700 | 0.41344800 |
| H | -0.18346500 | 2.41019000 | -0.50052700 |
| C | 1.35689100 | 1.25954500 | 0.45747500 |
| H | 1.47099100 | 0.48372400 | -0.30656800 |
| C | 2.39599400 | 2.35840800 | 0.24515800 |
| H | 2.26357600 | 3.13108600 | 1.01064000 |
| H | 2.20843300 | 2.82609100 | -0.72811500 |
| C | 3.83779900 | 1.85608300 | 0.26871000 |
| H | 3.96596500 | 1.06445700 | -0.48191300 |
| C | 4.80728300 | 2.99129600 | -0.04044100 |
| H | 4.64179200 | 3.81471400 | 0.66165400 |
| H | 4.60640000 | 3.35545500 | -1.05186700 |
| C | 6.27953800 | 2.59412800 | 0.04795000 |
| C | 7.19923600 | 3.67904000 | -0.49506000 |

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| H | 7.13490500 | 4.57367500 | 0.12731900 |
| H | 6.89656900 | 3.93607500 | -1.51362400 |
| C | 8.64132600 | 3.20569900 | -0.53609300 |
| H | 8.99946600 | 3.06041200 | 0.49247100 |
| C | 8.73471800 | 1.84412600 | -1.27739700 |
| H | 8.55087600 | 2.05349800 | -2.33802000 |
| C | 7.69791400 | 0.83965200 | -0.75437000 |
| H | 7.96004200 | 0.55714200 | 0.26998100 |
| C | 10.16714600 | 1.38492200 | -1.15513300 |
| C | -11.86018900 | -0.58757400 | 1.28773000 |
| H | -11.45512800 | -0.47453100 | 2.29495600 |
| H | -12.76021500 | -1.20179800 | 1.33082000 |
| H | -12.12590800 | 0.40184300 | 0.90845900 |
| C | -12.00741200 | -0.39474000 | -1.69453600 |
| H | -12.96354100 | -0.19156400 | -1.20496300 |
| H | -12.20042500 | -0.60173900 | -2.75010400 |
| H | -11.41109700 | 0.51930300 | -1.63896300 |
| C | -12.20834000 | -5.36778200 | -0.92704600 |
| H | -12.20145900 | -5.52501900 | -2.01005400 |
| H | -13.24228800 | -5.26108200 | -0.59893600 |
| H | -11.77411300 | -6.25064200 | -0.45596900 |
| O | 8.95523100 | -3.46062200 | 2.16783800 |
| H | 8.08265700 | -3.06298300 | 2.06451600 |
| O | 11.47170900 | -5.99585200 | -0.10179500 |
| H | 12.05546500 | -5.98029700 | 0.66778800 |
| O | 8.54624800 | -3.93674800 | -0.67437700 |

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| O | 7.86093200 | -1.96734700 | 0.21647300 |
| O | 6.68036700 | 2.33185100 | 1.36328000 |
| H | 5.96507100 | 1.83008300 | 1.78220600 |
| O | 6.40914600 | 1.43670700 | -0.76730600 |
| O | 11.11414200 | 2.01714900 | -1.55043200 |
| O | 10.33474000 | 0.22129500 | -0.50025500 |
| H | 11.28985300 | 0.07485700 | -0.44379100 |
| O | 4.18404900 | 1.32822100 | 1.55213800 |
| H | 3.40640800 | 0.87068700 | 1.90072600 |
| O | 1.55718700 | 0.60442500 | 1.71625400 |
| H | 1.10275400 | 1.15214700 | 2.37167400 |
| O | -0.15125400 | 2.65357900 | 1.56098700 |
| H | -1.05814600 | 2.94963000 | 1.66818200 |
| O | -3.24187900 | -0.40995100 | 1.94478300 |
| H | -4.04549300 | -0.79259100 | 2.32010900 |
| O | -5.88611800 | -0.95543300 | 2.10618500 |
| H | -6.67001700 | -1.48560400 | 2.30306700 |
| O | -8.49851400 | -1.63357300 | 1.70432600 |
| O | -9.68435300 | -0.36865100 | 0.28038700 |
| O | -13.35047800 | -2.76241400 | -0.49447100 |
| H | -13.92943200 | -2.20640200 | -1.02114000 |
| O | 9.38068200 | 4.20666200 | -1.19557200 |
| H | 10.26289400 | 3.85965700 | -1.37216000 |
| N | 11.64483200 | -4.29320600 | 2.12060300 |
| H | 10.96098500 | -4.48963600 | 2.84783300 |
| H | 12.22673300 | -3.53630600 | 2.46224100 |

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| C | 3.88351900 | 7.12727700 | -0.08800400 |
| H | 3.82447600 | 7.59819600 | -1.07265500 |
| H | 4.87760700 | 6.68615500 | 0.01390500 |
| H | 3.78673700 | 7.91447300 | 0.66401400 |
| C | 2.78747300 | 6.07900600 | 0.07912100 |
| H | 2.87820300 | 5.60329400 | 1.06258100 |
| H | 2.92700500 | 5.28162400 | -0.65947600 |
| C | 1.37896600 | 6.64922000 | -0.06997900 |
| H | 1.27895200 | 7.11576100 | -1.05784700 |
| H | 1.22883800 | 7.44839800 | 0.66590600 |
| C | 0.29966400 | 5.58444800 | 0.10571900 |
| H | 0.38596900 | 5.13482300 | 1.10081200 |
| H | 0.48504100 | 4.76814300 | -0.60524700 |
| C | -1.11785500 | 6.10952300 | -0.10730300 |
| H | -1.20148500 | 6.51799000 | -1.12167600 |
| H | -1.31048900 | 6.94405400 | 0.57720400 |
| C | -2.18951600 | 5.03764000 | 0.08562200 |
| H | -2.19435400 | 4.71592600 | 1.13595800 |
| H | -1.92863800 | 4.15543900 | -0.51457300 |
| C | -3.59315100 | 5.50207400 | -0.29668900 |
| H | -3.57266600 | 5.89301000 | -1.32095200 |
| H | -3.89007100 | 6.33876200 | 0.34656200 |
| C | -4.63549300 | 4.39000300 | -0.20959800 |
| H | -4.65388300 | 3.97935300 | 0.80821700 |
| H | -4.32927200 | 3.56511200 | -0.86569500 |
| C | -6.04069400 | 4.84266700 | -0.59976700 |

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| H | -6.00892500 | 5.29624200 | -1.59807000 |
| H | -6.37572400 | 5.62895700 | 0.08668500 |
| C | -7.05244500 | 3.69978100 | -0.59419900 |
| H | -7.09419800 | 3.24928100 | 0.40315200 |
| H | -6.70771500 | 2.91541100 | -1.28222800 |
| C | -8.45862100 | 4.13117500 | -1.00133200 |
| H | -8.43938200 | 4.56054900 | -2.00894000 |
| H | -8.81832000 | 4.91238700 | -0.32353000 |
| C | -9.45335800 | 2.98359500 | -0.97430900 |
| H | -10.41931400 | 3.31473100 | -1.37625000 |
| H | -9.08786100 | 2.16580600 | -1.61365100 |
| O | -9.59783300 | 2.54471200 | 0.36602700 |
| H | -9.92366400 | 1.63959700 | 0.35382300 |

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| C | 9.95267500 | -4.71177600 | 1.18332700 |
| H | 10.71426200 | -4.35528400 | 0.47851200 |
| C | 9.34521800 | -5.97577000 | 0.57657500 |
| H | 8.60717700 | -6.38231400 | 1.28276700 |
| C | 8.61962300 | -5.64523300 | -0.72164900 |
| H | 9.35525000 | -5.22152000 | -1.42473100 |
| C | 8.12251100 | -3.46150300 | 0.02834900 |
| H | 8.79615300 | -3.02939100 | -0.73010800 |

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| C | 8.88039300 | -3.63753600 | 1.34377400 |
| H | 9.33585800 | -2.66892400 | 1.59766300 |
| C | 7.95528700 | -6.85749600 | -1.33527600 |
| H | 7.19651400 | -7.24153600 | -0.65007900 |
| H | 8.70219700 | -7.63231400 | -1.50887100 |
| H | 7.47459200 | -6.59424700 | -2.27820600 |
| C | 6.23176400 | -2.25098000 | -0.80953700 |
| H | 6.10030700 | -3.13062500 | -1.44582700 |
| C | 4.90519800 | -1.85903200 | -0.23133800 |
| H | 4.91466000 | -1.10888400 | 0.55698000 |
| C | 3.74927900 | -2.38768400 | -0.64277800 |
| H | 3.75595300 | -3.12954000 | -1.44009200 |
| C | 2.45484500 | -2.05639600 | -0.07563500 |
| H | 2.43814400 | -1.36490500 | 0.76480700 |
| C | 1.29908700 | -2.58534200 | -0.51919200 |
| H | 1.32833100 | -3.27408500 | -1.36235600 |
| C | 0.00106700 | -2.31836600 | 0.05773500 |
| H | -0.03335100 | -1.65853300 | 0.92344600 |
| C | -1.13730100 | -2.85387400 | -0.42888400 |
| H | -1.07615000 | -3.50423800 | -1.30056500 |
| C | -2.45293800 | -2.64123400 | 0.12452500 |
| H | -2.54652500 | -2.01492800 | 1.01099500 |
| C | -3.56426800 | -3.18011200 | -0.41956400 |
| H | -3.46702000 | -3.78836000 | -1.31783400 |
| C | -4.89762400 | -3.01577000 | 0.10676100 |
| H | -5.00886100 | -2.45251600 | 1.03250100 |

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| C | -5.99145900 | -3.52006500 | -0.50095200 |
| H | -5.86684700 | -4.06011300 | -1.43826200 |
| C | -7.34061000 | -3.39016600 | -0.00185300 |
| H | -7.47065500 | -2.93036600 | 0.97622300 |
| C | -8.42778900 | -3.78925600 | -0.68888800 |
| H | -8.29662500 | -4.22832300 | -1.67666500 |
| C | 6.92133300 | -1.13992500 | -1.61077600 |
| H | 7.88647900 | -1.51299200 | -1.96202300 |
| H | 6.31750700 | -0.90361900 | -2.49143100 |
| C | -9.78865800 | -3.62948600 | -0.21094200 |
| H | -9.90139400 | -3.29273700 | 0.81738700 |
| C | -10.87422700 | -3.81684500 | -0.97122000 |
| H | -10.74265300 | -4.14426300 | -2.00414600 |
| C | -12.28922300 | -3.56685900 | -0.53574500 |
| H | -12.30054300 | -3.33735000 | 0.53505300 |
| C | -12.88153500 | -2.35291100 | -1.27672300 |
| H | -13.02524000 | -2.64852400 | -2.32838200 |
| C | -11.98586900 | -1.10044400 | -1.28996400 |
| H | -11.06693600 | -1.39468700 | -1.80658100 |
| C | -11.54506800 | -0.66388300 | 0.11070200 |
| H | -11.24325300 | -1.53320100 | 0.68712500 |
| C | -9.29889800 | -0.10475900 | 0.69396700 |
| C | -8.13452300 | 0.81585700 | 0.41896500 |
| H | -8.24406200 | 1.25007800 | -0.57544000 |
| H | -8.18853700 | 1.62915600 | 1.15197600 |
| C | -6.78438200 | 0.10639600 | 0.56581100 |

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| H | -6.72618400 | -0.70861900 | -0.16999500 |
| C | -5.63113500 | 1.07771400 | 0.33871300 |
| H | -5.74502200 | 1.52976300 | -0.65283100 |
| H | -5.69847200 | 1.87893500 | 1.08567600 |
| C | -4.24714100 | 0.43229900 | 0.42747400 |
| H | -4.19826400 | -0.39636300 | -0.29655900 |
| C | -3.14558500 | 1.43794900 | 0.10330500 |
| H | -3.26665000 | 2.26342500 | 0.81883800 |
| H | -3.30026100 | 1.84967000 | -0.90097700 |
| C | -1.75615800 | 0.81160000 | 0.21312800 |
| H | -1.67480600 | 0.29235300 | 1.17142500 |
| H | -1.63329200 | 0.06032300 | -0.57441200 |
| C | -0.61585800 | 1.81703200 | 0.10974300 |
| H | -0.67145600 | 2.35708200 | -0.84708900 |
| C | 0.75740000 | 1.15128700 | 0.22057600 |
| H | 0.81475200 | 0.31687200 | -0.48600100 |
| C | 1.89707500 | 2.13523400 | -0.04176200 |
| H | 1.82103800 | 2.97304700 | 0.66199600 |
| H | 1.77468000 | 2.54185900 | -1.05225400 |
| C | 3.28819600 | 1.50985800 | 0.06039300 |
| H | 3.36514500 | 0.66264600 | -0.63497800 |
| C | 4.36177900 | 2.53328800 | -0.29104100 |
| H | 4.25303100 | 3.41959700 | 0.34492800 |
| H | 4.21943100 | 2.83690600 | -1.33242200 |
| C | 5.79331300 | 2.02296000 | -0.13075100 |
| C | 6.80950800 | 3.01007500 | -0.68256100 |

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| H | 6.77828200 | 3.93288300 | -0.10144600 |
| H | 6.56656800 | 3.23436900 | -1.72587300 |
| C | 8.21075300 | 2.43413800 | -0.64532600 |
| H | 8.51626500 | 2.29855400 | 0.40143100 |
| C | 8.23014000 | 1.04383400 | -1.33633300 |
| H | 8.09459600 | 1.22338500 | -2.40962200 |
| C | 7.10484000 | 0.14116000 | -0.80627400 |
| H | 7.31408200 | -0.10292900 | 0.24000200 |
| C | 9.61981400 | 0.48737300 | -1.14864000 |
| C | -12.54262900 | 0.15336800 | 0.90945200 |
| H | -12.14784800 | 0.34381900 | 1.90915500 |
| H | -13.47749600 | -0.40164700 | 0.99412200 |
| H | -12.73829900 | 1.11115000 | 0.42403700 |
| C | -12.63320300 | 0.03366600 | -2.08317600 |
| H | -13.58443900 | 0.34342600 | -1.64216600 |
| H | -12.81882200 | -0.27623300 | -3.11475200 |
| H | -11.98255100 | 0.90993500 | -2.10652900 |
| C | -13.16847000 | -4.79906300 | -0.77193100 |
| H | -13.15027300 | -5.08342800 | -1.82875900 |
| H | -14.19946500 | -4.58682200 | -0.48884100 |
| H | -12.80558500 | -5.64665800 | -0.18879100 |
| O | 8.00832500 | -4.05910300 | 2.36833000 |
| H | 7.16976500 | -3.60532500 | 2.22396200 |
| O | 10.36378600 | -6.90903300 | 0.30126700 |
| H | 10.93143100 | -6.89159600 | 1.08285000 |
| O | 7.60743000 | -4.68178200 | -0.45012100 |

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| O | 7.05666300 | -2.61762000 | 0.30961000 |
| O | 6.12931500 | 1.78653600 | 1.20687900 |
| H | 5.35520700 | 1.38488300 | 1.62828600 |
| O | 5.86111600 | 0.82178100 | -0.89225600 |
| O | 10.62194700 | 1.03468200 | -1.53578200 |
| O | 9.68376100 | -0.65791600 | -0.44478100 |
| H | 10.62379400 | -0.86795900 | -0.35024500 |
| O | 3.55278300 | 1.03917100 | 1.38423900 |
| H | 2.72896000 | 0.67618700 | 1.73810100 |
| O | 0.87589400 | 0.57100000 | 1.52545800 |
| H | 0.46923400 | 1.20738500 | 2.13066700 |
| O | -0.63666600 | 2.74905400 | 1.19069400 |
| H | -1.53180700 | 3.07801300 | 1.30919100 |
| O | -3.97086700 | -0.05996600 | 1.72905500 |
| H | -4.80289800 | -0.36976500 | 2.11012800 |
| O | -6.63592100 | -0.43337100 | 1.87466900 |
| H | -7.46442600 | -0.87552700 | 2.10872100 |
| O | -9.27510600 | -0.96618500 | 1.54715900 |
| O | -10.34720200 | 0.14741900 | -0.07832600 |
| O | -14.14844300 | -2.10070200 | -0.67912900 |
| H | -14.67140900 | -1.56582900 | -1.28069100 |
| O | 9.04957900 | 3.36027600 | -1.30112900 |
| H | 9.90522400 | 2.93880100 | -1.44546700 |
| N | 10.62562800 | -5.09396300 | 2.42322300 |
| H | 9.91841100 | -5.18356400 | 3.14908400 |
| H | 11.26604000 | -4.36814900 | 2.72521400 |

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| C | -7.36309100 | 4.50765400 | 0.48025700 |
| H | -7.62126400 | 5.32106900 | -0.20239900 |
| H | -8.18818100 | 4.38783500 | 1.18580500 |
| H | -7.28812800 | 3.59254100 | -0.11400600 |
| C | -6.04390000 | 4.79772000 | 1.19129800 |
| H | -5.84321700 | 4.02477500 | 1.94209700 |
| H | -6.12102100 | 5.74233200 | 1.73993400 |
| C | -4.87152900 | 4.87329000 | 0.21716200 |
| H | -5.09976800 | 5.60573900 | -0.56672100 |
| H | -4.76181400 | 3.90656100 | -0.29135500 |
| C | -3.55025300 | 5.25282300 | 0.87942900 |
| H | -3.34177000 | 4.55815000 | 1.70586000 |
| H | -3.64776500 | 6.24212400 | 1.34191400 |
| C | -2.37878400 | 5.26439600 | -0.09957400 |
| H | -2.64677400 | 5.87161500 | -0.97239300 |
| H | -2.21675200 | 4.24864100 | -0.48618400 |
| C | -1.07936900 | 5.79807800 | 0.50019700 |
| H | -0.86356000 | 5.28720800 | 1.44491200 |
| H | -1.20473900 | 6.86018800 | 0.74166500 |
| C | 0.10942300 | 5.61925600 | -0.43820100 |
| H | -0.09187000 | 6.13455700 | -1.38573400 |
| H | 0.21118300 | 4.55290400 | -0.67426800 |
| C | 1.42587900 | 6.12241100 | 0.14524200 |
| H | 1.64206000 | 5.57432400 | 1.07080700 |
| H | 1.32468800 | 7.17764200 | 0.42688800 |
| C | 2.59761400 | 5.96414500 | -0.81963000 |

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| H | 2.37682400 | 6.49939500 | -1.75144600 |
| H | 2.69486300 | 4.90476000 | -1.09072100 |
| C | 3.92366100 | 6.45739700 | -0.24745000 |
| H | 4.12222400 | 5.96466100 | 0.70887800 |
| H | 3.85737500 | 7.53146400 | -0.03461000 |
| C | 5.09334200 | 6.19043200 | -1.19098000 |
| H | 4.93255200 | 6.70384100 | -2.14543300 |
| H | 5.13548900 | 5.11903300 | -1.40967200 |
| C | 6.43451200 | 6.62811700 | -0.62690900 |
| H | 7.24225900 | 6.28737500 | -1.28617000 |
| H | 6.47403700 | 7.72404400 | -0.56610000 |
| O | 6.57485500 | 6.06196400 | 0.66981000 |
| H | 7.48842900 | 6.15530700 | 0.94736600 |

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| C | -6.31899500 | 5.77983600 | 1.59150000 |
| H | -7.10874200 | 5.07644400 | 1.26606300 |
| C | -6.21531400 | 6.86373900 | 0.50385300 |
| H | -5.45087000 | 7.60580100 | 0.81403400 |
| C | -5.75791100 | 6.25057400 | -0.82590700 |
| H | -6.49931400 | 5.48283300 | -1.13680900 |
| C | -4.56246600 | 4.53815400 | 0.31000400 |
| H | -5.30005300 | 3.79424200 | -0.06901600 |

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|---|-------------|------------|-------------|
| C | -5.00401300 | 4.99370300 | 1.71117600 |
| H | -5.16540500 | 4.07991400 | 2.32197500 |
| C | -5.58310900 | 7.27512000 | -1.93095500 |
| H | -4.81525900 | 8.01136500 | -1.64677700 |
| H | -6.53239200 | 7.80273600 | -2.09848300 |
| H | -5.27438200 | 6.78301400 | -2.86465300 |
| C | -2.58372500 | 3.57804900 | -0.75611000 |
| H | -2.33923900 | 4.49575300 | -1.31761000 |
| C | -1.33106500 | 2.91859100 | -0.27152900 |
| H | -1.46157400 | 2.05357000 | 0.38737500 |
| C | -0.08004900 | 3.33098600 | -0.59474300 |
| H | 0.04416800 | 4.20003800 | -1.25468700 |
| C | 1.11049900 | 2.69006600 | -0.10567100 |
| H | 0.96982600 | 1.83644400 | 0.56821500 |
| C | 2.39479400 | 3.07026100 | -0.40031100 |
| H | 2.55863800 | 3.92121400 | -1.07480800 |
| C | 3.53979500 | 2.40633400 | 0.13697500 |
| H | 3.33928300 | 1.55799700 | 0.80352000 |
| C | 4.84869900 | 2.72557700 | -0.13854000 |
| H | 5.06270500 | 3.55652800 | -0.82360500 |
| C | 5.95710200 | 2.01728700 | 0.41166600 |
| H | 5.72928700 | 1.19945200 | 1.10847700 |
| C | 7.27932600 | 2.26926200 | 0.12342000 |
| H | 7.51811200 | 3.07542000 | -0.58271900 |
| C | 8.36952800 | 1.54020100 | 0.68192600 |
| H | 8.12479600 | 0.75080000 | 1.40547300 |

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|---|-------------|-------------|-------------|
| C | 9.69358500 | 1.75004900 | 0.37274900 |
| H | 9.94235100 | 2.52985800 | -0.35911400 |
| C | 10.77688100 | 1.00998300 | 0.93726900 |
| H | 10.52518400 | 0.25206700 | 1.69103000 |
| C | 12.09614700 | 1.16642800 | 0.59687600 |
| H | 12.36114800 | 1.91368300 | -0.16258000 |
| C | -3.46178900 | 2.68928600 | -1.66010700 |
| H | -4.31551600 | 3.28687700 | -2.01296100 |
| H | -2.87668100 | 2.42757400 | -2.55661800 |
| C | 13.16205100 | 0.37779900 | 1.15324400 |
| H | 12.87586000 | -0.34115400 | 1.93191100 |
| C | 14.45960000 | 0.42510800 | 0.75627300 |
| H | 14.74817700 | 1.14069300 | -0.02728600 |
| C | 15.55702800 | -0.45201400 | 1.29067000 |
| H | 15.15325700 | -1.06981500 | 2.11315700 |
| C | 16.07651300 | -1.42458900 | 0.19920500 |
| H | 16.63124500 | -0.81611000 | -0.54701800 |
| C | 14.96833800 | -2.17219100 | -0.58486900 |
| H | 14.34428800 | -1.37366000 | -1.02428600 |
| C | 14.01712700 | -2.97128300 | 0.32409700 |
| H | 13.74478100 | -2.36635300 | 1.19734600 |
| C | 11.60383900 | -2.94260500 | 0.17322900 |
| C | 10.41296500 | -3.13538400 | -0.74391500 |
| H | 10.72133500 | -2.97329800 | -1.78730000 |
| H | 10.09085200 | -4.18844500 | -0.65134600 |
| C | 9.23824700 | -2.21656500 | -0.36640900 |

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| H | 9.57013300 | -1.16173800 | -0.44867300 |
| C | 8.03002500 | -2.43166800 | -1.27820600 |
| H | 8.33704400 | -2.22386400 | -2.31763400 |
| H | 7.71614600 | -3.48994900 | -1.22702700 |
| C | 6.82884800 | -1.54053000 | -0.93437400 |
| H | 7.15954400 | -0.48279800 | -0.90598800 |
| C | 5.70389600 | -1.67348800 | -1.96455800 |
| H | 5.49089000 | -2.74595400 | -2.12843700 |
| H | 6.08892900 | -1.28087200 | -2.92000100 |
| C | 4.40488300 | -0.92962300 | -1.58052200 |
| H | 4.62578200 | -0.11068000 | -0.87694500 |
| H | 3.97779600 | -0.45041700 | -2.47724700 |
| C | 3.29996500 | -1.82157000 | -0.99869700 |
| H | 3.00830900 | -2.56376500 | -1.76830300 |
| C | 2.03498400 | -0.99352100 | -0.61686200 |
| H | 2.00492000 | -0.06827800 | -1.21934300 |
| C | 0.72701800 | -1.76612400 | -0.82600700 |
| H | 0.74506000 | -2.70008900 | -0.23593900 |
| H | 0.65871100 | -2.04668100 | -1.89245900 |
| C | -0.50842200 | -0.93825800 | -0.45755500 |
| H | -0.46904200 | 0.02375000 | -1.00610600 |
| C | -1.81767000 | -1.63980900 | -0.82161700 |
| H | -1.88781300 | -2.60115000 | -0.28626900 |
| H | -1.81486800 | -1.84783300 | -1.90340100 |
| C | -3.07494000 | -0.81778300 | -0.49108900 |
| C | -4.35937100 | -1.47729300 | -1.01117000 |

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| H | -4.55565700 | -2.39995300 | -0.44587600 |
| H | -4.22888200 | -1.74162000 | -2.07332700 |
| C | -5.55089700 | -0.53720300 | -0.87702300 |
| H | -5.72123400 | -0.32748200 | 0.19358000 |
| C | -5.24947500 | 0.79435100 | -1.59887200 |
| H | -5.06949000 | 0.59973500 | -2.66985500 |
| C | -3.93574900 | 1.39410200 | -1.00097000 |
| H | -4.09373700 | 1.55267700 | 0.08280300 |
| C | -6.39585900 | 1.77964100 | -1.54201100 |
| C | 14.48262800 | -4.34419700 | 0.78187700 |
| H | 13.73659700 | -4.79242200 | 1.45442200 |
| H | 15.43139300 | -4.23636100 | 1.32730600 |
| H | 14.63944300 | -5.02251800 | -0.06963400 |
| C | 15.55069100 | -3.00041300 | -1.73734500 |
| H | 16.22355000 | -3.79746300 | -1.38042100 |
| H | 16.12166700 | -2.35683500 | -2.42563500 |
| H | 14.75109900 | -3.48468000 | -2.31742200 |
| C | 16.72078400 | 0.38783400 | 1.85121700 |
| H | 17.13918400 | 1.04419100 | 1.06939000 |
| H | 17.52412700 | -0.26529800 | 2.22022600 |
| H | 16.37321300 | 1.02625500 | 2.67658100 |
| O | -4.03023600 | 5.83481500 | 2.32300100 |
| H | -3.16235200 | 5.46952100 | 2.06638300 |
| O | -7.48607400 | 7.48629100 | 0.32692600 |
| H | -7.82635500 | 7.58539800 | 1.24060300 |
| O | -4.47805300 | 5.61323200 | -0.61565100 |

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| O | -3.28836500 | 3.97170100 | 0.46715500 |
| O | -3.23497600 | -0.61456200 | 0.89874200 |
| H | -2.32947800 | -0.48449400 | 1.26464300 |
| O | -2.88025900 | 0.44226200 | -1.18312600 |
| O | -6.62293800 | 2.65408000 | -2.35775700 |
| O | -7.18750100 | 1.61523800 | -0.42836000 |
| H | -7.87768600 | 2.30710300 | -0.49166800 |
| O | -0.54042000 | -0.65892000 | 0.96227300 |
| H | 0.39502500 | -0.51382800 | 1.23688700 |
| O | 2.16588700 | -0.57085800 | 0.75930200 |
| H | 2.72225900 | -1.29238600 | 1.14806800 |
| O | 3.68926200 | -2.54256700 | 0.18011600 |
| H | 4.65870100 | -2.39678300 | 0.33683500 |
| O | 6.28498700 | -1.87618700 | 0.36214300 |
| H | 7.04519900 | -2.09692200 | 0.94718300 |
| O | 8.81322900 | -2.46963600 | 0.98817200 |
| H | 9.62966900 | -2.45750400 | 1.53757900 |
| O | 11.50391300 | -2.64668000 | 1.36332500 |
| O | 12.76924800 | -3.13916500 | -0.46346600 |
| O | 16.99415800 | -2.31973300 | 0.85757900 |
| H | 17.54135400 | -2.74446600 | 0.17759600 |
| O | -6.69240300 | -1.20280600 | -1.43926000 |
| H | -7.48124400 | -0.74735000 | -1.09957700 |
| N | -6.78447900 | 6.42607700 | 2.82638100 |
| H | -5.98633000 | 6.87942000 | 3.28332500 |
| H | -7.15335900 | 5.73705200 | 3.48551600 |

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| C | -20.43556800 | -7.76509500 | 0.98941700 |
| H | -20.61214200 | -7.75212000 | -0.06583500 |
| H | -21.37119400 | -7.80326000 | 1.50715400 |
| H | -19.85230400 | -8.62558800 | 1.24290300 |
| C | -19.67431100 | -6.49035100 | 1.39821500 |
| H | -19.49943100 | -6.50240000 | 2.45375700 |
| H | -20.25672300 | -5.62979900 | 1.14297200 |
| C | -18.32648400 | -6.43681600 | 0.65517000 |
| H | -18.50134400 | -6.42514200 | -0.40038000 |
| H | -17.74391800 | -7.29718100 | 0.91069600 |
| C | -17.56545600 | -5.16181300 | 1.06355800 |
| H | -17.39066900 | -5.17344500 | 2.11912600 |
| H | -18.14797900 | -4.30144100 | 0.80795800 |
| C | -16.21757700 | -5.10834000 | 0.32060300 |
| H | -16.39237300 | -5.09671400 | -0.73496300 |
| H | -15.63505100 | -5.96869700 | 0.57620900 |
| C | -15.45655900 | -3.83332400 | 0.72897700 |
| H | -15.28177700 | -3.84494700 | 1.78454300 |
| H | -16.03909000 | -2.97295900 | 0.47336900 |
| C | -14.10868800 | -3.77985600 | -0.01397600 |
| H | -14.28347600 | -3.76822200 | -1.06953400 |
| H | -13.52614900 | -4.64021200 | 0.24164100 |
| C | -13.34765700 | -2.50484000 | 0.39440900 |
| H | -13.17287500 | -2.51646300 | 1.44997400 |
| H | -13.93018800 | -1.64447500 | 0.13880000 |
| C | -11.99979200 | -2.45136400 | -0.34854700 |

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| H | -12.17457900 | -2.43973200 | -1.40411500 |
| H | -11.41726000 | -3.31172800 | -0.09293900 |
| C | -11.23876000 | -1.17634700 | 0.05983800 |
| H | -11.06397300 | -1.18798100 | 1.11539600 |
| H | -11.82129200 | -0.31598300 | -0.19577100 |
| C | -9.89089500 | -1.12287400 | -0.68312800 |
| H | -10.06568200 | -1.11124000 | -1.73868600 |
| H | -9.30836300 | -1.98323800 | -0.42751900 |
| C | -9.12985800 | 0.15213400 | -0.27474000 |
| H | -8.19335300 | 0.18929200 | -0.79095100 |
| H | -9.71239800 | 1.01249600 | -0.53033800 |
| O | -8.89626500 | 0.13658800 | 1.13596300 |
| H | -8.16487900 | 0.72182800 | 1.34614600 |

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| C | 7.07527400 | 4.37143800 | -1.19800600 |
| H | 7.76812100 | 3.61634400 | -0.78067300 |
| C | 7.03161800 | 5.53619300 | -0.19301200 |
| H | 6.36722200 | 6.32816700 | -0.59624600 |
| C | 6.44407600 | 5.07101900 | 1.14559000 |
| H | 7.08282900 | 4.25597900 | 1.54990400 |
| C | 5.13340600 | 3.41217600 | 0.05832400 |
| H | 5.76740500 | 2.62610300 | 0.52867400 |

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| C | 5.69212900 | 3.71742700 | -1.34182700 |
| H | 5.78669400 | 2.75008300 | -1.87981800 |
| C | 6.32260000 | 6.18542500 | 2.16770700 |
| H | 5.65286900 | 6.97386000 | 1.79056300 |
| H | 7.31269200 | 6.62385400 | 2.35500600 |
| H | 5.91587000 | 5.79644400 | 3.11244900 |
| C | 3.01182600 | 2.73940900 | 1.06832400 |
| H | 2.83769100 | 3.71557100 | 1.55208100 |
| C | 1.72274000 | 2.17826000 | 0.55624200 |
| H | 1.79428400 | 1.25897400 | -0.03472700 |
| C | 0.50766500 | 2.73885500 | 0.77738100 |
| H | 0.44274300 | 3.66157300 | 1.36948400 |
| C | -0.71754500 | 2.18941500 | 0.26322800 |
| H | -0.63392800 | 1.27931300 | -0.34282700 |
| C | -1.96762000 | 2.71940200 | 0.45610300 |
| H | -2.07456000 | 3.62927300 | 1.06158700 |
| C | -3.14757000 | 2.13898200 | -0.10187000 |
| H | -3.00434600 | 1.22853100 | -0.69746100 |
| C | -4.42757300 | 2.60963100 | 0.07457800 |
| H | -4.58699200 | 3.50555700 | 0.68898400 |
| C | -5.57522800 | 1.98051700 | -0.49116200 |
| H | -5.40010100 | 1.09533900 | -1.11733300 |
| C | -6.87625500 | 2.38671500 | -0.29832600 |
| H | -7.06399500 | 3.26210600 | 0.33727200 |
| C | -8.00761600 | 1.73452800 | -0.86988200 |
| H | -7.81130000 | 0.87389100 | -1.52358800 |

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| C | -9.31601100 | 2.10063500 | -0.65349700 |
| H | -9.51777900 | 2.95277100 | 0.00889700 |
| C | -10.44137400 | 1.43638800 | -1.22990300 |
| H | -10.23324800 | 0.60408700 | -1.91539600 |
| C | -11.75228400 | 1.75128500 | -0.97858300 |
| H | -11.97504500 | 2.57478400 | -0.28748500 |
| C | 3.74300700 | 1.83328200 | 2.07946900 |
| H | 4.63613300 | 2.36434100 | 2.44109700 |
| H | 3.08819900 | 1.69847000 | 2.95561300 |
| C | -12.86595100 | 1.03766900 | -1.54261100 |
| H | -12.61815600 | 0.23868800 | -2.25349000 |
| C | -14.16978700 | 1.24616700 | -1.22638600 |
| H | -14.42056000 | 2.04240600 | -0.51055100 |
| C | -15.32528200 | 0.44957500 | -1.76447700 |
| H | -14.94773900 | -0.26426100 | -2.51885900 |
| C | -16.00041500 | -0.38308200 | -0.64289600 |
| H | -16.52494300 | 0.33143200 | 0.02730000 |
| C | -15.01958500 | -1.18140100 | 0.25286800 |
| H | -14.33763700 | -0.42121000 | 0.67385900 |
| C | -14.11323600 | -2.13739300 | -0.54348700 |
| H | -13.73375400 | -1.62837500 | -1.43767500 |
| C | -11.72148400 | -2.34501100 | -0.25373300 |
| C | -10.60644300 | -2.59171000 | 0.74242000 |
| H | -10.94897600 | -2.32375300 | 1.75280900 |
| H | -10.39365300 | -3.67613300 | 0.73931800 |
| C | -9.32298600 | -1.82772400 | 0.37395500 |

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| H | -9.54476500 | -0.74129500 | 0.36610300 |
| C | -8.19281400 | -2.09873400 | 1.36728700 |
| H | -8.52894900 | -1.78584500 | 2.37076500 |
| H | -7.99088000 | -3.18449600 | 1.40527700 |
| C | -6.88775100 | -1.36248000 | 1.03575900 |
| H | -7.10236100 | -0.28130700 | 0.91757000 |
| C | -5.83761800 | -1.53489500 | 2.13665400 |
| H | -5.74839100 | -2.60882400 | 2.38388900 |
| H | -6.22728800 | -1.03675100 | 3.03958200 |
| C | -4.44897800 | -0.95767700 | 1.78063500 |
| H | -4.54527600 | -0.17356000 | 1.01227800 |
| H | -4.01998700 | -0.46100000 | 2.66688500 |
| C | -3.41663800 | -1.99782200 | 1.32532800 |
| H | -3.24531300 | -2.70825500 | 2.15848100 |
| C | -2.05296500 | -1.33344200 | 0.96389300 |
| H | -1.95576700 | -0.37493200 | 1.50405300 |
| C | -0.84689900 | -2.21866500 | 1.30037100 |
| H | -0.93372100 | -3.18615900 | 0.77386100 |
| H | -0.86357200 | -2.42673800 | 2.38532500 |
| C | 0.48673300 | -1.55047300 | 0.95054700 |
| H | 0.52164300 | -0.55228800 | 1.43047000 |
| C | 1.69367000 | -2.35411300 | 1.43666700 |
| H | 1.68870300 | -3.35382900 | 0.97165400 |
| H | 1.61330000 | -2.48183700 | 2.52788900 |
| C | 3.04641500 | -1.69120300 | 1.12628700 |
| C | 4.22516700 | -2.43929000 | 1.76355100 |

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| H | 4.35110700 | -3.41571100 | 1.27352200 |
| H | 4.01303000 | -2.61122600 | 2.83149800 |
| C | 5.51508900 | -1.63829100 | 1.63705100 |
| H | 5.76143100 | -1.52522100 | 0.56666900 |
| C | 5.32013600 | -0.23410200 | 2.24958900 |
| H | 5.06579700 | -0.33117100 | 3.31877700 |
| C | 4.10993900 | 0.45206000 | 1.53707900 |
| H | 4.33926300 | 0.51469800 | 0.45626600 |
| C | 6.56606500 | 0.62196000 | 2.19441000 |
| C | -14.69779400 | -3.48499000 | -0.93517400 |
| H | -13.97006300 | -4.05475700 | -1.53146200 |
| H | -15.60050600 | -3.32041400 | -1.54123000 |
| H | -14.96923000 | -4.08021900 | -0.05097600 |
| C | -15.74494700 | -1.85999000 | 1.42190800 |
| H | -16.47943900 | -2.60773900 | 1.08012500 |
| H | -16.27890800 | -1.11318800 | 2.03110700 |
| H | -15.03211900 | -2.38024800 | 2.07883800 |
| C | -16.36297700 | 1.36129500 | -2.44700400 |
| H | -16.74886700 | 2.11193500 | -1.73655000 |
| H | -17.21113900 | 0.76880700 | -2.81806700 |
| H | -15.90769400 | 1.89930900 | -3.29132100 |
| O | 4.84585300 | 4.60724200 | -2.06438300 |
| H | 3.93207000 | 4.35225000 | -1.83526600 |
| O | 8.35054300 | 6.03658600 | 0.01615200 |
| H | 8.74584700 | 6.03389100 | -0.88059100 |
| O | 5.11625700 | 4.55446800 | 0.90368200 |

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| O | 3.81610600 | 2.96921300 | -0.13508000 |
| O | 3.29821400 | -1.60665300 | -0.26223300 |
| H | 2.43161800 | -1.41144200 | -0.68841800 |
| O | 2.95139400 | -0.37104200 | 1.72015300 |
| O | 6.84256700 | 1.52535300 | 2.96192400 |
| O | 7.39185700 | 0.29715000 | 1.14250200 |
| H | 8.14744800 | 0.91750100 | 1.19985800 |
| O | 0.62101100 | -1.37947600 | -0.48043000 |
| H | -0.27841100 | -1.15968100 | -0.81844300 |
| O | -2.06747100 | -1.00041500 | -0.44269500 |
| H | -2.67663600 | -1.68746800 | -0.81440600 |
| O | -3.81930600 | -2.75868400 | 0.17644300 |
| H | -4.75845900 | -2.52618300 | -0.04617900 |
| O | -6.31681400 | -1.84507900 | -0.20138900 |
| H | -7.06514800 | -2.02864900 | -0.81394000 |
| O | -8.85831500 | -2.22043300 | -0.93349900 |
| H | -9.63958500 | -2.16463600 | -1.52938200 |
| O | -11.52977700 | -2.14786700 | -1.45301100 |
| O | -12.93229600 | -2.37461300 | 0.32527600 |
| O | -16.97293500 | -1.22493600 | -1.29273900 |
| H | -17.59630000 | -1.54104900 | -0.61917500 |
| O | 6.54910400 | -2.37474100 | 2.30833800 |
| H | 7.39823200 | -2.02822700 | 1.98584000 |
| N | 7.66948600 | 4.87547300 | -2.44383700 |
| H | 6.94848900 | 5.37382400 | -2.97597400 |
| H | 7.99643800 | 4.10638000 | -3.03280600 |

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| C | 19.02599300 | -7.04475100 | -1.16104000 |
| H | 19.14857700 | -6.97350200 | -0.10047300 |
| H | 19.97759800 | -7.21588300 | -1.61936900 |
| H | 18.36842800 | -7.85711900 | -1.39031200 |
| C | 18.42638600 | -5.73177000 | -1.69783900 |
| H | 18.30559800 | -5.80229500 | -2.75865600 |
| H | 19.08302200 | -4.91912900 | -1.46686900 |
| C | 17.05553100 | -5.48687800 | -1.04026500 |
| H | 17.17625800 | -5.41672100 | 0.02058400 |
| H | 16.39877700 | -6.29933800 | -1.27153800 |
| C | 16.45615700 | -4.17363300 | -1.57666000 |
| H | 16.33550700 | -4.24375500 | -2.63752500 |
| H | 17.11286600 | -3.36115600 | -1.34531700 |
| C | 15.08524800 | -3.92880300 | -0.91917700 |
| H | 15.20590600 | -3.85868700 | 0.14168800 |
| H | 14.42853900 | -4.74126500 | -1.15052700 |
| C | 14.48588600 | -2.61554600 | -1.45555700 |
| H | 14.36524100 | -2.68566000 | -2.51642000 |
| H | 15.14260100 | -1.80307600 | -1.22420500 |
| C | 13.11498300 | -2.37072100 | -0.79807400 |
| H | 13.23563500 | -2.30059700 | 0.26278100 |
| H | 12.45826100 | -3.18318300 | -1.02943600 |
| C | 12.51560800 | -1.05746300 | -1.33446600 |
| H | 12.39496400 | -1.12757800 | -2.39532900 |
| H | 13.17232400 | -0.24499400 | -1.10311400 |
| C | 11.14471300 | -0.81263200 | -0.67698100 |

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| H | 11.26536300 | -0.74251000 | 0.38388400 |
| H | 10.48799700 | -1.62510100 | -0.90833300 |
| C | 10.54533700 | 0.50062600 | -1.21337300 |
| H | 10.42468600 | 0.43050200 | -2.27422900 |
| H | 11.20205300 | 1.31309600 | -0.98202100 |
| C | 9.17444100 | 0.74545600 | -0.55587800 |
| H | 9.29509200 | 0.81558000 | 0.50497700 |
| H | 8.51772500 | -0.06701300 | -0.78723000 |
| C | 8.57505900 | 2.05870700 | -1.09227200 |
| H | 7.62255300 | 2.22882000 | -0.63544800 |
| H | 9.23178300 | 2.87117200 | -0.86093100 |
| O | 8.41381700 | 1.96499100 | -2.51005600 |
| H | 7.76046500 | 2.60524200 | -2.80129100 |

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| C | 5.76982000 | 6.10236400 | -1.69094600 |
| H | 6.48688000 | 6.21893700 | -0.86771500 |
| C | 4.83884600 | 7.31357100 | -1.64133200 |
| H | 4.12335100 | 7.23251500 | -2.47428700 |
| C | 4.03643600 | 7.31431100 | -0.34578300 |
| H | 4.74753500 | 7.37042100 | 0.49636100 |
| C | 4.10307300 | 4.95111500 | -0.23020600 |
| H | 4.74670200 | 4.98611000 | 0.66506000 |

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| C | 4.97906500 | 4.81544200 | -1.47449500 |
| H | 5.66286000 | 3.96793200 | -1.30487000 |
| C | 3.05409600 | 8.46032400 | -0.26563800 |
| H | 2.32883300 | 8.38161800 | -1.07974000 |
| H | 3.58711600 | 9.40775200 | -0.35860100 |
| H | 2.51413100 | 8.43659000 | 0.68337700 |
| C | 2.40640900 | 3.68161600 | 0.91067800 |
| H | 2.01039800 | 4.66518600 | 1.18245600 |
| C | 1.28800600 | 2.80325500 | 0.44476700 |
| H | 1.56984900 | 1.85728500 | -0.00966700 |
| C | -0.00103500 | 3.13219100 | 0.56449800 |
| H | -0.27017900 | 4.07813900 | 1.03447100 |
| C | -1.09509300 | 2.30980300 | 0.08551300 |
| H | -0.83403900 | 1.39801800 | -0.44588500 |
| C | -2.39246500 | 2.62890800 | 0.24549400 |
| H | -2.64506200 | 3.54248100 | 0.78400600 |
| C | -3.49727000 | 1.84758800 | -0.26013000 |
| H | -3.24953500 | 0.95348900 | -0.82921000 |
| C | -4.78757900 | 2.18168300 | -0.05673200 |
| H | -5.00604800 | 3.07781800 | 0.52462600 |
| C | -5.92477900 | 1.44748600 | -0.55462700 |
| H | -5.74266100 | 0.55760000 | -1.15514200 |
| C | -7.19855300 | 1.80996000 | -0.29724200 |
| H | -7.38024500 | 2.69048500 | 0.31922000 |
| C | -8.36152700 | 1.11073500 | -0.78422200 |
| H | -8.19183700 | 0.25228200 | -1.43123700 |

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| C | -9.62530800 | 1.45911400 | -0.46905500 |
| H | -9.78745000 | 2.30646500 | 0.19680800 |
| C | -10.80037200 | 0.77197900 | -0.94793000 |
| H | -10.64226000 | -0.03229000 | -1.66364500 |
| C | -12.05490400 | 1.04546700 | -0.54497300 |
| H | -12.21749100 | 1.83138200 | 0.19204900 |
| C | 3.21046900 | 3.11836000 | 2.08873100 |
| H | 3.98490500 | 3.84316800 | 2.35389600 |
| H | 2.55432100 | 3.01167100 | 2.95761200 |
| C | -13.21855800 | 0.30970100 | -0.99980700 |
| H | -13.04760500 | -0.39950300 | -1.80679900 |
| C | -14.43726800 | 0.40414000 | -0.45669600 |
| H | -14.59817600 | 1.10326000 | 0.36582200 |
| C | -15.62422300 | -0.42613500 | -0.85358300 |
| H | -15.38442500 | -0.97656700 | -1.77039400 |
| C | -15.95677900 | -1.46816600 | 0.23264900 |
| H | -16.32174700 | -0.91507500 | 1.11415700 |
| C | -14.76100700 | -2.31376400 | 0.70995400 |
| H | -14.01670100 | -1.59905400 | 1.07403600 |
| C | -14.07099300 | -3.07506800 | -0.42719800 |
| H | -13.93313400 | -2.41557000 | -1.27963900 |
| C | -11.68651000 | -3.07819300 | -0.67270900 |
| C | -10.37779400 | -3.49461000 | -0.04973100 |
| H | -10.51418000 | -3.64115200 | 1.02316600 |
| H | -10.10466600 | -4.46105100 | -0.48933200 |
| C | -9.25584000 | -2.48942600 | -0.33213500 |

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| H | -9.51989100 | -1.52350400 | 0.12344200 |
| C | -7.92905200 | -2.97036500 | 0.24008200 |
| H | -8.05237700 | -3.14723200 | 1.31429600 |
| H | -7.67552600 | -3.92786000 | -0.23109100 |
| C | -6.76861700 | -1.99678600 | 0.02835700 |
| H | -7.03405700 | -1.02842200 | 0.48222800 |
| C | -5.49342900 | -2.51157100 | 0.68737300 |
| H | -5.30225500 | -3.50756400 | 0.26297100 |
| H | -5.66299400 | -2.65127700 | 1.76160900 |
| C | -4.30181300 | -1.58628000 | 0.45693300 |
| H | -4.23230000 | -1.35013500 | -0.60711000 |
| H | -4.46513100 | -0.63962200 | 0.98152000 |
| C | -2.97257500 | -2.18083900 | 0.90136500 |
| H | -3.02746800 | -2.47866000 | 1.95959000 |
| C | -1.80465700 | -1.20913100 | 0.72453200 |
| H | -2.05950900 | -0.24045400 | 1.16536700 |
| C | -0.51364500 | -1.74173100 | 1.34100400 |
| H | -0.28503800 | -2.71671100 | 0.89769900 |
| H | -0.68000200 | -1.89974600 | 2.41277700 |
| C | 0.68193100 | -0.80965000 | 1.16217800 |
| H | 0.44661700 | 0.17713000 | 1.58247200 |
| C | 1.91504000 | -1.35838400 | 1.87021400 |
| H | 2.11786100 | -2.37509100 | 1.51941600 |
| H | 1.70812800 | -1.40275000 | 2.94329700 |
| C | 3.17905800 | -0.52926900 | 1.64568800 |
| C | 4.33473600 | -0.97706500 | 2.53204600 |

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| H | 4.65327500 | -1.98396900 | 2.25395000 |
| H | 4.00675900 | -0.99259100 | 3.57518500 |
| C | 5.51549300 | -0.02898900 | 2.41740300 |
| H | 5.90931800 | -0.07835200 | 1.39271200 |
| C | 5.04668900 | 1.42874300 | 2.67328300 |
| H | 4.76423100 | 1.49365100 | 3.72977000 |
| C | 3.84195100 | 1.76655200 | 1.78742000 |
| H | 4.15722300 | 1.73637900 | 0.74028700 |
| C | 6.25300300 | 2.30791300 | 2.48712900 |
| C | -14.72821800 | -4.36189400 | -0.88277200 |
| H | -14.18189900 | -4.78102600 | -1.73089100 |
| H | -15.75418000 | -4.14890900 | -1.18579300 |
| H | -14.74085400 | -5.10386100 | -0.08148500 |
| C | -15.14908200 | -3.22167800 | 1.87566300 |
| H | -15.94438100 | -3.92153000 | 1.60176500 |
| H | -15.49808200 | -2.62990300 | 2.72680500 |
| H | -14.29265500 | -3.81383900 | 2.20600800 |
| C | -16.84807400 | 0.45088300 | -1.13299000 |
| H | -17.10768400 | 1.04389900 | -0.24894900 |
| H | -17.70814900 | -0.16694300 | -1.39431900 |
| H | -16.64582100 | 1.14446100 | -1.95229700 |
| O | 4.18715800 | 4.59948500 | -2.62099100 |
| H | 3.43782300 | 4.05683400 | -2.33613400 |
| O | 5.59610900 | 8.49833900 | -1.71851000 |
| H | 6.26556700 | 8.31008500 | -2.39590600 |
| O | 3.29260700 | 6.10179200 | -0.26992400 |

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| O | 3.27451000 | 3.83604300 | -0.22749800 |
| O | 3.61943000 | -0.59664800 | 0.32047000 |
| H | 2.82315600 | -0.53346700 | -0.23721300 |
| O | 2.82115700 | 0.80250100 | 2.00441400 |
| O | 7.21677200 | 2.28852800 | 3.22449300 |
| O | 6.23933000 | 3.07322900 | 1.37998100 |
| H | 7.10652700 | 3.50978500 | 1.34456100 |
| O | 1.00465900 | -0.65376900 | -0.22249700 |
| H | 0.16639700 | -0.65089500 | -0.71740500 |
| O | -1.63533000 | -0.96967100 | -0.68086000 |
| H | -1.79247900 | -1.83580300 | -1.09428000 |
| O | -2.60942500 | -3.30632200 | 0.09756600 |
| H | -3.40159700 | -3.81253900 | -0.11181800 |
| O | -6.47518400 | -1.81419200 | -1.34724400 |
| H | -7.31252800 | -1.88031500 | -1.83545200 |
| O | -9.07880200 | -2.31793100 | -1.73381900 |
| H | -9.96460600 | -2.22474700 | -2.12825600 |
| O | -11.75728100 | -2.51334800 | -1.75315700 |
| O | -12.73518800 | -3.41073800 | 0.06586800 |
| O | -17.00664200 | -2.27447100 | -0.29342700 |
| H | -17.43606800 | -2.73633200 | 0.43452800 |
| O | 6.48717600 | -0.44540800 | 3.35081700 |
| H | 7.08214400 | 0.30002800 | 3.52419000 |
| N | 6.51240200 | 6.16475900 | -2.94564900 |
| H | 5.90300700 | 5.83242600 | -3.68984400 |
| H | 7.31519100 | 5.54408600 | -2.92359200 |

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|---|-------------|-------------|-------------|
| C | 8.75175300 | 0.64363800 | 0.87855300 |
| H | 8.30990300 | -0.09369600 | 1.55547500 |
| H | 7.93225700 | 1.17384200 | 0.38325100 |
| H | 9.29078700 | 1.36697700 | 1.49897500 |
| C | 9.67730700 | -0.02372600 | -0.13209100 |
| H | 10.08884600 | 0.72985100 | -0.81555300 |
| H | 9.10033400 | -0.71703300 | -0.75623600 |
| C | 10.82493000 | -0.78091000 | 0.53029400 |
| H | 10.41214300 | -1.53425300 | 1.21400000 |
| H | 11.40178600 | -0.08795400 | 1.15736300 |
| C | 11.75991800 | -1.45892000 | -0.46652700 |
| H | 12.17086900 | -0.70465600 | -1.15084700 |
| H | 11.18229100 | -2.15202200 | -1.09238400 |
| C | 12.90675700 | -2.21515100 | 0.19757900 |
| H | 12.49578900 | -2.96952100 | 0.88140900 |
| H | 13.48385600 | -1.52213500 | 0.82404900 |
| C | 13.84275300 | -2.89325900 | -0.79852700 |
| H | 14.25348400 | -2.13886600 | -1.48262500 |
| H | 13.26585500 | -3.58670400 | -1.42471800 |
| C | 14.98970400 | -3.64873100 | -0.13377000 |
| H | 14.57894000 | -4.40334200 | 0.55009700 |
| H | 15.56613500 | -2.95522300 | 0.49274000 |
| C | 15.92648800 | -4.32626700 | -1.12947700 |
| H | 16.33850300 | -3.57203500 | -1.81267700 |
| H | 15.35002000 | -5.01930100 | -1.75658500 |
| C | 17.07313600 | -5.08209000 | -0.46466100 |

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|---|-------------|-------------|-------------|
| H | 16.66176800 | -5.83828200 | 0.21764100 |
| H | 17.64788400 | -4.38885200 | 0.16362300 |
| C | 18.01136500 | -5.75254500 | -1.46305800 |
| H | 18.43565000 | -5.00256100 | -2.13833800 |
| H | 17.43779000 | -6.44612300 | -2.09305300 |
| C | 19.15403100 | -6.51053500 | -0.79404700 |
| H | 18.75433600 | -7.30017300 | -0.14591600 |
| H | 19.72338400 | -5.82921200 | -0.15097200 |
| C | 20.11311000 | -7.13798000 | -1.78799500 |
| H | 20.87355900 | -7.72677900 | -1.25290400 |
| H | 19.56186800 | -7.83044400 | -2.44413000 |
| O | 20.71136200 | -6.09267200 | -2.53707700 |
| H | 21.27052500 | -6.48427100 | -3.21633300 |

structures with protonation and deprotonation in basic and acidic groups

AmB-DSPE

0 1

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|---|--------------|------------|-------------|
| C | -10.52914200 | 2.22885100 | 0.78693000 |
| H | -10.84464100 | 2.28423000 | -0.25740600 |
| C | -10.63655000 | 3.58145900 | 1.46713500 |
| H | -10.30551400 | 3.48208300 | 2.50980900 |
| C | -9.68976000 | 4.56582500 | 0.76569800 |
| H | -10.01967500 | 4.65629000 | -0.28300700 |

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|---|--------------|------------|-------------|
| C | -8.25530500 | 2.80309900 | 0.15616500 |
| H | -8.63638100 | 2.90732100 | -0.86210500 |
| C | -9.10317200 | 1.73344500 | 0.83864200 |
| H | -9.00299100 | 0.79906700 | 0.28186100 |
| C | -9.68382600 | 5.92999800 | 1.42257600 |
| H | -9.37995700 | 5.84352000 | 2.46952600 |
| H | -10.67084700 | 6.39781200 | 1.36697200 |
| H | -8.97078000 | 6.58108900 | 0.91446000 |
| C | -6.12430200 | 2.87013100 | -0.90188500 |
| H | -6.12620200 | 3.96827400 | -0.88561500 |
| C | -4.74396200 | 2.36527700 | -0.62568400 |
| H | -4.62503600 | 1.28520600 | -0.59832100 |
| C | -3.68439600 | 3.16291900 | -0.46584500 |
| H | -3.81596900 | 4.24437900 | -0.49508500 |
| C | -2.33849100 | 2.66796400 | -0.26430800 |
| H | -2.20953000 | 1.58818900 | -0.27654200 |
| C | -1.25780500 | 3.44894900 | -0.07634900 |
| H | -1.37455800 | 4.53224000 | -0.05817100 |
| C | 0.06809700 | 2.91045600 | 0.09645300 |
| H | 0.14957900 | 1.82807700 | 0.04765500 |
| C | 1.18844700 | 3.63521000 | 0.29120200 |
| H | 1.13193100 | 4.72194100 | 0.34322000 |
| C | 2.48708300 | 3.02353100 | 0.41996400 |
| H | 2.52180500 | 1.93781800 | 0.35143100 |
| C | 3.64745800 | 3.68609100 | 0.60198000 |
| H | 3.63909600 | 4.77322300 | 0.67267000 |

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|---|-------------|------------|-------------|
| C | 4.92290200 | 3.02276600 | 0.70668600 |
| H | 4.91445100 | 1.93623000 | 0.64101700 |
| C | 6.10250700 | 3.65467700 | 0.86962600 |
| H | 6.11813700 | 4.74252500 | 0.92924300 |
| C | 7.36929400 | 2.97105300 | 0.96623000 |
| H | 7.33918500 | 1.88347000 | 0.94116400 |
| C | 8.56186400 | 3.58619800 | 1.07129700 |
| H | 8.60066300 | 4.67500800 | 1.08927100 |
| C | -6.65916800 | 2.38762100 | -2.26134800 |
| H | -7.62090300 | 2.85738600 | -2.47094600 |
| H | -5.96684300 | 2.71751400 | -3.04129700 |
| C | 9.82201500 | 2.87365500 | 1.13040100 |
| H | 9.75386100 | 1.78867500 | 1.16109000 |
| C | 11.02904700 | 3.45139000 | 1.11078900 |
| H | 11.09799500 | 4.53990700 | 1.07094900 |
| C | 12.32878200 | 2.70011900 | 1.10537500 |
| H | 12.11750700 | 1.64054000 | 1.27005000 |
| C | 13.04240100 | 2.81521500 | -0.25524400 |
| H | 13.39963800 | 3.85323900 | -0.35635900 |
| C | 12.14867500 | 2.53068700 | -1.47618000 |
| H | 11.29954300 | 3.21522700 | -1.39284000 |
| C | 11.54641200 | 1.12355500 | -1.43761600 |
| H | 11.22316100 | 0.89238500 | -0.42649700 |
| C | 9.23642100 | 0.61764300 | -1.78683400 |
| C | 8.07227500 | 0.69121800 | -2.74008300 |
| H | 8.27451700 | 1.43540800 | -3.51212600 |

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|---|-------------|-------------|-------------|
| H | 7.99463500 | -0.28955000 | -3.22412500 |
| C | 6.74991000 | 0.99150500 | -2.02521700 |
| H | 6.81572300 | 1.98098200 | -1.55038400 |
| C | 5.58657300 | 0.97340100 | -3.00393500 |
| H | 5.76675000 | 1.72436500 | -3.78053000 |
| H | 5.55287100 | -0.00840200 | -3.49121900 |
| C | 4.22390400 | 1.24522200 | -2.37117000 |
| H | 4.26281100 | 2.18835500 | -1.80955700 |
| C | 3.14502700 | 1.35157000 | -3.44286600 |
| H | 3.23783300 | 0.49350200 | -4.12034000 |
| H | 3.36475900 | 2.24323600 | -4.03753500 |
| C | 1.71271000 | 1.42629100 | -2.89204300 |
| H | 1.71756600 | 1.76378100 | -1.85346600 |
| H | 1.13815600 | 2.17224300 | -3.44973800 |
| C | 0.94974700 | 0.10941000 | -2.99179100 |
| H | 0.85756100 | -0.15566500 | -4.05455200 |
| C | -0.47209100 | 0.22220600 | -2.39269600 |
| H | -0.80455100 | 1.26592200 | -2.42958100 |
| C | -1.49468400 | -0.65154600 | -3.10905300 |
| H | -1.19480600 | -1.70335500 | -3.02699500 |
| H | -1.49433500 | -0.39063800 | -4.17355900 |
| C | -2.90620000 | -0.46123600 | -2.56352900 |
| H | -3.15601000 | 0.60719900 | -2.60413700 |
| C | -3.94459200 | -1.21681500 | -3.38264700 |
| H | -3.72630400 | -2.28887300 | -3.36022800 |
| H | -3.88105900 | -0.87421600 | -4.41974900 |

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|---|--------------|-------------|-------------|
| C | -5.37624300 | -1.00722200 | -2.88581400 |
| C | -6.43229800 | -1.59220400 | -3.82457400 |
| H | -6.36737700 | -2.68297600 | -3.81037800 |
| H | -6.25208300 | -1.24535900 | -4.84620000 |
| C | -7.81447100 | -1.13612500 | -3.38560000 |
| H | -7.98471700 | -1.50056800 | -2.36218800 |
| C | -7.86627200 | 0.40408800 | -3.34695600 |
| H | -7.59851000 | 0.77205500 | -4.34570000 |
| C | -6.80651700 | 0.87367600 | -2.35516300 |
| H | -7.02490200 | 0.45669700 | -1.36596200 |
| C | -9.32516400 | 0.81710900 | -3.08938800 |
| C | 12.41060300 | -0.00443300 | -1.96046100 |
| H | 11.88686100 | -0.95328400 | -1.84264700 |
| H | 13.34012700 | -0.03866500 | -1.39072400 |
| H | 12.64408100 | 0.13246200 | -3.01834500 |
| C | 12.87154400 | 2.83449400 | -2.78662200 |
| H | 13.77958600 | 2.23486200 | -2.90193200 |
| H | 13.15562600 | 3.88960000 | -2.83457400 |
| H | 12.22816200 | 2.62081100 | -3.64356800 |
| C | 13.25642100 | 3.16983800 | 2.22869900 |
| H | 13.47260400 | 4.23984700 | 2.13411400 |
| H | 14.20070100 | 2.62408900 | 2.19272700 |
| H | 12.79109300 | 3.00759700 | 3.20374700 |
| O | -8.77557900 | 1.57213200 | 2.20611900 |
| H | -7.86854400 | 1.22872100 | 2.27366300 |
| O | -12.00793100 | 3.94969300 | 1.39415200 |

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|---|--------------|-------------|-------------|
| H | -12.16060700 | 4.70223500 | 1.97625300 |
| O | -8.37239700 | 4.05460000 | 0.82961800 |
| O | -6.93993300 | 2.39478100 | 0.18302400 |
| O | -5.58039200 | -1.61910600 | -1.64192500 |
| H | -4.86267500 | -1.32660800 | -1.05632800 |
| O | -5.52472900 | 0.39798200 | -2.79342500 |
| O | -9.65622400 | 1.33799300 | -1.99981700 |
| O | -2.99649600 | -0.89770900 | -1.20181400 |
| H | -2.13114800 | -0.72838400 | -0.78784700 |
| O | -0.40456200 | -0.13020400 | -1.00869000 |
| H | 0.34125100 | -0.76353500 | -0.97866200 |
| O | 1.59789000 | -0.96311800 | -2.32511700 |
| H | 2.45730800 | -0.65840000 | -1.96263500 |
| O | 3.85283500 | 0.19965700 | -1.46645100 |
| H | 4.65984400 | -0.11608000 | -1.02201500 |
| O | 6.47762700 | 0.01332000 | -1.02958500 |
| H | 7.30699800 | -0.16794100 | -0.54800500 |
| O | 9.15602400 | 0.07728600 | -0.69325700 |
| O | 10.33869500 | 1.17147600 | -2.26391000 |
| O | 14.15843000 | 1.92880000 | -0.19507700 |
| H | 14.79034800 | 2.17622600 | -0.87846100 |
| O | -8.82753700 | -1.67627800 | -4.23786900 |
| H | -9.35728800 | -0.87556500 | -4.52304100 |
| N | -11.43367500 | 1.26461900 | 1.47889900 |
| H | -11.72259500 | 0.46465400 | 0.86568400 |
| H | -12.26850900 | 1.76789600 | 1.79078800 |

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|---|-------------|-------------|------------|
| C | 14.47347500 | -1.53173800 | 2.39427400 |
| H | 14.60439500 | -1.85578300 | 3.43409000 |
| H | 14.38864900 | -2.44820000 | 1.79785900 |
| C | 13.18286700 | -0.72976000 | 2.26681900 |
| H | 13.06826900 | -0.42022300 | 1.21958300 |
| H | 13.28080300 | 0.20223400 | 2.83925300 |
| C | 11.92559000 | -1.46814300 | 2.71670200 |
| H | 12.00964100 | -1.72844400 | 3.77967500 |
| H | 11.84388400 | -2.41807300 | 2.17374600 |
| C | 10.66273900 | -0.64524900 | 2.48283000 |
| H | 10.75248700 | 0.31528800 | 3.00843800 |
| H | 10.59066500 | -0.40235700 | 1.41532600 |
| C | 9.36476100 | -1.32838800 | 2.90377500 |
| H | 9.38923700 | -1.55129200 | 3.97816300 |
| H | 9.28174200 | -2.29483400 | 2.38980900 |
| C | 8.14228600 | -0.48015000 | 2.57482300 |
| H | 8.22499700 | 0.49627500 | 3.07478400 |
| H | 8.15531400 | -0.26074100 | 1.49934500 |
| C | 6.80552500 | -1.12037000 | 2.93450000 |
| H | 6.75310200 | -1.27864600 | 4.01933600 |
| H | 6.74599800 | -2.11738100 | 2.47754400 |
| C | 5.61008400 | -0.28896700 | 2.47691100 |
| H | 5.69289600 | 0.72900900 | 2.88018200 |
| H | 5.65157300 | -0.18214600 | 1.38544200 |
| C | 4.26570000 | -0.88486700 | 2.87943000 |
| H | 4.21528600 | -0.94705400 | 3.97434400 |

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|---|-------------|-------------|------------|
| H | 4.20103500 | -1.91778100 | 2.51390200 |
| C | 3.06285700 | -0.09755500 | 2.36444300 |
| H | 3.16388200 | 0.95858200 | 2.64578800 |
| H | 3.06126300 | -0.11847000 | 1.26605800 |
| C | 1.74170800 | -0.64246200 | 2.89890400 |
| H | 1.76761200 | -0.60794300 | 3.99611100 |
| H | 1.65634200 | -1.70438600 | 2.63375400 |
| C | 0.49632200 | 0.09326900 | 2.40855200 |
| H | 0.40367300 | -0.02006400 | 1.32224200 |
| H | 0.59987500 | 1.17005200 | 2.59277100 |
| C | -0.76736700 | -0.42909900 | 3.08610800 |
| H | -0.65768400 | -0.31133700 | 4.17256200 |
| H | -0.84426400 | -1.51007600 | 2.91025800 |
| C | -2.07719400 | 0.22841600 | 2.65171800 |
| H | -2.23993600 | 0.06359000 | 1.57894500 |
| H | -2.01738400 | 1.31573400 | 2.78555700 |
| C | -3.24663200 | -0.35287900 | 3.44097800 |
| H | -3.06174800 | -0.22250800 | 4.51374200 |
| H | -3.27871300 | -1.43356700 | 3.28047200 |
| C | -4.61950500 | 0.22099800 | 3.10739200 |
| H | -4.82775000 | 0.20346600 | 2.03058900 |
| H | -4.72252900 | 1.26721000 | 3.41182700 |
| C | -5.71095100 | -0.59081700 | 3.75490400 |
| O | -5.56702000 | -1.67604800 | 4.26173600 |
| C | 15.69127500 | -0.73141700 | 1.94103400 |
| H | 16.60674800 | -1.32843000 | 1.97605400 |

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| H | 15.55713000 | -0.36669200 | 0.91772300 |
| H | 15.83928300 | 0.14740400 | 2.57686800 |
| C | -8.06989600 | -0.73399800 | 4.07941200 |
| H | -7.78476100 | -1.45877900 | 4.84560600 |
| H | -8.77062400 | -0.00592900 | 4.48231500 |
| C | -8.69418200 | -1.42463600 | 2.87718700 |
| H | -8.79172100 | -0.72227100 | 2.05744400 |
| C | -10.06281000 | -2.02643700 | 3.19227600 |
| H | -10.01345900 | -3.11448700 | 3.13373200 |
| H | -10.39896400 | -1.75676600 | 4.19985300 |
| O | -6.91696600 | 0.02886200 | 3.68675700 |
| C | -7.01722700 | -2.11036400 | 1.38477700 |
| C | -6.18600000 | -3.24927900 | 0.87404600 |
| H | -6.53749300 | -4.19753000 | 1.28308300 |
| H | -6.29750900 | -3.25014700 | -0.21205800 |
| C | -4.72181000 | -2.97483900 | 1.24135700 |
| H | -4.57643300 | -3.16902600 | 2.30955600 |
| H | -4.53335800 | -1.90581200 | 1.09804000 |
| C | -3.69327800 | -3.73085800 | 0.41101000 |
| H | -3.85104900 | -4.81429400 | 0.48243800 |
| H | -3.82401500 | -3.45356000 | -0.64033400 |
| C | -2.28149200 | -3.36853700 | 0.86323100 |
| H | -2.08994900 | -3.80266200 | 1.85369600 |
| H | -2.23238700 | -2.28131800 | 1.00274600 |
| C | -1.17195700 | -3.77298500 | -0.09898900 |
| H | -1.36646600 | -3.30543600 | -1.07248500 |

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|---|-------------|-------------|-------------|
| H | -1.18632900 | -4.85771300 | -0.26461700 |
| C | 0.20055900 | -3.34183400 | 0.40722600 |
| H | 0.17119700 | -2.26294900 | 0.60662600 |
| H | 0.39384200 | -3.81188300 | 1.38092900 |
| C | 1.35537000 | -3.64591300 | -0.54141100 |
| H | 1.16571000 | -3.18103200 | -1.51432100 |
| H | 1.41541200 | -4.72863900 | -0.71223800 |
| C | 2.68814600 | -3.14088600 | 0.00242500 |
| H | 2.60151200 | -2.06992300 | 0.22576700 |
| H | 2.89145000 | -3.63083900 | 0.96457700 |
| C | 3.87501800 | -3.35760900 | -0.93208900 |
| H | 3.77144300 | -2.70821300 | -1.81054900 |
| H | 3.86165000 | -4.38852900 | -1.30931200 |
| C | 5.21156100 | -3.09590600 | -0.24395000 |
| H | 5.22021500 | -2.08084100 | 0.17157400 |
| H | 5.30223800 | -3.76983700 | 0.61859900 |
| C | 6.42591300 | -3.27447700 | -1.14787500 |
| H | 6.37040700 | -4.25110900 | -1.64676300 |
| H | 6.39967300 | -2.51499100 | -1.93825000 |
| C | 7.74588000 | -3.17160500 | -0.39048100 |
| H | 7.81765400 | -2.19397200 | 0.10004400 |
| H | 7.75335500 | -3.91188500 | 0.42059100 |
| C | 8.97629200 | -3.38110900 | -1.26539200 |
| H | 8.91904300 | -4.36834500 | -1.74247800 |
| H | 8.97134600 | -2.64743000 | -2.08347300 |
| C | 10.28493500 | -3.25918200 | -0.49156900 |

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|---|--------------|-------------|-------------|
| H | 10.24216300 | -3.90127400 | 0.39819200 |
| H | 10.38026100 | -2.23140600 | -0.12093300 |
| C | 11.51858100 | -3.62474300 | -1.31136000 |
| H | 11.45177000 | -4.67199300 | -1.63290300 |
| H | 11.53116200 | -3.03305500 | -2.23703000 |
| C | 12.82419900 | -3.40805700 | -0.55151100 |
| H | 12.83519200 | -4.05632700 | 0.33348200 |
| H | 12.85137700 | -2.38159000 | -0.17011300 |
| C | 14.06646400 | -3.66444200 | -1.39654300 |
| H | 14.98230700 | -3.50753600 | -0.81980000 |
| H | 14.08227500 | -4.68979500 | -1.77877100 |
| H | 14.09644400 | -2.99079200 | -2.25958900 |
| O | -7.83738300 | -2.46482200 | 2.39048500 |
| O | -6.89874800 | -0.96577500 | 1.00252300 |
| O | -11.07500900 | -1.51810000 | 2.31034500 |
| O | -12.15941100 | -1.02321600 | 0.20620400 |
| O | -11.71004600 | -3.51051500 | 0.72432900 |
| O | -9.76213600 | -1.87681500 | 0.14231600 |
| C | -12.77916000 | -1.33483200 | -1.04615900 |
| H | -13.13032900 | -2.37139700 | -1.00522300 |
| H | -13.64871600 | -0.67965400 | -1.13725800 |
| C | -11.86820100 | -1.08104400 | -2.23670300 |
| H | -11.43303000 | -0.08138100 | -2.19796500 |
| H | -12.43579900 | -1.16262000 | -3.16535700 |
| N | -10.73014600 | -2.04439500 | -2.29352000 |
| H | -11.06044100 | -3.01036500 | -2.30461100 |

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| H | -10.10116800 | -1.90091600 | -3.12659400 |
| P | -11.08992000 | -2.16846300 | 0.80844400 |
| O | -10.11760100 | 0.48784100 | -4.01976200 |
| H | -10.15180400 | -1.94820200 | -1.39377200 |
| H | -10.95013400 | 0.84526900 | 2.28026100 |

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|---|--------------|------------|-------------|
| C | -9.69960800 | 4.77016900 | -2.03789000 |
| C | -11.01741000 | 4.27929700 | -1.45191400 |
| C | -10.91315100 | 2.84195900 | -0.97858600 |
| C | -10.30857400 | 1.96727100 | -2.06871800 |
| C | -8.97236400 | 2.56147400 | -2.50421600 |
| C | -8.23906400 | 1.79642100 | -3.58638700 |
| O | -8.77151400 | 4.90733500 | -1.00520400 |
| O | -11.38876900 | 5.14036400 | -0.39236200 |
| O | -12.21339900 | 2.45239200 | -0.61877000 |
| O | -9.23518200 | 3.87314500 | -3.01396600 |
| O | -6.87269700 | 2.17184500 | -3.63922600 |
| H | -10.99068400 | 1.93428900 | -2.92808500 |
| H | -9.84901100 | 5.72509000 | -2.55192300 |
| H | -11.76853200 | 4.30939700 | -2.25328300 |
| H | -10.22930100 | 2.80946600 | -0.11607800 |
| H | -8.31198700 | 2.62694800 | -1.63127300 |

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| H | -8.33955000 | 0.72176800 | -3.40291000 |
| H | -8.69807200 | 2.02352900 | -4.55375000 |
| H | -12.14045200 | 4.71671300 | 0.04552300 |
| H | -12.23192100 | 1.48928100 | -0.46006100 |
| H | -6.34916700 | 1.51514900 | -3.13145600 |
| C | -10.71851200 | -0.41672300 | -2.18387200 |
| C | -11.58472900 | -1.19995400 | -1.20002500 |
| C | -10.72287500 | -1.84165700 | -0.13417600 |
| C | -9.65145600 | -2.67087700 | -0.81437500 |
| C | -8.82701800 | -1.81566600 | -1.77287900 |
| C | -7.76344200 | -2.60398500 | -2.53776700 |
| O | -10.14502100 | 0.67053900 | -1.51573700 |
| O | -12.54855000 | -0.33774600 | -0.62616700 |
| O | -11.57728000 | -2.62070000 | 0.66586500 |
| O | -9.72847600 | -1.25080200 | -2.73510800 |
| O | -6.47112900 | -2.26529500 | -2.05536200 |
| H | -10.14233700 | -3.45606400 | -1.40444500 |
| H | -11.32229100 | -0.07487100 | -3.03000900 |
| H | -12.08524800 | -2.00052800 | -1.76142200 |
| H | -10.23384400 | -1.04828800 | 0.45037500 |
| H | -8.32564800 | -1.01148200 | -1.22164300 |
| H | -7.92172600 | -3.68019200 | -2.42264900 |
| H | -7.85366900 | -2.34903800 | -3.59936500 |
| H | -12.91890900 | -0.81939000 | 0.12793700 |
| H | -11.04660800 | -3.11642700 | 1.31827800 |
| H | -5.90312000 | -3.07314200 | -1.93455200 |

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| C | -8.82148000 | -4.65047500 | 0.25145500 |
| C | -8.95935700 | -5.09783400 | 1.70495400 |
| C | -7.71856700 | -4.75289200 | 2.50133400 |
| C | -6.49477700 | -5.28871200 | 1.77828900 |
| C | -6.45191400 | -4.72200300 | 0.36279100 |
| C | -5.24870800 | -5.15577600 | -0.45277600 |
| O | -8.85086800 | -3.25121600 | 0.19589700 |
| O | -10.11624200 | -4.50044600 | 2.26022900 |
| O | -7.87554100 | -5.30789400 | 3.78259700 |
| O | -7.64004500 | -5.14668900 | -0.31889500 |
| O | -4.75929700 | -4.06313500 | -1.22042500 |
| H | -6.55208300 | -6.38360700 | 1.72442300 |
| H | -9.63951300 | -5.07225900 | -0.34029500 |
| H | -9.06201500 | -6.19175700 | 1.70145600 |
| H | -7.62853400 | -3.65639200 | 2.54843800 |
| H | -6.45223000 | -3.62748700 | 0.42925100 |
| H | -4.45950000 | -5.52516900 | 0.20677100 |
| H | -5.55540200 | -5.97836200 | -1.10922700 |
| H | -10.06128700 | -4.63766700 | 3.21634600 |
| H | -7.04526700 | -5.18813000 | 4.28271000 |
| H | -3.90131300 | -4.45511600 | -1.78061400 |
| C | -4.49304900 | -5.88380700 | 2.98525500 |
| C | -4.12812500 | -5.57613200 | 4.43130400 |
| C | -3.25247800 | -4.34125200 | 4.52666000 |
| C | -2.08323000 | -4.47011000 | 3.56055400 |
| C | -2.60534800 | -4.72338500 | 2.14979800 |

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| C | -1.55836800 | -4.83035900 | 1.05003500 |
| O | -5.36809300 | -4.88551800 | 2.52823400 |
| O | -5.32115300 | -5.42867600 | 5.18221000 |
| O | -2.84934300 | -4.23871500 | 5.86911700 |
| O | -3.34093800 | -5.95558900 | 2.19151800 |
| O | -1.36461600 | -3.54772800 | 0.50089100 |
| H | -1.46846400 | -5.32939000 | 3.86057800 |
| H | -4.97037800 | -6.86638700 | 2.91791600 |
| H | -3.54395300 | -6.42527800 | 4.81058400 |
| H | -3.84653300 | -3.46587700 | 4.22034300 |
| H | -3.27864200 | -3.90809200 | 1.86195000 |
| H | -0.61658700 | -5.24885200 | 1.42006200 |
| H | -1.95258300 | -5.51117200 | 0.28696700 |
| H | -5.05841000 | -5.06349300 | 6.03847600 |
| H | -2.06904900 | -3.65414500 | 5.92824400 |
| H | -0.41841200 | -3.31902200 | 0.45313400 |
| C | 0.05265900 | -3.37252000 | 3.82892200 |
| C | 0.44606800 | -2.55305500 | 5.05565100 |
| C | 0.19585300 | -1.08225000 | 4.80614400 |
| C | 0.88550500 | -0.65695800 | 3.52731700 |
| C | 0.49500500 | -1.55099600 | 2.35542800 |
| C | 1.32392100 | -1.26249200 | 1.12242200 |
| O | -1.33567800 | -3.27484600 | 3.66018300 |
| O | -0.29073000 | -3.01034800 | 6.17781900 |
| O | 0.67628800 | -0.37299000 | 5.92547800 |
| O | 0.74825600 | -2.91832500 | 2.70404400 |

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| O | 0.85834500 | -2.01811500 | 0.02607600 |
| H | 1.97170100 | -0.71007700 | 3.68627800 |
| H | 0.34893300 | -4.41762200 | 3.96325400 |
| H | 1.52111900 | -2.69815900 | 5.22523800 |
| H | -0.88564300 | -0.93268500 | 4.67344500 |
| H | -0.56468000 | -1.41562600 | 2.11383100 |
| H | 1.27762300 | -0.19492300 | 0.89676700 |
| H | 2.36545900 | -1.54454600 | 1.32083100 |
| H | -0.15062900 | -2.35491400 | 6.87583500 |
| H | 0.82943400 | 0.55249300 | 5.66151900 |
| H | 0.46998600 | -1.41776000 | -0.63716600 |
| C | 1.41886300 | 1.58667200 | 2.79810300 |
| C | 1.51721500 | 2.77134500 | 3.75763600 |
| C | 0.24372400 | 3.58832300 | 3.72170500 |
| C | -0.10243200 | 3.91486800 | 2.27905500 |
| C | -0.25820600 | 2.62553600 | 1.47671600 |
| C | -0.68013400 | 2.80061900 | 0.01970900 |
| O | 0.48681300 | 0.68661900 | 3.31874400 |
| O | 1.77773500 | 2.27749300 | 5.05977600 |
| O | 0.47260000 | 4.74501400 | 4.49262100 |
| O | 1.03835600 | 2.00773200 | 1.51137500 |
| O | -2.05957000 | 2.45260000 | -0.08450600 |
| H | 0.72685600 | 4.47460800 | 1.82781800 |
| H | 2.39722400 | 1.11057800 | 2.68062600 |
| H | 2.34089400 | 3.41559800 | 3.42073300 |
| H | -0.57328500 | 2.98326200 | 4.14185700 |

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| H | -0.99142100 | 1.96326200 | 1.94790000 |
| H | -0.52337200 | 3.83289100 | -0.31007600 |
| H | -0.07233500 | 2.13201300 | -0.60116700 |
| H | 1.67662200 | 3.03512600 | 5.65314200 |
| H | -0.32935500 | 5.29872600 | 4.47924700 |
| H | -2.51457300 | 3.01542900 | -0.74230900 |
| C | -1.10839500 | 6.02819200 | 1.85455800 |
| C | -1.96226400 | 6.94822400 | 2.72331700 |
| C | -3.43756300 | 6.71060300 | 2.47218700 |
| C | -3.69608200 | 6.76978400 | 0.97596000 |
| C | -2.82490200 | 5.73925800 | 0.26668500 |
| C | -3.04592900 | 5.60178500 | -1.23488400 |
| O | -1.26725800 | 4.71494200 | 2.30229000 |
| O | -1.61468000 | 6.74054000 | 4.07883900 |
| O | -4.15046400 | 7.69935300 | 3.17718100 |
| O | -1.46593300 | 6.13891200 | 0.49970100 |
| O | -3.57628300 | 4.30989100 | -1.49383200 |
| H | -3.42250800 | 7.76536800 | 0.60291200 |
| H | -0.05967400 | 6.33365300 | 1.91751700 |
| H | -1.73710200 | 7.98200600 | 2.42586300 |
| H | -3.69629400 | 5.70137400 | 2.82541400 |
| H | -2.99137800 | 4.75167300 | 0.70681800 |
| H | -3.73200300 | 6.36988400 | -1.60334600 |
| H | -2.07873000 | 5.73203100 | -1.73483000 |
| H | -2.29095700 | 7.18315300 | 4.60916100 |
| H | -5.09507900 | 7.62303000 | 2.95087000 |

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| H | -4.29556000 | 4.37238400 | -2.16435800 |
| C | -5.79382300 | 7.53554000 | 0.11036500 |
| C | -7.15334300 | 7.69512100 | 0.78121000 |
| C | -8.00330900 | 6.46086700 | 0.55954000 |
| C | -8.03471200 | 6.11373100 | -0.91954100 |
| C | -6.61875500 | 5.96535100 | -1.46796300 |
| C | -6.52043000 | 5.64441800 | -2.96133500 |
| O | -5.08007300 | 6.54502900 | 0.78612800 |
| O | -6.94691600 | 7.95201400 | 2.15716200 |
| O | -9.28903400 | 6.73676300 | 1.06178800 |
| O | -5.94783900 | 7.21550100 | -1.24986300 |
| O | -5.62686500 | 4.57342000 | -3.22325000 |
| H | -8.55400100 | 6.91623700 | -1.46055000 |
| H | -5.25297600 | 8.48680700 | 0.13400500 |
| H | -7.66103900 | 8.54443800 | 0.30358300 |
| H | -7.53655200 | 5.61900200 | 1.09266800 |
| H | -6.10566700 | 5.17090800 | -0.91518300 |
| H | -7.50068300 | 5.40013100 | -3.37407200 |
| H | -6.14482700 | 6.53849000 | -3.46732700 |
| H | -7.80911900 | 7.87010400 | 2.58670900 |
| H | -9.90562200 | 6.06136100 | 0.72556500 |
| H | -6.14315800 | 3.74868500 | -3.36426700 |
| C | -3.62730300 | -1.09557300 | -1.54188400 |
| H | -3.77951700 | -1.85710200 | -2.31297300 |
| C | -4.09618000 | 0.26039100 | -2.05195300 |
| H | -3.96013400 | 1.03470300 | -1.28799400 |

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| C | -3.19868500 | 0.61976200 | -3.25666400 |
| H | -3.30955600 | -0.18523700 | -4.00132300 |
| C | -1.40946500 | -0.63081800 | -2.42085900 |
| H | -1.66424700 | -1.33950700 | -3.20904600 |
| C | -2.14794000 | -1.07721700 | -1.17555300 |
| H | -1.84658000 | -2.09242100 | -0.91654200 |
| C | -3.51087200 | 1.95116100 | -3.89771900 |
| H | -3.34504600 | 2.76314900 | -3.18998900 |
| H | -4.53848000 | 1.98454200 | -4.26141200 |
| H | -2.84122600 | 2.10180500 | -4.74670100 |
| C | 0.81275800 | -1.04775600 | -3.27432800 |
| H | 0.71865100 | -0.29846700 | -4.06981000 |
| C | 2.19189000 | -1.01339800 | -2.69568800 |
| H | 2.38696300 | -1.71752700 | -1.89145400 |
| C | 3.15038000 | -0.16867100 | -3.08686600 |
| H | 2.96383000 | 0.53936100 | -3.89406100 |
| C | 4.45078700 | -0.13613500 | -2.44866200 |
| H | 4.59707800 | -0.82928500 | -1.62377000 |
| C | 5.46019100 | 0.69159900 | -2.77730000 |
| H | 5.33671600 | 1.39670800 | -3.59888200 |
| C | 6.71756900 | 0.69137500 | -2.06855200 |
| H | 6.79891900 | -0.02755400 | -1.25530800 |
| C | 7.76940100 | 1.48821000 | -2.34433500 |
| H | 7.70375900 | 2.20822200 | -3.15948800 |
| C | 9.00251200 | 1.43634600 | -1.59900000 |
| H | 9.06218700 | 0.69890400 | -0.79863500 |

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| C | 10.07761600 | 2.21681200 | -1.83202800 |
| H | 10.04225500 | 2.94771700 | -2.63921500 |
| C | 11.28783700 | 2.15334500 | -1.05170900 |
| H | 11.30826700 | 1.43442100 | -0.23281700 |
| C | 12.37962800 | 2.91393900 | -1.26983900 |
| H | 12.37894800 | 3.62046600 | -2.09915100 |
| C | 13.56841900 | 2.85208700 | -0.45473900 |
| H | 13.53338600 | 2.19168300 | 0.40998500 |
| C | 14.70580000 | 3.52957200 | -0.69566600 |
| H | 14.77169200 | 4.17472700 | -1.57103400 |
| C | 0.40983100 | -2.42404200 | -3.83581400 |
| H | -0.54965000 | -2.36034200 | -4.34680100 |
| H | 1.15560600 | -2.69882500 | -4.58780500 |
| C | 15.88447600 | 3.40872500 | 0.13995900 |
| H | 15.75243900 | 2.84357200 | 1.06051400 |
| C | 17.09717500 | 3.88164900 | -0.16717300 |
| H | 17.23302300 | 4.43276800 | -1.09922700 |
| C | 18.33268500 | 3.67021100 | 0.66059400 |
| H | 18.04439800 | 3.24049200 | 1.62677200 |
| C | 19.28963800 | 2.66847300 | -0.01475200 |
| H | 19.68974700 | 3.15678600 | -0.91901600 |
| C | 18.63305600 | 1.35578900 | -0.48171200 |
| H | 17.84138300 | 1.65009000 | -1.17745700 |
| C | 17.92016800 | 0.59989400 | 0.64473600 |
| H | 17.31805900 | 1.29125400 | 1.22775400 |
| C | 15.72108200 | -0.32028700 | 0.36107600 |

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| C | 14.89141100 | -1.30655300 | -0.42167800 |
| H | 15.36953900 | -1.50048400 | -1.38364000 |
| H | 14.88440200 | -2.24616600 | 0.14303500 |
| C | 13.44835400 | -0.83145600 | -0.60881400 |
| H | 13.45040100 | 0.11399400 | -1.17001800 |
| C | 12.62610500 | -1.86501100 | -1.36477100 |
| H | 13.08415900 | -2.02769100 | -2.34628100 |
| H | 12.66283900 | -2.81564900 | -0.81929000 |
| C | 11.16179700 | -1.48003900 | -1.56221100 |
| H | 11.10363900 | -0.48857100 | -2.03203900 |
| C | 10.44186500 | -2.48989200 | -2.44984300 |
| H | 10.67623800 | -3.50115800 | -2.09505400 |
| H | 10.86745800 | -2.40468100 | -3.45441900 |
| C | 8.91716700 | -2.29793300 | -2.50095400 |
| H | 8.65071200 | -1.27918200 | -2.20954600 |
| H | 8.56037200 | -2.42212300 | -3.52800400 |
| C | 8.14180100 | -3.29311300 | -1.63983800 |
| H | 8.30593000 | -4.30005700 | -2.04837700 |
| C | 6.61909300 | -3.00204200 | -1.65449700 |
| H | 6.36094600 | -2.43119000 | -2.55417100 |
| C | 5.77313700 | -4.26901400 | -1.60797700 |
| H | 6.01496700 | -4.83284100 | -0.69871800 |
| H | 6.03926700 | -4.89707100 | -2.46626200 |
| C | 4.27308000 | -3.98439400 | -1.65030600 |
| H | 4.05860900 | -3.35067200 | -2.52249700 |
| C | 3.46319200 | -5.26616100 | -1.79084400 |

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| H | 3.70430100 | -5.94975500 | -0.97124400 |
| H | 3.74696100 | -5.74774300 | -2.73183100 |
| C | 1.94849000 | -5.05461000 | -1.78168700 |
| C | 1.17335900 | -6.27957300 | -2.24632700 |
| H | 1.34093200 | -7.11966900 | -1.56771600 |
| H | 1.51854500 | -6.56498700 | -3.24446200 |
| C | -0.30424700 | -5.94885100 | -2.28474700 |
| H | -0.61279300 | -5.70931200 | -1.26514600 |
| C | -0.60103400 | -4.71311800 | -3.14988800 |
| H | -0.46248000 | -4.99401500 | -4.20178600 |
| C | 0.35840400 | -3.55173000 | -2.80369800 |
| H | 0.05121000 | -3.16661800 | -1.82983600 |
| C | -2.06826600 | -4.28287900 | -2.95692800 |
| C | 18.79240300 | -0.22090000 | 1.57237400 |
| H | 18.18461400 | -0.66059800 | 2.36646500 |
| H | 19.54891600 | 0.42833500 | 2.01516600 |
| H | 19.29064200 | -1.02906900 | 1.03262100 |
| C | 19.62300100 | 0.47716000 | -1.24482000 |
| H | 20.48271500 | 0.19744500 | -0.62831400 |
| H | 19.99777300 | 0.99766800 | -2.13088300 |
| H | 19.14367800 | -0.44715600 | -1.57494600 |
| C | 19.05826100 | 4.99205500 | 0.92696400 |
| H | 19.34094700 | 5.47355400 | -0.01579600 |
| H | 19.96536600 | 4.81859200 | 1.50740500 |
| H | 18.41241000 | 5.68276900 | 1.47381600 |
| O | -1.93095800 | -0.28632300 | -0.02722800 |

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| H | -2.01159000 | 0.67331200 | -0.23184900 |
| O | -5.48384200 | 0.22570700 | -2.36242800 |
| H | -5.78231900 | -0.69603400 | -2.52850700 |
| O | -1.84500900 | 0.66594000 | -2.80331500 |
| O | -0.04418600 | -0.62769100 | -2.17389600 |
| O | 1.48456000 | -4.73151900 | -0.49894700 |
| H | 1.96640900 | -3.93660800 | -0.21208500 |
| O | 1.70809400 | -4.00148700 | -2.70402300 |
| O | -2.48359100 | -3.22143100 | -3.44824900 |
| O | -2.80017600 | -5.06566300 | -2.24815600 |
| O | 3.84954200 | -3.30436900 | -0.46837500 |
| H | 4.57861700 | -2.71564300 | -0.20837700 |
| O | 6.31785900 | -2.15837500 | -0.54137000 |
| H | 7.01183200 | -2.40272700 | 0.10558000 |
| O | 8.55284900 | -3.30569400 | -0.27994200 |
| H | 9.27999500 | -2.65965400 | -0.15539900 |
| O | 10.47485900 | -1.42279700 | -0.30894700 |
| H | 11.09859800 | -1.07418100 | 0.35364400 |
| O | 12.82267300 | -0.62549600 | 0.65501800 |
| H | 13.43915300 | -0.10254200 | 1.19802300 |
| O | 15.26341200 | 0.37372000 | 1.25525400 |
| O | 16.99026400 | -0.31295800 | -0.01916800 |
| O | 20.34697300 | 2.43957500 | 0.91194000 |
| H | 21.09542700 | 2.05999400 | 0.43934300 |
| O | -1.00839800 | -7.07896000 | -2.76051100 |
| H | -1.93881600 | -6.84167600 | -2.62622800 |

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|---|-------------|-------------|-------------|
| N | -4.36198900 | -1.55415700 | -0.32468800 |
| H | -5.33302300 | -1.23403400 | -0.34324000 |
| H | -3.85108800 | -1.20017800 | 0.49378500 |
| H | -4.39002900 | -2.61176800 | -0.37769600 |

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| C | 8.44721900 | -1.52852600 | 1.20672000 |
| H | 8.93057300 | -0.54741500 | 1.12901400 |
| C | 9.12175600 | -2.60233000 | 0.37527400 |
| H | 8.58935700 | -3.55312900 | 0.51971100 |
| C | 9.00017800 | -2.22620000 | -1.11156700 |
| H | 9.51065900 | -1.26440600 | -1.26201000 |
| C | 6.99550800 | -1.03714400 | -0.66709700 |
| H | 7.57931000 | -0.12067200 | -0.75449900 |
| C | 6.99301500 | -1.40582100 | 0.80646400 |
| H | 6.53679200 | -0.56854900 | 1.33727000 |
| C | 9.58810900 | -3.27947300 | -2.02428200 |
| H | 9.10178000 | -4.24617100 | -1.85850600 |
| H | 10.66221700 | -3.38664300 | -1.85303400 |
| H | 9.44206500 | -2.99245800 | -3.06684600 |
| C | 5.36344300 | 0.04075100 | -2.13581100 |
| H | 5.60627100 | -0.44397800 | -3.09352900 |
| C | 3.88350100 | 0.17977800 | -1.98334600 |

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| H | 3.56363500 | 0.79977100 | -1.15237500 |
| C | 2.96708500 | -0.49167400 | -2.68825100 |
| H | 3.26331500 | -1.13773700 | -3.51736000 |
| C | 1.56473900 | -0.41890000 | -2.33020700 |
| H | 1.31815300 | 0.32078700 | -1.57536100 |
| C | 0.56653400 | -1.21905600 | -2.74841600 |
| H | 0.73724400 | -2.01000900 | -3.47759000 |
| C | -0.74496600 | -1.06823400 | -2.16016800 |
| H | -0.83039300 | -0.23408600 | -1.46602100 |
| C | -1.83195300 | -1.84021800 | -2.35472900 |
| H | -1.80313900 | -2.68528900 | -3.04137600 |
| C | -3.05902200 | -1.57614400 | -1.64256300 |
| H | -3.04607400 | -0.71658000 | -0.97119000 |
| C | -4.19801500 | -2.29091100 | -1.74205700 |
| H | -4.24266900 | -3.14381100 | -2.41835100 |
| C | -5.37738300 | -1.99005300 | -0.96974500 |
| H | -5.30638600 | -1.15136100 | -0.27689300 |
| C | -6.54204800 | -2.66517900 | -1.04128600 |
| H | -6.63821100 | -3.49324600 | -1.74262600 |
| C | -7.68724700 | -2.35005000 | -0.22242800 |
| H | -7.55256400 | -1.56489700 | 0.51959900 |
| C | -8.89605200 | -2.93281000 | -0.31935900 |
| H | -9.06571300 | -3.70120600 | -1.07272000 |
| C | 6.13694500 | 1.35561000 | -2.04776000 |
| H | 7.20578600 | 1.15421100 | -2.15222200 |
| H | 5.85612800 | 1.95225700 | -2.92107900 |

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| C | -10.01799700 | -2.54490400 | 0.51322900 |
| H | -9.78385900 | -1.85757600 | 1.32363300 |
| C | -11.28853100 | -2.91326400 | 0.31775600 |
| H | -11.52692200 | -3.58739700 | -0.50661500 |
| C | -12.45499000 | -2.41833800 | 1.12513800 |
| H | -12.07759000 | -1.88224600 | 2.00335800 |
| C | -13.30561900 | -1.42090700 | 0.31439200 |
| H | -13.79177600 | -1.98966000 | -0.49585700 |
| C | -12.51057700 | -0.28839400 | -0.36310500 |
| H | -11.78429300 | -0.78390200 | -1.01454300 |
| C | -11.67457100 | 0.53899100 | 0.61931000 |
| H | -11.13560700 | -0.12262200 | 1.29165400 |
| C | -9.39592500 | 1.13951700 | 0.15679800 |
| C | -8.49362800 | 1.91774900 | -0.76691300 |
| H | -8.97692700 | 2.02674800 | -1.73960600 |
| H | -8.38115800 | 2.92011800 | -0.33717400 |
| C | -7.10723500 | 1.28432400 | -0.90864200 |
| H | -7.21125800 | 0.28071600 | -1.34592700 |
| C | -6.21364200 | 2.13730500 | -1.79822100 |
| H | -6.67654200 | 2.21598400 | -2.78791900 |
| H | -6.16044500 | 3.14814100 | -1.37635200 |
| C | -4.78814000 | 1.61569700 | -1.96509800 |
| H | -4.81370400 | 0.58104900 | -2.33515400 |
| C | -4.00547400 | 2.48123100 | -2.95343400 |
| H | -4.20634300 | 3.53585100 | -2.73217200 |
| H | -4.41166900 | 2.28457800 | -3.95040300 |

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| C | -2.48836100 | 2.23298300 | -2.93092100 |
| H | -2.27506500 | 1.25597200 | -2.49123900 |
| H | -2.09275300 | 2.20628200 | -3.95084200 |
| C | -1.70564900 | 3.30214600 | -2.16170600 |
| H | -1.68374600 | 4.22511900 | -2.75837200 |
| C | -0.26476600 | 2.85069400 | -1.88799800 |
| H | 0.15907100 | 2.38992500 | -2.78873900 |
| C | 0.63454300 | 4.00214000 | -1.43836600 |
| H | 0.12719400 | 4.58067200 | -0.65938200 |
| H | 0.79761000 | 4.66975300 | -2.29285000 |
| C | 1.97132300 | 3.51383300 | -0.88770300 |
| H | 2.34808900 | 2.70258900 | -1.51935600 |
| C | 3.04875100 | 4.59581400 | -0.83921200 |
| H | 2.71636600 | 5.42365800 | -0.20451300 |
| H | 3.21081000 | 4.98576400 | -1.84789000 |
| C | 4.38332700 | 4.07480600 | -0.28992500 |
| C | 5.52115800 | 5.08062500 | -0.35012400 |
| H | 5.26978200 | 5.96889900 | 0.23497400 |
| H | 5.69122100 | 5.38233700 | -1.38817200 |
| C | 6.78587800 | 4.44375000 | 0.19951500 |
| H | 6.61268800 | 4.19987600 | 1.25787400 |
| C | 7.11086200 | 3.13766200 | -0.55394300 |
| H | 7.51734300 | 3.46853100 | -1.51894200 |
| C | 5.89516600 | 2.23894400 | -0.81477100 |
| H | 5.71249000 | 1.62673100 | 0.07311100 |
| C | 8.25696800 | 2.42891300 | 0.21292300 |

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| C | -12.41131400 | 1.59002400 | 1.42441000 |
| H | -11.72624800 | 2.07151900 | 2.12603000 |
| H | -13.21902400 | 1.11236200 | 1.98059700 |
| H | -12.83470900 | 2.35934600 | 0.77501000 |
| C | -13.41380500 | 0.57789100 | -1.23955200 |
| H | -14.21319500 | 1.05018000 | -0.66063200 |
| H | -13.87702300 | -0.02193800 | -2.02829900 |
| H | -12.84010100 | 1.37602300 | -1.71581100 |
| C | -13.32728400 | -3.57751000 | 1.61479500 |
| H | -13.70473400 | -4.16051200 | 0.76723700 |
| H | -14.18219300 | -3.20027300 | 2.17741800 |
| H | -12.75033600 | -4.25100300 | 2.25262600 |
| O | 6.40833700 | -2.64612300 | 1.13500500 |
| H | 5.43299000 | -2.68404900 | 0.92709000 |
| O | 10.45630100 | -2.68465900 | 0.84565100 |
| H | 10.87538000 | -3.47428200 | 0.48524800 |
| O | 7.61940600 | -2.08453900 | -1.44153600 |
| O | 5.69204500 | -0.89473100 | -1.07200700 |
| O | 4.24792400 | 3.68900200 | 1.05227200 |
| H | 3.32545000 | 3.37704000 | 1.14365600 |
| O | 4.70470400 | 2.96791200 | -1.12927500 |
| O | 8.06018700 | 1.23822100 | 0.61068000 |
| O | 1.78709100 | 3.01842900 | 0.44798900 |
| H | 1.68274400 | 2.05050400 | 0.41635900 |
| O | -0.30145300 | 1.81164000 | -0.91978800 |
| H | -0.83492900 | 2.15682500 | -0.18936700 |

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| O | -2.29272100 | 3.62469400 | -0.90995900 |
| H | -2.95445300 | 2.94144600 | -0.68679400 |
| O | -4.09336600 | 1.62097700 | -0.71319200 |
| H | -4.73222700 | 1.37886700 | -0.01777400 |
| O | -6.47371800 | 1.17828300 | 0.36375400 |
| H | -7.12557500 | 0.80069800 | 0.98072500 |
| O | -8.98621500 | 0.52482200 | 1.12882900 |
| O | -10.67120800 | 1.22481300 | -0.19369400 |
| O | -14.29617300 | -0.92151400 | 1.20769700 |
| H | -15.00531000 | -0.52361000 | 0.69150100 |
| O | 7.85022600 | 5.35427300 | 0.06312500 |
| H | 8.64702700 | 4.80201400 | 0.21905800 |
| N | 8.45404900 | -1.97057200 | 2.64240000 |
| H | 7.67744000 | -2.65154600 | 2.71669200 |
| H | 8.26445300 | -1.17753900 | 3.26041000 |
| C | -4.14439400 | 3.88462700 | 2.02244800 |
| H | -4.45498300 | 3.42631700 | 1.08001000 |
| H | -4.73078100 | 3.42015200 | 2.82246000 |
| C | -2.64769000 | 3.70178400 | 2.25711300 |
| H | -2.35919500 | 4.19064300 | 3.19570700 |
| H | -2.09247600 | 4.19615100 | 1.45430400 |
| C | -2.24173600 | 2.23123100 | 2.31125000 |
| H | -2.49063200 | 1.73944500 | 1.36498500 |
| H | -2.83186100 | 1.71624400 | 3.07974600 |
| C | -0.75318800 | 2.04767900 | 2.61412400 |
| H | -0.47632600 | 2.55263000 | 3.54245800 |

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| H | -0.13076600 | 2.49586400 | 1.82943300 |
| C | -0.31988000 | 0.61522000 | 2.77086100 |
| O | 0.47519500 | 0.21589800 | 3.58802800 |
| C | -0.65404400 | -1.59492100 | 1.97043900 |
| H | -0.45390100 | -1.86672300 | 3.00917500 |
| H | -1.56576800 | -2.08655400 | 1.62252200 |
| C | 0.50706700 | -2.02274700 | 1.09323900 |
| H | 0.45595700 | -1.51660800 | 0.12946500 |
| C | 0.52752400 | -3.52794200 | 0.88934900 |
| H | 0.63637500 | -4.04326500 | 1.84891400 |
| H | -0.39775100 | -3.84484700 | 0.40217500 |
| O | -0.93149000 | -0.19527800 | 1.87825700 |
| C | 2.36769100 | -0.57648800 | 1.40436100 |
| C | 3.75191700 | -0.46202300 | 1.96344800 |
| H | 3.97120800 | -1.34212200 | 2.57067000 |
| H | 4.39974900 | -0.48828400 | 1.08164500 |
| C | 3.94154100 | 0.84820200 | 2.72530300 |
| H | 3.26535400 | 0.86528700 | 3.58749400 |
| H | 3.64458900 | 1.66430800 | 2.06904500 |
| C | 5.37966200 | 1.09738000 | 3.17256700 |
| H | 5.72318400 | 0.25171900 | 3.79046400 |
| H | 6.04309700 | 1.15135500 | 2.30088000 |
| C | 5.51425900 | 2.40393800 | 3.94862800 |
| H | 4.89382700 | 2.39583000 | 4.85087500 |
| H | 5.19506800 | 3.23764600 | 3.31794200 |
| O | 1.76637800 | -1.72132200 | 1.71456700 |

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| O | 1.83384500 | 0.27579400 | 0.71724600 |
| O | 1.59210800 | -3.88738100 | 0.01998600 |
| O | 3.42310900 | -5.36513400 | -0.48925900 |
| O | 3.07268900 | -4.66560300 | 2.01309500 |
| O | 4.00145000 | -3.03049700 | 0.21575400 |
| C | 4.77461600 | -5.59985000 | -0.82832800 |
| H | 5.46417700 | -5.24115000 | -0.05367300 |
| H | 4.91372700 | -6.67942600 | -0.93204100 |
| C | 5.08647300 | -4.92702300 | -2.15736100 |
| H | 4.28874800 | -5.17074700 | -2.86025200 |
| H | 6.03737700 | -5.27878500 | -2.56735100 |
| N | 5.13814500 | -3.45321400 | -1.97976100 |
| H | 6.09249900 | -3.11748300 | -1.78845200 |
| H | 4.79053900 | -2.93303500 | -2.78151500 |
| P | 3.06297800 | -4.19786400 | 0.61292900 |
| O | 9.28259500 | 3.10628000 | 0.40785700 |
| H | -4.41361500 | 4.94351900 | 1.98154400 |
| H | 6.54986400 | 2.58614300 | 4.24907500 |
| H | 4.53866400 | -3.15282200 | -1.05887600 |
| H | 9.35968400 | -2.38954100 | 2.87177000 |

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| C | 5.72554000 | -2.31256900 | -1.83424800 |
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| C | 6.06105100 | -3.80888700 | -1.71207100 |
| C | 7.51679500 | -4.07533500 | -2.12742800 |
| C | 8.49359000 | -3.08995500 | -1.50623400 |
| C | 8.15122900 | -1.67451200 | -1.94994800 |
| C | 6.67277000 | -1.35709200 | -1.92214400 |
| H | 7.77872600 | -5.10707100 | -1.86747300 |
| H | 8.45159800 | -3.15185300 | -0.41291200 |
| H | 9.52178700 | -3.33756900 | -1.78819400 |
| H | 8.67789700 | -0.95017100 | -1.32036000 |
| H | 8.51888100 | -1.50202200 | -2.97213300 |
| H | 7.58880900 | -3.99821200 | -3.21954000 |
| C | 6.39094200 | 0.11941800 | -2.02028900 |
| H | 5.38673900 | 0.39074900 | -1.69715500 |
| H | 7.10633300 | 0.68865300 | -1.41899600 |
| H | 6.51038600 | 0.47171000 | -3.05245800 |
| C | 5.83420300 | -4.27961000 | -0.26348900 |
| H | 4.80590000 | -4.10186100 | 0.06317300 |
| H | 6.02077800 | -5.35502100 | -0.17956300 |
| H | 6.49592700 | -3.76586100 | 0.43810400 |
| C | 5.15307300 | -4.63052900 | -2.64156200 |
| H | 5.45665100 | -5.68209600 | -2.62674300 |
| H | 4.10355300 | -4.58249000 | -2.34194000 |
| H | 5.22077000 | -4.26998100 | -3.67166000 |
| C | 4.27915800 | -2.01973600 | -1.80946200 |
| H | 3.70279200 | -2.56802200 | -1.06658700 |
| C | 3.60513200 | -1.20337300 | -2.62936600 |

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| H | 4.16183300 | -0.65354400 | -3.38561100 |
| C | 2.15967900 | -0.93568800 | -2.58580700 |
| C | 1.28150000 | -1.85915500 | -2.14512000 |
| H | 1.67085800 | -2.84179500 | -1.88405600 |
| C | 1.77263100 | 0.43368300 | -3.07486900 |
| H | 2.22031500 | 1.20156300 | -2.43852900 |
| H | 2.15335500 | 0.59103700 | -4.09032900 |
| H | 0.69617500 | 0.59789800 | -3.09174000 |
| C | -0.14806200 | -1.69835500 | -1.97908800 |
| H | -0.57974100 | -0.72445200 | -2.18500600 |
| C | -0.94576200 | -2.69393300 | -1.55613000 |
| H | -0.49192500 | -3.66369600 | -1.35277600 |
| C | -2.38963600 | -2.61381700 | -1.33896500 |
| C | -3.03895900 | -3.72728600 | -0.96322400 |
| H | -2.45171200 | -4.63793000 | -0.83696700 |
| C | -3.06950700 | -1.29336200 | -1.57930500 |
| H | -2.53513500 | -0.47773200 | -1.08561200 |
| H | -3.08699500 | -1.05785700 | -2.64917500 |
| H | -4.09362300 | -1.27793700 | -1.20996700 |
| C | -4.50567500 | -3.90877000 | -0.71912100 |
| H | -4.98753000 | -4.33826800 | -1.61201500 |
| H | -5.00875700 | -2.96554400 | -0.50049200 |
| O | -4.74292100 | -4.73373900 | 0.41679500 |
| H | -4.45687000 | -5.63158200 | 0.21411600 |
| C | -11.26818800 | 1.70177700 | -1.66916000 |
| H | -11.24407500 | 1.95023600 | -2.73805600 |

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| C | -11.71994700 | 2.94748200 | -0.92137100 |
| H | -11.81340900 | 2.70207200 | 0.14515600 |
| C | -10.65223900 | 4.04467700 | -1.07359800 |
| H | -10.54891000 | 4.25869000 | -2.15077900 |
| C | -8.87581300 | 2.48917800 | -1.21108300 |
| H | -8.57691300 | 2.74928400 | -2.24354500 |
| C | -9.87254400 | 1.34079500 | -1.20948100 |
| H | -9.50233000 | 0.56215300 | -1.87281700 |
| C | -11.00857800 | 5.31676400 | -0.33487500 |
| H | -11.12359200 | 5.11076300 | 0.73310800 |
| H | -11.93830600 | 5.73771200 | -0.72474600 |
| H | -10.21669700 | 6.05775000 | -0.45561400 |
| C | -6.76946900 | 1.27464300 | -1.07598800 |
| H | -6.63982900 | 1.61888300 | -2.11236300 |
| C | -5.50002900 | 1.52395700 | -0.31959800 |
| H | -5.51029900 | 1.29218200 | 0.74266400 |
| C | -4.38509000 | 1.97417900 | -0.90303800 |
| H | -4.38797700 | 2.18195000 | -1.97356400 |
| C | -3.13011300 | 2.17595400 | -0.20574100 |
| H | -3.13163700 | 2.02114000 | 0.87120700 |
| C | -1.97667100 | 2.50481200 | -0.81936200 |
| H | -1.97411000 | 2.65959100 | -1.89872600 |
| C | -0.70897000 | 2.60654700 | -0.13580800 |
| H | -0.71132300 | 2.43910600 | 0.93672200 |
| C | 0.47066500 | 2.84260400 | -0.74413900 |
| H | 0.49080200 | 3.03010500 | -1.81741500 |

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| C | 1.73655200 | 2.82363000 | -0.05160900 |
| H | 1.71010400 | 2.54015400 | 0.99804400 |
| C | 2.92051200 | 3.08691200 | -0.64135500 |
| H | 2.93241700 | 3.36804200 | -1.69455300 |
| C | 4.20034600 | 3.02433100 | 0.02059000 |
| H | 4.20907700 | 2.74158700 | 1.07299100 |
| C | 5.36593800 | 3.28053300 | -0.60662400 |
| H | 5.34036100 | 3.54358900 | -1.66395700 |
| C | 6.66814000 | 3.22148700 | 0.01044400 |
| H | 6.70740100 | 2.99423800 | 1.07399100 |
| C | 7.81989600 | 3.39548900 | -0.66467800 |
| H | 7.77841600 | 3.59422900 | -1.73537000 |
| C | -7.14752000 | -0.22337900 | -1.13178100 |
| H | -7.98626900 | -0.37549800 | -1.80437400 |
| H | -6.30099900 | -0.74708400 | -1.58638000 |
| C | 9.13452700 | 3.27328000 | -0.06669900 |
| H | 9.16028900 | 3.16200300 | 1.01476300 |
| C | 10.27639200 | 3.21835100 | -0.76131100 |
| H | 10.23976500 | 3.31117900 | -1.84825100 |
| C | 11.63451700 | 2.97485000 | -0.16937300 |
| H | 11.56067000 | 3.01643400 | 0.92322500 |
| C | 12.15124700 | 1.57009800 | -0.53883700 |
| H | 12.36441700 | 1.57483400 | -1.62082000 |
| C | 11.14962200 | 0.42592900 | -0.29500300 |
| H | 10.26217400 | 0.68076800 | -0.88220600 |
| C | 10.66836100 | 0.34798000 | 1.15768400 |

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| H | 10.42741900 | 1.34403300 | 1.51835900 |
| C | 8.34698800 | 0.12064700 | 1.72051800 |
| C | 7.14696700 | -0.78658400 | 1.65605800 |
| H | 7.22549800 | -1.43989800 | 0.78587900 |
| H | 7.17358300 | -1.41636400 | 2.55338600 |
| C | 5.82511400 | -0.01767100 | 1.62048800 |
| H | 5.78223400 | 0.56906800 | 0.69338700 |
| C | 4.64563400 | -0.97755400 | 1.66156200 |
| H | 4.74412200 | -1.67013500 | 0.82304500 |
| H | 4.69625000 | -1.55826800 | 2.59039700 |
| C | 3.28200200 | -0.29466600 | 1.58820800 |
| H | 3.23730400 | 0.32365100 | 0.67873600 |
| C | 2.15651400 | -1.32193600 | 1.54080600 |
| H | 2.18494000 | -1.90413500 | 2.47034400 |
| H | 2.38876900 | -2.01191300 | 0.72339100 |
| C | 0.74346100 | -0.78380200 | 1.29807700 |
| H | 0.75093800 | -0.08531900 | 0.45363900 |
| H | 0.11466300 | -1.62382900 | 0.98576900 |
| C | 0.05695300 | -0.09228100 | 2.47151300 |
| H | 0.15442700 | -0.70844500 | 3.38016400 |
| C | -1.43615400 | 0.12703700 | 2.16843600 |
| H | -1.53372100 | 0.31961700 | 1.09170100 |
| C | -2.33890600 | -1.04351800 | 2.53197300 |
| H | -2.28228500 | -1.22140400 | 3.61199200 |
| H | -1.98911700 | -1.94534100 | 2.01806900 |
| C | -3.79194700 | -0.79555100 | 2.12778600 |

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|---|-------------|-------------|-------------|
| H | -3.82282400 | -0.58854600 | 1.05166600 |
| C | -4.68543700 | -1.99502800 | 2.41488500 |
| H | -4.64035100 | -2.23535000 | 3.48196600 |
| H | -4.32478900 | -2.86359700 | 1.85885400 |
| C | -6.15518300 | -1.74975700 | 2.06760300 |
| C | -7.00560800 | -3.00892300 | 2.13594500 |
| H | -7.06824000 | -3.35336400 | 3.17065700 |
| H | -6.54044100 | -3.79474600 | 1.53659200 |
| C | -8.40370500 | -2.73237300 | 1.61704400 |
| H | -8.88947700 | -2.00076900 | 2.27408000 |
| C | -8.36651700 | -2.12058000 | 0.20315100 |
| H | -7.94185700 | -2.85666200 | -0.49081500 |
| C | -7.42854100 | -0.88221300 | 0.21638500 |
| H | -7.84460600 | -0.15492600 | 0.91622000 |
| C | -9.80465800 | -1.86570600 | -0.23227700 |
| C | 11.59222100 | -0.33902800 | 2.14244600 |
| H | 11.17374700 | -0.28297900 | 3.14999600 |
| H | 12.56193100 | 0.16042100 | 2.12816000 |
| H | 11.72987400 | -1.39150700 | 1.88544100 |
| C | 11.68704700 | -0.90790900 | -0.81018300 |
| H | 12.62490900 | -1.18576400 | -0.31997700 |
| H | 11.86876300 | -0.86099000 | -1.88788700 |
| H | 10.97168700 | -1.71219300 | -0.62543200 |
| C | 12.63947400 | 4.03915000 | -0.61909400 |
| H | 12.71932000 | 4.05729800 | -1.71173100 |
| H | 13.62729900 | 3.82737700 | -0.20759800 |

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|---|--------------|-------------|-------------|
| H | 12.32271100 | 5.03173200 | -0.29109000 |
| O | -9.98598500 | 0.84684300 | 0.11285500 |
| H | -9.24425700 | 1.21661400 | 0.61387500 |
| O | -12.95998300 | 3.34925100 | -1.48001100 |
| H | -13.41162400 | 3.92123700 | -0.85065100 |
| O | -9.40037100 | 3.60691700 | -0.54876100 |
| O | -7.76009400 | 2.11242200 | -0.44673000 |
| O | -6.73570400 | -0.79674400 | 2.91001800 |
| H | -6.06153300 | -0.10623300 | 3.04805200 |
| O | -6.15294200 | -1.28227300 | 0.70856100 |
| O | -9.94329600 | -1.56486400 | -1.53052800 |
| O | -10.76395700 | -1.97726600 | 0.50292700 |
| O | -4.34294100 | 0.33253600 | 2.81742900 |
| H | -3.62297900 | 0.95271000 | 3.02647600 |
| O | -1.89346500 | 1.28007000 | 2.87353600 |
| H | -1.09057700 | 1.76705800 | 3.13162000 |
| O | 0.58097200 | 1.20344200 | 2.71907900 |
| H | 1.54549700 | 1.11173000 | 2.88731900 |
| O | 3.09396700 | 0.53737800 | 2.73681700 |
| H | 3.95269700 | 0.94086800 | 2.96238500 |
| O | 5.71158200 | 0.86098700 | 2.73830400 |
| H | 6.55782400 | 1.33561800 | 2.81879200 |
| O | 8.33756300 | 1.20623600 | 2.27899300 |
| O | 9.41418700 | -0.40390300 | 1.13023400 |
| O | 13.36304900 | 1.38710300 | 0.18631000 |
| H | 13.86173800 | 0.67047100 | -0.22040500 |

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|---|--------------|-------------|-------------|
| O | -9.11663600 | -3.95368800 | 1.62436400 |
| H | -10.04404800 | -3.70909900 | 1.50197300 |
| N | -12.09676000 | 0.50765000 | -1.50063500 |
| H | -12.12527600 | 0.26960100 | -0.51018300 |
| H | -10.84906500 | -1.19590400 | -1.66279400 |
| H | -13.04668000 | 0.70969800 | -1.79663000 |

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|---|-------------|------------|-------------|
| C | 4.36568000 | 2.56554300 | 1.22024000 |
| C | 3.06968400 | 2.78318500 | 1.98502700 |
| C | 2.01837500 | 3.63382200 | 1.25790900 |
| C | 4.08117400 | 1.97075100 | -0.18365700 |
| C | 2.61646400 | 2.02799400 | -0.53750400 |
| C | 1.97156900 | 0.94548600 | -0.96683000 |
| C | 0.49676300 | 0.87995100 | -1.21656000 |
| C | -0.24730800 | 2.02571000 | -0.53233800 |
| C | -1.69507400 | 2.09669400 | -1.00683100 |
| C | -2.56668700 | 0.86570800 | -0.78413800 |
| C | -4.01236400 | 1.39563000 | -0.89859400 |
| C | -3.95313500 | 2.95701900 | -0.95380800 |
| C | -4.32017100 | 3.56634900 | -2.33157500 |
| C | -5.50785000 | 2.86229800 | -3.02299800 |
| C | -6.77912200 | 2.74271300 | -2.18113800 |

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| C | -7.94354800 | 2.12914000 | -2.95465600 |
| C | -9.20322300 | 1.88905200 | -2.11584600 |
| C | -9.75064200 | 3.17887200 | -1.50271500 |
| C | -10.28278800 | 1.19314600 | -2.94342700 |
| C | -4.64249400 | 5.06315300 | -2.21387000 |
| C | -2.51516700 | 3.25167100 | -0.40350900 |
| C | -2.60699700 | 3.16276700 | 1.13259300 |
| C | -1.80994700 | 4.55459300 | -0.79842400 |
| C | -0.34604700 | 4.57047700 | -0.33620300 |
| C | 0.47405100 | 3.35780700 | -0.80996400 |
| C | 1.93647000 | 3.36404800 | -0.27679900 |
| C | 2.72672300 | 4.46346600 | -1.01719500 |
| O | 5.08461700 | 3.79310600 | 1.14644900 |
| H | 0.54780900 | 3.43105100 | -1.90666300 |
| H | -0.23102300 | 1.82839400 | 0.54825300 |
| H | -1.65975300 | 2.28512200 | -2.09189200 |
| H | 4.97083000 | 1.84272300 | 1.77672500 |
| H | 3.30102100 | 3.22539100 | 2.95893900 |
| H | 2.64813400 | 1.79108600 | 2.17220600 |
| H | 2.21507700 | 4.69729100 | 1.42323800 |
| H | 1.05271100 | 3.42018200 | 1.72650700 |
| H | 4.42507200 | 0.93560000 | -0.22834400 |
| H | 4.68263800 | 2.53207200 | -0.90633800 |
| H | 2.54454500 | 0.03659900 | -1.12524700 |
| H | 0.11045200 | -0.08023300 | -0.85571500 |
| H | 0.28901800 | 0.90245000 | -2.29741200 |

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|---|--------------|------------|-------------|
| H | -2.37369800 | 0.45870200 | 0.21024600 |
| H | -2.35344700 | 0.06835100 | -1.50135300 |
| H | -4.60714900 | 1.08116500 | -0.03879800 |
| H | -4.50317300 | 0.97709900 | -1.77637500 |
| H | -4.68500200 | 3.35885300 | -0.24352100 |
| H | -3.45941700 | 3.45671000 | -3.00509200 |
| H | -5.74393100 | 3.42315100 | -3.93618300 |
| H | -5.21400100 | 1.86519200 | -3.36751600 |
| H | -7.06585900 | 3.73206500 | -1.81260300 |
| H | -6.58524300 | 2.13047100 | -1.29234600 |
| H | -7.62108700 | 1.16913700 | -3.37850500 |
| H | -8.19713400 | 2.77285900 | -3.80881300 |
| H | -8.91224300 | 1.21354700 | -1.30194900 |
| H | -9.94307700 | 3.92299000 | -2.28390900 |
| H | -9.05598800 | 3.61882700 | -0.78338400 |
| H | -10.69511600 | 2.99856900 | -0.98096600 |
| H | -10.61994100 | 1.83974600 | -3.76101500 |
| H | -11.15844300 | 0.94576400 | -2.33426200 |
| H | -9.90635400 | 0.26652500 | -3.38694200 |
| H | -5.48001600 | 5.22852000 | -1.52931200 |
| H | -4.92626100 | 5.47437200 | -3.18750200 |
| H | -3.80427100 | 5.64816000 | -1.84224500 |
| H | -3.14976800 | 2.27461900 | 1.46424900 |
| H | -3.14642200 | 4.03505200 | 1.51562000 |
| H | -1.63028300 | 3.14006900 | 1.61765900 |
| H | -2.32211500 | 5.42435800 | -0.37282700 |

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| H | -1.83439100 | 4.66710200 | -1.88804100 |
| H | -0.32044800 | 4.63446400 | 0.75418000 |
| H | 0.11998100 | 5.49172400 | -0.69749100 |
| H | 2.21562100 | 5.42602400 | -0.93341500 |
| H | 2.82398500 | 4.22273700 | -2.08089900 |
| H | 3.72225700 | 4.58429100 | -0.58795300 |
| H | 5.98475300 | 3.54155100 | 0.89057400 |
| C | 10.56602800 | 2.02518200 | 0.63084200 |
| H | 10.90142000 | 2.21083800 | 1.65933200 |
| C | 10.05587500 | 3.34755500 | 0.07240600 |
| H | 9.77186100 | 3.19930200 | -0.97810600 |
| C | 8.80573500 | 3.78413500 | 0.85435800 |
| H | 9.09134300 | 3.89273000 | 1.91283200 |
| C | 8.14474700 | 1.54124400 | 1.29037200 |
| H | 8.24980300 | 1.61932300 | 2.38687300 |
| C | 9.42473700 | 1.03153600 | 0.65101000 |
| H | 9.75709400 | 0.15779100 | 1.20771800 |
| C | 8.20718800 | 5.08018800 | 0.35134600 |
| H | 7.91198600 | 4.97723200 | -0.69685100 |
| H | 8.93318600 | 5.89090400 | 0.44375000 |
| H | 7.32157900 | 5.34626300 | 0.93192900 |
| C | 6.92529700 | -0.53773200 | 1.70952400 |
| H | 7.09728500 | -0.29817800 | 2.76825200 |
| C | 5.48762100 | -0.88773200 | 1.49963700 |
| H | 5.20597000 | -1.13951800 | 0.48155500 |
| C | 4.55143200 | -0.83760600 | 2.45146700 |

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| H | 4.81982100 | -0.58904000 | 3.47793500 |
| C | 3.14901700 | -1.01162000 | 2.13985300 |
| H | 2.91679000 | -1.20687600 | 1.09719000 |
| C | 2.12517000 | -0.84807500 | 2.99804500 |
| H | 2.31669500 | -0.62740800 | 4.04740800 |
| C | 0.75845600 | -0.88672700 | 2.53967000 |
| H | 0.63134800 | -1.09965700 | 1.48003000 |
| C | -0.34093200 | -0.64650900 | 3.28190800 |
| H | -0.25270000 | -0.41433700 | 4.34220900 |
| C | -1.65155900 | -0.64337600 | 2.68405900 |
| H | -1.68647000 | -0.91209000 | 1.62929900 |
| C | -2.80951800 | -0.31377600 | 3.29212800 |
| H | -2.81438000 | -0.04585800 | 4.34764000 |
| C | -4.05544700 | -0.24332900 | 2.57009200 |
| H | -4.00701100 | -0.47730300 | 1.50762800 |
| C | -5.24923000 | 0.11836300 | 3.08263400 |
| H | -5.33699300 | 0.34592100 | 4.14401400 |
| C | -6.43074700 | 0.24488900 | 2.26417800 |
| H | -6.29003100 | 0.09707100 | 1.19487400 |
| C | -7.67341200 | 0.52684200 | 2.69602500 |
| H | -7.86679200 | 0.65819800 | 3.75968400 |
| C | 7.88801100 | -1.67076700 | 1.30731300 |
| H | 8.91019500 | -1.41633800 | 1.57423700 |
| H | 7.62057000 | -2.54422200 | 1.91036500 |
| C | -8.78799900 | 0.63465800 | 1.77512700 |
| H | -8.51670300 | 0.61304900 | 0.72271500 |

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| C | -10.08232300 | 0.71154800 | 2.10096500 |
| H | -10.37591200 | 0.71726400 | 3.15168500 |
| C | -11.19447900 | 0.76010200 | 1.09090600 |
| H | -10.76103100 | 0.96492400 | 0.10766100 |
| C | -11.92989600 | -0.58900100 | 0.98305900 |
| H | -12.46349300 | -0.75133400 | 1.93424600 |
| C | -11.01735200 | -1.81136400 | 0.77191100 |
| H | -10.28168600 | -1.77981500 | 1.58065400 |
| C | -10.20251000 | -1.73694700 | -0.52657400 |
| H | -9.79638700 | -0.73669300 | -0.65409800 |
| C | -7.83714100 | -2.18651300 | -0.51450300 |
| C | -6.80223500 | -3.27122400 | -0.34842900 |
| H | -7.21291100 | -4.07238200 | 0.26888500 |
| H | -6.60836200 | -3.68462100 | -1.34514100 |
| C | -5.48799100 | -2.74767200 | 0.23269500 |
| H | -5.67751700 | -2.33177800 | 1.23288900 |
| C | -4.45501400 | -3.86208000 | 0.34038300 |
| H | -4.83844900 | -4.63158700 | 1.01903000 |
| H | -4.32361100 | -4.32392200 | -0.64548300 |
| C | -3.08709500 | -3.39935000 | 0.83555300 |
| H | -3.20588000 | -2.84237700 | 1.77499900 |
| C | -2.14688700 | -4.57891200 | 1.08035400 |
| H | -2.23351900 | -5.28389900 | 0.24507700 |
| H | -2.50093700 | -5.10338900 | 1.97273400 |
| C | -0.67821100 | -4.15577900 | 1.25245100 |
| H | -0.62480900 | -3.10573800 | 1.54905400 |

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| H | -0.21071000 | -4.72556200 | 2.06121800 |
| C | 0.17612400 | -4.37030100 | -0.00052800 |
| H | 0.36222900 | -5.44529300 | -0.12175200 |
| C | 1.53326600 | -3.63575700 | 0.11159500 |
| H | 1.82895700 | -3.54598000 | 1.16288200 |
| C | 2.65304900 | -4.30658800 | -0.68115100 |
| H | 2.33527400 | -4.40847600 | -1.72585700 |
| H | 2.81099100 | -5.31622600 | -0.28491900 |
| C | 3.97402200 | -3.53742700 | -0.62707900 |
| H | 4.27849400 | -3.41017600 | 0.42099400 |
| C | 5.09132000 | -4.26558100 | -1.36957400 |
| H | 4.75180100 | -4.53618500 | -2.37430300 |
| H | 5.32528100 | -5.18804400 | -0.83019400 |
| C | 6.37080400 | -3.44110800 | -1.53176100 |
| C | 7.54026500 | -4.24556700 | -2.08218700 |
| H | 7.31998500 | -4.59274200 | -3.09390400 |
| H | 7.71352700 | -5.11737300 | -1.44420500 |
| C | 8.78694800 | -3.38195200 | -2.10728200 |
| H | 8.61513600 | -2.54447100 | -2.79221200 |
| C | 9.08630900 | -2.78942100 | -0.71825700 |
| H | 9.35655100 | -3.60605200 | -0.03780900 |
| C | 7.81352400 | -2.09819300 | -0.15684000 |
| H | 7.58534600 | -1.24538100 | -0.79931200 |
| C | 10.30473200 | -1.88371800 | -0.85700700 |
| C | -10.90666600 | -2.16854100 | -1.79709200 |
| H | -10.24175600 | -2.04117100 | -2.65388200 |

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| H | -11.79366900 | -1.55216700 | -1.94272600 |
| H | -11.20206200 | -3.21849700 | -1.74541200 |
| C | -11.79774700 | -3.11884700 | 0.90059500 |
| H | -12.61299100 | -3.18465900 | 0.17324300 |
| H | -12.23103300 | -3.21162900 | 1.90033000 |
| H | -11.14414500 | -3.97861500 | 0.73582300 |
| C | -12.18532900 | 1.88182700 | 1.41135700 |
| H | -12.63194400 | 1.73354400 | 2.40089300 |
| H | -12.98896600 | 1.90527300 | 0.67422200 |
| H | -11.67866200 | 2.84982200 | 1.41508200 |
| O | 9.15515400 | 0.68269300 | -0.69476300 |
| H | 8.19297300 | 0.62729800 | -0.78618700 |
| O | 11.10212100 | 4.29325900 | 0.20844000 |
| H | 10.94516100 | 5.02097000 | -0.40244000 |
| O | 7.78204100 | 2.78693100 | 0.74122100 |
| O | 7.09612300 | 0.68109000 | 0.94254000 |
| O | 6.17406000 | -2.35539600 | -2.39090000 |
| H | 5.30720600 | -1.97575100 | -2.15782200 |
| O | 6.71708600 | -3.00440000 | -0.21738100 |
| O | 10.84802000 | -1.50877400 | 0.30932200 |
| O | 10.78612500 | -1.55865000 | -1.92146400 |
| O | 3.81752600 | -2.24125300 | -1.21276000 |
| H | 2.89328500 | -1.96747200 | -1.05922700 |
| O | 1.32094400 | -2.30094200 | -0.36098700 |
| H | 0.64195600 | -2.42328500 | -1.05547600 |
| O | -0.44698200 | -3.91530000 | -1.19478300 |

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| H | -1.24636700 | -3.39665600 | -0.95637700 |
| O | -2.46712800 | -2.53490500 | -0.12219500 |
| H | -3.16222000 | -1.96324300 | -0.49879500 |
| O | -4.93867800 | -1.73231500 | -0.60174700 |
| H | -5.64716700 | -1.09745700 | -0.80785500 |
| O | -7.55549100 | -1.03251300 | -0.79885800 |
| O | -9.06812000 | -2.64257500 | -0.34321400 |
| O | -12.87239700 | -0.44119800 | -0.07625300 |
| H | -13.52913000 | -1.14257100 | -0.00793600 |
| O | 9.86471900 | -4.17866000 | -2.55833000 |
| H | 10.56538600 | -3.55666000 | -2.79591200 |
| N | 11.66649100 | 1.39639400 | -0.09774400 |
| H | 11.36378300 | 1.22271800 | -1.05470400 |
| H | 11.47146700 | -0.76643500 | 0.13433700 |
| H | 12.45637500 | 2.03319400 | -0.13503200 |

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| C | -4.82395700 | -0.23466700 | 3.60154400 |
| H | -5.05853900 | -1.13553800 | 3.02289000 |
| H | -5.50708000 | 0.55380700 | 3.27232900 |
| H | -5.03972100 | -0.45511400 | 4.65177000 |
| C | -3.36820400 | 0.17186800 | 3.40012500 |
| H | -3.15513200 | 1.08613500 | 3.96864200 |

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|---|-------------|-------------|------------|
| H | -3.21260300 | 0.42998700 | 2.34936100 |
| C | -2.37264200 | -0.91577500 | 3.78890500 |
| H | -2.64072800 | -1.84097900 | 3.25957500 |
| H | -2.46204700 | -1.14813500 | 4.85822600 |
| C | -0.92640900 | -0.56240200 | 3.44605500 |
| H | -0.60700900 | 0.31362200 | 4.02454500 |
| H | -0.88009600 | -0.25056100 | 2.39700000 |
| C | 0.04303400 | -1.72270800 | 3.67576700 |
| H | -0.45387700 | -2.66384700 | 3.40222500 |
| H | 0.27653200 | -1.81269300 | 4.74416400 |
| C | 1.33254200 | -1.62150300 | 2.86529200 |
| H | 1.81729600 | -0.65153300 | 3.03145600 |
| H | 1.07326400 | -1.63911700 | 1.79908500 |
| C | 2.31227800 | -2.75530100 | 3.15954300 |
| H | 1.75616100 | -3.69890000 | 3.24392500 |
| H | 2.77717600 | -2.59414300 | 4.14072300 |
| C | 3.39166400 | -2.92122600 | 2.09487200 |
| H | 3.90394500 | -1.96724600 | 1.91857200 |
| H | 2.90832900 | -3.17229700 | 1.14091100 |
| C | 4.41563600 | -4.00053600 | 2.43680900 |
| H | 3.89144600 | -4.93021200 | 2.69757400 |
| H | 4.96830600 | -3.70305900 | 3.33762200 |
| C | 5.39955600 | -4.26781700 | 1.30371400 |
| H | 5.88090700 | -3.32953300 | 1.01425400 |
| H | 4.84168300 | -4.60733600 | 0.41970600 |
| C | 6.46576200 | -5.30578800 | 1.63855300 |

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| H | 5.99574800 | -6.27720000 | 1.83733200 |
| H | 6.99444200 | -5.01408100 | 2.55382900 |
| C | 7.49900600 | -5.46371200 | 0.53306400 |
| H | 8.15379000 | -6.32065000 | 0.75289700 |
| H | 6.98777800 | -5.68500300 | -0.41679900 |
| O | 8.25004200 | -4.27202400 | 0.44632600 |
| H | 8.52270300 | -4.09444100 | -0.47240700 |
| C | 9.84403300 | 3.23351200 | 0.51074300 |
| H | 9.96457300 | 3.54657700 | 1.55574900 |
| C | 9.78866200 | 4.49371900 | -0.33954500 |
| H | 9.73090400 | 4.20189500 | -1.39706200 |
| C | 8.51792100 | 5.28582000 | 0.01301600 |
| H | 8.57439300 | 5.54344900 | 1.08412900 |
| C | 7.28571500 | 3.33645100 | 0.54323100 |
| H | 7.12910900 | 3.58296700 | 1.60972000 |
| C | 8.53517400 | 2.48898300 | 0.36213700 |
| H | 8.52295900 | 1.69861000 | 1.10819400 |
| C | 8.36783300 | 6.55008200 | -0.80561300 |
| H | 8.32445200 | 6.30487800 | -1.87063600 |
| H | 9.20669200 | 7.22584600 | -0.62335900 |
| H | 7.44453000 | 7.06578700 | -0.53683600 |
| C | 5.57532700 | 1.61947900 | 0.85658400 |
| H | 5.50282800 | 2.01683300 | 1.87910900 |
| C | 4.19956600 | 1.45591000 | 0.28804600 |
| H | 4.14152200 | 1.08586200 | -0.73171600 |
| C | 3.07818000 | 1.74960500 | 0.95202100 |

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| H | 3.13358200 | 2.12069500 | 1.97546000 |
| C | 1.76122700 | 1.63183800 | 0.35933900 |
| H | 1.72201300 | 1.24535000 | -0.65588800 |
| C | 0.61469100 | 1.99501100 | 0.96348900 |
| H | 0.64340300 | 2.39030100 | 1.97863900 |
| C | -0.67360900 | 1.89526400 | 0.32066700 |
| H | -0.67871200 | 1.46126500 | -0.67734900 |
| C | -1.83911200 | 2.27876300 | 0.87863500 |
| H | -1.83856400 | 2.70832100 | 1.87985300 |
| C | -3.11699900 | 2.12482400 | 0.22908000 |
| H | -3.12241200 | 1.65322300 | -0.75292700 |
| C | -4.29335300 | 2.47848900 | 0.78620200 |
| H | -4.29386500 | 2.92693800 | 1.77923600 |
| C | -5.57275800 | 2.29375400 | 0.15064900 |
| H | -5.57320000 | 1.84244200 | -0.84099500 |
| C | -6.75243000 | 2.63022200 | 0.71096300 |
| H | -6.76068200 | 3.06182900 | 1.71142400 |
| C | -8.02520900 | 2.45803700 | 0.05451200 |
| H | -8.00152400 | 2.08011700 | -0.96594200 |
| C | -9.22208700 | 2.71173400 | 0.61460200 |
| H | -9.26971600 | 3.06507900 | 1.64402700 |
| C | 6.35320000 | 0.28761000 | 0.91902200 |
| H | 7.30838500 | 0.42374100 | 1.41761200 |
| H | 5.77485900 | -0.39181000 | 1.55259000 |
| C | -10.47580300 | 2.49202100 | -0.07943600 |
| H | -10.39078900 | 2.23612500 | -1.13360200 |

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| C | -11.68613900 | 2.52264900 | 0.48856900 |
| H | -11.77020700 | 2.76242900 | 1.54986300 |
| C | -12.97008300 | 2.19480500 | -0.21850600 |
| H | -12.77086900 | 2.10175600 | -1.29224900 |
| C | -13.53628100 | 0.84214500 | 0.25626500 |
| H | -13.88174000 | 0.97813300 | 1.29466000 |
| C | -12.52042400 | -0.31499500 | 0.28198000 |
| H | -11.71419200 | 0.01152400 | 0.94608900 |
| C | -11.85169900 | -0.56357900 | -1.07445200 |
| H | -11.54085400 | 0.38155300 | -1.51073400 |
| C | -9.48401400 | -0.89079000 | -1.29121300 |
| C | -8.32253400 | -1.76874600 | -0.89900400 |
| H | -8.55997400 | -2.29088200 | 0.02976200 |
| H | -8.20752400 | -2.52369900 | -1.68559900 |
| C | -7.01440900 | -0.98439900 | -0.77112400 |
| H | -7.12225000 | -0.22890500 | 0.02016000 |
| C | -5.85608700 | -1.91068400 | -0.43124700 |
| H | -6.07730700 | -2.41586100 | 0.51517700 |
| H | -5.77916700 | -2.67990900 | -1.20905100 |
| C | -4.50463100 | -1.21195900 | -0.30737200 |
| H | -4.58161700 | -0.39700900 | 0.42601500 |
| C | -3.42479700 | -2.18745700 | 0.14776400 |
| H | -3.47941300 | -3.09035600 | -0.47271000 |
| H | -3.67050800 | -2.49295400 | 1.16962300 |
| C | -2.00401100 | -1.60626500 | 0.10229800 |
| H | -2.04053300 | -0.51360600 | 0.13542400 |

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| H | -1.45011400 | -1.91957800 | 0.99161500 |
| C | -1.17510100 | -2.04666200 | -1.10261000 |
| H | -0.99435500 | -3.12728000 | -1.02044200 |
| C | 0.19758500 | -1.31785000 | -1.13173200 |
| H | 0.41463300 | -0.90596900 | -0.14043100 |
| C | 1.35103700 | -2.21974900 | -1.55706100 |
| H | 1.16034200 | -2.59332000 | -2.57065600 |
| H | 1.38739500 | -3.08683900 | -0.88725200 |
| C | 2.70261300 | -1.51159800 | -1.50890900 |
| H | 2.87516300 | -1.14587700 | -0.48801800 |
| C | 3.84574700 | -2.44641700 | -1.88394100 |
| H | 3.66887300 | -2.85999900 | -2.88178400 |
| H | 3.86911700 | -3.27305200 | -1.16971800 |
| C | 5.21800500 | -1.77294700 | -1.89648400 |
| C | 6.35620200 | -2.76505900 | -2.09324800 |
| H | 6.30545900 | -3.19951000 | -3.09383100 |
| H | 6.26396500 | -3.56519800 | -1.35594000 |
| C | 7.69353100 | -2.07881300 | -1.90372500 |
| H | 7.83354200 | -1.33748200 | -2.69743000 |
| C | 7.77337400 | -1.34905600 | -0.55074200 |
| H | 7.71678300 | -2.08980700 | 0.25405400 |
| C | 6.54695400 | -0.40602000 | -0.42730200 |
| H | 6.59816400 | 0.32932000 | -1.23376000 |
| C | 9.14685600 | -0.70125100 | -0.45587400 |
| C | -12.64895100 | -1.35361900 | -2.09198800 |
| H | -12.09829800 | -1.41407000 | -3.03353600 |

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| H | -13.60201500 | -0.85152500 | -2.26395200 |
| H | -12.84145600 | -2.36933500 | -1.73989200 |
| C | -13.13315400 | -1.58196600 | 0.87630200 |
| H | -13.99453600 | -1.92936000 | 0.29791500 |
| H | -13.46473900 | -1.40562900 | 1.90365800 |
| H | -12.40220900 | -2.39346700 | 0.89321300 |
| C | -14.01375300 | 3.29818500 | -0.02342500 |
| H | -14.22035200 | 3.45013800 | 1.04182200 |
| H | -14.94815200 | 3.02925100 | -0.51799600 |
| H | -13.65485200 | 4.24544600 | -0.43217100 |
| O | 8.51808500 | 1.93261900 | -0.94121200 |
| H | 7.61828500 | 2.05212000 | -1.27959700 |
| O | 10.96129900 | 5.24132700 | -0.06267700 |
| H | 11.10723900 | 5.86551400 | -0.78124300 |
| O | 7.35217600 | 4.50194200 | -0.23234500 |
| O | 6.19079700 | 2.62723300 | 0.02559400 |
| O | 5.31615300 | -0.81208500 | -2.90871300 |
| H | 4.45405600 | -0.35921100 | -2.94820100 |
| O | 5.36099700 | -1.17754400 | -0.60834200 |
| O | 9.44960200 | -0.22421800 | 0.75351300 |
| O | 9.94538700 | -0.68083400 | -1.37348500 |
| O | 2.72965300 | -0.39303900 | -2.40182900 |
| H | 1.81350400 | -0.07711100 | -2.51295300 |
| O | 0.09088100 | -0.20175700 | -2.01620400 |
| H | -0.62946100 | -0.47452300 | -2.62354400 |
| O | -1.80937900 | -1.81064700 | -2.35053800 |

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| H | -2.68383800 | -1.39246500 | -2.19528700 |
| O | -4.09706600 | -0.65253200 | -1.55908600 |
| H | -4.89800300 | -0.34410500 | -2.02110500 |
| O | -6.69823700 | -0.33627200 | -2.00072500 |
| H | -7.50749800 | 0.11308900 | -2.30359400 |
| O | -9.36791100 | 0.08511600 | -2.01568500 |
| O | -10.63129300 | -1.31405100 | -0.78147000 |
| O | -14.65063300 | 0.55976100 | -0.58475300 |
| H | -15.20147500 | -0.10394000 | -0.15612400 |
| O | 8.70600900 | -3.07882200 | -2.01277200 |
| H | 9.54148600 | -2.58762600 | -2.05138600 |
| N | 10.91499700 | 2.28659100 | 0.19670100 |
| H | 10.81821400 | 1.99963100 | -0.77613300 |
| H | 10.23636500 | 0.36741600 | 0.66842300 |
| H | 11.81438900 | 2.74756500 | 0.29349800 |