

Supplementary Materials

Tailoring Carbene-Metal-Amides for Thermally Activated Delayed Fluorescence: A Computationally Guided Study on the Effect of Cyclic (Alkyl)(amino)carbenes

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Computational Results

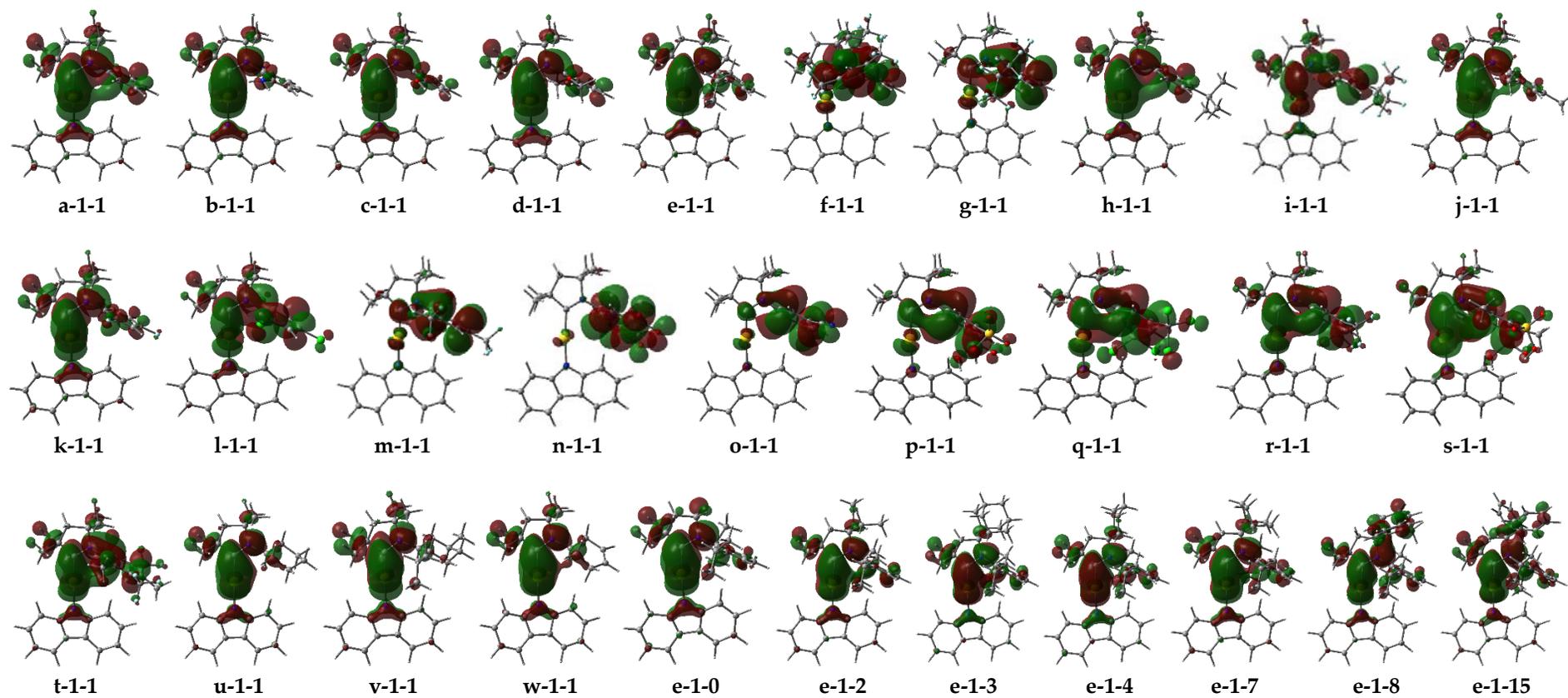


Figure S1. LUMO orbitals of complexes modified at positions 1 and 3

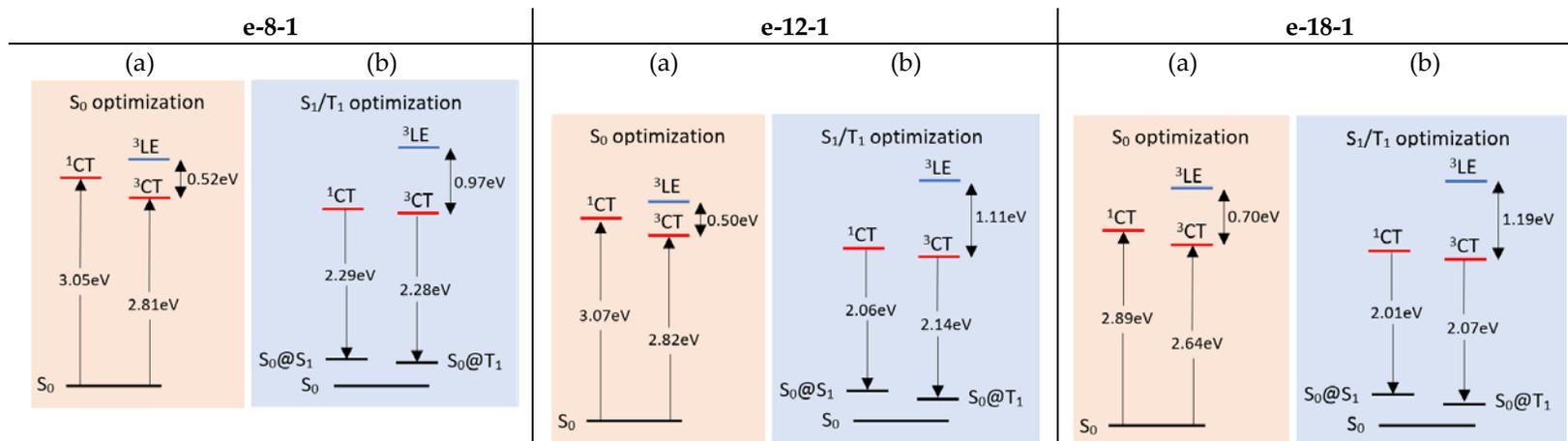


Figure S2. Schematic energy of **e-8-1**, **e-12-1**, and **e-18-1** complexes: (a) vertical excitation energies indicated by the upward arrows; (b) energy levels at optimized S₁ and T₁ geometries with fluorescence (left) and phosphorescence (right) indicated by the downward arrows.

Table S1. Calculated parameters for complexes modified at position **1**

	%Au in HOMO	%Au in LUMO	Overlap integral	Vertical excitations						Dipole moments (D)		Bond dissociation energy			
				¹ CT - S ₁ E (eV)	³ CT - T ₁ E (eV)	³ LE		ΔE_{ST} (eV)	Oscillator strength	S ₀	S ₁ @S ₀	Au-N bond		Au-C bond	
						E (eV)	Character					kJ/mol	eV	kJ/mol	eV
a-1-1	2.9	13.9	0.36	3.03	2.73	3.34	T ₂ (³ LE(Cz))	0.30	0.2073	11.7	-2.5	367.4	3.81	385.9	4.00
b-1-1	2.8	15.2	0.38	2.96	2.64	3.36	T ₂ (³ LE(Cz))	0.32	0.2061	9.6	-3.6	366.6	3.80	391.4	4.06
c-1-1	3.0	13.9	0.35	3.22	2.93	3.33	T ₂ (³ LE(Cz))	0.29	0.1900	10.7	-4.8	372.8	3.86	398.2	4.13
d-1-1	3.1	14.4	0.35	3.26	2.98	3.32	T ₂ (³ LE(Cz))	0.28	0.1791	10.2	-4.3	373.8	3.87	403.4	4.18
e-1-1	2.8	12.9	0.36	3.11	2.80	3.35	T ₂ (³ LE(Cz))	0.31	0.2005	10.8	-2.7	376.7	3.90	401.3	4.16
f-1-1	2.5	1.9	0.23	2.78	2.54	3.31	T ₆ (mixed ³ CT and ³ LE(Cz))	0.24	0.1331	9.0	-7.6	357.4	3.70	374.2	3.88
g-1-1	2.7	2.3	0.20	2.67	2.53	3.34	T ₅ (³ LE(Cz))	0.14	0.0699	10.4	-6.6	370.0	3.83	374.4	3.88
h-1-1	2.9	14.5	0.35	3.07	2.79	3.33	T ₂ (³ LE(Cz))	0.28	0.1820	11.4	-2.7	371.4	3.85	390.9	4.05
i-1-1	2.8	10.0	0.33	2.91	2.61	3.38	T ₃ (mixed ³ CT and ³ LE(Cz))	0.30	0.2037	12.2	-3.9	364.1	3.77	378.7	3.92
j-1-1	2.9	13.9	0.37	3.05	2.74	3.34	T ₂ (³ LE(Cz))	0.31	0.2033	11.3	-2.6	371.9	3.85	395.3	4.10
k-1-1	2.7	12.3	0.36	2.99	2.67	3.35	T ₂ (³ LE(Cz))	0.32	0.2146	11.2	-2.6	364.5	3.78	379.7	3.94
l-1-1	2.7	7.9	0.32	2.96	2.65	3.36	T ₄ (³ LE(Cz))	0.31	0.1910	11.1	-2.9	367.0	3.80	384.5	3.99
m-1-1	2.7	2.2	0.21	2.48	2.35	3.36	T ₆ (³ LE(Cz))	0.13	0.0661	10.9	-8.9	364.8	3.78	380.0	3.94
n-1-1	2.8	1.0	0.14	1.73	1.68	3.36	T ₆ (mixed ³ CT and ³ LE(Cz))	0.05	0.0219	12.6	-14.3	355.6	3.69	369.3	3.83
o-1-1	2.7	2.3	0.19	2.27	2.17	3.38	T ₆ (³ LE(Cz))	0.10	0.0483	12.7	-13.1	355.2	3.68	368.5	3.82
p-1-1	3.4	4.5	0.23	2.89	2.75	3.11	T ₂ (mixed ³ CT and ³ LE(Cz))	0.14	0.0645	9.4	-13.4	390.4	4.05	412.5	4.28
q-1-1	3.1	5.8	0.26	2.81	2.59	3.22	T ₃ (mixed ³ CT and ³ LE(Cz))	0.22	0.1008	11.0	-6.6	373.9	3.87	390.9	4.05
r-1-1	2.8	8.0	0.31	2.76	2.49	3.38	T ₅ (³ LE(Cz))	0.27	0.1539	11.8	-5.8	361.4	3.75	375.5	3.89
s-1-1	3.4	7.7	0.29	3.11	2.89	3.26	T ₂ (mixed ³ CT and ³ LE(Cz))	0.22	0.1095	8.8	-9.5	398.0	4.12	419.9	4.35
t-1-1	2.8	9.3	0.34	2.88	2.57	3.36	T ₃ (³ LE(Cz))	0.31	0.1916	11.3	-4.0	366.1	3.79	385.6	4.00
u-1-1	3.0	16.1	0.35	3.17	2.89	3.34	T ₂ (³ LE(Cz))	0.28	0.1916	11.8	-2.9	362.9	3.76	386.6	4.01
v-1-1	3.0	14.0	0.35	3.21	2.92	3.34	T ₂ (³ LE(Cz))	0.29	0.1991	11.4	-3.0	361.1	3.74	387.3	4.01
w-1-1	3.0	16.1	0.35	3.13	2.86	3.34	T ₂ (³ LE(Cz))	0.27	0.1841	11.6	-2.9	362.6	3.76	387.0	4.01

Table S2. Calculated parameters for complexes modified at position 2

	%Au in HOMO	%Au in LUMO	Overlap integral	Vertical excitations						Dipole		Bond dissociation energy			
				¹ CT - S ₁ E (eV)	³ CT - T ₁ E (eV)	³ LE		ΔE_{ST} (eV)	Oscillator strength	moments (D)		Au-N bond		Au-C bond	
						E (eV)	Character			S ₀	S _{1@S₀}	kJ/mol	eV	kJ/mol	eV
j-1-1	2.9	13.9	0.37	3.05	2.74	3.34	T ₂ (³ LE(Cz))	0.31	0.2033	11.3	-2.6	371.9	3.85	395.3	4.10
j-2-1	2.9	11.9	0.36	3.11	2.81	3.33	T ₂ (³ LE(Cz))	0.30	0.1976	11.2	-2.8	372.1	3.86	397.4	4.12
j-3-1	3.0	12.4	0.36	3.02	2.71	3.33	T ₂ (³ LE(Cz))	0.31	0.1922	10.8	-2.8	370.9	3.84	389.8	4.04
j-4-1	2.9	13.7	0.37	3.06	2.76	3.33	T ₂ (³ LE(Cz))	0.30	0.2015	11.3	-2.6	372.8	3.86	396.8	4.11
j-5-1	2.9	13.5	0.37	3.04	2.73	3.34	T ₂ (³ LE(Cz))	0.31	0.2058	11.2	-2.8	372.3	3.86	395.8	4.10
j-6-1	3.0	12.8	0.36	3.11	2.81	3.33	T ₂ (³ LE(Cz))	0.30	0.1935	11.0	-2.8	373.7	3.87	401.1	4.16
f-1-1	2.5	1.9	0.23	2.78	2.54	3.31	T ₆ (mixed ³ CT and ³ LE(Cz))	0.24	0.1331	9.0	-7.6	357.4	3.70	374.2	3.88
f-2-1	2.6	2.8	0.23	2.78	2.60	3.36	T ₅ (mixed ³ CT and ³ LE(Cz))	0.18	0.1030	9.1	-6.3	370.2	3.84	389.0	4.03
f-3-1	2.7	3.7	0.27	2.68	2.47	3.35	T ₅ (mixed ³ CT and ³ LE(Cz))	0.21	0.1228	8.7	-6.1	362.7	3.76	370.5	3.84
f-4-1	2.6	1.7	0.22	2.79	2.57	3.31	T ₅ (mixed ³ CT and ³ LE(Cz))	0.22	0.1288	8.9	-7.7	358.2	3.71	376.0	3.90
f-5-1	2.5	1.8	0.22	2.77	2.54	3.30	T ₆ (mixed ³ CT and ³ LE(Cz))	0.23	0.1330	8.8	-7.8	357.5	3.71	376.0	3.90
f-6-1	3.0	3.6	0.25	2.80	2.60	3.33	T ₃ (mixed ³ CT and ³ LE(Cz))	0.20	0.1160	8.8	-5.8	371.5	3.85	396.9	4.11
m-1-1	2.7	2.2	0.21	2.48	2.35	3.36	T ₆ (³ LE(Cz))	0.13	0.0661	10.9	-8.9	364.8	3.78	380.0	3.94
m-2-1	2.7	2.0	0.20	2.50	2.38	3.36	T ₆ (³ LE(Cz))	0.12	0.0596	10.8	-9.2	365.5	3.79	382.6	3.97
m-3-1	2.8	2.4	0.22	2.51	2.36	3.35	T ₆ (³ (Cz))	0.15	0.0742	10.7	-8.8	366.4	3.80	377.2	3.91
m-4-1	2.7	2.1	0.20	2.49	2.36	3.36	T ₆ (³ LE(Cz))	0.13	0.0648	11.0	-9.2	365.7	3.79	382.1	3.96
m-5-1	2.7	2.2	0.21	2.49	2.35	3.36	T ₆ (³ LE(Cz))	0.14	0.0666	10.9	-9.0	364.9	3.78	380.7	3.95
m-6-1	2.8	2.0	0.19	2.51	2.38	3.36	T ₆ (³ LE(Cz))	0.13	0.0512	10.6	-9.2	366.6	3.80	389.6	4.04
e-1-1	2.8	12.9	0.36	3.11	2.80	3.35	T ₂ (³ LE(Cz))	0.31	0.2005	10.8	-2.7	376.7	3.90	401.3	4.16
e-2-1	2.8	10.8	0.35	3.17	2.88	3.35	T ₂ (³ LE(Cz))	0.29	0.1952	10.7	-3.0	375.5	3.89	403.2	4.18
e-3-1	3.0	11.4	0.36	3.07	2.77	3.34	T ₂ (³ LE(Cz))	0.30	0.1927	10.5	-2.9	376.5	3.90	394.9	4.09
e-4-1	2.8	12.7	0.36	3.12	2.82	3.35	T ₂ (³ LE(Cz))	0.30	0.1994	10.8	-2.8	377.3	3.91	403.1	4.18
e-5-1	2.8	12.6	0.36	3.10	2.79	3.35	T ₂ (³ LE(Cz))	0.31	0.2029	10.7	-2.9	376.5	3.90	401.8	4.16
e-7-1	3.0	11.9	0.36	3.06	2.76	3.34	T ₂ (³ LE(Cz))	0.30	0.1920	10.6	-2.9	372.5	3.86	395.8	4.10
e-8-1	3.0	8.6	0.32	3.05	2.81	3.33	T ₂ (³ LE(Cz))	0.24	0.1516	9.7	-4.7	376.6	3.90	397.2	4.12

e-9-1	2.7	10.4	0.36	3.08	2.81	3.33	T ₂ (³ LE(Cz))	0.27	0.1726	10.7	-3.1	381.5	3.95	398.8	4.13
e-10-1	2.7	10.4	0.36	3.05	2.74	3.35	T ₂ (³ LE(Cz))	0.31	0.2068	10.7	-3.1	371.3	3.85	395.2	4.10
e-11-1	3.0	7.6	0.32	3.15	2.89	3.32	T ₂ (³ LE(Cz))	0.26	0.1713	11.0	-3.7	369.8	3.83	386.7	4.01
e-12-1	2.9	5.4	0.28	3.07	2.82	3.32	T ₂ (³ LE(Cz))	0.25	0.1659	10.8	-5.0	370.3	3.84	384.9	3.99
e-13-1	3.1	8.4	0.32	3.15	2.90	3.33	T ₂ (³ LE(Cz))	0.25	0.1669	10.7	-4.0	374.5	3.88	390.1	4.04
e-14-1	2.6	9.9	0.37	2.92	2.59	3.37	T ₃ (³ LE(Cz))	0.33	0.2199	10.1	-5.6	368.0	3.81	385.9	4.00
e-15-1	3.0	6.7	0.32	3.01	2.75	3.33	T ₂ (³ LE(Cz))	0.26	0.1672	10.4	-4.4	373.1	3.87	390.9	4.05
e-16-1	3.2	3.9	0.28	3.08	2.88	3.32	T ₂ (³ LE(Cz))	0.20	0.1233	10.3	-5.0	377.2	3.91	376.1	3.90
e-17-1	3.9	8.4	0.28	3.36	3.14	3.31	T ₂ (³ LE(Cz))	0.22	0.1212	11.1	-4.1	387.4	4.01	417.0	4.32
e-18-1	2.9	5.1	0.30	2.89	2.64	3.34	T ₂ (³ LE(Cz))	0.25	0.1567	10.2	-5.6	371.7	3.85	374.8	3.88
e-19-1	2.9	1.8	0.21	2.58	2.44	3.33	T ₄ (mixed ³ CT and ³ LE(Cz))	0.14	0.0696	10.0	-9.4	374.3	3.88	365.3	3.79
e-20-1	2.9	4.9	0.31	2.64	2.38	3.30	T ₄ (mixed ³ CT and ³ LE(Cz))	0.26	0.1514	10.7	-8.0	363.9	3.77	372.6	3.86

Table S3. Calculated parameters for complexes modified at position **3**

	%Au in HOMO	%Au in LUMO	Overlap integral	Vertical excitations						Dipole moments (D)		Bond dissociation energy			
				¹ CT - S ₁ E (eV)	³ CT - T ₁ E (eV)	³ LE		ΔE_{ST} (eV)	Oscillator strength	S ₀	S ₁ @S ₀	Au-N bond		Au-C bond	
						E (eV)	Character					kJ/mol	eV	kJ/mol	eV
e-1-0	2.8	13.5	0.37	3.03	2.71	3.35	T ₂ (³ LE(Cz))	0.32	0.1994	10.6	-2.6	369.4	3.83	392.1	4.06
e-1-1	2.8	12.9	0.36	3.11	2.80	3.35	T ₂ (³ LE(Cz))	0.31	0.2005	10.8	-2.7	376.7	3.90	401.3	4.16
e-1-2	2.8	12.9	0.36	3.11	2.80	3.35	T ₂ (³ LE(Cz))	0.31	0.2037	11.0	-2.7	374.8	3.88	402.8	4.18
e-1-3	2.7	12.0	0.36	3.08	2.77	3.34	T ₂ (³ LE(Cz))	0.31	0.2176	11.5	-2.6	372.9	3.87	393.7	4.08
e-1-4	2.8	13.0	0.36	3.12	2.82	3.35	T ₂ (³ LE(Cz))	0.30	0.2078	11.3	-2.5	377.3	3.91	402.7	4.17
e-1-7	2.8	12.3	0.36	3.06	2.75	3.35	T ₂ (³ LE(Cz))	0.31	0.2176	11.2	-2.6	372.9	3.86	395.1	4.09
e-1-8	2.8	10.2	0.34	3.08	2.80	3.35	T ₂ (³ LE(Cz))	0.28	0.2182	11.5	-3.7	375.0	3.89	393.2	4.08
e-1-15	2.7	10.5	0.35	2.98	2.68	3.35	T ₂ (³ LE(Cz))	0.30	0.2218	11.3	-3.2	371.9	3.85	386.7	4.01

X-Ray Crystallography

Crystals suitable for X-ray diffraction study were obtained by slow layer diffusion of hexanes/petroleum ether into dichloromethane solution for **e-2-1** at room temperature. Crystals were mounted in oil on glass fiber and fixed on the diffractometer in a cold nitrogen stream. Data were collected using XtaLAB AFC11 (RINC): quarter-chi single diffractometer at 100 K. Data were processed using the CrystAlisPro-CCD and –RED software. Multi-scan absorption correction was applied for all crystals. For the final refinement, the contribution of severely disordered CH₂Cl₂ molecules in the crystals **e-2-1** was accounted for by applying a solvent void mask calculated using BYPASS, implemented through Olex2. Structures were solved by direct method/intrinsic phasing and refined by the full-matrix least-squares against F² in an anisotropic (for non-hydrogen atoms) approximation. All hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms with C-H = 0.95–1.00 Å, and U_{iso} = 1.2–1.5 U_{eq} (parent atom). All calculations were performed using the SHELXL software and Olex2 graphical user interface.

e-2-1, CCDC number 2259783, C₃₅H₄₇AuN₂ (*M* = 676.67 g/mol): monoclinic, space group P2₁/c (no. 14), *a* = 9.71163(5) Å, *b* = 18.40218(10) Å, *c* = 17.11055(10) Å, β = 95.3962(5)°, *V* = 3044.36(3) Å³, *Z* = 4, *T* = 100.00(10) K, μ(Cu Kα) = 9.241 mm⁻¹, *D*_{calc} = 1.476 g/cm³, 20350 reflections measured (7.072° ≤ 2Θ ≤ 151.65°), 6090 unique (*R*_{int} = 0.0181, *R*_{sigma} = 0.0150) which were used in all calculations. The final *R*₁ was 0.0207 (*I* > 2σ(*I*)) and *wR*₂ was 0.0564 (all data).

Experimental Details

General Considerations. Unless stated otherwise, all reactions were carried out in air. Solvents were distilled and dried as required. Potassium *tert*-butoxide and carbazole were purchased from FluoroChem. The carbene complex (^{Et}L)AuCl [1] were obtained according to literature procedures. ¹H and ¹³C{¹H} NMR spectra were recorded using a Bruker Avance 500 MHz NMR spectrometer. ¹H NMR spectra were referenced to CD₂Cl₂ at δ 5.32 (¹³C, δ 53.84) ppm. All electrochemical experiments were performed using an Autolab PGSTAT 302N computer-controlled potentiostat. Cyclic voltammetry (CV) was performed using a three-electrode configuration consisting of either a glassy carbon macrodisk working electrode (GCE) (diameter of 3 mm; BASi, Indiana, USA) combined with a Pt wire counter electrode (99.99 %; GoodFellow, Cambridge, UK) and an Ag wire pseudo-reference electrode (99.99 %; GoodFellow, Cambridge, UK). The GCE was polished between experiments using alumina slurry (0.3 μm), rinsed in distilled water and subjected to brief sonication to remove any adhering alumina microparticles. The metal electrodes were then dried in an oven at 100 °C to remove residual traces of water, the GCE was left to air dry and residual traces of water were removed under vacuum. The Ag wire pseudoreference electrodes were calibrated to the ferrocene/ferrocenium couple in THF at the end of each run to allow for any drift in potential, following IUPAC recommendations [2]. All electrochemical measurements were performed at ambient temperatures under an inert Ar atmosphere in THF containing complex under study (0.14 mM) and supporting electrolyte [n-Bu₄N][PF₆] (0.13 mM). Data were recorded with Autolab NOVA software (v. 1.11). Elemental analyses were performed by the University of Manchester. UV-visible absorption spectra were recorded using a Perkin-Elmer Lambda 35 UV/vis spectrometer. Mass spectrometry data was obtained using APCI(ASAP) (Atmospheric Solids Analysis Probe) at the University of Manchester.

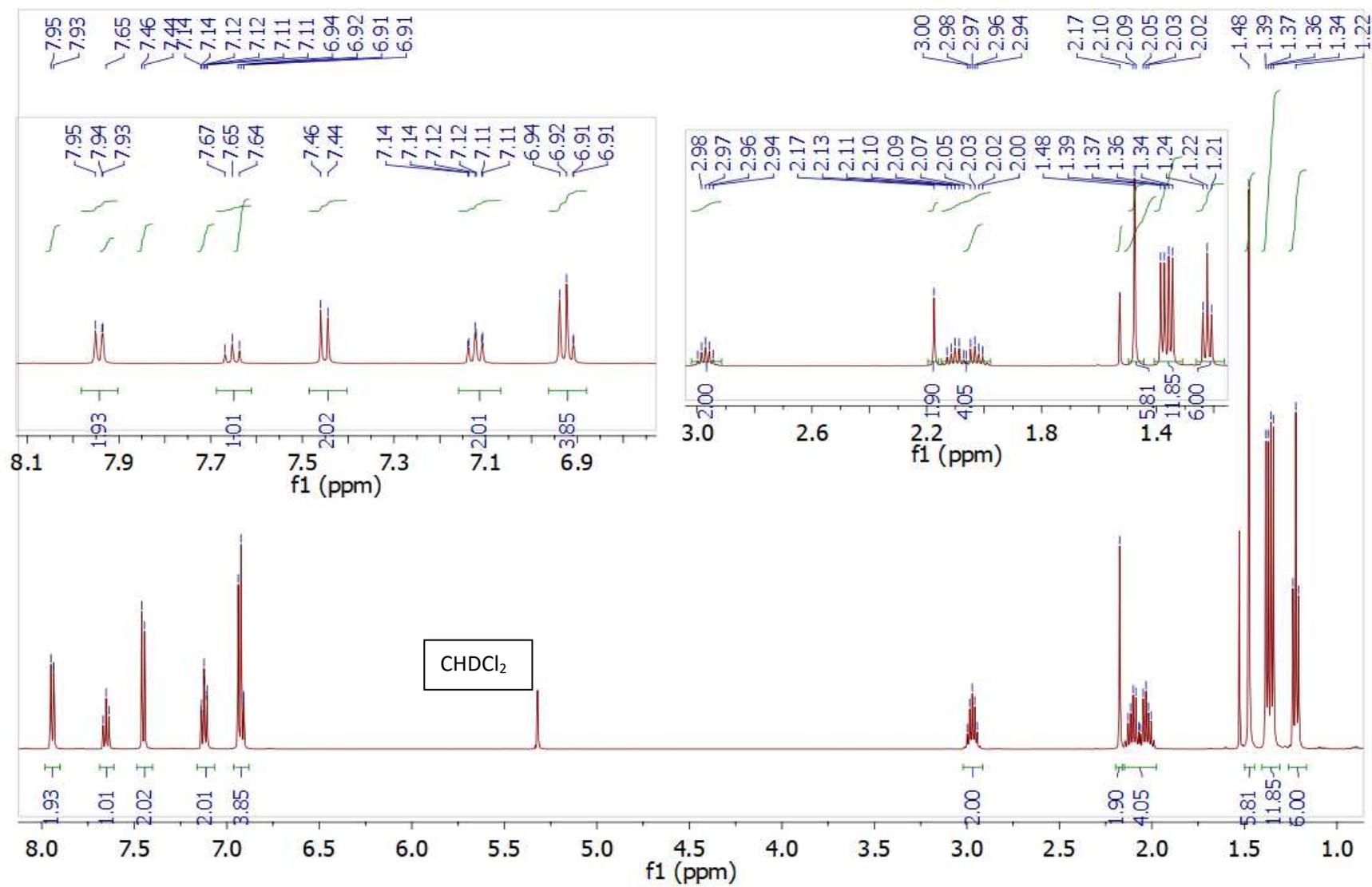


Figure S3. ^1H NMR (500 MHz, CD_2Cl_2) for e-2-1

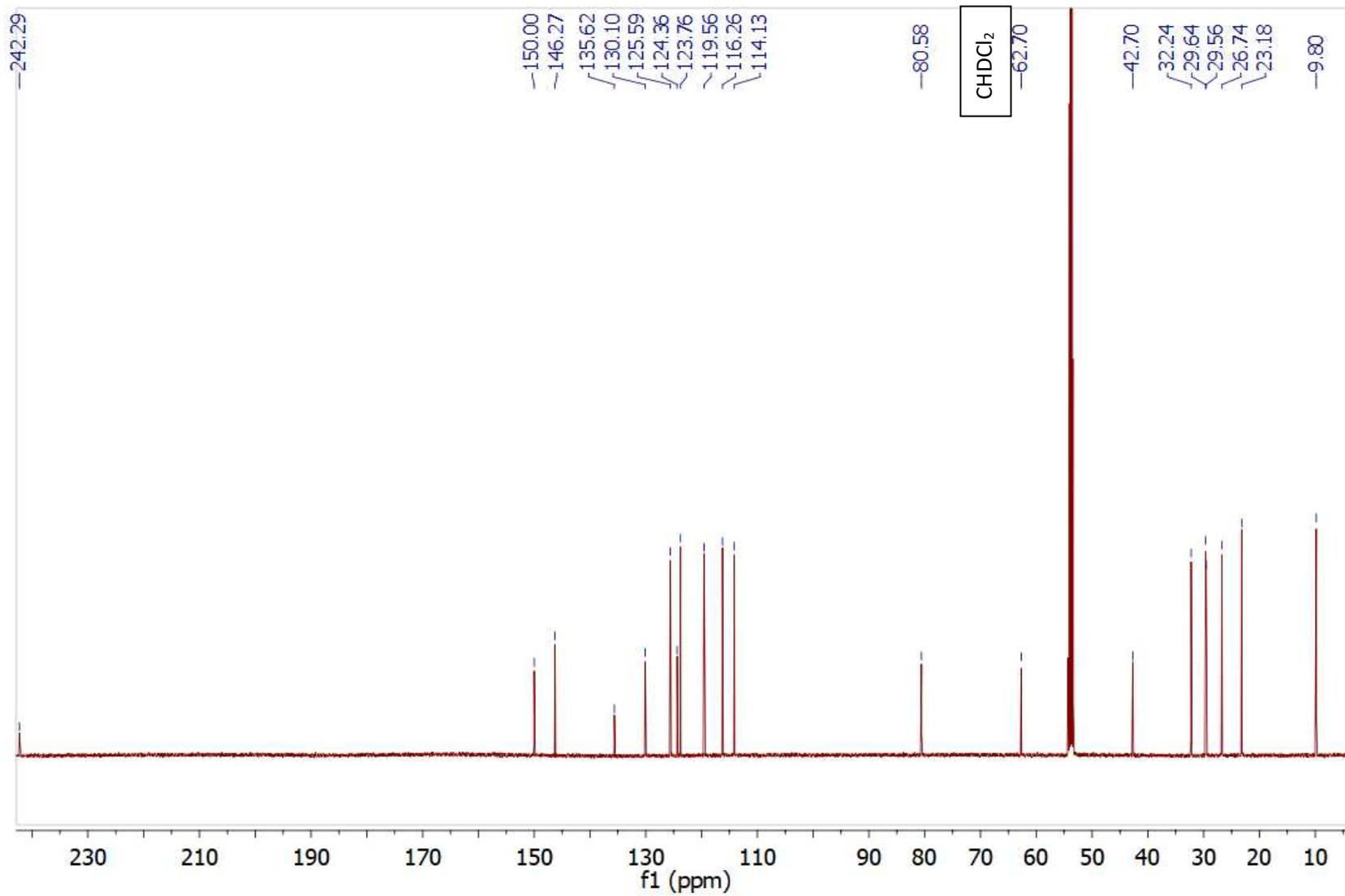


Figure S4. ^{13}C NMR (125 MHz, CD_2Cl_2) for e-2-1

Table S4. UV-vis data for **e-2-1** in various solvents

	λ_{abs} [nm], ($10^3 \epsilon/M^{-1} \text{ cm}^{-1}$)			
	DCM	THF	Toluene	MCH
e-2-1	387 (sh) (4.4)	379 (8.0)	392 (8.2)	408 (8.4)
	367 (11.3)	367 (12.5)	367 (10.1)	365 (7.3)

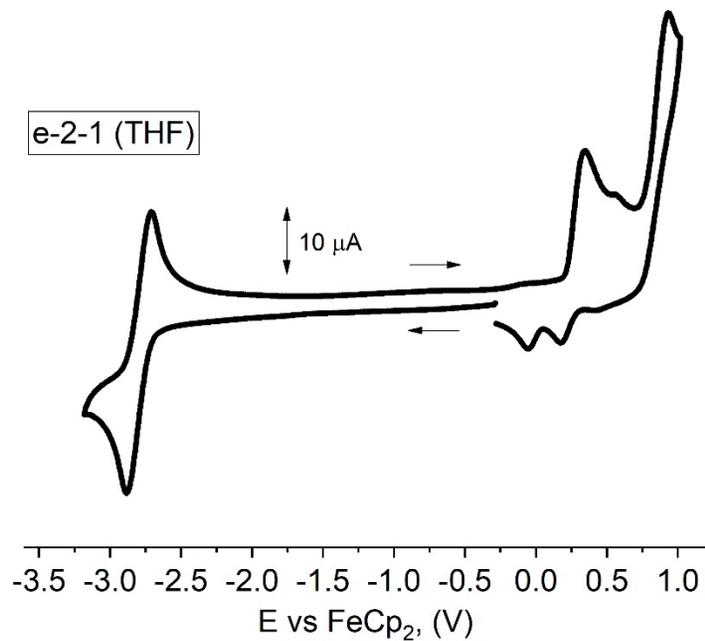


Figure S5. Full range cyclic voltammogram for **e-2-1**. Recorded using a glassy carbon electrode in THF solution (1.4 mM) with [n-Bu₄N]PF₆ as supporting electrolyte (0.13 M), scan rate 0.1 V s⁻¹.

Table S5. Formal electrode potentials (peak position E_p for irreversible and $E_{1/2}$ for quasi-reversible processes (*), V , vs. FeCp_2), onset potentials (E , V , vs. FeCp_2), peak-to-peak separation in parentheses for quasi-reversible processes (ΔE_p in mV), $E_{\text{HOMO}}/E_{\text{LUMO}}$ (eV) and band gap values (ΔE , eV) for the redox changes exhibited.^a

	Reduction		E_{LUMO} (eV)	Oxidation				E_{HOMO} (eV)	ΔE (eV)
	$E_{1\text{st}}$	$E_{\text{onset red}}$		$E_{1\text{st}}$	$E_{\text{onset ox}}$	$E_{2\text{nd}}$	$E_{3\text{rd}}$		
e-2-1	-2.79 (176)	-2.72	-2.67	0.15 (397)	0.22	0.37 (384)	0.93	-5.61	2.94

^a In tetrahydrofuran solution, recorded using a glassy carbon electrode, concentration 1.4 mM, supporting electrolyte [$n\text{Bu}_4\text{N}$][PF₆] (0.13 M), measured at 0.1 Vs⁻¹.

^b In difluorobenzene solution, recorded using a glassy carbon electrode, concentration 1.4 mM, supporting electrolyte [$n\text{Bu}_4\text{N}$][PF₆] (0.13 M), measured at 0.1 Vs⁻¹. $E_{\text{HOMO}} = -(E_{\text{onset ox Fe/Fc}^+} + 5.39)$ eV; $E_{\text{LUMO}} = -(E_{\text{onset red Fe/Fc}^+} + 5.39)$ eV [3].

Photophysical Characterization

UV-visible absorption spectra were recorded using a Varian Cary 5000 UV-Vis-NIR spectrometer. Photoluminescence measurements were recorded on an Edinburgh Instruments FLS980 spectrometer with a solids mount attachment where appropriate. Absolute photoluminescence quantum yields were recorded using a Hamamatsu Quantaaurus-QY C11347-11. Quantum yields have been measured in air for solid samples and under nitrogen for solutions. Time resolved luminescence data were collected on a time-correlated single photon counting (TCSPC) Edinburgh Instruments FLS980 spectrometer using F-900 software. A xenon flash lamp and EPL pulsed diode lasers were used as excitation sources. The collected data were analyzed using F-900 software.

Coordinates of optimized structures in zyz-format

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a-1-1

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Au      -0.02661400 -0.61993800 -0.07452500
N       -1.98046200 -0.20384200 -0.05935200
C       -4.27500500 -0.31421500  0.03955300
C       2.06245200  1.95972800  1.25555300
N       2.79966300  0.05385200 -0.06958700
C       4.23441200 -0.35346500 -0.00916100
C       1.65735300  3.28433300  1.34654800
H       1.37056600  3.69387900  2.30594700
C      -4.30423700 -3.08933000  0.09946400
H      -4.33587700 -4.17220700  0.12315500

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C	1.92175300	-0.91806600	-0.08267200
C	-2.47960200	1.08233600	-0.06651700
C	2.34101800	2.21068600	-1.13125300
C	1.59808900	4.07311500	0.20329200
C	-3.06647900	-1.05042800	0.00404800
C	2.40864700	1.43458900	0.01702500
C	-4.59221800	2.28258300	0.00093000
H	-5.67570300	2.28823800	0.04799100
C	-1.77042300	2.28404200	-0.12639400
H	-0.68550900	2.27736300	-0.18244800
C	-3.89206900	1.07603300	-0.00529200
C	-3.08090900	-2.44621300	0.03435000
H	-2.14971300	-3.00298700	0.00626700
C	4.11980700	-1.86016500	-0.27950500
H	4.79996500	-2.42995400	0.35627800
H	4.38734400	-2.06203700	-1.31998300
C	-5.49685300	-0.98335000	0.10527800
H	-6.42674500	-0.42591600	0.13266000
C	-2.48489300	3.46883700	-0.11742600
H	-1.95068100	4.41174600	-0.16378800
C	1.93367600	3.53549800	-1.03343700
H	1.86415500	4.14212500	-1.92671000
C	-5.50712300	-2.36769300	0.13495300
H	-6.44802800	-2.90125800	0.18565900
C	4.79197100	-0.02738300	1.37141100
H	4.76171300	1.04839700	1.55551200
H	5.83143300	-0.35389100	1.42803700
H	4.22709700	-0.53191000	2.15664100
C	-3.88695800	3.47375700	-0.05347200
H	-4.41833400	4.41732500	-0.04911800
C	5.04254600	0.36673400	-1.07698100
H	4.61503200	0.19895600	-2.06723700
H	6.06225900	-0.02185200	-1.07246400
H	5.08535800	1.44057200	-0.88601100

C	2.64657700	-2.23877200	-0.04363600
C	2.40354300	-2.84680900	1.34214600
H	1.33697100	-3.02165800	1.49434000
H	2.93143300	-3.80019300	1.41652600
H	2.75621300	-2.19262800	2.14174700
C	2.10493200	-3.18519400	-1.10950800
H	2.66276000	-4.12436200	-1.08867000
H	1.05026800	-3.39935400	-0.92530200
H	2.19467900	-2.74998300	-2.10662500
H	2.08791100	1.31754700	2.12809800
H	1.27123500	5.10247100	0.27398000
H	2.58223300	1.76947800	-2.09022200

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b-1-1

Au	-0.16753900	-0.71498500	-0.04359200
N	-2.09996300	-0.21758400	-0.02712100
C	-4.39848000	-0.22055000	0.00791000
C	2.02117600	1.88132900	1.22848400
N	2.65563700	-0.10284500	-0.06589300
C	4.09336200	-0.52732700	-0.04977600
C	1.74960200	3.25007100	1.26878500
H	1.56430700	3.72556100	2.22399000
C	-4.56160200	-2.99153100	-0.02941700
H	-4.64535600	-4.07174500	-0.04407900
C	1.77272800	-1.06937800	-0.05746100
C	-2.53740600	1.09239300	-0.00215300
C	2.08750700	1.98983700	-1.20862000
C	-3.22634300	-1.01312100	-0.02135700
C	2.27919700	1.28477000	-0.01330900
C	-4.59263100	2.38836700	0.04920700
H	-5.67555200	2.44385800	0.06711600
C	-1.77044800	2.25962400	0.00157100
H	-0.68512300	2.20829000	-0.01873100
C	-3.94922300	1.15076800	0.02083500

C	-3.30762100	-2.40658800	-0.04020200
H	-2.40366600	-3.00678000	-0.06321100
C	3.95095500	-2.03772200	-0.28715500
H	4.64582900	-2.60442200	0.33532700
H	4.17828200	-2.26320200	-1.33244300
C	-5.65206400	-0.83132500	0.01837000
H	-6.55473800	-0.23067800	0.04083400
C	-2.42931600	3.47591600	0.03051900
H	-1.84890600	4.39212800	0.03408200
C	1.81289600	3.35654500	-1.14437500
H	1.67808400	3.91461100	-2.06265200
C	-5.72900700	-2.21386700	-0.00027700
H	-6.69527900	-2.70249600	0.00745600
C	4.72307100	-0.18214300	1.29414500
H	4.67569200	0.89291400	1.47490100
H	5.77087700	-0.48670400	1.27715900
H	4.22505800	-0.68715900	2.12087400
C	-3.83097800	3.54542500	0.05442100
H	-4.31759300	4.51259900	0.07653800
C	4.86972600	0.16658500	-1.15782600
H	4.44918500	-0.05377500	-2.13789800
H	5.90365700	-0.18171500	-1.12911800
H	4.86655900	1.24920300	-1.01570600
C	2.48337600	-2.39533300	0.00714200
C	2.27781700	-2.93530300	1.42742800
H	1.21468800	-3.08780400	1.62379000
H	2.79515400	-3.89158000	1.53134800
H	2.67112700	-2.24994700	2.18189900
C	1.89964600	-3.38090000	-0.99791600
H	2.44583200	-4.32585600	-0.95269400
H	0.84781600	-3.57275700	-0.77556400
H	1.96735000	-2.99218000	-2.01624600
N	2.04779900	1.11933300	2.38971300
H	1.70319400	0.17138500	2.27806600

H	1.62419200	1.57558200	3.18646100
N	2.17901100	1.32951000	-2.42668300
H	1.79319200	1.84656000	-3.20497300
H	1.85014000	0.37069000	-2.41188800
C	1.67404000	3.97308100	0.08913600
H	1.45432300	5.03260800	0.13034200

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c-1-1

Au	-0.16255800	-0.67805100	-0.08318600
N	-2.10850500	-0.20929500	-0.06293800
C	-4.40623100	-0.26826300	0.01722000
C	2.01455100	1.82067400	1.26010600
N	2.69003600	-0.10650900	-0.07684300
C	4.11089000	-0.56691900	-0.03166900
C	1.61787000	3.14954200	1.36211700
H	1.37045300	3.56268300	2.33256000
C	-4.49926600	-3.04249200	0.00873900
H	-4.55593400	-4.12461800	0.00548100
C	1.77538100	-1.04280700	-0.08569600
C	-2.57770100	1.08635000	-0.04152800
C	2.19105600	2.05162800	-1.13447500
C	-3.21412200	-1.03102800	-0.02771800
C	2.33672300	1.27560300	0.01539100
C	-4.66127900	2.33610700	0.04027700
H	-5.74469000	2.36724700	0.07933500
C	-1.83986100	2.27197200	-0.06460100
H	-0.75520900	2.23839200	-0.10989100
C	-3.99090200	1.11297900	0.00924100
C	-3.26111100	-2.42677500	-0.03195000
H	-2.34266900	-3.00391900	-0.06734500
C	3.93225000	-2.07281200	-0.26992800
H	4.59642600	-2.65690600	0.36988900
H	4.17597100	-2.30665800	-1.30938200
C	-5.64373600	-0.91051400	0.05777200

H	-6.56086700	-0.33260700	0.09210400
C	-2.52500000	3.47350800	-0.03163000
H	-1.96753700	4.40414200	-0.04927200
C	1.79485500	3.38170700	-1.03452500
H	1.68631800	3.97683500	-1.93352400
C	-5.68588000	-2.29438600	0.05340000
H	-6.63905800	-2.80731300	0.08424800
C	4.71941200	-0.23757700	1.32593100
H	4.71145800	0.84092700	1.49815000
H	5.75581500	-0.57881600	1.34019500
H	4.17627800	-0.71776300	2.13825800
C	-3.92729600	3.51107700	0.02094200
H	-4.43601600	4.46680200	0.04477900
C	4.92197900	0.10271700	-1.12955100
H	4.49495600	-0.10052000	-2.11042100
H	5.94268300	-0.28237900	-1.09757200
H	4.96089000	1.18454700	-0.98138700
C	2.44896600	-2.38680600	-0.00753100
C	2.19641100	-2.90627200	1.41358200
H	1.12785100	-3.06440400	1.57075300
H	2.71842900	-3.85613900	1.55003700
H	2.54531100	-2.19921700	2.16868000
C	1.86302900	-3.36434300	-1.01860500
H	2.38163900	-4.32361300	-0.95067800
H	0.80163700	-3.52558700	-0.81832400
H	1.96432500	-2.98575000	-2.03732400
C	1.51786600	3.91901100	0.21310600
H	1.19839100	4.95023900	0.28946400
O	2.42253500	1.44839800	-2.32224000
H	2.15648800	2.02769200	-3.04702200
O	2.08808600	0.99704300	2.33102800
H	1.66990800	1.40856700	3.09757200

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d-1-1

Au	-0.26373000	-0.74333000	-0.28800600
N	-2.18706900	-0.18298000	-0.31705200
C	-4.47428300	-0.13940300	-0.07551200
C	1.69549300	1.53284200	1.37597600
N	2.59475500	-0.31448300	0.07025100
C	3.95183000	-0.85939700	0.38163000
C	1.35235000	2.87660700	1.50807500
H	0.88247700	3.23205500	2.41405800
C	-4.71271100	-2.89750100	-0.27554900
H	-4.82620400	-3.97236400	-0.35283700
C	1.64985700	-1.19949500	-0.11742500
C	-2.58572400	1.12807600	-0.16701900
C	2.47986600	1.94959400	-0.88010100
C	1.58990500	3.73902800	0.45086200
C	-3.32957000	-0.95198600	-0.26064800
C	2.29520100	1.07825000	0.19794600
C	-4.58904700	2.46368900	0.16885200
H	-5.66375900	2.54276500	0.29123900
C	-1.79002500	2.27636600	-0.16170100
H	-0.71708900	2.19885900	-0.31243100
C	-3.98865200	1.21707100	-0.00924500
C	-3.44953000	-2.33985000	-0.36021200
H	-2.56718100	-2.95517700	-0.50369200
C	3.75252200	-2.34002200	0.03429400
H	4.26193600	-2.98714200	0.75076200
H	4.17135200	-2.53946000	-0.95550300
C	-5.73827800	-0.72351200	0.00698000
H	-6.61945800	-0.10711300	0.14777500
C	-2.40612300	3.50176800	0.02318500
H	-1.80303300	4.40353900	0.02960100
C	2.13714900	3.29401500	-0.74549800
H	2.27686600	3.98376600	-1.56470900
C	-5.85292100	-2.09952600	-0.09352600
H	-6.82740600	-2.56772600	-0.03250300

C	4.26509700	-0.62184900	1.85463300
H	4.26615600	0.44735000	2.07757100
H	5.25743200	-1.01922700	2.07412000
H	3.53695400	-1.10374000	2.50452000
C	-3.79639300	3.60007300	0.18960400
H	-4.25048800	4.57332900	0.32847300
C	5.01894200	-0.19974400	-0.47576900
H	4.81126800	-0.33837100	-1.53546000
H	5.98454900	-0.65039200	-0.23930300
H	5.08141200	0.87055700	-0.26633100
C	2.23346300	-2.58193700	0.00709600
C	1.69796400	-3.15889900	1.32400700
H	0.61476900	-3.28249300	1.26556900
H	2.15558800	-4.13403300	1.50590600
H	1.91452200	-2.50339500	2.16978800
C	1.79721700	-3.47306700	-1.14966000
H	2.24047400	-4.46578900	-1.04106400
H	0.70993000	-3.57458700	-1.15932900
H	2.11055000	-3.05623000	-2.10859300
H	1.31934700	4.78272400	0.54887500
O	1.45362000	0.60918700	2.32963100
O	2.95416600	1.40081900	-2.01638500
C	0.30121300	0.80949600	3.13557200
H	-0.54671200	1.11361200	2.51414700
H	0.08255200	-0.14635600	3.60491300
H	0.48312800	1.55869200	3.90928500
C	3.03068800	2.21633100	-3.16585600
H	3.37511300	1.57799100	-3.97455700
H	2.04987500	2.62611100	-3.41895000
H	3.74065300	3.03538200	-3.02314200
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e-1-1			
Au	-0.39371800	-0.88896000	-0.04159300
N	-2.28825700	-0.24781800	-0.02118100

C	-4.57717000	-0.03395800	-0.00517000
C	1.97420800	1.59881500	1.27429900
N	2.45334700	-0.41214700	-0.05946800
C	3.86652200	-0.91234100	-0.08232500
C	1.78469400	2.97926500	1.31352100
H	1.64418300	3.46199900	2.27342900
C	-4.99894300	-2.77663100	-0.08302400
H	-5.18369600	-3.84388900	-0.11357600
C	1.52529200	-1.33362100	-0.06723300
C	-2.60045600	1.09640700	0.01795600
C	0.39824500	0.94516500	3.08185700
H	-0.32910000	0.62368900	2.33366600
H	0.17582700	1.98401000	3.33785200
H	0.26417700	0.33907000	3.97996600
C	2.00497000	1.72636600	-1.17414000
C	1.73262100	3.73299100	0.15288900
H	1.58484400	4.80420000	0.20677700
C	-3.48432600	-0.93302900	-0.03596000
C	2.15085200	1.00001000	0.01706700
C	0.47678300	1.21074400	-3.06233900
H	-0.24477700	0.77069100	-2.37039800
H	0.37784200	0.71568800	-4.03039700
H	0.21527700	2.26410800	-3.19037600
C	-4.52375100	2.58121900	0.06936000
H	-5.59660700	2.73942700	0.07899800
C	-1.72641400	2.18673600	0.04368300
H	-0.65063900	2.03290200	0.03265700
C	1.83660600	0.81985200	2.56845600
H	2.02257500	-0.23712400	2.36258600
C	1.91131400	1.07903100	-2.54159600
H	2.12891400	0.01243800	-2.44087900
C	-4.00112400	1.28857800	0.03014400
C	-3.69558700	-2.31230300	-0.07514800
H	-2.85155500	-2.99378000	-0.09918300

C	3.64569200	-2.40496900	-0.36415300
H	4.31878600	-3.02546600	0.23048600
H	3.84879900	-2.60756200	-1.41915600
C	-5.88276900	-0.52442300	-0.01359000
H	-6.72537200	0.15792900	0.00989900
C	2.80172400	1.29244700	3.65477300
H	3.84431100	1.25477400	3.33803100
H	2.69099100	0.67336700	4.54704500
H	2.57723700	2.32160800	3.94361600
C	-2.26738700	3.46015900	0.08276300
H	-1.60243600	4.31698200	0.10330800
C	1.81098400	3.10255300	-1.07818000
H	1.69101700	3.68111100	-1.98653000
C	-6.08864700	-1.89312400	-0.05241300
H	-7.09653700	-2.28890500	-0.05951300
C	2.88410500	1.69080100	-3.54855900
H	3.91373500	1.68301000	-3.18808600
H	2.61301800	2.72699500	-3.76208300
H	2.84251000	1.14329900	-4.49202000
C	4.54286500	-0.64212700	1.25487700
H	4.57765200	0.43164400	1.44810700
H	5.56801600	-1.01320100	1.21308000
H	4.03296000	-1.13364800	2.08362700
C	-3.65606900	3.66131500	0.09577700
H	-4.04954400	4.66973900	0.12636200
C	4.67155800	-0.23335200	-1.17926100
H	4.24882800	-0.42852600	-2.16449900
H	5.68827200	-0.62959400	-1.16051100
H	4.72248800	0.84603800	-1.01988500
C	2.16618200	-2.69573200	-0.06250200
C	1.95082700	-3.28935900	1.33375400
C	1.52031300	-3.59985400	-1.10595600
H	0.88368300	-3.37911400	1.54519700
H	2.39993400	-2.66782600	2.11156100

H	0.46496400	-3.75500700	-0.87304800
H	1.58700800	-3.15801700	-2.10273600
H	2.40443000	-4.28192300	1.38039700
H	2.02378200	-4.56933000	-1.12111300

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e-2-1

Au	-0.41221100	-0.74941600	0.02092500
N	-2.36243500	-0.30240300	0.01483000
C	-4.66107200	-0.31763800	0.00712800
C	1.74893300	2.10146200	1.11043500
N	2.37735000	0.00440300	0.00235200
C	3.83291400	-0.35220500	-0.00529100
C	1.40840900	3.44849000	1.01018400
H	1.25409700	4.02045000	1.91754200
C	-4.80699700	-3.08940600	0.05896200
H	-4.88441300	-4.17002800	0.07930700
C	1.54502900	-1.00233200	0.03126900
C	-2.80703000	1.00410300	-0.01062000
C	0.33786000	1.40776800	3.03332000
H	-0.33644100	0.88059800	2.35396600
H	-0.05418000	2.41880700	3.17086600
H	0.32318700	0.90184400	4.00124300
C	1.66133200	1.94344900	-1.33459900
C	1.22959600	4.05346000	-0.22313500
H	0.96841600	5.10255800	-0.28175100
C	-3.48379200	-1.10356700	0.02614600
C	1.93392300	1.37971500	-0.07819600
C	0.12265900	1.12898100	-3.11123100
H	-0.56029200	0.75046500	-2.34797500
H	0.03208100	0.50177100	-4.00024100
H	-0.19969800	2.13906400	-3.37562100
C	-4.86892900	2.29039600	-0.04315200
H	-5.95224600	2.34099100	-0.04828600
C	-2.04601500	2.17630200	-0.02899000

H	-0.96023200	2.13060000	-0.02264400
C	1.76580000	1.45864300	2.48228900
H	2.11307800	0.42908900	2.37969800
C	1.57438900	1.14395800	-2.62079200
H	1.86215900	0.11036200	-2.41218400
C	-4.22000000	1.05592600	-0.01718400
C	-3.55642700	-2.49746400	0.05217500
H	-2.64826300	-3.09114900	0.06697700
C	3.78129000	-1.87761000	0.17941900
H	4.16968300	-2.14784400	1.16329200
H	4.41039700	-2.37184000	-0.56361000
C	-5.91117800	-0.93595200	0.01433600
H	-6.81769600	-0.34083300	-0.00012600
C	2.67718300	2.18724200	3.46781300
H	3.69611800	2.28906500	3.09132900
H	2.71162600	1.64656300	4.41557400
H	2.29617300	3.18872600	3.67899000
C	-2.71133600	3.38969300	-0.05532700
H	-2.13506200	4.30861700	-0.07029300
C	1.32887700	3.29645900	-1.37862900
H	1.11326300	3.75195400	-2.33794700
C	-5.97948900	-2.31868000	0.04014600
H	-6.94285700	-2.81307300	0.04614900
C	2.47283600	1.69784000	-3.72590600
H	3.51961600	1.75772400	-3.42713900
H	2.14917000	2.70061500	-4.01362500
H	2.40401300	1.06673600	-4.61401400
C	4.57396000	0.34351600	1.12575300
H	4.49399900	1.42918000	1.03739500
H	5.62964600	0.07311700	1.06803400
H	4.19675200	0.03630300	2.10201300
C	-4.11324500	3.45172000	-0.06243100
H	-4.60527900	4.41617300	-0.08284700
C	4.45930800	0.05647700	-1.33104100

H	3.98457200	-0.44864600	-2.17365500
H	5.51653700	-0.21293800	-1.31994000
H	4.38291100	1.13610300	-1.47422000
C	2.30677300	-2.29910500	0.03521200
C	1.81867400	-3.18881600	1.18633000
C	2.03088700	-2.96734000	-1.32719600
H	0.81850400	-3.55583500	0.92986900
H	0.94694200	-3.00749000	-1.47322200
H	2.42631300	-2.31333800	-2.11419100
H	2.47761200	-4.06012400	1.24324600
C	2.62666100	-4.36168000	-1.45970400
H	2.51695900	-4.72825800	-2.48020800
H	3.69183000	-4.37244500	-1.21560300
H	2.12569500	-5.07048200	-0.79987100
C	1.77083400	-2.47860900	2.53307300
H	1.53966200	-3.17737200	3.33674400
H	2.72819300	-2.00585400	2.77470200
H	1.00197900	-1.70125000	2.53550900

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Au	0.39528100	0.44852800	-0.13882000
N	2.36117200	0.79909400	-0.06890800
C	4.44137100	1.77553900	-0.02073900
C	-0.45722700	-2.71329800	1.38024100
N	-1.85029900	-1.31410300	-0.08876400
C	-2.75736800	1.88574400	-1.33438200
H	-2.57529600	1.39659300	-2.29908300
C	-1.92718100	3.62284700	0.26443000
H	-1.13754400	4.35612400	0.45144000
C	-3.31265100	-1.61532300	-0.11982000
C	0.37755500	-3.82109300	1.51911600
H	0.71859400	-4.09929000	2.50934100
C	-2.99503700	1.51647600	1.12060700
H	-2.97340300	0.77460000	1.92709700

C	3.41498200	4.35266700	-0.15352400
H	3.03389600	5.36581600	-0.20260000
C	-1.52284800	-0.04732900	-0.17517500
C	3.30830300	-0.19983200	0.01593000
C	-1.69102300	2.95222700	-1.08703800
H	-1.75642500	3.69951900	-1.88550700
H	-0.68728100	2.52160300	-1.13289900
C	0.57478100	-1.24670100	3.10113000
H	1.07995100	-0.68636700	2.31185100
H	1.25835600	-2.02675500	3.44538000
H	0.38190300	-0.57291500	3.93837300
C	-0.38210800	-3.02923900	-1.05002700
C	0.80702300	-4.54335000	0.41834200
H	1.45397000	-5.40146900	0.54993400
C	-1.90830900	2.56860200	1.37174900
H	-2.10796000	3.04603700	2.33713500
H	-0.91870800	2.10772800	1.43715000
C	-3.28845000	4.31574500	0.24125900
H	-3.47221400	4.82133200	1.19534400
H	-3.30725700	5.07583200	-0.54699200
C	3.04442500	1.99584500	-0.08628000
C	-0.88127900	-2.37375300	0.08552700
C	-2.78303600	0.79402600	-0.24182300
C	0.72455600	-1.96578000	-3.00203800
H	1.11133400	-1.16754600	-2.36470900
H	0.58574200	-1.57089000	-4.01049000
H	1.48127700	-2.75326900	-3.04549600
C	5.71566600	-0.50609100	0.13217600
H	6.72129700	-0.10074800	0.15562200
C	3.10250500	-1.58020300	0.07576400
H	2.09538500	-1.98706500	0.05705200
C	-4.12497900	2.57946900	-1.35176000
H	-4.13536000	3.32097300	-2.15690700
H	-4.92645000	1.86452700	-1.56323600

C	-0.73661500	-1.86950900	2.60966700
H	-1.40747300	-1.05297400	2.32944200
C	-0.59516900	-2.52799000	-2.46462200
H	-1.31863600	-1.70840200	-2.44163700
C	4.61306700	0.34405700	0.04650200
C	2.52717900	3.29117300	-0.14976900
H	1.45321800	3.45112900	-0.19106600
C	-3.86347700	-0.26108000	-0.55770400
H	-4.82684200	-0.06343700	-0.09092900
H	-4.02215900	-0.27574200	-1.64158100
C	5.31725600	2.86070000	-0.02608900
H	6.38882000	2.70122900	0.02320900
C	-1.36901700	-2.66443600	3.75137000
H	-2.29698400	-3.15714400	3.46104300
H	-1.58063400	-2.00235600	4.59318700
H	-0.67987000	-3.43305600	4.10821500
C	4.21112000	-2.40419600	0.16210000
H	4.06996700	-3.47862600	0.21045600
C	0.45322900	-4.12689600	-0.85473400
H	0.85265700	-4.64378600	-1.71934500
C	4.80121000	4.14413000	-0.09385100
H	5.46920500	4.99634800	-0.09880300
C	-1.10859700	-3.61872500	-3.40378400
H	-2.00115700	-4.11312000	-3.01779600
H	-0.34385900	-4.38319500	-3.55715300
H	-1.34221900	-3.19347400	-4.38163600
C	-4.34486000	2.24164400	1.11886200
H	-5.18198300	1.54576400	1.02525000
H	-4.46435600	2.74918300	2.08188800
C	-3.79641100	-2.05339100	1.25647000
H	-3.29631200	-2.97735000	1.55209600
H	-4.86874700	-2.24916000	1.20749500
H	-3.61881700	-1.29552500	2.01946800
C	-4.37659900	3.27284900	-0.01027900

H	-5.35629500	3.75826400	-0.03100500
C	5.51091700	-1.87546800	0.18892400
H	6.35876700	-2.54577100	0.25622600
C	-3.63938500	-2.71532600	-1.11783700
H	-3.34888600	-2.43607200	-2.12994300
H	-4.71815500	-2.88121500	-1.10766400
H	-3.14744600	-3.65292400	-0.85004900

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Au	0.38344100	0.65876400	-0.06985600
N	2.37580100	0.48175300	-0.02651100
C	4.64986100	0.81731000	0.00620300
C	-1.34465800	-2.28444500	1.29328400
N	-2.27132700	-0.47218500	-0.08744400
C	-3.76040300	-0.32040600	-0.12601100
C	-0.83653700	-3.58044600	1.36511800
H	-0.59614300	-3.99630100	2.33648000
C	4.41016800	3.57962500	-0.13014000
H	4.33705000	4.65943600	-0.18334800
C	-1.58756900	0.64263500	-0.11186300
C	2.99721600	-0.74879300	0.04465800
C	0.01639600	-1.23922900	3.09077400
H	0.65337500	-0.77130400	2.33747200
H	0.47541800	-2.19053900	3.37103800
H	-0.00384700	-0.59942700	3.97521000
C	-1.31927000	-2.46695100	-1.15167700
C	-0.59695400	-4.32510000	0.22226800
H	-0.20225900	-5.33018600	0.30138200
C	3.37528000	1.43057100	-0.05040900
C	-1.64457400	-1.77055500	0.02185400
C	0.06364900	-1.64816700	-3.04520300
H	0.65593800	-1.03623100	-2.36120500
H	0.05250600	-1.16482900	-4.02413000
H	0.56572900	-2.61344400	-3.14797200

C	5.21722200	-1.73363700	0.13956800
H	6.29684700	-1.63250500	0.15825900
C	2.40638600	-2.01460700	0.09103700
H	1.32502100	-2.12078900	0.07138800
C	-1.40643700	-1.46762800	2.56987100
H	-1.83444300	-0.48889500	2.33948500
C	-1.36662400	-1.84468600	-2.53308100
H	-1.82833000	-0.85668300	-2.45750800
C	4.40343800	-0.60302000	0.06831300
C	3.25402200	2.81963500	-0.11904900
H	2.27259400	3.28056300	-0.16268300
C	-3.90090000	1.18020300	-0.42041700
H	-4.70216500	1.61957100	0.17614800
H	-4.15988200	1.32415000	-1.47369800
C	5.80193900	1.60323900	-0.00609500
H	6.78200200	1.14089600	0.03716700
C	-2.24238000	-2.13119600	3.66331300
H	-3.26179000	-2.34672700	3.34229000
H	-2.28815200	-1.48455800	4.54165500
H	-1.78440500	-3.07213000	3.97623700
C	3.23346900	-3.12214100	0.16174600
H	2.79041300	-4.11161400	0.19865900
C	-0.80824200	-3.75665800	-1.02323100
H	-0.54628500	-4.30972100	-1.91751900
C	5.67790600	2.98066900	-0.07412700
H	6.56324600	3.60406400	-0.08453100
C	-2.16002800	-2.68808400	-3.52996000
H	-3.16696100	-2.91215000	-3.17500500
H	-1.65322400	-3.63719300	-3.71757400
H	-2.23717700	-2.16663700	-4.48588400
C	-4.36622100	-0.72704700	1.21038200
H	-4.14551300	-1.77506800	1.42137200
H	-5.44986100	-0.61176300	1.15639700
H	-3.99555900	-0.11459100	2.03293400

C	4.63011000	-2.98791600	0.18618200
H	5.25104500	-3.87338100	0.24166300
C	-4.37180000	-1.18101000	-1.22042900
H	-3.99578500	-0.90231300	-2.20461700
H	-5.45331600	-1.03481300	-1.21494600
H	-4.16918600	-2.24035600	-1.04744600
C	-2.52790600	1.81447700	-0.13746700
C	-2.44444200	2.49283200	1.24365000
C	-2.10700200	2.82239100	-1.21044100
C	-3.27795300	3.76773600	1.30213900
H	-1.39158400	2.73263600	1.43348900
H	-2.75431400	1.78829100	2.02275300
C	-2.97986400	4.06930500	-1.16461500
H	-1.06092300	3.09736100	-1.02951400
H	-2.14555000	2.34203400	-2.19355800
C	-2.86868200	4.73740800	0.20041400
H	-3.16595600	4.22979900	2.28504500
H	-4.34133000	3.52619400	1.19055400
H	-2.68623500	4.75914000	-1.95792800
H	-4.02624500	3.79685600	-1.35296200
H	-3.48070000	5.64069000	0.24073200
H	-1.82892900	5.04523900	0.36117400

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Au	0.38751000	0.69019300	-0.05596900
N	2.37799100	0.49662000	-0.02135900
C	4.65547500	0.80883800	0.00081400
C	-1.36723900	-2.24903700	1.28771700
N	-2.27683500	-0.42233300	-0.08206900
C	-3.76615600	-0.25657400	-0.12187900
C	-0.86945000	-3.54935600	1.35338900
H	-0.63330700	-3.97226500	2.32273700
C	4.44353000	3.57439300	-0.10985600
H	4.38113800	4.65530800	-0.15277200

C	-1.58261300	0.68650700	-0.09277300
C	2.98735100	-0.74090400	0.03593000
C	0.00018500	-1.22524100	3.09245500
H	0.64319700	-0.76168000	2.34152000
H	0.44903200	-2.18195200	3.37068800
H	-0.01505200	-0.58798000	3.97881700
C	-1.34087100	-2.41915600	-1.15832000
C	-0.63452500	-4.28982400	0.20679700
H	-0.24770500	-5.29833000	0.28110000
C	3.38710600	1.43561500	-0.04293200
C	-1.66169600	-1.72665300	0.01855400
C	0.05046900	-1.59958400	-3.04543600
H	0.64637500	-0.99531400	-2.35776700
H	0.04394600	-1.11135900	-4.02198000
H	0.54593100	-2.56781700	-3.15234800
C	5.19785800	-1.74865200	0.10863300
H	6.27852600	-1.65840900	0.12139600
C	2.38419600	-2.00110900	0.07583300
H	1.30174500	-2.09667600	0.06273900
C	-1.42389400	-1.43778400	2.56819800
H	-1.84245400	-0.45364400	2.34222000
C	-1.38180300	-1.78849900	-2.53604400
H	-1.83621300	-0.79756200	-2.45481400
C	4.39502600	-0.60943700	0.05217900
C	3.27962900	2.82633300	-0.09865700
H	2.30297400	3.29793000	-0.13202000
C	-3.88747200	1.24545800	-0.41535700
H	-4.69160500	1.70902000	0.15976400
H	-4.11313200	1.38575800	-1.47710000
C	5.81559000	1.58284800	-0.01149000
H	6.79102900	1.11004800	0.02196600
C	-2.26823900	-2.09907500	3.65650300
H	-3.28931500	-2.30184500	3.33252100
H	-2.30848300	-1.45746200	4.53879100

H	-1.82058000	-3.04668900	3.96411300
C	3.20054200	-3.11746500	0.13175600
H	2.74772600	-4.10270100	0.16337400
C	-0.84004600	-3.71343700	-1.03604500
H	-0.58129800	-4.26389000	-1.93286700
C	5.70532400	2.96198700	-0.06669800
H	6.59694500	3.57636100	-0.07676600
C	-2.18056800	-2.61993400	-3.53864000
H	-3.18951800	-2.83839800	-3.18592300
H	-1.68079000	-3.57174400	-3.73130000
H	-2.25280800	-2.09236400	-4.49158000
C	-4.38098700	-0.66966700	1.20847600
H	-4.17616700	-1.72375000	1.40548900
H	-5.46257500	-0.53801200	1.15283500
H	-4.00496700	-0.07633500	2.04187900
C	4.59854000	-2.99740100	0.14818300
H	5.21093000	-3.88943500	0.19212200
C	-4.38164100	-1.10687200	-1.22241500
H	-4.00016700	-0.82750500	-2.20423800
H	-5.46174700	-0.95066100	-1.21945200
H	-4.18941600	-2.16877600	-1.05341200
C	-2.51620800	1.86206800	-0.09941600
C	-2.46055300	2.50749100	1.29447700
C	-2.09016400	2.91207400	-1.12603600
C	-3.15710200	3.83619200	1.30928600
H	-1.41071600	2.61788100	1.59345300
H	-2.91585400	1.83887200	2.03315100
C	-3.10282800	4.04873000	-1.17031800
H	-1.10560700	3.29253700	-0.83501000
H	-1.97877200	2.44691800	-2.11000700
C	-3.46247900	4.51643500	0.20799700
H	-3.41981100	4.24187800	2.28040300
H	-2.70052500	4.88305000	-1.74984700
H	-4.01060000	3.73407200	-1.70039300

H	-3.98745700	5.46183800	0.29482800
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Au	0.37798500	0.62023700	-0.12339300
N	2.36543300	0.40676500	-0.06359500
C	4.64147900	0.72984700	-0.03103700
C	-1.31383000	-2.20254200	1.37826900
N	-2.25822700	-0.48903000	-0.11282400
C	-3.74975900	-0.37817000	-0.16462800
C	-0.81470400	-3.49534300	1.53099300
H	-0.57128700	-3.84881000	2.52598600
C	4.41827600	3.49318800	-0.17569100
H	4.35115600	4.57331000	-0.22963800
C	-1.60186400	0.64676300	-0.16644200
C	2.97973600	-0.82594400	0.02239700
C	0.06321800	-1.06275700	3.10536100
H	0.71001500	-0.66636700	2.32015200
H	0.50430400	-1.99781500	3.45944700
H	0.05383200	-0.35701400	3.93841700
C	-1.30747200	-2.54705700	-1.04942000
C	-0.58903500	-4.31595900	0.43853600
H	-0.20168300	-5.31683200	0.58166700
C	3.37032600	1.35014400	-0.09186300
C	-1.61761500	-1.77061100	0.07693400
C	0.06286700	-1.82579300	-2.98933100
H	0.63907300	-1.15241300	-2.35094700
H	0.04560300	-1.41736700	-4.00178500
H	0.58560200	-2.78537200	-3.01716400
C	5.19319000	-1.82326200	0.12906800
H	6.27346800	-1.72905100	0.14570000
C	2.38068200	-2.08612200	0.09066300
H	1.29898000	-2.18224200	0.07860100
C	-1.36384700	-1.30680200	2.60202700
H	-1.78488800	-0.33960100	2.31357800

C	-1.36473800	-2.01509400	-2.46728800
H	-1.84519300	-1.03328300	-2.45339200
C	4.38665200	-0.68835800	0.04387600
C	3.25767500	2.73977700	-0.16200500
H	2.27940200	3.20881000	-0.19963700
C	-3.90340900	1.06996100	-0.62157400
H	-4.79111400	1.52709200	-0.18431900
H	-4.01380100	1.09808400	-1.71103400
C	5.79801700	1.50889200	-0.04671800
H	6.77524900	1.04088500	-0.00070200
C	-2.19847900	-1.89321500	3.74009600
H	-3.22298400	-2.11718800	3.44273500
H	-2.22942500	-1.19339000	4.57736300
H	-1.74732800	-2.81797200	4.10656500
C	3.20020200	-3.19814300	0.17581900
H	2.75044800	-4.18383300	0.23036100
C	-0.80471500	-3.82921700	-0.84047000
H	-0.55350200	-4.44180200	-1.69828500
C	5.68231600	2.88688200	-0.12007500
H	6.57136400	3.50489600	-0.13285600
C	-2.14001200	-2.93486000	-3.40963900
H	-3.13509200	-3.17341700	-3.03114500
H	-1.60400700	-3.87529400	-3.55459500
H	-2.24408300	-2.46701400	-4.39039200
C	-4.33911500	-0.62712600	1.21703900
H	-4.10709100	-1.64111200	1.54655900
H	-5.42427000	-0.52630600	1.16479600
H	-3.96007800	0.08076300	1.95525000
C	4.59784700	-3.07288100	0.19388100
H	5.21312700	-3.96150100	0.26079400
C	-4.35875500	-1.36562000	-1.14585300
H	-4.00019000	-1.19457700	-2.16020600
H	-5.44213600	-1.23300200	-1.14167700
H	-4.14042300	-2.39653000	-0.85893300

C	-2.59544600	1.77385900	-0.23836100
C	-2.24426800	2.98231200	-1.12898700
C	-2.63758400	2.63465700	1.05902900
C	-3.45121800	3.88707100	-0.84847200
C	-1.03008300	3.61823500	-0.44271600
H	-2.09620700	2.74232900	-2.18287800
C	-3.67728800	3.70056600	0.67484600
C	-1.27101300	3.32667000	1.05890800
H	-2.86499900	2.09175900	1.97813000
H	-3.24279700	4.92157200	-1.12307200
H	-4.32708300	3.56727400	-1.41705200
H	-0.09545000	3.17154700	-0.78654500
H	-0.98341100	4.68682300	-0.66050400
H	-3.50110400	4.61783800	1.23863900
H	-4.69757000	3.38198500	0.89326200
H	-0.49063400	2.67655800	1.46015100
H	-1.29448200	4.23101000	1.66858200

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Au	0.47878700	0.29923400	0.06794800
N	2.47656300	0.21189700	0.17352500
C	4.73220600	0.63874200	0.29369500
C	-1.30479000	-2.89173700	0.89561700
N	-2.10472900	-0.93644300	-0.34069900
C	-3.57315700	-0.84476100	-0.60694500
C	-0.71887000	-4.15564900	0.88380600
H	-0.62023800	-4.69797700	1.81689900
C	4.40874800	3.36422400	-0.12166500
H	4.30342600	4.42877700	-0.29472000
C	-1.48140900	0.19158200	-0.12307200
C	3.13801900	-0.98513900	0.35977300
C	-0.37899200	-1.97603000	3.01220900
H	0.29222600	-1.32517500	2.44751200
H	0.15722000	-2.90374900	3.22877200

H	-0.61788800	-1.48833900	3.95966300
C	-0.83853400	-2.70219100	-1.50509100
C	-0.22974500	-4.70818200	-0.28883900
H	0.22094700	-5.69260100	-0.27950400
C	3.44112700	1.19374400	0.11701400
C	-1.41511700	-2.20885200	-0.32501200
C	-2.46749200	1.34421500	-0.14407600
C	0.80507700	-1.63042300	-3.03641800
H	1.29734700	-1.17343300	-2.17612000
H	0.92567400	-0.96805000	-3.89581900
H	1.31928100	-2.56903500	-3.25726600
C	5.38405700	-1.87195700	0.63705500
H	6.45637200	-1.72621200	0.70843200
C	2.59325800	-2.26959000	0.44546200
H	1.52029300	-2.42159000	0.36324100
C	-1.66262700	-2.26988700	2.23083500
H	-2.15556300	-1.31216700	2.05265800
C	-0.68304700	-1.88663000	-2.77447700
H	-1.16189800	-0.91405400	-2.62880600
C	4.53429900	-0.78180900	0.44880100
C	3.28054300	2.56301400	-0.10469900
H	2.29294600	2.97595400	-0.28580700
C	-3.81887900	0.67372800	-0.49686600
H	-4.57141500	0.88861500	0.25924000
H	-4.21013100	1.06132900	-1.43546200
C	5.85512500	1.46525800	0.27418200
H	6.84621400	1.04680700	0.41130500
C	-2.58860100	-3.15199600	3.06586500
H	-3.49298200	-3.43364300	2.52422100
H	-2.88037500	-2.62846300	3.97858800
H	-2.07954000	-4.07025900	3.36693400
C	3.45572900	-3.33646900	0.62758300
H	3.04920400	-4.34000100	0.69334000
C	-0.26561300	-3.97216300	-1.46167700

H	0.18756000	-4.37321000	-2.36058700
C	5.68936000	2.82525600	0.07237800
H	6.55216700	3.47926300	0.05380300
C	-1.29317700	-2.57298100	-3.99631500
H	-2.34862800	-2.81206400	-3.86475600
H	-0.76454600	-3.50471100	-4.21049200
H	-1.19121600	-1.93191500	-4.87416600
C	-4.36942000	-1.66953700	0.39665400
H	-4.09043800	-2.72333200	0.32781600
H	-5.42977800	-1.58211200	0.15459900
H	-4.22488200	-1.34288000	1.42464200
C	4.84230800	-3.14401700	0.72692500
H	5.49138100	-3.99878100	0.87103400
C	-3.89061800	-1.38806100	-1.99396300
H	-3.35263200	-0.85633700	-2.77803700
H	-4.96129600	-1.28041100	-2.17509800
H	-3.63867200	-2.44869200	-2.05485300
C	-1.94418800	2.30049800	-1.21304800
C	-2.18744600	2.04407100	-2.56414400
C	-1.10662700	3.36335400	-0.87637200
C	-1.64989200	2.84059300	-3.56248900
H	-2.80168600	1.19995600	-2.85248800
C	-0.57991400	4.16940400	-1.88506000
C	-0.84480100	3.91985300	-3.22061200
H	-1.85726800	2.61734300	-4.60114800
H	0.06010300	4.99914000	-1.60434200
H	-0.42030000	4.55364000	-3.98843100
C	-2.44376800	1.94895600	1.25989300
C	-3.19146800	1.37308500	2.28986100
C	-1.62193000	3.03232600	1.56509500
C	-3.15602700	1.86994000	3.58264500
H	-3.82166900	0.51766900	2.08678400
C	-1.60602700	3.54245500	2.86288900
C	-2.36308900	2.97347800	3.87173800

H	-3.74967900	1.40100500	4.35693900
H	-0.97180700	4.39616900	3.07545800
H	-2.33186000	3.38098300	4.87400700
C	-0.70726100	3.62898600	0.54270400
H	-0.61106800	4.70517300	0.70831900
H	0.29410600	3.20751100	0.70496800

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Au	0.44694800	0.19723900	0.00016300
N	2.40869300	-0.17218300	0.00021800
C	4.70098500	-0.01981800	-0.00016200
C	-1.66345900	-2.59074800	1.22571800
N	-2.35434000	-0.57645500	0.00009300
C	-3.80432700	-0.20937600	0.00013200
C	-1.31070700	-3.93849800	1.19721500
H	-1.11771400	-4.45024200	2.13276400
C	4.67672600	2.75729300	-0.00013300
H	4.68976500	3.84095100	-0.00012700
C	-1.50727600	0.41843500	0.00015700
C	2.92747300	-1.44951900	0.00010000
C	-0.18847800	-1.83884900	3.08115400
H	0.49769600	-1.39802800	2.35500700
H	0.15696800	-2.85302500	3.29682400
H	-0.13488900	-1.25841700	4.00449000
C	-1.66338400	-2.59030500	-1.22617300
C	-1.16436000	-4.61870600	-0.00056600
H	-0.89053300	-5.66617800	-0.00076000
C	3.47880200	0.69461300	0.00004800
C	-1.90556600	-1.95235700	-0.00012100
C	-0.18841000	-1.83790200	-3.08145600
H	0.49789200	-1.39756600	-2.35514200
H	-0.13483200	-1.25698100	-4.00448300
H	0.15687400	-2.85200900	-3.29772300
C	5.06127100	-2.61261100	-0.00029300

H	6.14575100	-2.60054600	-0.00046400
C	2.23514800	-2.66416100	0.00017200
H	1.14765400	-2.68075100	0.00033300
C	-1.62752500	-1.86513300	2.55632100
H	-1.93417700	-0.82877200	2.39722900
C	-1.62741700	-1.86425800	-2.55652500
H	-1.93398600	-0.82792200	-2.39709500
C	4.34163500	-1.41773700	-0.00013000
C	3.46406600	2.09111500	0.00006900
H	2.51850800	2.62707400	0.00021600
C	-3.74644800	1.33156100	0.00049500
H	-4.25009800	1.73229400	0.88142700
H	-4.25063400	1.73281900	-0.87988600
C	5.91100100	0.67398000	-0.00036300
H	6.85262200	0.13588100	-0.00052300
C	-2.54164300	-2.50032300	3.60271500
H	-3.57653200	-2.57241200	3.26622500
H	-2.51836600	-1.91565300	4.52449200
H	-2.19911200	-3.50799100	3.84840200
C	2.97097500	-3.83645400	-0.00000400
H	2.45109200	-4.78833600	0.00003600
C	-1.31060100	-3.93806200	-1.19810500
H	-1.11749400	-4.44947900	-2.13381100
C	5.89416000	2.05865900	-0.00034700
H	6.82565200	2.61092600	-0.00049200
C	-2.54162100	-2.49906100	-3.60310000
H	-3.57652300	-2.57106200	-3.26664700
H	-2.19924000	-3.50672900	-3.84899600
H	-2.51823100	-1.91418100	-4.52474100
C	-4.49290600	-0.76327000	1.23817100
H	-4.42240100	-1.85259600	1.26457500
H	-5.54843100	-0.48858900	1.20788900
H	-4.05965300	-0.35763900	2.15380900
C	4.37424900	-3.81607400	-0.00023300

H	4.92168000	-4.75044700	-0.00035000
C	-4.49280400	-0.76275000	-1.23818800
H	-4.05939900	-0.35683500	-2.15363000
H	-5.54829600	-0.48795300	-1.20791300
H	-4.42240300	-1.85207100	-1.26496400
C	-2.26210400	1.72868600	0.00025700
C	-1.73583000	2.52476300	-1.17546100
C	-1.73555300	2.52479400	1.17582900
C	-1.94385400	2.30173700	-2.52404200
C	-0.87464200	3.53431600	-0.73239700
C	-1.94320300	2.30171300	2.52445800
C	-0.87447000	3.53433500	0.73255700
C	-1.27680500	3.10804600	-3.44264800
H	-2.61228000	1.51515100	-2.86234900
C	-0.19866600	4.32814200	-1.64957100
C	-1.27587700	3.10798300	3.44290100
H	-2.61156400	1.51514600	2.86293300
C	-0.19819900	4.32810700	1.64956400
C	-0.40778400	4.10558300	-3.00607000
H	-1.42701000	2.95552300	-4.50366700
H	0.47975700	5.10516000	-1.31766800
C	-0.40694700	4.10550600	3.00611400
H	-1.42580000	2.95543300	4.50395700
H	0.48017700	5.10509200	1.31749200
H	0.11166500	4.71467200	-3.73473600
H	0.11274200	4.71453500	3.73465900
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Au	-0.46589600	-0.58525600	-0.37938500
N	-2.43838600	-0.64458500	-0.06342800
C	-4.66658800	-1.19226300	0.07311300
C	1.29469500	2.10733700	1.49964700
N	2.06342300	0.80999900	-0.44086600
C	3.52518000	0.84926300	-0.78035400

C	0.68451400	3.25782500	1.99659500
H	0.60708600	3.38874400	3.06947600
C	-4.26748200	-3.75483800	-0.91654300
H	-4.13162700	-4.75884300	-1.30070500
C	1.47138500	-0.33596500	-0.66002100
C	-3.12519700	0.44402600	0.43542600
C	0.47608500	0.39754500	3.10862800
H	-0.20882500	0.01256900	2.34877100
H	-0.07050000	1.13503000	3.70207700
H	0.76454600	-0.42428600	3.76882700
C	0.76744500	2.86800000	-0.77096200
C	0.14823400	4.21114200	1.14742100
H	-0.32204400	5.09802200	1.55306900
C	-3.37064900	-1.63622800	-0.28334200
C	1.37210600	1.95624200	0.10727300
C	2.48988500	-1.32529000	-1.19024000
C	-0.84302900	2.38705400	-2.60678900
H	-1.25378400	1.54377600	-2.04770600
H	-0.95323800	2.18478100	-3.67402800
H	-1.44152800	3.26876600	-2.36449500
C	-5.37746100	1.13970000	1.02498500
H	-6.43907600	0.93502400	1.10992300
C	-2.61424600	1.68877300	0.81244700
H	-1.55064500	1.89635700	0.73162800
C	1.71887600	1.03344400	2.47998800
H	2.25012500	0.25277500	1.93427400
C	0.62850600	2.63517000	-2.26224100
H	1.19077900	1.73591500	-2.53211500
C	-4.50672300	0.16348600	0.54078400
C	-3.16886600	-2.92467500	-0.78110200
H	-2.17159900	-3.25652000	-1.05068500
C	3.62020600	-0.39311600	-1.66410300
H	4.60965700	-0.84726200	-1.61729700
H	3.42185700	-0.10610100	-2.70204500

C	-5.75956000	-2.04627000	-0.07199800
H	-6.75558300	-1.71365700	0.19897700
C	2.63722100	1.56297200	3.57993200
H	3.50630900	2.08697700	3.17920400
H	2.98948000	0.73735300	4.20101400
H	2.10148800	2.25634100	4.23191300
C	-3.49690700	2.64255800	1.28891200
H	-3.11658000	3.61420700	1.58557700
C	0.17094100	4.00081700	-0.22170300
H	-0.30777100	4.71442900	-0.88181600
C	-5.55598400	-3.32366800	-0.56604700
H	-6.39462800	-3.99838100	-0.68421300
C	1.15311400	3.81440600	-3.08200200
H	2.16856700	4.09731300	-2.80066700
H	0.51429900	4.68917800	-2.94265400
H	1.14090100	3.56951300	-4.14568000
C	4.37162700	0.74646200	0.48228900
H	4.16660000	1.59055600	1.14336800
H	5.42552600	0.78360300	0.20199500
H	4.19130600	-0.18459800	1.02116400
C	-4.87019200	2.37472200	1.39613300
H	-5.53609700	3.14092300	1.77320700
C	3.88915100	2.12165700	-1.52500400
H	3.34031700	2.20640000	-2.46190300
H	4.95521500	2.09473900	-1.75656400
H	3.69442600	3.00723100	-0.91616200
C	2.94039000	-2.28292900	-0.08645300
C	4.06065000	-3.08376700	-0.31529000
C	2.26562400	-2.42237000	1.12517700
C	4.50916400	-3.97984700	0.64368300
H	4.58793400	-3.01043900	-1.26066800
C	2.71655700	-3.31726200	2.09068100
H	1.37150200	-1.84170600	1.32185700
C	3.84110700	-4.09489400	1.85768400

H	5.38080300	-4.58995400	0.44242700
H	2.17608900	-3.40680300	3.02489300
H	4.19058500	-4.79102900	2.60930300
C	1.88957000	-2.13015600	-2.34418200
H	1.07665400	-2.76116500	-1.98170100
H	1.49141300	-1.46056100	-3.11049900
H	2.65450100	-2.76630100	-2.79437500

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Au	-0.49768100	-0.52476000	-0.24455800
N	-2.31962100	-1.34331600	-0.13430200
C	-4.13855100	-2.74803400	-0.10961400
C	-0.28983400	2.75340100	1.51965100
N	1.30325800	1.72390400	-0.06878300
C	2.67553000	2.31177700	-0.18573200
C	-1.39349800	3.58068100	1.72457400
H	-1.74564400	3.74361900	2.73631100
C	-2.61746600	-4.99488700	-0.69924200
H	-2.04083900	-5.88317600	-0.92859200
C	1.23590800	0.44145900	-0.33313500
C	-3.44270400	-0.59625300	0.15051900
C	-0.64654600	0.99931300	3.24942900
H	-0.91898200	0.27948400	2.47290000
H	-1.56779100	1.46901700	3.60358200
H	-0.19559300	0.45778700	4.08419700
C	-0.54901600	3.08675600	-0.89288700
C	-2.06059900	4.16521800	0.66254900
H	-2.91897500	4.80037200	0.84137200
C	-2.73790400	-2.64615800	-0.29282400
C	0.13591400	2.53737000	0.20403900
C	2.55836600	-0.02625400	-0.94654300
C	-1.27781600	1.85974100	-2.94080800
H	-1.37645000	0.92788500	-2.37985500
H	-1.03229000	1.62041500	-3.97798800

H	-2.25020700	2.35891700	-2.92765700
C	-5.84107600	-0.84016300	0.45255400
H	-6.73415700	-1.45498600	0.47760200
C	-3.52545200	0.77760700	0.38980800
H	-2.63136700	1.39398600	0.36247000
C	0.32029100	2.05703600	2.71477500
H	1.22510400	1.54914300	2.38526200
C	-0.21118900	2.77723600	-2.33842500
H	0.74777700	2.25092500	-2.36930400
C	-4.59787100	-1.41121600	0.17932300
C	-1.97245000	-3.77578800	-0.58887600
H	-0.89959400	-3.68821400	-0.72689800
C	3.30710700	1.31979800	-1.15543200
H	4.37662000	1.24207100	-0.96780000
H	3.15695800	1.66889700	-2.18362200
C	-4.76701200	-3.98770800	-0.22567500
H	-5.83911200	-4.07429300	-0.08666000
C	0.71190400	3.03632000	3.81930400
H	1.36283600	3.83009900	3.44575900
H	1.23242000	2.51024400	4.62155600
H	-0.17091200	3.50792100	4.25583600
C	-4.76898400	1.32199400	0.65908100
H	-4.85168900	2.38715700	0.84760800
C	-1.64597800	3.90413100	-0.63371700
H	-2.19604000	4.32495600	-1.46690000
C	-4.00485800	-5.10573400	-0.51993900
H	-4.47893200	-6.07482500	-0.61317900
C	-0.09216600	4.04275300	-3.18951800
H	0.56663100	4.78724600	-2.73922400
H	-1.07062800	4.50701900	-3.32771900
H	0.28968200	3.79279500	-4.18098700
C	3.37336100	2.27371400	1.16925800
H	2.86784300	2.91804200	1.89078700
H	4.39593500	2.63538500	1.04960000

H	3.41581200	1.25389800	1.56010400
C	-5.92212300	0.52239700	0.69164600
H	-6.88155900	0.97707300	0.90497000
C	2.65540000	3.73485000	-0.70967700
H	2.19185300	3.79573400	-1.69304200
H	3.68524400	4.08522900	-0.79670400
H	2.12462400	4.40032600	-0.02584700
C	3.43486700	-1.06049200	-0.21408400
C	4.62860300	-1.47013200	-0.85513900
C	3.14386400	-1.62366500	1.04501400
C	5.45967900	-2.40884500	-0.25006400
C	4.01093600	-2.56470400	1.60247900
C	5.17021300	-2.98576900	0.97541700
H	6.37234000	-2.69342800	-0.76642200
H	3.76034000	-2.97488700	2.57598200
C	2.06263000	-0.62979700	-2.28281700
H	1.53632700	-1.56472800	-2.08656800
H	1.35686700	0.05208300	-2.76740300
H	2.87886000	-0.82049500	-2.97283900
C	5.12998300	-1.00046900	-2.20583700
H	6.21820500	-0.93246600	-2.17816200
H	4.87650000	-1.73109200	-2.97813800
H	4.74927200	-0.03958100	-2.53563600
C	6.06472200	-4.02443000	1.58714500
H	5.78801400	-5.02368400	1.24340900
H	7.10693100	-3.85982800	1.31193200
H	5.98923000	-4.01883900	2.67468900
C	1.93941500	-1.30498000	1.89071400
H	1.68274600	-0.24865500	1.89361900
H	1.05120800	-1.84314500	1.55228300
H	2.13230600	-1.59791600	2.92325800
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Au	-0.66576800	-0.50437500	-0.28882800

N	-2.31990300	-1.62539200	-0.21981300
C	-3.88006600	-3.31210000	-0.27076600
C	-1.00690200	2.66479300	1.62704600
N	0.72202900	2.01881900	-0.01682800
C	1.97464400	2.83529100	-0.10074900
C	-2.22741400	3.28948700	1.88135000
H	-2.59282800	3.32948400	2.90074800
C	-2.00300200	-5.25160000	-0.92177600
H	-1.28529900	-6.02276100	-1.17555100
C	0.86779900	0.75518500	-0.32669800
C	-3.55390800	-1.08593100	0.07572800
C	-1.08779800	0.78529700	3.25579600
H	-1.28533500	0.08386800	2.44082400
H	-2.05245500	1.10315800	3.65969300
H	-0.54588100	0.25986000	4.04613000
C	-1.33683500	3.10156000	-0.76118900
C	-2.98835900	3.82382000	0.85650500
H	-3.93619500	4.30008100	1.07326100
C	-2.51456900	-2.97257600	-0.43109600
C	-0.56219600	2.60843100	0.30150500
C	2.24873500	0.55335300	-0.96374600
C	-1.87240400	1.87053000	-2.86234900
H	-1.80649800	0.91149800	-2.34381900
H	-1.60244100	1.72267600	-3.91044600
H	-2.91469600	2.19748500	-2.82199700
C	-5.88056500	-1.73631700	0.33558700
H	-6.65861300	-2.49179700	0.32650700
C	-3.86706200	0.24535300	0.36171100
H	-3.08905500	1.00352800	0.36865400
C	-0.28378400	1.99426100	2.77265900
H	0.67369600	1.62967100	2.40379900
C	-0.96854900	2.92660700	-2.22159700
H	0.06524600	2.57211500	-2.28239200
C	-4.55746300	-2.08197500	0.05980000

C	-1.57027500	-3.94770900	-0.75795100
H	-0.52580200	-3.67842200	-0.87612800
C	2.76966400	2.00759500	-1.10517900
H	3.83789000	2.10390600	-0.92205300
H	2.56867400	2.36147200	-2.12136200
C	-4.29315500	-4.63339900	-0.44046500
H	-5.33696300	-4.90157800	-0.31905400
C	-0.02036300	2.95336700	3.93185900
H	0.50067100	3.85626100	3.60580500
H	0.58383900	2.46239400	4.69691300
H	-0.95641700	3.26279200	4.40186100
C	-5.18610800	0.56486800	0.63254500
H	-5.44651500	1.59385300	0.85692800
C	-2.54970600	3.71197500	-0.45358000
H	-3.16934700	4.08598300	-1.25978000
C	-3.35399700	-5.59758700	-0.76538900
H	-3.65989800	-6.62752000	-0.90034800
C	-1.07462900	4.23352600	-3.00872200
H	-0.54212900	5.05446500	-2.52533600
H	-2.11864100	4.53407000	-3.11686300
H	-0.67130000	4.09954600	-4.01400800
C	2.65949100	2.86250700	1.26052600
H	2.04328800	3.38047600	1.99719000
H	3.60661800	3.39700100	1.17154200
H	2.86233600	1.85052900	1.61925000
C	-6.18988000	-0.41605500	0.62115600
H	-7.21339200	-0.13564000	0.83681800
C	1.71584300	4.25426500	-0.56975000
H	1.25821400	4.27618700	-1.55738600
H	2.67137300	4.77827900	-0.62622000
H	1.07295300	4.79020300	0.13114500
C	3.26721100	-0.36281300	-0.27718000
C	4.51053300	-0.60943200	-0.89756600
C	3.10076800	-1.03568700	0.94340300

C	5.45478600	-1.49615200	-0.40596600
C	4.02810200	-1.93608500	1.45633900
C	5.19806600	-2.17732100	0.76871300
H	6.38269500	-1.64269000	-0.94027500
H	3.82576800	-2.43024500	2.39596000
C	1.85548300	-0.05948700	-2.33046700
H	1.50179700	-1.08119400	-2.18815600
H	1.03024800	0.51608000	-2.75936400
H	2.68152400	-0.05101400	-3.03456900
Cl	5.02201200	0.21824300	-2.33201500
Cl	1.75291300	-0.76966000	1.98394300
Cl	6.34806600	-3.29219800	1.38428800

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Au	-0.67063700	-0.44651100	-0.38020200
N	-2.52978700	-1.18380200	-0.44342600
C	-4.38692600	-2.53760500	-0.41201600
C	-0.56248700	2.74503800	1.45478800
N	1.18818900	1.70891700	0.05066900
C	2.58621100	2.23020000	0.14741600
C	-1.62466200	3.64379700	1.55112800
H	-2.10613800	3.78431500	2.51177600
C	-2.91206500	-4.84908500	-0.85061200
H	-2.35398400	-5.76160500	-1.02356300
C	1.10426600	0.43398900	-0.23951300
C	-3.64006700	-0.39492100	-0.22856400
C	-1.33941900	0.97064000	3.01120700
H	-1.55083500	0.29152400	2.18097500
H	-2.25600000	1.52767900	3.22136600
H	-1.09728500	0.37690500	3.89587600
C	-0.45553200	3.20921000	-0.94901500
C	-2.09374600	4.32499100	0.44186000
H	-2.92314500	5.01437300	0.53699900
C	-2.97884100	-2.48132700	-0.55457500

C	0.03534600	2.56974300	0.20116100
C	2.48182400	-0.09208300	-0.65306100
C	-0.97117300	2.06858200	-3.10339100
H	-1.17813300	1.13008100	-2.58428900
H	-0.61063500	1.84105700	-4.10908000
H	-1.91453300	2.61338400	-3.19441000
C	-6.05178300	-0.56228200	0.01347400
H	-6.96181600	-1.15169100	0.03859200
C	-3.69181900	0.99019700	-0.05332900
H	-2.78131900	1.58232000	-0.08638000
C	-0.19572500	1.93215300	2.67731000
H	0.69048400	1.34095700	2.44514800
C	0.05263800	2.91942800	-2.34811800
H	0.98030900	2.34362500	-2.27246400
C	-4.81754300	-1.17714900	-0.19864900
C	-2.23685100	-3.64339500	-0.77662500
H	-1.15918100	-3.59090600	-0.89486900
C	3.30223900	1.22457000	-0.74577100
H	4.33557900	1.10738400	-0.42394200
H	3.29849100	1.58780500	-1.78018300
C	-5.04579800	-3.76416000	-0.49103900
H	-6.12369100	-3.81577600	-0.38300500
C	0.12692400	2.80546900	3.88816200
H	0.88448800	3.55856300	3.66134300
H	0.49242100	2.18313700	4.70834700
H	-0.76504300	3.32676000	4.24260300
C	-4.92663700	1.57790400	0.15880300
H	-4.98534700	2.65225600	0.29745500
C	-1.52365300	4.08929800	-0.79962000
H	-1.92585800	4.58239900	-1.67648200
C	-4.30643900	-4.91470200	-0.70877000
H	-4.80436000	-5.87414400	-0.77265300
C	0.34070400	4.19493600	-3.14077100
H	0.97313200	4.89291200	-2.58931600

H	-0.58778100	4.71339600	-3.38824800
H	0.83305500	3.94752300	-4.08288200
C	3.06493100	2.11993300	1.58909900
H	2.46934000	2.75215800	2.24998700
H	4.10502800	2.44472900	1.64876500
H	3.00682100	1.08461300	1.93231200
C	-6.10167200	0.81083700	0.19308700
H	-7.05374500	1.29937400	0.35926000
C	2.71399900	3.66309000	-0.33160600
H	2.40519200	3.77130300	-1.37016800
H	3.76151700	3.95945200	-0.25565900
H	2.12179500	4.34061200	0.28674200
C	3.21005300	-1.17460300	0.17757300
C	4.45486200	-1.63545100	-0.33418800
C	2.72733000	-1.75902000	1.36903900
C	5.11287700	-2.68930700	0.29235000
C	3.42367800	-2.82470300	1.94678700
C	4.59854200	-3.30884400	1.41583900
H	6.05668600	-3.03184000	-0.11547300
H	3.01888400	-3.27884500	2.84322200
H	5.11630200	-4.13997700	1.87736100
C	2.14087200	-0.68754900	-2.04255100
H	1.51031900	-1.56736600	-1.90641800
H	1.57365900	0.03801900	-2.63465900
H	3.02365300	-0.97628000	-2.60448900
C	5.21717400	-1.05368900	-1.52510500
H	4.65706800	-0.24015700	-1.97681100
C	1.49787000	-1.33555700	2.15398400
H	1.06165600	-0.45147000	1.69393400
C	6.55563100	-0.46467600	-1.07340500
H	7.06537800	0.00797300	-1.91571500
H	6.42207000	0.28113200	-0.28642700
H	7.21253800	-1.24222500	-0.67906800
C	5.45097700	-2.09868400	-2.61770300

H	5.92665100	-1.63798000	-3.48606500
H	6.10883100	-2.89492900	-2.26471500
H	4.51665200	-2.56259400	-2.93892100
C	1.84781000	-0.96063500	3.59686200
H	2.17700600	-1.83264700	4.16501800
H	2.64247900	-0.21319900	3.64847500
H	0.96525800	-0.55869600	4.10021600
C	0.42391600	-2.42386900	2.14636500
H	-0.49699100	-2.05718400	2.60648400
H	0.18572300	-2.74571300	1.13073300
H	0.76184200	-3.29817000	2.70883100

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Au	-1.00809900	-0.39558500	-0.63068900
N	-2.64372600	-1.50128900	-0.34587100
C	-4.28465100	-3.11048600	-0.35019500
C	-0.68766000	2.48078300	1.72320000
N	0.45662200	2.08743900	-0.41908200
C	1.66293100	2.92260700	-0.73712800
C	-1.74502500	3.07014600	2.41474000
H	-1.78562100	2.97081500	3.49288100
C	-2.74475600	-4.91361500	-1.79334100
H	-2.15868800	-5.63117500	-2.35506900
C	0.49574400	0.85685100	-0.85986900
C	-3.73989900	-1.00785300	0.33466200
C	-0.42913500	0.35563800	2.98271600
H	-0.86914300	-0.20377100	2.15279200
H	-1.24064700	0.61995000	3.66557300
H	0.26508400	-0.29673900	3.51560200
C	-1.71601100	3.22276500	-0.37688200
C	-2.75543800	3.74204800	1.74809500
H	-3.56816200	4.19188700	2.30421700
C	-2.97318500	-2.77465200	-0.76173700
C	-0.66479300	2.61629800	0.32752800

C	1.80566300	0.63542300	-1.59103800
C	-3.01549000	2.28526500	-2.28177900
H	-2.89224400	1.27237900	-1.89277100
H	-3.10418900	2.23303300	-3.36871700
H	-3.95272200	2.68118300	-1.88298400
C	-5.98429700	-1.65225300	1.00424800
H	-6.79222600	-2.37502500	1.03271500
C	-3.88896800	0.24177700	0.94135700
H	-3.08057900	0.96787700	0.91751400
C	0.28787500	1.62024000	2.50004900
H	1.09533400	1.31695400	1.83141200
C	-1.84750800	3.19406600	-1.88698500
H	-0.93377300	2.76814000	-2.31363500
C	-4.78428000	-1.95942900	0.36329900
C	-2.19774100	-3.68005400	-1.48715100
H	-1.19230200	-3.41409600	-1.79657600
C	2.28230500	2.07747600	-1.85022900
H	3.36748500	2.17956900	-1.88107000
H	1.87937600	2.40684900	-2.81317100
C	-4.81587100	-4.35964500	-0.66971700
H	-5.81992600	-4.62514800	-0.35774400
C	0.90835400	2.34578600	3.69248500
H	1.37169900	3.29209200	3.40806700
H	1.66821500	1.71293700	4.15460000
H	0.15376100	2.55899300	4.45258200
C	-5.08897800	0.52553100	1.57042500
H	-5.22171600	1.49097800	2.04678000
C	-2.74905900	3.79240400	0.36355200
H	-3.57467800	4.25948000	-0.16003000
C	-4.04415600	-5.25584900	-1.38990100
H	-4.44248300	-6.22979100	-1.64516300
C	-2.06553400	4.58884400	-2.47457300
H	-1.31602500	5.30534800	-2.13513400
H	-3.04618400	4.97399900	-2.18745900

H	-2.04013300	4.54693400	-3.56498200
C	2.55978200	3.04599400	0.48844600
H	2.02259200	3.53869300	1.30091800
H	3.42531100	3.65882300	0.23239500
H	2.91579700	2.07540000	0.83663000
C	-6.13232400	-0.41185800	1.60426200
H	-7.05924500	-0.16146600	2.10494600
C	1.27275700	4.31067600	-1.21307400
H	0.66906400	4.26683200	-2.11834200
H	2.18324900	4.86852500	-1.43773800
H	0.72117600	4.85320000	-0.44250100
C	2.78820200	-0.14520000	-0.72422800
C	4.10047400	-0.28776500	-1.16998000
C	2.44362900	-0.72457300	0.49385900
C	5.04185000	-0.96871400	-0.41325700
H	4.40116000	0.13956500	-2.12127500
C	3.40013600	-1.38558200	1.25539100
H	1.42451200	-0.67086500	0.86280100
C	4.70677000	-1.51771300	0.81545300
H	5.44439600	-2.03577500	1.41197900
C	1.55053200	-0.12826100	-2.89232400
H	1.19893200	-1.13849100	-2.67809200
H	0.78697000	0.38237500	-3.48339600
H	2.46669100	-0.18979100	-3.48321000
C	6.43781800	-1.08662300	-0.96328600
C	2.99518100	-1.89614200	2.61212300
F	7.26458400	-1.70148100	-0.11869600
F	3.88323200	-2.75357000	3.11485000
F	1.80876800	-2.50378700	2.58120600
F	2.88838400	-0.87900500	3.48599600
F	6.45095200	-1.77107600	-2.11336700
F	6.95607500	0.12017800	-1.23016200

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Au	-0.51337300	0.39482600	0.02856500
N	-2.49215600	0.49115000	-0.22999500
C	-4.68061000	1.15595000	-0.45235400
C	1.03905700	-2.78302300	-0.91362900
N	1.91795300	-1.05248000	0.57494300
C	3.37096500	-1.09951200	0.92449600
C	0.36989400	-3.99555900	-1.06770200
H	0.27784100	-4.42116500	-2.06016900
C	-4.05700800	3.85092600	-0.21033200
H	-3.83416400	4.90708500	-0.11546400
C	1.42051000	0.13385000	0.33889900
C	-3.27409900	-0.63412900	-0.38782500
C	0.28532000	-1.62355000	-2.98558300
H	-0.41023600	-1.01977100	-2.39805000
H	-0.25599500	-2.50041600	-3.35022100
H	0.60879700	-1.03696500	-3.84867500
C	0.48300900	-2.83911900	1.47631100
C	-0.20659000	-4.64187500	0.01410200
H	-0.72125200	-5.58388700	-0.12753700
C	-3.34145000	1.57568500	-0.26609000
C	1.14146500	-2.25715600	0.38458500
C	2.54745500	1.16228000	0.36385000
C	-1.13388700	-1.76219900	3.02889900
H	-1.50178800	-1.12651700	2.22087600
H	-1.25049100	-1.22749900	3.97384300
H	-1.76503900	-2.65365200	3.06388000
C	-5.59452700	-1.28444800	-0.69917100
H	-6.64254100	-1.02812200	-0.80941900
C	-2.86788500	-1.97090300	-0.41675400
H	-1.81775800	-2.23041700	-0.31062200
C	1.50220600	-2.04889400	-2.15852200
H	2.02381500	-1.13544400	-1.86423700
C	0.33213300	-2.15507400	2.82057000
H	0.92216800	-1.23407800	2.80890100

C	-4.63688600	-0.28443100	-0.52980200
C	-3.02638900	2.93018500	-0.14110000
H	-1.99737900	3.24097300	0.01219700
C	3.65318600	0.39690900	1.11693300
H	4.66451700	0.67611500	0.82557300
H	3.54772400	0.63338100	2.17841200
C	-5.70287600	2.10240500	-0.51892800
H	-6.73152700	1.79009600	-0.66219400
C	2.44026600	-2.88685300	-3.02603400
H	3.29676700	-3.26622300	-2.46747200
H	2.81073200	-2.28394300	-3.85813300
H	1.91105700	-3.74320900	-3.45053500
C	-3.83591400	-2.94591300	-0.58358200
H	-3.53839600	-3.98876000	-0.60772800
C	-0.17403900	-4.04993000	1.26628900
H	-0.69432700	-4.51625500	2.09467100
C	-5.38719100	3.44537300	-0.39905100
H	-6.17018700	4.19173900	-0.44887100
C	0.79599100	-3.03097900	3.98323000
H	1.82267900	-3.37786900	3.86141400
H	0.15482000	-3.91036600	4.07623300
H	0.72688400	-2.47738900	4.92155700
C	4.16797400	-1.78137400	-0.18076000
H	3.86984600	-2.82976500	-0.25434500
H	5.22843600	-1.74807900	0.07654900
H	4.03049700	-1.31270400	-1.15206700
C	-5.19129400	-2.60999100	-0.72418900
H	-5.92538000	-3.39541200	-0.85441300
C	3.59610300	-1.87616200	2.21310000
H	3.06588400	-1.42664000	3.05277000
H	4.66373700	-1.87101600	2.44022800
H	3.27698900	-2.91447600	2.10100100
C	2.83727600	1.43748200	-1.11541200
C	4.06483500	1.18183600	-1.71826800

C	1.80766100	1.95537200	-1.90901300
C	4.24801000	1.38829000	-3.08322800
H	4.89978200	0.81324100	-1.13769500
C	1.98389900	2.15625400	-3.26882400
H	0.85883700	2.20550700	-1.44709900
C	3.20515500	1.86000600	-3.86594400
H	5.21229400	1.17906100	-3.52910800
H	1.16640400	2.54661700	-3.86131300
H	3.34529200	2.01210300	-4.92853100
C	2.13790800	2.42202100	1.11126800
C	1.36851100	2.30251300	2.26912500
C	2.55200600	3.68681900	0.70852900
C	1.00652000	3.42338200	3.00113900
H	1.03719600	1.31846500	2.59247600
C	2.19866000	4.81213100	1.44569300
H	3.14658200	3.79643300	-0.19076200
C	1.42206400	4.68473300	2.58879500
H	0.39450900	3.31392800	3.88722200
H	2.52663000	5.79082700	1.11871700
H	1.13726200	5.56255800	3.15460700

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Au	0.68104100	0.42370000	-0.09764000
N	2.54123800	1.07119000	0.26182100
C	4.38299900	2.32742600	0.82311300
C	0.36789900	-3.10260200	0.35703900
N	-1.11117800	-1.61461600	-0.93030100
C	-2.43619000	-2.17294500	-1.32526000
C	1.38427400	-4.05667200	0.36056300
H	1.63737000	-4.54394200	1.29469900
C	2.93259900	4.69077900	0.96612900
H	2.38460400	5.62401700	1.02128800
C	-1.10078900	-0.37185600	-0.50977600
C	3.63825100	0.23796800	0.31062200

C	0.82354100	-2.06127300	2.56983400
H	1.23235900	-1.16358300	2.10022800
H	1.65166500	-2.75051700	2.75420300
H	0.39215400	-1.77941800	3.53337100
C	0.82205300	-2.71495100	-2.01760900
C	2.09306300	-4.36749300	-0.78752800
H	2.87699200	-5.11378800	-0.75914700
C	2.98954400	2.33736200	0.56845900
C	0.05179300	-2.48563500	-0.86718600
C	-2.56562000	0.13863100	-0.37899300
C	1.93109000	-0.94587300	-3.35830000
H	2.03902800	-0.33250600	-2.46055600
H	1.84171600	-0.28550100	-4.22408700
H	2.84638700	-1.53331200	-3.46943400
C	6.02672100	0.29139800	0.75521700
H	6.92865300	0.83376700	1.01718700
C	3.68690600	-1.13755400	0.07283800
H	2.78353300	-1.67986700	-0.18872300
C	-0.24392300	-2.72604700	1.69417500
H	-1.04172800	-1.99658700	1.53741100
C	0.71321100	-1.87068400	-3.26873500
H	-0.16996700	-1.24199600	-3.17520600
C	4.80570300	0.95871000	0.65324300
C	2.26060100	3.52711500	0.63459100
H	1.19731200	3.53130400	0.41685500
C	-3.31245900	-0.91107000	-1.23838900
H	-4.31882300	-1.12843000	-0.90680800
H	-3.41066100	-0.49209800	-2.24124800
C	5.03853900	3.51288300	1.15443900
H	6.10511700	3.51316500	1.35107400
C	-0.82084000	-3.93001100	2.44012800
H	-1.51335700	-4.51057000	1.82925500
H	-1.35272700	-3.58768300	3.33172400
H	-0.02294300	-4.60006100	2.76904700

C	4.90864300	-1.77850000	0.17907800
H	4.96365300	-2.84653900	-0.00311300
C	1.83154800	-3.67332200	-1.95622900
H	2.43813500	-3.85146700	-2.83624300
C	4.31110800	4.68909400	1.22757600
H	4.80678900	5.61724000	1.48342800
C	0.59928800	-2.69468200	-4.54953400
H	-0.22460600	-3.40869400	-4.51485000
H	1.51945700	-3.25312300	-4.73419800
H	0.44572100	-2.03370100	-5.40479800
C	-2.78896800	-3.33093200	-0.39993400
H	-2.06151100	-4.13428000	-0.53695200
H	-3.77210600	-3.72330600	-0.66544700
H	-2.78555200	-3.04106100	0.64847800
C	6.07394500	-1.07290800	0.51775200
H	7.01586000	-1.60192300	0.59346100
C	-2.41505700	-2.72476300	-2.74546400
H	-2.15895400	-1.96547400	-3.48453300
H	-3.41204000	-3.10311400	-2.97960000
H	-1.71033000	-3.55444600	-2.82593200
C	-2.72888700	-0.00791900	1.16003200
C	-3.60355700	-0.91799300	1.80766000
C	-1.86139500	0.74860900	1.98811900
C	-3.37225400	-1.24160000	3.14575800
C	-1.67122600	0.37981300	3.31788600
C	-2.36196900	-0.66813700	3.90350600
H	-4.03615900	-1.95968100	3.61857700
H	-0.95874400	0.94743100	3.90880900
C	-2.80480900	1.56107100	-0.91695300
C	-2.11788800	2.01724500	-2.06155100
C	-3.71370500	2.44719400	-0.30303100
C	-2.24291500	3.34286600	-2.46953400
C	-3.80632200	3.76300000	-0.75255800
C	-3.05352900	4.25163600	-1.80854300

H	-1.68981400	3.66477200	-3.34691300
H	-4.50784900	4.42607800	-0.25489300
C	-1.25554100	1.14940000	-2.94099900
H	-0.22822800	1.07373800	-2.57566900
H	-1.64631200	0.13726500	-3.03193000
H	-1.21958300	1.57514300	-3.94426700
C	-3.12904400	5.69000900	-2.23016300
H	-4.09458700	6.12648700	-1.97330600
H	-2.35703600	6.27929500	-1.73027100
H	-2.97609300	5.79531000	-3.30461800
C	-4.65473000	2.08523200	0.81810400
H	-5.11341000	1.11159800	0.66807900
H	-4.16836700	2.06770600	1.79536700
H	-5.45597800	2.82334100	0.85822900
C	-2.07216300	-1.12456600	5.30221100
H	-2.97131500	-1.49961600	5.79224100
H	-1.33935300	-1.93727500	5.29671300
H	-1.65728900	-0.31661600	5.90495900
C	-1.22315000	2.06518700	1.60955100
H	-0.27277300	2.18863400	2.13169200
H	-1.05050900	2.21607000	0.54834200
H	-1.89161300	2.86993200	1.93835300
C	-4.90467700	-1.49031800	1.27220800
H	-5.47182700	-0.77087200	0.68410900
H	-4.79940900	-2.38990400	0.67047600
H	-5.52786200	-1.75363400	2.12660900

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Au	-1.03498800	0.04267300	-0.07737100
N	-2.87292200	0.36705800	-0.80410700
C	-4.81702100	1.35596600	-1.52625300
C	0.22519500	-3.41152500	0.03864600
N	0.86481000	-1.48291200	1.41139800
C	2.08810300	-1.60727200	2.25839100

C	-0.53511600	-4.56944300	-0.11363000
H	-0.37001700	-5.19239300	-0.98504800
C	-3.82941600	3.92952000	-1.16697400
H	-3.46570500	4.94023800	-1.02394600
C	0.70289300	-0.33457300	0.80047600
C	-3.77875100	-0.62682200	-1.10105600
C	0.32569500	-2.68507400	-2.33740800
H	-0.35503200	-1.85136800	-2.14159300
H	-0.27508700	-3.54485800	-2.64552200
H	0.98424300	-2.41158700	-3.16546200
C	-1.05654500	-2.89947300	2.06132300
C	-1.51013000	-4.92044000	0.80492700
H	-2.08461100	-5.82839300	0.67111200
C	-3.50013800	1.56663000	-1.04619300
C	-0.00488800	-2.61732100	1.17649000
C	1.98894200	0.50963500	0.97514700
C	-2.94183600	-1.44395900	2.76441200
H	-2.94977700	-0.90843400	1.81253200
H	-3.32641600	-0.78104400	3.54371500
H	-3.63231200	-2.28618100	2.67985400
C	-6.05168900	-0.92006800	-1.91160400
H	-6.99105300	-0.50952600	-2.26573900
C	-3.61043600	-2.01030800	-0.98647400
H	-2.67061400	-2.42317300	-0.62582900
C	1.15661400	-3.02522000	-1.09627600
H	1.71095800	-2.12660800	-0.81989500
C	-1.53723500	-1.93844400	3.13027700
H	-0.86334600	-1.07666000	3.14134500
C	-4.99863200	-0.07511400	-1.55941300
C	-3.00556600	2.86100600	-0.85553300
H	-2.00423300	3.01413600	-0.45907700
C	2.56410700	-0.15013100	2.24747600
H	3.63453600	-0.04248900	2.36508100
H	2.07103100	0.35526600	3.08120700

C	-5.62632200	2.44912100	-1.83382900
H	-6.63491600	2.29834800	-2.20312200
C	2.16184500	-4.12286900	-1.44282000
H	2.74445200	-4.43970700	-0.57605000
H	2.85079300	-3.75449500	-2.20844400
H	1.65773600	-5.00274800	-1.84966700
C	-4.67136700	-2.82666400	-1.33674200
H	-4.56292900	-3.90230300	-1.25325200
C	-1.78261100	-4.07268100	1.86445100
H	-2.59600900	-4.30508300	2.54176600
C	-5.12903600	3.73025800	-1.65711900
H	-5.74799600	4.58759400	-1.89057500
C	-1.58302000	-2.57046700	4.52153700
H	-0.63112300	-3.01127200	4.81669600
H	-2.34144200	-3.35620400	4.55653700
H	-1.85955400	-1.81925500	5.26445500
C	3.02915600	-2.65774500	1.67900700
H	2.57046300	-3.64552000	1.77451400
H	3.96141300	-2.65566600	2.24690700
H	3.25732900	-2.49021800	0.62923500
C	-5.88410600	-2.29048100	-1.79888900
H	-6.69412700	-2.95741700	-2.06699600
C	1.73099300	-2.04064600	3.67274300
H	1.04383500	-1.33754100	4.14396900
H	2.64755600	-2.07540700	4.26522800
H	1.28771000	-3.03855300	3.67397100
C	2.70474600	0.20515400	-0.36036100
C	3.93994700	-0.44325100	-0.49967300
C	2.07740000	0.56269700	-1.57762900
C	4.37064400	-0.97614300	-1.72029600
C	2.48835500	0.05306600	-2.80324200
C	3.60167200	-0.77271700	-2.85876600
H	5.29645500	-1.52578700	-1.77444800
H	1.96086500	0.27199300	-3.71947200

C	1.73284400	1.99174300	1.18473300
C	0.60321200	2.43976200	1.89134400
C	2.55290000	2.97468100	0.64150400
C	0.23252800	3.77549200	1.90651600
C	2.21566200	4.32931500	0.65220300
C	1.03430400	4.71803700	1.26479200
H	-0.65507600	4.12319100	2.41380300
H	2.89233000	5.04330300	0.20480200
O	0.60115000	5.99910700	1.32319900
O	3.73352700	2.58061000	0.09465800
O	-0.09627200	1.49472000	2.57078400
O	3.89416500	-1.30708700	-4.06691900
O	1.08282600	1.46761300	-1.50260600
O	4.73846100	-0.53077900	0.59185500
C	5.02350400	-2.14046600	-4.16918500
H	4.94436100	-2.99869100	-3.49406700
H	5.05867500	-2.49357400	-5.19613800
H	5.94379200	-1.59254200	-3.94506700
C	5.91530400	-1.29615100	0.53017800
H	6.34884000	-1.27505000	1.52757400
H	5.70261300	-2.33417700	0.25188600
H	6.63167600	-0.87242400	-0.17906600
C	4.09476100	3.12142500	-1.15861100
H	3.20613400	3.31309900	-1.76668500
H	4.66486200	4.04774400	-1.04684000
H	4.71526800	2.37644900	-1.65924900
C	1.37497200	6.98492700	0.68505400
H	1.47901600	6.77571000	-0.38391700
H	0.85105500	7.92777400	0.81756100
H	2.37081800	7.05973000	1.13256900
C	-1.41226900	1.81936100	2.97485000
H	-1.40765100	2.59584700	3.74372500
H	-2.00982400	2.14755700	2.11799500
H	-1.84567200	0.91305100	3.38627000

C	0.25865100	1.67811800	-2.63332600
H	-0.16760000	0.73322500	-2.98399100
H	-0.54912100	2.33060700	-2.31053000
H	0.81950000	2.15511300	-3.44216700

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Au	0.71088900	0.34163100	-0.01111400
N	2.58180700	0.90207900	0.39932900
C	4.49479200	2.08389900	0.87516000
C	0.09000700	-3.17826800	0.52188700
N	-1.20070800	-1.61365400	-0.85834800
C	-2.55918800	-2.04342300	-1.30611700
C	1.05102400	-4.18453000	0.59849300
H	1.22997400	-4.66550300	1.55299800
C	3.15472700	4.51193200	1.01521300
H	2.65004100	5.46896000	1.07480700
C	-1.07306000	-0.36822600	-0.48131100
C	3.63948200	0.01776400	0.44383200
C	0.47404000	-2.10391800	2.73798100
H	1.00498500	-1.28109500	2.25375000
H	1.21398800	-2.85071700	3.03638200
H	-0.00756000	-1.72382800	3.64247300
C	0.69081700	-2.85872400	-1.83497400
C	1.79931900	-4.55372800	-0.50745900
H	2.53930900	-5.33978300	-0.42499300
C	3.09714600	2.15335200	0.66255600
C	-0.12132500	-2.57285100	-0.72855100
C	-2.47523500	0.28908600	-0.47295300
C	1.98175700	-1.21471700	-3.17743400
H	2.10360300	-0.57121600	-2.30367000
H	1.97980800	-0.58848300	-4.07189200
H	2.84952500	-1.87775200	-3.22627700
C	6.03912200	-0.02938100	0.81971900
H	6.97277300	0.47662600	1.03968700

C	3.61524800	-1.36555200	0.25191100
H	2.67931300	-1.87397600	0.03815200
C	-0.57349900	-2.72723800	1.81022400
H	-1.30597900	-1.94953200	1.58163100
C	0.68779500	-2.03137600	-3.10396500
H	-0.14098000	-1.32477500	-3.05384600
C	4.84839500	0.69194200	0.73174800
C	2.42137900	3.37294500	0.73288200
H	1.34889700	3.41324500	0.56989000
C	-3.27101400	-0.68525600	-1.37222500
H	-4.32883900	-0.74523600	-1.14622900
H	-3.17335000	-0.31337800	-2.39324900
C	5.21328200	3.24546900	1.15766000
H	6.28441400	3.20214400	1.32173400
C	-1.28328300	-3.86680300	2.54096200
H	-1.98970500	-4.39746000	1.90171300
H	-1.82534400	-3.47268300	3.40413000
H	-0.55861300	-4.59411000	2.91404100
C	4.80859500	-2.06057500	0.34288100
H	4.80818800	-3.13539300	0.19616700
C	1.63835200	-3.87194200	-1.70214100
H	2.27984100	-4.10342300	-2.54423400
C	4.54088400	4.45410400	1.22634400
H	5.08524200	5.36433200	1.44482300
C	0.54732200	-2.88008700	-4.36642600
H	-0.33212400	-3.52485100	-4.34159700
H	1.42485500	-3.51614700	-4.50208700
H	0.47656800	-2.23445600	-5.24377300
C	-3.12851800	-3.06795800	-0.33267800
H	-2.54882400	-3.99123700	-0.40338400
H	-4.16219400	-3.28652100	-0.60190000
H	-3.10428900	-2.73239000	0.70041900
C	6.01519200	-1.40103600	0.62348900
H	6.93310700	-1.97184600	0.68910500

C	-2.51137600	-2.68844500	-2.68394400
H	-2.12305700	-2.00359500	-3.43785100
H	-3.52706900	-2.97239400	-2.96585800
H	-1.89900100	-3.59185500	-2.66706500
C	-2.82136900	0.27456000	1.02396500
C	-3.81848700	-0.47840600	1.64433600
C	-2.03940300	1.00963200	1.92800100
C	-3.92482800	-0.65254400	3.01419500
C	-2.09038600	0.88229400	3.30075000
C	-3.02607100	0.01076100	3.82321300
H	-4.71096200	-1.27002500	3.42389100
H	-1.43386900	1.46541000	3.92990300
C	-2.45908600	1.68112800	-1.08228000
C	-1.72633200	1.92854800	-2.24294700
C	-3.17000700	2.78056300	-0.60844200
C	-1.63298000	3.15481900	-2.86815400
C	-3.12528400	4.03664500	-1.18519300
C	-2.34049500	4.20150400	-2.30860800
H	-1.03394100	3.28141200	-3.75782500
H	-3.69063900	4.85481900	-0.76357800
F	-2.27763000	5.40164400	-2.88113300
F	-1.09111000	0.89756900	-2.81885400
F	-3.95889100	2.64177900	0.46161500
F	-4.77875300	-1.07003900	0.92141200
F	-1.22476800	1.94768700	1.44824100
F	-3.09781700	-0.15274100	5.14151500

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Au	0.93412300	0.44504800	0.00430300
N	2.67395500	1.25127400	0.57061600
C	4.32475000	2.61832300	1.40169400
C	1.09725900	-3.13133500	-0.28515600
N	-0.51497300	-1.60513800	-1.35091900
C	-1.73434900	-2.21389700	-1.96066100

C	2.23872600	-3.92335800	-0.39996700
H	2.51988400	-4.55558700	0.43379500
C	2.57119900	4.71206800	1.90004700
H	1.90306900	5.54221300	2.09654000
C	-0.67970800	-0.48512000	-0.68995200
C	3.87341700	0.57334300	0.50832700
C	1.31075500	-2.52686700	2.12160500
H	1.61060700	-1.50563700	1.87439100
H	2.21847900	-3.12767600	2.21717100
H	0.80892200	-2.52054100	3.09275800
C	1.59024500	-2.20762700	-2.49982100
C	3.03314800	-3.89316100	-1.53336600
H	3.91474600	-4.51833600	-1.59743000
C	2.94561800	2.49184400	1.10632900
C	0.75019500	-2.32214100	-1.38178200
C	-2.21364300	-0.20235200	-0.57588900
C	2.45401300	-0.05252200	-3.37946500
H	2.39974300	0.39119900	-2.38268100
H	2.31070600	0.73777300	-4.12037000
H	3.45966500	-0.46202300	-3.50680100
C	6.22831300	0.86027100	1.03451400
H	7.04574800	1.46107200	1.41793900
C	4.11066200	-0.71813800	0.03248400
H	3.29214900	-1.31866400	-0.35225500
C	0.38483300	-3.12220400	1.05521600
H	-0.49615900	-2.47986100	0.98630700
C	1.40497800	-1.15235100	-3.56836700
H	0.42367300	-0.70275000	-3.42788000
C	4.92932700	1.36824400	1.01049700
C	2.06462600	3.54710500	1.35108100
H	1.01297800	3.45029200	1.10172300
C	-2.74905800	-1.08742400	-1.72194100
H	-3.76607000	-1.43454800	-1.59227100
H	-2.73689900	-0.45164400	-2.61030900

C	4.81303000	3.80192800	1.95426500
H	5.86791100	3.90571400	2.18363000
C	-0.05890800	-4.51639600	1.49916900
H	-0.67000200	-5.02079900	0.74941700
H	-0.63331500	-4.44382300	2.42674600
H	0.80779900	-5.14880200	1.70401600
C	5.40714000	-1.20124000	0.06449200
H	5.60830700	-2.20225800	-0.30214600
C	2.72379900	-3.01512400	-2.55785300
H	3.38571700	-2.92746900	-3.41105100
C	3.93461500	4.84294100	2.20400100
H	4.29928500	5.76809700	2.63247900
C	1.49041700	-1.70737000	-4.98858600
H	0.80558400	-2.54048800	-5.15302500
H	2.50161400	-2.05534800	-5.20958500
H	1.25534500	-0.92173300	-5.70917900
C	-2.00570400	-3.56453500	-1.31002600
H	-1.20951000	-4.25912700	-1.58824300
H	-2.95350800	-3.96209900	-1.67284400
H	-2.04272700	-3.51094200	-0.22542800
C	6.46252500	-0.42109700	0.56183400
H	7.46663400	-0.82643400	0.57489500
C	-1.56545900	-2.45710300	-3.45496000
H	-1.38690500	-1.53241900	-4.00405800
H	-2.48637300	-2.90682900	-3.83116600
H	-0.74765400	-3.15483000	-3.64227100
C	-2.44176000	-0.68206100	0.88117800
C	-3.14908600	-1.82926200	1.29314800
C	-1.76927600	-0.03057500	1.93961800
C	-2.94164600	-2.43911400	2.52309600
C	-1.54474300	-0.61744700	3.17544300
C	-2.07551300	-1.86610100	3.43409000
H	-3.48117100	-3.34395200	2.76619500
H	-0.96529700	-0.08952600	3.91983100

C	-2.64280600	1.24421800	-0.82062600
C	-1.97256500	2.08982400	-1.71629100
C	-3.77345400	1.81784700	-0.22167000
C	-2.27825400	3.43288300	-1.87340000
C	-4.11260800	3.15484300	-0.36316800
C	-3.33605200	3.96964100	-1.16441700
H	-1.70317800	4.03881200	-2.55910400
H	-4.98165200	3.54458000	0.14755800
Cl	-0.75537500	1.49492400	-2.78369500
Cl	-3.72309100	5.63333800	-1.32746800
Cl	-4.87805500	0.88745800	0.71986700
Cl	-1.27112800	1.61509800	1.83599500
Cl	-1.73121600	-2.66545000	4.91172600
Cl	-4.47411700	-2.52029500	0.41924200

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Au	-1.02929500	0.39667700	-0.11513600
N	-2.38099900	1.11286600	-1.38775700
C	-3.46100100	2.05561900	-3.18286900
C	-2.07580100	-2.66692100	1.45240100
N	-0.21278100	-1.22614400	2.13269000
C	0.83525500	-1.79694200	3.03320200
C	-3.39721000	-3.06732500	1.63995200
H	-3.78631100	-3.88475700	1.04440300
C	-1.11382700	3.05491200	-4.28082100
H	-0.20838100	3.44881100	-4.72635700
C	0.20447800	-0.44560800	1.17350800
C	-3.72798000	0.83003500	-1.28084700
C	-1.92265100	-3.01392700	-1.01664700
H	-2.05966500	-1.94240500	-1.17700100
H	-2.90359100	-3.49025800	-1.08678800
H	-1.29841900	-3.40557500	-1.82379100
C	-2.44803700	-0.86849700	3.08508800
C	-4.22585700	-2.41853500	2.54155600

H	-5.24913000	-2.74780700	2.67037600
C	-2.21626100	1.84715900	-2.54414600
C	-1.60531100	-1.60495300	2.24196200
C	1.73321000	-0.42058900	1.17713200
C	-2.79240600	1.59293400	3.02022200
H	-2.61225500	1.59604000	1.94242800
H	-2.47591100	2.55516000	3.42797400
H	-3.86945700	1.49270300	3.17657500
C	-5.82692300	1.21712300	-2.43818600
H	-6.38950000	1.64490600	-3.26058600
C	-4.37727900	0.08847100	-0.29160100
H	-3.81452600	-0.34859000	0.52928900
C	-1.27468700	-3.31728900	0.33867900
H	-0.27128300	-2.88268900	0.32120300
C	-2.04505100	0.45030300	3.71460900
H	-0.97700500	0.60616800	3.54193100
C	-4.44574800	1.39323300	-2.36004500
C	-1.03560300	2.34674500	-3.09474400
H	-0.08365500	2.18033900	-2.59882900
C	2.07435500	-1.01944000	2.55712500
H	2.97772400	-1.62832700	2.56099000
H	2.24854400	-0.18982900	3.24537600
C	-3.51707400	2.77534000	-4.37594100
H	-4.46638100	2.94094400	-4.87315300
C	-1.14991300	-4.83160100	0.50698300
H	-0.74765000	-5.11643300	1.47941800
H	-0.49557000	-5.23903100	-0.26706700
H	-2.12654600	-5.30842000	0.39638400
C	-5.74818100	-0.07655600	-0.39167000
H	-6.27004400	-0.65066800	0.36628100
C	-3.76112500	-1.31075300	3.23241000
H	-4.43452700	-0.75570900	3.87480900
C	-2.34403100	3.27196700	-4.91921100
H	-2.37168700	3.83112100	-5.84595400

C	-2.30753100	0.49548900	5.21818600
H	-1.82293900	-0.32542700	5.74869500
H	-3.37879900	0.44026400	5.42261500
H	-1.94531800	1.43755100	5.63343400
C	0.91099400	-3.31011500	2.86985900
H	-0.01610800	-3.76362500	3.22679800
H	1.73145400	-3.69201700	3.48001300
H	1.06747900	-3.62410100	1.84030400
C	-6.47216500	0.48455200	-1.45418800
H	-7.54407500	0.33986100	-1.50486700
C	0.52321200	-1.49941100	4.49296600
H	0.49217300	-0.42801600	4.69212600
H	1.30598300	-1.94004300	5.11279000
H	-0.43053700	-1.94559000	4.78149200
C	2.08755100	-1.29033900	-0.02704200
C	2.64282500	-2.55618400	0.08033400
C	1.71369900	-0.84371700	-1.29862400
C	2.74883500	-3.38149500	-1.03641700
H	2.98658700	-2.93934000	1.03209100
C	1.81783900	-1.67084400	-2.40271400
H	1.31756500	0.15924000	-1.42428400
C	2.32164800	-2.96050200	-2.28283500
H	2.38885800	-3.61154100	-3.14327700
C	2.25178900	1.00047000	1.04934100
C	1.56425900	2.02726200	1.70179500
C	3.41686600	1.30524200	0.36610600
C	2.03773900	3.32402400	1.66106500
H	0.64557800	1.81008900	2.23776500
C	3.88816100	2.61663500	0.33252700
H	3.96962700	0.52863200	-0.15138500
C	3.20715500	3.63384000	0.97176400
H	3.57269500	4.65196300	0.93895400
C	1.29893600	4.43887700	2.35284900
C	5.16450100	2.88592200	-0.41894500

C	3.30555800	-4.76185200	-0.82272300
C	1.30448800	-1.15087700	-3.72203700
F	4.55100900	-4.71830600	-0.33521600
F	2.56889600	-5.43802200	0.07493700
F	3.33206000	-5.48015000	-1.94241500
F	1.64182800	-1.95129600	-4.73565200
F	1.78998900	0.06570500	-3.98350500
F	-0.02637800	-1.05298500	-3.70772100
F	2.09683300	5.08049700	3.21586700
F	0.24386500	3.99255900	3.03950700
F	0.85959500	5.34856800	1.48074600
F	5.49881500	4.17537300	-0.40130100
F	5.06260300	2.50866200	-1.69769200
F	6.18595300	2.19612400	0.10620600

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Au	-0.10132700	1.51343000	-0.44816000
N	-0.17677800	3.25427900	0.51612000
C	-0.26303800	5.47897100	1.08722000
C	-1.10834700	-1.47836900	1.52086600
N	0.10804100	-1.39599900	-0.62447500
C	0.19645600	-2.64484300	-1.46119900
C	-1.08203900	-1.47851700	2.91646200
H	-2.02414200	-1.52007400	3.44925500
C	-0.29674600	6.32863700	-1.55474300
H	-0.31026100	6.67947800	-2.57965900
C	-0.00243100	-0.27310800	-1.29662500
C	-0.17853900	3.35033200	1.89338800
C	1.32290900	-1.33383300	1.51500800
C	0.11200500	-1.39585800	3.61175700
C	-0.22708500	4.54402600	0.02654100
C	0.10516300	-1.40325100	0.81976200
C	-0.24205900	5.01404700	3.66225700
H	-0.28259600	6.04766100	3.98752800

C	-0.13564400	2.31759900	2.83175500
H	-0.09372000	1.28220000	2.50466200
C	-0.23145900	4.70170200	2.30309000
C	-0.24375200	4.96929100	-1.30234900
H	-0.21519500	4.24502800	-2.11008400
C	0.41604400	-2.03562900	-2.85257500
H	-0.11990200	-2.59426500	-3.62173900
H	1.48332900	-2.06859200	-3.09153100
C	-0.31639900	6.84467900	0.80993500
H	-0.34434000	7.56805100	1.61726700
C	-0.14701200	2.64981400	4.17528800
H	-0.11442300	1.86092800	4.91908600
C	1.30337400	-1.32769300	2.91043800
H	2.24517500	-1.24901400	3.43950500
C	-0.33315800	7.26373500	-0.50952400
H	-0.37438900	8.32060000	-0.74108700
C	-1.08952600	-3.45602200	-1.35180400
H	-1.20865200	-3.85629400	-0.34290800
H	-1.02667500	-4.29958000	-2.04058200
H	-1.97524400	-2.86951700	-1.60046200
C	-0.19993200	3.98807800	4.59273400
H	-0.20761800	4.21760900	5.65085400
C	1.36406800	-3.52466200	-1.04177500
H	2.32033800	-3.02084600	-1.18632600
H	1.35524400	-4.42234600	-1.66216000
H	1.27494500	-3.83725900	0.00171900
C	-0.03542200	-0.57017200	-2.77108000
C	-1.47564200	-0.35999700	-3.25244000
H	-1.80457500	0.65941500	-3.03910700
H	-1.51964400	-0.52153600	-4.33156200
H	-2.17155600	-1.05164900	-2.77500800
C	0.89179400	0.37234000	-3.53041100
H	0.90011100	0.10648800	-4.58975900
H	0.55170900	1.40530800	-3.43108900

H	1.91416700	0.31077300	-3.15287500
C	2.65273800	-1.33996900	0.85192500
C	3.56830700	-2.31512700	1.23610200
C	3.02810700	-0.42127900	-0.13019600
C	4.81241800	-2.40231900	0.62482900
H	3.29577400	-3.03651600	1.99906100
C	4.27381100	-0.51618700	-0.73011900
H	2.35753300	0.38489900	-0.40434100
C	5.17426400	-1.51259000	-0.37073100
H	6.14357600	-1.57780600	-0.84693900
C	-2.44114300	-1.60934100	0.87264200
C	-3.21331300	-2.72704800	1.17098900
C	-2.96460100	-0.64624300	0.00932500
C	-4.45679800	-2.90929200	0.57850500
H	-2.82827400	-3.48011900	1.85069200
C	-4.20985300	-0.83331100	-0.56790500
H	-2.40409800	0.25757900	-0.19852400
C	-4.96371800	-1.97102400	-0.30256200
H	-5.93308700	-2.10967800	-0.76359200
C	-5.21643500	-4.16725300	0.90196900
C	-4.77895000	0.18697000	-1.51942900
F	-6.42540900	-4.18615100	0.34317400
F	-4.55577000	-5.25112100	0.47063000
F	-5.37459600	-4.31442200	2.22191700
F	-4.85034400	-0.30935600	-2.76513700
F	-4.04416100	1.29533700	-1.57328900
F	-6.02174800	0.53389100	-1.17374200
C	5.73606400	-3.51140400	1.05144100
C	4.66829400	0.44423800	-1.82146600
F	5.23773700	-4.70884800	0.71371300
F	5.90037400	-3.52376300	2.37856600
F	6.94122200	-3.40756300	0.49328300
F	5.94426900	0.81863400	-1.70920700
F	3.91601600	1.54271300	-1.82387000

F	4.53824800	-0.13020600	-3.02986200
H	0.11330900	-1.37284600	4.69344800
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Au	-0.60256000	0.88291700	-0.60111600
N	-1.70008400	2.41159600	0.07438000
C	-3.34725600	3.98726200	0.37525900
C	-0.20013100	-1.56027200	1.95001400
N	1.01596000	-1.50739900	-0.20504300
C	1.73936700	-2.70266000	-0.77643500
C	-0.21757000	-1.33408700	3.32534300
H	-1.12121700	-1.57097500	3.87311200
C	-3.97270500	4.09004400	-2.32635200
H	-4.23296500	4.14285100	-3.37668500
C	0.44345000	-0.72359000	-1.08741600
C	-1.77942800	2.70686400	1.41980400
C	2.03138500	-0.59914500	1.85807600
C	0.87651600	-0.79252100	3.97921700
C	-2.65245100	3.18512500	-0.55921800
C	0.95322100	-1.23239400	1.21620600
C	-3.03266700	4.09515200	2.97045100
H	-3.80015400	4.83461900	3.17009400
C	-1.02530900	2.17374400	2.46885100
H	-0.23770600	1.45008700	2.26944400
C	-2.78362500	3.67213600	1.66598300
C	-2.96707200	3.23272400	-1.91762000
H	-2.43330200	2.60647400	-2.62504700
C	1.42113300	-2.57326700	-2.27552400
H	0.78256000	-3.39896500	-2.59353300
H	2.33986000	-2.62886300	-2.86239400
C	-4.35782700	4.84498200	-0.05883200
H	-4.89597800	5.46344400	0.65085500
C	-1.29551200	2.60350600	3.75785300
H	-0.71851400	2.20161100	4.58373100

C	1.98216400	-0.41134600	3.24077900
H	2.81679100	0.08374100	3.72234800
C	-4.66485600	4.89388000	-1.40770500
H	-5.44668000	5.55438600	-1.76092300
C	1.18492900	-3.99180600	-0.19651200
H	1.25396700	-4.00186400	0.89450000
H	1.77106500	-4.82839400	-0.57990200
H	0.14868200	-4.13776200	-0.50118800
C	-2.29130600	3.55709500	4.01139000
H	-2.47755600	3.87711100	5.02881700
C	3.23678200	-2.63741800	-0.51245600
H	3.68130900	-1.72409600	-0.91376900
H	3.70171600	-3.49081400	-1.00849500
H	3.45908400	-2.70891000	0.55368900
C	0.71869400	-1.22085700	-2.47791300
C	-0.59151200	-1.33125500	-3.26783100
C	1.66864400	-0.18529100	-3.11503400
H	1.23481100	0.81138800	-2.98603500
H	-0.36670500	-1.79911600	-4.23051800
C	-1.67488800	-2.11360200	-2.53788400
H	-1.34002600	-3.11749600	-2.25808000
H	-1.97285000	-1.59388700	-1.62380500
H	-2.56444800	-2.22659800	-3.15756400
H	-0.94790400	-0.31620500	-3.47732300
C	1.96332200	-0.43713100	-4.58599300
H	1.08093300	-0.26657100	-5.20319700
H	2.74599600	0.23872200	-4.93091300
H	2.30429500	-1.46037700	-4.76237800
H	2.60458500	-0.19665000	-2.54344200
H	0.84793100	-0.62623400	5.04789400
C	3.21337100	-0.04491300	1.14946300
C	4.49319400	-0.39207100	1.56664500
C	3.07288600	0.86506200	0.10013100
C	5.61085200	0.11315600	0.91428400

H	4.62199000	-1.08993700	2.38749400
C	4.19459100	1.36889600	-0.53758200
H	2.08430400	1.18912900	-0.20663100
C	5.47435300	0.98892600	-0.14831600
H	6.34463500	1.38496800	-0.65530300
C	-1.48850800	-1.99673500	1.33426900
C	-1.79375100	-3.31599100	1.04016300
C	-2.47133200	-1.02166800	1.13593800
C	-3.02089200	-3.64426300	0.46960800
H	-1.08994400	-4.10487800	1.26974800
C	-3.68592000	-1.35789400	0.56163500
H	-2.28456600	0.00268500	1.44123400
C	-3.96836500	-2.67180700	0.20633500
H	-4.91398800	-2.92811600	-0.25209900
C	6.96743000	-0.34276100	1.37942300
C	4.05972100	2.33497500	-1.68612800
C	-3.25732700	-5.08514300	0.11677600
C	-4.66364300	-0.26306200	0.22104300
F	-3.12754800	-5.88300500	1.18347600
F	-4.46530200	-5.29459500	-0.40172900
F	-5.92614200	-0.70591400	0.24913400
F	-4.57096500	0.76697300	1.05600400
F	-2.35389800	-5.50946500	-0.78533600
F	-4.43606400	0.19455800	-1.01700900
F	7.12662800	-1.65877600	1.18089000
F	7.12865100	-0.13033800	2.69022800
F	7.95699700	0.28107700	0.74210700
F	4.84732500	3.40097300	-1.51949200
F	2.81102400	2.76808400	-1.83999000
F	4.43131100	1.76067100	-2.84295400
103			
f-3-1			
Au	-0.56658900	-0.78730900	0.53667000
N	-1.59980900	-2.49483000	0.44396900

C	-3.22802000	-4.09744200	0.70256700
C	0.06715700	0.40033500	-2.65128700
N	1.16281100	1.23009300	-0.59665600
C	1.91490200	2.53241200	-0.50533500
C	0.12030100	-0.36531300	-3.81485100
H	-0.74576300	-0.37334100	-4.46504300
C	-4.11823400	-3.04498200	3.11087100
H	-4.48292100	-2.64643500	4.04995200
C	0.43274100	0.92558600	0.45819500
C	-1.55616300	-3.33888400	-0.64560200
C	2.26817700	-0.44177600	-2.04423300
C	1.23517500	-1.12716300	-4.12465900
C	-2.61727700	-2.95002600	1.25981100
C	1.17279800	0.39842100	-1.78084000
C	-2.67143200	-5.29467700	-1.55678700
H	-3.42348900	-6.07278300	-1.48842500
C	-0.70354500	-3.27845600	-1.75032200
H	0.06579900	-2.51225400	-1.80667900
C	-2.54186700	-4.34760800	-0.54230700
C	-3.06691400	-2.41595000	2.46805600
H	-2.60434000	-1.52417700	2.88112100
C	1.71941600	2.84667600	0.97379500
H	1.66525500	3.92143500	1.13620200
H	2.58336700	2.47007000	1.53505000
C	-4.28618600	-4.71590200	1.36773200
H	-4.76002700	-5.59588400	0.94719500
C	-0.85539100	-4.22533800	-2.74993400
H	-0.20093300	-4.19559900	-3.61445100
C	2.28865700	-1.17857700	-3.22974400
H	3.13257100	-1.83137900	-3.41743000
C	-4.72471500	-4.18889900	2.57044800
H	-5.54519600	-4.65725500	3.09930000
C	1.30911200	3.58732200	-1.42050800
H	1.33355400	3.25307200	-2.46086500

H	1.91136000	4.49402900	-1.34918700
H	0.28802700	3.83975500	-1.14108600
C	-1.83100000	-5.22815800	-2.65760700
H	-1.92396100	-5.95734000	-3.45255600
C	3.39137400	2.40506000	-0.85165400
H	3.91478900	1.72556600	-0.17973500
H	3.83910200	3.39435900	-0.74220700
H	3.54051100	2.08501700	-1.88543300
C	3.39537300	-0.62438800	-1.09847600
C	4.70486400	-0.54812100	-1.55846800
C	3.17490700	-0.86628500	0.25919900
C	5.77141000	-0.65194200	-0.67362400
H	4.89894200	-0.36029100	-2.60920000
C	4.24445200	-0.95370200	1.13304700
H	2.16388400	-0.99244900	0.62862700
C	5.55451900	-0.83674500	0.68052500
H	6.38496800	-0.90239400	1.37092800
C	-1.24504200	1.03258800	-2.32149800
C	-1.52816900	2.37902500	-2.47607100
C	-2.26490300	0.18068000	-1.87837200
C	-2.76935500	2.88630300	-2.09424200
H	-0.79703200	3.04813400	-2.90687600
C	-3.49411800	0.69401400	-1.50364900
H	-2.08831600	-0.88929200	-1.83342100
C	-3.75155800	2.05863800	-1.58389100
H	-4.70996600	2.45729600	-1.27848200
C	-2.98264000	4.36866100	-2.21094800
C	-4.54133000	-0.21995100	-0.92142600
F	-4.23554700	4.72929800	-1.94245100
F	-2.18418900	5.03610900	-1.35616700
F	-2.68116800	4.81706200	-3.43479400
F	-5.77268500	0.15390200	-1.29261400
F	-4.51056500	-0.18066100	0.41658500
F	-4.36701600	-1.48305100	-1.29514800

C	7.16445500	-0.52796600	-1.22968400
C	4.00120300	-1.11048500	2.61066900
F	7.33303600	0.64794800	-1.84955000
F	7.41120600	-1.47925600	-2.13738500
F	8.09721100	-0.62040700	-0.28281600
F	4.86301500	-1.96408100	3.16729000
F	2.76823100	-1.53621400	2.87867800
F	4.15996900	0.06677200	3.24102800
H	1.25944100	-1.71500900	-5.03264200
C	0.47735700	2.06877600	1.44645000
C	-0.85870000	2.86433900	1.32903900
C	0.63433900	1.65843000	2.92633300
H	-1.03766300	3.11967600	0.28000000
C	-0.77058500	4.13934800	2.17155600
C	-2.04668000	2.04497100	1.84790800
H	1.54955500	1.06181900	3.02136500
C	0.75868700	2.94070600	3.75914800
C	-0.55590000	0.86560500	3.46423600
H	-1.72097700	4.67602500	2.08189700
H	0.00488100	4.81628000	1.80451200
C	-0.52216000	3.77207800	3.63607100
H	-2.19819600	1.13921300	1.25281300
H	-2.95368400	2.65107200	1.73891100
C	-1.83887600	1.68115700	3.31772000
H	1.62692400	3.52989400	3.44860200
H	0.91800600	2.66585000	4.80642200
H	-0.64836700	-0.09796800	2.95558700
H	-0.37457500	0.64867500	4.52245400
H	-0.41901200	4.68599300	4.22741000
C	-1.71027600	2.95746700	4.14774700
H	-2.69091600	1.09109800	3.66708900
H	-1.56414500	2.70285400	5.20274300
H	-2.62746700	3.55125300	4.07286100

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Au	0.06205600	1.50488900	0.20707300
N	0.10194700	3.24363000	-0.76411400
C	0.15735700	5.46901600	-1.33618800
C	1.07532100	-1.47557800	-1.76398200
N	-0.10429300	-1.40564300	0.40194100
C	-0.15780400	-2.65128400	1.24286800
C	1.02336900	-1.48136600	-3.15887200
H	1.95601400	-1.50985100	-3.70890800
C	0.24708500	6.31789700	1.30489300
H	0.28214200	6.66860400	2.32937600
C	-0.00036400	-0.27897300	1.06898900
C	0.07071000	3.33982900	-2.14072600
C	-1.35776200	-1.36677700	-1.71480500
C	-0.18434500	-1.42115900	-3.83264000
C	0.15370000	4.53335300	-0.27539600
C	-0.12678900	-1.41687700	-1.04154500
C	0.07923000	5.00426500	-3.91018600
H	0.10377500	6.03820100	-4.23607200
C	0.01398800	2.30682500	-3.07813000
H	-0.01185200	1.27117800	-2.75019500
C	0.10326100	4.69173100	-2.55119900
C	0.19856000	4.95827800	1.05306100
H	0.19489300	4.23312100	1.86067800
C	-0.33486800	-2.04642000	2.64300100
H	0.25207100	-2.59522700	3.38096100
H	-1.38696000	-2.11616500	2.93747400
C	0.20674800	6.83497600	-1.05935400
H	0.21000100	7.55891200	-1.86667100
C	-0.00901900	2.63932300	-4.42140200
H	-0.05297900	1.85032300	-5.16448200
C	-1.36392200	-1.36765700	-3.11030700
H	-2.31623300	-1.30508500	-3.62247100
C	0.25152000	7.25366600	0.25959200

H	0.29014000	8.31073700	0.49071500
C	1.13159600	-3.45094000	1.09853100
H	1.23400500	-3.84263600	0.08443900
H	1.09104600	-4.29987600	1.78243000
H	2.01546000	-2.85589800	1.33532000
C	0.02330400	3.97806500	-4.83964100
H	0.00403900	4.20771000	-5.89759700
C	-1.33164900	-3.53986700	0.86139200
H	-2.28583400	-3.03903600	1.02931700
H	-1.30146200	-4.43339600	1.48709500
H	-1.27017600	-3.85851500	-0.18228900
C	-2.67467000	-1.38114100	-1.02622300
C	-3.58699700	-2.37037800	-1.37993000
C	-3.04100700	-0.45278100	-0.04953800
C	-4.81825200	-2.46201600	-0.74315000
H	-3.32187000	-3.09885800	-2.13877100
C	-4.27374400	-0.55155700	0.57522700
H	-2.37336700	0.36312400	0.20167700
C	-5.17033800	-1.56233800	0.24679500
H	-6.12981100	-1.63068100	0.74236400
C	2.42144500	-1.58514600	-1.13917600
C	3.20673400	-2.68924700	-1.45431700
C	2.94348500	-0.61806700	-0.27939400
C	4.46177100	-2.85460600	-0.88185600
H	2.82299800	-3.44569200	-2.13102500
C	4.19991800	-0.78870100	0.27911400
H	2.37241100	0.27608800	-0.05856300
C	4.96726700	-1.91306000	-0.00326300
H	5.94553500	-2.03900700	0.44219000
C	5.23680900	-4.09774500	-1.22530400
C	4.76348500	0.23427000	1.23126400
F	6.44940800	-4.10663700	-0.67390900
F	4.59407300	-5.19613500	-0.80387900
F	5.38933200	-4.22635000	-2.54791800

F	4.81539500	-0.25263800	2.48299400
F	4.03602000	1.34778800	1.26812900
F	6.01338300	0.56992900	0.90070700
C	-5.73764100	-3.58724400	-1.13491800
C	-4.66341400	0.42349700	1.65543100
F	-5.22604200	-4.77329900	-0.77708500
F	-5.91715200	-3.62992900	-2.45946900
F	-6.93718800	-3.48089700	-0.56507900
F	-5.93098900	0.82077400	1.52262000
F	-3.89150700	1.50794900	1.66098800
F	-4.56238500	-0.14493800	2.86929600
H	-0.20546200	-1.40326400	-4.91423100
C	0.06496000	-0.56623100	2.54076200
C	1.51255800	-0.29444400	2.99579900
C	-0.88200400	0.35792400	3.31222100
C	1.67344000	-0.43411900	4.50459900
H	1.77726000	0.72564500	2.69134900
H	2.19629700	-0.97108300	2.47487000
C	-0.73617600	0.16157300	4.81479500
H	-0.64010900	1.39580500	3.05195100
H	-1.91060000	0.17642600	2.98619600
C	0.69327900	0.46528800	5.24676500
H	2.70454700	-0.19743700	4.77513500
H	1.50277400	-1.47474500	4.80378800
H	-1.44608400	0.80127600	5.34159500
H	-0.98654000	-0.87369500	5.07923200
H	0.80638300	0.34343000	6.32569500
H	0.91962600	1.51256600	5.01534500
93			
f-5-1			
Au	0.09804100	1.53712400	0.24000200
N	0.15440300	3.29348700	-0.69702300
C	0.22521400	5.52909000	-1.22647700
C	1.06285600	-1.42783600	-1.77160300

N	-0.11971400	-1.37500500	0.39018500
C	-0.20206800	-2.62954400	1.21896600
C	1.01749500	-1.39972800	-3.16628400
H	1.95176400	-1.43407700	-3.71321100
C	0.32500700	6.32658800	1.43011300
H	0.36451300	6.65725000	2.46105200
C	0.01318700	-0.25849200	1.07005000
C	0.12177800	3.41643200	-2.07164000
C	-1.36816000	-1.27880700	-1.72906100
C	-0.18619800	-1.29937800	-3.84281200
C	0.21636700	4.57351600	-0.18377300
C	-0.14082400	-1.36322600	-1.05298500
C	0.13999700	5.11412900	-3.80885000
H	0.17172600	6.15385600	-4.11507600
C	0.05649600	2.40194900	-3.02834000
H	0.02415400	1.36056800	-2.71974700
C	0.16363300	4.77559700	-2.45611400
C	0.26640400	4.97239700	1.15245700
H	0.25922200	4.23221800	1.94616000
C	-0.39178200	-2.02828200	2.61839300
H	0.14351600	-2.59520400	3.38239500
H	-1.45839500	-2.04490500	2.86874900
C	0.28475800	6.88915400	-0.92375100
H	0.29206700	7.62833000	-1.71709800
C	0.03396700	2.76004100	-4.36504200
H	-0.01643000	1.98580000	-5.12308300
C	-1.36796000	-1.24408500	-3.12418100
H	-2.31666300	-1.15343900	-3.63884400
C	0.33442900	7.28212000	0.40289800
H	0.38098100	8.33427100	0.65413200
C	1.07324600	-3.45295600	1.07791000
H	1.16584600	-3.84943000	0.06455800
H	1.01654300	-4.29897100	1.76411300
H	1.97071100	-2.87768800	1.30916300

C	0.07529700	4.10625700	-4.75762700
H	0.05634700	4.35623800	-5.81096800
C	-1.38375500	-3.49856300	0.81535500
H	-2.33463400	-2.99179300	0.98340000
H	-1.36688900	-4.40155700	1.42779900
H	-1.31695600	-3.80292200	-0.23223700
C	-2.68591200	-1.30498100	-1.04327500
C	-3.60544500	-2.27224600	-1.43810000
C	-3.04166900	-0.42415200	-0.01993900
C	-4.83185400	-2.39127900	-0.79747700
H	-3.34740100	-2.96614200	-2.23104500
C	-4.26849100	-0.55347900	0.61210800
H	-2.36943300	0.37665600	0.26593800
C	-5.17152400	-1.54323300	0.24134400
H	-6.12496300	-1.63657300	0.74381400
C	2.40181800	-1.58403400	-1.14116600
C	3.15457100	-2.70721900	-1.46775400
C	2.94794000	-0.64499700	-0.26514100
C	4.40009400	-2.91964600	-0.89027900
H	2.75172600	-3.44143600	-2.15766400
C	4.19636600	-0.86137700	0.29612400
H	2.40342200	0.26391300	-0.03716500
C	4.92952000	-2.00577200	0.00321800
H	5.90147400	-2.16727200	0.45090400
C	5.13773600	-4.18230200	-1.24499600
C	4.78874600	0.13310500	1.26094100
F	6.34887400	-4.23284000	-0.69276900
F	4.46161200	-5.26450400	-0.83420200
F	5.28750300	-4.30290100	-2.56860000
F	4.78822900	-0.35404600	2.51376700
F	4.11665200	1.28155500	1.28116400
F	6.06046100	0.40614200	0.95840600
C	-5.76249800	-3.48441000	-1.24932700
C	-4.62797700	0.35339600	1.75943900

F	-5.20486800	-4.69103400	-1.07973000
F	-6.04737300	-3.37230700	-2.55131500
F	-6.91411700	-3.47649000	-0.57971700
F	-5.92401700	0.66971700	1.75215000
F	-3.92810100	1.48602900	1.74667300
F	-4.38350500	-0.25114500	2.93624600
H	-0.20233700	-1.25365400	-4.92367100
C	0.07826700	-0.57011200	2.53525700
C	1.53240400	-0.38006700	2.99613900
C	-0.80041400	0.38159800	3.34889900
C	1.64027300	-0.41506000	4.49184300
H	1.91124900	0.57374400	2.60694600
H	2.16832200	-1.15842300	2.56314800
C	-0.79632700	-0.02636700	4.81559100
H	-0.40058100	1.39508400	3.23745300
H	-1.81761700	0.38785000	2.94913600
C	0.59749700	-0.28136600	5.30637200
H	2.63324400	-0.56475000	4.90214800
H	-1.26340200	0.75595400	5.41809400
H	-1.41446700	-0.92026100	4.96636700
H	0.74810700	-0.34327400	6.37881800

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Au	-0.48277500	1.02065500	0.38919200
N	-1.54630600	2.64393500	-0.07852500
C	-3.25050300	4.18701800	-0.10004800
C	2.03912000	-0.36605900	-2.22021600
N	1.00836300	-1.41006200	-0.22774000
C	1.67917200	-2.67333500	0.25251000
C	1.97105400	-0.03761900	-3.57568300
H	2.81994400	0.46230400	-4.02639600
C	-3.62082200	4.05915200	2.64814100
H	-3.78209200	4.02229400	3.71882400
C	0.48530900	-0.66763700	0.72068200

C	-1.76719100	3.02900300	-1.38417300
C	-0.23468100	-1.21301500	-2.35304700
C	0.83205200	-0.28698800	-4.31971800
C	-2.44944300	3.33921600	0.69960500
C	0.94539500	-1.00867100	-1.61750900
C	-3.19651200	4.48761300	-2.69978200
H	-3.99514500	5.21762700	-2.76999800
C	-1.11075900	2.58985000	-2.53727100
H	-0.29422900	1.87439700	-2.46622700
C	-2.81067800	3.98092300	-1.45957800
C	-2.63630600	3.26928200	2.08086800
H	-2.01847000	2.61158000	2.68511900
C	1.22258200	-2.70886400	1.71969500
H	2.04001100	-3.02329200	2.36991400
H	0.41915400	-3.43781400	1.82611800
C	-4.23520800	4.97625300	0.49327800
H	-4.85415500	5.62969700	-0.11141100
C	-1.51652700	3.10128800	-3.75887400
H	-1.01762300	2.77413600	-4.66459900
C	-0.27200700	-0.84480300	-3.69688400
H	-1.19567300	-0.98901700	-4.24364800
C	-4.41505000	4.90980100	1.86456900
H	-5.17589700	5.51578500	2.34009200
C	3.19507500	-2.59132500	0.11581300
H	3.49525000	-2.59899300	-0.93322000
H	3.62358000	-3.47573500	0.58966200
H	3.61184000	-1.70540100	0.59749400
C	-2.55149000	4.04369400	-3.84381000
H	-2.84459200	4.42842300	-4.81246100
C	1.19070900	-3.89240100	-0.50945000
H	0.14922100	-4.10596900	-0.27442800
H	1.78543200	-4.75473100	-0.20402900
H	1.31114000	-3.76630400	-1.58884100
C	-1.51742000	-1.69999800	-1.76530600

C	-1.80109200	-3.04779600	-1.60153600
C	-2.51275200	-0.76381300	-1.46979200
C	-3.01307700	-3.45079400	-1.05074100
H	-1.08656200	-3.79546000	-1.91668200
C	-3.73098900	-1.17911700	-0.95323100
H	-2.33694400	0.29080600	-1.66147200
C	-3.98349200	-2.52373500	-0.71294000
H	-4.92388400	-2.83919300	-0.28123600
C	3.25995200	0.06332500	-1.49129700
C	4.51166600	-0.31922400	-1.95786300
C	3.18373500	0.90123000	-0.37672100
C	5.66580300	0.08036600	-1.29482500
H	4.58910300	-0.96205600	-2.82861400
C	4.34124700	1.30366400	0.26733400
H	2.21805100	1.24698600	-0.02428000
C	5.59309700	0.88783000	-0.17438000
H	6.49093200	1.20206900	0.34205100
C	6.98814800	-0.40687000	-1.82222800
C	4.28766700	2.21220000	1.46733500
F	8.01831800	0.07310400	-1.12730600
F	7.05992600	-1.74447900	-1.77904500
F	7.16027400	-0.05461500	-3.10138200
F	4.85290900	1.62477200	2.53362400
F	3.04273100	2.54162000	1.80345200
F	4.96525800	3.34348600	1.25013600
C	-3.23940900	-4.92264200	-0.84685200
C	-4.80648100	-0.15206200	-0.70073800
F	-2.19177900	-5.48977900	-0.22531900
F	-3.38459100	-5.56804700	-2.01010400
F	-4.32223100	-5.17185200	-0.11076900
F	-5.45461500	0.14498000	-1.83402600
F	-4.30649600	0.98205800	-0.21982500
F	-5.72077400	-0.60071400	0.16726000
H	0.78943000	-0.01077000	-5.36491300

C	0.70890400	-1.30425500	2.06200500
C	1.76684900	-0.45552600	2.79640400
C	-0.59820100	-1.25858800	2.87869200
C	2.00954400	-0.92616100	4.22771900
H	1.41662700	0.58489800	2.82069800
H	2.70940800	-0.45901800	2.23414900
C	-0.35719900	-1.77351400	4.29185100
H	-0.81770800	-0.18240400	2.96817000
C	0.69584900	-0.93230600	4.99818300
H	2.38713800	-1.95725000	4.20165800
H	-1.29704600	-1.75534600	4.85098300
H	-0.03403700	-2.82238600	4.25543300
H	0.86579800	-1.29338900	6.01607400
H	0.33682500	0.10208400	5.08060400
C	3.04803800	-0.04532900	4.90531600
H	4.01103700	-0.09633700	4.39565800
H	2.72108500	0.99845300	4.89557200
H	3.19395900	-0.34361700	5.94530800
C	-1.82865200	-1.88972200	2.18007600
H	-1.63558900	-1.90657600	1.09635900
C	-3.03771600	-0.99122600	2.43129700
H	-3.17139600	-0.84329100	3.50814800
H	-2.90771400	-0.00726400	1.96909300
H	-3.95680200	-1.43646300	2.04440100
C	-2.18080800	-3.31297600	2.61358800
H	-2.47034300	-3.33806900	3.66683400
H	-3.03872000	-3.66592700	2.03534100
H	-1.37486000	-4.03513200	2.47329500

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Au	1.06841900	0.06866800	1.10852700
N	2.84680900	0.08005800	0.19300700
C	5.07428700	0.13564200	-0.37340100
C	-1.61519300	-1.31212400	-1.07299100

N	-1.82881500	-0.03988300	1.06335700
C	-3.14755000	-0.04889500	1.80552400
C	-1.67566900	-1.31886800	-2.46675800
H	-1.63458200	-2.25955600	-2.99633400
C	5.91415300	0.20244200	2.27101600
H	6.26155300	0.22912500	3.29697900
C	-0.76184600	0.07850500	1.82044000
C	2.94701800	0.06477400	-1.18217100
C	-1.75538200	1.10621500	-1.11949500
C	-1.78931100	-0.14828800	-3.18684700
C	4.13397200	0.12522200	0.68423900
C	-1.72768900	-0.09299600	-0.37434700
C	4.61714300	0.08818700	-2.94887100
H	5.65243000	0.11214700	-3.27078700
C	1.91807300	0.03012900	-2.12761900
H	0.87990200	0.01161200	-1.80612000
C	4.30082000	0.09618100	-1.59071200
C	4.55542500	0.15826000	2.01456600
H	3.82728900	0.14913900	2.81892000
C	-2.69270800	0.50145300	3.15997200
H	-3.25241000	0.04630100	3.97896400
H	-2.86557000	1.58088900	3.18507500
C	6.43957000	0.17971000	-0.09158400
H	7.16629900	0.18820400	-0.89647100
C	2.25436800	0.02241200	-3.47021000
H	1.46682100	-0.00440800	-4.21607100
C	-1.80134300	1.05513000	-2.51162900
H	-1.85375300	1.97391100	-3.07779000
C	6.85398400	0.21314000	1.22894400
H	7.91037300	0.24792600	1.46402100
C	-3.71695800	-1.45867400	1.92704700
H	-3.94204900	-1.87732200	0.94702700
H	-4.65611100	-1.39123800	2.47839500
H	-3.05570100	-2.13480000	2.46099200

C	3.59462300	0.05046300	-3.88356100
H	3.82824300	0.04412600	-4.94079700
C	-4.19879400	0.81720200	1.13325000
H	-3.92054300	1.86763800	1.11358300
H	-5.12346500	0.73232500	1.70589800
H	-4.40722500	0.47317400	0.11798100
C	-1.40764500	-2.68593100	-0.45333100
C	-1.71701400	2.52276300	-0.55671600
C	-1.18183600	0.23394900	3.25568700
C	-0.81667800	-1.05526000	3.99939900
H	0.26477100	-1.20104100	3.97422500
H	-1.13527500	-0.97415700	5.04086100
H	-1.28160300	-1.93727700	3.55865000
C	-0.43752400	1.40647700	3.88997400
H	-0.80206200	1.56242900	4.90822800
H	0.63423000	1.20324700	3.92690400
H	-0.59244100	2.32396600	3.31871000
H	-1.84626000	-0.17185100	-4.26602400
C	-2.57032100	-3.67090600	-0.84151500
C	-0.03917500	-3.34132600	-0.84796800
C	-2.93590400	3.38232400	-1.06588500
C	-0.39312200	3.28217600	-0.91406500
F	0.94697800	-2.67734500	-0.28088300
F	0.17667000	-3.37744900	-2.15509500
F	-0.02910300	-4.59044500	-0.38632600
F	-2.28948100	-4.33288200	-1.96126800
F	-2.77142900	-4.54556600	0.12748400
F	-3.71276700	-3.01585700	-1.04916500
F	-2.63798700	4.02573500	-2.19257600
F	-4.00174900	2.62614900	-1.31570600
F	-3.27264800	4.27426600	-0.15014200
F	-0.10508200	3.25258800	-2.20665600
F	-0.52281400	4.55306200	-0.53837700
F	0.61438300	2.75327800	-0.24926900

F	-1.74973100	2.58138000	0.80379800
F	-1.35463500	-2.66218300	0.90357100
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Au	-0.60150400	-1.02500100	-0.02242300
N	-2.22325400	0.14473000	0.01301700
C	-4.40226900	0.87932700	0.05438500
C	2.53468600	0.35586800	1.20284200
N	2.23921700	-1.63937500	-0.16370000
C	3.35479300	-2.62770300	-0.22038700
C	2.70903700	1.72418100	1.31412700
H	2.73612300	2.16867100	2.30146400
C	-5.41706300	-1.64175200	0.61597200
H	-5.83177300	-2.61848400	0.83554300
C	1.02831700	-2.13275000	-0.11216900
C	-2.22992300	1.49947800	-0.24588400
C	2.60704700	0.55260100	-1.19278200
C	2.82420600	2.54048700	0.18444200
C	-3.53743700	-0.23180600	0.19276400
C	2.48529900	-0.22798100	-0.05670900
C	-3.78346800	3.35715800	-0.49362200
H	-4.79411500	3.75051900	-0.48864200
C	-1.14516600	2.34182500	-0.50520600
H	-0.13095900	1.94973000	-0.50404900
C	-3.55125100	2.00645400	-0.23600400
C	-4.04801500	-1.50071900	0.47509300
H	-3.37828700	-2.34844700	0.58065400
C	2.57846900	-3.92984500	-0.46388500
H	2.98818100	-4.75243800	0.12524500
H	2.65455600	-4.20469600	-1.51912500
C	-5.77946200	0.71465600	0.20090800
H	-6.44766700	1.56242400	0.09605900
C	-1.40155000	3.67701200	-0.76744800
H	-0.57546400	4.34520500	-0.98767500

C	2.77424500	1.92805000	-1.06660500
H	2.84026500	2.52316700	-1.96711000
C	-6.28175500	-0.54471400	0.48119400
H	-7.34858600	-0.68877500	0.59807200
C	4.11278800	-2.61434200	1.10170400
H	4.56751700	-1.63719000	1.27606400
H	4.90861500	-3.35995300	1.06941100
H	3.45341600	-2.84766100	1.93911500
C	-2.70841300	4.18767800	-0.76224300
H	-2.87292000	5.23736300	-0.97112600
C	4.29941700	-2.29079500	-1.36339800
H	3.75735300	-2.23049100	-2.30901000
H	5.05299300	-3.07559400	-1.44722500
H	4.81005200	-1.34221300	-1.18727100
C	2.99185200	4.04427800	0.36331100
C	1.10815000	-3.63795100	-0.11290800
C	0.72865200	-4.10862800	1.29544100
H	-0.29181500	-3.80140900	1.53217700
H	0.78809600	-5.19833600	1.34154600
H	1.39218400	-3.69320400	2.05635000
C	0.13357200	-4.23472500	-1.12222900
H	0.23353700	-5.32265400	-1.13454300
H	-0.89391000	-3.97975400	-0.85474700
H	0.32629200	-3.85671900	-2.12805500
C	4.35976300	4.31840600	0.99715700
H	4.48828900	5.39264100	1.15275100
H	4.45092200	3.82124200	1.96542000
H	5.16711100	3.96332300	0.35261500
C	1.89543100	4.58339500	1.28928600
H	1.98321300	4.18065000	2.29950300
H	1.97945500	5.67067300	1.35905100
H	0.90148000	4.33434600	0.91178200
C	2.90833300	4.79313300	-0.96342600
H	2.99888100	5.86496300	-0.77636700

H	3.71330300	4.50567600	-1.64381000
H	1.95122000	4.61634100	-1.46145600
H	2.40408500	-0.26464600	2.08179400
H	2.53573000	0.09165100	-2.17049400

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Au	2.20805600	0.49235300	0.04756400
N	2.68298000	-1.44509000	0.07607800
C	3.92000000	-3.38291700	0.00503900
C	-1.39342700	1.99188500	1.06711700
N	0.55632800	2.91114100	-0.09660000
C	0.45637600	4.39528200	-0.24371400
C	-2.51643900	1.18057300	1.06763000
H	-3.09487100	1.11194500	1.97555900
C	6.34375700	-2.04398300	0.18885800
H	7.29936300	-1.53826200	0.26057000
C	1.76624100	2.40974700	-0.03966200
C	1.81252600	-2.51222300	-0.02775300
C	-0.93516100	1.33531700	-1.19435800
C	-2.87990300	0.44458000	-0.06390000
C	3.95880100	-1.97244200	0.09504200
C	-0.61271400	2.08320800	-0.07448600
C	1.83405700	-4.94077300	-0.18826200
H	2.37491800	-5.87994500	-0.22688800
C	0.41656500	-2.49842600	-0.08333300
H	-0.12825600	-1.55886600	-0.03180100
C	2.52358400	-3.73416100	-0.07706600
C	5.17804800	-1.29820500	0.18750000
H	5.20141100	-0.21494400	0.25998800
C	1.92844400	4.76034900	-0.48593500
H	2.20884300	5.66373500	0.05853000
H	2.08234700	4.95083700	-1.55122900
C	5.10637900	-4.11561100	0.00832900
H	5.08302500	-5.19767200	-0.05986600

C	-0.24775800	-3.70808300	-0.19499700
H	-1.33014000	-3.71876500	-0.23747000
C	-2.05241800	0.51273100	-1.18590900
H	-2.24013000	-0.07734700	-2.06729300
C	6.31374600	-3.44364300	0.10009500
H	7.24351600	-3.99857000	0.10420800
C	-0.11469200	5.02848300	1.01926700
H	-1.15599100	4.73860800	1.16819500
H	-0.08295700	6.11408700	0.91590400
H	0.46214300	4.74980800	1.90239500
C	0.45095700	-4.92314800	-0.24906200
H	-0.09969000	-5.85143900	-0.33575300
C	-0.42865000	4.72693900	-1.43594900
H	-0.06753100	4.22662700	-2.33671100
H	-0.41102300	5.80425700	-1.60758300
H	-1.46282500	4.42580400	-1.25692800
C	-4.10863100	-0.47285400	0.01566000
C	2.76298600	3.54137600	-0.05704100
C	3.31660900	3.67340600	1.36627900
H	3.81820300	2.75023300	1.66249600
H	4.03905700	4.49188400	1.39829000
H	2.52744400	3.87894300	2.09195900
C	3.90958300	3.24992200	-1.01885100
H	4.58970800	4.10431400	-1.05140100
H	4.46835300	2.37036500	-0.69196400
H	3.54043100	3.06097100	-2.02867000
C	-5.41972300	0.33410900	0.26512800
C	-3.90312700	-1.47600900	1.19942100
C	-4.31689000	-1.30933300	-1.28005500
H	-1.10769500	2.52358600	1.96488300
H	-0.29065000	1.37387300	-2.06379700
F	-2.64028800	-1.87301600	1.25631900
F	-4.66540400	-2.55490800	1.09269700
F	-4.20144000	-0.88943000	2.36141100

F	-6.39895900	-0.45964900	0.68482400
F	-5.26384600	1.28642500	1.17927500
F	-5.81579900	0.92819500	-0.85623400
F	-5.46716200	-1.96893900	-1.26668400
F	-4.32883000	-0.55065000	-2.37416400
F	-3.32864200	-2.19346200	-1.40408200

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Au	-0.22353800	-0.84962700	-0.03635500
N	-2.14127100	-0.28767100	-0.02433600
C	-4.43895300	-0.20501800	0.00789800
C	2.06430900	1.66947800	1.22221300
N	2.62810700	-0.34838700	-0.05582400
C	4.04174200	-0.83697400	-0.04282300
C	1.75774800	3.02693400	1.23036000
H	1.55348700	3.50549200	2.18301800
C	-4.70333500	-2.96830000	-0.00372500
H	-4.82675500	-4.04483700	-0.00844400
C	1.70254400	-1.27324600	-0.04874800
C	-2.53075600	1.03601500	-0.01288500
C	2.12772500	1.75192500	-1.21628700
C	1.65151900	3.76916500	0.05991400
C	-3.29597600	-1.04033700	-0.01242000
C	2.29824500	1.05580800	-0.01461800
C	-4.53404200	2.41080300	0.02292000
H	-5.61401100	2.50877400	0.03909500
C	-1.71991600	2.17289700	-0.02092900
H	-0.63872600	2.07391700	-0.04026800
C	-3.93956300	1.14860000	0.00795600
C	-3.42878300	-2.43018300	-0.01830000
H	-2.54725100	-3.06292000	-0.03452100
C	3.83607100	-2.33960000	-0.28349600
H	4.49976600	-2.93690300	0.34458000
H	4.06355800	-2.57418300	-1.32668300

C	-5.71420900	-0.76935900	0.02250100
H	-6.59431800	-0.13582800	0.03812900
C	-2.33037800	3.41447400	-0.00543100
H	-1.71551100	4.30876000	-0.01220000
C	1.81800000	3.10716700	-1.15061600
H	1.66345800	3.64879200	-2.07861700
C	-5.84178300	-2.14813000	0.01667900
H	-6.82530800	-2.60104400	0.02770200
C	4.68863400	-0.52770200	1.30140300
H	4.71393100	0.55035000	1.47487500
H	5.71558600	-0.89602900	1.29342300
H	4.15693600	-1.00515500	2.12443000
C	-3.72858300	3.53808800	0.01667100
H	-4.17811200	4.52325900	0.02809400
C	4.85283900	-0.18093600	-1.14928700
H	4.44396400	-0.41934500	-2.13064300
H	5.87645700	-0.55649200	-1.10464100
H	4.88053200	0.90419900	-1.02655100
C	2.04964700	0.91796200	2.52520700
H	2.98933400	1.03230100	3.06958900
H	1.25281700	1.30948600	3.15712800
H	1.86430900	-0.14681600	2.38348800
C	2.18930700	1.08808800	-2.56412400
H	1.39368200	1.48072100	-3.19713000
H	3.13852700	1.28898000	-3.06549900
H	2.05851700	0.00802400	-2.49817100
C	1.32128700	5.23330200	0.10195300
H	2.23099800	5.83507500	0.16276700
H	0.78142500	5.53925500	-0.79450800
H	0.70865500	5.47141300	0.97192300
C	2.35149200	-2.63145600	-0.00318900
C	2.11366800	-3.19830900	1.40047600
H	1.04329100	-3.28992100	1.59434600
H	2.57154500	-4.18718800	1.47545600

H	2.54574900	-2.55923700	2.17378600
C	1.72910700	-3.56056300	-1.03921300
H	2.23713600	-4.52768100	-1.02477500
H	0.67029000	-3.71592700	-0.82245100
H	1.81204700	-3.13991800	-2.04393000
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Au	-0.23784700	-0.69846200	0.02063700
N	-2.21508900	-0.40572300	0.01253600
C	-4.50222700	-0.63795500	-0.02702100
C	1.73949900	2.23014600	1.15947900
N	2.51701600	0.19309100	0.02988500
C	3.98526200	-0.08923400	0.01467300
C	1.24522000	3.52871500	1.07054900
H	1.02637700	4.06296000	1.98986400
C	-4.38585200	-3.41142500	-0.04557700
H	-4.36078300	-4.49472800	-0.05295400
C	1.73150400	-0.85222600	0.02964500
C	-2.78188200	0.85213500	0.01293100
C	1.66729600	2.08931800	-1.27537900
C	0.97605800	4.13517600	-0.14984100
C	-3.25555000	-1.30916400	-0.01129800
C	1.99428400	1.53828100	-0.02926200
C	-4.95444800	1.94025500	-0.01555100
H	-6.03764500	1.88976200	-0.03418900
C	-2.13415900	2.08915800	0.03458000
H	-1.04958500	2.13878500	0.05558100
C	-4.19286900	0.77110500	-0.01147800
C	-3.19694100	-2.70420100	-0.02058100
H	-2.23713500	-3.21051200	-0.00794900
C	4.00894300	-1.62047100	0.15247600
H	4.39937600	-1.90093100	1.13270000
H	4.66964400	-2.06087200	-0.59703300
C	-5.68817100	-1.37141300	-0.05213800

H	-6.64668200	-0.86415200	-0.06429000
C	-2.90881900	3.23556600	0.02981700
H	-2.42214900	4.20544700	0.04842700
C	1.17366300	3.38954600	-1.30652000
H	0.89695200	3.81474000	-2.26619100
C	-5.62585500	-2.75463200	-0.06143200
H	-6.53811100	-3.33771400	-0.08081700
C	4.67557700	0.60462700	1.17834500
H	4.54625100	1.68803700	1.12456500
H	5.74346800	0.38411900	1.13654800
H	4.28767900	0.24525600	2.13224000
C	-4.31081500	3.16695000	0.00477300
H	-4.89084600	4.08145400	0.00218100
C	4.59228500	0.38812300	-1.29791100
H	4.15160900	-0.13321200	-2.14861800
H	5.66421400	0.18491700	-1.28686600
H	4.44810200	1.46334300	-1.42544400
C	1.89962300	1.61093700	2.52005900
H	2.81501700	1.95020700	3.00982500
H	1.06071500	1.90382000	3.15131300
H	1.92024700	0.52277000	2.47614300
C	1.75327600	1.32156200	-2.56598500
H	0.90474700	1.58372800	-3.19749700
H	2.66377900	1.56326400	-3.11842700
H	1.72532400	0.24353700	-2.40778800
C	0.44415300	5.53760500	-0.21837300
H	1.25653300	6.25507500	-0.35492400
H	-0.24356300	5.65432900	-1.05655400
H	-0.08183700	5.80280800	0.69897000
C	2.55814500	-2.10933800	-0.02043700
C	2.11724400	-3.08498200	1.07793900
C	2.32287000	-2.72129300	-1.41723200
H	1.24295000	-2.80461000	-1.57510900
H	2.82863000	-3.91580500	1.09610900

C	2.01546100	-2.44938700	2.45802900
H	2.92805100	-1.90501700	2.72139200
H	1.18085100	-1.74597900	2.49699100
H	1.85074500	-3.20323100	3.22754200
H	1.14371100	-3.50004300	0.79340000
C	2.98379200	-4.07847800	-1.61288600
H	2.51200500	-4.84164000	-0.99352800
H	2.89816200	-4.39804800	-2.65132900
H	4.04661800	-4.05199000	-1.35990900
H	2.69361300	-2.01298900	-2.16798900

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Au	-0.26612500	-0.35991200	-0.15960800
N	-2.12362100	-1.08913700	-0.10762100
C	-3.93438500	-2.49819900	0.04011300
C	-0.03917300	2.84188900	1.31796600
N	1.66359800	1.75045800	-0.07316200
C	3.12645200	-1.23411300	-1.29017600
H	2.90439600	-0.75953200	-2.25395200
C	2.53328700	-3.11936100	0.24375200
H	1.86921100	-3.97659500	0.38652200
C	3.05187900	2.28868600	-0.03228000
C	-1.12505900	3.70555100	1.40923700
H	-1.57891400	3.86525800	2.38239100
C	3.20613300	-0.88607300	1.17768700
H	3.03298700	-0.17635500	1.99502600
C	-2.35688400	-4.78194100	0.13259000
H	-1.75851200	-5.68450700	0.17196600
C	1.54797200	0.44703100	-0.16126500
C	-3.27079000	-0.32477200	-0.10748700
C	2.23944400	-2.46462000	-1.10431700
H	2.45470600	-3.17233300	-1.91239400
H	1.18103600	-2.20211100	-1.18157100
C	-0.05401700	3.16289900	-1.10148700

C	-1.67467600	4.32644900	0.29236300
C	2.29944000	-2.10859700	1.36666000
H	2.53952900	-2.56869600	2.33124000
H	1.24495700	-1.82027600	1.40042700
C	3.98924000	-3.58034400	0.26500100
H	4.21647800	-4.07198100	1.21702200
H	4.16253500	-4.30812600	-0.53484000
C	-2.52257500	-2.40488000	-0.01405300
C	0.51783000	2.61786800	0.05169800
C	2.93142800	-0.17658700	-0.18033500
C	-5.68741200	-0.55445300	-0.00432200
H	-6.57756800	-1.17038900	0.06230700
C	-3.37891700	1.06514200	-0.17851900
H	-2.48542600	1.67792300	-0.24598400
C	4.58892500	-1.69521300	-1.26228100
H	4.75083400	-2.40716900	-2.07784700
H	5.27019400	-0.85497000	-1.42942100
C	-4.42160500	-1.14125200	-0.01999900
C	-1.72869400	-3.55275800	0.03555600
H	-0.64549300	-3.47160600	0.00100500
C	3.84012800	1.04575200	-0.43768700
H	4.79582800	1.00430000	0.08203600
H	4.05394400	1.09531500	-1.51077000
C	-4.54566700	-3.74780100	0.13772100
H	-5.62640000	-3.82815900	0.17933300
C	-4.64377900	1.62572400	-0.16009100
H	-4.74822200	2.70427800	-0.21844500
C	-1.13693100	4.02604100	-0.95226000
H	-1.59701700	4.43905900	-1.84466700
C	-3.75540500	-4.88431200	0.18225800
H	-4.21613300	-5.86129900	0.25816400
C	4.65575400	-1.38155700	1.22024800
H	5.37083000	-0.55685300	1.17177900
H	4.81997100	-1.88409500	2.17925500

C	3.38453200	2.78233200	1.37100900
H	2.72151000	3.60251500	1.65465800
H	4.41008800	3.15481300	1.38121400
H	3.29792300	1.98655100	2.11062900
C	4.89979400	-2.36812300	0.07719200
H	5.94617400	-2.68566600	0.08930100
C	-5.79397400	0.82513300	-0.07409200
H	-6.77075500	1.29262700	-0.06309500
C	3.23473600	3.43445000	-1.01571100
H	3.04634400	3.11114500	-2.03866700
H	4.26609700	3.78586800	-0.95356700
H	2.57389000	4.27043700	-0.77643900
C	-2.84990400	5.25079000	0.43029900
H	-2.53210400	6.23709500	0.77568200
H	-3.36214500	5.37986800	-0.52312000
H	-3.56601700	4.86317600	1.15622400
C	0.39165000	2.79620800	-2.49010600
H	-0.48393600	2.59958000	-3.10933600
H	0.94997700	3.60973500	-2.95835600
H	1.01324100	1.90121300	-2.50185600
C	0.42925800	2.13482600	2.56063200
H	1.07019400	2.77367600	3.17191700
H	-0.43514000	1.85920600	3.16446200
H	0.97672300	1.21996700	2.33317400

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Au	-0.20218000	-0.58480100	-0.07523400
N	-2.19882000	-0.67152300	-0.04215800
C	-4.39743100	-1.34233400	0.01772300
C	1.15371300	2.50487600	1.23070500
N	2.33666900	0.80476700	-0.08554200
C	3.83033600	0.79746800	-0.07518000
C	0.42560100	3.69044400	1.26492900
H	0.07943200	4.05737800	2.22611000

C	-3.74729600	-4.04064600	-0.04151300
H	-3.51345600	-5.09848800	-0.06448800
C	1.75958000	-0.36966700	-0.09911100
C	-2.99743800	0.45262400	-0.00117400
C	1.18274900	2.65453800	-1.20530300
C	0.08344500	4.38298800	0.10940200
C	-3.04515000	-1.75913200	-0.03115400
C	1.57122800	2.02571300	-0.01718000
C	-5.33818700	1.09954300	0.08391200
H	-6.39087500	0.84040000	0.11412100
C	-2.60078200	1.79154100	0.00368800
H	-1.54654800	2.04966900	-0.02996200
C	-4.36577300	0.09997700	0.03771500
C	-2.71806500	-3.11623900	-0.06097400
H	-1.67874000	-3.42659600	-0.09877100
C	4.12461400	-0.68841600	-0.33121600
H	4.93938800	-1.03772600	0.30532700
H	4.43887400	-0.82678500	-1.36994500
C	-5.41876000	-2.29189000	0.03664100
H	-6.45687000	-1.98020600	0.07403400
C	-3.58165300	2.76628000	0.05050100
H	-3.29145200	3.81204700	0.05419300
C	0.45229600	3.83555000	-1.11362500
H	0.12948000	4.31766400	-2.03113200
C	-5.09030900	-3.63675300	0.00700700
H	-5.87240000	-4.38556100	0.02110900
C	4.34351500	1.27804800	1.27634700
H	4.01658100	2.30210300	1.46971100
H	5.43446400	1.26369700	1.26698000
H	3.99619400	0.63670800	2.08682700
C	-4.94349200	2.42759000	0.09074100
H	-5.68873100	3.21252000	0.12647000
C	4.38640500	1.69350100	-1.17069100
H	4.07524100	1.34801000	-2.15610400

H	5.47647400	1.66705100	-1.12713900
H	4.06310400	2.72816500	-1.03496500
C	1.38369100	1.76172400	2.51821600
H	2.23128900	2.16784300	3.07424900
H	0.50009100	1.85468900	3.14930600
H	1.56074300	0.69877000	2.35401600
C	1.45310300	2.07374700	-2.56573700
H	0.57467500	2.20722500	-3.19690500
H	2.29010100	2.57576800	-3.05578600
H	1.67177600	1.00680100	-2.52185400
C	-0.70153500	5.66105700	0.17943000
H	-0.03448600	6.52322600	0.25111100
H	-1.31709000	5.79222200	-0.71087000
H	-1.35257200	5.67304900	1.05399100
C	2.80764400	-1.44718600	-0.08451400
C	2.74714100	-2.12728600	1.29664200
C	2.51542700	-2.49381900	-1.16373500
C	3.69621300	-3.31672800	1.38638400
H	1.71675500	-2.46658200	1.45581600
H	2.96511100	-1.39493500	2.08137700
C	3.49963400	-3.65315300	-1.08588800
H	1.49482700	-2.86525500	-1.01157600
H	2.53784600	-2.01521400	-2.14830000
C	3.41263800	-4.32447900	0.27929200
H	3.60072800	-3.78418200	2.36843700
H	4.73442700	-2.97500400	1.30304100
H	3.29469300	-4.36982800	-1.88324300
H	4.52092100	-3.28443500	-1.24605600
H	4.10610600	-5.16544500	0.34228700
H	2.40254700	-4.72907800	0.41233300
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Au	-0.20917100	-0.61443800	-0.06090400
N	-2.20664500	-0.66242500	-0.03385000

C	-4.41916700	-1.28687000	0.01136800
C	1.22208200	2.45621800	1.22699500
N	2.35927200	0.72500300	-0.08589600
C	3.85419800	0.68334700	-0.08584300
C	0.51737800	3.65572900	1.26022400
H	0.18536500	4.03441000	2.22183000
C	-3.82567300	-3.99830600	-0.03340900
H	-3.61392700	-5.06087200	-0.05058800
C	1.75499900	-0.43607400	-0.08383600
C	-2.98190400	0.47855300	-0.00304300
C	1.23716600	2.59300300	-1.21004700
C	0.18083800	4.34906100	0.10335200
C	-3.07580400	-1.73225900	-0.02557900
C	1.62109800	1.96274900	-0.02148000
C	-5.30934800	1.17408300	0.06113800
H	-6.36734400	0.93677700	0.08404900
C	-2.55763700	1.80896300	0.00048700
H	-1.49805500	2.04544700	-0.02476500
C	-4.35747800	0.15455400	0.02636900
C	-2.77699200	-3.09594200	-0.04812700
H	-1.74435000	-3.42846100	-0.07646700
C	4.10741100	-0.80969500	-0.34194600
H	4.92867200	-1.19377900	0.26663200
H	4.37690000	-0.95277000	-1.39288000
C	-5.46051400	-2.21451300	0.02566000
H	-6.49205600	-1.88087000	0.05397600
C	-3.51851400	2.80398000	0.03555000
H	-3.20672400	3.84351400	0.03787100
C	0.53081100	3.78876700	-1.11930800
H	0.21118000	4.27264800	-2.03697900
C	-5.16019900	-3.56602900	0.00325300
H	-5.95795400	-4.29818500	0.01395100
C	4.39203800	1.16591300	1.25533400
H	4.09409100	2.20109100	1.43651700

H	5.48198800	1.12270900	1.23595900
H	4.03657000	0.54804400	2.07961500
C	-4.88730800	2.49371200	0.06599100
H	-5.61636100	3.29403900	0.09280500
C	4.41985300	1.56052800	-1.19206900
H	4.09072800	1.21774600	-2.17252600
H	5.50934200	1.50832400	-1.15910900
H	4.12269200	2.60327500	-1.05840700
C	1.44894900	1.71580600	2.51675000
H	2.31193500	2.10573200	3.06054800
H	0.57504800	1.83318600	3.15713500
H	1.59999900	0.64778100	2.35799100
C	1.48591100	1.99959300	-2.56904300
H	0.60642100	2.14869900	-3.19520600
H	2.33040200	2.48065500	-3.06716400
H	1.68163900	0.92842500	-2.52050100
C	-0.57891300	5.64232300	0.17263000
H	0.10477300	6.49079400	0.25055800
H	-1.18695100	5.78805700	-0.72051400
H	-1.23426200	5.66492400	1.04379100
C	2.78168800	-1.53166900	-0.05070000
C	2.74357400	-2.16492000	1.34917000
C	2.46697900	-2.62423000	-1.07345900
C	3.54568800	-3.43186100	1.39789200
H	1.69897500	-2.35857200	1.62335400
H	3.12359400	-1.45370700	2.09068300
C	3.56758400	-3.67693300	-1.07918300
H	1.50890700	-3.07907700	-0.80109000
H	2.34312000	-2.18110700	-2.06613200
C	3.93130400	-4.09769700	0.31311500
H	3.81699100	-3.80366500	2.38012800
H	3.24585600	-4.54765100	-1.65551600
H	4.45954600	-3.29800600	-1.59368200
H	4.52880700	-4.99630500	0.42450700

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j-6-1

Au	0.33831100	-0.39612800	-0.15938600
N	2.25175100	-0.96847000	-0.19084200
C	4.20382300	-2.17834300	-0.08982200
C	-0.36452000	3.06362300	-1.14554900
N	-1.80111400	1.53292700	0.12126200
C	-3.25059600	1.85464200	0.28520300
C	0.63039400	4.03651700	-1.15533500
H	0.96657200	4.42255600	-2.11257500
C	2.87931400	-4.61841900	-0.02383200
H	2.38093400	-5.58021700	0.00315800
C	-1.51629800	0.26687700	-0.04707400
C	3.31148500	-0.08571200	-0.18984300
C	-0.13557200	2.92638700	1.27891100
C	1.23923300	4.48518500	0.01075600
C	2.78951200	-2.23526200	-0.12605000
C	-0.77448700	2.54960600	0.09201700
C	5.74016700	-0.05881400	-0.11929100
H	6.69141200	-0.57782000	-0.07499600
C	3.27083500	1.30953800	-0.23554000
H	2.31752800	1.82826200	-0.28133300
C	4.54357700	-0.77642200	-0.13120300
C	2.12259100	-3.46185300	-0.09187100
H	1.03732600	-3.49555900	-0.12097600
C	-3.87266900	0.44785100	0.33876700
H	-4.77472600	0.39969400	-0.27385500
H	-4.16190800	0.22185300	1.36575800
C	4.94577300	-3.35725000	-0.02247200
H	6.02939800	-3.32280600	0.00512500
C	4.46942500	2.00058900	-0.22016600
H	4.45792900	3.08516000	-0.25582200
C	0.85484600	3.90199900	1.21140000
H	1.36985300	4.17929300	2.12582700

C	4.28133100	-4.57194500	0.01012100
H	4.84427300	-5.49547800	0.06256500
C	-3.74808000	2.68403900	-0.89070600
H	-3.19406600	3.62292500	-0.96168400
H	-4.80218600	2.92018500	-0.73735400
H	-3.64987600	2.14221300	-1.83156900
C	5.69900600	1.32529500	-0.16326700
H	6.62077000	1.89364100	-0.15409500
C	-3.47704200	2.62079300	1.57926600
H	-3.16455300	2.02665000	2.43920000
H	-4.54187100	2.83745100	1.68009800
H	-2.93169100	3.56750400	1.57878200
C	-0.89224900	2.56194700	-2.46150500
H	-1.71648900	3.17644300	-2.82900900
H	-0.09785400	2.59876300	-3.20627000
H	-1.23819400	1.53014900	-2.39741300
C	-0.40835100	2.27263800	2.60446000
H	0.52713800	2.16472800	3.15285200
H	-1.08464300	2.87181600	3.21779300
H	-0.84083300	1.27977300	2.48805200
C	2.31304500	5.53370100	-0.03121400
H	1.88291900	6.53435300	0.05306000
H	3.01720000	5.40559300	0.79125500
H	2.86672700	5.49012600	-0.96951500
C	-2.78851500	-0.53359400	-0.13745900
C	-2.94780300	-0.89882700	-1.62724900
C	-2.66656900	-1.83222000	0.67820000
C	-4.12935200	-1.82576600	-1.89240800
H	-2.02668800	-1.39757800	-1.95815800
H	-3.04646600	0.01508900	-2.22504200
C	-3.86572000	-2.74002000	0.43170600
H	-1.78939400	-2.33993800	0.24623400
C	-3.99189900	-3.08339600	-1.04518000
H	-5.05411400	-1.31556200	-1.59026700

H	-3.76075600	-3.65172300	1.02682700
H	-4.78405400	-2.24494000	0.77380200
H	-4.84451800	-3.74533000	-1.22012100
H	-3.09335700	-3.62413700	-1.37055600
C	-4.21571600	-2.15961300	-3.37395100
H	-5.06223700	-2.81710500	-3.58056500
H	-4.32623900	-1.25947900	-3.98212600
H	-3.30531500	-2.67265900	-3.69587200
C	-2.34780600	-1.60005800	2.17581300
C	-3.53332200	-1.75417800	3.12888000
H	-3.87302800	-2.79225100	3.15652500
H	-3.22599800	-1.48649600	4.14153400
H	-4.39292400	-1.13521200	2.86718300
C	-1.24132800	-2.55613900	2.61144600
H	-1.56248500	-3.59016300	2.44700700
H	-0.32511400	-2.39061300	2.03870900
H	-1.01073500	-2.44343400	3.67255600
H	-1.96749300	-0.57316500	2.27803700

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k-1-1

Au	-0.23949000	-0.81266100	-0.08092700
N	-2.15445900	-0.25105200	-0.06855900
C	-4.45166600	-0.20153500	0.02027400
C	2.05977900	1.61705100	1.21782700
N	2.63544700	-0.37343100	-0.08482600
C	4.03545300	-0.89475700	-0.03065500
C	1.73216700	2.95311900	1.33441200
H	1.49687100	3.38976100	2.29376800
C	-4.67618500	-2.96774900	0.05880900
H	-4.78395400	-4.04579100	0.07404400
C	1.67473600	-1.26933900	-0.08233000
C	-2.56289800	1.06678800	-0.06812800
C	2.26616200	1.81871800	-1.14038100
C	1.68725000	3.69838900	0.16870400

C	-3.29823100	-1.02055000	-0.01564900
C	2.34982900	1.01954200	-0.00581100
C	-4.58551300	2.41172600	0.00016600
H	-5.66605300	2.49306900	0.04293100
C	-1.77279500	2.21671700	-0.11542700
H	-0.69131200	2.13024700	-0.16768600
C	-3.97217400	1.15900500	-0.01261400
C	-3.41032900	-2.41181400	0.00385300
H	-2.52068700	-3.03294700	-0.02456300
C	3.78863300	-2.39170200	-0.26362900
H	4.42446300	-3.00218000	0.37993500
H	4.02443000	-2.64011100	-1.30139700
C	-5.71785600	-0.78319900	0.07571400
H	-6.60631500	-0.16199800	0.10341900
C	-2.40020400	3.44992100	-0.10015000
H	-1.80172100	4.35375500	-0.13555900
C	1.94401000	3.16089400	-1.08050000
H	1.87361900	3.75826100	-1.97756200
C	-5.82531600	-2.16355100	0.09468900
H	-6.80152800	-2.63005200	0.13736400
C	4.64243600	-0.58345900	1.33165600
H	4.69285300	0.49577000	1.49407200
H	5.65896700	-0.97754500	1.36784800
H	4.06425900	-1.02811000	2.14086400
C	-3.79859800	3.55128800	-0.04194700
H	-4.26278100	4.52946800	-0.03201700
C	4.87750000	-0.26471000	-1.12838100
H	4.44052900	-0.44499300	-2.11017600
H	5.87658500	-0.70237000	-1.10308000
H	4.97844400	0.81289500	-0.97778200
C	2.29161100	-2.63960500	-0.00324600
C	2.01400700	-3.15553000	1.41477000
H	0.93934600	-3.26043700	1.57317100
H	2.48681900	-4.13195200	1.54113400

H	2.40123200	-2.47726200	2.17735400
C	1.66415600	-3.58682700	-1.01926800
H	2.14249300	-4.56681100	-0.95484800
H	0.59725700	-3.70468100	-0.81902500
H	1.78097600	-3.20922200	-2.03659100
F	2.48549700	1.25670100	-2.32407700
F	1.36784400	4.98617300	0.25096600
F	2.08801200	0.85621700	2.30697600

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l-1-1

Au	-0.43711500	-0.96666600	-0.03528600
N	-2.30474200	-0.26405200	-0.02392400
C	-4.59318600	-0.04112000	0.00003100
C	2.06436700	1.35094000	1.18839600
N	2.45706600	-0.73063800	-0.06172700
C	3.82438300	-1.35062800	-0.05252200
C	1.86878900	2.72279900	1.23256900
H	1.72584700	3.21996300	2.18133200
C	-5.02720600	-2.78245400	-0.03636600
H	-5.21656900	-3.84920400	-0.05092900
C	1.43950100	-1.56018100	-0.04725300
C	-2.61184600	1.08075000	-0.00299800
C	2.11301200	1.41819600	-1.20396100
C	1.81979900	3.43309500	0.04399100
C	-3.50443000	-0.94482800	-0.02281400
C	2.24515500	0.68055000	-0.02463700
C	-4.52768400	2.57469400	0.03697800
H	-5.59974200	2.73767700	0.04996100
C	-1.73550800	2.16750800	0.00179700
H	-0.66250000	1.99921400	-0.01455400
C	-4.01110200	1.27920000	0.01343600
C	-3.72189400	-2.32354200	-0.04118300
H	-2.88134100	-3.00995500	-0.05940500
C	3.46159700	-2.82291600	-0.29328200

H	4.07508600	-3.48549800	0.31986500
H	3.64152300	-3.07256900	-1.34197400
C	-5.90084400	-0.52575400	0.00465100
H	-6.74027100	0.16061200	0.02210300
C	-2.26775200	3.44472500	0.02554200
H	-1.60126500	4.30056100	0.02956800
C	1.91712000	2.79016600	-1.17973000
H	1.81281300	3.33994000	-2.10418900
C	-6.11283000	-1.89395800	-0.01351000
H	-7.12240100	-2.28538500	-0.01042200
C	4.51244300	-1.11664000	1.28678700
H	4.63532100	-0.04879100	1.48149200
H	5.50439800	-1.56944200	1.24948500
H	3.95920400	-1.55939500	2.11283700
C	-3.65564200	3.65133200	0.04347600
H	-4.04442600	4.66174700	0.06180000
C	4.69484100	-0.77762500	-1.16028800
H	4.27030000	-0.97156300	-2.14312000
H	5.67748700	-1.24883600	-1.10715700
H	4.83244600	0.29975200	-1.03818800
C	1.96114000	-2.96935700	0.01594900
C	1.69181700	-3.46649200	1.44194100
H	0.61781600	-3.49131900	1.63441800
H	2.09441500	-4.47551800	1.55448000
H	2.15214400	-2.81889700	2.19068000
C	1.23988400	-3.86675300	-0.98270600
H	1.65638700	-4.87583800	-0.94172700
H	0.17490300	-3.91753900	-0.74716000
H	1.34623500	-3.48708300	-2.00076200
Cl	1.57455600	5.13012400	0.08645100
Cl	1.98143200	0.47468800	2.65930300
Cl	2.09427500	0.62263400	-2.72146100

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m-1-1

Au	-1.00023600	-1.08602200	0.02324300
N	-2.61186000	0.08695500	0.04059700
C	-4.74840000	0.93605700	0.01831700
C	2.05653500	0.59905900	1.19419800
N	1.85383100	-1.55536700	-0.00325600
C	3.04229400	-2.47370500	-0.05223100
C	2.24614700	1.97638800	1.16117700
H	2.29584600	2.52867800	2.09063900
C	-5.92563300	-1.57702500	-0.02577500
H	-6.40352200	-2.54923500	-0.04329800
C	0.67158400	-2.12568400	-0.01505400
C	-2.53441400	1.46469700	0.05507400
C	1.98718200	0.56815600	-1.21112500
C	2.33000500	2.64375000	-0.04621300
C	-3.95374400	-0.23451500	0.01701500
C	1.97870800	-0.12977700	0.00208200
C	-3.95914400	3.43164700	0.05265700
H	-4.94345900	3.88650400	0.04296500
C	-1.39147900	2.26558500	0.07756500
H	-0.40864600	1.80382100	0.08797200
C	-3.82318700	2.04355200	0.04247200
C	-4.54437300	-1.49871500	-0.00521000
H	-3.92749000	-2.39153600	-0.00601500
C	2.34407000	-3.79038700	-0.41818100
H	2.79500900	-4.63543900	0.10484900
H	2.44617600	-3.96200400	-1.49315300
C	-6.13903300	0.83378800	-0.00234900
H	-6.75503000	1.72620500	-0.00123100
C	-1.54689800	3.64062900	0.08696900
H	-0.67030600	4.27982000	0.10514800
C	2.17098300	1.94513500	-1.22882900
H	2.16448900	2.47113700	-2.17521800
C	-6.72189700	-0.42192500	-0.02422400
H	-7.80027200	-0.51776600	-0.04037300

C	3.74007400	-2.51902200	1.30158900
H	4.12478800	-1.53441700	1.57511100
H	4.59123000	-3.19752000	1.22927000
H	3.08376100	-2.87206700	2.09390400
C	-2.82263700	4.22422500	0.07464800
H	-2.91580100	5.30280800	0.08242600
C	4.05107400	-2.02921200	-1.10119800
H	3.62758600	-2.02225600	-2.10286900
H	4.88436500	-2.73329000	-1.09350100
H	4.45470400	-1.03971400	-0.87243900
C	1.88835900	0.03611100	2.59463100
C	1.75173300	-0.02320500	-2.59155300
C	2.58319300	4.12985100	-0.07602700
C	0.85312000	-3.61722900	-0.07354500
C	0.47628700	-4.18585000	1.29910000
H	-0.56225400	-3.94415400	1.53234000
H	0.58746200	-5.27208200	1.27969900
H	1.10314100	-3.78545600	2.09648000
C	-0.06002100	-4.21590100	-1.13932400
H	0.12377000	-5.28980100	-1.21918200
H	-1.10741600	-4.05807600	-0.87494300
H	0.11964600	-3.75676300	-2.11337100
F	2.12047400	4.72755200	1.02134100
F	3.89474000	4.38688000	-0.14724800
F	2.00886300	4.70205000	-1.13333100
F	3.06540600	0.00901700	3.23838700
F	1.08265900	0.82799200	3.30094300
F	2.85835700	0.10842000	-3.33929700
F	1.40957100	-1.31022700	-2.62412600
F	0.78457900	0.65565500	-3.20503100
F	1.37692000	-1.18975000	2.64583800
71			
m-2-1			
Au	-1.00708600	-0.92245100	0.05278600

N	-2.63394000	0.23074700	0.05958300
C	-4.77938100	1.05470700	-0.00278400
C	2.06945600	0.84062900	1.16296600
N	1.85332300	-1.33451700	0.01749700
C	3.06241200	-2.22808600	-0.01000300
C	2.24145400	2.21946400	1.12084900
H	2.31901100	2.77277300	2.04797400
C	-5.92745400	-1.47228900	-0.00579000
H	-6.39419500	-2.45007800	-0.00726100
C	0.68443800	-1.93538000	0.03373300
C	-2.57193500	1.60924000	0.04746500
C	1.92091100	0.79727000	-1.23486600
C	2.28060600	2.88439200	-0.08887000
C	-3.97153600	-0.10646500	0.02956300
C	1.95597000	0.09773800	-0.01969100
C	-4.01891800	3.55930800	-0.01242700
H	-5.00820400	4.00229700	-0.04331300
C	-1.43863700	2.42405900	0.07109000
H	-0.45059800	1.97508100	0.11105800
C	-3.86703900	2.17292300	0.00782700
C	-4.54748300	-1.37770100	0.02793500
H	-3.92030000	-2.26297000	0.05310500
C	2.40355000	-3.59699100	0.22644000
H	2.57952900	-3.90978100	1.25773600
H	2.84119500	-4.35319800	-0.42820000
C	-6.16847900	0.93588200	-0.03659600
H	-6.79454800	1.82092500	-0.06156200
C	-1.60999700	3.79704200	0.04939000
H	-0.74107700	4.44673100	0.06850500
C	2.09457400	2.17654900	-1.26041600
H	2.05593300	2.69821700	-2.20783100
C	-6.73677600	-0.32666400	-0.03794300
H	-7.81375300	-0.43529500	-0.06388700
C	4.04900400	-1.86580600	1.08986300

H	4.41970300	-0.84391700	0.97743500
H	4.90615200	-2.53650400	1.01373400
H	3.61477500	-1.98392700	2.08035300
C	-2.89198900	4.36542800	0.00701400
H	-2.99752100	5.44278600	-0.00867400
C	3.77274300	-2.12139200	-1.35398200
H	3.13595400	-2.41799300	-2.18463700
H	4.64472900	-2.77655300	-1.33801300
H	4.12833900	-1.10313400	-1.52780000
C	1.98011900	0.29898700	2.57779600
C	1.66395600	0.20894200	-2.61208000
C	2.51741200	4.37272500	-0.12948700
C	0.89565700	-3.42462100	-0.03027300
C	0.00844200	-4.16493400	0.97944500
H	-1.02316600	-4.11441000	0.61200000
H	0.29960700	-5.21905600	0.95962800
C	0.50703300	-3.85379100	-1.46596900
H	-0.47363500	-3.42599000	-1.69728600
H	1.21353200	-3.40638300	-2.16773100
F	2.05044400	4.97142000	0.96580000
F	3.82588100	4.64387600	-0.20446100
F	1.93435900	4.93231600	-1.18847600
F	3.17855200	0.36257300	3.17820200
F	1.14988000	1.05574300	3.29538100
F	2.79470500	0.20274500	-3.33521000
F	1.18231000	-1.02877100	-2.61885500
F	0.79114200	0.97162900	-3.26897500
F	1.55079600	-0.95392200	2.67618800
C	0.47848000	-5.36300300	-1.66779900
H	-0.34902800	-5.82670200	-1.13155300
H	0.35760800	-5.59664100	-2.72545500
H	1.40441000	-5.83427500	-1.32806800
C	0.06430400	-3.63878300	2.40520900
H	-0.35818300	-2.63512100	2.46860300

H	-0.50742900	-4.28414100	3.07193600
H	1.08724200	-3.59746300	2.78754400
80			
m-3-1			
Au	0.55724600	0.81920500	0.10026500
N	-0.35145900	2.59084000	0.07579600
C	-0.78836100	4.84631300	-0.00210900
C	-1.54192300	-1.76952100	-1.25711200
N	0.58051500	-2.03746300	-0.01617800
C	1.24305400	-3.37922900	-0.03693600
C	-2.93174000	-1.73235400	-1.25934100
H	-3.45850200	-1.61834500	-2.19819500
C	1.90111600	5.53228800	-0.08485000
H	2.94506000	5.82012200	-0.12001000
C	1.36684800	-0.98884800	0.09132700
C	-1.71842600	2.76994900	0.08913400
C	-1.56612900	-1.88828400	1.14569600
C	-3.63747600	-1.80369100	-0.07271000
C	0.21417800	3.84783400	0.01709500
C	-0.84287800	-1.89986900	-0.05224400
C	-3.38776500	4.53257200	0.04676300
H	-3.65391300	5.58319900	0.01193800
C	-2.71503700	1.79499400	0.14037600
H	-2.43902300	0.74611000	0.18215600
C	-2.04835800	4.14306200	0.04329400
C	1.56655500	4.19062900	-0.02823400
H	2.33000900	3.41705600	-0.02288500
C	2.63083300	-2.97611700	0.45408000
H	3.39758400	-3.60189800	0.00113100
H	2.67749700	-3.12372300	1.53832800
C	-0.42806200	6.19208500	-0.05964700
H	-1.18943200	6.96405700	-0.07402600
C	-4.03777200	2.20106900	0.14098000
H	-4.82747800	1.45814600	0.18091200

C	-2.95494600	-1.85223700	1.12881400
H	-3.49821700	-1.83481300	2.06532700
C	0.91454500	6.52952400	-0.09904000
H	1.20960000	7.57033300	-0.14355100
C	1.25000800	-3.95866200	-1.44701700
H	0.23234200	-4.10551900	-1.81488800
H	1.73406900	-4.93596900	-1.41629200
H	1.78984400	-3.32759300	-2.14940800
C	-4.37587900	3.56209500	0.09428300
H	-5.41877800	3.85274200	0.09684700
C	0.55256800	-4.37119800	0.88780300
H	0.53557100	-4.03109400	1.92075200
H	1.10742200	-5.30995200	0.85368100
H	-0.46813000	-4.58035800	0.55857600
C	-0.92377300	-1.58908600	-2.63203100
C	-0.98317700	-1.82891100	2.54784000
C	-5.14480000	-1.81223600	-0.08932600
F	-5.62643900	-1.13489900	-1.13066100
F	-5.61347500	-3.06301000	-0.17650700
F	-5.64910700	-1.27665900	1.02223400
F	-1.12983300	-2.68078200	-3.38554600
F	-1.51587600	-0.57271600	-3.25750900
F	-1.36406100	-2.90883900	3.24781000
F	0.34473600	-1.76192400	2.62735300
F	-1.46937700	-0.76308700	3.18189100
F	0.38278500	-1.34536900	-2.63443100
C	2.80128300	-1.46583400	0.16725100
C	3.53760500	-1.14845600	-1.16722400
C	3.60951200	-0.79636700	1.30394100
H	2.96616200	-1.56268200	-2.00321500
C	4.94065300	-1.76290800	-1.13925400
C	3.69715300	0.36338400	-1.36848100
H	3.08307500	-0.97994600	2.24777000
C	4.99837000	-1.44559900	1.34379000

C	3.79764800	0.70642000	1.10032300
H	5.44148700	-1.51847700	-2.08180300
H	4.90627500	-2.85334900	-1.07657900
C	5.73800700	-1.18265800	0.02939600
H	2.72351200	0.85672500	-1.44355000
H	4.21570000	0.52973300	-2.31850200
C	4.51012300	0.96841400	-0.22420900
H	4.92522700	-2.52208900	1.52772700
H	5.56377200	-1.01623400	2.17673900
H	2.83957300	1.23227300	1.13335600
H	4.40123500	1.09366000	1.92826600
H	6.72343500	-1.65496900	0.06713200
C	5.89401000	0.32301800	-0.17912800
H	4.60680000	2.04655100	-0.38058600
H	6.48135000	0.75673900	0.63701500
H	6.43149000	0.51477100	-1.11388600

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m-4-1

Au	0.70108600	1.03239300	-0.01635400
N	-0.54597200	2.58810300	-0.04292000
C	-1.49275400	4.68321300	-0.02492000
C	-0.83516700	-2.09256400	-1.19177400
N	1.30079800	-1.79553100	0.01835700
C	2.27010300	-2.94001700	0.07239900
C	-2.20246500	-2.34554000	-1.16717000
H	-2.74646000	-2.41851200	-2.09999700
C	0.96338100	5.97487100	0.03195900
H	1.91245400	6.49706700	0.05442400
C	1.81969500	-0.58939500	0.03142000
C	-1.91844200	2.44746200	-0.06397500
C	-0.82170100	-2.02574000	1.21380500
C	-2.87230500	-2.46242100	0.03605300
C	-0.28674900	3.94315400	-0.01782300
C	-0.11741000	-1.98355600	0.00474500

C	-3.94931200	3.77965300	-0.07106900
H	-4.44923600	4.74188900	-0.06373800
C	-2.66565500	1.26879400	-0.08996300
H	-2.15922100	0.30844000	-0.09811100
C	-2.55639300	3.70810600	-0.05438900
C	0.94886400	4.59146200	0.01077900
H	1.86901000	4.01599100	0.01600100
C	3.55562700	-2.18614600	0.43991300
H	4.41445300	-2.60814100	-0.08398500
H	3.73820000	-2.28533700	1.51431600
C	-1.45461800	6.07701300	-0.00354800
H	-2.37438600	6.65134500	-0.00898200
C	-4.04625300	1.36030500	-0.10571200
H	-4.64395900	0.45494400	-0.12659600
C	-2.18878400	-2.27286700	1.22300400
H	-2.72017000	-2.29163700	2.16620800
C	-0.22716000	6.71712500	0.02476200
H	-0.18110700	7.79877300	0.04155200
C	2.35433200	-3.63298300	-1.28212100
H	1.38855000	-4.05612900	-1.56591000
H	3.06620900	-4.45617400	-1.20619000
H	2.68817800	-2.95896500	-2.06839000
C	-4.68837400	2.60772600	-0.09639400
H	-5.77006800	2.65098100	-0.10918100
C	1.86839300	-3.96815900	1.11961300
H	1.83729400	-3.54501800	2.12098000
H	2.61033800	-4.76795000	1.11554300
H	0.89955100	-4.41713500	0.88683200
C	-0.27355900	-1.89417000	-2.58889800
C	-0.25021200	-1.76371200	2.59788600
C	-4.34571200	-2.78177200	0.05654200
F	-4.95672700	-2.34516400	-1.04427900
F	-4.54519700	-4.10347900	0.12547900
F	-4.94951600	-2.23419300	1.11056100

F	-0.19489900	-3.06627000	-3.23790300
F	-1.09634300	-1.11941700	-3.29484600
F	-0.33346000	-2.87589200	3.34459900
F	1.01852400	-1.36027000	2.63841900
F	-0.97839400	-0.83069700	3.20798100
F	0.92955500	-1.33140700	-2.63350600
C	3.31439400	-0.70179700	0.10362000
C	3.88733100	-0.26959800	-1.26084500
C	3.85821600	0.23844200	1.18570500
C	5.41153400	-0.24115100	-1.24840900
H	3.50278200	0.73403000	-1.47726700
H	3.51548300	-0.92605700	-2.05181600
C	5.38032300	0.21476100	1.21246300
H	3.50998800	1.25393500	0.96213100
H	3.43355500	-0.03973900	2.15471900
C	5.93521200	0.65802900	-0.13555000
H	5.77357900	0.09701300	-2.22125200
H	5.80373200	-1.25474500	-1.10587100
H	5.74706700	0.85927100	2.01323500
H	5.73216200	-0.80015400	1.43738400
H	7.02686300	0.65558900	-0.12525700
H	5.61739700	1.68929300	-0.32809800

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m-5-1

Au	-0.23801200	-1.25575300	0.01656200
N	-2.22126500	-1.45777300	0.03126500
C	-4.38047600	-2.24753400	0.01678100
C	0.90792600	2.03150500	1.19548200
N	2.20007400	0.30299100	-0.00719300
C	3.69821400	0.41199100	-0.05036500
C	0.12918400	3.18335100	1.16887600
H	-0.20577000	3.62059300	2.10054100
C	-3.58507900	-4.90625500	-0.02058600
H	-3.29405000	-5.94979700	-0.03509800

C	1.70113600	-0.91151000	-0.01520900
C	-3.08128400	-0.37864000	0.04489700
C	0.88378700	1.97979300	-1.21059900
C	-0.24991800	3.74528300	-0.03571000
C	-3.00801100	-2.59149100	0.01322800
C	1.34075800	1.44671600	0.00000300
C	-5.45398500	0.13984200	0.04779600
H	-6.49118200	-0.17646600	0.04187000
C	-2.76208700	0.98004500	0.06320300
H	-1.72153500	1.29032000	0.06963500
C	-4.42813200	-0.80516800	0.03699700
C	-2.60668100	-3.92798500	-0.00554000
H	-1.55192000	-4.18322100	-0.00774800
C	4.05917400	-1.03676600	-0.40657000
H	4.95755300	-1.37033000	0.11630400
H	4.24951400	-1.09921000	-1.48255200
C	-5.34979400	-3.24994200	0.00155800
H	-6.40363100	-2.99442800	0.00441700
C	-3.79364000	1.90233400	0.07341400
H	-3.56539700	2.96299500	0.08836500
C	0.10130300	3.12779600	-1.22202100
H	-0.25246100	3.52199000	-2.16637800
C	-4.94838900	-4.57491300	-0.01704300
H	-5.68896400	-5.36469200	-0.02884200
C	4.24312800	0.85804100	1.30085900
H	3.87246700	1.85182600	1.56084100
H	5.33012900	0.91845000	1.23220800
H	3.98580700	0.16787500	2.10113700
C	-5.13399500	1.48803700	0.06584000
H	-5.92185400	2.23052300	0.07421200
C	4.15627800	1.40786300	-1.10602200
H	3.84077200	1.12113100	-2.10642500
H	5.24664500	1.44074700	-1.09363600
H	3.79440400	2.41578000	-0.88790100

C	1.15599700	1.48953300	2.59267100
C	1.10811000	1.39086000	-2.59374400
C	-1.05329900	5.02103000	-0.05829000
F	-1.80039400	5.14896400	1.03764800
F	-0.24816000	6.08847100	-0.11877600
F	-1.85958800	5.07193400	-1.11785300
F	2.04811200	2.25151500	3.24382300
F	0.02565400	1.53510200	3.29658500
F	1.85564600	2.22667500	-3.33104300
F	1.70283400	0.19957600	-2.62922800
F	-0.06203300	1.26408300	-3.21646500
F	1.59476800	0.23527800	2.63718600
C	2.83041300	-1.89626000	-0.06168800
C	2.93219100	-2.57991700	1.31143900
C	2.56305400	-2.97774800	-1.11204100
C	3.85416900	-3.76263300	1.26049300
H	1.92828000	-2.88459000	1.63168600
H	3.28139900	-1.86597600	2.06295700
C	3.76237600	-3.90955900	-1.22225900
H	1.67562400	-3.53947300	-0.80279100
H	2.33429300	-2.51280500	-2.07496000
C	4.24345500	-4.34404700	0.12953700
H	4.21466700	-4.14204100	2.21052700
H	3.49674000	-4.78527800	-1.81899200
H	4.58048900	-3.42138300	-1.76645500
H	4.93246400	-5.18084400	0.17096400

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m-6-1

Au	0.50584900	0.94326300	-0.20533400
N	-0.54887000	2.63169400	-0.30601700
C	-1.23096600	4.82623200	-0.25072600
C	-1.35697400	-2.10240300	-1.10031000
N	0.76399500	-1.91166800	0.16315400
C	1.60348300	-3.13920800	0.38319100

C	-2.74332200	-2.20103200	-1.12368800
H	-3.25093900	-2.31121500	-2.07307100
C	1.36533700	5.80776700	-0.31172700
H	2.37102500	6.21003800	-0.33682500
C	1.42572400	-0.78769300	-0.01674800
C	-1.92790300	2.65877000	-0.26245800
C	-1.43646500	-1.81095600	1.28228300
C	-3.47594000	-2.12398200	0.04502100
C	-0.12521500	3.94452500	-0.29753400
C	-0.67207300	-1.95045200	0.11615500
C	-3.77885100	4.22918500	-0.17705200
H	-4.15665400	5.24523600	-0.14920900
C	-2.81379300	1.57978900	-0.25260700
H	-2.43080700	0.56415000	-0.29187400
C	-2.40586700	3.98795700	-0.22707300
C	1.18086100	4.43635000	-0.32956800
H	2.02355300	3.75288500	-0.37368900
C	2.98003700	-2.48453800	0.59229200
H	3.77462100	-3.09883900	0.16621400
H	3.15902200	-2.39686500	1.66550300
C	-1.02141000	6.20469200	-0.23450000
H	-1.86305000	6.88751100	-0.19875800
C	-4.17188800	1.83977600	-0.20089900
H	-4.87621800	1.01432100	-0.19500400
C	-2.82336300	-1.90551500	1.24103400
H	-3.38992000	-1.78209400	2.15498100
C	0.27534900	6.68968600	-0.26419900
H	0.45397500	7.75752400	-0.25215100
C	1.52741000	-4.06942900	-0.82240800
H	0.50732400	-4.43562900	-0.95983900
H	2.16401400	-4.93476100	-0.63320500
H	1.85493100	-3.59767900	-1.74512100
C	-4.65562900	3.15628600	-0.16251800
H	-5.72332100	3.33122200	-0.12343500

C	1.14844600	-3.92197200	1.60686500
H	1.24212600	-3.34443700	2.52304300
H	1.78090100	-4.80626000	1.69901200
H	0.11681100	-4.26708300	1.50045200
C	-0.73881500	-2.14964600	-2.48701600
C	-0.91886700	-1.51334900	2.67706000
C	-4.97566800	-2.27150500	0.00543800
F	-5.48397800	-1.77308900	-1.12145500
F	-5.32906100	-3.56093100	0.06448700
F	-5.55642500	-1.65177400	1.03162400
F	-0.74287600	-3.40514400	-2.96097900
F	-1.46794500	-1.41959400	-3.33132900
F	-1.10321700	-2.57770500	3.47375800
F	0.36586900	-1.18387300	2.74919800
F	-1.61206700	-0.50768400	3.20872000
F	0.50767100	-1.69970600	-2.56206300
C	2.90472600	-1.08026600	-0.02990200
C	3.33423200	-1.06583500	-1.51576400
C	3.69564900	0.03228400	0.68867400
C	4.83715700	-1.23990800	-1.71238900
H	3.02911300	-0.10334300	-1.94790700
H	2.80659700	-1.83949400	-2.07406200
C	5.19715000	-0.17099500	0.52060100
H	3.43299900	0.94221900	0.12514500
C	5.59107100	-0.16364400	-0.94707800
H	5.13476700	-2.21553900	-1.30430600
H	5.72882900	0.61586900	1.06309700
H	5.49557300	-1.12326000	0.97837800
H	6.66886200	-0.30477000	-1.06525700
H	5.34426500	0.81232400	-1.38528100
C	5.17355500	-1.20895600	-3.19581100
H	6.24482900	-1.34111100	-3.35812300
H	4.64570000	-1.99185100	-3.74405900
H	4.88492000	-0.24567800	-3.62519900

C	3.27796200	0.29592100	2.15248000
H	2.25594700	-0.07184400	2.27571500
C	4.15738500	-0.36897200	3.21204000
H	4.28912200	-1.44241900	3.06719700
H	5.15215600	0.08308100	3.22727500
H	3.71738400	-0.21827400	4.19935000
C	3.25784500	1.80088400	2.40538600
H	4.24231700	2.23073400	2.19238000
H	2.52269300	2.29888300	1.76762900
H	3.01461100	2.02492400	3.44554700

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n-1-1

Au	0.51996800	-1.14621200	0.30076600
N	2.25956000	-0.18214300	0.43002300
C	4.45113500	0.44083000	0.11699900
C	-1.71909800	0.78288800	-1.29097300
N	-2.35208100	-1.22976300	-0.08389800
C	-3.60620900	-1.98518100	-0.38791400
C	-1.62662600	2.16104700	-1.34405600
C	5.35746300	-2.18046900	0.01883800
H	5.73046100	-3.19688600	-0.02082300
C	-1.26484700	-1.94974500	0.08452300
C	2.32377800	1.19719300	0.40689500
C	-2.76927700	0.98274200	0.87216100
C	-2.09061400	2.98300400	-0.33315900
C	3.55046600	-0.64105800	0.25521400
C	-2.29664200	0.19865800	-0.16834900
C	3.92162400	3.00456400	0.12988000
H	4.93563200	3.35456300	-0.02795400
C	1.28048900	2.11271900	0.55728200
H	0.27488800	1.75832900	0.76732800
C	3.65060400	1.63880700	0.20737400
C	4.00415000	-1.95953300	0.20472800
H	3.30635100	-2.78344100	0.31292700

C	-3.16058900	-3.41595100	-0.05654400
H	-3.55801100	-4.12969900	-0.78007300
H	-3.54122300	-3.69262900	0.92988500
C	5.81096800	0.19541500	-0.06989200
H	6.50785200	1.01919200	-0.17670900
C	1.56839900	3.46403300	0.46776700
H	0.77096600	4.19108400	0.58107100
C	-2.66022400	2.36038100	0.75949500
C	6.25849700	-1.11402800	-0.11759700
H	7.31149300	-1.32097700	-0.26111600
C	-3.95568100	-1.78127100	-1.85743700
H	-4.16520800	-0.72921300	-2.06401900
H	-4.84970100	-2.35631300	-2.10164700
H	-3.14428200	-2.10887800	-2.50866900
C	2.87999600	3.91073900	0.25037600
H	3.07713500	4.97306400	0.18540700
C	-4.75693200	-1.52160300	0.49054200
H	-4.49267500	-1.58132700	1.54784000
H	-5.61539400	-2.17207000	0.31673800
H	-5.05931100	-0.49972200	0.25311700
C	-1.62112000	-3.40741200	-0.03150800
C	-1.00008000	-3.92250500	-1.33559100
H	0.08646100	-3.82735000	-1.29898300
H	-1.25732000	-4.97608300	-1.46381200
H	-1.35797300	-3.37122300	-2.20695600
C	-1.04813100	-4.19504200	1.14253200
H	-1.33788500	-5.24478200	1.05819400
H	0.04153400	-4.13149600	1.14511400
H	-1.41554600	-3.80925700	2.09519500
H	-1.32306000	0.17775700	-2.09610600
H	-1.99913400	4.05776300	-0.39214500
H	-3.19384000	0.54826700	1.76595300
N	-0.99230600	2.78134300	-2.52147700
O	-0.86944700	3.98675500	-2.50945800

O	-0.65094900	2.03827500	-3.41764800
N	-3.16705200	3.19463300	1.86398100
O	-3.02411200	4.39370800	1.76342900
O	-3.69743100	2.61854400	2.79239700

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Au	-0.27025800	-0.96494000	-0.18917600
N	-2.13327300	-0.26159100	-0.23115500
C	-4.40702500	0.00533100	-0.01991100
C	1.91399600	1.23404900	1.30325400
N	2.61155600	-0.67451800	-0.02563100
C	3.97663200	-1.26384800	0.13063000
C	1.66294300	2.59857700	1.43305000
C	-4.88222800	-2.72470800	0.13550500
H	-5.08767800	-3.78671000	0.19706600
C	1.61479600	-1.52668100	-0.11278400
C	-2.41873500	1.08918300	-0.25888400
C	2.59524900	1.57495200	-0.98453900
C	1.87935000	3.45892500	0.35832000
C	-3.33867600	-0.91920500	-0.08780400
C	2.38396000	0.73485600	0.09580800
C	-4.30135600	2.61802400	-0.12247900
H	-5.36507600	2.80146300	-0.01992900
C	-1.53166100	2.15771300	-0.40105100
H	-0.46989700	1.96886900	-0.53482100
C	-3.80730000	1.31390500	-0.12753100
C	-3.57582100	-2.29203200	-0.00906800
H	-2.75045300	-2.99463400	-0.06275400
C	3.68637700	-2.73724700	-0.18768000
H	4.24204200	-3.40102600	0.47683200
H	3.99808800	-2.95300100	-1.21276400
C	-5.71597700	-0.45252000	0.12634300
H	-6.54037800	0.24982800	0.17927900
C	-2.04171300	3.44428800	-0.39010400

H	-1.36919600	4.28763200	-0.50505800
C	2.34356600	2.94222700	-0.84745900
C	-5.94824500	-1.81540100	0.20312900
H	-6.95907500	-2.18646700	0.31622600
C	4.45551700	-1.03327800	1.55912600
H	4.55126900	0.03437100	1.76925200
H	5.43659400	-1.49120300	1.69105700
H	3.76912200	-1.47178800	2.28472100
C	-3.41753400	3.67758800	-0.24874700
H	-3.78842200	4.69460000	-0.24485100
C	4.95577500	-0.64277600	-0.85259700
H	4.58994200	-0.73024900	-1.87728200
H	5.90742400	-1.17184800	-0.78416500
H	5.14050000	0.40912400	-0.62564800
C	2.16386200	-2.92737100	-0.06126200
C	1.74790300	-3.52385100	1.28878200
H	0.65995200	-3.56816200	1.36203700
H	2.14821100	-4.53641600	1.37299700
H	2.11952300	-2.93474200	2.12924900
C	1.58220300	-3.77705500	-1.18649100
H	2.01284300	-4.78024100	-1.15118100
H	0.49878500	-3.85692600	-1.07988300
H	1.79789500	-3.34107300	-2.16363500
H	1.67881200	4.51678000	0.45839700
H	1.72598600	0.55721100	2.12750900
H	2.93210600	1.17521800	-1.93162700
C	1.18513900	3.12037000	2.68223400
C	2.56904200	3.81745600	-1.96306200
N	0.82606200	3.53974300	3.69278300
N	2.76583200	4.51506000	-2.85807100
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Au	-0.75525400	1.41857100	0.55221500
N	-2.27977900	0.15012200	0.87165900

C	-4.25670400	-0.91064800	0.34850900
C	1.32871800	-0.18846400	-1.46021300
N	1.95010900	1.87230000	-0.32775400
C	3.04082500	2.76295700	-0.82810700
C	1.32158600	-1.57273700	-1.51881600
C	-5.68993000	1.45858600	0.23541000
H	-6.26831400	2.37329600	0.18796000
C	0.84862900	2.46520400	0.06432000
C	-2.04717400	-1.20457300	0.81564100
C	2.70112600	-0.29563000	0.52186800
C	2.01038900	-2.33839700	-0.58900200
C	-3.62179400	0.32848400	0.59348100
C	2.02587700	0.44367600	-0.43506700
C	-3.17963300	-3.29411000	0.29152800
H	-4.07011900	-3.84162100	0.00484400
C	-0.84483000	-1.88449800	1.02873100
H	0.04579700	-1.32914400	1.31095300
C	-3.22724400	-1.91184000	0.47347800
C	-4.34160300	1.52318000	0.53356800
H	-3.84736900	2.46991100	0.72198900
C	2.51204000	4.13426400	-0.38334200
H	2.68496300	4.89084400	-1.15045900
H	3.03896500	4.44849600	0.52107600
C	-5.61891300	-0.95322300	0.04771800
H	-6.11186600	-1.90022600	-0.14075900
C	-0.82074900	-3.25959800	0.84882100
H	0.10653400	-3.81187900	0.97803200
C	2.67821900	-1.68331800	0.43209900
C	-6.32935300	0.23186800	-0.00559900
H	-7.38708300	0.21882300	-0.23533800
C	3.14032100	2.60838100	-2.34099500
H	3.41220400	1.58535000	-2.60985200
H	3.91459700	3.27470000	-2.72315200
H	2.19716100	2.85685600	-2.82959700

C	-1.97533000	-3.96432700	0.46875600
H	-1.92247900	-5.03483500	0.32116600
C	4.36865600	2.41174700	-0.17701100
H	4.29198300	2.44162500	0.91138300
H	5.11727400	3.14235400	-0.48675400
H	4.71716800	1.42366700	-0.48346900
C	1.01412300	3.95397200	-0.07189700
C	0.10695100	4.40336800	-1.22356200
H	-0.93613800	4.18010100	-0.99231000
H	0.21297500	5.48105200	-1.36436500
H	0.35923700	3.90600600	-2.16173300
C	0.58875700	4.66160200	1.21044000
H	0.73596000	5.73848600	1.10325500
H	-0.46626400	4.47107800	1.41558700
H	1.17208200	4.31597900	2.06581900
H	0.76967800	0.39610000	-2.18265700
H	1.99319500	-3.41928300	-0.64414800
H	3.20679600	0.18891000	1.34810300
S	0.32957100	-2.37562600	-2.73648800
O	0.49634200	-1.68293300	-3.96166700
O	0.55750600	-3.77323100	-2.61552100
S	3.37616100	-2.61862200	1.74464400
O	3.35032400	-3.99090100	1.37747800
O	4.54885600	-1.96582900	2.19532700
O	2.31118700	-2.39046000	2.88624500
H	1.55668100	-2.99781700	2.79365500
O	-1.11850000	-2.03950000	-2.25962600
H	-1.40603300	-2.59766500	-1.50448300
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Au	1.49041900	1.18840800	-0.56938800
N	2.50231700	-0.48585000	-0.98576000
C	4.06462800	-2.13999700	-0.63984700
C	-1.03918600	0.34071200	1.35933000

N	-0.87667400	2.54971700	0.37897600
C	-1.54603100	3.74870300	0.96629900
C	-1.55421200	-0.95440900	1.36267900
C	6.16814800	-0.34161400	-0.43569400
H	7.00254000	0.34490900	-0.35540000
C	0.36914100	2.70938300	-0.00138500
C	1.85882500	-1.70797700	-1.00958700
C	-2.44976300	0.90234800	-0.51763700
C	-2.52691300	-1.30553000	0.44512000
C	3.84004900	-0.74898100	-0.76524300
C	-1.48263400	1.24951800	0.41879700
C	2.31000500	-4.07808000	-0.70574800
H	3.00113900	-4.89232700	-0.51800900
C	0.49996400	-1.96745000	-1.20604600
H	-0.19252900	-1.15464800	-1.41330000
C	2.77120900	-2.76365900	-0.78188200
C	4.89703400	0.15672800	-0.65969500
H	4.71581200	1.22198000	-0.75775800
C	-0.54660100	4.84918500	0.58393800
H	-0.42102400	5.56761100	1.39589200
H	-0.92275100	5.39195200	-0.28708500
C	5.35423000	-2.62087200	-0.41327900
H	5.53414800	-3.68597500	-0.31754700
C	0.06350300	-3.27819400	-1.12133000
H	-0.98959100	-3.49908100	-1.25943400
C	-2.98264800	-0.37483800	-0.49025500
C	6.40071100	-1.72003900	-0.31337700
H	7.40799600	-2.07750200	-0.14018300
C	-1.67825300	3.54300400	2.47103800
H	-2.30793200	2.67748100	2.68896900
H	-2.14221400	4.42268900	2.91916800
H	-0.70406400	3.38880300	2.93713500
C	0.95701200	-4.32922300	-0.86450900
H	0.58369800	-5.34365100	-0.80153200

C	-2.91738400	3.97377300	0.34991200
H	-2.85114600	4.04361800	-0.73744900
H	-3.32290000	4.91335200	0.72851900
H	-3.61259400	3.17513000	0.61563800
C	0.77268700	4.14240500	0.22130300
C	1.79099600	4.15399600	1.36720200
H	2.67472400	3.57561100	1.09165300
H	2.09274200	5.18382200	1.57040500
H	1.38080900	3.72659500	2.28393900
C	1.42228400	4.71715800	-1.03333800
H	1.68826700	5.76324700	-0.86529600
H	2.32790700	4.15963100	-1.27907900
H	0.74579700	4.66454500	-1.88843700
C	-1.00397800	-1.92088200	2.39718900
C	-3.99040600	-0.84235800	-1.52397000
H	-2.92556300	-2.31074000	0.43246700
H	-0.26951400	0.63160200	2.06541200
H	-2.75180400	1.61874700	-1.26768800
Cl	-1.44632600	-1.31306700	4.01176300
Cl	0.75295600	-1.98768400	2.28456700
Cl	-1.64332900	-3.54772900	2.22581500
Cl	-5.30799000	-1.72821900	-0.74470000
Cl	-4.70175500	0.48991800	-2.43377200
Cl	-3.17114700	-1.92472200	-2.65965900

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Au	0.86404900	1.20772100	-0.30502100
N	2.39917400	-0.05891700	-0.44081600
C	4.44527900	-1.08231000	-0.20910200
C	-1.70765300	-0.27011600	1.30161600
N	-1.94764800	1.80457700	0.06391500
C	-3.05018300	2.77314700	0.34524400
C	-1.84532100	-1.64928900	1.38999000
C	5.81692500	1.32512400	-0.04343200

H	6.36993900	2.25456700	0.02201600
C	-0.75030500	2.31925200	-0.10067900
C	2.21008400	-1.42641900	-0.46804100
C	-2.71999600	-0.31805300	-0.88710500
C	-2.42718000	-2.36737600	0.35986400
C	3.75417800	0.15022000	-0.28482500
C	-2.14819700	0.38808200	0.16369300
C	3.45727200	-3.50451400	-0.30882000
H	4.39366600	-4.03927500	-0.19450200
C	1.01384800	-2.12946900	-0.62306600
H	0.08252400	-1.59177700	-0.77723200
C	3.43803800	-2.10987600	-0.32236900
C	4.44261700	1.36122100	-0.20033300
H	3.90466100	2.30170300	-0.25996400
C	-2.35640800	4.09990200	0.00783900
H	-2.62825900	4.87981500	0.72123800
H	-2.67245500	4.43017200	-0.98499800
C	5.83064800	-1.09519000	-0.05027200
H	6.36749200	-2.03553000	0.00848900
C	1.05335300	-3.51268900	-0.59996700
H	0.13341800	-4.07490800	-0.72427800
C	-2.85789100	-1.69293400	-0.77607800
C	6.51087300	0.10810100	0.03131700
H	7.58667500	0.11439700	0.15373100
C	-3.44879200	2.65120800	1.81144100
H	-3.83884000	1.65364400	2.02513400
H	-4.23227700	3.37602000	2.03637200
H	-2.60089700	2.84190700	2.47074600
C	2.26598400	-4.20008700	-0.44034800
H	2.26820100	-5.28266900	-0.42895500
C	-4.25457500	2.50895500	-0.54404100
H	-3.97104100	2.51228700	-1.59809400
H	-4.98917900	3.29998600	-0.38572300
H	-4.72994000	1.55612800	-0.30328700

C	-0.84273700	3.81854400	-0.00003100
C	-0.15338700	4.22719700	1.30709400
H	0.89873000	3.93802700	1.28438800
H	-0.21871200	5.31102300	1.42480700
H	-0.61409800	3.75688200	2.17771600
C	-0.12781300	4.48152300	-1.17293300
H	-0.22709600	5.56688800	-1.09967300
H	0.93307600	4.22490300	-1.16345500
H	-0.54887800	4.15820700	-2.12669200
C	-1.33755000	-2.34417100	2.62774400
C	-3.46264600	-2.50126100	-1.89396300
H	-2.51749500	-3.44427800	0.42409100
H	-1.22449300	0.29106500	2.09336300
H	-3.02364500	0.19507500	-1.78943100
F	-0.13108700	-1.89854900	2.97144600
F	-2.15258400	-2.11304300	3.66893000
F	-1.26525800	-3.66287400	2.46371700
F	-3.71817400	-1.75589700	-2.97029900
F	-2.65133800	-3.49341300	-2.26634700
F	-4.61627600	-3.06246500	-1.51116300

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Au	1.33815700	1.17875500	-0.56758000
N	2.40423500	-0.48946000	-0.91417600
C	3.99012400	-2.07560500	-0.38644400
C	-1.21340800	0.10920600	1.44804900
N	-1.05983500	2.34570300	0.46568300
C	-1.83329100	3.48258500	1.06354200
C	-1.77947700	-1.17614300	1.40501800
C	6.06215100	-0.23487400	-0.36239300
H	6.88591100	0.46857200	-0.34974200
C	0.13705700	2.63316400	0.02319000
C	1.78164200	-1.71354100	-0.81135100
C	-2.30189600	0.60525300	-0.69789200

C	-2.73922100	-1.53415100	0.44741500
C	3.74474600	-0.71040300	-0.65995500
C	-1.56972500	0.99949900	0.42981900
C	2.26225300	-4.03414000	-0.25444200
H	2.95966100	-4.81333700	0.03108500
C	0.42861000	-2.01522700	-0.99184500
H	-0.27057900	-1.23247800	-1.27294800
C	2.70815000	-2.73000400	-0.46729300
C	4.78699700	0.21860000	-0.64477900
H	4.59067000	1.26426300	-0.85489500
C	-0.97493500	4.67125300	0.60833200
H	-0.90191300	5.43029200	1.38907200
H	-1.43730800	5.13496400	-0.26747600
C	5.28501500	-2.51209600	-0.10283400
H	5.47979900	-3.55779100	0.10705500
C	0.00665600	-3.31961000	-0.78352800
H	-1.04441500	-3.56921500	-0.88506600
C	-2.88833300	-0.66795300	-0.65312000
C	6.31531100	-1.58961300	-0.09359200
H	7.32658400	-1.90983600	0.12234400
C	-1.88953200	3.32517900	2.57959200
H	-2.37268500	2.38446000	2.85330100
H	-2.48043200	4.14247100	2.99507100
H	-0.89943100	3.35452700	3.03256200
C	0.91178100	-4.32535300	-0.40303300
H	0.55005100	-5.33055400	-0.23040300
C	-3.25689800	3.53915800	0.52840200
H	-3.28592300	3.70927700	-0.54649800
H	-3.77456200	4.36728200	1.01443100
H	-3.80222700	2.62147600	0.75976100
C	-0.24602700	0.52020200	2.52242300
H	-0.73034500	0.51508900	3.49876100
H	0.58360700	-0.18220100	2.57224100
H	0.16824500	1.50402400	2.32843300

C	-2.37387600	1.52009700	-1.89092000
H	-1.83951000	1.07268100	-2.72793900
H	-3.39789200	1.68516800	-2.22237700
H	-1.91225400	2.47846600	-1.67700400
C	-3.61649600	-2.74999100	0.60653900
H	-3.86809200	-2.88319900	1.65506300
H	-4.53788600	-2.62823500	0.04601200
H	-3.12309600	-3.66259400	0.27869700
C	0.40219700	4.10070600	0.21672200
C	1.45156700	4.23881700	1.32468300
H	2.37510800	3.73431400	1.03427800
H	1.66638400	5.29656700	1.49053400
H	1.11175900	3.80487900	2.26708200
C	0.94121500	4.70981800	-1.07365100
H	1.09057700	5.78385100	-0.94265900
H	1.89550600	4.25152200	-1.33954400
H	0.24544800	4.55567900	-1.90170000
S	-1.18520000	-2.37522700	2.58471300
O	-1.31817300	-1.83300200	3.88922600
O	-1.70129000	-3.66260300	2.27667500
S	-3.83663400	-1.24155000	-2.04136700
O	-5.21002400	-1.28173900	-1.69447300
O	-3.40744400	-0.58358000	-3.22791700
O	-3.36111400	-2.74077000	-2.18020900
H	-2.59388900	-2.78180000	-2.77597300
O	0.35073500	-2.39992100	2.28067300
H	0.55158500	-2.95153100	1.49142900
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Au	1.22002900	1.04765100	-0.06351600
N	2.58956400	-0.40064000	-0.03344000
C	4.55974100	-1.58386400	0.03059400
C	-2.06759600	0.13226700	1.22944900
N	-1.47874300	2.09888900	-0.09639400

C	-2.43516600	3.25156400	-0.11384300
C	-2.52947500	-1.18913000	1.26719800
C	6.12666200	0.70450300	0.13221000
H	6.75482000	1.58643400	0.17212500
C	-0.20549500	2.40718500	-0.09893100
C	2.28954700	-1.74796100	-0.06857700
C	-2.14041300	0.03629600	-1.22332500
C	-2.71581700	-1.94111900	0.10088900
C	3.96475800	-0.30071200	0.02550300
C	-1.92628000	0.73151500	-0.02743500
C	3.38565800	-3.91803100	-0.06148200
H	4.28563800	-4.52229300	-0.03334100
C	1.03385000	-2.35571800	-0.13755600
H	0.13308500	-1.74809600	-0.16985300
C	3.46891200	-2.52627700	-0.03134000
C	4.75181700	0.85092800	0.07654400
H	4.28758800	1.83206300	0.07220800
C	-1.47541000	4.41881300	-0.38828900
H	-1.73187800	5.29228300	0.21388500
H	-1.54661200	4.70615200	-1.44055000
C	5.94747200	-1.70861300	0.08738200
H	6.41063100	-2.68912300	0.09183600
C	0.97453900	-3.73829900	-0.16877600
H	0.01053800	-4.23050400	-0.22937800
C	-2.59311300	-1.28550600	-1.13132400
C	6.72537700	-0.56424600	0.13800300
H	7.80424200	-0.64455700	0.18246000
C	-3.14735400	3.36533400	1.22812000
H	-3.72988400	2.46466000	1.43467800
H	-3.83492000	4.21141800	1.19101800
H	-2.44566900	3.52812600	2.04583600
C	2.13960300	-4.51874600	-0.13007300
H	2.05978500	-5.59817500	-0.15649100
C	-3.47000100	3.08555800	-1.21587100

H	-2.99938900	3.05274800	-2.19764700
H	-4.14675700	3.94102700	-1.19146800
H	-4.06355500	2.17997500	-1.07092700
C	-1.58199600	0.83715200	2.47050100
H	-2.39534500	1.26316700	3.05567300
H	-1.04857300	0.13550400	3.10977000
H	-0.88582200	1.63072400	2.20923200
C	-1.73711000	0.65249600	-2.53840800
H	-1.19736600	-0.07798500	-3.13965500
H	-2.59452100	0.98664900	-3.12031300
H	-1.07259600	1.49820700	-2.37694000
C	-2.88288100	-3.44168900	0.16847700
H	-3.92768500	-3.74195600	0.22796500
H	-2.44489000	-3.90997900	-0.70889800
H	-2.36346300	-3.83572900	1.03887000
C	-0.05542800	3.90493500	-0.09185100
C	0.44152500	4.30318800	1.30236900
H	1.40161900	3.82777100	1.51194600
H	0.56890500	5.38704700	1.34523500
H	-0.26216100	4.00902000	2.08417500
C	0.96006800	4.34744800	-1.13965600
H	1.02474100	5.43777600	-1.15666300
H	1.94664200	3.94032800	-0.90919000
H	0.67362300	4.00149800	-2.13545600
C	-2.90664400	-2.06345400	-2.39624000
C	-2.78889600	-1.84650700	2.61078200
F	-3.78687300	-2.73496000	2.55289800
F	-3.16202400	-0.96461200	3.54603500
F	-3.92119600	-2.91783000	-2.21880800
F	-3.28698900	-1.27649300	-3.40839400
F	-1.85421700	-2.77261100	-2.82363100
F	-1.70998000	-2.48485400	3.07925400

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Au	-0.18147800	-0.57498200	0.10857500
N	-2.11708200	-0.06865600	0.11049500
C	-4.40528900	-0.15213900	-0.10708600
N	2.74794400	-0.23023500	0.02439600
C	4.09867700	-0.87424300	-0.00506300
C	-4.43348100	-2.89511300	-0.52646700
H	-4.46422500	-3.96555700	-0.69176000
C	1.73969600	-1.06266500	0.08593400
C	-2.61467700	1.20855500	0.26146800
C	-3.20034500	-0.89324000	-0.11128600
C	-4.72872700	2.41490800	0.25186100
H	-5.80878000	2.42695000	0.15455300
C	-1.91820800	2.39320400	0.51439800
H	-0.83789900	2.38035400	0.63231900
C	-4.02415400	1.21738900	0.13427700
C	-3.21429500	-2.27353000	-0.32311100
H	-2.28607800	-2.83665600	-0.32517200
C	3.72192300	-2.34522600	-0.24231500
H	4.36354100	-3.01766600	0.33000400
H	3.85080600	-2.58199800	-1.30212300
C	-5.62344400	-0.79870300	-0.31479300
H	-6.55059900	-0.23611300	-0.31235300
C	-2.63677300	3.57077900	0.62673200
H	-2.11219300	4.49821200	0.82481000
C	-5.63324700	-2.16740600	-0.52325000
H	-6.57094200	-2.68394100	-0.68569500
C	4.83189500	-0.69262100	1.32396600
H	5.18581300	0.32730300	1.46186700
H	5.70276300	-1.35031000	1.33128500
H	4.19473500	-0.95839200	2.16793500
C	-4.03324400	3.58761000	0.49502300
H	-4.56716100	4.52490400	0.58899800
C	4.95874400	-0.35508700	-1.14902700
H	4.43682900	-0.45063000	-2.10224400

H	5.86664900	-0.95994800	-1.19427000
H	5.25644100	0.68420600	-1.00802700
C	2.24158000	-2.48228000	0.13166100
C	2.02509300	-3.01196800	1.55292000
H	0.96213500	-2.99638200	1.80094100
H	2.38436100	-4.04173800	1.61407800
H	2.55560900	-2.41590500	2.29704200
C	1.47428800	-3.36163200	-0.85095200
H	1.90039300	-4.36784800	-0.85484200
H	0.42255000	-3.42931600	-0.56404000
H	1.52482600	-2.95862300	-1.86440300
C	2.48938500	1.22347000	-0.06532700
C	3.40517900	2.12155100	0.75266600
C	2.39134700	1.68908900	-1.51520200
H	1.48713900	1.33269000	0.36439700
C	2.84879900	3.54405700	0.70538400
H	4.42146100	2.12318900	0.34416500
H	3.45806400	1.76938800	1.78506600
C	1.84661100	3.11225600	-1.55218600
H	3.37748200	1.66474000	-1.98938200
H	1.73461300	1.00406200	-2.05917200
C	2.73036000	4.04249300	-0.72995400
H	3.48246600	4.20854300	1.29551500
H	1.85623500	3.55141300	1.17172200
H	1.77343400	3.45834500	-2.58447400
H	0.82883900	3.11489900	-1.14370800
H	2.33519100	5.05986100	-0.74614200
H	3.73011900	4.08072600	-1.18019200

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Au	0.56228300	-0.73527200	-0.20301200
N	2.40862500	0.03488600	-0.18986000
C	4.68877000	0.27635500	-0.01470900
N	-2.39564000	-0.77213300	-0.24258300

C	-3.63170400	-1.61567300	-0.34477200
C	5.14172600	-2.46131300	0.03780300
H	5.33835500	-3.52666000	0.05951100
C	-1.28134500	-1.45983900	-0.18904800
C	2.70221800	1.38209400	-0.17388700
C	3.60983200	-0.63521100	-0.09271300
C	4.60924900	2.88751900	-0.02846200
H	5.67779500	3.05300400	0.05482700
C	1.82628500	2.46866200	-0.25026400
H	0.75552400	2.30757300	-0.35080300
C	4.09798600	1.59096300	-0.06544500
C	3.83703800	-2.01277300	-0.06584900
H	3.00380700	-2.70623700	-0.12753200
C	-3.09683300	-2.96586400	0.14453600
H	-3.58929600	-3.79849800	-0.36093400
H	-3.29556000	-3.05658500	1.21716800
C	5.99635600	-0.19762800	0.08912800
H	6.82825300	0.49555200	0.14891800
C	2.35512800	3.74731800	-0.21078900
H	1.68987800	4.60083500	-0.27046700
C	6.21792100	-1.56408900	0.11483000
H	7.22735600	-1.94762000	0.19490700
C	-4.10646800	-1.70019200	-1.79695400
H	-4.56500300	-0.77185200	-2.13229000
H	-4.85667200	-2.48950500	-1.87167300
H	-3.28393100	-1.94095800	-2.47016300
C	3.73678900	3.96106200	-0.09918200
H	4.11984200	4.97342600	-0.07148400
C	-4.77326500	-1.13664700	0.53812500
H	-4.44722600	-1.00083200	1.57094800
H	-5.55038100	-1.90368200	0.52507100
H	-5.21644100	-0.20905600	0.17436700
C	-1.58136800	-2.93390000	-0.08571700
C	-1.12592800	-3.64617600	-1.36118800

H	-0.05449700	-3.49470700	-1.50816700
H	-1.31646000	-4.71747400	-1.26529900
H	-1.64348700	-3.28344900	-2.24951400
C	-0.81851100	-3.51679700	1.10380700
H	-1.11715200	-4.55705000	1.25584100
H	0.25843000	-3.48181700	0.92608200
H	-1.03068400	-2.95606800	2.01774700
C	-2.37568600	0.70423000	-0.22659900
C	-3.11463700	1.33164200	-1.40123300
C	-2.83012200	1.33062700	1.10342000
H	-1.31277100	0.94714900	-0.34370800
C	-2.83127900	2.82917600	-1.47369300
H	-4.19850900	1.19753800	-1.28640900
H	-2.81470000	0.84495600	-2.33406700
C	-2.52061300	2.82740600	1.01675400
H	-3.92157400	1.23871400	1.16894400
C	-3.23437200	3.48123700	-0.15708200
H	-1.74754900	2.96047600	-1.60096800
H	-2.79493200	3.31362600	1.95659500
H	-1.43904500	2.96320200	0.89525800
H	-3.01860100	4.55233500	-0.19014400
H	-4.32144600	3.37780100	-0.03599900
C	-3.55392000	3.45834400	-2.65381100
H	-4.63527400	3.33426800	-2.54184300
H	-3.34547800	4.52751800	-2.71828400
H	-3.25719600	2.99642100	-3.59726100
C	-2.22547100	0.67371000	2.35723300
H	-2.20815200	-0.41224600	2.19343800
C	-3.11034200	0.94084000	3.57068000
H	-2.69227600	0.47701700	4.46579300
H	-3.18761500	2.01422400	3.76362900
H	-4.12222800	0.55282600	3.42524100
C	-0.79730100	1.12777700	2.64601900
H	-0.34685300	0.49804400	3.41475800

H	-0.15214400	1.08052600	1.76442000
H	-0.78812500	2.15733500	3.01294200
60			
w-1-1			
Au	-0.10897100	-0.57446600	0.15996600
N	-2.06144500	-0.14015700	0.16386400
C	-4.33767000	-0.27554800	-0.13560900
N	2.78653500	-0.07219200	0.00965600
C	4.17207600	-0.62791000	-0.06211400
C	-4.28114600	-3.00841300	-0.61419300
H	-4.27881000	-4.07539600	-0.80300600
C	1.83452700	-0.96387000	0.11874400
C	-2.59655400	1.12118100	0.32503400
C	-3.11483800	-0.98634100	-0.11354200
C	-4.73922000	2.27435300	0.26385900
H	-5.81505000	2.26152800	0.12761800
C	-1.94021100	2.31618800	0.63266900
H	-0.86686000	2.33010800	0.80143900
C	-4.00034800	1.09760300	0.14723300
C	-3.08589400	-2.36134500	-0.35566000
H	-2.14386900	-2.90069100	-0.33779100
C	3.88484600	-2.12768800	-0.24063900
H	4.58427000	-2.73693000	0.33483400
H	4.00025400	-2.39303200	-1.29513200
C	-5.53105900	-0.94750300	-0.39898500
H	-6.47190700	-0.40841200	-0.41656100
C	-2.69283500	3.47284600	0.74216900
H	-2.19932900	4.40701000	0.98383700
C	-5.49862700	-2.31107700	-0.63666300
H	-6.41674600	-2.84716400	-0.84191800
C	4.94393800	-0.36154600	1.22908100
H	5.18949100	0.69090700	1.35620100
H	5.88072300	-0.92044800	1.19514600
H	4.37854500	-0.69497800	2.09975100

C	-4.08313400	3.45845900	0.55653900
H	-4.64410300	4.37980800	0.65077400
C	4.93443600	-0.08514800	-1.26364600
H	4.36195700	-0.23149300	-2.18108400
H	5.87200800	-0.63714900	-1.35374000
H	5.17797500	0.97269700	-1.16410400
C	2.42654100	-2.34705400	0.18208700
C	2.28441400	-2.85334200	1.62116300
H	1.23001900	-2.89817300	1.90007700
H	2.70988000	-3.85661800	1.69591200
H	2.79648500	-2.20627700	2.33505700
C	1.68710400	-3.29574500	-0.75641800
H	2.17230900	-4.27475900	-0.74822400
H	0.64953900	-3.41769000	-0.43765500
H	1.68579200	-2.91692600	-1.78046300
C	2.42697200	1.35406400	-0.12478700
C	3.32480900	2.35927700	0.57569500
C	2.21495600	1.75966900	-1.58043000
H	1.44949100	1.42452100	0.36366200
C	2.76040500	3.73699600	0.34857900
H	4.35336900	2.31851700	0.20370100
H	3.36680100	2.14989800	1.64803500
C	1.36395400	3.02303700	-1.59572700
H	3.17933000	1.95157800	-2.06083500
H	1.71498600	0.94942400	-2.11678400
C	1.86922600	4.02249400	-0.59762700
H	3.09895200	4.51847700	1.01965700
H	1.35623900	3.46758800	-2.59348600
H	0.32042600	2.76856900	-1.37041600
H	1.48088300	5.03297600	-0.66733000
68			
e-1-0			
Au	-0.24879400	-0.89696700	-0.11303200
N	-2.10862000	-0.16966700	-0.15113700

C	-4.38442700	0.14911000	-0.09375200
C	2.09631000	1.46247200	1.36839400
N	2.60395400	-0.54410200	0.06212800
C	3.95762800	-1.10502500	0.16950800
C	1.94754600	2.84734700	1.40355600
H	1.70674700	3.32797600	2.34457900
C	-4.93399500	-2.57117600	-0.14836300
H	-5.16838300	-3.62886200	-0.16982400
C	1.64480400	-1.42782500	-0.04025900
C	-2.35819600	1.18803400	-0.11376500
C	0.49247200	0.90063500	3.20146000
H	-0.27939900	0.70701600	2.45273700
H	0.38487700	1.93538600	3.53491200
H	0.31487900	0.25235100	4.06139000
C	2.51999100	1.61921500	-1.04365800
C	2.07751500	3.61084200	0.25416100
H	1.94754600	4.68471400	0.30116800
C	-3.33505500	-0.79957800	-0.13985100
C	2.40042000	0.87825600	0.13567900
C	1.45142400	1.06387200	-3.21380200
H	0.60738700	0.61806200	-2.68157200
H	1.56725900	0.55903800	-4.17476900
H	1.20815500	2.11194900	-3.40610200
C	-4.21019200	2.75916200	-0.02849400
H	-5.27430000	2.96618900	0.00202100
C	-1.43474600	2.23683100	-0.11496700
H	-0.36782600	2.03373100	-0.15792200
C	1.89087700	0.65761600	2.63296700
H	1.96498900	-0.40463800	2.38394600
C	2.73726400	0.96523500	-2.39110300
H	2.95368500	-0.09600100	-2.23396200
C	-3.74783000	1.44396000	-0.07451100
C	-3.61059800	-2.16777100	-0.16677500
H	-2.79977700	-2.88790900	-0.20256600

C	3.74182300	-2.53020300	-0.31941100
H	4.41556700	-3.24951700	0.14612000
H	3.88782900	-2.57147400	-1.40215800
C	-5.71116900	-0.28016400	-0.07552600
H	-6.52064300	0.44069100	-0.04045600
C	2.96428800	0.98510300	3.67006100
H	3.96850000	0.79603500	3.28347900
H	2.82069100	0.38624400	4.57132100
H	2.90962700	2.03839400	3.95578900
C	-1.91618100	3.53354000	-0.06581300
H	-1.21302500	4.35946900	-0.06531800
C	2.34893300	2.99841200	-0.96032700
H	2.41423200	3.59595000	-1.86212500
C	-5.98089900	-1.63802700	-0.10307000
H	-7.00596100	-1.98672300	-0.08993400
C	3.91571500	1.57844500	-3.14367000
H	4.83506000	1.53238000	-2.55605900
H	3.72320500	2.62604200	-3.38439200
H	4.07928000	1.05014300	-4.08452100
C	-3.29354800	3.79820400	-0.02185600
H	-3.63958700	4.82368600	0.01437600
C	2.26367100	-2.80527700	0.00788600
C	2.09871100	-3.30111200	1.44921400
C	1.59510100	-3.76540600	-0.96237700
H	1.04448400	-3.30806500	1.73236700
H	2.63887500	-2.66468200	2.15581000
H	0.54547800	-3.90365300	-0.69563900
H	1.63688800	-3.38298300	-1.98421300
H	2.49155300	-4.31673300	1.53197600
H	2.09407600	-4.73677200	-0.93296400
H	4.64716400	-0.51655200	-0.43819300
H	4.28231400	-1.04242300	1.21410300

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Au	-0.64709800	-0.88168500	-0.06108500
N	-2.54884900	-0.26337800	0.00846100
C	-4.83970100	-0.08047900	0.07391100
C	1.71278700	1.63032800	1.24559200
N	2.20028200	-0.38870000	-0.08019700
C	3.62089500	-0.88842900	-0.10837700
C	1.52499700	3.01177000	1.27044300
H	1.41162400	3.50845700	2.22683900
C	-5.22661300	-2.82743100	-0.03023600
H	-5.39782100	-3.89663100	-0.07051700
C	1.27478800	-1.31248800	-0.12937400
C	-2.87798200	1.07578100	0.07081900
C	0.15208400	0.98323100	3.06478500
H	-0.57213500	0.62944600	2.32825800
H	-0.08636100	2.02523500	3.29237700
H	0.03061900	0.39961700	3.97947900
C	1.66548800	1.71975500	-1.20342400
C	1.43777900	3.74782100	0.10064500
H	1.29462700	4.82017100	0.14204900
C	-3.73584400	-0.96425900	0.00927600
C	1.86209700	1.01507000	-0.00595500
C	0.12884900	1.18391300	-3.08428300
H	-0.58889500	0.74202400	-2.38982200
H	0.03135500	0.68569000	-4.05091200
H	-0.13886400	2.23531200	-3.21560000
C	-4.81905700	2.53416000	0.17966800
H	-5.89346500	2.67795200	0.21333100
C	-2.01803100	2.17733400	0.09084900
H	-0.94097800	2.03765200	0.05547000
C	1.59078000	0.86636000	2.54989800
H	1.78587800	-0.19076100	2.35505000
C	1.56489400	1.06330500	-2.56627100
H	1.79306300	-0.00187300	-2.46398000
C	-4.28055200	1.24912100	0.11406500

C	-3.92963700	-2.34569000	-0.04304700
H	-3.07723300	-3.01527000	-0.09253500
C	3.38497900	-2.34441400	-0.53383700
H	4.07169700	-3.02979200	-0.03520200
H	3.55873000	-2.42870500	-1.61132800
C	-6.13858900	-0.58839600	0.08599500
H	-6.98950300	0.08215600	0.13547300
C	2.55266000	1.36349800	3.62800000
H	3.59288000	1.35994500	3.30021700
H	2.47017100	0.73890000	4.51935300
H	2.30060000	2.38454800	3.92307400
C	-2.57459700	3.44291900	0.15630200
H	-1.92064100	4.30826700	0.17272700
C	1.46915800	3.09621800	-1.12202400
H	1.31854900	3.66074300	-2.03459000
C	-6.32708800	-1.95916500	0.03393200
H	-7.32957400	-2.36842900	0.04245700
C	2.53007300	1.68219700	-3.57819500
H	3.55570200	1.71716100	-3.20600400
H	2.22973000	2.70507400	-3.81554100
H	2.51606000	1.11421900	-4.51016900
C	4.23321300	-0.75591800	1.28795000
H	4.20147900	0.30049500	1.56829000
H	3.60385900	-1.28788500	2.00485200
C	-3.96522200	3.62537400	0.20095200
H	-4.37118500	4.62801800	0.25178200
C	4.48275800	-0.16435200	-1.15067800
H	3.92231300	-0.14118400	-2.08820300
H	5.33394000	-0.82758600	-1.33858300
C	1.91432700	-2.66901300	-0.23341200
C	1.70393000	-3.39498800	1.09864500
C	1.26084900	-3.47194400	-1.35425100
H	0.63651700	-3.51670300	1.29245100
H	2.13828500	-2.84799300	1.93751000

H	0.20952400	-3.65863500	-1.12696800
H	1.31309000	-2.93261200	-2.30317700
H	2.16743100	-4.38302900	1.05259700
H	1.77254600	-4.43036900	-1.47064800
C	5.66117300	-1.27640100	1.39272600
H	6.34760700	-0.73336700	0.74267100
H	6.02361000	-1.17095800	2.41525800
H	5.72517300	-2.33399600	1.13158300
C	5.01013700	1.22464700	-0.80403900
H	4.21528800	1.93397400	-0.57192200
H	5.68967400	1.19793100	0.04882600
H	5.57104300	1.62384600	-1.65068100

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Au	1.17895200	-0.82071300	-0.08414700
N	3.10714000	-0.28923500	-0.05218100
C	5.40338600	-0.20855300	0.01876100
C	-1.15801300	1.79447500	-1.14900500
N	-1.70457200	-0.32706500	0.00878000
C	-0.85299400	3.15092500	-1.05715900
H	-0.72966000	3.72308600	-1.96868700
C	5.66467000	-2.97266500	0.00572200
H	5.78712400	-4.04929900	0.00140000
C	-0.75007100	-1.22719200	-0.05926100
C	3.49657100	1.03381600	-0.02830700
C	0.24791500	1.00249900	-3.04240700
H	0.85731900	0.37925900	-2.38632200
H	0.72570500	1.98409400	-3.10467000
H	0.24508500	0.56002500	-4.04082900
C	-1.02867800	1.65244300	1.29283100
C	-0.67414600	3.76917800	0.16982500
H	-0.44343600	4.82585500	0.21886200
C	4.26034000	-1.04320700	-0.02219900
C	-1.31990700	1.07523800	0.04736400

C	0.50513800	0.90550400	3.10763700
H	1.21074400	0.53428000	2.36148400
H	0.59677300	0.29529100	4.00837500
H	0.79617100	1.92756500	3.36171000
C	5.49812400	2.40801700	0.04638500
H	6.57759000	2.50699600	0.07993100
C	2.68396500	2.16994100	-0.04118600
H	1.60237000	2.07148700	-0.07548700
C	-1.18716200	1.15965500	-2.52798500
H	-1.63801900	0.16645000	-2.44455200
C	-0.93690100	0.87435400	2.59149900
H	-1.19794400	-0.17027400	2.39758300
C	4.90503500	1.14581200	0.01561600
C	4.39105600	-2.43304700	-0.02845000
H	3.50861700	-3.06412500	-0.05960600
C	-2.74913200	-2.35715700	0.46532800
H	-3.46372300	-3.07818000	0.07517500
H	-2.73687400	-2.46619300	1.55608600
C	6.67751200	-0.77459500	0.05252500
H	7.55815500	-0.14241000	0.08358600
C	-1.96933700	1.97340100	-3.56289900
H	-2.95786900	2.27517400	-3.21811200
H	-2.08790200	1.38670600	-4.47546100
H	-1.41753100	2.87578000	-3.83476400
C	3.29411300	3.41175400	-0.00880600
H	2.67878700	4.30513000	-0.01763600
C	-0.73054900	3.01367100	1.32837900
H	-0.51440400	3.47849000	2.28301800
C	6.80336800	-2.15361100	0.04568700
H	7.78610200	-2.60763200	0.07143600
C	-1.87142800	1.42845100	3.66786300
H	-2.90659000	1.49527300	3.33007100
H	-1.55448200	2.43045000	3.96581100
H	-1.83603500	0.79683400	4.55761700

C	4.69152900	3.53492300	0.03441700
H	5.14030000	4.52018600	0.05866500
C	-1.33758200	-2.60572500	-0.05595100
C	-1.29148500	-3.13391100	-1.49355500
C	-0.54780800	-3.54207100	0.85133300
H	-0.25572700	-3.19779000	-1.83297700
H	-1.83487500	-2.48924100	-2.18619900
H	0.46288900	-3.68911800	0.46499800
H	-0.46806200	-3.13265400	1.86105400
H	-1.73326000	-4.13244500	-1.52866600
H	-1.04763200	-4.51242200	0.90671400
C	-3.11430600	-0.89685800	0.14194400
C	-3.94203600	-0.30017900	1.29859600
C	-3.96099200	-0.73092600	-1.14101700
H	-3.35231100	-0.37519200	2.21672700
C	-5.20877200	-1.16124100	1.44982500
C	-4.40224100	1.14354900	1.07306000
H	-3.38641900	-1.07933800	-2.00337900
C	-5.25087000	-1.55453600	-1.02599300
C	-4.38048800	0.72760700	-1.35598600
H	-5.78357000	-0.77857700	2.29932700
H	-4.95523300	-2.19910700	1.67884500
C	-6.06235200	-1.08630200	0.18228600
H	-3.56164000	1.83583400	1.00387600
H	-5.00040100	1.44892400	1.93952000
C	-5.24308300	1.22336400	-0.19798800
H	-5.04843500	-2.62526200	-0.96829100
H	-5.83584700	-1.39679100	-1.93835300
H	-3.50959300	1.37483800	-1.43509500
H	-4.92967100	0.79636300	-2.30122400
H	-6.94382900	-1.72218500	0.29977000
C	-6.49059000	0.35974400	-0.05006700
H	-5.52800400	2.26267000	-0.38073500
H	-7.10690700	0.42648500	-0.95286600

H	-7.09386600	0.71585100	0.79171100
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Au	0.76221800	-0.87459900	0.03496500
N	2.68401000	-0.31836500	0.00674700
C	4.98024700	-0.20597200	0.00116200
C	-1.49867500	1.70694600	-1.27193200
N	-2.06307200	-0.27739400	0.06984300
C	-1.24506500	3.07684800	-1.31687300
H	-1.09204300	3.55022100	-2.27954600
C	5.27992200	-2.96421700	0.09177200
H	5.41718600	-4.03847200	0.12741600
C	-1.17427900	-1.23662800	0.07263200
C	3.05575100	1.01043000	-0.03594200
C	0.02901100	0.98037700	-3.09302700
H	0.74860500	0.63000500	-2.35025200
H	0.29467300	2.00728900	-3.35591400
H	0.12773000	0.36530100	-3.98963800
C	-1.49372000	1.83974600	1.17572500
C	-1.14540500	3.82990900	-0.15893100
H	-0.94897400	4.89307100	-0.21695500
C	3.84844100	-1.05571800	0.02998600
C	-1.69220400	1.11911800	-0.01166300
C	0.03390300	1.27420200	3.05072800
H	0.73305600	0.81051800	2.35137700
H	0.12471700	0.77415700	4.01702900
H	0.33357800	2.31738800	3.17818000
C	5.04291100	2.40882800	-0.08213000
H	6.12175000	2.51951700	-0.08667000
C	2.23087800	2.13816600	-0.06999800
H	1.14942800	2.03197700	-0.06453800
C	-1.40855700	0.91994200	-2.56562400
H	-1.63883100	-0.12721800	-2.35531100
C	-1.40944300	1.19255100	2.54404500

H	-1.66543600	0.13430000	2.44801200
C	4.46360000	1.14058700	-0.04169600
C	3.99839500	-2.44284200	0.07570700
H	3.12480800	-3.08605700	0.09829400
C	-3.33795400	-2.22185600	0.37405400
H	-4.02571000	-2.81555300	-0.23076800
H	-3.55997900	-2.43175700	1.42469000
C	6.26280300	-0.75354500	0.01797700
H	7.13486000	-0.10918800	-0.00387500
C	-2.36238200	1.43125500	-3.64433900
H	-3.40328600	1.43391200	-3.31928000
H	-2.28284300	0.80876500	-4.53759800
H	-2.09988300	2.45108300	-3.93439700
C	2.82756700	3.38634300	-0.10984100
H	2.20103000	4.27149800	-0.13656700
C	-1.23694400	3.20529200	1.07407700
H	-1.07783000	3.77857400	1.97977800
C	6.40780600	-2.12985700	0.06308700
H	7.39713400	-2.56985300	0.07675300
C	-2.34913300	1.84022800	3.55994000
H	-3.38377700	1.86019800	3.21457500
H	-2.04418200	2.86943900	3.76156100
H	-2.31013100	1.29818700	4.50669400
C	4.22386400	3.52605600	-0.11608000
H	4.66166500	4.51602700	-0.14754300
C	-1.87000500	-2.57008800	0.07559800
C	-1.68210200	-3.17878900	-1.31815300
C	-1.26045400	-3.49438600	1.12335100
H	-0.62006600	-3.30916900	-1.53426200
H	-2.11258300	-2.54388500	-2.09606900
H	-0.21234800	-3.69322500	0.89086400
H	-1.30884100	-3.04513300	2.11791100
H	-2.17278600	-4.15396800	-1.35772900
H	-1.80282100	-4.44259900	1.14348200

C	-3.49745000	-0.71739100	0.11058100
C	-4.24729200	-0.01203900	1.23726500
C	-4.17800600	-0.38907800	-1.21884400
C	-5.71848300	-0.41162500	1.25196200
H	-4.16783400	1.07224300	1.09344700
H	-3.77610000	-0.25599200	2.19222300
C	-5.66157600	-0.74218400	-1.21456000
H	-4.06847300	0.68847900	-1.38705500
H	-3.66664000	-0.90159900	-2.03771900
C	-6.38384800	-0.05007900	-0.06795100
H	-6.22071300	0.07552300	2.08965900
H	-5.80349100	-1.49258900	1.41763000
H	-6.10009100	-0.46632300	-2.17552700
H	-5.78598700	-1.82632300	-1.11504500
H	-7.44046600	-0.32397200	-0.05780800
H	-6.33258700	1.03569200	-0.21026000

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Au	-0.83150500	-0.84837600	-0.05632300
N	-2.75014600	-0.28374200	-0.04376000
C	-5.04606100	-0.16432200	-0.03116100
C	1.40879600	1.58742000	1.32048900
N	2.03131600	-0.33883800	-0.07563100
C	1.14104800	2.95180200	1.40649500
H	0.94743000	3.38923400	2.37898300
C	-5.35425300	-2.92206300	-0.11343200
H	-5.49492000	-3.99597300	-0.14585100
C	1.09419600	-1.25842400	-0.08817600
C	-3.11793700	1.04576300	-0.00375400
C	-0.12796300	0.81120200	3.11011100
H	-0.85927400	0.56644400	2.33723200
H	-0.35065000	1.81762300	3.47342400
H	-0.25536200	0.11714000	3.94289600
C	1.51418800	1.81559800	-1.11897300

C	1.08397800	3.74752300	0.27258100
H	0.87397700	4.80582800	0.36312300
C	-3.91689100	-1.01770900	-0.06171900
C	1.66381700	1.05570100	0.04715100
C	0.12458400	1.25255400	-3.09401800
H	-0.59308900	0.74368000	-2.44629300
H	0.10487700	0.77955900	-4.07782200
H	-0.20606800	2.28818200	-3.20717000
C	-5.09844600	2.45182000	0.04721000
H	-6.17670600	2.56773400	0.05563100
C	-2.28759800	2.16892700	0.02348100
H	-1.20714700	2.05501200	0.01155300
C	1.30938400	0.74615200	2.58064800
H	1.52837200	-0.29389800	2.32447300
C	1.53893600	1.21030600	-2.50768900
H	1.83664300	0.16103000	-2.42697200
C	-4.52501800	1.18088500	0.00698200
C	-4.07110900	-2.40445800	-0.10319200
H	-3.19938900	-3.05035200	-0.12714200
C	3.15767600	-2.32063500	-0.54079300
H	3.87084200	-3.01641900	-0.10022300
H	3.23073100	-2.41166100	-1.63038700
C	-6.33023200	-0.70816800	-0.04188400
H	-7.20031800	-0.06122000	-0.01845400
C	2.26417400	1.18348700	3.69223300
H	3.31359700	1.04611900	3.43161700
H	2.06245300	0.60339500	4.59481800
H	2.11114800	2.23657600	3.93947200
C	-2.87833300	3.41988300	0.06414000
H	-2.24830600	4.30271100	0.08605400
C	1.23597200	3.17374800	-0.97964400
H	1.11548000	3.78179300	-1.86850400
C	-6.47945400	-2.08420300	-0.08288400
H	-7.47014900	-2.52123400	-0.09180600

C	2.51151700	1.92273100	-3.44620800
H	3.52633700	1.95464200	-3.04599400
H	2.18997600	2.95088500	-3.62608300
H	2.53775700	1.41617600	-4.41283500
C	-4.27404300	3.56541900	0.07619800
H	-4.70742700	4.55733300	0.10767400
C	1.72541500	-2.62020700	-0.10651400
C	1.66192500	-3.15680000	1.32820800
C	0.99632900	-3.56873400	-1.04713700
H	0.62813900	-3.18896700	1.67834000
H	2.23932000	-2.53239100	2.01408800
H	-0.02642000	-3.73469200	-0.70210100
H	0.94992400	-3.15984500	-2.05859600
H	2.07331000	-4.16845200	1.35400300
H	1.51450800	-4.53000700	-1.08277400
C	3.43234300	-0.85877400	-0.15964900
C	4.33344600	-0.60741400	1.07520100
C	4.41408800	-0.17513000	-1.13615600
C	5.62420500	-1.31310200	0.62884900
C	4.64405000	0.89598300	1.01177700
H	3.93461500	-0.95008400	2.03136600
C	5.64566600	-1.06620000	-0.90591600
C	4.74541600	1.18135700	-0.50544300
H	4.08209300	-0.14424200	-2.17417100
H	6.48785800	-0.87638000	1.13120100
H	5.62078600	-2.37759800	0.86363800
H	3.86397500	1.50720200	1.45629500
H	5.57029700	1.11351500	1.54623300
H	6.55426500	-0.56452500	-1.23905100
H	5.56890800	-2.00477300	-1.45655100
H	4.05054600	1.96692400	-0.79790400
H	5.74489800	1.50222800	-0.80461400

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Au	-1.40559800	-0.88686500	0.00057900
N	-3.27438300	-0.17076300	0.00068800
C	-5.55277600	0.13422100	0.00010700
C	1.05823300	1.57647800	1.22585100
N	1.45545800	-0.51516400	0.00020900
C	2.87044800	-1.05301000	0.00026800
C	0.96231200	2.96679800	1.19669800
H	0.85915300	3.50451800	2.13154300
C	-6.08384900	-2.59037700	0.00071300
H	-6.31102500	-3.64988300	0.00095800
C	0.49776700	-1.40283400	0.00050100
C	-3.53262000	1.18570300	0.00017100
C	-0.59329200	1.04994700	3.00588800
H	-1.30166400	0.65361900	2.27592000
H	-0.81926000	2.11029000	3.14614200
H	-0.75385200	0.53954000	3.95781100
C	1.05715800	1.57555600	-1.22682100
C	0.95500300	3.66304500	-0.00118000
H	0.88610900	4.74366400	-0.00159200
C	-4.49648700	-0.80807600	0.00055400
C	1.19713800	0.90798600	-0.00027800
C	-0.59526200	1.04794000	-3.00590300
H	-1.30351700	0.65211700	-2.27555500
H	-0.75611100	0.53698000	-3.95748200
H	-0.82118700	2.10821300	-3.14676100
C	-5.39738400	2.74550100	-0.00077600
H	-6.46342800	2.94480800	-0.00106500
C	-2.61713700	2.24228200	-0.00001600
H	-1.54753200	2.04939900	0.00032600
C	0.86033100	0.87562500	2.55458900
H	1.05074600	-0.19287400	2.42212500
C	0.85849300	0.87382700	-2.55499300
H	1.04895700	-0.19459600	-2.42193900
C	-4.92481100	1.43318300	-0.00017600

C	-4.76294900	-2.17843300	0.00085500
H	-3.94676700	-2.89343700	0.00120000
C	2.59831900	-2.57882100	0.00105000
H	3.05641700	-3.05071200	0.86548500
H	3.05662800	-3.05157200	-0.86282200
C	-6.87685600	-0.30366400	-0.00003200
H	-7.69146200	0.41229000	-0.00039300
C	1.79384600	1.41216300	3.63600200
H	2.82897900	1.44258000	3.29839600
H	1.73803300	0.78548500	4.52823300
H	1.49871500	2.42280400	3.92856800
C	-3.10889000	3.53607200	-0.00062600
H	-2.41108300	4.36657000	-0.00079500
C	0.96117300	2.96588000	-1.19854800
H	0.85712000	3.50294500	-2.13367200
C	-7.13742800	-1.66360900	0.00027400
H	-8.16033900	-2.01886500	0.00018800
C	1.79159200	1.40967500	-3.63714000
H	2.82681000	1.44052000	-3.29985600
H	1.49620900	2.42005700	-3.93035200
H	1.73564000	0.78232900	-4.52889400
C	-4.48869400	3.79147900	-0.00101000
H	-4.84263400	4.81491900	-0.00147300
C	1.07032200	-2.78857200	0.00118300
C	0.57283100	-3.52045100	1.24907100
C	0.57242600	-3.52241200	-1.24529400
H	-0.51275600	-3.62757600	1.21533700
H	0.82384300	-2.97297200	2.16090500
H	-0.51312800	-3.62977900	-1.21083100
H	0.82268200	-2.97632100	-2.15815900
H	1.02607000	-4.51310900	1.30020300
H	1.02583100	-4.51505000	-1.29521800
C	3.61592700	-0.59677900	-1.26200600
C	3.50487500	-1.30345900	-2.46250500

C	4.45501800	0.51910000	-1.23566500
C	4.25714400	-0.96999200	-3.57762700
H	2.81906000	-2.13713800	-2.54198300
C	5.22465600	0.84162500	-2.35306800
C	5.14726700	0.09480100	-3.51617100
H	4.15300200	-1.54722300	-4.48725600
H	5.89493400	1.69180900	-2.29444100
H	5.75988500	0.34969700	-4.37134500
C	3.61665100	-0.59565400	1.26165200
C	3.50665400	-1.30131200	2.46286600
C	4.45575300	0.52014700	1.23361000
C	4.25982600	-0.96684100	3.57706300
H	2.82098100	-2.13497700	2.54370400
C	5.22637200	0.84364600	2.35009000
C	5.14989800	0.09790200	3.51394600
H	4.15642100	-1.54326000	4.48729200
H	5.89666800	1.69371600	2.29010200
H	5.76324000	0.35352700	4.36838300
C	4.54405700	1.36110400	-0.00141500
H	5.47048100	1.93811600	-0.00182000
H	3.71952000	2.08834500	-0.00167900

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Au	-1.31104100	-0.79069900	-0.31683000
N	-3.23606900	-0.27076400	-0.15330800
C	-5.53240300	-0.17976300	-0.09921600
C	0.80268400	1.18262600	1.77472100
N	1.54928600	-0.27466500	-0.11471400
C	2.96426200	-0.68993800	-0.53095100
C	0.55404400	2.48156600	2.22089700
H	0.28327000	2.63012300	3.25947900
C	-5.82075700	-2.80637900	-0.95069600
H	-5.95366900	-3.82935100	-1.28229700
C	0.62005300	-1.12248400	-0.49860900

C	-3.61289800	0.99232900	0.25615900
C	-0.95223500	-0.00442300	3.10603700
H	-1.57657200	-0.17404800	2.22857800
H	-1.27343000	0.93388000	3.56483100
H	-1.13403500	-0.81043400	3.82005200
C	1.10230200	2.09086200	-0.48214900
C	0.60089800	3.56845300	1.36569300
H	0.40403800	4.56495300	1.74048800
C	-4.39738900	-0.98023600	-0.37289200
C	1.16755400	1.02030900	0.42594900
C	-0.24490500	2.02414500	-2.55972500
H	-0.92313400	1.28950500	-2.11908300
H	-0.22903200	1.88118300	-3.64234300
H	-0.65297700	3.01700000	-2.35218800
C	-5.60421700	2.30852500	0.70986000
H	-6.68326500	2.40646300	0.75671400
C	-2.79128900	2.07394000	0.58452400
H	-1.70972800	1.98361600	0.52558100
C	0.54038200	0.05713900	2.76333300
H	0.82295800	-0.89428800	2.30271500
C	1.17123700	1.91130100	-1.98627400
H	1.54978800	0.91069500	-2.20859800
C	-5.02090600	1.10541600	0.31249000
C	-4.54140600	-2.30125800	-0.80010300
H	-3.66509000	-2.90738900	-1.00562200
C	2.58952100	-1.68038000	-1.63528800
H	3.35689700	-2.42392500	-1.83861400
H	2.40326200	-1.12386500	-2.55842600
C	-6.81253500	-0.71022200	-0.25677100
H	-7.68723600	-0.10369400	-0.04904100
C	1.31203800	0.24041700	4.07727100
H	2.35335400	0.53354600	3.93362200
H	1.28846100	-0.68449800	4.65659300
H	0.83906300	1.01554100	4.68420800

C	-3.39194700	3.25699900	0.97857200
H	-2.76884800	4.10629000	1.23769300
C	0.83400700	3.36250500	0.01588900
H	0.78501700	4.19685700	-0.67317500
C	-6.95180900	-2.02065700	-0.68209300
H	-7.93930900	-2.44626300	-0.80949400
C	2.08608400	2.92421600	-2.67002200
H	3.06950000	2.96597400	-2.20212500
H	1.64782900	3.92447300	-2.64082100
H	2.21375300	2.65837800	-3.72120500
C	-4.78853500	3.37797500	1.04354500
H	-5.22940800	4.31718900	1.35370900
C	1.25801700	-2.29090100	-1.19613700
C	1.37768400	-3.43824600	-0.18582200
C	0.43101700	-2.74612100	-2.39153600
H	0.37879600	-3.78766200	0.08241200
H	1.89286500	-3.13985800	0.72790400
H	-0.53304100	-3.13895500	-2.06318800
H	0.24147300	-1.91552800	-3.07561400
H	1.92744500	-4.26752400	-0.63732300
H	0.96347300	-3.53220000	-2.93302000
C	3.85591200	0.46542900	-0.98149100
C	4.49046800	0.43627000	-2.22034600
C	4.18073600	1.49507000	-0.09411200
C	5.41674100	1.41350100	-2.57205600
H	4.28572700	-0.36144100	-2.92258800
C	5.09329100	2.47697900	-0.44738500
H	3.72516200	1.52766200	0.88840800
C	5.71982700	2.43822600	-1.68892900
H	5.90166900	1.36555100	-3.53876300
H	5.32326300	3.26882600	0.25388700
H	6.44014900	3.19909000	-1.96072300
C	3.73267600	-1.37298200	0.60372100
C	4.72088900	-2.31731400	0.32749600

C	3.53451400	-0.99775300	1.92418700
C	5.44021100	-2.91018900	1.35646100
H	4.95394600	-2.58945400	-0.69402300
C	4.24618100	-1.58979500	2.95916200
H	2.82392500	-0.21779400	2.13937200
C	5.19598900	-2.56220300	2.67935800
H	6.19758000	-3.64698100	1.12040300
H	4.05762600	-1.28367000	3.98124100
H	5.75228800	-3.03250400	3.47977300

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Au	-0.13313400	1.48592600	-0.47994800
N	0.04228400	3.26197300	0.53549400
C	0.18859500	5.47342400	1.13221500
C	-1.14636900	-1.36559800	1.60002800
N	-0.04862800	-1.40713700	-0.59414800
C	-0.00812500	-2.68587600	-1.39642500
C	-1.08518900	-1.44884200	2.99550100
H	-2.00369900	-1.44538300	3.56664200
C	-0.29220600	6.34289900	-1.47141600
H	-0.47574800	6.70710100	-2.47299400
C	-0.20663500	-0.33093300	-1.31004000
C	0.29818900	3.30864700	1.86912000
C	1.32253900	-1.42159900	1.46499800
C	0.16578000	-1.56851700	3.62265100
C	-0.02681000	4.55227900	0.07568100
C	0.03360000	-1.36421900	0.84918400
C	0.66822000	4.90968500	3.64322600
H	0.75747100	5.92217400	4.01655700
C	0.45426100	2.21987900	2.74091300
H	0.36831700	1.20138400	2.38045000
C	0.40475800	4.65540500	2.31888400
C	-0.26820900	4.97474100	-1.23056900
H	-0.42845500	4.24956000	-2.01837000

C	0.13580200	-2.12185400	-2.81642000
H	-0.40696000	-2.72596300	-3.54553700
H	1.19557200	-2.12065100	-3.09014800
C	0.16108100	6.82621500	0.87575800
H	0.32332100	7.55134200	1.66342700
C	0.72063500	2.50081100	4.07111000
H	0.84900300	1.68513200	4.76915400
C	1.32021100	-1.57021100	2.88316200
H	2.27544200	-1.63111100	3.38982500
C	-0.08198700	7.25394600	-0.43822400
H	-0.10575700	8.31392600	-0.65315200
C	-1.30097000	-3.46726700	-1.18664500
H	-1.35990000	-3.83276200	-0.15987400
H	-1.29537600	-4.33082600	-1.85338600
H	-2.19160800	-2.87264500	-1.39391600
C	0.82604700	3.81863400	4.51745900
H	1.03593300	4.00873900	5.56156700
C	1.15947200	-3.58024100	-1.01061000
H	2.12121400	-3.11243200	-1.21819400
H	1.08624000	-4.49695500	-1.59955000
H	1.11407000	-3.85001700	0.04649300
C	-0.36142200	-0.66959800	-2.76558400
C	-1.83765100	-0.50768700	-3.14583500
H	-2.17282100	0.51196400	-2.93769600
H	-1.95468900	-0.69468300	-4.21557100
H	-2.48672500	-1.19557600	-2.60411600
C	0.47380400	0.26436900	-3.63421600
H	0.41234300	-0.05306600	-4.67753300
H	0.09888400	1.28835000	-3.56180300
H	1.52155700	0.25719700	-3.33343000
C	2.58516400	-1.43794900	0.75857100
C	3.62374600	-2.28658300	1.23182600
C	2.88999700	-0.68031000	-0.40183500
C	4.82567000	-2.39743800	0.57602000

H	3.44354100	-2.91085800	2.09729900
C	4.10594000	-0.80923000	-1.04540000
H	2.19154200	0.05567600	-0.77205800
C	5.10367200	-1.66974000	-0.59008000
H	6.05601200	-1.75408000	-1.09321000
C	-2.50730200	-1.42911500	1.00023800
C	-3.29699700	-2.54041700	1.28259700
C	-3.05163400	-0.42305400	0.20215900
C	-4.56617200	-2.67469900	0.73203500
H	-2.89741200	-3.32514700	1.91609100
C	-4.32145600	-0.56112000	-0.33883700
H	-2.48429700	0.47749700	0.00909700
C	-5.08803000	-1.69320800	-0.09342500
H	-6.07479100	-1.79723500	-0.52578000
C	-5.33565300	-3.93164700	1.02778100
C	-4.90218800	0.50953100	-1.22036400
F	-6.55916800	-3.91441900	0.49566900
F	-4.70424700	-5.01101100	0.54391100
F	-5.47107500	-4.12615000	2.34476800
F	-5.10005900	0.05977900	-2.46913600
F	-4.11032000	1.58252800	-1.30906800
F	-6.09229000	0.92618500	-0.77336400
C	5.88566300	-3.33250600	1.07845500
C	4.34601700	-0.02595300	-2.30144800
F	6.18904500	-4.27289100	0.16903600
F	5.53166500	-3.97247400	2.19804400
F	7.03123300	-2.68463000	1.34268100
F	5.63881800	0.24347000	-2.50066700
F	3.69266400	1.14684500	-2.31224000
F	3.92551200	-0.69805400	-3.39385800
H	0.22068100	-1.65563400	4.70101700

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Au	0.09566000	1.54334900	0.38922400
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N	0.06219900	3.44723400	-0.38138000
C	0.72882600	5.46770200	-1.25983500
C	1.12873300	-1.52170400	-1.64946600
N	-0.08461700	-1.44525500	0.49255800
C	-0.14479900	-2.64803800	1.35884100
C	1.10329800	-1.58062000	-3.04273700
H	2.04524600	-1.62813900	-3.57648200
C	3.41792500	4.74529300	-1.20930600
H	4.46891200	4.49093900	-1.19664000
C	0.12162700	-0.26374000	1.17939700
C	-1.05770900	4.21135800	-0.58201500
C	-1.29654800	-1.48662100	-1.63427300
C	-0.09768600	-1.58393500	-3.73647300
C	1.13796400	4.19472700	-0.78389000
C	-0.07883800	-1.47684600	-0.92850500
C	-1.71270200	6.39432500	-1.39847300
H	-1.48106000	7.36750000	-1.81341500
C	-2.38156000	3.85996400	-0.30809800
H	-2.61284700	2.88958300	0.11166400
C	-0.72254400	5.47872400	-1.12648100
C	2.48382900	3.82403800	-0.75371500
H	2.77343300	2.85128700	-0.37896300
C	-0.36276400	-1.99331600	2.72924400
H	0.06698000	-2.59043800	3.53709600
H	-1.44193600	-1.90858000	2.90211700
C	1.66707500	6.36885700	-1.70820900
H	1.37859900	7.34628500	-2.07469600
C	-3.36838600	4.79679100	-0.58757200
H	-4.40341600	4.55797900	-0.38479800
C	-1.28546700	-1.54600300	-3.03205300
H	-2.23145500	-1.54388200	-3.56036300
C	3.01952200	5.99540300	-1.67931200
H	3.76849300	6.69436100	-2.02754300
C	1.14455100	-3.46922800	1.28909400

H	1.23664300	-3.94359200	0.30845700
H	1.11120100	-4.26011800	2.04134500
H	2.03437500	-2.86373600	1.45958800
C	-3.04320900	6.04122600	-1.12360600
H	-3.83220500	6.75186200	-1.33162600
C	-1.29572600	-3.58180600	1.00131200
H	-2.26622500	-3.10914500	1.15683000
H	-1.24152100	-4.46748800	1.63761600
H	-1.22321000	-3.91485000	-0.03806000
C	0.22669900	-0.57577700	2.65308400
C	1.68124700	-0.51619700	3.13870900
H	2.07689600	0.49111100	2.98549100
H	1.73671800	-0.75214100	4.20624700
H	2.32616000	-1.21237600	2.60274300
C	-0.58356900	0.40527300	3.49718700
H	-0.55648200	0.11787100	4.55226100
H	-0.16793500	1.41204000	3.40594600
H	-1.62385400	0.43540200	3.16709900
C	-2.61440000	-1.52723900	-0.95571500
C	-3.55330200	-2.46686400	-1.37717700
C	-2.96091800	-0.67605200	0.09650900
C	-4.79379500	-2.56513800	-0.75924800
H	-3.30104700	-3.15789800	-2.17431500
C	-4.20041300	-0.78492400	0.70539800
H	-2.25069800	0.06958500	0.44093800
C	-5.13249400	-1.73126600	0.29121700
H	-6.09918100	-1.80558600	0.76966700
C	2.46431700	-1.63302000	-1.00121800
C	3.21536000	-2.77880300	-1.23888900
C	3.01579700	-0.63057300	-0.20114200
C	4.46038400	-2.95350100	-0.64485200
H	2.80835500	-3.56188600	-1.87013600
C	4.26286400	-0.80999500	0.37764400
H	2.45503300	0.27730900	-0.02061300

C	4.99188700	-1.97647900	0.17784000
H	5.96076000	-2.10842700	0.64200500
C	5.19178700	-4.24065100	-0.90006400
C	4.87015100	0.25580500	1.24698200
F	6.40122600	-4.25828100	-0.33687900
F	4.51169200	-5.29160800	-0.42081500
F	5.35557100	-4.45952500	-2.21169700
F	5.03088200	-0.16608900	2.50731100
F	4.12811700	1.36681700	1.29020400
F	6.08677100	0.61054700	0.80724600
C	-5.74828500	-3.61520100	-1.25580600
C	-4.52870000	0.10100800	1.87493000
F	-5.23861700	-4.84606800	-1.11435600
F	-6.01052100	-3.45919800	-2.56076600
F	-6.91459500	-3.58935500	-0.60835700
F	-5.84172200	0.33779700	1.96880400
F	-3.91537800	1.28889500	1.79629500
F	-4.15244600	-0.45461700	3.03591800
H	-0.10393800	-1.61882700	-4.81808800

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Au	-0.25877400	1.54128300	-0.44710900
N	-0.39872400	3.34802400	0.51619800
C	-0.65736700	5.57451100	1.02225900
C	-0.93949200	-1.44961800	1.59848400
N	0.21734200	-1.37296500	-0.57552100
C	0.37432800	-2.58729700	-1.41354600
C	-0.87947900	-1.42563100	2.99165200
H	-1.80152200	-1.52877800	3.55149300
C	-1.07052300	6.25137400	-1.65149300
H	-1.23424900	6.54387100	-2.67969400
C	-0.15629600	-0.24732700	-1.28072400
C	-0.26033000	3.49038100	1.87170800
C	1.47512200	-1.20110200	1.51636800

C	0.33458300	-1.28881600	3.65297600
C	-0.63861600	4.58864400	-0.00068100
C	0.24551900	-1.34428900	0.84532300
C	-0.29615400	5.19107400	3.58906900
H	-0.40245000	6.21817400	3.91555200
C	-0.00690500	2.47771600	2.79883900
H	0.09758500	1.44851300	2.47463200
C	-0.40631500	4.84599700	2.26139600
C	-0.84427900	4.91677100	-1.34289700
H	-0.82426900	4.14364500	-2.10012800
C	0.48897400	-1.94705200	-2.80380700
H	0.10669200	-2.60741800	-3.58584500
H	1.54843200	-1.75318800	-3.00671900
C	-0.88250700	6.89186700	0.69792000
H	-0.90151600	7.66403100	1.45693100
C	0.10132700	2.84477500	4.13410300
H	0.29747900	2.08639300	4.88053800
C	1.49951700	-1.18631900	2.91676000
H	2.45346600	-1.07536700	3.41864100
C	-1.08983100	7.22238700	-0.65133300
H	-1.26853100	8.25517000	-0.91992200
C	-0.83016400	-3.52268100	-1.29025700
H	-0.84902700	-3.98618400	-0.30054800
H	-0.74635100	-4.32003800	-2.03169800
H	-1.77626700	-3.00328500	-1.44154800
C	-0.04013700	4.17544400	4.52423000
H	0.04876000	4.43324300	5.57137600
C	1.61767500	-3.39672200	-1.06528900
H	2.53523800	-2.84125100	-1.26237200
H	1.62941000	-4.30292300	-1.67425100
H	1.60459800	-3.70299300	-0.01525800
C	-0.24870700	-0.59789100	-2.74422300
C	-1.70766500	-0.69820700	-3.20833100
H	-2.20680500	0.26247000	-3.05714800

H	-1.75241200	-0.94876500	-4.27290300
H	-2.26827700	-1.45309000	-2.65732200
C	0.44445500	0.44997800	-3.61242100
H	0.43032600	0.14973400	-4.66407200
H	-0.07177000	1.40995200	-3.52306400
H	1.48085000	0.59154500	-3.30006700
C	2.77258400	-1.15839500	0.79997600
C	3.80219100	-1.98910500	1.23681300
C	3.01022600	-0.33611500	-0.30499500
C	5.02782300	-2.01223400	0.58207200
H	3.63523500	-2.65765000	2.07457800
C	4.23484900	-0.37104100	-0.95046000
H	2.23101100	0.33199500	-0.65813300
C	5.25861600	-1.21062800	-0.52087400
H	6.21240100	-1.22737600	-1.02973600
C	-2.26747700	-1.73199900	0.98542400
C	-2.86137700	-2.95865800	1.25803300
C	-2.95546200	-0.82091800	0.18142500
C	-4.08126200	-3.30419500	0.68586900
H	-2.34749600	-3.67095000	1.89518700
C	-4.17623000	-1.17167900	-0.37548900
H	-2.53014200	0.15368700	-0.01398000
C	-4.74339400	-2.41982000	-0.14678300
H	-5.69110300	-2.68546400	-0.59735100
C	-4.63294300	-4.67146300	0.97078100
C	-4.92627400	-0.20820900	-1.25342100
F	-5.83047200	-4.86309700	0.41490900
F	-3.81873400	-5.63150200	0.50837300
F	-4.76164400	-4.88488200	2.28742800
F	-5.07235000	-0.69015400	-2.49614700
F	-4.31746700	0.97429800	-1.35262000
F	-6.16335600	0.01650100	-0.78739300
C	6.08956100	-2.93944200	1.10443100
C	4.44700100	0.47147900	-2.17809600

F	7.20248100	-2.90442800	0.36981900
F	5.66279000	-4.20912800	1.12685200
F	6.43117000	-2.63071600	2.36347500
F	5.73145200	0.81028300	-2.33409900
F	3.73467400	1.59990000	-2.14640000
F	4.08529200	-0.18891300	-3.29086200
H	0.36797900	-1.27120400	4.73493300

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Au	0.07529500	1.52570400	0.28624000
N	-0.14732100	3.32412900	-0.67815000
C	-0.37648600	5.54704300	-1.20199800
C	1.09767700	-1.25916700	-1.86965300
N	0.05092600	-1.37154700	0.34434800
C	0.05574400	-2.66478900	1.12364200
C	1.00599500	-1.29876500	-3.26638700
H	1.91087700	-1.26643200	-3.85799900
C	0.04651900	6.34596300	1.43417000
H	0.20667500	6.68293100	2.44919200
C	0.19664700	-0.30536900	1.07679200
C	-0.39600900	3.40563200	-2.01150800
C	-1.36754000	-1.35432200	-1.68044100
C	-0.25784600	-1.41265300	-3.86757000
C	-0.13421700	4.59989700	-0.17470700
C	-0.06527500	-1.29599700	-1.09495100
C	-0.81534900	5.04949400	-3.73460500
H	-0.94075500	6.06967100	-4.07516200
C	-0.50778400	2.34111800	-2.91897300
H	-0.38928600	1.31513000	-2.59039500
C	-0.55095700	4.76156600	-2.41728200
C	0.07899600	4.98684100	1.14735100
H	0.26107900	4.24214700	1.91193400
C	-0.07742300	-2.12974000	2.55628500
H	0.49077800	-2.72823100	3.27088200

H	-1.13382700	-2.15809900	2.84511800
C	-0.40462400	6.89040800	-0.90007000
H	-0.58836400	7.63493100	-1.66457400
C	-0.77601500	2.65558800	-4.24116600
H	-0.87129200	1.85913100	-4.96621400
C	-1.39553300	-1.45356900	-3.10338600
H	-2.36086200	-1.51043700	-3.59088600
C	-0.19036400	7.28251800	0.42999000
H	-0.21037900	8.33473100	0.68051600
C	1.36202500	-3.41338200	0.87826400
H	1.40681400	-3.76918500	-0.15262900
H	1.39035200	-4.28197800	1.53773800
H	2.24359100	-2.80044400	1.07103100
C	-0.92663300	3.98277700	-4.64515000
H	-1.13683900	4.19925700	-5.68405100
C	-1.09574100	-3.58128900	0.73987300
H	-2.06558400	-3.14676700	0.97912600
H	-0.98425000	-4.51002100	1.30331900
H	-1.06514300	-3.82318400	-0.32454600
C	-2.61020200	-1.43091400	-0.94307700
C	-3.63582300	-2.29159300	-1.42377800
C	-2.90562000	-0.73504400	0.25874500
C	-4.80900800	-2.47907500	-0.73514600
H	-3.46349100	-2.86758000	-2.32362200
C	-4.09163900	-0.94402700	0.93730800
H	-2.22396000	0.01101900	0.64042500
C	-5.07130100	-1.82116500	0.47619500
H	-5.99944500	-1.96977300	1.00847800
C	2.47001400	-1.33367700	-1.29765100
C	3.26097000	-2.42664200	-1.64226800
C	3.02127300	-0.36282900	-0.46064100
C	4.53753100	-2.58111400	-1.11562400
H	2.85507600	-3.18360400	-2.30487300
C	4.30005200	-0.52012000	0.05497300

H	2.45329700	0.52581700	-0.21874000
C	5.06709300	-1.63649400	-0.25280900
H	6.06092400	-1.75503700	0.15885200
C	5.30828500	-3.81886500	-1.48123800
C	4.88987900	0.50999400	0.97827800
F	6.53370100	-3.82760100	-0.95324900
F	4.68055600	-4.92377600	-1.05408900
F	5.43959200	-3.94181100	-2.80727600
F	5.02131800	0.03177100	2.22693200
F	4.14036700	1.61325000	1.05747900
F	6.11250200	0.88283500	0.58529600
C	-5.85530500	-3.42145100	-1.25169000
C	-4.30919000	-0.23384700	2.24011100
F	-5.49674700	-4.03191800	-2.38615400
F	-7.01318300	-2.78760100	-1.49750100
F	-6.13874500	-4.38483800	-0.36026600
F	-5.60188600	-0.08586700	2.53834300
F	-3.75721200	0.98986400	2.25992300
F	-3.75657000	-0.90814800	3.27286200
H	-0.33671800	-1.46478700	-4.94679200
C	0.38233700	-0.66547500	2.51800600
C	1.85937300	-0.46917800	2.89155800
C	-0.44804100	0.23799600	3.43168000
C	2.06644600	-0.56588200	4.37486700
H	2.19417300	0.50982000	2.52262200
H	2.48385900	-1.20976600	2.38453400
C	-0.34977800	-0.24562300	4.87137000
H	-0.05292300	1.25755600	3.35296400
H	-1.48660100	0.26032700	3.09776800
C	1.07664800	-0.49508800	5.26072500
H	3.08641300	-0.71573600	4.71295400
H	-0.79416400	0.49262100	5.54308900
H	-0.94361300	-1.15810000	5.00562800
H	1.29797600	-0.60812300	6.31680100

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Au	0.07811000	1.56135600	0.20850800
N	0.02506800	3.47774500	-0.52855200
C	0.66671300	5.50121100	-1.41816900
C	1.08434000	-1.43441900	-1.90125100
N	-0.10523600	-1.42598100	0.25565300
C	-0.13834000	-2.64586200	1.09910500
C	1.04050600	-1.45134400	-3.29504400
H	1.97544000	-1.47443500	-3.84257300
C	3.35483300	4.77522500	-1.45694600
H	4.40535100	4.51956700	-1.47867900
C	0.13223800	-0.26257600	0.95950300
C	-1.09922300	4.24435900	-0.68880600
C	-1.34194300	-1.42291600	-1.85391200
C	-0.17016400	-1.44690500	-3.97276900
C	1.08899200	4.22547200	-0.96210100
C	-0.11486000	-1.42318000	-1.16533600
C	-1.77642900	6.43211300	-1.47361600
H	-1.55672200	7.40675500	-1.89154200
C	-2.41431300	3.89362200	-0.37371800
H	-2.63351600	2.92151800	0.04883600
C	-0.77961900	5.51387000	-1.23773800
C	2.43439200	3.85288400	-0.97620800
H	2.73496700	2.87812900	-0.61522100
C	-0.33696800	-2.02048700	2.48570200
H	0.10822900	-2.62735100	3.27789600
H	-1.41498100	-1.94599500	2.67641800
C	1.59127900	6.40323800	-1.89228200
H	1.29265000	7.38273300	-2.24481400
C	-3.40790400	4.83314000	-0.61711000
H	-4.43635000	4.59504000	-0.38253600
C	-1.34925300	-1.44255600	-3.25287600
H	-2.30199500	-1.43505100	-3.76890500

C	2.94340300	6.02784000	-1.90842200
H	3.68183400	6.72739600	-2.27727900
C	1.15860900	-3.45068300	0.99376600
H	1.23756500	-3.91383800	0.00682300
H	1.15039500	-4.24876900	1.73898400
H	2.04320900	-2.83404000	1.15306000
C	-3.09793700	6.07958500	-1.15773800
H	-3.89210300	6.79224300	-1.33708600
C	-1.28565100	-3.58375200	0.74259200
H	-2.25814400	-3.12488700	0.92497700
H	-1.21062300	-4.48164000	1.35935200
H	-1.22833200	-3.89425300	-0.30467200
C	-2.64686700	-1.49332000	-1.15380100
C	-3.58701300	-2.42757100	-1.58455600
C	-2.97710800	-0.67896300	-0.06755900
C	-4.81219700	-2.55760500	-0.94195200
H	-3.34527400	-3.09259900	-2.40660600
C	-4.20039400	-0.82071000	0.56694800
H	-2.26673700	0.06361200	0.28382100
C	-5.13323500	-1.76258300	0.14356000
H	-6.08636200	-1.86423000	0.64354200
C	2.42708300	-1.56455500	-1.27046100
C	3.16590400	-2.71058900	-1.54172400
C	2.99411400	-0.58647500	-0.45048600
C	4.41201700	-2.91354900	-0.95849400
H	2.74715000	-3.47366800	-2.18956000
C	4.24319200	-0.79320100	0.11673900
H	2.44635700	0.32445700	-0.24874200
C	4.95747400	-1.96298400	-0.11414000
H	5.92745000	-2.11648800	0.34091800
C	5.12755300	-4.20193800	-1.24837400
C	4.86525900	0.24447300	1.00903400
F	6.33809000	-4.24811300	-0.68904500
F	4.43627800	-5.25687200	-0.79410900

F	5.28566100	-4.38964800	-2.56559000
F	4.95857900	-0.18148100	2.27595700
F	4.17185000	1.38791400	1.02487900
F	6.11189500	0.54358200	0.61729200
C	-5.77818200	-3.58602900	-1.46120800
C	-4.50499300	0.02140100	1.77447600
F	-5.21190000	-4.79732600	-1.53448900
F	-6.19452900	-3.28423600	-2.69924800
F	-6.86375900	-3.69682000	-0.69327600
F	-5.81899300	0.20826800	1.93598500
F	-3.93756500	1.23251300	1.70069500
F	-4.05457700	-0.54990200	2.90207900
H	-0.19015400	-1.45027100	-5.05478800
C	0.23973800	-0.59692100	2.42458800
C	1.69433300	-0.51717600	2.91869500
C	-0.57390200	0.36389400	3.29827200
C	1.80159900	-0.62955000	4.41194900
H	2.11595900	0.43740400	2.57750200
H	2.30370700	-1.29353900	2.44786500
C	-0.60382900	-0.10218500	4.74839500
H	-0.11112500	1.35550900	3.23507500
H	-1.58625800	0.45350200	2.89490700
C	0.76767100	-0.46626800	5.23298400
H	2.77902300	-0.86630500	4.82089500
H	-1.02649800	0.67881500	5.38620000
H	-1.27672100	-0.96306900	4.85471400
H	0.90835800	-0.58949600	6.30216200

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Au	0.26627800	1.56749400	0.24879600
N	0.41593000	3.39667000	-0.66888300
C	0.70600700	5.63176800	-1.11685700
C	0.85720200	-1.37615200	-1.86823600
N	-0.25189300	-1.34296600	0.32981500

C	-0.39805600	-2.57056000	1.14970200
C	0.76769700	-1.30796000	-3.25839700
H	1.67572600	-1.40543500	-3.84166700
C	1.21518500	6.21927500	1.56144000
H	1.41676000	6.47720100	2.59216000
C	0.15888000	-0.23794300	1.04481900
C	0.23945900	3.58253700	-2.01455100
C	-1.55300000	-1.10290700	-1.72602700
C	-0.45896000	-1.13638500	-3.88790200
C	0.69804300	4.61625000	-0.12333500
C	-0.31067800	-1.27952600	-1.08846400
C	0.25865800	5.33262000	-3.68156100
H	0.37639400	6.36665900	-3.98107600
C	-0.06316700	2.60327200	-2.96242900
H	-0.17928900	1.56733300	-2.66490300
C	0.40199400	4.94601200	-2.36856600
C	0.95184800	4.89927700	1.22081800
H	0.93953900	4.10409500	1.95511300
C	-0.49021700	-1.95315500	2.55176200
H	-0.10280100	-2.62405000	3.32236500
H	-1.54723200	-1.75558700	2.76932400
C	0.96833400	6.93404600	-0.76094000
H	0.98007600	7.72826100	-1.49699300
C	-0.20409900	3.01193000	-4.28240200
H	-0.43853800	2.28032600	-5.04436100
C	-1.60743400	-1.04478100	-3.12440400
H	-2.57049000	-0.90961200	-3.60240300
C	1.22380300	7.21943800	0.59032900
H	1.43210000	8.23987900	0.88362500
C	0.80327800	-3.50569200	0.99545600
H	0.79891100	-3.96857000	0.00539400
H	0.73775700	-4.30310500	1.73858300
H	1.75216300	-2.98483800	1.12432300
C	-0.04677500	4.35062100	-4.63759800

H	-0.16203100	4.64134300	-5.67348700
C	-1.64692400	-3.37307400	0.80557100
H	-2.56194800	-2.82483400	1.03241100
H	-1.64578600	-4.29362100	1.39263800
H	-1.65233200	-3.65413500	-0.25159600
C	-2.83192100	-1.07790700	-0.97571300
C	-3.87572500	-1.88981200	-1.41458400
C	-3.03619500	-0.29844600	0.16631900
C	-5.08175400	-1.93769200	-0.72575500
H	-3.73419500	-2.52571800	-2.28189400
C	-4.24111700	-0.35958500	0.84709500
H	-2.24627400	0.35666400	0.52078400
C	-5.27811900	-1.18139300	0.41527900
H	-6.21594100	-1.21925500	0.95167400
C	2.18936700	-1.70506300	-1.28758600
C	2.74685600	-2.93680500	-1.60920700
C	2.91098200	-0.84082700	-0.46036500
C	3.96182600	-3.33637700	-1.06231500
H	2.20653200	-3.61220900	-2.26440700
C	4.12731900	-1.24533800	0.07088000
H	2.51722100	0.13935500	-0.23026400
C	4.65612600	-2.50055000	-0.20612600
H	5.60107900	-2.80754400	0.22333900
C	4.47207400	-4.70748300	-1.40039200
C	4.91247600	-0.33605300	0.97548900
F	5.66747500	-4.95281800	-0.86129200
F	3.63391800	-5.66006900	-0.96605700
F	4.58539000	-4.87715800	-2.72482200
F	4.97805000	-0.82235600	2.22458600
F	4.38727300	0.88759900	1.05204900
F	6.17864500	-0.20339700	0.55617200
C	-6.15957300	-2.84386500	-1.25212600
C	-4.41040400	0.43344300	2.11385000
F	-5.73902400	-4.11372000	-1.32510800

F	-6.52933900	-2.49377400	-2.49218200
F	-7.25459700	-2.82839100	-0.49042000
F	-5.69434400	0.71099800	2.36232800
F	-3.74890400	1.59266800	2.07516000
F	-3.94937200	-0.24358400	3.18011400
H	-0.51522000	-1.08470400	-4.96784600
C	0.25208000	-0.60649200	2.50030900
C	1.71311600	-0.70653900	2.96942200
C	-0.42916900	0.43380700	3.39586600
C	1.82986300	-0.84166400	4.46010500
H	2.24363000	0.19073800	2.62437000
H	2.21563100	-1.54863300	2.48578300
C	-0.49216000	-0.04093800	4.84161100
H	0.14889600	1.36388300	3.33274600
H	-1.42897700	0.64907200	3.01025100
C	0.83512100	-0.56715300	5.29990200
H	2.77946200	-1.19428700	4.85061900
H	-0.81207100	0.77655500	5.49341000
H	-1.26012100	-0.81798300	4.94920400
H	0.97776800	-0.71625100	6.36551500

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r-1-1 coplanar S1

Au	0.97647400	1.15378900	-0.02922600
N	2.51878000	-0.19971300	0.12573100
C	4.56902500	-1.23693300	0.17945100
C	-2.29741400	-0.07463900	1.15987000
N	-1.82219600	1.83092900	-0.25274100
C	-2.92696200	2.83143300	-0.35921700
C	-2.66229800	-1.45804600	1.28928300
C	5.93709300	1.17360100	0.44282400
H	6.49122800	2.09700600	0.54532900
C	-0.62035800	2.32085400	-0.22304700
C	2.30472900	-1.52882200	0.00264000
C	-2.09953300	-0.36332300	-1.25677000

C	-2.72485700	-2.25951600	0.15986100
C	3.87763500	-0.00109400	0.22416000
C	-2.08378200	0.41781500	-0.11217100
C	3.51581600	-3.61841100	-0.09974700
H	4.42940500	-4.19971600	-0.08663800
C	1.06449200	-2.17278800	-0.15514700
H	0.14582000	-1.60101500	-0.17122100
C	3.53454800	-2.25175600	0.02870900
C	4.54919300	1.21017800	0.35478900
H	3.99603500	2.14064200	0.38473800
C	-2.13213000	4.10719200	-0.67749100
H	-2.53998700	4.97167700	-0.15068600
H	-2.18987700	4.30998400	-1.75016100
C	5.94475300	-1.25543300	0.26775700
H	6.49641300	-2.18685600	0.23495900
C	1.07305200	-3.54959300	-0.29407200
H	0.13801700	-4.07503700	-0.43208100
C	-2.44374000	-1.75000000	-1.09755200
C	6.62453400	-0.03692900	0.40079800
H	7.70421300	-0.03732400	0.47108700
C	-3.68369900	2.91657700	0.96159500
H	-4.18864200	1.97528500	1.17859900
H	-4.43343700	3.70649200	0.88820000
H	-3.01480000	3.15011400	1.79125100
C	2.27287200	-4.26202900	-0.26269100
H	2.25110500	-5.33828700	-0.37069200
C	-3.88014800	2.43974500	-1.47614800
H	-3.34591900	2.32093900	-2.42029300
H	-4.62956200	3.22475500	-1.59413200
H	-4.38836500	1.50328300	-1.24357700
C	-0.67046200	3.82433100	-0.28823400
C	-0.30400900	4.36220700	1.09840100
H	0.70850100	4.05357400	1.36705100
H	-0.34533900	5.45375100	1.08651900

H	-0.98417000	3.99761300	1.86932900
C	0.32262700	4.35954400	-1.31395800
H	0.23919000	5.44683500	-1.37927500
H	1.34430300	4.10600500	-1.02215100
H	0.13466000	3.93764100	-2.30302700
C	-2.98254200	-1.97401700	2.63467500
C	-2.43553500	-2.61155200	-2.29697100
H	-3.00291200	-3.30046200	0.26177900
H	-2.22930300	0.57322900	2.02325800
H	-1.91873100	0.06983800	-2.23061700
F	-1.95720800	-1.82450400	3.50615700
F	-4.01722100	-1.31955400	3.21335500
F	-3.30095000	-3.27498900	2.63706900
F	-1.20365500	-2.69238500	-2.86259500
F	-2.81359000	-3.87244800	-2.04442800
F	-3.23435000	-2.15161000	-3.28280100

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Au	0.93085700	1.03580600	-0.17116600
N	2.70326700	0.08731200	0.26866300
C	4.56620400	-0.64177200	1.40656500
C	-3.39312500	-0.24259600	0.64382200
N	-2.03479000	1.50750100	-0.39836500
C	-3.02101900	2.61668900	-0.35244000
C	-3.66296400	-1.59103300	0.81575800
C	3.87349000	0.77767600	3.70065600
H	3.62802900	1.31789800	4.60483000
C	-0.75309600	1.97098700	-0.62049600
C	3.41448300	-0.73218200	-0.56612700
C	-1.62071700	-0.82448300	-0.86758400
C	-2.92754600	-2.57735100	0.17565800
C	3.38547100	0.14501800	1.45466300
C	-2.35985900	0.17621800	-0.20923900
C	5.43333100	-2.06787700	-0.60675900

H	6.33129000	-2.45575300	-0.14196000
C	3.08967300	-1.09137900	-1.87642000
H	2.18609100	-0.71391100	-2.33574800
C	4.58524900	-1.22233600	0.07007000
C	3.03045000	0.86080900	2.60007600
H	2.12527100	1.45299500	2.61019000
C	-2.32988600	3.64251300	-1.26130500
H	-2.59443600	4.66372800	-0.97653900
H	-2.67226800	3.48078800	-2.28805600
C	5.39094000	-0.71223600	2.50544000
H	6.29654800	-1.30598100	2.49237900
C	3.95588900	-1.94588100	-2.54479900
H	3.73228300	-2.24810600	-3.55865800
C	-1.90042100	-2.15923600	-0.67005000
C	5.03338300	0.00629600	3.65694500
H	5.67234100	-0.04062900	4.52885600
C	-3.16208700	3.15271000	1.07182300
H	-3.68876400	2.45324300	1.72204200
H	-3.72472900	4.08847100	1.06105000
H	-2.17736900	3.33886600	1.50209900
C	5.10790100	-2.42603100	-1.92439900
H	5.76412200	-3.09274500	-2.46802200
C	-4.37664100	2.24672300	-0.93911400
H	-4.24824600	1.71718400	-1.88506100
H	-4.92743600	3.16911000	-1.13457000
H	-4.98565900	1.63243300	-0.27743500
C	-0.81951600	3.37248700	-1.17707000
C	-0.08771500	4.38084600	-0.28602500
H	0.96201800	4.09294400	-0.18998500
H	-0.13242400	5.38137400	-0.72664100
H	-0.51564600	4.42452800	0.71621400
C	-0.18137600	3.42985300	-2.56931400
H	-0.29785000	4.42599700	-3.00867900
H	0.88539000	3.20328600	-2.50183300

H	-0.64474800	2.69723700	-3.23365200
C	-4.80431000	-1.96482200	1.71959200
C	-1.11830800	-3.18439200	-1.44089800
H	-3.13153600	-3.62538000	0.33747300
H	-3.96398000	0.47693600	1.21187400
H	-0.84273300	-0.52399600	-1.55752500
F	-4.79983500	-1.24956900	2.85360600
F	-5.99090600	-1.73635300	1.13455100
F	-4.78109100	-3.25484100	2.06365700
F	0.12885200	-2.77080000	-1.71061300
F	-1.01656300	-4.34118300	-0.77768200
F	-1.68933300	-3.46661100	-2.62205200

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Au	1.10589400	0.87357500	0.10861600
N	2.77689000	-0.27179600	-0.24229400
C	4.92742200	-0.88746300	-0.78075700
C	-1.79712300	-0.51815900	0.85989600
N	-1.77136900	1.77699800	0.09837500
C	-2.56125200	3.02792200	-0.08858000
C	-2.31983600	-1.79207100	0.81660700
C	5.68740900	1.74545700	-1.28257500
H	6.00969300	2.75816900	-1.48346500
C	-0.45766900	2.03277900	0.44572300
C	2.86902600	-1.62973900	-0.11753600
C	-3.38860200	0.16932200	-0.80200900
C	-3.37617800	-2.12947200	-0.03257400
C	4.00702700	0.18355500	-0.63909600
C	-2.31673400	0.50607700	0.03824500
C	4.46327200	-3.43110300	-0.36850600
H	5.45045300	-3.80820600	-0.60552600
C	1.85328600	-2.50996800	0.26319700
H	0.86575600	-2.13393300	0.49531000
C	4.17475000	-2.08777000	-0.43559600

C	4.37758200	1.50622400	-0.88624900
H	3.65551300	2.30415800	-0.76733300
C	-1.59252000	4.10248900	0.45252000
H	-2.10910900	4.78799600	1.12999300
H	-1.20150700	4.68969200	-0.38258600
C	6.22152700	-0.63244700	-1.17359800
H	6.94250700	-1.43224200	-1.28936100
C	2.16130800	-3.86164900	0.32713800
H	1.39642200	-4.56773100	0.61941000
C	-3.89640900	-1.12150800	-0.82435900
C	6.59449300	0.69689700	-1.42448300
H	7.60882100	0.91171500	-1.73404300
C	-3.86402300	2.99196400	0.70077000
H	-4.53367200	2.20353800	0.35517000
H	-4.37942900	3.94666500	0.58081000
H	-3.66891200	2.83718500	1.76320700
C	3.44282300	-4.31558800	0.01756800
H	3.65723900	-5.37464200	0.07480900
C	-2.82489500	3.33017900	-1.56541800
H	-1.90751000	3.18036600	-2.13879800
H	-3.12062400	4.37763400	-1.65926500
H	-3.62196000	2.73025300	-2.00237500
C	-0.42969500	3.36968800	1.13120700
C	-0.71364900	3.16405200	2.62626600
H	0.09541800	2.59169200	3.08536400
H	-0.80177700	4.12578000	3.14240500
H	-1.64334500	2.60765300	2.76984400
C	0.88950600	4.10780700	0.96331900
H	0.84266500	5.09795800	1.42436600
H	1.69913000	3.54747800	1.43893900
H	1.12986800	4.22314200	-0.09673900
C	-1.77209000	-2.87043400	1.70560100
C	-5.05813000	-1.38987000	-1.74005100
H	-3.77380800	-3.13392500	-0.06201500

H	-1.00961900	-0.26962100	1.55979400
H	-3.82392200	0.90343500	-1.46216600
F	-0.84147800	-2.42345800	2.55452200
F	-2.72949300	-3.45503900	2.43372800
F	-1.19584000	-3.85362500	0.98467600
F	-4.81258500	-0.97192600	-2.98993900
F	-5.36615600	-2.68688900	-1.80811700
F	-6.16181800	-0.74195700	-1.33586800

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e-8-1 coplanar S1

Au	0.50034700	-0.27315100	0.02869900
N	2.58398500	-0.14848200	-0.06019800
C	4.81681300	-0.61197200	-0.32964500
C	-1.33447000	2.86565800	-0.91900900
N	-2.13318900	0.94329400	0.37271200
C	-3.58031000	0.80155200	0.61597000
C	-0.75228800	4.13243600	-0.93986100
H	-0.66312100	4.65501800	-1.88613200
C	4.44590000	-3.30502600	0.30071100
H	4.33395500	-4.35297900	0.54476100
C	-1.48074700	-0.20603000	0.01435600
C	3.20916600	1.00996200	-0.40268600
C	-0.45496200	1.92766700	-3.05243500
H	0.21658400	1.26621300	-2.50081600
H	0.08030000	2.85353900	-3.28453800
H	-0.71852500	1.44024800	-3.99382600
C	-0.89728000	2.75019800	1.48238400
C	-0.27747200	4.72396100	0.22113600
H	0.15619700	5.71631500	0.18999700
C	3.52758200	-1.12876000	-0.01914300
C	-1.46757100	2.20568800	0.31712100
C	-2.43449900	-1.37629900	0.09979300
C	0.69885700	1.73965700	3.11264400
H	1.21880900	1.24744100	2.28820300

H	0.78949200	1.10840200	3.99934200
H	1.20197500	2.68849400	3.31968900
C	5.41087300	1.87432000	-0.91255900
H	6.47830900	1.75343900	-1.05196000
C	2.61866900	2.27242400	-0.54960100
H	1.55213200	2.40396400	-0.39891800
C	-1.71588300	2.22331200	-2.23753000
H	-2.18888000	1.26322000	-2.02605800
C	-0.77759600	1.97472100	2.77969800
H	-1.24145000	0.99626200	2.63119000
C	4.60640500	0.80747300	-0.58206100
C	3.33174000	-2.47592600	0.30015300
H	2.33912300	-2.83649500	0.54523200
C	-3.78673500	-0.72533700	0.49437300
H	-4.55718800	-0.94711200	-0.24250300
H	-4.14638900	-1.13322200	1.43797600
C	5.90731600	-1.45245500	-0.32524600
H	6.90034900	-1.08698400	-0.55715000
C	-2.66862100	3.08889000	-3.06073300
H	-3.55576200	3.37747400	-2.49544000
H	-2.98901200	2.54742200	-3.95362600
H	-2.17237800	4.00361600	-3.39478700
C	3.44952500	3.33221400	-0.88516300
H	3.02591600	4.32103100	-1.00515200
C	-0.32872500	4.02271400	1.41472300
H	0.09513100	4.45817300	2.31301800
C	5.71081800	-2.80616900	-0.00964600
H	6.56062100	-3.47617800	-0.00484000
C	-1.43795800	2.68832400	3.95937900
H	-2.48787400	2.91614200	3.77830900
H	-0.92340300	3.62975400	4.16931300
H	-1.36961800	2.07141500	4.85811000
C	-4.40854900	1.58537400	-0.40182600
H	-4.16986800	2.65038200	-0.34078900

H	-5.46995700	1.46131600	-0.17652300
H	-4.23419300	1.25373900	-1.42408100
C	4.81967300	3.13977800	-1.06547100
H	5.44409300	3.98447300	-1.32596300
C	-3.97016300	1.32783400	1.99413700
H	-3.42854900	0.82496700	2.79509700
H	-5.04025700	1.17680600	2.15216200
H	-3.76612000	2.39946400	2.05565300
C	-1.87859500	-2.29836400	1.18042400
C	-2.06632200	-1.99728000	2.53464000
C	-1.05666000	-3.38068800	0.85797600
C	-1.47628300	-2.74341700	3.53893100
H	-2.66840300	-1.14052900	2.81150900
C	-0.46970100	-4.13372100	1.87435700
C	-0.66721900	-3.82797300	3.21034300
H	-1.64359900	-2.47905500	4.57572400
H	0.15630000	-4.97698000	1.59770200
H	-0.20447800	-4.42609600	3.98493900
C	-2.46922500	-2.03572300	-1.27683800
C	-3.25064000	-1.49720600	-2.30603600
C	-1.66097300	-3.13200200	-1.57895700
C	-3.25604900	-2.03355200	-3.58108700
H	-3.86836200	-0.63032400	-2.11008300
C	-1.67534100	-3.67553000	-2.86449900
C	-2.46393400	-3.14244700	-3.86751300
H	-3.87911200	-1.59134400	-4.34865800
H	-1.04542400	-4.53553000	-3.06892400
H	-2.46426000	-3.58057900	-4.85747900
C	-0.71818500	-3.70348900	-0.56583200
H	-0.64152200	-4.78709900	-0.69478200
H	0.28311400	-3.30172100	-0.77898200

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Au	-0.54491000	-0.03320600	-0.09402100
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N	-2.56270300	-0.39122000	-0.09416500
C	-4.72153400	-0.60900900	0.67622000
C	2.29226600	-2.70438900	-0.56835900
N	2.42032300	-0.40549600	0.26348500
C	3.74429100	0.23912300	0.29281600
C	2.23188800	-4.06950100	-0.29472600
H	2.28244500	-4.77549000	-1.11670500
C	-4.06016800	0.38448600	3.19096400
H	-3.83214400	0.77525200	4.17329600
C	1.36537800	0.41895100	-0.04807100
C	-3.33293600	-0.86995500	-1.12212200
C	0.95215900	-2.61043000	-2.65638200
H	0.12723100	-2.20798600	-2.06502000
H	0.83519200	-3.69621500	-2.71836500
H	0.89224400	-2.20082200	-3.66793400
C	1.99987400	-2.25509300	1.81248000
C	2.08833000	-4.53436100	1.00278700
H	2.05361100	-5.59896900	1.19937600
C	-3.39295200	-0.21814100	0.98468300
C	2.24449500	-1.79875800	0.50571200
C	1.87581300	1.83537600	-0.24884200
C	0.22688200	-1.49783900	3.38261800
H	-0.44242200	-1.41100800	2.52436700
H	-0.05183600	-0.74118800	4.12123800
H	0.08071000	-2.48358500	3.83360000
C	-5.61436600	-1.51809300	-1.60815600
H	-6.64880700	-1.65898200	-1.31984600
C	-2.91730400	-1.16699600	-2.42128300
H	-1.88490900	-1.01542800	-2.70831900
C	2.29299500	-2.24909500	-2.01342500
H	2.37105000	-1.16036200	-2.02492800
C	1.68503300	-1.31170400	2.95531300
H	1.78602600	-0.28969100	2.58456100
C	-4.68209300	-1.03968400	-0.71599000

C	-3.05189600	0.29149600	2.23972700
H	-2.03642100	0.61100900	2.44030400
C	3.40807000	1.71284300	-0.02676200
H	3.95291400	2.04226300	-0.91073700
H	3.73051800	2.35983300	0.78842800
C	-5.70753300	-0.51107700	1.63136400
H	-6.72804500	-0.80545900	1.41933800
C	3.42924400	-2.85491800	-2.83497700
H	4.40770400	-2.66068000	-2.39504200
H	3.42007900	-2.44638100	-3.84814000
H	3.30960900	-3.93809700	-2.91900400
C	-3.87204800	-1.64431900	-3.31013900
H	-3.58515400	-1.88271800	-4.32531200
C	1.94529200	-3.62873100	2.04164500
H	1.77180000	-3.98926600	3.04991300
C	-5.36320000	-0.01302400	2.89692800
H	-6.12785000	0.07037000	3.65811400
C	2.59243200	-1.51319300	4.16778800
H	3.64922900	-1.42747100	3.91488800
H	2.43298200	-2.50181600	4.60598500
H	2.36150200	-0.77366200	4.93816200
C	4.70061500	-0.37052300	-0.73177900
H	4.85906600	-1.42943700	-0.51227100
H	5.66608000	0.13680200	-0.67394400
H	4.32899700	-0.28334000	-1.75179600
C	-5.19616000	-1.82115700	-2.91261800
H	-5.91813900	-2.19795400	-3.62516900
C	4.41925900	0.08273200	1.65456100
H	3.82659200	0.50968700	2.46252800
H	5.39031400	0.58237500	1.63913000
H	4.58454800	-0.97577100	1.87109800
C	1.20023600	2.70395000	0.80905800
C	1.62694700	2.64030800	2.14135400
C	0.08177900	3.48490000	0.51941100

C	0.98016700	3.32385500	3.15394700
H	2.47764400	2.02037300	2.39440600
C	-0.56639100	4.17835700	1.54401100
C	-0.13379600	4.10672000	2.85551400
H	1.34236700	3.24965400	4.17203700
H	-1.43132100	4.78349200	1.29045200
H	-0.64726400	4.65649700	3.63421800
C	1.52325600	2.26320100	-1.67000000
C	2.26694100	1.77617000	-2.75157600
C	0.41415200	3.06082500	-1.94793700
C	1.94508400	2.08027900	-4.06112100
H	3.11371100	1.12870000	-2.56167700
C	0.09533300	3.37120100	-3.27201200
C	0.84647400	2.89404500	-4.32987400
H	2.54790200	1.68691000	-4.87039700
H	-0.76752700	4.00242000	-3.46061500
H	0.58537000	3.15061100	-5.34880600
C	-0.49697100	3.54413400	-0.86127400
H	-0.82868300	4.56354000	-1.08080000
H	-1.40434700	2.92454000	-0.87705000

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e-8-1 coplanar T1

Au	0.52775000	-0.27908200	0.04165300
N	2.54986900	-0.13327200	-0.20589400
C	4.80482600	-0.54317700	-0.37043300
C	-1.48087100	2.81482600	-0.80676900
N	-2.11144400	0.89697400	0.56231000
C	-3.50614000	0.69788700	0.99051700
C	-0.92254700	4.08627900	-0.91592800
H	-0.93975200	4.58792000	-1.87766200
C	4.47102600	-3.25025600	0.20768200
H	4.37370400	-4.30293700	0.43622300
C	-1.41587800	-0.26334500	0.31220600
C	3.17324300	1.05416600	-0.48654300

C	-0.84669800	1.80782800	-3.00151700
H	-0.09759300	1.19036300	-2.50003800
H	-0.36589000	2.72444400	-3.35788500
H	-1.21763200	1.25439400	-3.86819300
C	-0.80606000	2.75222700	1.53814500
C	-0.34424800	4.70933200	0.18035200
H	0.06853900	5.70688100	0.08816600
C	3.51928600	-1.09333200	-0.12287100
C	-1.47899100	2.17176100	0.44678400
C	-2.39407000	-1.41927600	0.21310400
C	0.96802500	1.82842500	3.03263700
H	1.41511800	1.30923700	2.18305500
H	1.16070600	1.24033300	3.93254100
H	1.46668800	2.79488500	3.14759300
C	5.37650000	1.96312900	-0.88484600
H	6.44999700	1.86025000	-0.98507000
C	2.56567100	2.30414500	-0.63017100
H	1.49158400	2.41431700	-0.52263300
C	-2.00105300	2.13559700	-2.05354200
H	-2.44235100	1.18756100	-1.75177300
C	-0.53920200	2.01800600	2.83806700
H	-0.98663200	1.02458500	2.76175000
C	4.57507500	0.87906000	-0.60772100
C	3.33922800	-2.44581600	0.17409200
H	2.34765500	-2.83085100	0.38301800
C	-3.71322400	-0.81867300	0.76248300
H	-4.54310100	-0.99979500	0.08120800
H	-3.99349000	-1.29399700	1.69993600
C	5.91415600	-1.35645100	-0.33473500
H	6.90653900	-0.96464000	-0.52073900
C	-3.05489200	2.96459400	-2.78438100
H	-3.86103700	3.27990400	-2.11981400
H	-3.48696800	2.38039900	-3.60123600
H	-2.61146300	3.86259700	-3.22281000

C	3.39198500	3.38670000	-0.90465900
H	2.95608600	4.37061100	-1.01847000
C	-0.26975100	4.03268500	1.38633900
H	0.23080600	4.49497400	2.23016900
C	5.73478500	-2.71854300	-0.04571400
H	6.59870600	-3.36944700	-0.01429500
C	-1.09415400	2.75260500	4.05897400
H	-2.15862100	2.96793100	3.97551000
H	-0.57277000	3.70346800	4.19786600
H	-0.93411900	2.15763100	4.96072600
C	-4.47193500	1.56974100	0.19283700
H	-4.21639400	2.62554600	0.31846000
H	-5.48875300	1.42032700	0.56174400
H	-4.45547400	1.34347200	-0.87194200
C	4.77019000	3.22125200	-1.03292000
H	5.38952700	4.08211800	-1.24862600
C	-3.69499000	1.04624200	2.46507000
H	-3.01775200	0.46956300	3.09781700
H	-4.72203000	0.82653200	2.76611700
H	-3.51325000	2.11032800	2.62658800
C	-1.82729300	-2.56160100	1.05179500
C	-2.00474800	-2.59538000	2.43748700
C	-0.99533900	-3.52180500	0.47447600
C	-1.42152800	-3.57324900	3.22590100
H	-2.59101100	-1.82462000	2.92299100
C	-0.41063200	-4.50688900	1.27209400
C	-0.62051600	-4.54735900	2.63939200
H	-1.58611400	-3.57087100	4.29621000
H	0.21856400	-5.25314500	0.79629100
H	-0.16489100	-5.32300100	3.24201500
C	-2.50771000	-1.79849700	-1.26595900
C	-3.40366300	-1.15184500	-2.12557000
C	-1.65467700	-2.75423800	-1.82836000
C	-3.43445600	-1.40781000	-3.48745600

H	-4.09506000	-0.41913000	-1.73369300
C	-1.70189300	-3.02315900	-3.19318100
C	-2.57507800	-2.35231900	-4.03522300
H	-4.14048800	-0.87776900	-4.11570000
H	-1.03309000	-3.77780800	-3.59480200
H	-2.59619000	-2.57241300	-5.09489700
C	-0.64913200	-3.47186300	-0.98386600
H	-0.49456500	-4.48437100	-1.36754000
H	0.31528400	-2.95380400	-1.09205200

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Au	0.70209400	0.53262400	-0.24661900
N	2.49519400	1.59947400	-0.04981700
C	4.19329600	3.13710500	-0.20942200
C	0.85038700	-2.83315800	1.47259500
N	-0.82955200	-1.97127300	-0.08664200
C	-2.11094200	-2.67748100	-0.26998500
C	2.05728600	-3.49992500	1.69012900
H	2.38865000	-3.67117400	2.70879700
C	2.45991700	5.12011100	-1.13274400
H	1.81211500	5.90782800	-1.49375100
C	-0.88685300	-0.65552800	-0.47418100
C	3.64720800	0.98552700	0.32668000
C	0.88164000	-1.17320200	3.33125800
H	1.09001000	-0.36903000	2.61950500
H	1.83709300	-1.54609200	3.71254700
H	0.32103300	-0.75451300	4.17079200
C	1.22268300	-3.01681100	-0.93312900
C	2.83929500	-3.92420300	0.62960000
H	3.77137800	-4.44583900	0.81141000
C	2.80418200	2.87915500	-0.39000500
C	0.41875600	-2.62047500	0.15422400
C	-2.24325500	-0.35609000	-1.06927800
C	1.77940100	-1.72799600	-3.01022100

H	1.73876000	-0.77929600	-2.47178700
H	1.50103500	-1.55036300	-4.05193100
H	2.81115600	-2.09125200	-2.99345900
C	6.00672200	1.43824000	0.62316900
H	6.86634800	2.09678700	0.59128900
C	3.79919100	-0.35024900	0.72298900
H	2.94638500	-1.01989300	0.73972300
C	0.08839600	-2.29602800	2.66222800
H	-0.83916500	-1.86374500	2.29049700
C	0.84561900	-2.76128700	-2.37888900
H	-0.16853500	-2.35377200	-2.39651900
C	4.75283000	1.88105300	0.26681600
C	1.92985700	3.86760000	-0.85405400
H	0.87941500	3.64119200	-0.98635000
C	-2.77959300	-1.78935100	-1.32545500
H	-3.86241800	-1.88075200	-1.27234300
H	-2.46159100	-2.10549700	-2.32461900
C	4.69758100	4.38718700	-0.49155800
H	5.74962000	4.61084400	-0.36192100
C	-0.25107100	-3.39159800	3.66975300
H	-0.78174900	-4.22043400	3.19552900
H	-0.87834800	-2.99249000	4.46946700
H	0.65378600	-3.79679900	4.13000800
C	5.07312000	-0.77371600	1.07495700
H	5.22348900	-1.80035800	1.38369100
C	2.42546100	-3.66829900	-0.66996400
H	3.04555100	-3.98396500	-1.50164400
C	3.81918600	5.37876100	-0.95552200
H	4.20561200	6.36395400	-1.18161000
C	0.88323800	-4.04367000	-3.21380900
H	0.33010100	-4.86000600	-2.74687200
H	1.91269200	-4.38138900	-3.35513300
H	0.46269200	-3.85989400	-4.20457500
C	-2.93350000	-2.69161200	1.01876900

H	-2.46145000	-3.32385100	1.77381400
H	-3.92910200	-3.09219200	0.81357900
H	-3.04104400	-1.68535700	1.42662800
C	6.15829100	0.10223500	1.03090900
H	7.14056900	-0.25458700	1.31216400
C	-1.92543300	-4.10591700	-0.75080600
H	-1.40271000	-4.13913400	-1.70593000
H	-2.90459000	-4.57156100	-0.87803300
H	-1.36110500	-4.69212200	-0.02096300
C	-3.27385900	0.48774800	-0.26867200
C	-4.52174600	0.80646200	-0.84701200
C	-3.08493000	1.06811600	0.99606900
C	-5.44293200	1.67673300	-0.28561700
C	-3.98686500	1.94961700	1.58320300
C	-5.15686900	2.26826000	0.92911400
H	-6.37497600	1.87676500	-0.79530000
H	-3.76505700	2.36466900	2.55636600
C	-1.92724800	0.43627600	-2.35940000
H	-1.36194200	1.32851500	-2.08042100
H	-1.28458900	-0.17510400	-2.99761100
H	-2.80249900	0.74213200	-2.92698400
Cl	-5.08573000	0.09157500	-2.33002000
Cl	-1.74599500	0.70124000	2.03006200
Cl	-6.27311300	3.37021700	1.63663900

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Au	0.84565600	0.19911500	-0.36611100
N	2.59270300	1.28235700	-0.38911500
C	4.18163600	2.83481000	0.22394500
C	0.53771600	-2.52245100	2.23169500
N	-1.03658000	-1.95625000	0.45099900
C	-2.41308700	-2.46748200	0.40529300
C	1.65983300	-3.22933200	2.66192000
H	2.00397500	-3.10455100	3.68326700

C	2.55963900	3.89973200	2.21775500
H	1.94777100	4.33412800	2.99656500
C	-0.87105000	-0.78789600	-0.27869600
C	3.68468400	1.11762800	-1.20151500
C	0.79639400	-0.41505600	3.55382000
H	1.15351400	0.09159500	2.65285800
H	1.66697500	-0.78007700	4.10578600
H	0.27849700	0.31375600	4.18340500
C	0.79093600	-3.52910800	0.02455100
C	2.34258900	-4.07338800	1.80320000
H	3.21328700	-4.61673000	2.14941700
C	2.88370700	2.31566000	0.46618200
C	0.09366300	-2.68786900	0.91203100
C	-2.14961500	-0.49604900	-1.04079400
C	1.39100100	-3.04546900	-2.36466300
H	1.42384400	-1.97169800	-2.17213600
H	1.10520700	-3.20738000	-3.40727200
H	2.39043600	-3.46433200	-2.21437300
C	5.89223400	2.03997700	-1.58453500
H	6.68736600	2.73815300	-1.35363300
C	3.84228400	0.18894700	-2.23172300
H	3.04817200	-0.50744900	-2.46131300
C	-0.13990200	-1.56432000	3.18397900
H	-0.99365900	-1.13635400	2.66073100
C	0.38592400	-3.70897100	-1.42526100
H	-0.57302300	-3.20671800	-1.57007000
C	4.71076600	2.04414500	-0.87922800
C	2.06065900	2.84680000	1.46145700
H	1.06776100	2.44618300	1.61821500
C	-2.91671900	-1.83842200	-0.89775500
H	-3.99977100	-1.73404700	-0.87906600
H	-2.65608300	-2.48215800	-1.74426900
C	4.66110000	3.87828500	0.98223600
H	5.64938100	4.28830400	0.81422600

C	-0.64097300	-2.27581000	4.43855300
H	-1.29732600	-3.11186000	4.18614800
H	-1.19369400	-1.58368600	5.07772400
H	0.19382000	-2.67411700	5.02144300
C	5.03983700	0.19829000	-2.93501000
H	5.19264700	-0.50866800	-3.73911800
C	1.90904700	-4.21399100	0.49323400
H	2.45081500	-4.86688400	-0.18274800
C	3.83674700	4.40725100	1.98647200
H	4.19956700	5.22785500	2.59133100
C	0.23999500	-5.18534000	-1.79845400
H	-0.37864100	-5.73071700	-1.08395000
H	1.21676900	-5.67410200	-1.82942900
H	-0.20482200	-5.28308500	-2.79108400
C	-3.23518000	-1.96062200	1.59259600
H	-2.87189000	-2.39586000	2.52639400
H	-4.28259100	-2.24598400	1.46785900
H	-3.17803200	-0.87459600	1.67346000
C	6.04922500	1.10579700	-2.61920700
H	6.97268100	1.09039000	-3.18296700
C	-2.48604400	-3.98537900	0.38999100
H	-2.00652300	-4.40751400	-0.49161100
H	-3.53332500	-4.29350900	0.38977600
H	-2.00964100	-4.40252900	1.28123900
C	-3.04915900	0.69533100	-0.60495600
C	-4.20705200	1.00882500	-1.35194000
C	-2.81952200	1.59374900	0.45112900
C	-4.98512400	2.13900100	-1.15534700
C	-3.57791500	2.73963200	0.67082900
C	-4.64687700	3.02260200	-0.15016700
H	-5.85027800	2.31204700	-1.77975300
H	-3.32988600	3.38813400	1.49920000
C	-1.68666600	-0.19702600	-2.48568300
H	-1.00127700	0.65286500	-2.45802800

H	-1.12738800	-1.06111400	-2.85309000
H	-2.48862700	0.02792400	-3.18396600
Cl	-4.84504300	-0.03366900	-2.59085600
Cl	-1.62850300	1.35527500	1.69048000
Cl	-5.58139900	4.44584500	0.10112900

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Au	0.72985700	0.50692800	-0.34399600
N	2.46355200	1.58548300	-0.22161500
C	4.07138300	3.22912900	-0.22180100
C	0.93254700	-2.68376000	1.62352800
N	-0.77733600	-1.98427500	0.01948700
C	-2.05170400	-2.70120800	-0.11006300
C	2.14102100	-3.33060900	1.88674600
H	2.48716000	-3.40505100	2.91212300
C	2.22672100	5.19338500	-0.93815500
H	1.53378700	5.97651500	-1.21457600
C	-0.86269100	-0.66401700	-0.40356000
C	3.66010400	1.00712500	0.11621100
C	0.98338100	-0.87024000	3.33473800
H	1.20071700	-0.13588300	2.55368200
H	1.93315500	-1.21532300	3.75418200
H	0.42290800	-0.37209200	4.12993800
C	1.26732900	-3.09679900	-0.75656600
C	2.90081900	-3.86768200	0.86121600
H	3.83028900	-4.38028200	1.07942400
C	2.70050000	2.91587800	-0.42410400
C	0.47577800	-2.59996800	0.29823900
C	-2.22080800	-0.42733300	-1.03364400
C	1.83599500	-1.97890700	-2.92231000
H	1.81766300	-0.99500400	-2.44932400
H	1.55377100	-1.86542600	-3.97189200
H	2.86034200	-2.36200200	-2.88770900
C	5.98496500	1.57139700	0.45753200

H	6.80345900	2.28031700	0.48142500
C	3.88156400	-0.33892600	0.41289000
H	3.06477700	-1.05156500	0.38982900
C	0.18208100	-2.04208000	2.76750700
H	-0.74653800	-1.64099500	2.36469100
C	0.88576600	-2.94697200	-2.21561400
H	-0.12056800	-2.52199800	-2.25702900
C	4.70516500	1.96449600	0.13705000
C	1.76860100	3.89185000	-0.78231700
H	0.73033700	3.62222900	-0.92581500
C	-2.73153100	-1.88251500	-1.21175900
H	-3.81249500	-1.99191800	-1.15645700
H	-2.40415800	-2.24712700	-2.19128000
C	4.50760400	4.52426900	-0.38104400
H	5.54684900	4.79062800	-0.23290100
C	-0.15199700	-3.04567200	3.86868200
H	-0.68829600	-3.91090900	3.47272300
H	-0.77204500	-2.57694200	4.63568500
H	0.75605200	-3.41184300	4.35497800
C	5.17910200	-0.71669800	0.73477900
H	5.38517800	-1.75259300	0.97076900
C	2.46905300	-3.73361100	-0.45044500
H	3.07507000	-4.13075500	-1.25750900
C	3.57135100	5.50590400	-0.74225400
H	3.90137400	6.52839700	-0.87078000
C	0.90188400	-4.28664000	-2.95546800
H	0.34164800	-5.06008400	-2.42833700
H	1.92667800	-4.64643500	-3.07609100
H	0.47875600	-4.17052200	-3.95536500
C	-2.86074700	-2.63418700	1.18678200
H	-2.37329100	-3.21431900	1.97367400
H	-3.85950000	-3.04740400	1.02634600
H	-2.96089800	-1.60343800	1.53106000
C	6.21247600	0.21868400	0.75715500

H	7.21391300	-0.10327600	1.01145100
C	-1.87423900	-4.15739700	-0.50204000
H	-1.37598600	-4.25089000	-1.46601700
H	-2.85398900	-4.63360100	-0.57407700
H	-1.28933600	-4.69405700	0.24954900
C	-3.28023900	0.43378100	-0.28882700
C	-4.54083400	0.66388800	-0.88366800
C	-3.11925500	1.10223600	0.93732100
C	-5.50665300	1.51573100	-0.37023000
C	-4.06751200	1.96893900	1.47376100
C	-5.25379800	2.18633600	0.80935400
H	-6.44506900	1.64186000	-0.89147800
H	-3.86574600	2.45314400	2.41884900
C	-1.92199900	0.29657400	-2.36604600
H	-1.38369200	1.21981200	-2.13923400
H	-1.25642400	-0.33360500	-2.96102800
H	-2.80079100	0.54392200	-2.95640900
Cl	-5.06529000	-0.13669200	-2.33736400
Cl	-1.76138500	0.89043000	1.99112300
Cl	-6.42769900	3.26428800	1.45930300

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e-18-1 coplanar S1

Au	0.76750000	0.36271500	-0.13727600
N	2.77399200	0.78162000	0.26865600
C	4.71842100	1.74877600	1.01537000
C	-0.15852100	-3.17925600	0.40701200
N	-1.28325100	-1.49622000	-0.98639100
C	-2.64936600	-1.77887400	-1.46877300
C	0.73714200	-4.24271900	0.49697200
H	0.83914800	-4.76282600	1.44309200
C	3.62166600	4.31185800	0.89239800
H	3.22170600	5.31648400	0.85982100
C	-1.10579300	-0.26506500	-0.42345400
C	3.66894600	-0.21542700	0.50686800

C	0.13090000	-2.16570700	2.66622900
H	0.64492500	-1.29860900	2.24277400
H	0.88107600	-2.91520200	2.93479100
H	-0.38056400	-1.85270500	3.57985000
C	0.53759500	-2.85282900	-1.91409800
C	1.49717200	-4.64201400	-0.59301800
H	2.17201300	-5.48532300	-0.50829700
C	3.37569300	1.95899700	0.59243500
C	-0.30204200	-2.52530700	-0.83337700
C	-2.43900400	0.47244900	-0.42732800
C	1.98704400	-1.31549800	-3.23539800
H	2.15357000	-0.68407400	-2.36015500
H	2.05000700	-0.68827000	-4.12738400
H	2.79201800	-2.05496100	-3.28258700
C	5.95406900	-0.55225400	1.23071800
H	6.91477200	-0.18366500	1.56942900
C	3.46158700	-1.59165600	0.34296300
H	2.50088000	-1.96895300	0.00976600
C	-0.87671200	-2.74209900	1.66935600
H	-1.56999900	-1.93954400	1.41583000
C	0.62275700	-2.00843500	-3.17039300
H	-0.13748900	-1.22897900	-3.10282500
C	4.91335000	0.30717300	0.95864500
C	2.81596400	3.23922100	0.53460300
H	1.78460400	3.36535500	0.22898200
C	-3.26689300	-0.37312900	-1.42989600
H	-4.33231200	-0.38674600	-1.23033100
H	-3.12502000	0.07417300	-2.41341800
C	5.50016400	2.82713200	1.36546300
H	6.52619300	2.69656800	1.68752100
C	-1.65855400	-3.87851000	2.32727100
H	-2.33145800	-4.37333500	1.62560500
H	-2.25212900	-3.48560800	3.15688200
H	-0.98282100	-4.63454900	2.73517000

C	4.52319200	-2.43851100	0.62812200
H	4.39381400	-3.50694700	0.51207900
C	1.41236200	-3.93150300	-1.77851200
H	2.05133400	-4.19834000	-2.61318300
C	4.94080000	4.11276200	1.29979800
H	5.54532600	4.96693500	1.57540200
C	0.41718200	-2.81971300	-4.44899800
H	-0.51762200	-3.37985400	-4.44269300
H	1.23390800	-3.53330100	-4.58557700
H	0.41495100	-2.15770500	-5.31743200
C	-3.34252000	-2.81610700	-0.58719900
H	-2.82039800	-3.77262300	-0.67770200
H	-4.37316300	-2.95267600	-0.91924800
H	-3.35413900	-2.53561400	0.46281700
C	5.74890700	-1.93148600	1.06154400
H	6.56065000	-2.61491100	1.27429600
C	-2.65424400	-2.31987800	-2.89339500
H	-2.18356800	-1.62198300	-3.58693400
H	-3.68625200	-2.48285600	-3.21211800
H	-2.13268900	-3.27849800	-2.93648700
C	-2.87480000	0.37224600	1.04628000
C	-3.95365300	-0.34372600	1.56837400
C	-2.06716500	0.94226200	2.04460900
C	-4.11392000	-0.65110800	2.91468500
C	-2.18527400	0.70764200	3.39446200
C	-3.20450500	-0.13879900	3.80851200
H	-4.95533600	-1.24742700	3.23769900
H	-1.50924500	1.17408600	4.09582700
C	-2.32235100	1.90021600	-0.94753500
C	-1.60770000	2.16563000	-2.12105400
C	-2.89630600	3.03209800	-0.37224400
C	-1.41218000	3.42390400	-2.65581000
C	-2.73768600	4.32151800	-0.85391200
C	-1.98189800	4.49368000	-1.99280100

H	-0.84124000	3.55352200	-3.56349600
H	-3.20351900	5.15471400	-0.34818000
F	-1.80946400	5.72548800	-2.48101300
F	-1.09243800	1.14223400	-2.81528000
F	-3.66706800	2.90701500	0.71379400
F	-4.94829800	-0.77193300	0.76969200
F	-1.12249000	1.81167300	1.66837800
F	-3.32719800	-0.41845000	5.11069100

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e-18-1 rotated S1

Au	0.83678200	-0.08940600	0.11801700
N	2.78831000	-0.20881500	0.72801200
C	5.07893200	0.02337400	0.68346400
C	-1.61077700	-3.08743200	-0.27253700
N	-1.59836300	-0.88754600	-1.34885200
C	-2.80930900	-0.46298600	-2.06861900
C	-1.26434500	-4.43562100	-0.31182300
H	-1.61305300	-5.09235900	0.47793800
C	5.03297200	1.26057000	-1.80961800
H	5.04465400	1.74470100	-2.77672400
C	-1.01784200	0.07420800	-0.54750300
C	3.28931700	-0.73151100	1.89064400
C	-1.49723000	-2.62538300	2.17309900
H	-0.62060200	-1.98698300	2.03415300
H	-1.16055700	-3.64752100	2.36752600
H	-2.05128400	-2.27321200	3.04689700
C	-0.29418200	-2.73375200	-2.29835200
C	-0.47979000	-4.94676000	-1.33433500
H	-0.23259400	-6.00104800	-1.35698100
C	3.85722800	0.24965200	-0.00058100
C	-1.16982000	-2.24658600	-1.31192500
C	-1.95751100	1.28225400	-0.51156000
C	1.92568200	-1.84249200	-2.98832600
H	2.12961500	-1.61474700	-1.94037800

H	2.44243500	-1.10851800	-3.61247600
H	2.34675300	-2.82710100	-3.21009200
C	5.39651000	-1.09640100	3.02571300
H	6.47585900	-1.02658500	3.08084700
C	2.56741100	-1.30594400	2.93822000
H	1.48921600	-1.37291900	2.88074200
C	-2.38256400	-2.57414900	0.92725300
H	-2.62672500	-1.52580500	0.75549200
C	0.42157200	-1.82299000	-3.27664800
H	0.06462100	-0.80471100	-3.10719800
C	4.70405000	-0.62506500	1.93406100
C	3.82241200	0.87191600	-1.25039600
H	2.87430600	1.03488900	-1.74849200
C	-2.79938900	1.04843800	-1.79314100
H	-3.79352200	1.47949000	-1.76352200
H	-2.26336000	1.52455900	-2.61333000
C	6.26963500	0.41504200	0.11486500
H	7.21448000	0.25253300	0.61862300
C	-3.67526500	-3.34795000	1.18012700
H	-4.29974700	-3.40220700	0.28737200
H	-4.24888300	-2.86212900	1.97408500
H	-3.46378400	-4.36996900	1.50482100
C	3.28115800	-1.77601400	4.03266000
H	2.75356500	-2.22752800	4.86174000
C	0.01827000	-4.09258000	-2.30347900
H	0.68139100	-4.47845400	-3.07033300
C	6.23603900	1.03657200	-1.14210200
H	7.16399700	1.35006200	-1.60197200
C	0.19964200	-2.21570000	-4.73679300
H	-0.85518600	-2.24674600	-5.00673000
H	0.62415700	-3.20380900	-4.93318500
H	0.70238700	-1.50684400	-5.39871400
C	-4.05460200	-1.20697700	-1.58788300
H	-3.94754600	-2.27013100	-1.82080300

H	-4.93578700	-0.82807800	-2.10894900
H	-4.22205000	-1.11279000	-0.51834500
C	4.67069900	-1.67490100	4.07798300
H	5.20172900	-2.05006600	4.94289000
C	-2.69445700	-0.71503300	-3.56876500
H	-1.82378000	-0.20876700	-3.98782300
H	-3.58971700	-0.34093400	-4.07102300
H	-2.61792400	-1.78655900	-3.76677200
C	-2.74009600	1.13533600	0.80860500
C	-4.10704300	0.91174300	0.97122300
C	-2.04066300	1.10496400	2.02469400
C	-4.70215500	0.49751300	2.15808000
C	-2.56818600	0.73539700	3.24089200
C	-3.91026400	0.39162900	3.27570400
H	-5.76427600	0.30143700	2.19121500
H	-1.95258100	0.72570200	4.12827700
C	-1.20477600	2.60465400	-0.63950900
C	-0.21923900	2.77346100	-1.62147500
C	-1.41147900	3.74396300	0.13719600
C	0.53819300	3.91700000	-1.78860700
C	-0.68573800	4.91939000	0.02407300
C	0.29338900	4.97938100	-0.94131300
H	1.28262900	3.97210200	-2.56949200
H	-0.89772200	5.75515400	0.67476900
F	1.01189200	6.09771400	-1.07741500
F	0.01385400	1.79393600	-2.50728300
F	-2.37585100	3.75385800	1.06470300
F	-4.96750400	1.11278800	-0.04167400
F	-0.76469500	1.50470400	2.02834500
F	-4.44934100	-0.00609500	4.43320200

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e-18-1 coplanar T1

Au	0.76566700	0.35585400	-0.04712400
N	2.69679100	0.80059500	0.44277400

C	4.66122600	1.85318200	1.00408900
C	-0.10291200	-3.19838200	0.40121400
N	-1.22686000	-1.52943000	-1.00769200
C	-2.57316100	-1.82558300	-1.52144000
C	0.81347300	-4.24317800	0.50775400
H	0.89856000	-4.77223200	1.45076500
C	3.45404600	4.36703900	0.97764200
H	3.01310000	5.35463700	0.97650500
C	-1.05827900	-0.26227300	-0.48625100
C	3.66633600	-0.15981000	0.57728700
C	0.09781100	-2.22242400	2.68863200
H	0.62928500	-1.35114800	2.29658600
H	0.83435800	-2.97610300	2.98208600
H	-0.45142600	-1.91777400	3.58307900
C	0.65174200	-2.83098500	-1.89272300
C	1.61370500	-4.61313500	-0.56359800
H	2.30358500	-5.44323700	-0.46863300
C	3.28224300	2.00811500	0.70113000
C	-0.22889100	-2.53414600	-0.83571100
C	-2.41706300	0.43312600	-0.47729700
C	2.10040600	-1.25749100	-3.17304600
H	2.23655500	-0.63181800	-2.28857400
H	2.16844900	-0.61973200	-4.05721200
H	2.92006700	-1.98115800	-3.21289700
C	6.01588600	-0.38950300	1.09343200
H	6.98236900	0.02331700	1.35519400
C	3.50778700	-1.53681200	0.40890900
H	2.54135500	-1.95510800	0.15009800
C	-0.86765900	-2.78726100	1.64458800
H	-1.55537500	-1.98473200	1.37520200
C	0.74793600	-1.97497400	-3.14024300
H	-0.02768600	-1.20993200	-3.08079300
C	4.91442300	0.41810400	0.92053300
C	2.66637200	3.26100000	0.68652800

H	1.61137400	3.34340600	0.45706000
C	-3.20846000	-0.42609500	-1.49890300
H	-4.27921700	-0.45110400	-1.33017900
H	-3.04372300	0.02138900	-2.47878800
C	5.42599900	2.96082700	1.28962300
H	6.48001100	2.87294800	1.52251800
C	-1.66132500	-3.94066800	2.25764200
H	-2.30458400	-4.43173700	1.52666200
H	-2.28666900	-3.56725800	3.07289600
H	-0.99090500	-4.69584900	2.67620000
C	4.63051600	-2.33525300	0.58621000
H	4.54250100	-3.40669600	0.46169000
C	1.54781400	-3.89050900	-1.74318400
H	2.21513300	-4.13505500	-2.56255800
C	4.80885100	4.22163500	1.27360300
H	5.39887500	5.10073500	1.49723000
C	0.58357200	-2.78037400	-4.42859700
H	-0.34134500	-3.35630700	-4.44541900
H	1.41525400	-3.47909800	-4.55226600
H	0.58799500	-2.11255000	-5.29266700
C	-3.28155200	-2.87604900	-0.66800900
H	-2.74675500	-3.82624100	-0.75350600
H	-4.30185900	-3.02196200	-1.02728400
H	-3.32209300	-2.60641800	0.38403300
C	5.86196200	-1.77441300	0.92187500
H	6.72029600	-2.42008400	1.05434200
C	-2.53805300	-2.35907100	-2.94997800
H	-2.05399600	-1.65283800	-3.62583000
H	-3.55897500	-2.53004900	-3.29923900
H	-2.00563900	-3.31233200	-2.98422100
C	-2.88965200	0.31573200	0.98447100
C	-3.96721100	-0.41916600	1.47689600
C	-2.11997800	0.89656800	2.00460600
C	-4.15734800	-0.73461600	2.81806600

C	-2.26569400	0.65330200	3.35076900
C	-3.27971200	-0.21039300	3.73600500
H	-4.99538700	-1.34799500	3.11667500
H	-1.61555600	1.12841300	4.07053600
C	-2.34120000	1.86966500	-0.98642900
C	-1.62238800	2.17333800	-2.14936000
C	-2.96407800	2.97608600	-0.41163200
C	-1.46636300	3.44503400	-2.66767400
C	-2.84722600	4.27568400	-0.87806500
C	-2.08278300	4.48707400	-2.00406800
H	-0.89034800	3.60310700	-3.56764500
H	-3.35148900	5.08513900	-0.37069100
F	-1.94857200	5.72952000	-2.47843500
F	-1.06481600	1.18340000	-2.85687100
F	-3.74715400	2.81633500	0.66179800
F	-4.93382400	-0.86345300	0.65472900
F	-1.18813300	1.79267700	1.65789900
F	-3.43083500	-0.49679400	5.03360500

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Carbazole fragment

N	0.00007100	-1.69133800	0.00010400
C	0.73099100	0.51379400	0.00000100
C	3.40236100	-0.25621400	-0.00003900
H	4.45025500	-0.52704200	-0.00005800
C	-1.09108900	-0.86151200	0.00002800
C	1.09102500	-0.86158500	0.00001900
C	-1.70139500	1.49024700	0.00003500
H	-1.44319800	2.54266800	0.00003700
C	-2.43095000	-1.25107400	-0.00006500
H	-2.68877800	-2.30208600	-0.00016600
C	-0.73098300	0.51379600	0.00010000
C	2.43101700	-1.25105700	-0.00002200
H	2.68902000	-2.30202900	-0.00002000
C	1.70134800	1.49027700	-0.00001800

H	1.44304000	2.54266600	0.00000700
C	-3.40239000	-0.25624700	-0.00005400
H	-4.45028600	-0.52704100	-0.00010300
C	3.04536400	1.09164500	-0.00003300
H	3.82274400	1.84522100	-0.00003700
C	-3.04539000	1.09156900	-0.00001000
H	-3.82275200	1.84517100	-0.00003200

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Au-Carbazole fragment

Au	-1.88698800	-0.00020200	-0.04737400
N	0.03709700	-0.00010400	0.28714700
C	2.18124000	-0.72254700	-0.00757100
C	1.48617600	-3.40990600	0.04991600
H	1.23294700	-4.46266500	0.06387900
C	0.83590400	1.12328000	0.13995900
C	0.83619200	-1.12315900	0.13998600
C	3.17968100	1.68969500	-0.11037900
H	4.21790700	1.39544600	-0.21245800
C	0.47739600	2.46763200	0.16437800
H	-0.56261700	2.75884300	0.26442500
C	2.18103100	0.72302100	-0.00755500
C	0.47822300	-2.46769800	0.16439300
H	-0.56166600	-2.75934800	0.26445900
C	3.18023200	-1.68883500	-0.11041400
H	4.21831900	-1.39409900	-0.21250000
C	1.48501500	3.41022500	0.04992300
H	1.23147800	4.46290600	0.06388200
C	2.82768400	-3.02775800	-0.08333000
H	3.59239200	-3.78914900	-0.16761200
C	2.82664000	3.02848500	-0.08330300
H	3.59110400	3.79013100	-0.16756000

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a-1-1 carbene fragment

C	-1.82793800	-0.97569600	0.83999900
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N	0.19554900	-0.09318900	-0.18370900
C	0.82417200	1.14596200	0.38709600
C	-3.20774000	-1.12295900	0.86910600
H	-3.67002000	-1.70999900	1.65245900
C	0.97268900	-1.08457200	-0.54764900
C	-2.01131500	0.36288900	-1.15424200
C	-3.99198200	-0.52544300	-0.11070900
C	-1.23301900	-0.22963700	-0.16896300
C	2.29488700	0.88700100	0.05154200
H	2.94890100	1.17434800	0.87850500
H	2.58008700	1.48429000	-0.81939700
C	-3.39196900	0.21261700	-1.12341900
H	-3.99848600	0.66556100	-1.89738900
C	0.54573600	1.20532600	1.88523000
H	-0.52740300	1.27897100	2.07577400
H	1.02863100	2.08523500	2.31446000
H	0.92781700	0.31801400	2.39241200
C	0.29348800	2.40646300	-0.27928900
H	0.41607000	2.35361500	-1.36294200
H	0.85742100	3.26664300	0.08724000
H	-0.76107400	2.56920100	-0.04822800
C	2.39129700	-0.61366400	-0.28996800
C	2.91427700	-1.44387100	0.88566600
H	2.89324800	-2.50525700	0.63482600
H	3.94363500	-1.15477100	1.11506500
H	2.30973500	-1.29888400	1.78378300
C	3.26452900	-0.87231900	-1.51190600
H	4.28925800	-0.53829600	-1.32482900
H	3.27913100	-1.93781700	-1.74570600
H	2.88367800	-0.33802100	-2.38509500
H	-1.19347100	-1.44794900	1.58070500
H	-5.06794400	-0.64303300	-0.09061700
H	-1.53074500	0.91788500	-1.95002100

a-1-1 carbene-Au fragment

Au	1.22505900	-1.34095900	0.00114400
C	-2.02660300	-0.67642300	1.04566300
N	-0.67046800	0.96276200	-0.13767700
C	-0.86150200	2.40345600	0.21087600
C	-3.09452600	-1.56218800	1.07890300
H	-3.28731100	-2.13735300	1.97506900
C	0.57046700	0.57187700	-0.32913600
C	-2.57094600	-0.111105400	-1.23743100
C	-3.90161800	-1.72135300	-0.04138900
C	-1.77568300	0.04926900	-0.11207600
C	0.51432800	2.96837500	-0.16062400
H	0.83471400	3.73572300	0.54691200
H	0.45755900	3.42842000	-1.15115300
C	-3.63754100	-0.99994300	-1.19910600
H	-4.25633400	-1.13475600	-2.07683200
C	-1.18791600	2.52498200	1.69518000
H	-2.13642100	2.03275500	1.92027400
H	-1.27840400	3.57867200	1.96498600
H	-0.40801300	2.07368900	2.30984100
C	-1.97951800	3.02053500	-0.61404800
H	-1.79636900	2.88290400	-1.68138200
H	-2.02282600	4.09157300	-0.40803800
H	-2.94792000	2.58442300	-0.36185300
C	1.48247200	1.77046600	-0.20176900
C	2.30578900	1.64189000	1.08412100
H	2.95666300	0.76801200	1.02903700
H	2.91934000	2.53819600	1.20812100
H	1.67305600	1.52750500	1.96589000
C	2.43323200	1.82652400	-1.39353200
H	3.08497500	2.70036900	-1.31324100
H	3.05097700	0.92646700	-1.41685800
H	1.88232300	1.88952100	-2.33409400
H	-1.36462600	-0.55748600	1.89529400

H	-4.73056700	-2.41700500	-0.01576800
H	-2.33980000	0.44629800	-2.13662200

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b-1-1 carbene fragment

C	1.69341000	1.27282500	-0.19216900
N	-0.33752900	-0.09327200	-0.12001900
C	-0.98295300	-0.29508200	1.22867400
C	3.08741900	1.36010600	-0.19790100
H	3.55894600	2.33469300	-0.15382300
C	-1.11186200	0.08962300	-1.16163700
C	1.85992500	-1.14298300	-0.41709200
C	1.09252100	0.00896000	-0.21648800
C	-2.44207300	-0.48324300	0.80671100
H	-3.12422200	0.03411000	1.48563400
H	-2.69448800	-1.54748000	0.83012100
C	3.25260700	-1.03851600	-0.42324200
H	3.85224400	-1.93154100	-0.55358800
C	-0.75849200	0.93290300	2.10392900
H	0.30862400	1.10537800	2.25654800
H	-1.22497100	0.76411200	3.07659400
H	-1.18646100	1.83203000	1.66243100
C	-0.41679900	-1.51363800	1.94136300
H	-0.56851100	-2.42290600	1.36132600
H	-0.92208900	-1.62258600	2.90328400
H	0.65323800	-1.39724300	2.12681200
C	-2.53523300	0.04044000	-0.63986700
C	-3.05777500	1.47912600	-0.70426200
H	-3.02869500	1.84556000	-1.73183100
H	-4.09019200	1.51653600	-0.34641400
H	-2.46063600	2.15351900	-0.08506200
C	-3.40172700	-0.84676700	-1.52445300
H	-4.42835300	-0.87392400	-1.14819200
H	-3.41214900	-0.46711400	-2.54735800
H	-3.01996100	-1.87039600	-1.54525600

N	0.90038500	2.41276900	-0.15198100
H	0.01921900	2.31498200	-0.64601600
H	1.38695600	3.26377600	-0.39645000
N	1.23127600	-2.36812600	-0.59755000
H	1.81369800	-3.08081400	-1.01345000
H	0.31736500	-2.30699500	-1.03038300
C	3.84817000	0.20562500	-0.29062300
H	4.92869500	0.28043700	-0.29572400

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b-1-1 carbene-Au fragment

Au	1.37288300	-1.32628000	-0.06385300
C	-1.97797600	-0.65379800	1.15673800
N	-0.54640400	0.94604600	-0.03181400
C	-0.76708300	2.40011900	0.27086600
C	-3.11726400	-1.46142600	1.16453800
H	-3.39907200	-1.97003700	2.07857900
C	0.69256900	0.59423400	-0.28896900
C	-2.31662200	-0.24377600	-1.22314300
C	-1.63990500	0.01633200	-0.02573700
C	0.59596200	2.98113000	-0.12574700
H	0.90930700	3.76963200	0.56140500
H	0.52365800	3.41698100	-1.12636600
C	-3.45053000	-1.05578600	-1.19380100
H	-3.99331900	-1.24553100	-2.11195800
C	-1.10507100	2.59523700	1.74381300
H	-2.02451800	2.06660400	1.99881300
H	-1.25159700	3.66100600	1.93021900
H	-0.31372900	2.23117200	2.39770900
C	-1.90195100	2.95852300	-0.57397200
H	-1.70885300	2.82655600	-1.63760900
H	-2.00295600	4.02423800	-0.36002100
H	-2.84662700	2.46790100	-0.33013100
C	1.58672500	1.80310000	-0.15046100
C	2.37057100	1.67135100	1.16055800

H	3.03728100	0.80854300	1.11708900
H	2.96485900	2.57498600	1.31848100
H	1.70716300	1.53848900	2.01793500
C	2.56817900	1.88000400	-1.31387200
H	3.20561100	2.76189400	-1.21235400
H	3.19926200	0.98879700	-1.32848000
H	2.04147100	1.94417900	-2.26876500
N	-1.19581500	-0.49882800	2.29430100
H	-0.19967900	-0.42737000	2.09885500
H	-1.37621500	-1.19501100	3.00532200
N	-1.86202600	0.31906300	-2.40987300
H	-2.24240600	-0.10842200	-3.24268600
H	-0.85574500	0.42987800	-2.46162500
C	-3.84966800	-1.63321500	0.00154300
H	-4.72951200	-2.26447800	0.01752400

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c-1-1 carbene fragment

C	1.67645700	1.25440700	-0.11703400
N	-0.35347200	-0.10592500	-0.11366100
C	-1.03136400	-0.33436300	1.20688900
C	3.05884700	1.38036900	-0.21978500
H	3.51324700	2.36293900	-0.15913000
C	-1.08692700	0.09321600	-1.18265300
C	1.86434700	-1.12386600	-0.40453600
C	1.06894600	-0.00005800	-0.18390500
C	-2.48363800	-0.47757400	0.74406300
H	-3.16915200	0.04986400	1.41214300
H	-2.76484600	-1.53452800	0.74491600
C	3.24763900	-1.00386400	-0.50783700
H	3.85019900	-1.88982500	-0.67440900
C	-0.80689800	0.85579000	2.13242400
H	0.25845600	0.98980200	2.33512200
H	-1.31346900	0.67071900	3.08186000
H	-1.19144500	1.77812600	1.69964300

C	-0.50617900	-1.59528800	1.87687600
H	-0.64132400	-2.46321000	1.23297500
H	-1.05014600	-1.75553500	2.81014900
H	0.55635100	-1.49916400	2.11555700
C	-2.52308900	0.06893700	-0.69720700
C	-2.98709300	1.52876100	-0.74737700
H	-2.95348500	1.89802500	-1.77340900
H	-4.01317800	1.60509500	-0.37661000
H	-2.34589400	2.17222800	-0.14070700
C	-3.39968800	-0.77309600	-1.61409900
H	-4.43663100	-0.76386500	-1.26529800
H	-3.36810000	-0.37856700	-2.63092000
H	-3.05554100	-1.80922600	-1.64023500
C	3.83421300	0.24772200	-0.41055400
H	4.90928000	0.34263600	-0.49301800
O	1.23906300	-2.31806000	-0.53329800
H	1.88440900	-3.00356900	-0.74342300
O	0.86859600	2.33084500	0.03537400
H	1.39087100	3.14069000	-0.00778600

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c-1-1 carbene-Au fragment

Au	1.23511000	-1.40327100	-0.11269700
C	-1.84819800	-0.52746600	1.19729400
N	-0.49021300	1.04646000	-0.07123300
C	-0.61491400	2.51372600	0.19474700
C	-2.86811800	-1.46922600	1.26938900
H	-3.04490000	-1.99578600	2.19932300
C	0.72065700	0.58490200	-0.25538600
C	-2.37345300	-0.12608100	-1.12092500
C	-1.60900000	0.16275100	0.00783400
C	0.80951300	2.98066300	-0.13184500
H	1.15109800	3.73906500	0.57554100
H	0.82561400	3.42186000	-1.13200400
C	-3.39913000	-1.06273600	-1.04955000

H	-3.98978900	-1.27771200	-1.93272000
C	-1.01349400	2.74942600	1.64637600
H	-1.97955200	2.28571800	1.85801100
H	-1.10384600	3.82346200	1.81886800
H	-0.27994900	2.33874800	2.33784700
C	-1.65533500	3.13395100	-0.72404100
H	-1.40424000	2.96357100	-1.76984200
H	-1.69623100	4.20854900	-0.53650200
H	-2.64598200	2.71564500	-0.52947500
C	1.69798100	1.72239200	-0.11021000
C	2.40313300	1.52592700	1.23791100
H	3.00221000	0.61391900	1.21649200
H	3.05629600	2.38054500	1.43208000
H	1.68688800	1.43222400	2.05660900
C	2.73146200	1.70418000	-1.22911100
H	3.43794900	2.52824500	-1.10089300
H	3.28180600	0.76118400	-1.20986400
H	2.25510900	1.80389400	-2.20626900
C	-3.63493700	-1.72714500	0.14398700
H	-4.42620400	-2.46375900	0.19542400
O	-2.05194000	0.50886600	-2.27256700
H	-2.56410200	0.14302600	-3.00386100
O	-1.04389900	-0.24477900	2.24958000
H	-1.01464400	-0.99347200	2.85799500

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d-1-1 carbene fragment

C	1.39547000	1.34023700	-0.15220200
N	-0.53141100	-0.15720000	-0.06972400
C	-1.22439200	-0.31796400	1.25339100
C	2.77258700	1.54962400	-0.22796300
H	3.18174900	2.54923600	-0.24324400
C	-1.25149200	-0.10003100	-1.16375100
C	1.74942700	-1.04975600	-0.23011800
C	3.61766900	0.45260500	-0.29559200

C	0.88256500	0.04015900	-0.12307500
C	-2.65251200	-0.59994800	0.77886700
H	-3.38809100	-0.06795600	1.38757600
H	-2.86117200	-1.67023500	0.86436000
C	3.12750300	-0.84418700	-0.30513300
H	3.80928800	-1.67861000	-0.38057800
C	-1.10452700	0.95836500	2.07885400
H	-0.05588000	1.18328900	2.28808200
H	-1.61935500	0.81675800	3.03139400
H	-1.54270100	1.81180600	1.56360800
C	-0.63490100	-1.47675700	2.04396300
H	-0.70444800	-2.40663500	1.48142500
H	-1.18651300	-1.58512200	2.98030200
H	0.41464200	-1.29142200	2.28735500
C	-2.69439600	-0.18029700	-0.70383300
C	-3.25311000	1.23487600	-0.88640800
H	-3.21795600	1.51912000	-1.93917000
H	-4.29096200	1.27244700	-0.54342000
H	-2.67076000	1.96795300	-0.32345200
C	-3.49185700	-1.15399100	-1.56059800
H	-4.53491900	-1.18680600	-1.23192000
H	-3.46306100	-0.84520300	-2.60675600
H	-3.07868600	-2.16267700	-1.49225800
H	4.68691700	0.61290200	-0.35368900
O	0.48815600	2.33910000	-0.11916100
O	1.17257300	-2.26901700	-0.27615300
C	0.95190500	3.66376500	-0.22245400
H	1.50124800	3.81748300	-1.15525900
H	0.07153800	4.30100200	-0.21530100
H	1.59624000	3.92783500	0.62143600
C	2.00420000	-3.39269900	-0.43825500
H	1.34955800	-4.25926600	-0.47677900
H	2.57522100	-3.33010500	-1.36869700
H	2.69732300	-3.50004600	0.40140400

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d-1-1 carbene-Au fragment

Au	1.36171100	-1.20958100	-0.61054700
C	-1.40331300	-0.83963700	1.35943100
N	-0.42079800	1.05942600	0.20955900
C	-0.54662400	2.43436900	0.78633600
C	-2.33854100	-1.86956500	1.42809400
H	-2.29435500	-2.59654200	2.22634600
C	0.75363800	0.72923100	-0.26158900
C	-2.43371200	-0.03223800	-0.68028700
C	-3.31789800	-1.95361200	0.45169300
C	-1.46413500	0.08918600	0.31724100
C	0.77768900	3.05591700	0.32435000
H	1.21174800	3.68952400	1.10054800
H	0.59822800	3.67829600	-0.55644400
C	-3.38073600	-1.05179100	-0.60151000
H	-4.14248200	-1.15925000	-1.35968500
C	-0.68379300	2.35574100	2.30215300
H	-1.57290000	1.78342600	2.57579000
H	-0.78975000	3.36662700	2.70027300
H	0.18100400	1.88147200	2.76209500
C	-1.75709700	3.14961900	0.20798900
H	-1.69411900	3.20861300	-0.87745900
H	-1.79888200	4.15993500	0.61943500
H	-2.68066800	2.63174600	0.47779900
C	1.70068300	1.88287500	-0.05517000
C	2.63674700	1.47718800	1.09087600
H	3.25787200	0.63377600	0.78402300
H	3.28005300	2.32199700	1.34995300
H	2.07713200	1.17092700	1.97729100
C	2.52369600	2.15260600	-1.30806300
H	3.21503100	2.98080700	-1.13257500
H	3.09889100	1.26266700	-1.57215400
H	1.88157000	2.40958100	-2.15269800

H	-4.04820900	-2.75112300	0.50373000
O	-0.40022500	-0.68097300	2.24669100
O	-2.35639600	0.84787500	-1.69996600
C	0.06878700	-1.83644400	2.91611500
H	0.24114800	-2.64236600	2.19770500
H	1.01336900	-1.56226900	3.37929600
H	-0.63209300	-2.16127300	3.68961600
C	-3.23669000	0.68105400	-2.78821200
H	-2.97795900	1.44601100	-3.51518500
H	-3.11566700	-0.30600800	-3.24160800
H	-4.27780600	0.81215400	-2.48027700

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e-1-1 carbene fragment

C	1.27722400	1.43127400	-0.05080100
N	-0.60405200	-0.14046500	0.03339300
C	-1.29570000	-0.29243500	1.36643600
C	2.65466200	1.64149200	-0.03055300
H	3.03505700	2.65599400	-0.06125700
C	-1.32488000	-0.20534500	-1.05756800
C	0.42665500	3.03023200	-1.73490900
H	0.15408100	2.19633300	-2.38400900
H	1.44275400	3.34881500	-1.98409000
H	-0.25070300	3.86483200	-1.93013900
C	1.69002100	-0.97921900	-0.06957800
C	3.54122400	0.57689500	-0.00443000
H	4.60852100	0.75923700	0.01510400
C	0.81243500	0.11077200	-0.01521200
C	1.43538700	-2.76728800	-1.76044700
H	0.91267800	-2.06941400	-2.41703600
H	1.07454900	-3.77838900	-1.96223500
H	2.50261200	-2.73155100	-1.99596500
C	0.34977400	2.60899600	-0.26610100
H	-0.67289000	2.28025400	-0.08284100
C	1.20442000	-2.39620900	-0.29438300

H	0.12678200	-2.42370900	-0.12651200
C	-2.67360500	-0.76838100	0.90129800
H	-3.47511700	-0.30663800	1.48312500
H	-2.74787400	-1.85197000	1.03455600
C	0.64980900	3.79033200	0.65119500
H	0.65203900	3.49829600	1.70327100
H	-0.09997000	4.57178600	0.51309400
H	1.62262100	4.23159800	0.42291700
C	3.05845600	-0.72172700	-0.05045800
H	3.75415000	-1.55178100	-0.09572000
C	1.86746600	-3.40921200	0.63381000
H	1.76167800	-3.12493600	1.68277200
H	2.93387600	-3.50367100	0.41712600
H	1.42019000	-4.39567600	0.49612200
C	-1.33805500	1.04147800	2.10576700
H	-0.32729200	1.42831500	2.25824700
H	-1.79336200	0.88948000	3.08608100
H	-1.92524900	1.78916800	1.57285600
C	-0.59341300	-1.30479000	2.26191700
H	-0.58860800	-2.30199600	1.82279500
H	-1.12715900	-1.35995600	3.21266200
H	0.43644400	-1.00308200	2.46879400
C	-2.75410200	-0.42716400	-0.60083400
C	-3.50404300	0.88092800	-0.86619300
C	-3.39355100	-1.54965700	-1.40892900
H	-3.46182300	1.12907700	-1.92789300
H	-3.07064000	1.71566000	-0.30994000
H	-3.40839500	-1.29141500	-2.46880100
H	-2.83060000	-2.47957100	-1.29411800
H	-4.55133100	0.77816400	-0.56920900
H	-4.41977400	-1.72583900	-1.07367400

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e-1-1 carbene-Au fragment

Au	-1.62915200	-0.76276200	-0.97998200
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C	1.86984900	0.92099000	-0.99139500
N	0.34210400	0.51941900	0.88273100
C	0.61427700	1.23733200	2.17608800
C	2.96619500	0.50536900	-1.74332600
H	3.32967300	1.14357700	-2.54041400
C	-0.91343700	0.43450700	0.53079800
C	0.44563700	1.96318200	-2.73715200
H	-0.24299700	1.11688000	-2.67857500
H	1.17975200	1.75427500	-3.51981600
H	-0.11651900	2.85347300	-3.02723100
C	1.96417200	-1.20198800	0.23029000
C	3.57591000	-0.71615200	-1.50943800
H	4.42956900	-1.01945700	-2.10242300
C	1.41924700	0.07416200	0.03150900
C	0.75580000	-3.37588000	0.32327400
H	0.01328300	-3.00163100	-0.38548600
H	0.27580000	-4.10745000	0.97677100
H	1.54201400	-3.88750500	-0.23815900
C	1.15003100	2.19144000	-1.39793300
H	0.37642600	2.40663500	-0.65922500
C	1.35300800	-2.23703800	1.15392800
H	0.53139400	-1.77087200	1.70352600
C	-0.80185600	1.34106700	2.75333200
H	-0.96803100	2.31094000	3.22687500
H	-0.94022600	0.56856500	3.51476100
C	2.07982900	3.39894400	-1.49552800
H	2.63211100	3.57253700	-0.57066600
H	1.50308500	4.29700400	-1.72538100
H	2.80687800	3.26572300	-2.29967000
C	3.05957400	-1.56879200	-0.54782000
H	3.49634800	-2.55122700	-0.41036800
C	2.36462300	-2.80727900	2.14754200
H	2.87238000	-2.03047300	2.72035400
H	3.12766100	-3.38747800	1.62354400

H	1.86592800	-3.48256100	2.84566300
C	1.24908200	2.59447300	1.89571500
H	2.18795300	2.46895000	1.35221400
H	1.46880900	3.08310300	2.84631000
H	0.59288600	3.24724800	1.32022700
C	1.55186900	0.44677000	3.07353900
H	1.13115500	-0.52139300	3.34289800
H	1.71509700	1.01371400	3.99189900
H	2.52010100	0.29506200	2.59095000
C	-1.77176800	1.08559400	1.58448500
C	-2.32741100	2.37522800	0.97198400
C	-2.92965700	0.17859300	1.98642200
H	-2.91029300	2.13976100	0.07925900
H	-1.53152100	3.06668400	0.68647300
H	-3.59063000	0.00433000	1.13570400
H	-2.56448300	-0.79116000	2.33230900
H	-2.97485300	2.87574300	1.69604300
H	-3.50032500	0.64615500	2.79321400

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e-2-1 carbene fragment

C	-1.98439600	-1.01330900	-0.06970200
N	0.24820600	-0.03080400	0.15501600
C	0.84603500	-0.06972500	1.53964000
C	-3.36288800	-0.83777700	-0.16273500
H	-4.00505700	-1.70946000	-0.21552100
C	1.04870700	-0.09363200	-0.87780500
C	-1.47300500	-2.83518300	-1.66035700
H	-0.94817000	-2.11724900	-2.29445200
H	-2.51452400	-2.88948200	-1.98928200
H	-1.01918700	-3.82032100	-1.79362200
C	-1.70928700	1.41462700	-0.14768400
C	-3.91947400	0.43031700	-0.21999100
H	-4.99369200	0.54978900	-0.28743000
C	-1.17478700	0.12753600	-0.00789900

C	-0.83569800	2.99101300	-1.84198400
H	-0.47386300	2.14805100	-2.43336300
H	-0.19262100	3.85418600	-2.02884300
H	-1.84776900	3.24039300	-2.17293300
C	-1.39984200	-2.40394900	-0.19444600
H	-0.34320500	-2.35681700	0.06686300
C	-0.83702000	2.63529600	-0.35401400
H	0.18757500	2.37513900	-0.09011200
C	2.31958300	-0.33543400	1.20972500
H	2.59793300	-1.34493500	1.52138700
H	2.96643700	0.35805300	1.75304600
C	-2.07589500	-3.42795200	0.71095800
H	-2.06546800	-3.11042400	1.75569400
H	-1.56352000	-4.38937900	0.63823800
H	-3.11557100	-3.59164000	0.41870000
C	-3.09372800	1.54304300	-0.23857200
H	-3.52654400	2.53051400	-0.35031800
C	-1.26371900	3.83260100	0.48927100
H	-1.31135600	3.58436800	1.55144000
H	-2.24590900	4.20146800	0.18535200
H	-0.55553500	4.65341900	0.35966600
C	0.22771000	-1.17512300	2.38603200
H	-0.85356800	-1.04529500	2.47868500
H	0.66116800	-1.13509300	3.38714600
H	0.43211700	-2.16320000	1.97124300
C	0.63396000	1.26094600	2.25421300
H	1.15541400	2.07716000	1.75247200
H	1.02555000	1.18442300	3.27018800
H	-0.42956200	1.50457800	2.31715900
C	2.45681400	-0.16864600	-0.31991900
C	3.20590800	-1.33405900	-0.97487100
C	3.11461300	1.17573900	-0.68355100
H	3.41351000	-1.06372200	-2.01548900
H	2.94584100	1.35651700	-1.74917600

H	2.58327200	1.97230700	-0.14772000
H	4.17246900	-1.45914500	-0.47553900
C	4.60307500	1.24774400	-0.36977800
H	4.98550700	2.25594200	-0.53307100
H	4.80982600	0.97854100	0.66924800
H	5.17419700	0.57135600	-1.00718900
C	2.42374500	-2.64045100	-0.93658800
H	3.01119700	-3.46994800	-1.33192200
H	2.13194000	-2.90272300	0.08562500
H	1.51126100	-2.55347900	-1.53093900

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e-2-1 carbene-Au fragment

Au	0.92503000	-0.21157400	-1.77061300
C	-2.27181000	-1.02590900	0.29198200
N	-0.21761800	0.09614700	1.01392800
C	-0.00184600	0.22065700	2.49850800
C	-3.57366900	-0.93424200	-0.19285600
H	-4.15332500	-1.84125400	-0.31946700
C	0.85604900	-0.01116000	0.28694100
C	-1.44423300	-3.07825200	-0.83986600
H	-0.81583500	-2.46551800	-1.49208700
H	-2.40023700	-3.24277100	-1.34423200
H	-0.96172900	-4.04841200	-0.69959800
C	-2.04375600	1.39910300	0.01282900
C	-4.12330100	0.28837700	-0.54261800
H	-5.13879600	0.34103100	-0.91455400
C	-1.54216300	0.16145500	0.43943900
C	-0.97808800	3.01630800	-1.54774700
H	-0.51102800	2.18860900	-2.08697400
H	-0.33248700	3.89347900	-1.62758600
H	-1.92909800	3.25024500	-2.03336000
C	-1.66681800	-2.39711400	0.51214200
H	-0.68625200	-2.27259700	0.97309700
C	-1.20657200	2.66024100	-0.07664100

H	-0.22716600	2.46224600	0.36378000
C	1.51593400	0.00816200	2.60698900
H	1.72649200	-0.94546500	3.09553100
H	1.96753200	0.79245900	3.21831500
C	-2.52166600	-3.28570100	1.41296500
H	-2.74156100	-2.81202500	2.37114000
H	-2.00728700	-4.22949300	1.60464400
H	-3.47236400	-3.52615600	0.93189800
C	-3.35327800	1.43663000	-0.46155400
H	-3.76301700	2.38244400	-0.79676500
C	-1.84366500	3.84705800	0.64433500
H	-2.05794000	3.63456700	1.69235800
H	-2.78200200	4.13038200	0.16205300
H	-1.18002800	4.71275100	0.59757500
C	-0.79391000	-0.82795200	3.26396400
H	-1.86339300	-0.73633000	3.06145200
H	-0.63492900	-0.67103500	4.33227600
H	-0.46937600	-1.83971800	3.01834500
C	-0.43594700	1.60127000	2.97117900
H	0.14289400	2.39306700	2.49366000
H	-0.28287900	1.66824300	4.04949500
H	-1.49637500	1.76135300	2.76595900
C	2.07368800	0.02461600	1.16913000
C	2.97385400	-1.17887800	0.86014200
C	2.79719400	1.34691300	0.84561900
H	3.43868800	-1.00960900	-0.11731400
H	2.93395300	1.39807400	-0.23930200
H	2.13115100	2.17600100	1.11571900
H	3.77518100	-1.20456500	1.60491200
C	4.13601200	1.50326500	1.55246100
H	4.53923800	2.50324000	1.39204500
H	4.04543300	1.35060600	2.63101400
H	4.86777400	0.78866400	1.17458700
C	2.22791400	-2.50677900	0.84228300

H	2.91863400	-3.34433600	0.74497000
H	1.65305400	-2.66008600	1.76171600
H	1.53352100	-2.54519100	-0.00210600

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e-3-1 carbene fragment

C	2.45253700	1.41294200	-0.19241700
N	0.64825700	-0.14594400	0.36518800
C	-2.50803600	-1.41169600	-0.34539700
H	-1.95512700	-2.35987400	-0.35565600
C	-3.63433400	0.30705400	-1.76872400
H	-3.88344100	0.59272800	-2.79477000
C	0.32273000	-0.32367000	1.82412800
C	3.78854100	1.61752600	-0.53114900
H	4.15493800	2.63059200	-0.65070000
C	-2.39530700	0.99208000	0.29619100
H	-1.77080700	1.77656100	0.74028700
C	-0.33373200	-0.14952100	-0.49882200
C	-2.87310500	-1.01792800	-1.77713100
H	-3.50190000	-1.80181000	-2.21525900
H	-1.96645900	-0.92732100	-2.37771200
C	1.18979400	3.02280100	-1.58172300
H	0.76421400	2.18725900	-2.14083700
H	2.10115000	3.35249200	-2.08861400
H	0.47659200	3.85057000	-1.58662600
C	2.82956500	-0.99911200	-0.34301800
C	4.64398600	0.54882400	-0.74788900
H	5.68048700	0.72681000	-1.00623200
C	-2.75801700	1.39030100	-1.13856200
H	-3.30465700	2.34030700	-1.11498600
H	-1.85127400	1.53230400	-1.73123800
C	-4.91674800	0.14487700	-0.95386300
H	-5.48423200	1.08237400	-0.95317600
H	-5.55056100	-0.62639100	-1.40569900
C	2.00521500	0.09340000	-0.04889300

C	-1.60718600	-0.34428700	0.30566500
C	2.13042200	-2.75950800	-1.93399400
H	1.46533400	-2.04668200	-2.42516900
H	1.71710800	-3.76401000	-2.04938500
H	3.10128700	-2.72910600	-2.43614300
C	-3.78859800	-1.56590100	0.47690400
H	-4.40848000	-2.35722400	0.04163500
H	-3.55384700	-1.86502100	1.50468200
C	1.50638400	2.59480100	-0.14719600
H	0.56748000	2.26909500	0.30043400
C	2.28850300	-2.40937900	-0.45315300
H	1.28987400	-2.43161500	-0.01454800
C	-1.13441600	-0.77011900	1.71328600
H	-1.73164500	-0.35956000	2.52876900
H	-1.18554000	-1.86231500	1.78931300
C	2.04403200	3.76972800	0.66318900
H	2.31893300	3.47097500	1.67682800
H	1.28931000	4.55579900	0.72927800
H	2.92629800	4.20720400	0.19052200
C	4.15737600	-0.74732500	-0.67968000
H	4.81120600	-1.57952200	-0.91444700
C	3.15758000	-3.44076600	0.25952700
H	3.32577200	-3.17335100	1.30470000
H	4.13237200	-3.53624000	-0.22400800
H	2.68145900	-4.42277600	0.22630400
C	-3.69278700	0.85141600	1.09585400
H	-3.49389500	0.62822400	2.14778900
H	-4.22980700	1.80624500	1.06811300
C	0.49266400	0.99314100	2.57694500
H	1.51313300	1.36926000	2.46654900
H	0.30832000	0.82265100	3.63922000
H	-0.20379500	1.75680000	2.23104000
C	-4.56193500	-0.24558700	0.48050200
H	-5.47694900	-0.35917900	1.06942400

C	1.21153300	-1.36518900	2.49080200
H	1.08548100	-2.35260000	2.04782900
H	0.93845800	-1.43396800	3.54556900
H	2.26543000	-1.08148700	2.43231000

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e-3-1 carbene-Au fragment

Au	-0.12521200	-1.72112100	0.79545200
C	-2.26275600	1.37584800	1.05486000
N	-0.62170300	0.77218300	-0.65572500
C	2.60848100	-0.62128200	-1.26080600
H	2.06580600	-1.22865800	-1.99515300
C	3.83117400	-0.67315700	0.92096100
H	4.14356500	-1.31179400	1.75136900
C	-0.23098600	1.81401000	-1.65662100
C	-3.58067300	1.36559100	1.50428300
H	-3.82590800	1.87815100	2.42729300
C	2.44203700	1.31873400	0.29197300
H	1.79312000	2.10483600	0.69001900
C	0.35723300	0.04002300	-0.17383900
C	3.10400200	-1.51403200	-0.12345400
H	3.78947100	-2.25910800	-0.54313900
H	2.27521800	-2.05936600	0.33741500
C	-0.98138700	1.14843800	3.17430600
H	-0.70746900	0.12716900	2.89711300
H	-1.89441300	1.10569100	3.77425200
H	-0.18615400	1.57034300	3.79343600
C	-2.93711300	-0.05411600	-0.81773700
C	-4.57090100	0.69314600	0.80737800
H	-5.59138700	0.70041900	1.16926300
C	2.88184500	0.40628700	1.44186600
H	3.38946200	1.01586400	2.19760500
H	2.01112500	-0.05873300	1.91607600
C	5.05488800	-0.02833600	0.27234000
H	5.60444400	0.57209000	1.00594200

H	5.73228300	-0.80716700	-0.09416100
C	-1.96822700	0.70036600	-0.13943200
C	1.66672200	0.50521900	-0.78465900
C	-2.85863300	-2.43691700	-1.55493300
H	-2.26388200	-2.69620900	-0.67617000
H	-2.58745200	-3.11072900	-2.37056100
H	-3.91382400	-2.59911900	-1.31986900
C	3.83613100	0.02491100	-1.91550600
H	4.48752500	-0.76516400	-2.30289400
H	3.54736700	0.64928900	-2.76722400
C	-1.20271500	2.01226100	1.93115200
H	-0.26208200	2.02953800	1.38059700
C	-2.62484300	-0.98314600	-1.97497900
H	-1.56491700	-0.88253300	-2.22250100
C	1.18905700	1.35929400	-1.97847200
H	1.82939700	2.21081300	-2.20490300
H	1.16626900	0.71945100	-2.86784200
C	-1.54730300	3.44290800	2.33883100
H	-1.75159600	4.07869200	1.47568600
H	-0.71988700	3.88080300	2.90081800
H	-2.42639400	3.46407000	2.98665500
C	-4.24150400	-0.02549000	-0.32946000
H	-5.00492300	-0.60070000	-0.84060800
C	-3.47258500	-0.68300100	-3.21193500
H	-3.41117600	0.35909900	-3.52535100
H	-4.52294700	-0.90865900	-3.01279300
H	-3.15736300	-1.31432300	-4.04524100
C	3.69076000	1.95356600	-0.32489200
H	3.43388600	2.67776400	-1.10207700
H	4.22168300	2.50637300	0.45793700
C	-0.30124600	3.20829300	-1.03982200
H	-1.31302900	3.41077900	-0.68126600
H	-0.06060200	3.94433100	-1.80875200
H	0.39716000	3.33928000	-0.21459000

C	4.60091900	0.86099700	-0.88439800
H	5.47117000	1.31977900	-1.36250600
C	-1.13202100	1.80003900	-2.88020900
H	-1.10432200	0.83915300	-3.39206400
H	-0.78392400	2.56608500	-3.57566800
H	-2.16371400	2.03296500	-2.60756700

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e-4-1 carbene fragment

C	2.03659800	1.33042500	-0.16042800
N	0.05729000	-0.08136200	0.16023400
C	-0.49442900	-0.16338500	1.56002500
C	3.42039000	1.42809700	-0.29275000
H	3.87467200	2.40782400	-0.38564700
C	-0.78233900	-0.09009900	-0.84440300
C	1.14215200	2.97495400	-1.77646800
H	0.73647500	2.15887700	-2.37684700
H	2.14808600	3.20739300	-2.13723300
H	0.51638200	3.85958900	-1.91552300
C	2.25224700	-1.10572300	-0.17277800
C	4.21725100	0.29542400	-0.33952100
H	5.29143100	0.39073800	-0.43861600
C	1.47519700	0.05248600	-0.04674500
C	1.67419400	-2.88624600	-1.79037800
H	1.14150100	-2.15536000	-2.40147900
H	1.21328700	-3.86642800	-1.93202900
H	2.70909200	-2.94116300	-2.13923400
C	1.18824900	2.57724400	-0.29980900
H	0.16761200	2.33508400	-0.00430800
C	1.63328900	-2.48073900	-0.31583200
H	0.58129300	-2.41780800	-0.03390600
C	-1.95397900	-0.51517200	1.25892800
H	-2.63233000	0.02974900	1.91954000
H	-2.11802300	-1.58381500	1.43347800
C	1.67762600	3.74004200	0.55778600

H	1.76616600	3.46086900	1.60963200
H	0.98342800	4.57928100	0.48236500
H	2.65384200	4.09650700	0.22143300
C	3.63080600	-0.96015500	-0.30639100
H	4.24913000	-1.84456800	-0.40911900
C	2.30882400	-3.53403500	0.55674900
H	2.33807000	-3.23086300	1.60532400
H	3.33525800	-3.71685400	0.23097100
H	1.77249400	-4.48245500	0.48596200
C	-0.34086500	1.17557900	2.27515800
H	0.70971500	1.47482700	2.31079700
H	-0.69909600	1.07389300	3.30121500
H	-0.91657800	1.96537000	1.79211100
C	0.20832200	-1.22757500	2.39268700
H	0.07529200	-2.22491400	1.97431300
H	-0.22047700	-1.22543000	3.39666800
H	1.27758000	-1.01913600	2.48068700
C	-2.16544700	-0.19624300	-0.23621000
C	-2.86135700	1.15558700	-0.47104200
C	-2.96199700	-1.28826900	-0.95371500
C	-4.32452400	1.13561800	-0.04214100
H	-2.79477500	1.37938800	-1.54170200
H	-2.31644400	1.95038100	0.04994000
C	-4.40933000	-1.32764600	-0.48092900
H	-2.92836400	-1.08044400	-2.02878600
H	-2.46800000	-2.25381800	-0.79925600
C	-5.08220200	0.01450800	-0.74340700
H	-4.78495900	2.10331400	-0.25506900
H	-4.39464200	0.98891300	1.04205400
H	-4.94977300	-2.13424700	-0.98144500
H	-4.44151200	-1.54440800	0.59467200
H	-6.12537700	-0.00326600	-0.41939900
H	-5.08354800	0.20446700	-1.82352600

e-4-1 carbene-Au fragment

Au	-0.40251400	-1.68608100	-0.96682400
C	2.13763000	1.20853900	-0.90275400
N	0.24691100	0.79065400	0.60201400
C	-0.20146400	1.91500800	1.49222300
C	3.50182400	1.09080200	-1.15887400
H	3.90931100	1.54346500	-2.05545400
C	-0.70334700	0.06291500	0.08159600
C	1.20614800	0.95994100	-3.19127700
H	0.85322900	-0.04241300	-2.93683000
H	2.20158700	0.87082600	-3.63430600
H	0.53746000	1.38715200	-3.94167100
C	2.44299800	-0.18233700	1.09280900
C	4.33426600	0.38243500	-0.30816300
H	5.39253300	0.30531400	-0.52377800
C	1.63835200	0.61084200	0.26325000
C	2.00700400	-2.51783600	1.83080100
H	1.48580300	-2.72354600	0.89270700
H	1.57685700	-3.14568000	2.61404700
H	3.05689500	-2.79762600	1.71022700
C	1.25615200	1.85669700	-1.95207700
H	0.23923300	1.92480200	-1.56172200
C	1.89326600	-1.04047100	2.21513100
H	0.83011300	-0.81806500	2.33555800
C	-1.68822600	1.58055200	1.66417200
H	-2.29747600	2.48516600	1.61627000
H	-1.85117400	1.12703300	2.64660800
C	1.72567200	3.25653300	-2.34281300
H	1.81148500	3.92183800	-1.48243900
H	1.02509500	3.70101300	-3.05248200
H	2.70120000	3.21521800	-2.83246800
C	3.80003400	-0.26819500	0.79172200
H	4.44028500	-0.87711300	1.41952400
C	2.60953600	-0.79962100	3.54334900

H	2.61453600	0.25268700	3.83019900
H	3.64784800	-1.13386900	3.48350500
H	2.12926200	-1.37315100	4.33863400
C	0.02884300	3.25158200	0.79754400
H	1.08818100	3.38318100	0.56758400
H	-0.27626300	4.05504700	1.46991400
H	-0.54719900	3.33951400	-0.12402600
C	0.55080200	1.92255300	2.81278000
H	0.38403800	1.00556500	3.37706500
H	0.19198400	2.76072800	3.41288300
H	1.62327700	2.05378300	2.65157500
C	-2.03818400	0.56070200	0.56273400
C	-2.75013600	1.18609900	-0.65125700
C	-2.89071200	-0.59715400	1.09086900
C	-4.16904500	1.63042300	-0.31455300
H	-2.77601800	0.42647400	-1.44168800
H	-2.16199100	2.02605200	-1.03641100
C	-4.28642300	-0.12053900	1.46962700
H	-2.95799300	-1.35831200	0.30503500
H	-2.37992900	-1.06296700	1.94012200
C	-4.98380000	0.47408700	0.25223700
H	-4.64565600	2.03705600	-1.20907500
H	-4.14157900	2.44315500	0.42082600
H	-4.86530500	-0.95066700	1.87904200
H	-4.22062500	0.63962800	2.25885100
H	-5.99244000	0.80698700	0.50629800
H	-5.08349800	-0.30382100	-0.51356800

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e-5-1 carbene fragment

C	1.97628800	1.33290300	-0.11985200
N	-0.00388100	-0.08898800	0.12188600
C	-0.60295400	-0.18003900	1.50388400
C	3.36290400	1.44056400	-0.20501300
H	3.81371400	2.42384400	-0.27433000

C	-0.80842600	-0.09306600	-0.91132600
C	1.12475300	2.98704700	-1.74971600
H	0.74621000	2.17375100	-2.37133300
H	2.14029100	3.23057500	-2.07435900
H	0.49709900	3.86829000	-1.90145200
C	2.20781800	-1.10179600	-0.14628000
C	4.16816500	0.31315300	-0.23505300
H	5.24439500	0.41598900	-0.29748800
C	1.41984600	0.05032200	-0.03613700
C	1.70326500	-2.87520900	-1.79619200
H	1.19077100	-2.14337800	-2.42316800
H	1.25348300	-3.85683800	-1.96151100
H	2.75107300	-2.92285700	-2.10524900
C	1.12435700	2.57545500	-0.27612100
H	0.09587000	2.32391600	-0.01743800
C	1.60319400	-2.47923700	-0.32184700
H	0.54095100	-2.42374600	-0.08006800
C	-2.05152900	-0.52436900	1.14775600
H	-2.76710000	0.00325700	1.78360200
H	-2.21120000	-1.59874500	1.28971800
C	1.57611700	3.73309500	0.60860700
H	1.62893700	3.44453000	1.66028200
H	0.87995900	4.56902700	0.51626200
H	2.56142100	4.09819100	0.31025600
C	3.58917100	-0.94623200	-0.23250500
H	4.21632000	-1.82583800	-0.32233800
C	2.25120800	-3.53423800	0.56937800
H	2.23678300	-3.23877000	1.62041200
H	3.29102900	-3.70731800	0.28311800
H	1.72503600	-4.48584800	0.47067700
C	-0.45691300	1.14453300	2.24679600
H	0.59637900	1.42644900	2.32289200
H	-0.84993600	1.02850200	3.25838600
H	-1.00289400	1.95411700	1.76338300

C	0.06685900	-1.26148600	2.34211300
H	-0.05631700	-2.25105200	1.90283900
H	-0.39544400	-1.27356800	3.33100100
H	1.13345700	-1.05961100	2.46919700
C	-2.20957600	-0.17457400	-0.34466200
C	-2.85848900	1.20037100	-0.55914900
C	-3.04275800	-1.21302100	-1.09416500
C	-4.34150100	1.16213600	-0.33503800
H	-2.62980600	1.54333900	-1.57539700
H	-2.40297100	1.93666700	0.11237000
C	-4.43951400	-1.31934800	-0.49498200
H	-3.10364800	-0.90701800	-2.14259700
H	-2.53377600	-2.18173500	-1.06874000
C	-5.04741200	0.03558700	-0.28578300
H	-4.84621000	2.11379700	-0.20132800
H	-5.08492600	-1.91674700	-1.14448500
H	-4.40609300	-1.85733500	0.46112300
H	-6.11492400	0.08376000	-0.09572300

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e-5-1 carbene-Au fragment

Au	-0.38388600	-1.69490900	-1.01270800
C	2.05582900	1.33116800	-0.83919900
N	0.18022500	0.75096500	0.62274800
C	-0.31898500	1.79754600	1.57921100
C	3.42342600	1.28415000	-1.09851100
H	3.81305600	1.80581500	-1.96500200
C	-0.74147200	0.04562500	0.01842900
C	1.10900500	1.17415800	-3.12871000
H	0.77868100	0.15352600	-2.92101500
H	2.10334500	1.12753300	-3.58066900
H	0.42670400	1.62324000	-3.85377700
C	2.41489900	-0.16332300	1.07037600
C	4.28334400	0.56124900	-0.28794900
H	5.34417700	0.54047300	-0.50380100

C	1.57904600	0.64452300	0.28701000
C	2.10090600	-2.55677400	1.67895300
H	1.60389200	-2.74135700	0.72374600
H	1.69409700	-3.24643800	2.42159900
H	3.16600700	-2.77391600	1.56278000
C	1.14796500	2.00843700	-1.84655300
H	0.13338900	2.02905600	-1.44544000
C	1.90125700	-1.10979100	2.13734000
H	0.82606200	-0.95155100	2.25288000
C	-1.79516000	1.40143200	1.69689700
H	-2.44990600	2.27503600	1.73200200
H	-1.94099300	0.83661600	2.62315100
C	1.57375200	3.44008600	-2.16419600
H	1.65037200	4.05679700	-1.26726900
H	0.85210600	3.90354600	-2.83982000
H	2.54398000	3.45573100	-2.66557500
C	3.77502100	-0.17403800	0.76987700
H	4.43931300	-0.79158600	1.36340200
C	2.59108100	-0.90495100	3.48574500
H	2.53559400	0.12725400	3.83295100
H	3.64692400	-1.17736600	3.41800000
H	2.13741400	-1.54923500	4.24152700
C	-0.11037200	3.18895800	0.99154600
H	0.95009400	3.36245800	0.79554900
H	-0.44822900	3.93074600	1.71693600
H	-0.66730300	3.33841100	0.06700700
C	0.40653300	1.73301300	2.91311200
H	0.26503600	0.77036900	3.40332500
H	0.00471200	2.50982800	3.56621600
H	1.47576600	1.91627800	2.78470300
C	-2.09662800	0.49009700	0.49416000
C	-2.77021400	1.23266500	-0.67055900
C	-2.98776500	-0.69356300	0.87403500
C	-4.22084300	1.49524600	-0.39132200

H	-2.65157400	0.63187200	-1.58121400
H	-2.25275600	2.17881200	-0.86244400
C	-4.31635400	-0.19755000	1.42990800
H	-3.15225600	-1.29840800	-0.02297300
H	-2.46967900	-1.33059100	1.59698900
C	-4.90814400	0.87202300	0.56170600
H	-4.71337600	2.24106700	-1.00646100
H	-5.01713800	-1.03160800	1.51627400
H	-4.18929200	0.18575000	2.45035200
H	-5.94955300	1.13057600	0.72297900

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e-7-1 carbene fragment

C	1.87216400	1.47793100	-0.06936600
N	0.13742500	-0.21614700	0.26022000
C	-0.30949100	-0.48473900	1.67587300
C	3.21648600	1.78437300	-0.27051100
H	3.52012900	2.82371500	-0.32000100
C	-0.77741400	-0.17525200	-0.67755000
C	0.64527700	3.07479100	-1.50828200
H	0.32737500	2.24501500	-2.14218800
H	1.57823800	3.48242100	-1.90781900
H	-0.11446500	3.85926900	-1.54629500
C	2.43191600	-0.89524300	-0.26073900
C	4.16223000	0.78525600	-0.43852200
H	5.20314400	1.04291300	-0.58977900
C	1.50726000	0.12598300	-0.01323900
C	2.01014900	-2.63140700	-1.97047700
H	1.34917900	-1.94337500	-2.50085600
H	1.67859600	-3.65471000	-2.16034100
H	3.02027400	-2.51863100	-2.37365900
C	0.84891400	2.59511900	-0.06971500
H	-0.10590600	2.19093600	0.26712400
C	2.00258600	-2.33206800	-0.47012000
H	0.97134000	-2.43524300	-0.13085500

C	-1.72503400	-0.99292900	1.40889900
H	-2.41211300	-0.68820800	2.20107200
H	-1.72212500	-2.08817800	1.37295600
C	1.22670800	3.76003200	0.83999100
H	1.42275300	3.43017000	1.86224000
H	0.41799900	4.49305800	0.86465400
H	2.11874400	4.27463000	0.47580500
C	3.76448500	-0.54234900	-0.45926100
H	4.49446100	-1.31907400	-0.65676400
C	2.86893500	-3.33322100	0.28739000
H	2.91775000	-3.09967600	1.35282600
H	3.88966000	-3.34433400	-0.10143400
H	2.46736000	-4.34209900	0.17298100
C	-0.29822400	0.80969400	2.48364700
H	0.69944400	1.25608600	2.48189200
H	-0.57009600	0.59021200	3.51768400
H	-1.01039500	1.53630300	2.09125100
C	0.57205400	-1.50219900	2.38462300
H	0.53928700	-2.47825400	1.90139600
H	0.21416000	-1.62307500	3.40888200
H	1.61006200	-1.16273300	2.42786300
C	-2.08545000	-0.44324700	0.02153800
C	-3.08900000	-1.28437300	-0.78580300
C	-2.98952700	0.82023800	-0.01216800
C	-4.34201200	-1.18083800	0.09119500
C	-3.30526800	-0.43711000	-2.04404900
H	-2.76687400	-2.30811900	-0.98512200
C	-4.29973500	0.28772900	0.58604700
C	-3.21445800	1.01674800	-1.51518500
H	-2.59070100	1.70152500	0.49451400
H	-5.24783700	-1.41495900	-0.47087600
H	-4.28820800	-1.87640100	0.93239500
H	-2.51927100	-0.62498500	-2.77410300
H	-4.26933000	-0.65869600	-2.50726300

H	-5.14921900	0.87526300	0.23212500
H	-4.30343000	0.34102700	1.67632400
H	-2.37185200	1.53842900	-1.97036600
H	-4.12142200	1.59529200	-1.70310900

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e-7-1 carbene-Au fragment

Au	0.32224200	-1.75389200	0.74365600
C	-1.85879800	1.42109200	1.09022800
N	-0.31710500	0.73371500	-0.67239300
C	0.05450500	1.72607800	-1.73146700
C	-3.15381800	1.45646600	1.60057500
H	-3.34450500	2.00302800	2.51693300
C	0.68861400	0.05579000	-0.15419500
C	-0.47789500	1.21876700	3.14620100
H	-0.23592400	0.18735300	2.87791700
H	-1.36129900	1.20705900	3.79031900
H	0.35434500	1.63809700	3.71664100
C	-2.65306400	-0.05078700	-0.70104900
C	-4.19126300	0.78740400	0.97150200
H	-5.19319700	0.83177500	1.37973300
C	-1.63708500	0.70328600	-0.09618500
C	-2.65018800	-2.45983700	-1.34243000
H	-2.02145400	-2.69338000	-0.48053500
H	-2.42501000	-3.17239400	-2.13882200
H	-3.69695800	-2.59233000	-1.05626500
C	-0.74335800	2.05860400	1.89519800
H	0.17101400	2.04442500	1.30038900
C	-2.40919400	-1.02937000	-1.83291400
H	-1.35894900	-0.95915100	-2.12707600
C	1.46879800	1.25363200	-2.06410400
H	2.10324700	2.09100500	-2.35854100
H	1.43053300	0.54695200	-2.90024100
C	-1.03983000	3.50568300	2.28166100
H	-1.27168300	4.12247200	1.41158900

H	-0.17775200	3.94024700	2.79175300
H	-1.88641700	3.56307300	2.96931700
C	-3.93264700	0.02461000	-0.15474600
H	-4.73205100	-0.54868600	-0.61016300
C	-3.30358400	-0.76340500	-3.04414000
H	-3.23109100	0.26170300	-3.40711600
H	-4.34927200	-0.95309500	-2.79006000
H	-3.04027300	-1.43877300	-3.86074400
C	0.02096700	3.14225400	-1.16402200
H	-0.97385300	3.36965700	-0.77406300
H	0.24346100	3.85096500	-1.96345200
H	0.75097800	3.28491700	-0.36790900
C	-0.87896400	1.66977500	-2.92754700
H	-0.87415100	0.68788300	-3.39918900
H	-0.54663500	2.40373100	-3.66416200
H	-1.90039900	1.92269600	-2.63484300
C	1.96014100	0.51745500	-0.81065400
C	3.06051100	-0.53328100	-1.05020500
C	2.85240800	1.35477600	0.15256300
C	4.16815700	0.35534800	-1.62573800
C	3.50454500	-0.94448200	0.36222000
H	2.75978300	-1.36574900	-1.68813800
C	4.09166100	1.61341600	-0.72181900
C	3.23801500	0.32187200	1.21113500
H	2.39713300	2.25922400	0.55809700
H	5.13975600	-0.13838200	-1.58434500
H	3.97198300	0.60927400	-2.67000400
H	2.93440700	-1.79713700	0.73498200
H	4.55998300	-1.22640400	0.35779700
H	4.97691900	1.72822000	-0.09330700
H	3.99637500	2.52673400	-1.31159200
H	2.41316200	0.15085400	1.90814900
H	4.10865400	0.64471500	1.78444600

e-8-1 carbene fragment

C	-2.72257600	-1.15989000	-0.39589500
N	-0.82155100	0.09864800	0.47109200
C	-0.67579100	0.13735900	1.96579500
C	-4.00681300	-1.16934000	-0.93310800
H	-4.48516900	-2.11814000	-1.14682000
C	0.25128700	0.07883500	-0.27536100
C	-1.45613100	-2.89409700	-1.63230800
H	-0.83244800	-2.11471900	-2.07484000
H	-2.30117100	-3.08613600	-2.29959600
H	-0.86412000	-3.80908200	-1.55077700
C	-2.73724600	1.28591300	-0.50067100
C	-4.66617800	0.01536200	-1.22565300
H	-5.66706500	-0.00877700	-1.63851200
C	-2.12819500	0.08111000	-0.13367200
C	1.43810600	0.01108900	0.69038400
C	-1.59124300	2.95722400	-1.91837400
H	-0.97526000	2.16285600	-2.34339700
H	-1.02291700	3.88957800	-1.93794600
H	-2.47875200	3.08218900	-2.54470800
C	-1.95360000	-2.45735700	-0.25308600
H	-1.06426200	-2.26913000	0.34807000
C	-1.99579300	2.60709300	-0.48490600
H	-1.07160800	2.47980900	0.07989500
C	0.84976300	0.04464200	2.11732600
H	1.12392200	-0.83933400	2.68834600
H	1.22448900	0.88750800	2.69221700
C	-2.75877000	-3.56557300	0.41618800
H	-3.15141300	-3.24939600	1.38518700
H	-2.12878800	-4.44419700	0.56936000
H	-3.60257100	-3.87608300	-0.20412100
C	-4.02347400	1.22811200	-1.03468500
H	-4.51460500	2.14858300	-1.32913700
C	-2.79916100	3.74116700	0.14342300

H	-3.12204300	3.49675300	1.15729600
H	-3.68975400	3.96936500	-0.44647100
H	-2.19520200	4.64968100	0.18490100
C	-1.41351600	-1.01333900	2.64143200
H	-2.47384600	-1.00578600	2.37712000
H	-1.33358500	-0.89432500	3.72356900
H	-0.99480000	-1.98467600	2.37817900
C	-1.23458200	1.44556100	2.51459700
H	-0.69544000	2.30940600	2.12317100
H	-1.13815000	1.44627200	3.60195600
H	-2.29371400	1.54895100	2.26600100
C	2.32862400	1.19724000	0.33075300
C	2.31362900	2.40156300	1.03295700
C	3.12889700	1.10901100	-0.81260700
C	3.10780800	3.47474700	0.64654200
H	1.67588600	2.52976400	1.89775100
C	3.93740300	2.17740900	-1.18349500
C	3.93707700	3.36061600	-0.45885200
H	3.07780000	4.39504400	1.21626400
H	4.56572000	2.07714900	-2.06203300
H	4.57024400	4.18583700	-0.75935200
C	2.09042500	-1.31997900	0.30970400
C	1.83562200	-2.51174000	0.98721200
C	2.88432200	-1.36903800	-0.84028600
C	2.38992000	-3.71524700	0.56810200
H	1.19024800	-2.52587500	1.85592600
C	3.45270000	-2.57165700	-1.24495200
C	3.21383500	-3.74680900	-0.54725000
H	2.17835200	-4.62310400	1.11902300
H	4.08020300	-2.58190200	-2.12966200
H	3.65954100	-4.67726900	-0.87551100
C	3.06410300	-0.12664400	-1.65779000
H	3.94854500	-0.20652500	-2.29384600
H	2.18988800	-0.03488700	-2.31392100

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e-8-1 carbene-Au fragment

Au	-0.31812800	-0.00009300	-1.74839300
C	2.84185900	1.22706400	0.01461500
N	0.95531000	0.00022800	0.98720900
C	0.83595600	0.00032200	2.48322700
C	4.12034100	1.19951200	-0.53723400
H	4.60040200	2.13570400	-0.79799000
C	-0.15626000	0.00023500	0.30877700
C	1.82168200	3.08137600	-1.29230200
H	1.24831800	2.35447200	-1.87277000
H	2.75396200	3.28910600	-1.82435600
H	1.24823200	4.00904000	-1.23339700
C	2.84263100	-1.22587000	0.01522500
C	4.76869600	0.00098400	-0.78725400
H	5.76334900	0.00118400	-1.21512100
C	2.24673900	0.00049400	0.33856700
C	-1.33854000	-0.00015600	1.26062700
C	1.82293100	-3.08076300	-1.29110100
H	1.24911600	-2.35417000	-1.87151900
H	1.24991300	-4.00867900	-1.23196800
H	2.75518600	-3.28810000	-1.82335400
C	2.11766200	2.55503500	0.11403600
H	1.15408800	2.39327700	0.60173100
C	2.11903900	-2.55413500	0.11510900
H	1.15553700	-2.39265700	0.60302600
C	-0.69308500	-0.00008600	2.67181400
H	-1.00758500	0.87074300	3.24386800
H	-1.00717200	-0.87115100	3.24374000
C	2.90499300	3.60060300	0.90168400
H	3.17831400	3.25341500	1.89914900
H	2.31562400	4.51420800	1.00322700
H	3.82569600	3.86465700	0.37626700
C	4.12110000	-1.19783300	-0.53658400

H	4.60175200	-2.13385700	-0.79685200
C	2.90693000	-3.59926400	0.90274000
H	3.18015400	-3.25186500	1.90016300
H	3.82771500	-3.86296900	0.37729400
H	2.31797700	-4.51312100	1.00441200
C	1.51521100	1.22614900	3.08127100
H	2.58079600	1.22523400	2.84170800
H	1.41040100	1.18630400	4.16675700
H	1.08235200	2.16137800	2.73020000
C	1.51602700	-1.22479400	3.08175500
H	1.08360900	-2.16050800	2.73143200
H	1.41150200	-1.18433800	4.16724900
H	2.58154900	-1.22341600	2.84192000
C	-2.12385200	-1.27301500	0.95043100
C	-1.71096800	-2.49956800	1.47505100
C	-3.20428800	-1.25690200	0.06933200
C	-2.37059800	-3.68007700	1.17283800
H	-0.85366800	-2.54333800	2.13455400
C	-3.87764800	-2.44442800	-0.21426900
C	-3.47380000	-3.65170100	0.32909900
H	-2.02656500	-4.61458600	1.59745900
H	-4.72628100	-2.40962700	-0.88880500
H	-4.00730300	-4.56308800	0.09112300
C	-2.12482600	1.27213800	0.95069500
C	-1.71294500	2.49890100	1.47561700
C	-3.20527400	1.25535300	0.06962000
C	-2.37355100	3.67894200	1.17370600
H	-0.85568900	2.54323500	2.13514100
C	-3.87960800	2.44239800	-0.21368000
C	-3.47674100	3.64987000	0.32997400
H	-2.03028500	4.61362600	1.59856400
H	-4.72822900	2.40707000	-0.88820400
H	-4.01100600	4.56087100	0.09223100
C	-3.61867800	-0.00086100	-0.63024200

H	-4.69866100	-0.00128000	-0.79917200
H	-3.14497800	-0.00055700	-1.62396800

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e-9-1 carbene fragment

C	-2.76824100	-1.22290600	-0.43208700
N	-0.83117800	0.00000800	0.43904300
C	-0.65233300	0.00001500	1.93356800
C	-4.06689000	-1.19891600	-0.93527400
H	-4.55768100	-2.13474800	-1.17642200
C	0.22404300	0.00001200	-0.33657200
C	-1.59424000	-2.92967600	-1.78757000
H	-0.97672500	-2.14682500	-2.23149100
H	-2.47473200	-3.08088900	-2.41836800
H	-1.02045600	-3.85935500	-1.77034600
C	-2.76823500	1.22291300	-0.43209900
C	-4.72433700	0.00000400	-1.16177600
H	-5.73521100	0.00000400	-1.55016800
C	-2.15494500	0.00000400	-0.13322700
C	-1.59429300	2.92970100	-1.78761300
H	-0.97680700	2.14685400	-2.23158000
H	-1.02050200	3.85937600	-1.77040200
H	-2.47481600	3.08093200	-2.41836400
C	-2.01709300	-2.53580700	-0.37123700
H	-1.10069900	-2.37843600	0.19568900
C	-2.01707800	2.53581000	-0.37126600
H	-1.10065600	2.37842300	0.19561100
C	0.87963800	0.00001500	2.04863600
H	1.22491200	-0.88049500	2.59346400
H	1.22491100	0.88053200	2.59345200
C	-2.81016900	-3.65526800	0.29471200
H	-3.14957600	-3.37212000	1.29329900
H	-2.19253200	-4.55142400	0.38232000
H	-3.68859500	-3.92459200	-0.29590700
C	-4.06688500	1.19892300	-0.93528500

H	-4.55767100	2.13475400	-1.17644600
C	-2.81011200	3.65526400	0.29474400
H	-3.14947000	3.37210100	1.29334300
H	-3.68856600	3.92460500	-0.29582500
H	-2.19246400	4.55141300	0.38233600
C	-1.28459600	-1.23607100	2.56274300
H	-2.34854900	-1.29827200	2.32119600
H	-1.18495900	-1.17112200	3.64762400
H	-0.79317900	-2.15345700	2.23554400
C	-1.28459000	1.23611100	2.56273100
H	-0.79317300	2.15349100	2.23551700
H	-1.18494300	1.17117600	3.64761200
H	-2.34854400	1.29831400	2.32119100
C	1.42776900	0.00000600	0.60539600
C	2.30165300	1.17102100	0.21912300
C	2.30163000	-1.17102800	0.21912700
C	2.04190600	2.52142700	0.37041500
C	3.48064400	0.73222800	-0.39304700
C	2.04185600	-2.52142900	0.37042300
C	3.48062900	-0.73226000	-0.39304500
C	2.97731900	3.44137300	-0.09598900
H	1.12711300	2.85940300	0.84875700
C	4.41137900	1.64958100	-0.86439200
C	2.97725100	-3.44139500	-0.09598000
H	1.12705600	-2.85938500	0.84876600
C	4.41134600	-1.64963400	-0.86438900
C	4.14974100	3.00625700	-0.71071600
H	2.79386100	4.50251500	0.01683800
H	5.32596600	1.31675600	-1.34150500
C	4.14968100	-3.00630400	-0.71070900
H	2.79377200	-4.50253300	0.01685100
H	5.32593800	-1.31682700	-1.34150300
H	4.86529400	3.73517800	-1.07022800
H	4.86522000	-3.73524000	-1.07021900

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e-9-1 carbene-Au fragment

Au	0.35792300	0.00079900	-1.71082100
C	-2.85536800	-1.22594500	0.03558200
N	-0.96980200	-0.00020900	1.01544300
C	-0.85294900	-0.00049600	2.51325200
C	-4.13279300	-1.19822000	-0.51859300
H	-4.61198700	-2.13433900	-0.78099800
C	0.14521100	-0.00004700	0.34150500
C	-1.82572900	-3.06957600	-1.27666700
H	-1.24680900	-2.33834600	-1.84614400
H	-2.75427200	-3.27142800	-1.81737600
H	-1.25474900	-3.99912700	-1.22201300
C	-2.85536500	1.22576200	0.03582500
C	-4.78086100	-0.00002200	-0.76975400
H	-5.77463000	0.00001500	-1.19959600
C	-2.25943100	-0.00012500	0.36212100
C	-1.82595800	3.06989400	-1.27596000
H	-1.24710200	2.33885100	-1.84574400
H	-1.25495000	3.99941200	-1.22104400
H	-2.75455200	3.27196400	-1.81650000
C	-2.13263500	-2.55460400	0.13153400
H	-1.17422600	-2.39302200	0.62809600
C	-2.13269500	2.55443500	0.13210300
H	-1.17421800	2.39274300	0.62849300
C	0.67334400	-0.00067400	2.71118900
H	0.98648600	-0.88197500	3.27300800
H	0.98667600	0.88025200	3.27349200
C	-2.92277000	-3.60604300	0.90812700
H	-3.19646000	-3.26774000	1.90853000
H	-2.33528800	-4.52161500	1.00240100
H	-3.84295600	-3.86434500	0.37918900
C	-4.13279100	1.19812700	-0.51836600
H	-4.61199600	2.13429700	-0.78056400

C	-2.92281700	3.60557100	0.90913600
H	-3.19634600	3.26692700	1.90946600
H	-3.84309900	3.86395300	0.38040500
H	-2.33540800	4.52116800	1.00362500
C	-1.51543800	-1.23688300	3.10248400
H	-2.57524800	-1.26969100	2.84145300
H	-1.43178200	-1.19539100	4.18968900
H	-1.03630700	-2.15490400	2.75924900
C	-1.51524700	1.23578100	3.10293100
H	-1.03595200	2.15385300	2.76006500
H	-1.43164000	1.19385700	4.19012500
H	-2.57503900	1.26886500	2.84187000
C	1.30831000	-0.00039600	1.30768800
C	2.19547000	1.17412000	0.95246700
C	2.19515700	-1.17496100	0.95189200
C	1.92744600	2.52277800	1.09719700
C	3.38486000	0.73192800	0.36514200
C	1.92672200	-2.52361100	1.09590900
C	3.38466200	-0.73280900	0.36478000
C	2.87109700	3.44222500	0.64724000
H	1.00119000	2.86043700	1.55322700
C	4.32231700	1.64940600	-0.09012400
C	2.87011400	-3.44310200	0.64549500
H	1.00033500	-2.86122200	1.55171900
C	4.32186200	-1.65032500	-0.09094000
C	4.05456100	3.00572100	0.05582800
H	2.68388400	4.50326200	0.75200600
H	5.24375800	1.31729500	-0.55338400
C	4.05371900	-3.00663700	0.05433300
H	2.68258600	-4.50413900	0.74970400
H	5.24340000	-1.31824400	-0.55402900
H	4.77419500	3.73460200	-0.29498500
H	4.77314800	-3.73554700	-0.29683900

e-10-1 carbene fragment

C	1.48797800	1.79030100	0.06808500
N	0.39142700	-0.40438900	0.11170900
C	-0.06653100	-0.91308500	1.45723200
C	2.67114000	2.52654100	0.03114800
H	2.62187000	3.60855300	0.07150600
C	-0.34230000	-0.68342900	-0.93418100
C	-0.07046400	3.00471600	-1.41899700
H	-0.01646400	2.17208800	-2.12367300
H	0.69238800	3.73850900	-1.69406800
H	-1.05097200	3.48036200	-1.50720100
C	2.80755000	-0.25572000	-0.18215400
C	3.90097300	1.89956800	-0.08696200
H	4.80988600	2.48782900	-0.11095500
C	1.58272500	0.39551700	0.00939100
C	-1.49278800	-1.54259300	-0.41026100
C	3.05243800	-1.91495900	-2.00150900
H	2.21594900	-1.45657100	-2.53247100
H	3.09707900	-2.97511300	-2.26124200
H	3.97830100	-1.44041600	-2.33832700
C	0.15784700	2.51102700	0.01088000
H	-0.63423800	1.79602800	0.23132400
C	2.88945500	-1.73666100	-0.49088100
H	1.94041200	-2.20198300	-0.21638500
C	-1.02708100	-1.99888600	0.98885900
H	-1.83849800	-2.15737200	1.70053200
H	-0.47673200	-2.94058600	0.88441900
C	0.05053500	3.66454400	1.00303700
H	0.26460800	3.34233200	2.02411900
H	-0.95691100	4.08431300	0.97983600
H	0.74466900	4.47006800	0.75262900
C	3.96278300	0.52023800	-0.21749800
H	4.92157500	0.03838100	-0.36963000
C	4.01032100	-2.44352000	0.26485400

H	3.95084000	-2.25847800	1.33957200
H	4.99130600	-2.10906000	-0.07965600
H	3.95811600	-3.52065000	0.09491700
C	-0.77068200	0.19967300	2.22728000
H	-0.08658500	1.03344100	2.40519600
H	-1.09255400	-0.18619200	3.19637100
H	-1.64997400	0.56503600	1.69430900
C	1.07733400	-1.44441500	2.30741300
H	1.58232500	-2.28751300	1.83717900
H	0.67147300	-1.78633300	3.26142800
H	1.81209600	-0.66283900	2.51417600
C	-2.77332600	-0.71602100	-0.36980500
C	-3.89111300	-1.20305500	0.30951700
C	-2.88252900	0.51110900	-1.02414000
C	-5.07374600	-0.47840300	0.35771400
H	-3.83738300	-2.16675800	0.80523500
C	-4.06470600	1.24244600	-0.97257700
H	-2.03515700	0.88644600	-1.58564000
C	-5.16300700	0.75492900	-0.27786200
H	-5.92712900	-0.87685300	0.89266500
H	-4.12490200	2.19587200	-1.48383100
H	-6.08271600	1.32484900	-0.23715400
C	-1.69351000	-2.73542400	-1.34677800
H	-2.00459800	-2.39200700	-2.33349800
H	-0.75735900	-3.29050200	-1.45410900
H	-2.45647400	-3.41078800	-0.95036400

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e-10-1 carbene-Au fragment

Au	0.34708900	-1.88163000	-0.88462700
C	1.09019200	1.96186600	-1.03631900
N	0.31377700	0.56041300	0.81402400
C	-0.19732700	1.22694000	2.05891300
C	2.14838600	2.54515200	-1.72891800
H	1.93226500	3.19818200	-2.56658300

C	-0.39703600	-0.45950100	0.39391000
C	-0.50472700	1.39011900	-2.85190900
H	-0.26598700	0.33210100	-2.71335000
H	0.15289600	1.78775800	-3.62966500
H	-1.53754500	1.47595700	-3.20040900
C	2.71841500	0.78016600	0.36376900
C	3.46370300	2.28424100	-1.38152100
H	4.27318400	2.74985600	-1.92960500
C	1.39634200	1.11773500	0.04149900
C	-1.55074400	-0.68139100	1.35850500
C	3.71996100	-1.48429100	0.66437500
H	3.04850200	-1.89505800	-0.09290000
H	3.95267000	-2.27058400	1.38569700
H	4.65178700	-1.18648600	0.17638900
C	-0.32004000	2.16882900	-1.54838900
H	-1.02082700	1.75391700	-0.82438600
C	3.08756900	-0.28569800	1.37629300
H	2.17114100	-0.63822000	1.85764200
C	-1.09668100	0.11734100	2.59427600
H	-1.91153000	0.51621100	3.19741800
H	-0.49961300	-0.54663100	3.22770500
C	-0.67159200	3.63933900	-1.75960600
H	-0.50105500	4.23502500	-0.86113600
H	-1.72314500	3.73243400	-2.03856000
H	-0.07918800	4.07400900	-2.56794800
C	3.74007900	1.39268100	-0.35829800
H	4.76927700	1.14533600	-0.12471600
C	4.05440300	0.23450600	2.44059700
H	3.69626500	1.14368200	2.92441200
H	5.02592700	0.45699000	1.99303600
H	4.21631300	-0.52632300	3.20683300
C	-0.96744200	2.49206300	1.69339300
H	-0.31420400	3.19006500	1.16467900
H	-1.31040500	2.97494300	2.61009100

H	-1.83816600	2.27721400	1.07300300
C	0.91905600	1.59370000	3.01980300
H	1.45767200	0.71400800	3.36937200
H	0.48247400	2.09201000	3.88720500
H	1.62564400	2.28398000	2.55316500
C	-2.83919800	-0.15938300	0.71885800
C	-3.92058300	0.21875300	1.51465900
C	-2.99404600	-0.12092600	-0.66751000
C	-5.10798600	0.65999200	0.94578700
H	-3.84479400	0.16244300	2.59443200
C	-4.17931400	0.32808800	-1.23888700
H	-2.18148800	-0.45218200	-1.30495100
C	-5.23858500	0.72841100	-0.43585000
H	-5.93272800	0.95021900	1.58482600
H	-4.27290000	0.35566400	-2.31781300
H	-6.16133700	1.07891500	-0.88047600
C	-1.73889300	-2.16424100	1.68160000
H	-2.02737300	-2.71283900	0.78397800
H	-0.81016300	-2.59589600	2.06163100
H	-2.52351000	-2.27773700	2.43417300

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e-11-1 carbene fragment

C	2.62096200	1.59203800	0.07933600
N	0.87457200	-0.15350900	0.18949400
C	0.38629200	-0.54624500	1.55649100
C	3.97308300	1.90617700	-0.05657400
H	4.28142100	2.94395100	-0.00486900
C	0.03198700	-0.27119300	-0.80774600
C	1.42142900	3.31695700	-1.22420200
H	1.12700400	2.54615200	-1.93979100
H	2.35696500	3.76774800	-1.56687800
H	0.65145600	4.09232100	-1.20779700
C	3.17941000	-0.76047200	-0.27932200
C	4.91851900	0.92028000	-0.27967900

H	5.96456500	1.18224500	-0.37892500
C	2.24467500	0.24901100	-0.00346400
C	-1.17062900	-1.06865200	-0.26667500
C	2.60568000	-2.37039900	-2.07180900
H	1.88294600	-1.65793800	-2.47519000
H	2.27210800	-3.38450300	-2.30663100
H	3.56885900	-2.20391200	-2.56226900
C	1.60730500	2.70981500	0.16697300
H	0.65479600	2.27640000	0.46576400
C	2.75413700	-2.18749900	-0.56031700
H	1.76943400	-2.34913200	-0.11435700
C	-0.73256700	-1.50054900	1.16474000
H	-1.53969500	-1.45060800	1.89512800
H	-0.34981400	-2.52834500	1.14394000
C	1.97608300	3.78064400	1.18866500
H	2.15932000	3.34845500	2.17499800
H	1.16802700	4.50929900	1.27653900
H	2.87399800	4.32551000	0.88910800
C	4.51748900	-0.40165700	-0.40707100
H	5.25438300	-1.16558600	-0.62406800
C	3.70789300	-3.22807600	0.01848300
H	3.89919700	-3.05541200	1.08002400
H	4.66801100	-3.22111500	-0.50185400
H	3.28556300	-4.22765100	-0.09943100
C	-0.17459300	0.68306500	2.26431900
H	0.61030000	1.41751500	2.46072600
H	-0.60501500	0.38337600	3.22176300
H	-0.96275700	1.14658700	1.66345700
C	1.46034000	-1.17686100	2.42719200
H	1.88552100	-2.07365600	1.97635300
H	1.01256200	-1.45926400	3.38208000
H	2.26813100	-0.46976400	2.62776700
C	-2.56330300	-0.42034300	-0.27597700
C	-3.65604000	-1.16628900	0.21533200

C	-2.82563900	0.87563500	-0.76879600
C	-4.93405100	-0.60840800	0.23478000
C	-4.12261000	1.38387400	-0.73565100
C	-5.19740700	0.66731400	-0.23133800
H	-5.75101800	-1.20948200	0.62567300
H	-4.29146400	2.38502100	-1.12150400
C	-1.16743700	-2.25727500	-1.25381900
H	-1.40636100	-1.89373600	-2.25323400
H	-0.17189300	-2.70942300	-1.29361100
H	-1.88240200	-3.02971800	-0.97713300
C	-3.60533400	-2.59759900	0.70807900
H	-4.25865900	-2.70696800	1.57542600
H	-3.98726100	-3.26937600	-0.06542200
H	-2.62110100	-2.95740800	0.98628400
C	-6.57628300	1.25991000	-0.17506400
H	-6.78147400	1.86540200	-1.05889200
H	-7.33679700	0.48145500	-0.10777800
H	-6.68784200	1.90789900	0.69751600
C	-1.77823500	1.78765000	-1.34881200
H	-0.98337900	1.99329400	-0.63125800
H	-1.29369600	1.35884700	-2.22434700
H	-2.23287800	2.74097700	-1.62221300

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e-11-1 carbene-Au fragment

Au	0.57060100	0.30272200	-1.97803600
C	2.39426200	1.46449000	1.09903800
N	0.65811900	-0.28628800	0.94242000
C	0.04730200	-0.85015700	2.19160300
C	3.74016000	1.81164100	0.99855600
H	4.02915900	2.84399900	1.15837300
C	-0.14032100	-0.25826000	-0.09434700
C	1.26590600	3.47204200	0.14526100
H	1.01883700	2.89970800	-0.75348400
H	2.21256800	3.98904300	-0.03221300

H	0.49070000	4.22504800	0.30707700
C	2.99378000	-0.83770800	0.51784900
C	4.70152900	0.87078500	0.67443200
H	5.74160600	1.16070500	0.59446100
C	2.04073100	0.13183700	0.86816500
C	-1.37709600	-1.11159500	0.20182600
C	2.83165800	-2.52663100	-1.32732200
H	2.22008500	-1.84905200	-1.92873100
H	2.56358600	-3.55749000	-1.57131700
H	3.87747800	-2.37335900	-1.60657500
C	1.38063600	2.55454500	1.36207700
H	0.41173800	2.08304300	1.51416900
C	2.64596700	-2.27241600	0.16916100
H	1.59195600	-2.44348600	0.40651200
C	-1.02562100	-1.74225400	1.58118800
H	-1.88366400	-1.80516200	2.24863300
H	-0.62388000	-2.75129900	1.43318500
C	1.70853200	3.35663900	2.61942900
H	1.82597400	2.70947800	3.49176400
H	0.91344100	4.07556400	2.82614500
H	2.63624700	3.91945600	2.49552800
C	4.32434900	-0.44027100	0.43105700
H	5.07375500	-1.17056500	0.14875900
C	3.49081000	-3.27137800	0.96253300
H	3.49000600	-3.05873200	2.03297000
H	4.52839900	-3.25002400	0.62245800
H	3.11965700	-4.28622800	0.80673000
C	-0.58333600	0.27796700	3.00218300
H	0.17520100	0.97220600	3.36950300
H	-1.09678000	-0.15104700	3.86430400
H	-1.31768100	0.82508500	2.40486900
C	1.04275300	-1.59663100	3.05917500
H	1.45386600	-2.46708100	2.55180300
H	0.52768500	-1.94120100	3.95756000

H	1.86310200	-0.94462800	3.36697100
C	-2.77048200	-0.45819800	0.20687200
C	-3.88464900	-1.28447400	0.47932100
C	-3.01342500	0.90914600	-0.03856500
C	-5.16774000	-0.74221200	0.50254700
C	-4.31948800	1.39815200	-0.00864800
C	-5.41771600	0.59652600	0.25339500
H	-6.00032200	-1.40390800	0.72565100
H	-4.47302100	2.45681600	-0.19459900
C	-1.30087600	-2.15337400	-0.93913500
H	-1.53057200	-1.67062400	-1.88954100
H	-0.28619400	-2.55779500	-1.01245400
H	-1.98821200	-2.97955800	-0.77899700
C	-3.85076000	-2.77775700	0.73195400
H	-4.61221400	-3.03420000	1.46979500
H	-4.09952900	-3.31951700	-0.18423000
H	-2.90286100	-3.16802000	1.08706300
C	-6.81356600	1.14956500	0.24895500
H	-7.24370200	1.10806600	-0.75439600
H	-7.46637300	0.57896500	0.91024400
H	-6.82570600	2.19236800	0.56742400
C	-1.95414200	1.93153800	-0.34782300
H	-1.11687900	1.89368700	0.34686100
H	-1.53305200	1.79702300	-1.34756800
H	-2.38367100	2.93235600	-0.29125000

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e-12-1 carbene fragment

C	2.99972600	1.58952100	0.17703900
N	1.28213100	-0.18392500	0.18254900
C	0.81237400	-0.67074200	1.52581700
C	4.34728300	1.93134000	0.06161200
H	4.63984900	2.96828500	0.18106800
C	0.42842500	-0.22629100	-0.81104900
C	1.82226200	3.42428300	-0.99005300

H	1.55904600	2.72648600	-1.78783700
H	2.76147700	3.91584600	-1.25865700
H	1.04482300	4.18955800	-0.92012400
C	3.59298800	-0.72642400	-0.33615900
C	5.30664400	0.97630500	-0.22613900
H	6.34858200	1.25964600	-0.30835400
C	2.64524000	0.24903100	0.00824000
C	-0.75712300	-1.07815800	-0.30268500
C	3.03122100	-2.21319500	-2.23456400
H	2.30142200	-1.48014000	-2.58490800
H	2.70594400	-3.21125800	-2.53936300
H	3.99071200	-2.00376700	-2.71555500
C	1.97039100	2.68453100	0.34019700
H	1.01078900	2.21984100	0.55905000
C	3.18482500	-2.13576900	-0.71438700
H	2.20434400	-2.34099300	-0.27667600
C	-0.30318400	-1.60873100	1.08619300
H	-1.09842700	-1.63357200	1.82981100
H	0.08260800	-2.62807900	0.97687000
C	2.30400900	3.65661100	1.46775500
H	2.46498900	3.13697000	2.41493600
H	1.48922400	4.37081300	1.60116000
H	3.20678700	4.22961700	1.24422300
C	4.92516100	-0.34040400	-0.44143600
H	5.67293600	-1.07672100	-0.71036300
C	4.15447200	-3.20199100	-0.21438100
H	4.34818800	-3.10262300	0.85604500
H	5.11203900	-3.14458600	-0.73621300
H	3.74521700	-4.19635200	-0.40170800
C	0.25595100	0.50723200	2.31853600
H	1.04281600	1.22814200	2.55148000
H	-0.16391100	0.14584500	3.25917000
H	-0.53289000	1.01490700	1.75610900
C	1.89930300	-1.35124800	2.34088600

H	2.32523400	-2.21242700	1.82615800
H	1.46298100	-1.70062500	3.27871000
H	2.70417000	-0.65330900	2.58060200
C	-2.14555900	-0.44208300	-0.24967700
C	-3.26527000	-1.20539700	0.13981800
C	-2.45389200	0.88666500	-0.57922400
C	-4.56413100	-0.72143900	0.15707200
C	-3.74662500	1.39973100	-0.57491900
C	-4.80090700	0.58764500	-0.21529100
H	-5.37504500	-1.36722100	0.46264400
H	-3.91065200	2.43284700	-0.84665200
C	-0.75308800	-2.18981300	-1.37659500
H	-1.04712300	-1.76831300	-2.33742000
H	0.26523600	-2.57287200	-1.48454200
H	-1.40541600	-3.02142500	-1.12235800
Cl	-3.13007100	-2.84832400	0.67778200
Cl	-1.24573000	2.04647500	-0.98369100
Cl	-6.40501300	1.20630100	-0.20966800

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e-12-1 carbene-Au fragment

Au	-0.81044600	-0.63274900	-1.91936200
C	-2.72084900	-1.27339600	1.27574600
N	-1.00681200	0.45487100	0.86499000
C	-0.42032500	1.20973000	2.02265300
C	-4.06529100	-1.63972500	1.24385800
H	-4.34469200	-2.63736600	1.56270300
C	-0.19175400	0.25900400	-0.13749900
C	-1.62196300	-3.41481900	0.63321600
H	-1.41033300	-3.00365000	-0.35791900
H	-2.57127800	-3.95429900	0.58049600
H	-0.83940700	-4.13270600	0.89241900
C	-3.34452900	0.90882900	0.35285800
C	-5.03675700	-0.76556700	0.78922900
H	-6.07529900	-1.07074100	0.76627500

C	-2.38330300	0.01291300	0.84578500
C	1.02989800	1.16752700	0.04420700
C	-3.15890700	2.24901000	-1.75120000
H	-2.53004000	1.48124500	-2.20975400
H	-2.89363900	3.22253700	-2.17063700
H	-4.19769900	2.03639000	-2.01751500
C	-1.69378700	-2.30537700	1.68269100
H	-0.71892100	-1.82169500	1.71334700
C	-3.00251500	2.26659700	-0.22995400
H	-1.95469500	2.48848200	-0.00713700
C	0.66889400	1.99881500	1.30579300
H	1.51595900	2.17058200	1.96736200
H	0.28276600	2.97434700	0.99373500
C	-1.98384200	-2.89285800	3.06241200
H	-2.08729800	-2.11577500	3.82310900
H	-1.17866100	-3.56611600	3.36279300
H	-2.91019300	-3.47173400	3.05303000
C	-4.67229700	0.49354900	0.33853600
H	-5.42950300	1.16437000	-0.05019400
C	-3.86772000	3.38013700	0.36212100
H	-3.88114600	3.35857900	1.45334000
H	-4.89968800	3.28990000	0.01656800
H	-3.50142100	4.35539600	0.03582800
C	0.18310700	0.21685100	3.01024700
H	-0.59060900	-0.41106200	3.45568900
H	0.67932100	0.76752300	3.81106700
H	0.91941900	-0.42485300	2.51937800
C	-1.43020700	2.08418400	2.74139300
H	-1.82832100	2.86460500	2.09583400
H	-0.93140800	2.56511700	3.58457400
H	-2.25849900	1.48871900	3.13101900
C	2.41479900	0.52436200	0.14674500
C	3.56126100	1.33908100	0.24932800
C	2.69496700	-0.85076300	0.13183600

C	4.85746100	0.84926100	0.25852300
C	3.98518500	-1.36982200	0.13327400
C	5.06504000	-0.51463900	0.18113200
H	5.69025100	1.53425400	0.33049400
H	4.12736800	-2.44082800	0.10647700
C	0.95789200	2.02153500	-1.24506300
H	1.22126900	1.40960500	-2.10815700
H	-0.07094500	2.36325900	-1.39137800
H	1.60568300	2.89151800	-1.19140800
Cl	3.47037800	3.06136700	0.42490000
Cl	1.46478700	-2.05540200	0.17149400
Cl	6.66412100	-1.14120600	0.17631200

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e-13-1 carbene fragment

C	3.07929000	1.06524000	0.33083700
N	1.03698000	-0.31263700	0.18232400
C	0.44764400	-0.78774600	1.48063300
C	4.47312000	1.11746100	0.30306900
H	4.97009100	2.05973900	0.50222900
C	0.19885200	-0.07892100	-0.80047100
C	2.31987000	3.05947600	-0.88250500
H	1.88117200	2.42354300	-1.65528000
H	3.35282100	3.28261700	-1.16377400
H	1.76860300	4.00208500	-0.84493700
C	3.20272400	-1.29101000	-0.31013000
C	5.22564500	-0.00405900	0.00007900
H	6.30695300	0.05387100	-0.01039900
C	2.46255600	-0.15935400	0.06405200
C	-1.14376800	-0.70801700	-0.37632500
C	2.39546000	-2.45658000	-2.33638300
H	1.84000100	-1.56076400	-2.62299800
H	1.88016300	-3.33466400	-2.73405200
H	3.38951000	-2.40726600	-2.78941900
C	2.29055000	2.34768700	0.47188800

H	1.25443400	2.09354000	0.69359700
C	2.52258700	-2.54766700	-0.81429900
H	1.50926200	-2.58049700	-0.40536300
C	-0.81948100	-1.44469800	0.95606400
H	-1.61772500	-1.37189700	1.69469700
H	-0.62845000	-2.50710700	0.76047600
C	2.79187800	3.26317500	1.58316400
H	2.84214700	2.74261600	2.54210600
H	2.11815900	4.11645700	1.69047800
H	3.78539200	3.65886700	1.36096900
C	4.59007800	-1.19346400	-0.32776000
H	5.18154300	-2.05480200	-0.61346200
C	3.23637800	-3.83235100	-0.40731900
H	3.42148300	-3.86877700	0.66869500
H	4.19646500	-3.93299400	-0.91801400
H	2.63279200	-4.69839800	-0.68450700
C	0.11750200	0.42936900	2.33877300
H	1.02600500	0.97122300	2.61461200
H	-0.37909900	0.10668100	3.25587200
H	-0.55465000	1.10507000	1.80150400
C	1.35137600	-1.72367600	2.26508400
H	1.61366700	-2.61843300	1.70041600
H	0.82404500	-2.03758400	3.16810300
H	2.27115900	-1.21912000	2.56829200
C	-2.40777800	0.16286500	-0.27181900
C	-3.63736600	-0.48320900	0.02602000
C	-2.42921300	1.55581600	-0.48764900
C	-4.82181400	0.24786600	0.03083200
C	-3.64722400	2.24066000	-0.49026800
C	-4.84466400	1.60250200	-0.24643800
H	-5.75124900	-0.26251600	0.25671300
H	-3.64306500	3.30563800	-0.69137600
H	-5.77844700	2.15064500	-0.25582700
C	-1.32398700	-1.68629800	-1.56296700

H	-1.45450100	-1.10924100	-2.47861400
H	-0.42388500	-2.29728100	-1.68127200
H	-2.17535200	-2.35238400	-1.44238900
C	-3.80648400	-1.95646500	0.39066300
H	-2.84596300	-2.46280600	0.36238900
C	-1.20924700	2.42642100	-0.72273700
H	-0.31411000	1.83385800	-0.53730600
C	-4.34389100	-2.10613600	1.81547700
H	-4.40256200	-3.16158800	2.09086200
H	-3.70681200	-1.59411000	2.53992100
H	-5.34646500	-1.68208200	1.90189900
C	-4.72891100	-2.68079600	-0.59138100
H	-4.77469100	-3.74606500	-0.35407800
H	-5.74544400	-2.28587400	-0.53776600
H	-4.38544400	-2.56871700	-1.62141700
C	-1.17217000	3.62637300	0.22509100
H	-1.94515400	4.35968600	-0.01433800
H	-1.31431500	3.31984600	1.26437400
H	-0.20880900	4.13625500	0.14784100
C	-1.13355300	2.86917700	-2.18080800
H	-0.28506300	3.53891200	-2.33926500
H	-1.01391000	2.00085100	-2.83181600
H	-2.04531300	3.39956600	-2.46944400

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e-13-1 carbene-Au fragment

Au	-0.84933900	-0.61796700	-1.89813600
C	-2.75294500	-0.75036300	1.33959300
N	-0.74033000	0.58211300	0.82475300
C	0.00526200	1.24665200	1.94261400
C	-4.14446700	-0.82458900	1.38046900
H	-4.61068700	-1.73089100	1.74950700
C	0.01096400	0.18074600	-0.16832800
C	-2.17319000	-3.06917300	0.67309900
H	-1.87478800	-2.72578900	-0.32194000

H	-3.23041200	-3.34374400	0.63246100
H	-1.60382700	-3.96753000	0.92328500
C	-2.95221000	1.48500200	0.35643400
C	-4.93318200	0.22075000	0.93372200
H	-6.01238400	0.14147200	0.96941500
C	-2.17548900	0.42496900	0.84986500
C	1.40103000	0.80994100	-0.03111000
C	-2.57544300	2.66384200	-1.81562800
H	-2.13159800	1.76501200	-2.25190100
H	-2.13544500	3.54352400	-2.29155200
H	-3.64529800	2.65471900	-2.04098000
C	-1.95087500	-1.97587300	1.71940400
H	-0.89337600	-1.71223100	1.71215000
C	-2.36128900	2.71697300	-0.30215200
H	-1.28243600	2.72637300	-0.12066400
C	1.20839600	1.77479800	1.17440400
H	2.07916000	1.82217700	1.82675900
H	0.99386300	2.78520400	0.80709300
C	-2.29303500	-2.49504400	3.11403600
H	-2.20788000	-1.71419700	3.87286300
H	-1.61924500	-3.31234200	3.38220000
H	-3.31318300	-2.88408200	3.14912000
C	-4.33637700	1.35811600	0.41246300
H	-4.95487500	2.15939600	0.02533300
C	-2.95835700	4.01113000	0.25281800
H	-2.94571600	4.04030700	1.34380200
H	-3.99565400	4.12480900	-0.06921400
H	-2.40630700	4.87308500	-0.12666600
C	0.42644400	0.18308100	2.94956800
H	-0.44403000	-0.28373200	3.41498500
H	1.02796200	0.64651900	3.73339500
H	1.02915000	-0.58611900	2.46091300
C	-0.79348700	2.32650000	2.64664500
H	-1.04850300	3.14720900	1.97899400

H	-0.18569700	2.72865300	3.45907100
H	-1.71114400	1.92072300	3.07766200
C	2.65411500	-0.07750000	0.12692000
C	3.90887900	0.58890200	0.18970200
C	2.64990500	-1.48777700	0.18166900
C	5.08579600	-0.15244700	0.22398700
C	3.86355800	-2.18152500	0.20327700
C	5.07968700	-1.53465600	0.20846600
H	6.03304900	0.37267900	0.26408700
H	3.83842300	-3.26461200	0.21725600
H	6.00667800	-2.09384900	0.21852700
C	1.49578800	1.56416900	-1.38133200
H	1.56650400	0.83798500	-2.19207900
H	0.58726200	2.15263600	-1.54665200
H	2.35236400	2.23051300	-1.42747800
C	4.12775300	2.09967000	0.26677700
H	3.17723500	2.62376900	0.23719900
C	1.42670700	-2.38591900	0.25021600
H	0.52774700	-1.77338600	0.30560900
C	4.79793700	2.48383400	1.58794200
H	4.89021800	3.56944800	1.66461000
H	4.22806100	2.12313100	2.44727200
H	5.80068000	2.05783100	1.65762600
C	4.96141000	2.61308700	-0.90863300
H	5.03934100	3.70182100	-0.87075100
H	5.97456000	2.20779400	-0.87705400
H	4.52282900	2.32916600	-1.86691900
C	1.45568400	-3.27715800	1.49505000
H	2.25352400	-4.02003900	1.43225500
H	1.61223400	-2.70184400	2.41021700
H	0.51264100	-3.82060400	1.58871700
C	1.29291100	-3.24332300	-1.00731200
H	0.37368700	-3.83275100	-0.96881800
H	1.25647700	-2.62201700	-1.90397800

H 2.13766500 -3.93247000 -1.09413700

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e-14-1 carbene fragment

C	2.84232000	1.53293300	0.56225200
N	1.73846400	-0.59845900	0.04365900
C	1.26055800	-1.42204500	1.21659900
C	4.03067600	2.23950200	0.74205300
H	3.98645900	3.27839500	1.04695200
C	1.02307400	-0.60987000	-1.04908800
C	1.34042400	3.06012200	-0.66304600
H	1.38854800	2.39549800	-1.52892300
H	2.13532000	3.80476000	-0.76030400
H	0.38106500	3.58188300	-0.66767200
C	4.15906100	-0.40505500	-0.15081200
C	5.25972200	1.64514600	0.50709300
H	6.17195200	2.20937600	0.65565100
C	2.93370500	0.19481200	0.16507500
C	-0.11615900	-1.59382100	-0.78338200
C	4.41369200	-1.55827400	-2.32484300
H	3.58286700	-0.97818100	-2.73129400
H	4.45905500	-2.51997000	-2.84099400
H	5.34287300	-1.01782300	-2.52503600
C	1.51999500	2.26719300	0.63388500
H	0.71575600	1.53244900	0.68124100
C	4.23915200	-1.76282800	-0.81870500
H	3.28672500	-2.27854900	-0.67658600
C	0.31540100	-2.36613100	0.48269200
H	-0.51505200	-2.68426000	1.11561000
H	0.86937700	-3.25919200	0.17449400
C	1.39089700	3.18066300	1.84815900
H	1.57561300	2.64318200	2.78082800
H	0.38533300	3.60365600	1.88641700
H	2.09347300	4.01523300	1.79537800
C	5.31880500	0.34094600	0.03868900

H	6.27915500	-0.09925900	-0.20249800
C	5.35111600	-2.64270000	-0.25640100
H	5.28654300	-2.72919400	0.83041300
H	6.33604700	-2.24071400	-0.50319300
H	5.29369400	-3.64359200	-0.68824500
C	0.53764100	-0.52515900	2.21666800
H	1.21382300	0.24376100	2.59913700
H	0.19947000	-1.12940500	3.06025400
H	-0.33269200	-0.04023200	1.77142500
C	2.38955400	-2.14099200	1.93870900
H	2.91350700	-2.84256400	1.29076200
H	1.96414100	-2.70597900	2.77020600
H	3.11123000	-1.43062900	2.34786100
C	-1.41913600	-0.83695600	-0.58139300
C	-2.56126700	-1.52578300	-0.17877300
C	-1.52247100	0.53705800	-0.78621200
C	-3.75992200	-0.86035400	0.03332100
H	-2.52011100	-2.59947100	-0.02449800
C	-2.72252300	1.19767000	-0.55212100
H	-0.65886100	1.09378200	-1.13457200
C	-3.85428200	0.51242800	-0.14006300
H	-4.78506400	1.03187700	0.03862900
C	-0.24871100	-2.52634600	-1.98949600
H	-0.54459300	-1.96362700	-2.87477600
H	0.71310200	-3.00446200	-2.19278900
H	-0.98983400	-3.30707300	-1.79921100
C	-4.94972100	-1.67065800	0.46865000
C	-2.74653400	2.69408700	-0.69694200
F	-6.03855900	-0.92113700	0.64525900
F	-3.98705100	3.18513600	-0.70220600
F	-2.14674400	3.09621600	-1.82139800
F	-2.09348800	3.28485600	0.31944000
F	-5.25339400	-2.61554200	-0.43079600
F	-4.70949300	-2.30774900	1.62351400

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e-14-1 carbene-Au fragment

Au	1.58150300	0.50636700	-1.97703800
C	2.09404400	1.15396100	1.85939600
N	1.29904700	-0.83077900	0.66043200
C	0.67900200	-1.94872100	1.44752800
C	3.15408300	1.85504700	2.42974600
H	2.95058400	2.78414700	2.94915200
C	0.67928900	-0.52222000	-0.45671300
C	0.69252100	2.96221500	0.90760100
H	0.96506100	2.64645600	-0.10354000
H	1.40877700	3.72406500	1.22642100
H	-0.29865200	3.41897700	0.88112400
C	3.70286600	-0.48461800	1.00123800
C	4.45752900	1.40003700	2.32022200
H	5.26742400	1.95749700	2.77367000
C	2.38485200	-0.04383000	1.19035800
C	-0.47370300	-1.49316800	-0.65705100
C	4.82403600	-1.14435000	-1.12651600
H	4.22477600	-0.42065700	-1.68331500
H	5.06646700	-1.97790500	-1.78909900
H	5.76021700	-0.66365400	-0.83089100
C	0.71486500	1.77959900	1.87835300
H	-0.00708800	1.04482900	1.52022200
C	4.07677300	-1.65206900	0.10930800
H	3.15740600	-2.13194400	-0.23872600
C	-0.14813500	-2.61230400	0.35124600
H	-1.02454000	-3.11655900	0.75895400
H	0.46898100	-3.35977400	-0.15686200
C	0.27334900	2.23080900	3.26823500
H	0.32877400	1.42171400	3.99898500
H	-0.75674000	2.59088100	3.22828500
H	0.89270500	3.05404700	3.63084300
C	4.72591700	0.25273500	1.59205700

H	5.75164000	-0.07097900	1.45807400
C	4.94543400	-2.68129800	0.83364400
H	4.50952900	-3.00841600	1.77807200
H	5.92956700	-2.25990500	1.05104000
H	5.10034200	-3.55685900	0.20004400
C	-0.18114200	-1.37018500	2.56705400
H	0.43090800	-0.76189300	3.23685600
H	-0.61128900	-2.18871500	3.14633600
H	-0.99683800	-0.75731100	2.18067600
C	1.70955000	-2.88424400	2.05232200
H	2.29963700	-3.38541300	1.28665500
H	1.18837500	-3.64711000	2.63329000
H	2.38010600	-2.34559600	2.72558800
C	-1.79881900	-0.79160000	-0.37209400
C	-2.94326900	-1.55198500	-0.15066700
C	-1.92429500	0.59769500	-0.38546900
C	-4.16925200	-0.94569600	0.08593100
H	-2.89165000	-2.63542900	-0.16939600
C	-3.15351800	1.19387000	-0.13483200
H	-1.06027100	1.21709700	-0.60343100
C	-4.28806600	0.43390500	0.10899200
H	-5.24177000	0.90584800	0.29996900
C	-0.51456100	-2.02643600	-2.09158400
H	-0.72663800	-1.21927100	-2.79376100
H	0.44847200	-2.46562900	-2.35941500
H	-1.29278000	-2.78920800	-2.17902800
C	-5.35991200	-1.83312300	0.32613600
C	-3.23895600	2.69483200	-0.06579000
F	-6.48325800	-1.13837900	0.50460100
F	-4.47025200	3.13859400	-0.32901200
F	-2.40233600	3.28512600	-0.92023500
F	-2.92016200	3.13741100	1.16310100
F	-5.56004800	-2.66904800	-0.70048200
F	-5.18355000	-2.59859500	1.41250200

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e-15-1 carbene fragment

C	2.51790700	1.29874100	-0.42435700
N	0.73702200	-0.16667400	0.38960900
C	0.41388200	-0.11492600	1.85926200
C	3.84871500	1.45450600	-0.80793800
H	4.20499000	2.43830300	-1.09122200
C	-0.24598100	-0.26639200	-0.46717200
C	1.25051100	2.69354300	-2.03110300
H	0.82840500	1.78823800	-2.47177100
H	2.16094000	2.95747900	-2.57687600
H	0.52969800	3.50680900	-2.14622900
C	2.91711700	-1.10597500	-0.19166000
C	4.71016300	0.37004900	-0.86334800
H	5.74160200	0.51197400	-1.16131100
C	2.08901100	0.01482800	-0.06683800
C	-1.53188200	-0.27033200	0.37583500
C	2.13285900	-3.07035700	-1.47387900
H	1.44384500	-2.42771500	-2.02658400
H	1.71128400	-4.07719400	-1.42186700
H	3.07463900	-3.12173700	-2.02701500
C	1.56166200	2.46749800	-0.55034700
H	0.61812600	2.20388100	-0.07224000
C	2.37272300	-2.51362400	-0.06917700
H	1.39894200	-2.46368500	0.42060400
C	-1.04119100	-0.58047200	1.80588800
H	-1.64876900	-0.15155400	2.60282400
H	-1.06304200	-1.66659300	1.93203900
C	2.08554000	3.74708600	0.09369700
H	2.34927600	3.59486500	1.14225500
H	1.32420600	4.52790800	0.04115400
H	2.97151100	4.11942300	-0.42596600
C	4.23796100	-0.90339700	-0.58258600
H	4.89707500	-1.75695500	-0.69121200

C	3.27178600	-3.43841100	0.74373100
H	3.48359800	-3.02439700	1.73186100
H	4.22483300	-3.60925700	0.23832600
H	2.79382300	-4.41151100	0.87228300
C	0.60251100	1.30138300	2.39449100
H	1.64534000	1.60863100	2.27882700
H	0.36273100	1.31449400	3.45961700
H	-0.03475700	2.02584000	1.89082200
C	1.29476400	-1.04675400	2.68148900
H	1.14225700	-2.09401200	2.42189800
H	1.04434000	-0.92359300	3.73684200
H	2.35174800	-0.79906600	2.55532000
C	-2.11215700	1.12498500	0.16284400
C	-2.54173400	1.95422600	1.19513100
C	-2.23720200	1.58664200	-1.15245600
C	-3.05979000	3.21863400	0.92854400
H	-2.47539800	1.62738300	2.22519300
C	-2.74691900	2.84836900	-1.42016000
H	-1.92099900	0.93745900	-1.95975500
C	-3.15612800	3.67424200	-0.37813300
H	-3.38779600	3.84529500	1.74873500
H	-2.82769500	3.18708000	-2.44576800
H	-3.55427000	4.65974200	-0.58477600
C	-2.48882400	-1.34757900	-0.10804500
C	-1.96734600	-2.57237800	-0.52498100
C	-3.86930300	-1.17724200	-0.09705000
C	-2.80510900	-3.60525900	-0.91940700
H	-0.88830800	-2.70493100	-0.55269300
C	-4.71285500	-2.21204100	-0.48748400
H	-4.28807000	-0.22597700	0.21158600
C	-4.18449800	-3.42761900	-0.89997900
H	-2.38327700	-4.54703000	-1.24834900
H	-5.78567900	-2.06396600	-0.47299200
H	-4.84145500	-4.23075600	-1.20968100

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e-15-1 carbene-Au fragment

Au	-0.07245500	-1.04135100	-1.60523500
C	2.41024200	1.58405000	-0.20507100
N	0.76926500	0.20917400	0.96586700
C	0.45908900	0.54775100	2.39321000
C	3.71701400	1.76400500	-0.65116700
H	3.98131400	2.69304700	-1.14305700
C	-0.25709100	-0.05116400	0.19613200
C	1.08509800	2.64063400	-2.02486000
H	0.73564100	1.65711200	-2.35001000
H	1.98730900	2.88937900	-2.59037900
H	0.31568300	3.37993300	-2.26041900
C	3.01849100	-0.68160800	0.51331900
C	4.67033200	0.76970900	-0.50011900
H	5.68251900	0.93067300	-0.84946200
C	2.09753500	0.37052900	0.42614300
C	-1.53800400	0.12573800	1.01139000
C	2.74649200	-3.04453400	-0.22848600
H	2.11722800	-2.71531300	-1.05863000
H	2.43080800	-4.04611900	0.07173300
H	3.77965200	-3.10730200	-0.58014900
C	1.37652000	2.64730200	-0.52310200
H	0.44070400	2.39915100	-0.02103800
C	2.64714300	-2.08253700	0.95845400
H	1.60307700	-2.07502400	1.28420800
C	-1.00643700	0.11203800	2.45983700
H	-1.58905300	0.71288400	3.15664700
H	-1.04582900	-0.92027500	2.81482100
C	1.80010600	4.04394700	-0.07412000
H	2.06640600	4.07165500	0.98395200
H	0.98223100	4.74842800	-0.24157000
H	2.66043100	4.39768100	-0.64709500
C	4.31335100	-0.44788300	0.05526500

H	5.04350300	-1.24701100	0.11314400
C	3.53111500	-2.59389100	2.09549800
H	3.54219600	-1.92358500	2.95513700
H	4.56121800	-2.71060600	1.75054000
H	3.18628400	-3.57539700	2.42704200
C	0.69415500	2.03210900	2.65291800
H	1.74726100	2.27486600	2.49202100
H	0.45181600	2.24813500	3.69531700
H	0.08639400	2.67320900	2.01802200
C	1.32776000	-0.24082300	3.35934800
H	1.18900500	-1.31576900	3.24446100
H	1.05167600	0.03209200	4.37962400
H	2.38260700	0.00318100	3.21670300
C	-2.09540000	1.46859500	0.53247600
C	-2.41155000	2.52144400	1.38514100
C	-2.29751300	1.64389700	-0.84104300
C	-2.88234100	3.73146900	0.88169600
H	-2.28928200	2.42075800	2.45564900
C	-2.76327000	2.84839900	-1.34494700
H	-2.08148700	0.81982700	-1.51387800
C	-3.04901500	3.90364700	-0.48428300
H	-3.11820300	4.53778700	1.56495000
H	-2.90279800	2.96252400	-2.41264600
H	-3.40917600	4.84669900	-0.87560400
C	-2.52233300	-1.01311300	0.78686200
C	-2.04486000	-2.32491100	0.80822400
C	-3.88462200	-0.79997400	0.61512100
C	-2.90639400	-3.39859600	0.65211700
H	-0.97920900	-2.50193100	0.93313600
C	-4.75410900	-1.87655800	0.46526700
H	-4.27304400	0.21112600	0.59190400
C	-4.26887400	-3.17562000	0.47997800
H	-2.51550100	-4.40811900	0.65514600
H	-5.81300500	-1.69382400	0.33137200

H -4.94509500 -4.01166300 0.35371500

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e-16-1 carbene fragment

C 3.08624900 0.52242400 -0.46073900
N 1.09776100 -0.62822900 0.40711000
C 0.88544000 -0.57682100 1.89044000
C 4.42629000 0.46699300 -0.84109000
H 4.93206500 1.38780400 -1.10846500
C 0.06819100 -0.43361800 -0.38119600
C 2.19974400 2.19869400 -2.04703800
H 1.56161900 1.45951100 -2.53714200
H 3.17002000 2.21526500 -2.55119000
H 1.73852100 3.18315600 -2.15663100
C 3.10077500 -1.91006100 -0.25764300
C 5.11154300 -0.73429200 -0.90698900
H 6.15437500 -0.75249700 -1.19836600
C 2.44729300 -0.67811500 -0.11223800
C -1.14456800 -0.08205700 0.54066900
C 2.08666600 -3.71736400 -1.59837400
H 1.57264200 -2.95026700 -2.18122500
H 1.46993500 -4.61944900 -1.58372300
H 3.02817200 -3.95202800 -2.10275900
C 2.37202000 1.85577100 -0.56542100
H 1.37235400 1.76577000 -0.14040900
C 2.35977600 -3.22537500 -0.17519800
H 1.39689300 -3.03759600 0.29216300
C -0.64963500 -0.53144300 1.93795200
H -1.01694600 0.04899000 2.77505500
H -1.01782300 -1.54783600 2.09413300
C 3.09915800 2.98646800 0.15880200
H 3.31396000 2.73252800 1.19879200
H 2.47729000 3.88586000 0.14682500
H 4.04500300 3.23196900 -0.33044200
C 4.43860300 -1.91582700 -0.64428700

H	4.94907900	-2.86460500	-0.76306900
C	3.08807900	-4.29730000	0.62890200
H	3.33567900	-3.95367000	1.63479500
H	4.01605600	-4.59871200	0.13799500
H	2.46373500	-5.18900700	0.71503200
C	1.62481200	0.62945800	2.46189200
H	2.70034500	0.49523000	2.32042900
H	1.43701700	0.70252800	3.53503900
H	1.33225600	1.56236100	1.98339600
C	1.42516700	-1.81076500	2.60457400
H	0.92109600	-2.72608500	2.29224200
H	1.26485000	-1.68891000	3.67792700
H	2.49910700	-1.91831600	2.43518800
C	-1.15082400	1.43605300	0.25684500
C	-0.96534100	2.45912000	1.21543400
C	-1.27238600	1.82543700	-1.10256600
C	-0.67352000	3.75433600	0.78013000
C	-0.99582300	3.13735700	-1.47431900
C	-0.62189500	4.10843700	-0.55818500
H	-0.50522600	4.52096300	1.53132100
H	-1.05990300	3.39789800	-2.52691600
C	-2.46156000	-0.78694500	0.16319400
C	-2.43599300	-2.13400200	-0.26030100
C	-3.72015400	-0.15883200	0.24667200
C	-3.60835100	-2.78256000	-0.63285900
C	-4.86982900	-0.85096400	-0.14216100
C	-4.84499700	-2.15533100	-0.60206600
H	-3.54593900	-3.81799000	-0.95535000
H	-5.82448600	-0.33792500	-0.06994900
C	-1.17640900	-2.95195800	-0.33306100
H	-0.50065500	-2.57960200	-1.10437800
H	-0.62930400	-2.93850200	0.61115700
H	-1.41868800	-3.99089200	-0.55939900
C	-6.09345400	-2.86026600	-1.04818500

H	-6.98354600	-2.37870500	-0.64247300
H	-6.17848100	-2.85006500	-2.13732900
H	-6.09244100	-3.90426700	-0.73155500
C	-3.96639900	1.24547800	0.73918900
H	-3.42815200	1.46430500	1.65698900
H	-3.67665400	2.00291400	0.00722400
H	-5.03030100	1.36820400	0.94345400
C	-0.20051600	5.47990600	-0.99669900
H	-0.34589000	6.21395000	-0.20351000
H	0.86162300	5.48739500	-1.26190300
H	-0.75661100	5.80440500	-1.87703500
C	-1.80276700	0.93353700	-2.19790900
H	-1.52614200	1.34747200	-3.16884800
H	-1.42914300	-0.08350600	-2.13652100
H	-2.89642600	0.90073300	-2.14845700
C	-1.18022800	2.35827100	2.71373400
H	-2.04139100	1.74580800	2.97652800
H	-0.32751100	1.96958300	3.26703400
H	-1.37729400	3.36036100	3.09512600

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e-16-1 carbene-Au fragment

Au	0.39475300	-0.85035700	-1.77713100
C	2.96443200	0.82277900	0.05927600
N	0.98644500	-0.27718200	1.01642300
C	0.70031700	-0.02860800	2.46317900
C	4.31606800	0.76628100	-0.27342000
H	4.79797300	1.66150800	-0.64897800
C	-0.03388800	-0.24204000	0.19737600
C	2.18870500	2.36906100	-1.73231700
H	1.66316900	1.56345700	-2.25240800
H	3.20298200	2.43457400	-2.13478800
H	1.67703300	3.31142900	-1.94255000
C	3.05971800	-1.56369200	0.60235600
C	5.04374800	-0.40566900	-0.15849600

H	6.09373400	-0.42350200	-0.42226600
C	2.36102400	-0.34816500	0.54980900
C	-1.30540100	0.18833000	0.99214800
C	2.32516600	-3.71937000	-0.40355800
H	1.82722000	-3.16405700	-1.20308200
H	1.77828200	-4.64880500	-0.22619600
H	3.33185000	-3.97700500	-0.74389400
C	2.22643400	2.11916100	-0.22244300
H	1.19267900	2.03142200	0.11695400
C	2.39645900	-2.89514800	0.88431900
H	1.37412200	-2.70064900	1.20107900
C	-0.83603600	-0.04076800	2.45043800
H	-1.25842900	0.64488700	3.17269100
H	-1.17549500	-1.03460600	2.74632300
C	2.86649800	3.32238000	0.47133700
H	3.01439300	3.15966800	1.53991800
H	2.22853000	4.20106800	0.34242300
H	3.83951200	3.55261400	0.03033300
C	4.40764500	-1.56380800	0.25270400
H	4.95552000	-2.49854600	0.28139100
C	3.10719300	-3.70706700	1.96601200
H	3.23428800	-3.15067600	2.89523600
H	4.09718700	-4.01863400	1.62534300
H	2.54008000	-4.61456300	2.18347500
C	1.37927400	1.26867400	2.88734000
H	2.46162100	1.15358500	2.79316300
H	1.15570500	1.46977000	3.93657800
H	1.07089900	2.11910400	2.28325700
C	1.24967900	-1.12906400	3.36113000
H	0.82166200	-2.10647700	3.13878400
H	1.00232300	-0.87911000	4.39484400
H	2.33642300	-1.18503600	3.27811900
C	-1.36308200	1.66833800	0.52943000
C	-1.19240700	2.80036600	1.36501100

C	-1.49628900	1.90608100	-0.86125200
C	-0.88052900	4.03012500	0.78215000
C	-1.17776600	3.15578600	-1.38686700
C	-0.79095100	4.21969100	-0.58876100
H	-0.72694100	4.88176700	1.43883100
H	-1.24117200	3.28928100	-2.46277000
C	-2.57232600	-0.63362100	0.69416200
C	-2.47982500	-2.02550000	0.47940000
C	-3.85455000	-0.04808700	0.65147700
C	-3.61162200	-2.75482200	0.12439000
C	-4.95630900	-0.82315200	0.29196400
C	-4.86107600	-2.17177300	-0.01010000
H	-3.50319200	-3.82218200	-0.04400400
H	-5.93065300	-0.34438400	0.25964600
C	-1.21444400	-2.82734500	0.63197400
H	-0.57382100	-2.75822300	-0.25281800
H	-0.62394600	-2.50898400	1.48981500
H	-1.46547100	-3.87813900	0.78006200
C	-6.05670700	-2.96658000	-0.44823100
H	-6.98021100	-2.53847600	-0.05719200
H	-6.13432300	-2.97886800	-1.53782500
H	-5.98678000	-4.00216800	-0.11369400
C	-4.17060700	1.38511900	1.00058300
H	-3.65841200	1.71051400	1.90211100
H	-3.90555900	2.08692000	0.20748200
H	-5.24195200	1.47553000	1.18106600
C	-0.34104900	5.52514600	-1.17413800
H	-0.59270500	6.36182400	-0.52143200
H	0.74504800	5.53060600	-1.30951100
H	-0.79170600	5.69770700	-2.15176900
C	-2.12894500	0.94948800	-1.84114900
H	-1.69304200	1.08470000	-2.83168100
H	-2.04924000	-0.10173200	-1.58500900
H	-3.19760300	1.18763000	-1.90651300

C	-1.46195700	2.89583700	2.85623600
H	-2.33160000	2.31860500	3.16616200
H	-0.63076300	2.59683600	3.49126300
H	-1.67940400	3.93808300	3.08960700

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e-17-1 carbene fragment

C	3.44711600	-0.55378600	-0.50163500
N	1.23481400	-1.05773800	0.44508100
C	1.11630700	-0.90312100	1.93358800
C	4.68968700	-1.02152000	-0.92833200
H	5.45005400	-0.30305300	-1.21441200
C	0.22497000	-0.70069800	-0.31209000
C	3.12727000	1.33108100	-2.07988800
H	2.34633700	0.78080800	-2.60841100
H	4.08711700	1.11566800	-2.55769600
H	2.92441400	2.40031900	-2.17996100
C	2.70356600	-2.87106500	-0.30418200
C	4.95769800	-2.37720000	-1.02207500
H	5.93174200	-2.71827300	-1.35054800
C	2.48230000	-1.49953500	-0.12451700
C	-0.78667500	-0.00330500	0.64579800
C	1.04322400	-4.15738400	-1.59440200
H	0.65304900	-3.24269600	-2.04689500
H	0.24451600	-4.90312700	-1.56407200
H	1.84570200	-4.54735200	-2.22682100
C	3.16138200	0.93233200	-0.60246700
H	2.16830200	1.13030400	-0.19693600
C	1.57064900	-3.86510500	-0.18770700
H	0.76333300	-3.38210300	0.35990500
C	-0.35334100	-0.49110100	2.04668900
H	-0.53317900	0.21784300	2.84618200
H	-0.93944600	-1.38835300	2.25133500
C	4.17753400	1.79846700	0.13833900
H	4.28959000	1.50325100	1.18273300

H	3.85483400	2.84379400	0.10785400
H	5.16140000	1.74325500	-0.33480800
C	3.95493100	-3.29323900	-0.74390300
H	4.13712900	-4.35197400	-0.88860800
C	1.95449100	-5.15193700	0.53319600
H	2.38313400	-4.94970000	1.51702800
H	2.68077400	-5.73187900	-0.04098500
H	1.07301100	-5.78488400	0.66699100
C	2.12177000	0.12253000	2.44496200
H	3.13825300	-0.26759000	2.34396200
H	1.93116900	0.31794400	3.50273800
H	2.05965700	1.06440500	1.90403900
C	1.37855700	-2.21926000	2.65742400
H	0.63697500	-2.97468400	2.39203000
H	1.31623100	-2.04643800	3.73409300
H	2.37801800	-2.60148100	2.43325800
C	-0.43124200	1.43612400	0.24524100
C	0.09083800	2.43719100	1.07540400
C	-0.51905700	1.76448000	-1.12333900
C	0.70325900	3.58424600	0.55827000
C	0.07031300	2.90214400	-1.65753500
C	0.72954600	3.78525300	-0.81781500
H	1.13321900	4.31409700	1.22576300
H	0.02085700	3.11764800	-2.71583200
C	-2.23682900	-0.36412700	0.38589200
C	-2.60674900	-1.69715500	0.13015400
C	-3.26697000	0.56710000	0.39357500
C	-3.90369600	-2.04735700	-0.21254100
C	-4.58323500	0.24805900	0.04615300
C	-4.88891900	-1.06261300	-0.27495400
H	-4.18977200	-3.06314000	-0.44201900
H	-5.33252200	1.02672100	0.06930200
O	-6.12742200	-1.48795400	-0.63214000
O	-2.98022800	1.83702300	0.79423600

O	-1.62299200	-2.62937200	0.25445800
O	1.34523900	4.84030300	-1.40979700
O	-1.29414400	0.97222800	-1.90719500
O	-0.02577800	2.27599000	2.41861800
C	2.03572100	5.74864700	-0.58919600
H	2.82160900	5.24631300	-0.01502200
H	2.48853200	6.48464000	-1.24843600
H	1.35807800	6.25670100	0.10420000
C	0.65822200	3.14982200	3.27827200
H	0.50751100	2.77232300	4.28741800
H	1.73174100	3.16804300	3.05734400
H	0.26237200	4.16787400	3.21638800
C	-3.39339100	2.89257300	-0.04877100
H	-3.33719300	2.59149400	-1.09801900
H	-4.41147400	3.21800800	0.18481700
H	-2.70517900	3.72231500	0.12012800
C	-7.14951300	-0.52648800	-0.70735400
H	-6.90556200	0.25585700	-1.43282300
H	-8.04768700	-1.04767000	-1.02887100
H	-7.33150500	-0.06196600	0.26687500
C	-1.98592000	-3.98498800	0.15385700
H	-2.79822600	-4.22643800	0.84547500
H	-2.29323500	-4.24126200	-0.86432100
H	-1.10606800	-4.56861200	0.41883700
C	-0.77369400	0.53512200	-3.14469500
H	0.12318500	-0.06267000	-2.96536100
H	-1.53931200	-0.09012800	-3.59883600
H	-0.55330000	1.36916100	-3.81651400

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e-17-1 carbene-Au fragment

Au	0.35992100	-1.41885200	-1.59055400
C	3.32049800	0.62845500	-0.29214300
N	1.42629000	-0.33304200	0.92901000
C	1.26220900	0.07409400	2.36099200

C	4.64440300	0.52446000	-0.71301100
H	5.10048500	1.36748700	-1.21925500
C	0.33481600	-0.36859700	0.20390600
C	2.32526000	1.89320800	-2.18262800
H	1.74258200	1.02046000	-2.49266800
H	3.28178200	1.87230100	-2.71214000
H	1.78856200	2.79915100	-2.47525700
C	3.44024300	-1.69064400	0.48177800
C	5.37570300	-0.63525300	-0.51859500
H	6.40672500	-0.69081200	-0.84501200
C	2.74860100	-0.47635200	0.36114800
C	-0.83644300	0.19323700	1.05565200
C	2.70034000	-3.94561100	-0.25466900
H	2.09998100	-3.52394300	-1.06542100
H	2.25499400	-4.89426000	0.05717800
H	3.70058900	-4.16125400	-0.63890700
C	2.55097600	1.88102600	-0.66887300
H	1.56750100	1.85672800	-0.19800300
C	2.78608800	-2.98081400	0.93233300
H	1.76714800	-2.74476400	1.24920400
C	-0.26225600	0.02695400	2.48040200
H	-0.65659500	0.72685100	3.20576400
H	-0.53235800	-0.98263300	2.79344700
C	3.25320600	3.16762900	-0.23822700
H	3.47980400	3.17436300	0.82989700
H	2.60931700	4.02331300	-0.46166500
H	4.18978500	3.31024700	-0.78261300
C	4.76394400	-1.73875900	0.05039100
H	5.31147000	-2.66991900	0.14209400
C	3.53460200	-3.67069400	2.07277600
H	3.70632500	-3.01566000	2.92634700
H	4.50628900	-4.03145500	1.72650400
H	2.97029400	-4.54108200	2.41589700
C	1.92979100	1.42542000	2.59804300

H	3.01365000	1.31858900	2.50259500
H	1.70482500	1.76089500	3.61242900
H	1.60094500	2.18868700	1.89663400
C	1.90440600	-0.92440600	3.31160400
H	1.47663800	-1.92061200	3.19667700
H	1.72297000	-0.58956500	4.33524500
H	2.98419400	-0.96955700	3.15701200
C	-0.89779500	1.63100200	0.49560000
C	-0.66510400	2.81340300	1.20864600
C	-1.16163200	1.80589000	-0.88303300
C	-0.41358600	4.03381300	0.56804600
C	-0.93045600	3.00634500	-1.54219800
C	-0.49214300	4.10449800	-0.81601600
H	-0.17445800	4.90976500	1.14911100
H	-1.06819000	3.11008400	-2.60819400
C	-2.13591400	-0.57987000	0.90852600
C	-2.12416300	-1.98368000	0.81969000
C	-3.38036900	0.03384100	0.81700900
C	-3.26436200	-2.70710300	0.50559500
C	-4.54824200	-0.66805000	0.51024400
C	-4.47441500	-2.04010000	0.33066700
H	-3.25575500	-3.78078400	0.39450300
H	-5.48344500	-0.13062800	0.44601000
O	-5.53955100	-2.81864400	0.01969900
O	-3.44749800	1.37014400	1.05899100
O	-0.93891800	-2.59364200	1.07905200
O	-0.19781000	5.21832000	-1.52859700
O	-1.70226300	0.75291400	-1.52005800
O	-0.70464000	2.76281500	2.56368100
C	0.24568400	6.35461300	-0.82815400
H	1.15251800	6.13702700	-0.25445700
H	0.46574100	7.11474100	-1.57292000
H	-0.52551800	6.72960600	-0.14819900
C	-0.30717000	3.88373600	3.31095000

H	-0.34211300	3.58513100	4.35648200
H	0.71381600	4.19062400	3.05838400
H	-0.98505100	4.72844000	3.15914800
C	-4.23490700	2.16325300	0.19892700
H	-4.19210400	1.78172200	-0.82550200
H	-5.27739400	2.20295700	0.52777300
H	-3.81405700	3.16937700	0.22332900
C	-6.78055000	-2.18679500	-0.16987800
H	-6.73114900	-1.45026700	-0.97784800
H	-7.49090300	-2.96518600	-0.43625500
H	-7.11780900	-1.68905100	0.74470500
C	-0.79950400	-3.94512500	0.69423000
H	-1.47706200	-4.58863300	1.26171300
H	-0.98181200	-4.05567600	-0.37887600
H	0.22558600	-4.23009300	0.91329800
C	-1.77976700	0.76278600	-2.92857300
H	-0.79473900	0.94249700	-3.37007500
H	-2.12070700	-0.22725400	-3.21995200
H	-2.48759500	1.52251400	-3.27653100

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e-18-1 carbene fragment

C	3.09178100	0.76860500	-0.50596600
N	1.18028600	-0.45131700	0.41769600
C	0.96040400	-0.37069700	1.90285900
C	4.41404300	0.75363200	-0.94657200
H	4.87734100	1.68462700	-1.25308600
C	0.15147800	-0.37985200	-0.38473400
C	2.01308200	2.35775100	-2.07217800
H	1.42612700	1.55012600	-2.51535200
H	2.94601700	2.45994900	-2.63312000
H	1.45366400	3.29184300	-2.16633400
C	3.19627000	-1.66486700	-0.26798600
C	5.13104100	-0.42929000	-1.02689700
H	6.15873500	-0.41876500	-1.36815100

C	2.51992000	-0.44913700	-0.11555400
C	-1.07551200	-0.13729300	0.54262000
C	2.09109000	-3.49064300	-1.51051200
H	1.46027500	-2.75563100	-2.01455200
H	1.54045800	-4.43121100	-1.43785900
H	2.98431900	-3.65857600	-2.11878000
C	2.30219100	2.05915900	-0.59969500
H	1.33598400	1.91774800	-0.11535000
C	2.48290900	-2.99079700	-0.11877500
H	1.55483000	-2.82113000	0.42370900
C	-0.56089300	-0.53714300	1.94395000
H	-1.02592000	-0.01884100	2.77576200
H	-0.77485100	-1.60266600	2.05725600
C	3.00047900	3.24132800	0.06583100
H	3.25880200	3.02618500	1.10455800
H	2.34573100	4.11606600	0.04794500
H	3.91902600	3.50910300	-0.46153900
C	4.51418600	-1.63136300	-0.71565100
H	5.05394400	-2.56219400	-0.84472600
C	3.29796900	-4.03723200	0.63260700
H	3.62108000	-3.67080400	1.60951700
H	4.18801800	-4.32848000	0.07042700
H	2.70146000	-4.93898900	0.78362900
C	1.49953200	0.95257800	2.43944600
H	2.58797600	0.96896100	2.33877700
H	1.25066800	1.04090100	3.49782600
H	1.09925500	1.82099000	1.92241900
C	1.66598200	-1.48872200	2.66159300
H	1.26487600	-2.47148000	2.41462700
H	1.52581500	-1.32478100	3.73182200
H	2.73949600	-1.47934500	2.45799100
C	-1.30140300	1.34968800	0.26945800
C	-1.26680700	2.39088000	1.19368400
C	-1.49575100	1.77263600	-1.05384600

C	-1.27981000	3.73450300	0.85762700
C	-1.52544500	3.09537000	-1.45340500
C	-1.38753100	4.06209100	-0.47785700
H	-1.23310500	4.49082000	1.62754200
H	-1.66205100	3.35056400	-2.49417700
C	-2.26613000	-0.98803600	0.14265900
C	-2.08661100	-2.32115500	-0.22255600
C	-3.59331100	-0.56943300	0.14206600
C	-3.10134400	-3.17398500	-0.60969100
C	-4.65959600	-1.36732800	-0.23591800
C	-4.38550900	-2.66463100	-0.61635000
H	-2.89247700	-4.19610300	-0.88952800
H	-5.66806100	-0.98041700	-0.22353300
F	-5.39300200	-3.45738400	-0.98685900
F	-0.84957200	-2.83209200	-0.16675100
F	-3.89060700	0.67284900	0.54024800
F	-1.23626600	2.12858800	2.50793000
F	-1.72131400	0.86317700	-1.99766900
F	-1.39586700	5.34831100	-0.83169400

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e-18-1 carbene-Au fragment

Au	0.25295100	-1.14264300	-1.62354300
C	2.86831100	1.33090500	-0.20124300
N	1.13259900	0.03408600	0.92711800
C	0.85997900	0.32039600	2.36957000
C	4.18782200	1.44309600	-0.63158000
H	4.51381900	2.36940400	-1.09048100
C	0.08880100	-0.09488200	0.14119300
C	1.63957600	2.53504200	-1.99580600
H	1.18489600	1.60342400	-2.34401300
H	2.56868600	2.69194200	-2.54992700
H	0.96348000	3.36317800	-2.22248700
C	3.32705700	-0.98869800	0.44814800
C	5.07764100	0.38904800	-0.50322400

H	6.10179100	0.49853600	-0.83725500
C	2.47110900	0.12085600	0.38997500
C	-1.18389400	0.16810900	0.98727900
C	2.94037900	-3.30692400	-0.38130400
H	2.34799700	-2.91449700	-1.21066000
H	2.55748100	-4.29598000	-0.12080400
H	3.97540100	-3.42171700	-0.71454500
C	1.91644400	2.47552600	-0.49232300
H	0.96219800	2.27982500	-0.00261100
C	2.87157600	-2.38155600	0.83720700
H	1.82548600	-2.32799100	1.14390300
C	-0.64462200	0.03645600	2.43237000
H	-1.15823200	0.65090900	3.16135900
H	-0.77528800	-1.00211800	2.73303400
C	2.43455400	3.82211800	0.00811300
H	2.70227700	3.78784800	1.06584900
H	1.66651500	4.58752100	-0.12915700
H	3.31679500	4.13971100	-0.55219300
C	4.63897300	-0.81970200	0.00985900
H	5.31696300	-1.66455600	0.04926800
C	3.71043700	-2.98876300	1.96202400
H	3.75247700	-2.35906000	2.85042700
H	4.73583000	-3.15443000	1.62269100
H	3.30266300	-3.96033200	2.24823200
C	1.28090900	1.74799300	2.70579500
H	2.36546500	1.83917200	2.60798000
H	1.00673500	1.96847600	3.73815800
H	0.82013400	2.49324200	2.06240800
C	1.62486600	-0.61439000	3.29262200
H	1.37057600	-1.65873400	3.11171300
H	1.36664300	-0.36966000	4.32489500
H	2.70062600	-0.47607600	3.17161300
C	-1.55795300	1.59330500	0.54798800
C	-1.59085800	2.74137800	1.33851300

C	-1.82228700	1.84601600	-0.80673400
C	-1.71048900	4.02975300	0.84037200
C	-1.95831600	3.09983100	-1.36605700
C	-1.86680300	4.18721900	-0.51943700
H	-1.70370500	4.87389500	1.51444800
H	-2.14458600	3.21028400	-2.42430500
C	-2.26186100	-0.87149000	0.72415000
C	-1.93285400	-2.22960200	0.74900700
C	-3.60834400	-0.61779000	0.47743700
C	-2.81710500	-3.25828600	0.49989100
C	-4.54861800	-1.60039400	0.22095800
C	-4.12643100	-2.91307500	0.22670900
H	-2.48900700	-4.28696000	0.51859200
H	-5.57748300	-1.33565500	0.02582400
F	-5.01120200	-3.87859900	-0.02115700
F	-0.67747200	-2.57517100	1.06824200
F	-4.06112700	0.64060300	0.49236300
F	-1.52288900	2.66357900	2.67499800
F	-2.01275600	0.81093700	-1.61843300
F	-1.97410400	5.41550300	-1.02386900

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e-19-1 carbene fragment

C	3.46857400	-0.20885000	-0.47461500
N	1.31550400	-0.96736400	0.43591300
C	1.12349600	-0.85708000	1.92133400
C	4.77370600	-0.51370600	-0.85832300
H	5.43240800	0.29277600	-1.15931400
C	0.33292500	-0.62452300	-0.36019500
C	2.87530000	1.54622000	-2.11551900
H	2.10553200	0.92264800	-2.57700700
H	3.82434100	1.36251200	-2.62588500
H	2.61410100	2.59792100	-2.25890900
C	3.05279600	-2.59884000	-0.19169700
C	5.23331600	-1.81920700	-0.88686800

H	6.25327700	-2.03165600	-1.18197100
C	2.63224000	-1.26595900	-0.08493400
C	-0.79056600	-0.05153400	0.57856700
C	1.68464500	-4.20190900	-1.47131700
H	1.26760100	-3.36571600	-2.03632100
H	0.93914100	-5.00005100	-1.42502400
H	2.55796100	-4.57998100	-2.00985600
C	3.00057900	1.22546800	-0.62375500
H	2.00537300	1.31997700	-0.18977900
C	2.08687700	-3.75512900	-0.06393900
H	1.18884500	-3.38998500	0.42914700
C	-0.38528000	-0.58865000	1.96609500
H	-0.69553100	0.00970100	2.81491100
H	-0.88286100	-1.55862700	2.05644600
C	3.91852700	2.23381400	0.06298300
H	4.07359200	1.99077100	1.11610500
H	3.48067700	3.23390800	-0.00167500
H	4.89706900	2.27557800	-0.42081800
C	4.36438700	-2.85410000	-0.58260200
H	4.69785300	-3.88127200	-0.67241000
C	2.63281500	-4.93076100	0.73921000
H	2.98010400	-4.62173300	1.72694100
H	3.46700500	-5.41155800	0.22364800
H	1.85561500	-5.68633200	0.86977500
C	2.04044900	0.23260400	2.46863900
H	3.07914900	-0.09777900	2.38510800
H	1.81848000	0.40728900	3.52194400
H	1.94356300	1.17560600	1.93584500
C	1.46194800	-2.14403000	2.66439800
H	0.80306600	-2.96668900	2.38499600
H	1.34467200	-1.96441000	3.73511200
H	2.49940100	-2.43463300	2.48493800
C	-0.55006600	1.43259500	0.24268800
C	-0.11958700	2.45321600	1.10968700

C	-0.61604000	1.82004900	-1.11512000
C	0.41682600	3.65203100	0.65801500
C	-0.10934700	3.02182100	-1.58569000
C	0.46670600	3.90761400	-0.69770400
H	0.76866000	4.38239600	1.37309000
H	-0.14999700	3.24116600	-2.64332100
C	-2.21375900	-0.49954400	0.24697300
C	-2.49452600	-1.77346800	-0.26596400
C	-3.34985300	0.28999900	0.47238400
C	-3.76091800	-2.18876100	-0.64593000
C	-4.63214400	-0.09077000	0.10036700
C	-4.82794900	-1.32581600	-0.48379800
H	-3.90317400	-3.17930700	-1.05423300
H	-5.46334000	0.57548200	0.28273200
Cl	-1.26171600	-2.96657600	-0.41856000
Cl	-6.40524400	-1.80936400	-0.96641500
Cl	-3.26315700	1.80372300	1.29487600
Cl	-1.39813700	0.86434800	-2.31559300
Cl	1.21161400	5.34452300	-1.27567200
Cl	-0.31321700	2.41139200	2.82984600

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e-19-1 carbene-Au fragment

Au	0.50271400	-1.12203800	-1.77948500
C	3.36441200	0.20001100	0.04225800
N	1.23110100	-0.55269400	1.00367300
C	0.95639100	-0.25007800	2.44454600
C	4.68955100	-0.08042000	-0.28382400
H	5.30835900	0.71549700	-0.68149800
C	0.24994600	-0.36866400	0.15711100
C	2.84841700	1.80885900	-1.79100800
H	2.19575600	1.09053700	-2.29446100
H	3.85861700	1.69204200	-2.19098600
H	2.51096900	2.82177400	-2.02594600
C	3.07922100	-2.15533600	0.65303100

C	5.22027100	-1.35007200	-0.13564500
H	6.25331200	-1.54240200	-0.39648300
C	2.58300600	-0.84634000	0.56031500
C	-0.95280200	0.26065800	0.93985700
C	1.97279500	-4.18582600	-0.27513200
H	1.52755300	-3.58229600	-1.07069600
H	1.30495900	-5.02188000	-0.05184800
H	2.91727300	-4.59504300	-0.64394900
C	2.84449900	1.59016500	-0.27577800
H	1.80952200	1.66974500	0.06137300
C	2.21401400	-3.35230900	0.98533900
H	1.24795100	-2.98175700	1.32193400
C	-0.56512100	-0.07120800	2.39678900
H	-0.94565600	0.61785200	3.13996300
H	-1.01012700	-1.04655600	2.60527000
C	3.66106200	2.69170500	0.40034400
H	3.74348400	2.54630300	1.47858600
H	3.19611400	3.66393100	0.21409600
H	4.67276300	2.73115600	-0.00995100
C	4.40897700	-2.38007100	0.30739900
H	4.80161300	-3.38847300	0.36608200
C	2.81032000	-4.24030900	2.07638300
H	3.06870600	-3.68335000	2.97780400
H	3.71589700	-4.73553400	1.71903200
H	2.10003800	-5.02383900	2.34806200
C	1.79394100	0.95088300	2.86948800
H	2.84959300	0.66862700	2.85859800
H	1.52455200	1.24309200	3.88456800
H	1.66793000	1.80988700	2.21611400
C	1.32386500	-1.39884200	3.37355700
H	0.74222400	-2.29825900	3.17211800
H	1.11890000	-1.08221800	4.39817900
H	2.38798500	-1.62757300	3.29887900
C	-0.78685200	1.72409700	0.46124900

C	-0.39858400	2.83352100	1.23507500
C	-0.87545200	2.00407700	-0.92142000
C	0.14287900	3.98655100	0.68039500
C	-0.34648900	3.14746200	-1.50061100
C	0.23094900	4.10685200	-0.69241100
H	0.46627300	4.78865800	1.32900400
H	-0.39415700	3.27344200	-2.57309400
C	-2.32702800	-0.33762400	0.64098900
C	-2.50671800	-1.70201300	0.36811400
C	-3.51699900	0.40322800	0.68257100
C	-3.72397500	-2.25382300	-0.00070200
C	-4.75126900	-0.11884000	0.32558400
C	-4.84242300	-1.44467300	-0.05078800
H	-3.78906000	-3.30859500	-0.22676400
H	-5.62823400	0.51214500	0.35256400
Cl	-1.22707400	-2.84099400	0.56036000
Cl	-6.35759000	-2.10102800	-0.52260500
Cl	-3.56188800	2.03752600	1.23317300
Cl	-1.76366300	1.00305200	-1.99885800
Cl	0.99051600	5.48038600	-1.38768000
Cl	-0.68971400	2.98301300	2.93552700

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e-20-1 carbene fragment

C	-1.22526000	3.87172800	0.45475400
N	-1.28222800	1.66847600	-0.60933900
C	-0.92851700	1.57283700	-2.07081600
C	-1.92340000	4.98747800	0.91360300
H	-1.37220500	5.81687800	1.34111600
C	-0.87187900	0.72904000	0.19594700
C	0.52248300	3.47355100	2.16941900
H	0.01872200	2.55130700	2.46648900
H	0.14665000	4.28905100	2.79328000
H	1.59371200	3.36557400	2.35896400
C	-3.37115300	2.81172700	-0.07896700

C	-3.30743000	5.03762500	0.86135300
H	-3.83078700	5.91453600	1.22130700
C	-1.97197900	2.81986900	-0.08694800
C	-0.08979800	-0.26268600	-0.68724000
C	-4.56403500	0.86704400	0.88850300
H	-3.68250300	0.64193200	1.49391900
H	-5.09358000	-0.06589900	0.67888500
H	-5.22370800	1.51223500	1.47470000
C	0.26868500	3.77348100	0.69037200
H	0.65677500	2.92439900	0.12672600
C	-4.16244800	1.56409400	-0.41343900
H	-3.50835100	0.87566300	-0.95209700
C	-0.51497400	0.10171600	-2.12530000
H	0.23255000	-0.09367000	-2.89402000
H	-1.39609100	-0.49714800	-2.37294300
C	1.02801500	5.02232600	0.25344800
H	0.82869500	5.27412900	-0.79016500
H	2.10194900	4.86643100	0.37069400
H	0.75653500	5.88526500	0.86534300
C	-4.02459800	3.94685000	0.39205400
H	-5.10782300	3.96614000	0.41426700
C	-5.37969200	1.83933600	-1.28900600
H	-5.10478000	2.37468600	-2.20049800
H	-6.12246000	2.43767300	-0.75740700
H	-5.86029000	0.90046300	-1.56971300
C	0.19795600	2.54718100	-2.40267300
H	-0.12330500	3.57226800	-2.20113200
H	0.43651600	2.46984500	-3.46481200
H	1.10531000	2.34883200	-1.83389500
C	-2.10690600	1.88666400	-2.98254000
H	-2.91541000	1.16374900	-2.88079900
H	-1.76330100	1.86113300	-4.01801700
H	-2.49800400	2.88697500	-2.78256000
C	1.37077000	-0.00546500	-0.34346200

C	2.37677900	0.09628400	-1.29137300
C	1.71448400	0.14358400	1.00826500
C	3.68989300	0.36954900	-0.90992300
H	2.16310700	-0.02000600	-2.34689800
C	3.01665100	0.42872500	1.37322000
H	0.94097100	0.05387800	1.76011500
C	4.02237500	0.54861400	0.41737900
H	5.03917400	0.77534600	0.71074400
C	-0.50905700	-1.67816600	-0.33513000
C	-1.85490700	-1.91495400	-0.06217400
C	0.37137600	-2.75056600	-0.30571800
C	-2.30641800	-3.19175700	0.22602300
H	-2.55791600	-1.08595600	-0.06460700
C	-0.09093300	-4.03122500	-0.01760200
H	1.42728200	-2.59836600	-0.50205300
C	-1.42863900	-4.26742700	0.25226000
H	-1.78016700	-5.26390600	0.47956800
C	-3.76783200	-3.36925500	0.53489200
C	0.90537000	-5.15866800	-0.02364700
C	4.72261900	0.48586100	-1.99667900
C	3.39000100	0.62692100	2.81789200
F	4.80846100	-0.64306400	-2.71112100
F	4.40531700	1.46110100	-2.86118200
F	5.93678100	0.75400700	-1.51811900
F	3.97274900	1.82057300	3.00320500
F	4.27008900	-0.29541100	3.22526400
F	2.33594700	0.56532700	3.62946000
F	-4.11651000	-4.65364000	0.61820100
F	-4.53606600	-2.80326600	-0.40813200
F	-4.09843700	-2.78704900	1.69404500
F	0.37343500	-6.30731500	0.39666200
F	1.95422100	-4.88725600	0.76160600
F	1.39209600	-5.37003500	-1.25428900

e-20-1 carbene-Au fragment

Au	0.99459700	1.07379300	-1.60201200
C	-1.98734200	3.18840100	-0.18588200
N	-0.31546700	1.83555900	0.96346200
C	-0.52540800	1.53264500	2.41590700
C	-2.39425500	4.43051500	-0.66528400
H	-3.37661400	4.52527800	-1.11337500
C	0.04388300	0.83058100	0.20332500
C	-2.91334900	1.63236000	-1.89350100
H	-1.91135600	1.38066100	-2.25246100
H	-3.28672400	2.47371500	-2.48275200
H	-3.57284500	0.77815700	-2.06849900
C	0.18697700	4.17549000	0.38684600
C	-1.55785900	5.53378700	-0.59990700
H	-1.89515300	6.49255900	-0.97298900
C	-0.71042900	3.09950300	0.38993200
C	0.09876800	-0.43588800	1.06368600
C	2.52230000	4.25440500	-0.48180800
H	2.24847700	3.56146300	-1.28043500
H	3.57386100	4.09679000	-0.23341600
H	2.41181300	5.27539800	-0.85611100
C	-2.89087300	1.98931700	-0.40562100
H	-2.47486400	1.12838400	0.11947800
C	1.65105200	4.04637100	0.76031400
H	1.82856600	3.02634400	1.11353300
C	0.09172700	0.13118500	2.49799800
H	-0.40937700	-0.50317600	3.22810100
H	1.12970400	0.22762100	2.82334600
C	-4.31122900	2.21071700	0.11029000
H	-4.32250900	2.53255500	1.15306000
H	-4.88200600	1.28199200	0.03211100
H	-4.83266800	2.96637600	-0.48139700
C	-0.27304300	5.39692600	-0.10108300
H	0.40121100	6.24552100	-0.11248000

C	2.07718300	5.03971500	1.84068900
H	1.46857400	4.97193600	2.74234700
H	2.00150500	6.06244000	1.46416200
H	3.12021400	4.87040800	2.11457700
C	-2.00866500	1.60124600	2.76789400
H	-2.37949000	2.61615800	2.60734900
H	-2.13112800	1.35924300	3.82521000
H	-2.62276700	0.91687800	2.18627200
C	0.20969200	2.52004200	3.30745100
H	1.28393500	2.51416800	3.12211300
H	0.04001500	2.24497200	4.35000700
H	-0.17569200	3.53013500	3.15665200
C	-1.17075100	-1.17486100	0.64670300
C	-2.18953900	-1.51039500	1.52172400
C	-1.35223300	-1.43856600	-0.71820800
C	-3.38929400	-2.03794400	1.04414500
H	-2.09509400	-1.34104100	2.58665500
C	-2.54206000	-1.96707100	-1.18032000
H	-0.55939600	-1.19227800	-1.41746100
C	-3.58440300	-2.26014400	-0.30374300
H	-4.52436000	-2.64868000	-0.67233300
C	1.35865900	-1.24129100	0.79834200
C	2.58290000	-0.56362400	0.77674200
C	1.35390400	-2.61193600	0.61423200
C	3.76093700	-1.24930200	0.56545500
H	2.60575300	0.51277400	0.91503500
C	2.55115100	-3.29781500	0.40343400
H	0.42287400	-3.16721600	0.62540600
C	3.75727400	-2.62949500	0.37218600
H	4.68320800	-3.16265400	0.19996100
C	5.08185500	-0.52987100	0.53182400
C	2.48517100	-4.79021600	0.22565000
C	-4.48091100	-2.29356000	2.04558600
C	-2.73305400	-2.23157800	-2.65117000

F	-4.07104900	-3.11265100	3.02089700
F	-4.85722600	-1.14969200	2.64049000
F	-5.56542500	-2.83180100	1.49169300
F	-3.97840800	-1.92502600	-3.03727900
F	-2.54323800	-3.52362200	-2.94333600
F	-1.89092200	-1.52321000	-3.40062700
F	5.90217900	-0.98409000	1.49005800
F	4.94710000	0.78525200	0.71431100
F	5.71044100	-0.71618900	-0.63198200
F	3.67105100	-5.31650600	-0.08052000
F	1.62812500	-5.12787700	-0.74425600
F	2.05570700	-5.39162500	1.34388800

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f-1-1 carbene fragment

C	-1.19515400	-1.31153800	1.20560000
N	0.02207500	0.20966800	-0.30187200
C	0.03189500	-0.17514600	-1.76296600
C	-1.17047300	-2.35985500	2.12681300
H	-2.11271500	-2.74047100	2.50295600
C	-0.02155400	1.48496300	0.00443700
C	1.23418300	-1.29867700	1.20938100
C	0.02665600	-2.88534800	2.58168700
C	0.01731700	-0.80073700	0.72086700
C	0.25659600	1.19796700	-2.40243500
H	-0.36810000	1.33055300	-3.28856200
H	1.30118000	1.28570900	-2.71461500
C	1.21955000	-2.34429500	2.13277300
H	2.16449200	-2.71282300	2.51404700
C	-1.29986400	-0.80413500	-2.15346000
H	-1.45059200	-1.75433700	-1.63517100
H	-1.29615400	-1.00547900	-3.22599500
H	-2.14081800	-0.14547900	-1.92700300
C	1.15776200	-1.14542600	-2.08504300
H	2.13213000	-0.70263800	-1.87459800

H	1.11767500	-1.38846900	-3.14845100
H	1.05956700	-2.07861200	-1.52350000
C	-0.04523100	2.23835400	-1.30675400
C	-1.44465400	2.84345200	-1.44946900
H	-1.67797500	3.47511600	-0.59062100
H	-1.49074400	3.45371800	-2.35501300
H	-2.21314000	2.07009100	-1.52291300
C	0.99040200	3.35688800	-1.27829100
H	0.96794100	3.91609800	-2.21751200
H	0.78961300	4.04285900	-0.45413100
H	1.99757300	2.95287900	-1.14933500
C	2.55575700	-0.76194800	0.79853500
C	3.54172200	-1.63902800	0.36249700
C	2.85661100	0.60131100	0.88546300
C	4.79582900	-1.16782700	-0.01020600
H	3.32298600	-2.69888400	0.28472600
C	4.11356100	1.05500700	0.52298800
H	2.10532300	1.29490400	1.24566300
C	5.09293500	0.18006300	0.06208600
H	6.07006500	0.54870300	-0.22196200
C	-2.52456500	-0.78440400	0.80555900
C	-3.49241500	-1.66133300	0.33012700
C	-2.84997000	0.56762400	0.94596100
C	-4.75039200	-1.19760400	-0.03682600
H	-3.25606700	-2.71438800	0.21778100
C	-4.11190300	1.01376700	0.58991200
H	-2.10979500	1.26045800	1.32952800
C	-5.07098400	0.14194700	0.08436900
H	-6.05139900	0.50493600	-0.19559400
C	-5.74177900	-2.19274300	-0.57387400
C	-4.48874700	2.46456800	0.73191000
F	-6.91026300	-1.62970900	-0.88096500
F	-5.27870700	-2.78972700	-1.68044900
F	-5.98290500	-3.16656700	0.31320600

F	-4.68497000	3.03520300	-0.46568700
F	-3.55653700	3.17349100	1.36588100
F	-5.63408000	2.60217700	1.41160000
C	5.80724600	-2.16470200	-0.50538900
C	4.46834600	2.51529500	0.61793600
F	5.37768700	-2.78009900	-1.61540000
F	6.02964600	-3.12396700	0.40196000
F	6.98020400	-1.59887700	-0.78932800
F	5.59385100	2.69489300	1.32004500
F	3.51112300	3.23615300	1.19795600
F	4.68854200	3.03934300	-0.59714100
H	0.03000200	-3.69167800	3.30317000

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f-1-1 carbene-Au fragment

Au	-0.02859100	-2.28609800	-1.18927800
C	-1.15071400	1.34683800	-1.37261700
N	0.04529900	0.21740700	0.45830000
C	0.15540600	0.86787500	1.81461100
C	-1.11526400	2.06764200	-2.56591800
H	-2.05431500	2.35914000	-3.02068400
C	-0.21604600	-1.06976800	0.47205300
C	1.28200300	1.27784800	-1.38353000
C	0.08713000	2.38634900	-3.17384300
C	0.05779200	0.95628100	-0.77828800
C	0.31261400	-0.37230900	2.69998100
H	-0.19395900	-0.24586300	3.65864700
H	1.37724000	-0.53544200	2.89658100
C	1.27404000	1.99270200	-2.58152900
H	2.22179900	2.21804500	-3.05531300
C	-1.11959300	1.65437500	2.10096500
H	-1.21024400	2.50139400	1.41671500
H	-1.07158800	2.04723600	3.11756700
H	-2.01409500	1.03695900	2.00648200
C	1.34250500	1.81001700	1.93199100

H	2.29246300	1.28512300	1.82667200
H	1.31583800	2.26772100	2.92250300
H	1.28933800	2.61301900	1.19253900
C	-0.23556300	-1.56326300	1.89399300
C	-1.68130300	-1.92916400	2.24555300
H	-2.05396100	-2.68217400	1.54741400
H	-1.71419000	-2.34452200	3.25536100
H	-2.34977500	-1.06756500	2.20832100
C	0.63830900	-2.80487800	2.04674000
H	0.67940100	-3.09343600	3.10001700
H	0.23024000	-3.63398400	1.46646700
H	1.65616400	-2.61661700	1.70005000
C	2.60073700	0.94610400	-0.78750500
C	3.53198400	1.96906900	-0.63730700
C	2.94282300	-0.33829500	-0.35899200
C	4.76030200	1.72933700	-0.03492600
H	3.28249900	2.97464100	-0.95905000
C	4.17179100	-0.56423700	0.24079900
H	2.25615300	-1.16413100	-0.51967700
C	5.08881900	0.46524600	0.42113700
H	6.04352200	0.27743200	0.89366100
C	-2.48909700	1.07813300	-0.78095400
C	-3.28647200	2.15938600	-0.42381500
C	-2.99312700	-0.21350800	-0.61244000
C	-4.53835300	1.96048200	0.14675000
H	-2.91577100	3.16944800	-0.56467500
C	-4.24610400	-0.39832600	-0.05053000
H	-2.40772900	-1.06796000	-0.93262600
C	-5.02548300	0.68191300	0.34895700
H	-5.99949700	0.52333200	0.79370900
C	-5.32830100	3.17212500	0.55810600
C	-4.80279000	-1.78225400	0.15589300
F	-6.53297800	2.85532500	1.03162100
F	-4.68947400	3.86334200	1.51301700

F	-5.50344300	4.01183200	-0.46918900
F	-4.96710400	-2.04416200	1.46196600
F	-4.01326800	-2.72892700	-0.34621900
F	-6.00690700	-1.91130600	-0.41294300
C	5.70721300	2.88729800	0.12571700
C	4.51519400	-1.93433600	0.76293800
F	5.16624700	3.85305800	0.88101800
F	5.99972100	3.44391500	-1.05576900
F	6.85554500	2.52677500	0.69777000
F	5.81547600	-2.20522900	0.62230300
F	3.82799000	-2.89586900	0.15091300
F	4.24165100	-2.02467300	2.07661200
H	0.09826400	2.92923200	-4.10961500

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f-2-1 carbene fragment

C	-1.14106600	-1.64455700	1.14564300
N	0.01290900	-0.13406000	-0.40572700
C	0.18782900	-0.56771500	-1.84334800
C	-1.09766300	-2.71209800	2.03986500
H	-2.03208700	-3.11570600	2.41119300
C	-0.27770600	1.12147500	-0.16576100
C	1.28276200	-1.56491800	1.15608100
C	0.11360300	-3.22667600	2.47481500
C	0.05608900	-1.11295800	0.64740600
C	0.07510100	0.77912500	-2.57228800
H	-0.71509800	0.73784200	-3.32319400
H	1.00758800	0.99315100	-3.10031000
C	1.29122500	-2.63123000	2.05712900
H	2.24230600	-2.96780000	2.45262400
C	-0.92877400	-1.53007100	-2.22239300
H	-0.89969400	-2.43292700	-1.60563500
H	-0.80547100	-1.83013000	-3.26450900
H	-1.90592000	-1.05612600	-2.11447100
C	1.53649600	-1.22610500	-2.08973400

H	2.35748000	-0.55037600	-1.83885600
H	1.61103400	-1.47259600	-3.15052100
H	1.64623700	-2.15361000	-1.52248000
C	-0.19856100	1.84896400	-1.49179800
C	-1.48921100	2.64188300	-1.71964000
C	1.01274000	2.78999100	-1.33874000
H	0.89741900	3.35994100	-0.41242700
H	-1.37088700	3.28179500	-2.59866800
C	-2.72165000	1.76214000	-1.89677800
H	-2.74021300	1.27733000	-2.87504300
H	-2.74974600	0.97562000	-1.13836100
H	-3.63911700	2.34451900	-1.80348000
H	-1.62343000	3.29919100	-0.85488000
C	1.24460000	3.73190000	-2.51188500
H	0.48126000	4.50884300	-2.56080500
H	2.21224500	4.22551700	-2.41354700
H	1.23892100	3.19712000	-3.46539500
H	1.89781100	2.15504900	-1.20582600
H	0.13735200	-4.05444000	3.17120900
C	2.57886800	-0.92011000	0.83399000
C	3.67550400	-1.69601300	0.47773700
C	2.73626500	0.46563800	0.93095100
C	4.89870500	-1.10255300	0.18967300
H	3.57003900	-2.77253700	0.39313200
C	3.96345200	1.04355600	0.65083100
H	1.89549500	1.08311600	1.22724700
C	5.05411500	0.26944700	0.26756000
H	6.00723900	0.73251700	0.04794600
C	-2.47119600	-1.05195400	0.84017700
C	-3.41960700	-1.73401700	0.09008600
C	-2.81319900	0.17915400	1.40281800
C	-4.67806700	-1.18097400	-0.12289300
H	-3.17550700	-2.69765200	-0.34408500
C	-4.07901600	0.70825500	1.20317100

H	-2.07991400	0.72277400	1.98437800
C	-5.02087400	0.04091300	0.43084100
H	-6.00177300	0.46522300	0.26733000
C	6.03793300	-1.99424600	-0.22198700
C	4.15581700	2.53475000	0.74078800
C	-5.64514100	-1.94687300	-0.98168000
C	-4.39063800	2.06538500	1.77249600
F	-5.88111500	-3.16822800	-0.48479100
F	-6.81970600	-1.32841200	-1.10217900
F	-5.70612600	2.28958900	1.83985000
F	-3.89164200	2.21228400	3.00261000
F	-5.15562000	-2.12611300	-2.21706500
F	-3.86338900	3.04012200	1.01860000
F	5.75348100	-2.65330500	-1.35323800
F	6.28922700	-2.92323200	0.70902300
F	7.16568900	-1.31405200	-0.42715700
F	5.25108700	2.83994400	1.44663900
F	3.12186800	3.14727000	1.31380200
F	4.32220800	3.07810000	-0.47512500

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f-2-1 carbene-Au fragment

Au	-0.48606000	-2.00712300	-0.71182700
C	-1.01361300	1.60264300	-1.48984800
N	0.14277900	0.70361600	0.49158300
C	0.43841700	1.54215700	1.71677500
C	-0.95724300	2.20653100	-2.74403800
H	-1.88808000	2.46806400	-3.23212800
C	-0.20839800	-0.53358600	0.72382800
C	1.40900000	1.41333100	-1.50833800
C	0.25527800	2.45329400	-3.36668800
C	0.18178500	1.24945800	-0.84603200
C	0.14009600	0.54599700	2.84854900
H	-0.74063600	0.86930400	3.40635500
H	0.97487100	0.50833800	3.55110500

C	1.42460500	2.03733300	-2.75653300
H	2.37565600	2.15322300	-3.26234900
C	-0.49539900	2.73915200	1.76801200
H	-0.40257000	3.35850200	0.87179400
H	-0.23330800	3.35217700	2.63182000
H	-1.53002400	2.41520100	1.88434000
C	1.87949900	2.02850100	1.75070800
H	2.59149300	1.20174700	1.70499700
H	2.03172400	2.55930100	2.69197500
H	2.08520800	2.72694100	0.93770100
C	-0.09420000	-0.82692600	2.19398100
C	-1.35699500	-1.53206500	2.69888700
C	1.14798000	-1.73056600	2.34601300
H	1.06057600	-2.56373400	1.64120200
H	-1.29254200	-1.60928000	3.78820100
C	-2.63993100	-0.82448800	2.28618500
H	-2.64950600	0.22644500	2.59498800
H	-2.74902800	-0.85627600	1.20030300
H	-3.51665000	-1.30310400	2.72284600
H	-1.35710400	-2.55191100	2.29869900
C	1.35606200	-2.26216700	3.75613700
H	0.58085500	-2.97905100	4.02802400
H	2.31807800	-2.77039500	3.82520500
H	1.34786300	-1.46063900	4.49922600
H	2.02408700	-1.14748600	2.03704600
H	0.28440300	2.92725900	-4.33879800
C	2.70387000	0.90231100	-0.99178800
C	3.80551600	1.74800900	-0.93497800
C	2.85619400	-0.42969700	-0.60017600
C	5.02345900	1.29140300	-0.44671100
H	3.70618100	2.78453600	-1.24040600
C	4.07791500	-0.87480900	-0.12201100
H	2.02054000	-1.11894700	-0.68681600
C	5.16992600	-0.01860200	-0.02682700

H	6.11815500	-0.37602000	0.35308200
C	-2.37143500	1.27083100	-0.96578800
C	-3.10079500	2.14220900	-0.17115600
C	-2.97547600	0.08374700	-1.38832700
C	-4.37840800	1.79968400	0.26160400
H	-2.68585200	3.10219700	0.10875800
C	-4.25613700	-0.23768600	-0.96809400
H	-2.43354200	-0.59066100	-2.04279500
C	-4.96509800	0.60800500	-0.12325900
H	-5.95832100	0.34511600	0.21471800
C	6.16525500	2.26783000	-0.37206400
C	4.25708100	-2.30064500	0.33131300
C	-5.07851400	2.75405400	1.18681000
C	-4.85191800	-1.56490200	-1.35684200
F	-5.15474900	3.98361900	0.66325900
F	-6.31621800	2.36353100	1.48496700
F	-6.18737800	-1.50361700	-1.42064000
F	-4.40816500	-1.98372700	-2.54088800
F	-4.40546800	2.87490000	2.34401700
F	-4.54716400	-2.50814500	-0.45728500
F	5.86816800	3.29749800	0.43302900
F	6.43928400	2.78902700	-1.57408900
F	7.28248800	1.70740800	0.08959400
F	5.35907500	-2.84308900	-0.19779500
F	3.22487700	-3.07194100	0.00604800
F	4.40374700	-2.36496000	1.66626500

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f-3-1 carbene fragment

C	-1.16373500	-2.05873200	1.14729500
N	0.04881500	-0.32379200	-0.11679000
C	0.04997100	-0.46430500	-1.61623300
C	-1.13208100	-3.21115100	1.93518700
H	-2.07237300	-3.64563400	2.25331600
C	0.04172500	0.88237000	0.39697000

C	1.26453200	-2.02994800	1.15865800
C	0.06706700	-3.77672000	2.33116300
C	0.04459000	-1.47644000	0.74188500
C	0.30444000	0.98768100	-2.02222100
H	-0.32424200	1.26548100	-2.86916700
H	1.34642800	1.09631600	-2.34029400
C	1.25617800	-3.18039100	1.94761400
H	2.20390900	-3.59083300	2.27535600
C	-1.29769200	-0.97946200	-2.10565300
H	-1.47714900	-2.00138700	-1.76399100
H	-1.29770000	-0.98760400	-3.19697600
H	-2.11737800	-0.34328500	-1.76273400
C	1.15073700	-1.39641800	-2.09833400
H	2.13651100	-1.01250600	-1.83251700
H	1.09745400	-1.47078100	-3.18604400
H	1.03566100	-2.40321600	-1.68701700
C	2.59015800	-1.46748500	0.79349600
C	3.53534000	-2.30967600	0.21815800
C	2.94238200	-0.13925500	1.05483400
C	4.79771500	-1.83677700	-0.12003200
H	3.27547100	-3.34146400	0.00619400
C	4.21091300	0.31371300	0.72912700
H	2.22425500	0.52518200	1.52334400
C	5.14684100	-0.52287800	0.12900500
H	6.13236500	-0.15342800	-0.12296600
C	-2.50495300	-1.53036800	0.78622600
C	-3.41144600	-2.38952600	0.17313800
C	-2.91244600	-0.23057900	1.09651800
C	-4.68798700	-1.95765700	-0.15888300
H	-3.10858800	-3.40291000	-0.06868100
C	-4.20251500	0.17815600	0.78708100
H	-2.22292900	0.44422500	1.59234200
C	-5.09577400	-0.67128900	0.14417400
H	-6.09683300	-0.33814500	-0.09411200

C	-5.60350800	-2.92170700	-0.86195500
C	-4.67485500	1.56576300	1.13436500
F	-6.83036700	-2.42725600	-1.02670200
F	-5.13214300	-3.23989700	-2.07525800
F	-5.71706200	-4.06970200	-0.18249900
F	-5.96068900	1.56214900	1.50429300
F	-4.58231900	2.39458000	0.08370500
F	-3.97269100	2.10277400	2.13105300
C	5.75965800	-2.78968200	-0.77458100
C	4.63041600	1.73070900	1.01892600
F	5.30046400	-3.20131200	-1.96409300
F	5.93691100	-3.88936600	-0.03156500
F	6.95800100	-2.24171500	-0.97590400
F	5.80234500	1.76373500	1.66532800
F	3.74090200	2.38327400	1.76446700
F	4.79948500	2.43086300	-0.11253300
H	0.07499800	-4.66336000	2.95123200
C	0.06276800	1.85214300	-0.76528200
C	-1.27856900	2.62863600	-0.78771800
C	1.19025300	2.89051400	-0.57798700
H	-2.10032600	1.90916600	-0.90439700
C	-1.29682800	3.62407600	-1.95049200
C	-1.46150700	3.41720200	0.51412100
H	2.14600200	2.35097800	-0.55567800
C	1.18083800	3.86322100	-1.75963900
C	1.00832800	3.67801500	0.71874700
H	-2.25445000	4.15601700	-1.94036700
H	-1.22517000	3.11495200	-2.91572700
C	-0.14741000	4.62085800	-1.79721000
H	-1.47984800	2.74183500	1.37180500
H	-2.42027500	3.94463400	0.47776400
C	-0.32357500	4.42448200	0.68001200
H	1.33318900	3.32905200	-2.70373200
H	2.01028500	4.56966800	-1.64992900

H	1.03419700	3.00188500	1.57585100
H	1.83530000	4.38925400	0.82301100
H	-0.14946800	5.31171800	-2.64534600
C	-0.32641200	5.39976800	-0.49548800
H	-0.46222300	4.97383600	1.61539200
H	0.48466100	6.12720700	-0.38008600
H	-1.27032900	5.95537700	-0.52090300

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f-3-1 carbene-Au fragment

Au	0.07811900	1.23068900	-1.87366400
C	0.60036600	-2.30307500	-1.04673000
N	-0.35427400	-0.57887100	0.40817800
C	-0.60571600	-0.79454300	1.87542700
C	0.43295700	-3.32615000	-1.97689900
H	1.31087600	-3.84971500	-2.33515400
C	0.21211200	0.57027100	0.08560600
C	-1.80220200	-1.91763300	-1.07902200
C	-0.82584800	-3.65785800	-2.45230900
C	-0.52672100	-1.61388200	-0.57632500
C	-0.42021100	0.63060300	2.37806700
H	-0.02460600	0.63577300	3.39225600
H	-1.39807900	1.12721100	2.40074400
C	-1.92850000	-2.94888900	-2.01052400
H	-2.91149200	-3.16709600	-2.41023600
C	0.41480100	-1.76940700	2.45094600
H	0.31082000	-2.74935700	1.97869200
H	0.22007600	-1.89153100	3.51747200
H	1.43904300	-1.42246300	2.32820000
C	-1.99127000	-1.33370900	2.20023100
H	-2.78579600	-0.65456000	1.89238500
H	-2.05237700	-1.45283100	3.28358900
H	-2.15585800	-2.31537300	1.75003400
C	-3.03234400	-1.19908500	-0.66479800
C	-4.15571900	-1.93249000	-0.29656400

C	-3.09606200	0.19374100	-0.60112400
C	-5.29889400	-1.29359800	0.16707200
H	-4.12766800	-3.01650800	-0.32960100
C	-4.23546900	0.81892000	-0.12274000
H	-2.25235800	0.79024100	-0.93397500
C	-5.34716400	0.08571900	0.27542800
H	-6.23182700	0.58147700	0.65137100
C	1.99901900	-1.97503400	-0.63914800
C	2.65538900	-2.71789200	0.33148000
C	2.70980200	-0.98006100	-1.31557000
C	3.97068600	-2.42274900	0.67870300
H	2.14155900	-3.52714800	0.83658700
C	4.03186700	-0.72230700	-0.99135700
H	2.22007300	-0.41643900	-2.10249500
C	4.66946200	-1.42387600	0.02615700
H	5.69521300	-1.20228700	0.28999700
C	4.59211200	-3.20861800	1.79880700
C	4.82992700	0.28189300	-1.78083200
F	5.87292400	-2.89631500	1.99165900
F	3.94617800	-2.98680600	2.95484000
F	4.52446100	-4.52578800	1.57198600
F	5.63298900	-0.33269900	-2.66081600
F	5.62203400	1.01465300	-0.98801300
F	4.05600100	1.11870600	-2.46977500
C	-6.46719800	-2.14804700	0.57722100
C	-4.23539400	2.31343200	0.05738100
F	-6.13548200	-2.97343300	1.57954200
F	-6.88293600	-2.92137500	-0.43323000
F	-7.50817300	-1.42194200	0.98414900
F	-5.45440700	2.83587600	-0.09812200
F	-3.41366100	2.92618100	-0.79139100
F	-3.83056900	2.63698100	1.29977900
H	-0.94230000	-4.44806800	-3.18211200
C	0.45635600	1.37100600	1.34544400

C	1.98584500	1.31884200	1.63436200
C	0.05402400	2.86263100	1.30070900
H	2.33208200	0.27807300	1.59220500
C	2.27307400	1.91884700	3.01162700
C	2.75612200	2.12885000	0.58582600
H	-1.01274000	2.91906700	1.05035400
C	0.30013300	3.44971200	2.69806600
C	0.86022900	3.69219300	0.30316500
H	3.35417700	1.89080300	3.18545200
H	1.81209300	1.33412100	3.81159900
C	1.79064600	3.37082200	3.04758600
H	2.56287200	1.73535700	-0.41645000
H	3.82856700	2.02602500	0.78491500
C	2.34599700	3.59895600	0.63224300
H	-0.29738300	2.93419800	3.45553200
H	-0.01819200	4.49699300	2.70024500
H	0.67882700	3.36048400	-0.72392300
H	0.52333300	4.73250100	0.36956500
H	1.94941700	3.78180200	4.04850100
C	2.59433100	4.17278800	2.02527100
H	2.92247500	4.15766900	-0.10949600
H	2.29338300	5.22549900	2.05205900
H	3.66081100	4.12542500	2.27114700

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f-4-1 carbene fragment

C	1.14577600	-1.83398500	-1.08155000
N	-0.04815800	-0.05635100	0.13405400
C	-0.05149000	-0.16536700	1.63836900
C	1.10626000	-3.02858200	-1.80233600
H	2.04272600	-3.47905600	-2.10942700
C	0.00420200	1.14053400	-0.40180100
C	-1.28375400	-1.79906400	-1.07632700
C	-0.09828900	-3.61510300	-2.15093100
C	-0.05954400	-1.23435900	-0.68933100

C	-0.22946000	1.30785700	2.02229600
H	0.43094700	1.57559900	2.84997600
H	-1.25771000	1.47876400	2.35619000
C	-1.28388500	-2.99212000	-1.79934200
H	-2.23427500	-3.41360800	-2.10469000
C	1.26807700	-0.74635100	2.13074500
H	1.39645600	-1.77620600	1.78821900
H	1.26712300	-0.75433000	3.22201700
H	2.11993700	-0.15428100	1.78885500
C	-1.20007300	-1.02736100	2.13889400
H	-2.16365700	-0.60244900	1.85399700
H	-1.15687400	-1.07184900	3.22868600
H	-1.13287600	-2.05018100	1.75783600
C	-2.59713100	-1.18300100	-0.76148000
C	-3.58898500	-1.95609200	-0.16976500
C	-2.88341400	0.14674100	-1.08764600
C	-4.83401700	-1.40986100	0.12230900
H	-3.38189900	-2.98825700	0.09259500
C	-4.13116300	0.67431300	-0.80146700
H	-2.12750700	0.75591400	-1.57030800
C	-5.11590900	-0.09202700	-0.18514200
H	-6.08599400	0.33383300	0.03619800
C	2.48224600	-1.25840900	-0.78354400
C	3.44117100	-2.04925600	-0.16111900
C	2.82306200	0.04409700	-1.15889100
C	4.70464500	-1.54282400	0.11947000
H	3.19313200	-3.06374500	0.13322900
C	4.09075500	0.53178300	-0.88558100
H	2.09056600	0.66700600	-1.65957600
C	5.04021300	-0.24868300	-0.23416900
H	6.02556500	0.14573500	-0.02267900
C	5.68298200	-2.43514900	0.83226500
C	4.48121600	1.93277600	-1.27626800
F	6.88095300	-1.86678500	0.96946100

F	5.24563800	-2.75213100	2.05871500
F	5.85543100	-3.59036400	0.17767100
F	4.62501700	2.71854500	-0.19791500
F	3.58289700	2.50841400	-2.07308500
F	5.65747800	1.94659400	-1.91540600
C	-5.85034300	-2.28541200	0.80224900
C	-4.46964900	2.09925400	-1.15121500
F	-5.44722700	-2.63053700	2.03282300
F	-6.03990600	-3.42630000	0.12785700
F	-7.03515200	-1.68659800	0.92331900
F	-5.59853700	2.16620700	-1.86787600
F	-3.50895000	2.69418500	-1.85496000
F	-4.67520300	2.83309500	-0.04706600
H	-0.11293700	-4.53647200	-2.71802300
C	0.04713200	2.12286700	0.74352400
C	1.45118200	2.75193500	0.73446300
C	-0.99710200	3.21929400	0.51617400
C	1.58137600	3.90000400	1.72833100
H	1.64966500	3.12061100	-0.27839200
H	2.19894800	1.97956500	0.94508600
C	-0.87368500	4.33409000	1.54639400
H	-0.85449300	3.62594700	-0.49105700
H	-1.99676700	2.77214700	0.54332200
C	0.51452400	4.95900000	1.48096700
H	2.58297400	4.33004300	1.65503900
H	1.47653800	3.52144200	2.75203200
H	-1.64709600	5.08628100	1.37829100
H	-1.04019100	3.92778200	2.55247500
H	0.60849000	5.77268200	2.20349200
H	0.66281900	5.39339100	0.48516300

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f-4-1 carbene-Au fragment

Au	-0.00740400	-1.77143700	-1.79358600
C	-1.07039300	1.82219200	-1.23765300

N	0.08492400	0.33153900	0.34444000
C	0.17344900	0.69353600	1.80408800
C	-1.00701900	2.76652100	-2.26199400
H	-1.93505400	3.15647800	-2.66238000
C	-0.17364800	-0.93006000	0.09313000
C	1.36166400	1.72024500	-1.23155300
C	0.20849800	3.18318800	-2.77750800
C	0.12446700	1.30325200	-0.71838700
C	0.28637300	-0.70033100	2.43187500
H	-0.26126700	-0.74882500	3.37461800
H	1.33892100	-0.91495500	2.64628900
C	1.38138300	2.66121400	-2.26118700
H	2.33915600	2.96252600	-2.66788100
C	-1.09482500	1.43092100	2.21978400
H	-1.16673800	2.39396200	1.70881900
H	-1.05608100	1.62166600	3.29324100
H	-1.99404900	0.85276900	1.99995400
C	1.37484300	1.56631200	2.12845700
H	2.31617500	1.05281800	1.92968900
H	1.33993600	1.81151000	3.19144500
H	1.34976400	2.50464200	1.56862300
C	2.66678400	1.25159800	-0.70049100
C	3.60706200	2.20599000	-0.32578900
C	2.98786600	-0.09961200	-0.55096400
C	4.82369700	1.82637300	0.22693600
H	3.37399800	3.26032700	-0.43080500
C	4.20560400	-0.46511200	0.00059800
H	2.29422000	-0.86248400	-0.89158800
C	5.13124900	0.48988100	0.40705200
H	6.07710600	0.19229900	0.83954900
C	-2.42147400	1.46094500	-0.72949000
C	-3.21454200	2.46451500	-0.18445700
C	-2.94053900	0.16728100	-0.81623200
C	-4.47735100	2.17669100	0.31969500

H	-2.83182300	3.47816200	-0.12519800
C	-4.20446800	-0.10550400	-0.31715600
H	-2.35787200	-0.61811500	-1.28497700
C	-4.97990000	0.88894200	0.26870000
H	-5.96278700	0.66142000	0.66075600
C	-5.26098300	3.29687400	0.94608800
C	-4.77356400	-1.49867300	-0.37807900
F	-6.48481600	2.91691900	1.31198700
F	-4.64207500	3.76602300	2.03916700
F	-5.39047500	4.33105800	0.10666900
F	-4.89909000	-2.02221900	0.85284200
F	-4.01465000	-2.32861000	-1.08915600
F	-5.99763800	-1.50041500	-0.91769000
C	5.77922600	2.91029600	0.64542000
C	4.53363700	-1.91878000	0.21799900
F	5.24420600	3.68401100	1.60000600
F	6.07806600	3.71787900	-0.37913100
F	6.92377200	2.42082500	1.12125800
F	5.82473400	-2.17250500	-0.01397900
F	3.81253700	-2.72298000	-0.55894800
F	4.29441200	-2.27564500	1.49248900
H	0.24062000	3.90225000	-3.58525100
C	-0.22732400	-1.70126900	1.38028400
C	-1.68753500	-2.14066900	1.59767600
C	0.65123400	-2.95402500	1.29355900
C	-1.84231900	-3.03628000	2.82132400
H	-2.00418800	-2.68496400	0.69917600
H	-2.33597100	-1.26402500	1.68443500
C	0.52514000	-3.79893200	2.55390800
H	0.33169100	-3.53844900	0.42317200
H	1.68888100	-2.65702500	1.11479300
C	-0.91974000	-4.24567000	2.74022300
H	-2.88600100	-3.34669100	2.90649800
H	-1.60995000	-2.46807000	3.72967900

H	1.19257300	-4.66004600	2.48948000
H	0.84475500	-3.21608000	3.42720900
H	-1.02321700	-4.86428600	3.63405700
H	-1.21251300	-4.86419300	1.88401100

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f-5-1 carbene fragment

C	1.15426700	-1.78535500	-1.09951500
N	-0.04275300	-0.00372700	0.10541700
C	-0.03953300	-0.10352000	1.61260600
C	1.11838300	-2.98044900	-1.81972800
H	2.05630800	-3.42983600	-2.12390800
C	-0.00348400	1.19039300	-0.43874700
C	-1.27515100	-1.75633000	-1.09605800
C	-0.08433000	-3.56921300	-2.17046400
C	-0.05262500	-1.18647300	-0.71143500
C	-0.24185700	1.36913600	1.98167500
H	0.38846400	1.66893900	2.82221200
H	-1.28500700	1.52466000	2.27612000
C	-1.27160200	-2.94972500	-1.81852800
H	-2.22085200	-3.37486300	-2.12231800
C	1.28403700	-0.67008500	2.11109300
H	1.41378900	-1.70539300	1.78597200
H	1.28381500	-0.66000700	3.20227400
H	2.13570700	-0.08446500	1.75954200
C	-1.17705700	-0.97722100	2.11906900
H	-2.14643500	-0.56637200	1.83371500
H	-1.13147000	-1.01532900	3.20899300
H	-1.09730500	-2.00116200	1.74346500
C	-2.59131100	-1.14991400	-0.77430600
C	-3.57175800	-1.93181800	-0.17498900
C	-2.89192400	0.17703600	-1.09844700
C	-4.81929600	-1.39694300	0.12669000
H	-3.35328100	-2.96204100	0.08572100
C	-4.14222500	0.69335100	-0.80233400

H	-2.14568000	0.79213300	-1.58840700
C	-5.11524900	-0.08162200	-0.17831800
H	-6.08744900	0.33541700	0.05025600
C	2.48991900	-1.21273500	-0.79214800
C	3.43880700	-2.00785700	-0.15961100
C	2.84041600	0.08806500	-1.16437400
C	4.70094100	-1.50717200	0.13558300
H	3.18273200	-3.02111200	0.13199700
C	4.10820000	0.56928300	-0.87867400
H	2.11681300	0.71259500	-1.67596500
C	5.04629300	-0.21494300	-0.21534500
H	6.03134900	0.17473500	0.00584600
C	5.66686600	-2.40326400	0.86069700
C	4.51293300	1.96631700	-1.26915900
F	6.86629100	-1.84102000	1.00919900
F	5.21459200	-2.71472400	2.08303300
F	5.83966900	-3.56077900	0.21046100
F	4.62128000	2.76212300	-0.19384900
F	3.64168500	2.53502900	-2.10078200
F	5.70921500	1.97353300	-1.86902800
C	-5.82255300	-2.28192000	0.81392800
C	-4.49434200	2.11632700	-1.14622300
F	-5.40620800	-2.62498000	2.04060000
F	-6.00791800	-3.42348700	0.13959700
F	-7.01128800	-1.69326900	0.94549800
F	-5.64500700	2.17952400	-1.82706200
F	-3.55674500	2.71054100	-1.88124100
F	-4.66549000	2.85367600	-0.03821700
H	-0.09632600	-4.49060200	-2.73756500
C	0.05638500	2.17375600	0.70407400
C	1.47079400	2.77082700	0.70309300
C	-0.94321400	3.31190700	0.49820500
C	1.56970500	3.98515500	1.57703700
H	1.75135700	3.02035600	-0.32696300

H	2.19255900	2.01659100	1.03723800
C	-0.89901500	4.28508000	1.66973800
H	-0.69148900	3.82645500	-0.43351200
H	-1.95075100	2.90087400	0.38130000
C	0.51051100	4.65230800	2.02658900
H	2.56835200	4.31496700	1.84492000
H	-1.46619100	5.18734600	1.42753400
H	-1.39870200	3.85175900	2.54539300
H	0.65670300	5.51065200	2.67428300

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f-5-1 carbene-Au fragment

Au	-0.01107000	-1.82332000	-1.80609700
C	-1.09014300	1.76823400	-1.27541500
N	0.07111300	0.29059700	0.31143400
C	0.17813300	0.64827600	1.77187600
C	-1.03305200	2.69438800	-2.31620900
H	-1.96304600	3.08071300	-2.71557800
C	-0.21553800	-0.96846800	0.06304700
C	1.34183800	1.66479200	-1.28068500
C	0.18013700	3.09842600	-2.84775900
C	0.10690500	1.25552500	-0.75585700
C	0.32454300	-0.74890900	2.38221500
H	-0.16699900	-0.82486100	3.35419500
H	1.39112400	-0.95990600	2.52212100
C	1.35588800	2.58636700	-2.32789200
H	2.31119700	2.88116400	-2.74502900
C	-1.09337400	1.36923000	2.20873300
H	-1.16826000	2.34403100	1.72071100
H	-1.05339600	1.53450000	3.28628400
H	-1.99257200	0.79736400	1.97534300
C	1.36777300	1.54089400	2.08763000
H	2.31796300	1.04265800	1.89345700
H	1.32885200	1.79437200	3.14851400
H	1.32657400	2.47459600	1.52101000

C	2.64713800	1.21526700	-0.73423100
C	3.58491800	2.18553300	-0.39299100
C	2.96750000	-0.12709000	-0.52135100
C	4.79591700	1.83168300	0.18700900
H	3.35242100	3.23420900	-0.54479600
C	4.17787300	-0.46683900	0.06375400
H	2.27804000	-0.90550900	-0.83425000
C	5.10012600	0.50470400	0.43477300
H	6.03972000	0.22807200	0.89328000
C	-2.43494400	1.42121900	-0.74136200
C	-3.20420400	2.43361400	-0.17969300
C	-2.96875100	0.13224600	-0.81395700
C	-4.45645300	2.15913300	0.35764600
H	-2.80985400	3.44338500	-0.13236500
C	-4.22254100	-0.12664100	-0.28286000
H	-2.40595900	-0.65834400	-1.29728000
C	-4.97225900	0.87646100	0.32212500
H	-5.94698800	0.65907300	0.73955300
C	-5.21208400	3.28755100	1.00333700
C	-4.81313200	-1.51102900	-0.33298300
F	-6.43140700	2.92140200	1.39721500
F	-4.56232900	3.74760700	2.08227500
F	-5.34874500	4.32429800	0.16834600
F	-4.92847000	-2.03027500	0.90035900
F	-4.07702600	-2.35353000	-1.05407200
F	-6.04444500	-1.49540700	-0.85524200
C	5.74964600	2.93364000	0.56058400
C	4.48075100	-1.91011900	0.36736100
F	5.20206500	3.76305500	1.45933600
F	6.07122900	3.67968500	-0.50301900
F	6.88290500	2.46691800	1.08404900
F	5.79005000	-2.16534000	0.31550100
F	3.86767400	-2.74209400	-0.47193100
F	4.07337800	-2.23041200	1.60989200

H	0.20819900	3.80215900	-3.66904900
C	-0.24603800	-1.73746700	1.35132300
C	-1.69540000	-2.16019500	1.63435100
C	0.59175200	-3.01622100	1.25545900
C	-1.76783900	-3.13857400	2.76993700
H	-2.11291000	-2.60023900	0.71982500
H	-2.31505900	-1.28683700	1.86054500
C	0.64861700	-3.70816100	2.61038800
H	0.12793100	-3.67253000	0.51281600
H	1.59555500	-2.78071500	0.89336600
C	-0.71522700	-3.81256500	3.22495100
H	-2.73946900	-3.27911200	3.23152100
H	1.07965400	-4.70569400	2.49668900
H	1.32553100	-3.17296000	3.28836100
H	-0.83629100	-4.48409900	4.06844000

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f-6-1 carbene fragment

C	-0.83808200	-2.30929700	0.99981500
N	0.13383800	-0.44063200	-0.23835600
C	0.22284900	-0.54764400	-1.74459700
C	-0.70005000	-3.54184900	1.63280100
H	-1.59358100	-4.06448800	1.95250200
C	-0.27728800	0.69923100	0.27649100
C	1.57589300	-2.11567300	0.88797400
C	0.55491000	-4.07938100	1.87415700
C	0.30522100	-1.61781600	0.56991500
C	-0.04613400	0.90868900	-2.13285600
H	-0.66560500	0.96774300	-3.03020800
H	0.90602900	1.39349500	-2.35492800
C	1.68033800	-3.35288900	1.52746600
H	2.66710000	-3.72312000	1.77950200
C	-0.80639100	-1.52554800	-2.29812600
H	-0.68064800	-2.51629700	-1.85223900
H	-0.65377100	-1.62449900	-3.37427600

H	-1.82934100	-1.18923800	-2.13389900
C	1.60581000	-0.98984400	-2.19837100
H	2.38090600	-0.33053500	-1.80216900
H	1.64120900	-0.94203900	-3.28858700
H	1.82094900	-2.01955100	-1.90186700
C	2.82661500	-1.35789000	0.65048300
C	3.92018400	-1.98136800	0.06202100
C	2.95025900	-0.03259500	1.07646500
C	5.11117100	-1.29067400	-0.12594900
H	3.83715800	-3.00878300	-0.27639200
C	4.15189700	0.63484500	0.90659100
H	2.10985300	0.45960300	1.55342900
C	5.23933900	0.02062000	0.29348500
H	6.17152100	0.55501100	0.16476100
C	-2.20836500	-1.74130100	0.86815500
C	-3.12358700	-2.25421700	-0.03732900
C	-2.60697400	-0.70816300	1.72322800
C	-4.39804100	-1.70012000	-0.13996500
H	-2.83910900	-3.06869200	-0.69418900
C	-3.89199700	-0.20204000	1.64612900
H	-1.90015500	-0.30119200	2.43315100
C	-4.79324900	-0.67406000	0.69665400
H	-5.78451400	-0.24576600	0.61784500
C	-5.30238200	-2.21555600	-1.22287900
C	-4.34055400	0.91129200	2.55329200
F	-6.50600300	-1.64428800	-1.19787300
F	-4.77293200	-1.98045000	-2.43502600
F	-5.47813000	-3.53926100	-1.13486400
F	-5.48692700	0.60026600	3.17187300
F	-4.57486300	2.03901800	1.86427800
F	-3.44009200	1.19742500	3.49095400
C	6.24569800	-2.00528100	-0.80764500
C	4.32849200	2.04726400	1.39478400
F	5.94320000	-2.29120700	-2.08112500

F	6.51666700	-3.17110100	-0.20757500
F	7.36711900	-1.28487100	-0.81498900
F	5.45058700	2.17270400	2.11370600
F	3.31433500	2.45007400	2.15709900
F	4.43431500	2.90853900	0.37137300
H	0.65392900	-5.03722100	2.36760800
C	-0.68454400	1.56373700	-0.90007800
C	-2.22331500	1.43958400	-0.90072100
C	-0.34253800	3.04413700	-0.68821200
C	-2.91106200	2.29376600	-1.95731000
H	-2.58079100	1.76954900	0.08259500
H	-2.52562000	0.39160700	-1.00429600
C	-1.00682800	3.91530300	-1.75213300
H	-0.81661800	3.29101300	0.27302100
C	-2.52058400	3.74992000	-1.74345800
H	-2.56306900	1.98887700	-2.95319400
H	-0.73993400	4.96360500	-1.58648900
H	-0.61792700	3.64709700	-2.74311600
H	-2.98577400	4.38231000	-2.50511000
H	-2.91708900	4.07205700	-0.77102600
C	-4.41747200	2.09022200	-1.88214700
H	-4.68571400	1.04581400	-2.06788700
H	-4.78092900	2.35811100	-0.88504300
H	-4.94155800	2.71081500	-2.61174800
C	1.16635400	3.33572300	-0.51632000
H	1.64964200	2.39892200	-0.19472400
C	1.34495800	4.37390600	0.58778900
H	0.98259500	3.99667700	1.54552400
H	2.39085900	4.66397400	0.70159900
H	0.77253400	5.27339200	0.33705500
C	1.88366500	3.84058200	-1.76921200
H	1.52771100	4.83940300	-2.03453200
H	2.95425300	3.91771500	-1.57286700
H	1.74783700	3.20373100	-2.64410600

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f-6-1 carbene-Au fragment

Au	-0.31891700	1.27759200	-1.69298100
C	1.54771400	-2.16071500	-0.92917100
N	0.24478300	-0.67486800	0.55480500
C	0.48703900	-0.92159100	2.02638300
C	1.58514700	-3.24954900	-1.80154500
H	2.54634700	-3.56573400	-2.18862100
C	-0.08351800	0.54919600	0.23498200
C	-0.87485500	-2.32913800	-0.88916600
C	0.42636500	-3.88391700	-2.21016300
C	0.30826500	-1.73362900	-0.42716600
C	0.19065200	0.46228100	2.62630800
H	1.02332200	0.78505200	3.25358800
H	-0.68930800	0.40876400	3.26546400
C	-0.79680800	-3.40236800	-1.77419200
H	-1.71932000	-3.84728000	-2.12649600
C	1.91448700	-1.36706900	2.30327200
H	2.12276400	-2.34268000	1.86024800
H	2.03590400	-1.45842800	3.38391400
H	2.64348000	-0.64113700	1.93603600
C	-0.48305700	-1.96490300	2.55161100
H	-1.51032800	-1.60350900	2.47937900
H	-0.26305400	-2.14942500	3.60445000
H	-0.38560900	-2.91165400	2.01361800
C	-2.24456000	-1.82834300	-0.57126600
C	-2.98287100	-2.31986100	0.49559000
C	-2.85048600	-0.92402500	-1.44701800
C	-4.26798800	-1.84715200	0.73978600
H	-2.56178000	-3.07370400	1.14794600
C	-4.15023100	-0.49691100	-1.22208200
H	-2.29779500	-0.55682500	-2.30586600
C	-4.86362500	-0.93476900	-0.11330500
H	-5.86561700	-0.57346900	0.07575900

C	2.83940700	-1.48694900	-0.64301500
C	3.92241100	-2.23983300	-0.20514300
C	3.01168300	-0.11726300	-0.85813800
C	5.14449900	-1.63437200	0.06072300
H	3.80504900	-3.30531400	-0.03635800
C	4.23848400	0.47153500	-0.60071000
H	2.18988900	0.47904500	-1.24535700
C	5.31302800	-0.27487400	-0.12740000
H	6.26382700	0.19989500	0.07781100
C	6.26540700	-2.49786100	0.57101900
C	4.46399200	1.94199400	-0.83657500
F	7.38586800	-1.80603300	0.77473800
F	5.93556100	-3.08218900	1.73126500
F	6.54863000	-3.48507300	-0.28742700
F	4.88076000	2.54443300	0.28894800
F	3.36764100	2.57095000	-1.24803100
F	5.41882000	2.14393300	-1.75180500
C	-4.99291300	-2.36831800	1.94908700
C	-4.81214300	0.40762000	-2.22970900
F	-4.21158400	-2.31466800	3.03932800
F	-5.35018200	-3.64961500	1.79969000
F	-6.09841200	-1.67179200	2.21479600
F	-5.33008500	-0.30583200	-3.24017600
F	-3.95628700	1.27671000	-2.76279300
F	-5.81900700	1.10157100	-1.68839200
H	0.47273900	-4.72063300	-2.89443400
C	-0.02856900	1.42958000	1.45011400
C	1.18332100	2.36679500	1.27384600
C	-1.30220200	2.29171500	1.51565000
C	1.28836200	3.40631900	2.38585000
H	1.08966600	2.88256900	0.30931400
H	2.10386000	1.76783400	1.22906900
C	-1.20779800	3.28994600	2.66174600
H	-1.27018300	2.87261400	0.58066600

C	-0.00608200	4.20470800	2.47353300
H	1.42539100	2.88751300	3.34459900
H	-2.13011500	3.87590700	2.71491100
H	-1.12185000	2.75475700	3.61700600
H	0.06345600	4.93253200	3.28669300
H	-0.12768100	4.77318200	1.54225500
C	2.48570400	4.31379300	2.14705200
H	3.42041200	3.75154100	2.14283400
H	2.39188900	4.81129900	1.17750600
H	2.55229000	5.08493800	2.91719500
C	-2.63316100	1.50406600	1.47680900
H	-2.44568500	0.54648800	0.96795600
C	-3.62506900	2.29954400	0.63206000
H	-3.72725700	3.31265700	1.03446100
H	-3.27836500	2.38000500	-0.40187900
H	-4.61687100	1.84273600	0.63618100
C	-3.27734600	1.19896600	2.82901400
H	-3.54223300	2.12134100	3.35194400
H	-4.20412900	0.64080700	2.66943400
H	-2.65374900	0.60321200	3.49734000

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g-1-1 carbene fragment

C	1.24935900	-0.97343400	0.27660900
N	-0.01947600	1.15743200	0.18104700
C	-0.09671600	1.97118200	1.45992900
C	1.24678700	-2.34778700	0.51250100
H	2.18282300	-2.88552400	0.56108200
C	-0.05106200	1.78511000	-0.96962000
C	-1.16965700	-1.00537900	0.27647300
C	0.06492300	-3.04426000	0.66489200
C	0.03162600	-0.27160900	0.23402100
C	-0.55805300	3.30456700	0.87165000
H	-0.09352100	4.14850800	1.38702100
H	-1.64261700	3.39292600	0.98555800

C	-1.13504000	-2.37858500	0.50500400
H	-2.05670500	-2.94128100	0.54784200
C	1.26789600	2.06618100	2.13591200
H	1.64772600	1.07377600	2.38877900
H	1.15283800	2.62253100	3.06793900
H	2.00153800	2.57918500	1.51999100
C	-1.06916900	1.39181900	2.47806500
H	-2.09052800	1.36109500	2.10820400
H	-1.05744300	2.03117600	3.36259400
H	-0.76870100	0.38961600	2.79456700
C	2.60565400	-0.37565800	-0.06917600
C	-2.54744600	-0.43634900	-0.04555700
C	-0.20603900	3.25245900	-0.63026900
C	1.11889400	3.94299800	-0.96488200
H	1.35044800	3.80954600	-2.02257000
H	1.03927200	5.01302800	-0.75552800
H	1.95193900	3.53884100	-0.38823700
C	-1.31374900	3.85454100	-1.48912000
H	-1.46031600	4.90734700	-1.23088000
H	-1.05271500	3.78370600	-2.54580600
H	-2.25722400	3.32654200	-1.33435500
H	0.07830400	-4.10693900	0.86286500
C	3.72754500	-0.77085600	0.94916700
C	3.02189500	-0.79602600	-1.51218600
C	-3.65085500	-0.90608500	0.96589700
C	-2.96256300	-0.82886600	-1.49673900
F	2.19203400	-0.24786300	-2.37868200
F	3.00146900	-2.11434600	-1.68568800
F	4.25428700	-0.36368800	-1.76527600
F	4.26464100	-1.95741900	0.66505600
F	4.69489500	0.12939200	0.93403300
F	3.24140600	-0.83211600	2.18721900
F	-4.17262000	-2.08345700	0.62099600
F	-3.15442000	-1.02861900	2.19419900

F	-4.63243000	-0.02139600	1.00874200
F	-2.88556600	-2.13864800	-1.71031000
F	-4.21625400	-0.44322000	-1.72135600
F	-2.17030800	-0.21783000	-2.35610900
F	-2.62424900	0.92232200	-0.04816200
F	2.62554100	0.98023400	-0.11042000

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g-1-1 carbene-Au fragment

Au	0.31533800	2.32863600	-0.89352100
C	1.20307000	-1.40283000	-0.44030700
N	-0.07489600	0.11218900	1.07396100
C	-0.10278100	-0.19507800	2.55412900
C	1.19843600	-2.46522600	-1.34394000
H	2.13394300	-2.89995000	-1.66270500
C	-0.36895300	1.36629900	0.75479600
C	-1.21663100	-1.39210400	-0.49574200
C	0.01858300	-2.97563500	-1.84165700
C	-0.01491200	-0.88826100	0.04817400
C	-0.88130600	1.02677200	3.05892400
H	-0.54523700	1.32413500	4.05407200
H	-1.94504000	0.78432300	3.11729300
C	-1.17734100	-2.41920800	-1.43634200
H	-2.09827300	-2.80694900	-1.84639600
C	1.28161000	-0.24650700	3.19796000
H	1.85842400	-1.10299700	2.85735600
H	1.13507200	-0.35941600	4.27398000
H	1.85689300	0.65840600	3.02568300
C	-0.79510800	-1.51937200	2.83700700
H	-1.83666300	-1.51813400	2.52667400
H	-0.76736900	-1.70050600	3.91257600
H	-0.27458800	-2.34778100	2.34861800
C	2.58689800	-0.91397600	-0.04484400
C	-2.62885500	-0.92576600	-0.15014000
C	-0.66723400	2.13960800	2.01573700

C	0.50739300	3.06902400	2.34908100
H	0.56325400	3.86982200	1.61004900
H	0.35294900	3.50909200	3.33776900
H	1.46644400	2.55081100	2.33648500
C	-1.91827500	2.99254700	1.81788800
H	-2.14564500	3.54025500	2.73637200
H	-1.75070000	3.71177700	1.01316600
H	-2.77974600	2.37669400	1.55536600
H	0.02987700	-3.79559700	-2.54604500
C	3.37068300	-2.03164100	0.72889900
C	3.45276200	-0.42178500	-1.25319800
C	-3.56542400	-2.13496300	0.21755500
C	-3.28375000	-0.10616900	-1.30513700
F	2.90743300	0.65753700	-1.77645300
F	3.60084000	-1.31816600	-2.22375500
F	4.66398300	-0.11180400	-0.79614200
F	4.03642100	-2.82281700	-0.10990200
F	4.23249700	-1.49643900	1.57566700
F	2.53691900	-2.80704400	1.42381200
F	-4.13190900	-2.66899900	-0.86402700
F	-2.88591300	-3.09619900	0.83709200
F	-4.52879800	-1.73216100	1.02850700
F	-3.19356100	-0.72079500	-2.47856500
F	-4.57293400	0.08689000	-1.03301300
F	-2.69805500	1.07158100	-1.40004900
F	-2.70755100	-0.09343600	0.92376900
F	2.55905100	0.17674700	0.76051100

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h-1-1 carbene fragment

C	-0.53653500	-0.74222400	0.84863300
N	1.55936200	-0.05072300	-0.18618900
C	2.29184800	1.13805700	0.36715600
C	-1.92022600	-0.76753000	0.87718500
H	-2.41776700	-1.30691400	1.67526500

C	2.24956300	-1.10937600	-0.53562800
C	-0.60954200	0.57547300	-1.15230300
C	-2.68326000	-0.12342400	-0.10193800
C	0.12478700	-0.06386200	-0.16813200
C	3.73474600	0.75196800	0.03359600
H	4.41289300	0.99544600	0.85522400
H	4.06662100	1.31038800	-0.84657700
C	-2.00030800	0.54294900	-1.11612100
H	-2.54786400	1.04267300	-1.90411200
C	2.02246500	1.23972900	1.86461500
H	0.95913600	1.40293800	2.05462500
H	2.57645900	2.08264800	2.28212800
H	2.33170600	0.33050300	2.38248900
C	1.86742100	2.42974000	-0.31527200
H	1.98096200	2.35152100	-1.39837500
H	2.50329900	3.24421200	0.03780800
H	0.83104700	2.68359600	-0.08415700
C	-4.20474000	-0.18415900	-0.02791300
C	3.70363400	-0.75621600	-0.28612400
C	4.15934000	-1.61117500	0.89957900
H	4.04798400	-2.67033800	0.66344400
H	5.21032400	-1.40693900	1.12224700
H	3.57265500	-1.40383800	1.79727000
C	4.54817100	-1.10426300	-1.50613900
H	5.59789300	-0.85453500	-1.32600300
H	4.47280700	-2.17043700	-1.72475000
H	4.21038000	-0.55226500	-2.38602900
C	-4.67624500	0.43359600	1.29262600
H	-5.76690600	0.39058000	1.35421100
H	-4.26839600	-0.10111200	2.15236500
H	-4.36729100	1.47878800	1.36368900
C	-4.66089000	-1.64581900	-0.08699000
H	-4.25574700	-2.22546400	0.74434900
H	-5.75173800	-1.69633800	-0.03451700

H	-4.33697600	-2.11541400	-1.01807400
C	-4.87208400	0.57094700	-1.17342100
H	-5.95671400	0.49810100	-1.06728500
H	-4.60430300	1.63017100	-1.16669500
H	-4.60107900	0.14981100	-2.14428000
H	0.05044300	-1.25994700	1.59834800
H	-0.09423900	1.08076500	-1.95973700

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h-1-1 carbene-Au fragment

Au	1.41035600	-1.69252000	-0.00669100
C	-1.21618000	0.32779600	1.01628200
N	0.73254900	1.21662300	-0.14775900
C	1.19424500	2.59573300	0.19748500
C	-2.56070700	0.00117500	1.03700700
H	-2.97609200	-0.44366500	1.93367200
C	1.67456000	0.31653200	-0.31890100
C	-1.45164100	1.10118500	-1.24617900
C	-3.38249700	0.21457200	-0.07445400
C	-0.66253100	0.88532100	-0.13070000
C	2.68470700	2.49028800	-0.14503700
H	3.29856300	3.03806000	0.57277100
H	2.85753600	2.92445400	-1.13379500
C	-2.80199500	0.76744200	-1.21328000
H	-3.39700800	0.93752700	-2.10039900
C	0.92667000	2.86027000	1.67496300
H	-0.14568200	2.83411400	1.88017300
H	1.30161000	3.84944500	1.94369400
H	1.41858200	2.11822100	2.30516200
C	0.48155300	3.63806700	-0.64913900
H	0.60255000	3.42347100	-1.71263300
H	0.91602200	4.61832500	-0.44454600
H	-0.58379300	3.68024300	-0.41527500
C	-4.85407200	-0.17582400	-0.00218100
C	3.02102400	0.98711600	-0.17420100

C	3.67846200	0.51121900	1.12546600
H	3.87208300	-0.56150300	1.07868700
H	4.62500400	1.04057900	1.26334000
H	3.04577600	0.69553800	1.99542100
C	3.91772100	0.60950000	-1.34908000
H	4.88824500	1.10345700	-1.25464100
H	4.07167300	-0.47139700	-1.36477200
H	3.46806000	0.90619900	-2.29876800
C	-5.53084800	0.59333500	1.13718500
H	-6.58598800	0.31405000	1.19637800
H	-5.06905200	0.37061900	2.10071500
H	-5.46802100	1.67082500	0.96955700
C	-4.96659700	-1.67936400	0.27190100
H	-4.49545700	-1.95083500	1.21812200
H	-6.01975700	-1.96784700	0.32313900
H	-4.48769200	-2.25541800	-0.52233000
C	-5.60056000	0.13211200	-1.29659200
H	-6.64655400	-0.16146100	-1.18518900
H	-5.57457100	1.19870800	-1.53239900
H	-5.18560100	-0.42190900	-2.14164700
H	-0.57705700	0.13148800	1.86933300
H	-1.00724300	1.51257300	-2.14413800

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i-1-1 carbene fragment

C	1.12453300	-0.74575700	0.78039700
N	3.22460100	-0.00877700	-0.19811700
C	3.99524500	1.15773400	0.35440300
C	-0.25858500	-0.74360700	0.82975600
H	-0.74433000	-1.36157200	1.56818400
C	3.87801500	-1.09813100	-0.52776200
C	1.06279700	0.74141600	-1.09267700
C	-1.01045100	0.02484100	-0.06575300
C	1.79363200	0.00958800	-0.17157900
C	5.42377500	0.71737000	0.02577800

H	6.10758700	0.94271400	0.84761500
H	5.77655700	1.25829400	-0.85701200
C	-0.32476400	0.74256100	-1.04555300
H	-0.84566400	1.30332200	-1.80405000
C	3.72010000	1.26458300	1.85039000
H	2.66155900	1.46298800	2.03513100
H	4.29810300	2.08772200	2.27412900
H	3.99557900	0.34445900	2.36780100
C	3.62597000	2.46648800	-0.32727500
H	3.73162800	2.38481400	-1.41088800
H	4.30172100	3.24928900	0.02273200
H	2.60557400	2.77278700	-0.08870000
C	-2.54313400	-0.04542600	-0.01155500
C	5.34195200	-0.79126600	-0.28397500
C	5.76988300	-1.65389300	0.90710900
H	5.62668800	-2.71030400	0.67665100
H	6.82643900	-1.48026200	1.12830900
H	5.19075700	-1.42377800	1.80414300
C	6.17253900	-1.17596500	-1.50280600
H	7.22986800	-0.96072100	-1.32412100
H	6.06139600	-2.24031200	-1.71417900
H	5.85362200	-0.61845500	-2.38612200
C	-3.11240600	0.39358500	1.37389300
C	-2.97438200	-1.52136100	-0.28774000
C	-3.22519000	0.85284200	-1.08391500
H	1.70248400	-1.35236200	1.46659400
H	1.57443800	1.29143700	-1.87125100
F	-2.22723600	-2.05382900	-1.24558600
F	-4.24374500	-1.62493400	-0.66219800
F	-2.81911800	-2.26080400	0.81209500
F	-4.36719400	-0.01897100	1.52991500
F	-2.41462200	-0.08717700	2.39621300
F	-3.09540700	1.71958400	1.47604300
F	-4.53694800	0.93835100	-0.89955400

F	-2.75735000	2.09857100	-1.07075800
F	-3.01430900	0.34895800	-2.30005500

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i-1-1 carbene-Au fragment

Au	-2.70821500	-1.68809400	0.14362800
C	-0.14422500	0.58471200	-1.08956100
N	-2.15974400	1.20734600	0.11043600
C	-2.69806500	2.59010000	0.27351900
C	1.21205200	0.31510700	-1.12226100
H	1.65132600	0.02043300	-2.06188900
C	-3.03015400	0.27962000	-0.25197100
C	-0.01013100	0.98497200	1.26890200
C	1.99326900	0.40615300	0.03566000
C	-0.75744500	0.94328900	0.10327900
C	-4.20695300	2.31747600	0.23349300
H	-4.73374200	3.09050000	-0.33015800
H	-4.59983300	2.32084500	1.25376000
C	1.35151600	0.71501100	1.23427400
H	1.88231900	0.73075700	2.17177800
C	-2.20392300	3.44910800	-0.88564000
H	-1.11384700	3.51961800	-0.87175900
H	-2.61207300	4.45707800	-0.79575100
H	-2.51107400	3.03370900	-1.84628700
C	-2.27490100	3.22016400	1.59223600
H	-2.52361600	2.56899100	2.43224800
H	-2.81203900	4.16220600	1.71844900
H	-1.20577500	3.43877800	1.60885400
C	3.48420900	0.04755100	-0.03600200
C	-4.39284000	0.91559900	-0.37834400
C	-4.72064700	0.96463200	-1.87531200
H	-4.76441500	-0.04840500	-2.27878600
H	-5.69114800	1.44529200	-2.02243100
H	-3.97086700	1.52245500	-2.43949700
C	-5.47497300	0.11882500	0.34087100

H	-6.43096500	0.64329200	0.26008800
H	-5.57744300	-0.87307000	-0.10233500
H	-5.23136300	-0.00941200	1.39709500
C	4.26500500	0.94560600	-1.04612300
C	3.60622900	-1.44342900	-0.48725000
C	4.20258000	0.18512600	1.33794000
H	-0.74774900	0.50105600	-1.98525700
H	-0.49290600	1.19129400	2.21428200
F	2.67910800	-2.18495700	0.10189900
F	4.78994100	-1.97045700	-0.19961200
F	3.43316300	-1.54028800	-1.80696400
F	5.43363800	0.40058100	-1.37012900
F	3.60193100	1.14735800	-2.17899700
F	4.49765000	2.14054100	-0.51014700
F	5.51966100	0.06863700	1.22361600
F	3.97292600	1.36453100	1.91080400
F	3.77739900	-0.76429200	2.17082600

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j-1-1 carbene fragment

C	1.41195600	1.22357600	-0.15330800
N	-0.66962700	-0.07633300	-0.09948700
C	-1.36455100	-0.21093500	1.22912400
C	2.80303700	1.24865800	-0.18405500
H	3.30445000	2.21223000	-0.18686900
C	-1.40202200	0.05977900	-1.17714400
C	1.50076400	-1.20358500	-0.30205100
C	3.56296100	0.08690100	-0.24530400
C	0.76815500	-0.02012300	-0.16372300
C	-2.81256200	-0.39648000	0.76792400
H	-3.50648200	0.17289800	1.39126600
H	-3.08822000	-1.45227900	0.84509400
C	2.89032300	-1.12516300	-0.32945600
H	3.45985900	-2.04282300	-0.44632500
C	-1.15875500	1.04921800	2.06115400

H	-0.09789600	1.19858800	2.27646700
H	-1.68643100	0.94269800	3.01080200
H	-1.54279200	1.93251700	1.55045300
C	-0.84947700	-1.40734500	2.01480800
H	-1.02978700	-2.33734000	1.47625800
H	-1.37836600	-1.45871800	2.96866100
H	0.21940400	-1.31506500	2.22292200
C	0.66395000	2.52830900	-0.18263900
H	0.53746500	2.94761400	0.81739500
H	1.22350700	3.25479800	-0.77219300
H	-0.32201300	2.41374100	-0.63305600
C	0.85083500	-2.54674200	-0.49029400
H	1.39272300	-3.11053600	-1.25027200
H	0.87331200	-3.13467100	0.42968700
H	-0.18550100	-2.45338100	-0.81275800
C	5.06417700	0.14238000	-0.24115800
H	5.45097600	0.11068500	0.78014800
H	5.49158700	-0.70332400	-0.78053900
H	5.42609800	1.06278700	-0.70031100
C	-2.84438500	0.04313700	-0.70924600
C	-3.37074200	1.47099600	-0.87765600
H	-3.28378500	1.78445300	-1.91914500
H	-4.42223500	1.51767300	-0.58118900
H	-2.81137200	2.18122900	-0.26360700
C	-3.66682200	-0.90330900	-1.57498200
H	-4.70697700	-0.92385500	-1.23690600
H	-3.64102000	-0.58075700	-2.61687700
H	-3.27016900	-1.92046800	-1.52465200

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j-1-1 carbene-Au fragment

Au	1.07339100	-1.65461000	-0.07606900
C	-1.84951100	0.07367100	1.17739500
N	0.00399900	1.13326000	-0.02772600
C	0.26551700	2.58396400	0.24022100

C	-3.15120000	-0.41790800	1.16422100
H	-3.55731700	-0.83122000	2.08260300
C	1.05932500	0.38937200	-0.25588600
C	-2.05146800	0.52356100	-1.21106900
C	-3.92492900	-0.43312300	0.01061300
C	-1.32886000	0.58891000	-0.01532200
C	1.75574700	2.68026100	-0.11378300
H	2.29260100	3.31902400	0.59059000
H	1.86330900	3.11753100	-1.11034000
C	-3.34711000	0.01927500	-1.16934500
H	-3.90959900	-0.04457800	-2.09613500
C	-0.03266400	2.92515600	1.69467600
H	-1.08585800	2.74458500	1.92074500
H	0.17374600	3.98410500	1.85964700
H	0.58024500	2.34316400	2.38226900
C	-0.59335400	3.46117800	-0.65810400
H	-0.37362400	3.27853000	-1.70953100
H	-0.37537900	4.50825100	-0.44021200
H	-1.65703800	3.28787800	-0.47920600
C	-1.04827000	-0.04046700	2.44541700
H	-1.31827700	0.73604100	3.16478300
H	-1.24659500	-1.00657500	2.90952800
H	0.02382000	0.01540900	2.25948400
C	-1.46923300	0.91597900	-2.54089600
H	-1.78022000	0.19848500	-3.30033200
H	-1.82327400	1.89981800	-2.85652000
H	-0.37974300	0.93278200	-2.52291900
C	-5.33697100	-0.94416600	0.03397500
H	-6.03728700	-0.13601500	0.25758800
H	-5.61916700	-1.36673500	-0.93049600
H	-5.46535700	-1.71117700	0.79792300
C	2.29878200	1.23956000	-0.12257100
C	2.98696800	0.87053100	1.19612600
H	3.30380700	-0.17352900	1.17724200

H	3.86273000	1.50904300	1.33804100
H	2.31964800	1.00188300	2.05105300
C	3.25233000	0.97403300	-1.28136800
H	4.14198800	1.60239900	-1.19051000
H	3.55742100	-0.07445400	-1.27810300
H	2.77296000	1.18802100	-2.23948800

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j-2-1 carbene fragment

C	1.93009000	1.16812800	-0.12037300
N	-0.24663300	0.03847700	0.04623100
C	-0.85294300	-0.01846600	1.42215600
C	3.31431400	1.08182300	-0.24574000
H	3.89201600	2.00172400	-0.25811200
C	-1.04614200	0.06193100	-0.99053600
C	1.80669900	-1.25222300	-0.33140700
C	3.96865100	-0.13419300	-0.38761600
C	1.18490200	-0.01517400	-0.11570900
C	-2.34185900	0.13547100	1.09241500
H	-2.70064700	1.11233100	1.42590200
H	-2.93303100	-0.61999700	1.61633600
C	3.19213700	-1.28498000	-0.45373200
H	3.67439400	-2.24187800	-0.63186900
C	-0.33837900	1.11148300	2.30083800
H	0.74532300	1.05352500	2.42920000
H	-0.80309400	1.03452000	3.28583000
H	-0.59660100	2.08273300	1.87657100
C	-0.53539100	-1.35346100	2.08382200
H	-0.94096500	-2.18406500	1.50453500
H	-0.98383600	-1.37660400	3.07883600
H	0.54357900	-1.48863500	2.19229900
C	1.29863700	2.53195100	-0.06599000
H	1.39470700	2.97887900	0.92585500
H	1.80105400	3.19425000	-0.77180400
H	0.24155900	2.49975900	-0.32452600

C	1.03720100	-2.53334500	-0.50159900
H	1.54493600	-3.16869700	-1.22756800
H	0.97200100	-3.09372200	0.43316800
H	0.02509000	-2.34907200	-0.86162600
C	5.46596700	-0.20422300	-0.48686300
H	5.91255200	-0.37677100	0.49519400
H	5.78044600	-1.02099900	-1.13736200
H	5.87909900	0.72610100	-0.87734900
C	-2.45814500	-0.00365100	-0.44032800
C	-3.31297800	1.10210900	-1.06871900
C	-2.99099200	-1.39274800	-0.83997600
H	-2.80238600	-1.53134100	-1.90853600
H	-4.28126400	1.13231600	-0.55799100
C	-2.64739300	2.47059500	-1.01478700
H	-2.33918700	2.72651900	0.00436700
H	-1.75557300	2.47887300	-1.64420900
H	-3.31819700	3.25732500	-1.36201500
H	-3.50811800	0.83309300	-2.11210000
C	-4.46869500	-1.60369600	-0.53800400
H	-5.09481900	-0.96579000	-1.16332000
H	-4.75934100	-2.63776200	-0.72689100
H	-4.70310800	-1.37829200	0.50555600
H	-2.39426000	-2.15166300	-0.31909500

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j-2-1 carbene-Au fragment

Au	0.53983400	-1.85678400	-0.07288900
C	-2.17681300	0.48069900	1.18043200
N	-0.06724400	1.08160000	0.08199200
C	0.39153000	2.50607800	0.19244300
C	-3.53081600	0.17651900	1.07597900
H	-4.08522500	-0.03670200	1.98494000
C	0.86902300	0.18205000	-0.01920700
C	-2.06322500	0.58671200	-1.25334800
C	-4.17682100	0.09585200	-0.15035800

C	-1.46690500	0.73826600	0.00448000
C	1.91559100	2.33253000	0.28903600
H	2.26016300	2.59971400	1.29019200
H	2.42095200	2.99652700	-0.41578900
C	-3.41819100	0.27812000	-1.30082600
H	-3.88532800	0.14539200	-2.27196900
C	-0.19548500	3.16724100	1.42885500
H	-1.28737000	3.17287400	1.39235900
H	0.15144400	4.20104800	1.47454700
H	0.12919000	2.65554900	2.33570500
C	-0.02759800	3.27881200	-1.05054200
H	0.42737600	2.85386100	-1.94637700
H	0.30302500	4.31424200	-0.95373100
H	-1.11399700	3.27387800	-1.16530000
C	-1.52838700	0.43782700	2.53604800
H	-1.72907400	1.34644300	3.10807000
H	-1.93023500	-0.40291800	3.10146000
H	-0.44928200	0.30644200	2.46810600
C	-1.29328100	0.66883300	-2.54255200
H	-1.71761000	-0.03213000	-3.26082700
H	-1.34607600	1.66562200	-2.98512600
H	-0.24315300	0.40769100	-2.40693200
C	-5.64498800	-0.20818300	-0.23451500
H	-6.22913600	0.71392000	-0.27964800
H	-5.87635400	-0.78744200	-1.12867200
H	-5.98141500	-0.76957900	0.63712400
C	2.21619000	0.85078600	-0.01780200
C	3.13729500	0.19875500	1.02058500
C	2.77839700	0.65873500	-1.44107300
H	2.71549000	-0.40671100	-1.68495700
H	4.05028500	0.79852100	1.08575100
C	2.50023000	0.05489900	2.39616900
H	2.06267600	0.99757000	2.74151500
H	1.70824900	-0.69777000	2.37063800

H	3.23361200	-0.25738100	3.13968100
H	3.42113400	-0.79106500	0.64659400
C	4.20793400	1.15350700	-1.60980900
H	4.90852700	0.53784300	-1.04508200
H	4.50539100	1.11427700	-2.65780900
H	4.32160500	2.18638600	-1.27053700
H	2.11684600	1.18042700	-2.14360700

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j-3-1 carbene fragment

C	-2.61893300	-1.07538800	0.66472000
N	-0.72950700	0.38051500	0.09658000
C	2.48442800	0.65169100	-1.18725400
H	1.99464100	1.39516400	-1.82920500
C	3.45658300	-1.64939500	-1.10688100
H	3.65643600	-2.55500000	-1.68689900
C	-0.36015000	1.46299200	1.06881600
C	-3.95815200	-1.41398900	0.49789600
H	-4.35699900	-2.24912000	1.06652000
C	2.23589500	-0.72402800	0.87381800
H	1.57505400	-0.97553900	1.71274000
C	0.23211100	-0.25854200	-0.51965700
C	2.78253100	-0.60882700	-1.99995200
H	3.44855700	-0.35041300	-2.83159100
H	1.85565000	-1.01065500	-2.41220800
C	-2.88988400	0.63888100	-1.04142100
C	-4.78588500	-0.74212000	-0.39396000
C	2.53223000	-1.99037000	0.06299500
H	3.01918700	-2.72414500	0.71596800
H	1.60286900	-2.42568900	-0.31004600
C	4.77020800	-1.07915700	-0.57398800
H	5.27612300	-1.82096400	0.05432500
H	5.43886500	-0.83936400	-1.40837600
C	-2.10514300	-0.00633600	-0.08079600
C	1.53466800	0.33672700	-0.01502800

C	3.79550500	1.22140400	-0.64232400
H	4.45141500	1.48962200	-1.47767800
H	3.60967500	2.13580300	-0.06764700
C	1.12949400	1.61025400	0.75789300
H	1.70254900	1.77645900	1.67146100
H	1.28250500	2.48399500	0.11489100
C	-4.22411300	0.26244600	-1.17064500
H	-4.83234300	0.75653100	-1.92302400
C	3.56241800	-0.17911500	1.40947700
H	3.40852800	0.69515000	2.04819900
H	4.03537500	-0.94872300	2.02986800
C	-0.62797900	1.00222800	2.49681300
H	-1.69180000	0.79783400	2.64117000
H	-0.33663500	1.79255600	3.19122800
H	-0.05942300	0.10361400	2.73765800
C	4.48269100	0.18001100	0.24265900
H	5.41967200	0.59068900	0.63066300
C	-1.13682100	2.74540200	0.81240200
H	-0.92561300	3.14081600	-0.18070100
H	-0.83600500	3.49441100	1.54770600
H	-2.21307200	2.58376200	0.91241800
C	-6.23718000	-1.10636700	-0.52773400
H	-6.84621100	-0.54214800	0.18246200
H	-6.60879700	-0.88417600	-1.52840100
H	-6.39799300	-2.16615700	-0.32766600
C	-2.33632400	1.66958300	-1.98647700
H	-2.73870100	1.50114300	-2.98591100
H	-2.61961600	2.68082900	-1.68714400
H	-1.24951100	1.62159700	-2.04616300
C	-1.76761900	-1.91326300	1.57932500
H	-1.80630200	-1.55927100	2.61119800
H	-2.13064000	-2.94114800	1.57355000
H	-0.72437100	-1.91941500	1.26039400

j-3-1 carbene-Au fragment

Au	-0.27385000	-1.85195400	-0.20900700
C	-2.41036400	0.83762300	1.37636900
N	-0.64459200	1.03423200	-0.29741400
C	2.68883100	-0.06223000	-1.08180400
H	2.27445800	-0.30099000	-2.06853900
C	3.62320800	-1.03664900	1.02370000
H	3.85717500	-1.96745600	1.54728600
C	-0.17725700	2.37125400	-0.77463400
C	-3.74840300	0.63658100	1.68678200
H	-4.05391800	0.67726100	2.72779000
C	2.23326100	1.05192100	1.09971700
H	1.49205500	1.59774500	1.69269800
C	0.28942700	0.12461700	-0.10628700
C	3.07203300	-1.35476600	-0.36221300
H	3.83441600	-1.86991500	-0.95755600
H	2.21217600	-2.02667800	-0.28419500
C	-2.92865000	0.40286500	-0.96480200
C	-4.69687700	0.35039800	0.70794700
C	2.56474900	-0.26468700	1.81136700
H	2.93819600	-0.03589700	2.81564700
H	1.66462400	-0.87818000	1.91889700
C	4.88745500	-0.19214000	0.87646600
H	5.30966900	0.03774900	1.86118800
H	5.64267300	-0.75140000	0.31364100
C	-2.02401500	0.78013200	0.02940000
C	1.64452100	0.77146600	-0.31369600
C	3.95921200	0.78507500	-1.23254600
H	4.69343000	0.22204600	-1.81796600
H	3.75365900	1.71044100	-1.78014500
C	1.28072600	2.05089500	-1.09795100
H	1.92333700	2.90431100	-0.88516400
H	1.37343300	1.82938800	-2.16699500
C	-4.26073200	0.21078900	-0.60089700

H	-4.96768700	-0.08975200	-1.36850100
C	3.51854500	1.87351800	0.98307900
H	3.32916800	2.86040200	0.55277600
H	3.91886400	2.03993700	1.98931200
C	-0.33350900	3.43013400	0.31303200
H	-1.36787300	3.46922200	0.66363400
H	-0.07964100	4.40605800	-0.10422600
H	0.32531000	3.24556100	1.16053100
C	4.54325700	1.10588200	0.14729100
H	5.44501200	1.71324200	0.02720500
C	-0.94751400	2.83155300	-2.00352700
H	-0.82907900	2.13311500	-2.83014300
H	-0.55537700	3.80088200	-2.31693800
H	-2.01080500	2.95001600	-1.78170000
C	-6.14345500	0.17051100	1.06905000
H	-6.64808800	1.13685100	1.14039400
H	-6.66615200	-0.42124500	0.31764000
H	-6.24971500	-0.32577200	2.03427200
C	-2.51698200	0.10017200	-2.37850700
H	-3.00511900	-0.81937500	-2.70227600
H	-2.81402500	0.89487700	-3.06647400
H	-1.44158300	-0.05444100	-2.46240300
C	-1.40467100	1.00327600	2.47961900
H	-0.87997400	1.95706100	2.43158800
H	-1.89881600	0.93793800	3.44818300
H	-0.65029400	0.21259000	2.42229100

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j-4-1 carbene fragment

C	2.11722500	1.24256000	-0.18385500
N	0.10041300	-0.13534000	0.05383400
C	-0.46317000	-0.30320700	1.43673600
C	3.49734100	1.32091300	-0.34466500
H	3.95969400	2.30295200	-0.38639000
C	-0.73319900	-0.01816100	-0.95018000

C	2.28295900	-1.17874100	-0.36071900
C	4.29133000	0.18939900	-0.48667900
C	1.52266200	-0.02483700	-0.14385500
C	-1.94461100	-0.52356200	1.11399200
H	-2.58145900	0.03126600	1.80705100
H	-2.19296400	-1.58418400	1.22378400
C	3.65985500	-1.04708800	-0.51775900
H	4.24992500	-1.94171900	-0.69548500
C	-0.21934900	0.95546700	2.26058000
H	0.85155400	1.14038200	2.37484900
H	-0.64974900	0.82321000	3.25503300
H	-0.68154500	1.82795000	1.79762000
C	0.15558800	-1.49159900	2.15690300
H	-0.04787200	-2.42107600	1.62568400
H	-0.28055900	-1.56750200	3.15499500
H	1.23624200	-1.37030000	2.26583200
C	1.32142300	2.51802200	-0.13216500
H	1.27615500	2.92868800	0.87839900
H	1.79433000	3.26720600	-0.76745300
H	0.30151100	2.36794100	-0.48652400
C	1.66867800	-2.54460900	-0.49907200
H	2.16041700	-3.08507300	-1.30848300
H	1.79509400	-3.13467300	0.41108800
H	0.60472500	-2.48855900	-0.72651300
C	5.78315900	0.30210100	-0.62283100
H	6.26558600	0.27531200	0.35708200
H	6.18882800	-0.52147800	-1.21107300
H	6.06569100	1.24000700	-1.10185600
C	-2.12425600	-0.09342300	-0.35610600
C	-2.73718600	1.31115100	-0.49413800
C	-2.97710700	-1.08235500	-1.15357600
C	-4.20366900	1.34701600	-0.07814500
H	-2.64477700	1.61111900	-1.54395500
H	-2.15262300	2.02890000	0.09208900

C	-4.42994400	-1.06729100	-0.69614100
H	-2.91827600	-0.80291700	-2.21119200
H	-2.54485400	-2.08475900	-1.06323400
C	-5.01802500	0.32831800	-0.86642200
H	-4.60341500	2.35380900	-0.22091900
H	-4.29458400	1.12414200	0.99149800
H	-5.01148700	-1.80208100	-1.25755600
H	-4.48843700	-1.35759900	0.36092700
H	-6.06462400	0.35034500	-0.55377100
H	-4.99365600	0.59563200	-1.92978200

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j-4-1 carbene-Au fragment

Au	0.25605300	-1.88837100	-0.08720400
C	-2.25493500	0.37332000	1.19304800
N	-0.25321200	1.05493000	-0.04556800
C	0.27505800	2.43513100	0.19230000
C	-3.62491900	0.13025800	1.20048000
H	-4.08885200	-0.18770100	2.12936700
C	0.64370800	0.12394000	-0.25584800
C	-2.39984800	0.81630400	-1.20106900
C	-4.40232200	0.24075400	0.05451500
C	-1.66359200	0.76668400	-0.01306800
C	1.75994100	2.24575400	-0.14850700
H	2.39341400	2.78405900	0.55884500
H	1.96242800	2.65244800	-1.14423000
C	-3.76559900	0.56011300	-1.13854300
H	-4.34139800	0.58564900	-2.05895300
C	0.04362300	2.85473800	1.63835200
H	-1.02461300	2.87410900	1.86544900
H	0.44094000	3.86084400	1.78357000
H	0.54126500	2.18257900	2.33737100
C	-0.40064000	3.43809700	-0.73015400
H	-0.21521100	3.19402000	-1.77577800
H	0.00934500	4.43016000	-0.53253600

H	-1.47861800	3.47133100	-0.55560200
C	-1.47242800	0.13064300	2.45469000
H	-1.58672300	0.95296300	3.16473900
H	-1.83905000	-0.77659000	2.93490900
H	-0.41042700	-0.01347400	2.25817900
C	-1.77025100	1.07102300	-2.54269500
H	-2.22448900	0.41748500	-3.28749800
H	-1.93024400	2.10062100	-2.87008400
H	-0.69801300	0.87579000	-2.53597300
C	-5.88397000	-0.00053400	0.09989500
H	-6.42018600	0.92551600	0.32007700
H	-6.25181000	-0.37463700	-0.85569000
H	-6.14176100	-0.72193300	0.87549100
C	2.01933100	0.72692300	-0.14841300
C	2.65841400	0.22876900	1.16212600
C	2.88804300	0.27088900	-1.32358800
C	4.10147800	0.69820600	1.30645600
H	2.62707800	-0.86677700	1.15111700
H	2.05357900	0.55141400	2.01636300
C	4.31792200	0.77634100	-1.18484700
H	2.87855400	-0.82557400	-1.34070200
H	2.43539000	0.61150600	-2.26078500
C	4.93581700	0.26041100	0.10890200
H	4.52070100	0.30255600	2.23399000
H	4.13848700	1.79087200	1.38874900
H	4.91038200	0.46500500	-2.04754500
H	4.32287800	1.87412600	-1.17669600
H	5.96580300	0.60867800	0.21231500
H	4.96647800	-0.83482000	0.07547700

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j-5-1 carbene fragment

C	2.06521300	1.23406900	-0.16689300
N	0.03443500	-0.12947500	0.00920100
C	-0.57053900	-0.29284700	1.37741800

C	3.44958800	1.30490700	-0.28939900
H	3.91868700	2.28429400	-0.31510700
C	-0.76882600	-0.00916000	-1.01925300
C	2.22150100	-1.18778600	-0.34655800
C	4.24045700	0.16906700	-0.41354200
C	1.46250700	-0.02997200	-0.14777700
C	-2.04084400	-0.50916700	1.00727400
H	-2.71564400	0.02706700	1.67951000
H	-2.27862100	-1.57551700	1.08221900
C	3.60294100	-1.06360200	-0.46546300
H	4.19254200	-1.96112400	-0.62951100
C	-0.33665200	0.95800500	2.21589600
H	0.73299900	1.12650500	2.36336900
H	-0.79788700	0.82380600	3.19605400
H	-0.77077200	1.84208800	1.74929600
C	0.02081000	-1.48805900	2.11005300
H	-0.17119900	-2.41402700	1.56861900
H	-0.44531800	-1.56613900	3.09429700
H	1.09831800	-1.37269200	2.25170900
C	1.27592200	2.51425800	-0.13164100
H	1.21394400	2.92557100	0.87778900
H	1.76548800	3.26025400	-0.75799300
H	0.26183300	2.37106200	-0.50533800
C	1.60331100	-2.54962800	-0.50452200
H	2.11504500	-3.09231600	-1.29990800
H	1.69951600	-3.14127700	0.40829600
H	0.54686700	-2.48661700	-0.76273700
C	5.73600700	0.27369900	-0.50914600
H	6.19090600	0.25361200	0.48399200
H	6.15380100	-0.55689200	-1.07867400
H	6.03624600	1.20601600	-0.98834400
C	-2.17333300	-0.05122500	-0.45695200
C	-2.73741000	1.37233000	-0.57223000
C	-3.06660600	-0.98146200	-1.27587400

C	-4.22037200	1.40885700	-0.34769700
H	-2.48711300	1.77187000	-1.56222600
H	-2.23883400	2.02906100	0.14966500
C	-4.46898000	-1.04416600	-0.68344700
H	-3.10568000	-0.59969500	-2.30020100
H	-2.61906100	-1.97925700	-1.31931300
C	-4.99385200	0.32687400	-0.37722600
H	-4.66633100	2.37765900	-0.14551500
H	-5.14796200	-1.55352800	-1.37257700
H	-4.47097700	-1.64969900	0.23198400
H	-6.05689100	0.42629300	-0.18190200

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j-5-1 carbene-Au fragment

Au	0.24123300	-1.91747800	-0.09957600
C	-2.20130300	0.41236200	1.19241200
N	-0.17886500	1.04043100	-0.03783100
C	0.39288200	2.40277800	0.21254300
C	-3.57786100	0.21003500	1.19719600
H	-4.05202900	-0.10037800	2.12345200
C	0.68845300	0.08222100	-0.25345000
C	-2.33062700	0.87640400	-1.19872300
C	-4.35043300	0.35137900	0.05127100
C	-1.59748400	0.79622200	-0.01060100
C	1.86946500	2.16667300	-0.13398800
H	2.53922900	2.67946000	0.55979000
H	2.06876400	2.55526100	-1.13784400
C	-3.70342400	0.66032700	-1.13899500
H	-4.27736400	0.70951300	-2.05959900
C	0.16750500	2.82494500	1.65883600
H	-0.90130500	2.88280600	1.87709700
H	0.59981600	3.81556700	1.80967800
H	0.63285900	2.13505400	2.36199500
C	-0.25079500	3.43115100	-0.70542600
H	-0.07172200	3.18751600	-1.75222600

H	0.18905300	4.40903700	-0.50162900
H	-1.32746900	3.49620700	-0.53178400
C	-1.42712800	0.13861500	2.45291500
H	-1.51665500	0.96009500	3.16744300
H	-1.82147500	-0.75965000	2.92797200
H	-0.36962900	-0.03662000	2.25625300
C	-1.69214200	1.12227200	-2.53773300
H	-2.16530000	0.48898000	-3.28821200
H	-1.81993100	2.15890000	-2.85696700
H	-0.62643100	0.89420300	-2.53128400
C	-5.83855300	0.15330400	0.09363400
H	-6.34755100	1.09275500	0.32147100
H	-6.21631000	-0.20160600	-0.86538600
H	-6.11806800	-0.56688300	0.86280000
C	2.07875900	0.64257100	-0.12293700
C	2.68219500	0.14499900	1.20005200
C	2.97796500	0.16165000	-1.26188900
C	4.14767600	0.45286900	1.28258900
H	2.50823000	-0.93508700	1.28408500
H	2.15436100	0.60014000	2.04529200
C	4.35069700	0.81603900	-1.17104700
H	3.06550200	-0.92674500	-1.18239800
H	2.50563000	0.37968100	-2.22452600
C	4.89190700	0.76889900	0.22642700
H	4.60494500	0.40878300	2.26552200
H	5.04625500	0.32070200	-1.85320200
H	4.30091000	1.85897300	-1.50938300
H	5.94377900	0.99676400	0.36442400

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j-6-1 carbene fragment

C	-2.68094900	-1.33360600	-0.41016100
N	-0.62534900	-0.14016500	0.20435800
C	-0.12499100	-0.31582100	1.61116600
C	-4.05395100	-1.31125700	-0.63609500

H	-4.54888600	-2.23817200	-0.91142700
C	0.25055200	-0.07175500	-0.76703600
C	-2.74887000	1.07168500	-0.05373100
C	-4.79886400	-0.14137400	-0.55360900
C	-2.04136800	-0.13532000	-0.06762500
C	1.39052100	-0.20000800	1.40311900
H	1.90774700	-1.01961600	1.90707000
H	1.76297400	0.72969700	1.84364200
C	-4.12097100	1.04087100	-0.28737300
H	-4.66812000	1.97928900	-0.28599200
C	-0.52936900	-1.68327300	2.14740500
H	-1.61667500	-1.78998900	2.16743500
H	-0.15656800	-1.79305100	3.16754200
H	-0.10408300	-2.48232400	1.53818100
C	-0.67019900	0.76530400	2.53166100
H	-0.35208900	1.75554900	2.20297600
H	-0.28600100	0.60063600	3.54026800
H	-1.76188000	0.73579200	2.57313100
C	-1.93972400	-2.62687500	-0.61132700
H	-1.96889600	-3.25411000	0.28181300
H	-2.40558700	-3.19006700	-1.42022900
H	-0.89651000	-2.45486200	-0.87563400
C	-2.08130200	2.40647200	0.13112200
H	-2.54887400	3.14150000	-0.52473200
H	-2.18386700	2.77111900	1.15525400
H	-1.02035300	2.36326500	-0.11163000
C	-6.28575500	-0.15252700	-0.76707600
H	-6.81154300	-0.33249100	0.17357100
H	-6.63473300	0.80242400	-1.16090000
H	-6.57863800	-0.94001600	-1.46210900
C	1.61441300	-0.21957800	-0.12501900
C	2.15270500	-1.57861900	-0.60342900
C	2.56100300	0.89724800	-0.60918700
C	3.58267500	-1.85611800	-0.15354200

H	2.11489100	-1.59314700	-1.70005600
H	1.48776800	-2.37958900	-0.25385800
C	3.96828400	0.63263400	-0.07813600
H	2.60883700	0.78945200	-1.70282500
C	4.48448800	-0.70757700	-0.58506200
H	3.60609400	-1.90601800	0.94334900
H	4.64667800	1.43155400	-0.38506600
H	3.96418000	0.63048000	1.01977700
H	5.50715900	-0.88665000	-0.23972500
H	4.51653300	-0.68732700	-1.68311200
C	4.07108100	-3.18428800	-0.71136700
H	5.09165800	-3.39940900	-0.38754400
H	3.43094500	-4.01058300	-0.39475000
H	4.06451100	-3.15564800	-1.80484300
C	1.97469500	2.30283500	-0.31184200
C	2.95718700	3.29575300	0.30038500
H	3.76957300	3.52450000	-0.39446000
H	2.44530400	4.23419200	0.52394300
H	3.40102000	2.92433200	1.22652700
C	1.36455200	2.89848000	-1.57782600
H	2.15298900	3.10036700	-2.30938000
H	0.65203600	2.20481200	-2.02917300
H	0.85443200	3.84182800	-1.36482200
H	1.16035200	2.17371400	0.41480800

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j-6-1 carbene-Au fragment

Au	0.18360600	-1.60809100	-1.00898600
C	2.65090700	1.32194300	-0.75905800
N	0.60803800	0.90883900	0.53037500
C	0.05950600	2.00646500	1.38886800
C	4.02427600	1.15959200	-0.90440400
H	4.51106500	1.61032400	-1.76399100
C	-0.27291200	0.18616500	-0.10941300
C	2.74067500	-0.10451000	1.21536700

C	4.77970100	0.41119000	-0.00943200
C	2.02747600	0.72518400	0.34431200
C	-1.45437200	1.76420000	1.27366900
H	-1.97668500	2.69845300	1.05694200
H	-1.83612500	1.39217200	2.22376000
C	4.11362300	-0.23173900	1.02504400
H	4.66933400	-0.88464500	1.69133300
C	0.47614700	3.36130900	0.83364500
H	1.56439300	3.45170400	0.79889100
H	0.08673000	4.14677500	1.48346600
H	0.07321400	3.51288000	-0.16855300
C	0.54961300	1.86439100	2.82091100
H	0.22351500	0.91413500	3.24744500
H	0.12831000	2.67291300	3.42117200
H	1.63896800	1.92859000	2.87422400
C	1.89375200	2.06587300	-1.82412900
H	1.84173200	3.13621200	-1.61594400
H	2.40135700	1.94331800	-2.78050600
H	0.87680000	1.68808100	-1.93591500
C	2.08427500	-0.92628700	2.28913900
H	2.56661000	-1.90222700	2.34011200
H	2.17587700	-0.45944500	3.27212900
H	1.02804200	-1.09245600	2.08120600
C	6.26640900	0.27922500	-0.17455600
H	6.78625400	1.09158900	0.33866100
H	6.62732700	-0.65992200	0.24490300
H	6.55114000	0.31978400	-1.22616900
C	-1.65668800	0.71727200	0.16124900
C	-2.10678400	1.35928000	-1.16563300
C	-2.62702000	-0.42312900	0.51870000
C	-3.54875100	1.85289100	-1.13856300
H	-2.00332000	0.60582800	-1.95850500
H	-1.43056300	2.18551500	-1.42010100
C	-4.06238000	0.08787900	0.56908200

H	-2.55911100	-1.11448500	-0.33492500
C	-4.47163600	0.70205800	-0.76111500
H	-3.64320800	2.62712100	-0.36462700
H	-4.73228600	-0.73673100	0.83033300
H	-4.16324900	0.83837100	1.36446100
H	-5.50803500	1.05014500	-0.72799300
H	-4.41312800	-0.06171800	-1.54776500
C	-3.92860700	2.45418100	-2.48303100
H	-4.95803300	2.81783900	-2.47605600
H	-3.27393600	3.28679100	-2.74898800
H	-3.84468700	1.69745000	-3.26806300
C	-2.21234000	-1.23128300	1.77378300
C	-2.96371600	-0.88796800	3.06142200
H	-4.01580900	-1.17199700	2.97966300
H	-2.53933000	-1.45571500	3.89194500
H	-2.93060100	0.16843100	3.33161500
C	-2.39336900	-2.72033300	1.49529700
H	-3.43955600	-2.92200400	1.24066900
H	-1.76775700	-3.03933600	0.65793500
H	-2.14087100	-3.32248600	2.37081800
H	-1.14225800	-1.04700600	1.94677500

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k-1-1 carbene fragment

C	-1.41279100	-1.18695800	-0.01615800
N	0.66690200	0.10278800	-0.11482800
C	1.37446400	0.36919700	1.18400200
C	-2.78854600	-1.30780800	-0.07340500
H	-3.26909800	-2.26959700	0.02986800
C	1.37334200	-0.16671200	-1.18904400
C	-1.54842200	1.14941100	-0.36922200
C	-3.51829200	-0.15173600	-0.28058500
C	-0.75409100	0.03071100	-0.14869500
C	2.81882400	0.46220900	0.68491200
H	3.50677500	-0.05376600	1.35878500

H	3.12194300	1.51183800	0.63906100
C	-2.92819000	1.08884700	-0.43576200
H	-3.51683800	1.97682200	-0.61372900
C	1.13751600	-0.78546400	2.14991200
H	0.07460800	-0.88103500	2.38641600
H	1.67186800	-0.59240300	3.08177000
H	1.48538700	-1.73125700	1.73565700
C	0.88551900	1.66648200	1.80939300
H	1.01612800	2.50353500	1.12387600
H	1.45832800	1.86433200	2.71726400
H	-0.16962800	1.59910100	2.08768900
C	2.81813500	-0.14203800	-0.73484800
C	3.27126500	-1.60617100	-0.73928000
H	3.20043400	-2.01921400	-1.74619800
H	4.30927400	-1.67118900	-0.40211900
H	2.65342300	-2.22119100	-0.08130700
C	3.67910400	0.65609200	-1.70530700
H	4.72240000	0.65300100	-1.37703700
H	3.62422800	0.22012400	-2.70373500
H	3.34208300	1.69291300	-1.76704400
F	-0.95335900	2.32672700	-0.54177200
F	-4.84780000	-0.23812300	-0.34014500
F	-0.68180300	-2.28392700	0.16181600

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k-1-1 carbene-Au fragment

Au	1.01231600	-1.66139700	-0.07674800
C	-1.81861900	0.07476300	1.12892000
N	0.02827300	1.14836500	-0.06712800
C	0.32021900	2.58067000	0.24535500
C	-3.08412300	-0.47546600	1.18619300
H	-3.46224700	-0.91022200	2.09961200
C	1.06530500	0.36947400	-0.30758800
C	-2.09566700	0.59712000	-1.16948500
C	-3.83344900	-0.46604700	0.02363900

C	-1.29555300	0.63349900	-0.03402400
C	1.81159800	2.64331300	-0.10977800
H	2.36477300	3.25681100	0.60392500
H	1.92757200	3.09216900	-1.09982300
C	-3.36827100	0.05952400	-1.16832900
H	-3.96744400	0.04008400	-2.06671600
C	0.02839100	2.86985900	1.71233800
H	-1.03135500	2.71894700	1.93080800
H	0.27154200	3.91178000	1.92714700
H	0.61094200	2.22897100	2.37282200
C	-0.52255900	3.49093300	-0.63464700
H	-0.35740700	3.27524900	-1.69008700
H	-0.24662500	4.52876500	-0.44081500
H	-1.58675900	3.37846000	-0.41245700
C	2.32073100	1.18923600	-0.14124300
C	2.97551600	0.77643800	1.18324000
H	3.30981200	-0.26075600	1.13084200
H	3.83725600	1.42143600	1.37345400
H	2.28148300	0.85771400	2.02180700
C	3.29281400	0.92721500	-1.28533300
H	4.19882400	1.52374800	-1.15238600
H	3.56714000	-0.12953800	-1.30315400
H	2.84645300	1.18270500	-2.24808200
F	-1.60424900	1.08686000	-2.30409700
F	-5.05715700	-0.99090400	0.05141800
F	-1.06224500	0.06763500	2.22051600

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l-1-1 carbene fragment

C	-1.10098400	-1.18271500	-0.10837900
N	1.00207800	0.09094800	-0.03537900
C	1.74887800	0.16209600	1.27474000
C	-2.48624300	-1.24643300	-0.13143600
H	-2.98496500	-2.20499900	-0.15142600
C	1.68106000	0.01191300	-1.15575700

C	-1.18953000	1.20073600	-0.16858800
C	-3.21159200	-0.06769400	-0.15215000
C	-0.42144700	0.03764700	-0.07618500
C	3.17139400	0.37225000	0.74839200
H	3.89544700	-0.21729100	1.31570200
H	3.44535100	1.42599000	0.85027700
C	-2.57530900	1.16118900	-0.19260700
H	-3.14349100	2.07799600	-0.26044500
C	1.58781400	-1.13280400	2.06258400
H	0.53757900	-1.31760600	2.30228400
H	2.13574700	-1.04197900	3.00228000
H	1.97541900	-1.99114700	1.51674300
C	1.26554900	1.31904400	2.13652700
H	1.42286600	2.27644800	1.64375200
H	1.82574600	1.31593400	3.07341600
H	0.20485300	1.21634400	2.38183000
C	3.13806400	-0.01080400	-0.74560900
C	3.61213500	-1.44769100	-0.98869700
H	3.51178500	-1.70311700	-2.04435600
H	4.66213500	-1.54359500	-0.69963100
H	3.02572400	-2.16785000	-0.41372500
C	3.95444200	0.94574600	-1.60505300
H	5.00618500	0.92122900	-1.30597800
H	3.88138400	0.66421100	-2.65637700
H	3.59125800	1.97053500	-1.50068600
Cl	-4.92975300	-0.13160300	-0.16937400
Cl	-0.23215000	-2.65952000	-0.20543400
Cl	-0.42944800	2.72920500	-0.34241000

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l-1-1 carbene-Au fragment

Au	1.12702300	-1.74460400	-0.18250400
C	-1.58726500	0.18696800	1.19763400
N	0.38697300	1.12530800	0.07013000
C	0.81060500	2.52541700	0.41067400

C	-2.91541600	-0.21085200	1.18579500
H	-3.36868300	-0.61185600	2.08105200
C	1.34513300	0.28510400	-0.26741000
C	-1.71329800	0.72687400	-1.12916100
C	-3.63521100	-0.11458600	0.00707000
C	-0.97404500	0.70909700	0.05589000
C	2.28081800	2.47483500	-0.02763900
H	2.92035100	3.02933600	0.66188200
H	2.37605700	2.93017100	-1.01720000
C	-3.04116100	0.33270500	-1.16169400
H	-3.59388200	0.35892700	-2.08990800
C	0.63926600	2.82138300	1.89546800
H	-0.41113300	2.75768200	2.18721800
H	0.98096300	3.84053300	2.08539100
H	1.21459700	2.13968100	2.51879300
C	0.00398800	3.54241100	-0.38361900
H	0.13421800	3.40658000	-1.45551900
H	0.34567900	4.54379400	-0.11647300
H	-1.06026200	3.47627500	-0.14327400
C	2.66942300	0.98734400	-0.11326200
C	3.31693900	0.47456000	1.17943200
H	3.56518200	-0.58319700	1.07959100
H	4.23148900	1.04028500	1.37467000
H	2.64716700	0.57649900	2.03573500
C	3.58321200	0.68466300	-1.29417800
H	4.53656300	1.20593500	-1.17664300
H	3.77309800	-0.38913000	-1.35043300
H	3.12597000	1.00175000	-2.23365800
Cl	-5.28402300	-0.59563400	-0.01649500
Cl	-0.68493700	-0.06343200	2.63305300
Cl	-0.96391900	1.16893400	-2.60739900

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m-1-1 carbene fragment

C	0.65257900	1.21494400	-0.13990100
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N	-1.50095400	0.00438500	-0.00673800
C	-2.20640900	-0.02063300	1.32999100
C	2.04273700	1.19528500	-0.13275900
H	2.58781700	2.12943200	-0.17355300
C	-2.21342900	-0.02224000	-1.10856200
C	0.63447700	-1.18694000	-0.12769100
C	2.72754600	-0.00406100	-0.10049900
C	-0.07590600	0.02009400	-0.08710800
C	-3.61405700	-0.39083000	0.85757500
H	-4.37762600	0.15241200	1.41885600
H	-3.77621700	-1.46115000	1.01520800
C	2.02280300	-1.19334300	-0.12497500
H	2.55134000	-2.13792400	-0.15755500
C	-2.13574200	1.34688900	1.99906600
H	-1.10135700	1.62346800	2.21584200
H	-2.66872300	1.30023300	2.95029500
H	-2.58750500	2.12669700	1.38952000
C	-1.60779500	-1.04877300	2.27924500
H	-1.68537800	-2.06111200	1.88944500
H	-2.15702500	-1.01030000	3.22158600
H	-0.56045400	-0.82785500	2.50255400
C	0.06903900	2.61165300	-0.25588200
C	0.03525400	-2.58005800	-0.21973200
C	4.23134600	-0.02229800	-0.03311500
C	-3.65647300	-0.08462400	-0.65461000
C	-4.28765800	1.27514600	-0.96723800
H	-4.20500100	1.49086700	-2.03330600
H	-5.34574500	1.25856000	-0.69326000
H	-3.80317500	2.08642100	-0.42193000
C	-4.39081400	-1.17093600	-1.43321600
H	-5.42739400	-1.24239200	-1.09190400
H	-4.38625700	-0.94028100	-2.49922000
H	-3.91324600	-2.14290100	-1.29187300
F	4.76269900	1.07925100	-0.56571700

F	4.65664100	-0.09425900	1.23417700
F	4.73815000	-1.07545500	-0.67748000
F	0.22609900	3.28774600	0.89389100
F	0.73956300	3.29851800	-1.18901700
F	0.32717400	-3.27989400	0.88932300
F	-1.27909200	-2.64705000	-0.39315800
F	0.59775800	-3.23709300	-1.24031200
F	-1.21369900	2.66706800	-0.58249500

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m-1-1 carbene-Au fragment

Au	-1.48810400	-1.03283600	-1.51751300
C	1.24777800	1.32508300	-0.20547600
N	-0.86768800	0.61314600	0.85897200
C	-1.30353700	1.23040000	2.15993900
C	2.59545400	1.09908000	-0.45922200
H	3.16058800	1.82811100	-1.02507100
C	-1.82199200	0.28055300	0.01429200
C	1.11850600	-0.80584100	0.90525500
C	3.20854200	-0.05709200	-0.01438600
C	0.50247300	0.39344500	0.52602700
C	-2.79574600	0.88290600	2.12673100
H	-3.40045200	1.69303300	2.53892300
H	-2.96685200	-0.01199800	2.73122100
C	2.46632600	-1.01746000	0.64618200
H	2.92635000	-1.95022600	0.94661300
C	-1.03723700	2.73143700	2.13257000
H	0.03338300	2.93363800	2.05769400
H	-1.39219800	3.16718300	3.06770200
H	-1.54484600	3.22451200	1.30629300
C	-0.57985600	0.64019000	3.36104200
H	-0.79989700	-0.41479300	3.50093200
H	-0.90886000	1.17372200	4.25422000
H	0.50187100	0.77553200	3.28007200
C	0.71639800	2.61386900	-0.80647800

C	0.44644500	-1.98980000	1.58185000
C	4.68360700	-0.26215200	-0.24107600
C	-3.15220100	0.57369200	0.65765100
C	-3.77551600	1.76284200	-0.08053300
H	-3.91156100	1.51347000	-1.13430700
H	-4.75114700	1.98958200	0.35586400
H	-3.15307100	2.65637800	-0.02236400
C	-4.08252100	-0.63082400	0.54684500
H	-5.01142700	-0.42370300	1.08470200
H	-4.31646900	-0.83813400	-0.49857400
H	-3.61907200	-1.52290300	0.97321300
F	5.09554700	0.33288000	-1.36137300
F	5.39904300	0.25347100	0.76634200
F	4.99356600	-1.55617200	-0.32373200
F	1.11547600	3.67294100	-0.08390100
F	1.21989700	2.78115700	-2.03227500
F	0.94558900	-2.14605000	2.82090400
F	-0.87637200	-1.92487100	1.69960600
F	0.73040400	-3.10750900	0.91410700
F	-0.60469400	2.68155700	-0.91675400

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m-2-1 carbene fragment

C	1.02890500	1.18481200	-0.08050300
N	-1.16119500	0.05708200	0.10518200
C	-1.78115900	0.07345400	1.48518200
C	2.41675500	1.13246400	-0.12517200
H	2.98182200	2.05554500	-0.14865500
C	-1.94750200	0.03566000	-0.94767000
C	0.94517400	-1.21046700	-0.16020300
C	3.07232500	-0.08214600	-0.15913200
C	0.26245600	0.01071000	-0.04733100
C	-3.24974000	0.29541500	1.10666100
H	-3.52522200	1.33329300	1.30968100
H	-3.90545100	-0.34181600	1.70504800

C	2.33393400	-1.24845400	-0.20176200
H	2.83599200	-2.20372100	-0.28480200
C	-1.22956300	1.19900900	2.34780000
H	-0.15349200	1.09539800	2.51079400
H	-1.71331200	1.15274600	3.32517700
H	-1.43532600	2.17696600	1.91719400
C	-1.53040400	-1.24791500	2.20223800
H	-1.93804100	-2.09725000	1.65761400
H	-2.00437700	-1.21067300	3.18450100
H	-0.46134000	-1.41115500	2.36043700
C	0.49909200	2.60604900	-0.11161900
C	0.32133400	-2.59074500	-0.27504300
C	4.57659700	-0.13569200	-0.14225000
C	-3.36237500	-0.00860200	-0.40112400
C	-4.26967800	0.97516300	-1.14911200
H	-4.44973000	0.56756300	-2.14949100
H	-5.23842000	1.00304700	-0.63956600
C	-3.86167500	-1.45043800	-0.64488900
H	-3.62661500	-1.72204300	-1.67807600
H	-3.29138600	-2.13124400	-0.00929700
F	5.11338400	0.94763500	-0.70654200
F	5.04304500	-0.20071700	1.11079100
F	5.03767300	-1.20722800	-0.78987900
F	0.79571900	3.24282100	1.03289900
F	1.10982900	3.28716900	-1.08957500
F	0.51673200	-3.28953300	0.85532100
F	-0.97468800	-2.61727200	-0.54236600
F	0.93287200	-3.27559900	-1.24976800
F	-0.80402900	2.72799600	-0.31230200
C	-5.34933800	-1.64386600	-0.37850900
H	-5.96199700	-1.12385000	-1.11522500
H	-5.60868900	-2.70217200	-0.42196800
H	-5.63275500	-1.27380000	0.61045200
C	-3.70723700	2.38233400	-1.27250800

H	-2.79625800	2.37743200	-1.87138100
H	-4.42660100	3.04884300	-1.74984900
H	-3.46268100	2.80940200	-0.29641000

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m-2-1 carbene-Au fragment

Au	-1.23709800	0.61568800	-1.82996900
C	1.43358900	1.00544000	0.72664400
N	-0.66804300	-0.26003200	0.95901700
C	-1.11648700	-0.59004400	2.36016900
C	2.79612300	1.05113500	0.45698800
H	3.32682100	1.98810000	0.56530800
C	-1.61032200	-0.10711600	0.06168100
C	1.39469700	-1.30978600	0.08652800
C	3.46310600	-0.07898300	0.03005100
C	0.71843100	-0.19176000	0.59586000
C	-2.63381600	-0.38998600	2.22201700
H	-2.92462500	0.54156500	2.71148900
H	-3.17349100	-1.20314700	2.71215900
C	2.75666900	-1.24793100	-0.17922600
H	3.26116100	-2.12185900	-0.57053900
C	-0.49774500	0.34255300	3.38949000
H	0.59324100	0.27820600	3.38572800
H	-0.84100000	0.03612900	4.37895800
H	-0.79721900	1.37664900	3.23271000
C	-0.73085200	-2.02337200	2.70398700
H	-1.18142300	-2.74355000	2.02340500
H	-1.07478700	-2.24382800	3.71551600
H	0.35392600	-2.15234300	2.68782700
C	0.86410900	2.35706100	1.11672400
C	0.78527700	-2.65847200	-0.25495900
C	4.95103800	-0.04980100	-0.20299500
C	-2.94868900	-0.32707900	0.71368600
C	-3.95286500	0.77318300	0.34540000
H	-4.21785500	0.63854900	-0.70930900

H	-4.86015900	0.59288300	0.92969000
C	-3.45560600	-1.68653500	0.17591700
H	-3.36030600	-1.67453000	-0.91452100
H	-2.79085000	-2.47397400	0.53828400
F	5.38421100	1.18174100	-0.47111700
F	5.61229600	-0.47773000	0.87963700
F	5.30295200	-0.84140800	-1.21696400
F	1.30746600	2.71389000	2.33413900
F	1.29829900	3.28883700	0.26650700
F	1.13782300	-3.57754500	0.65873200
F	-0.53787600	-2.67778000	-0.34738300
F	1.26424000	-3.08469500	-1.42579500
F	-0.45971200	2.43148800	1.13811200
C	-4.88902200	-2.01177500	0.57479100
H	-5.60525300	-1.36405300	0.06982200
H	-5.12908500	-3.04078300	0.30684900
H	-5.04266200	-1.90547400	1.65201500
C	-3.47131200	2.19866600	0.56666500
H	-2.66663500	2.44900500	-0.12662200
H	-4.28574800	2.90460000	0.40267900
H	-3.10219400	2.35513900	1.58366400

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m-3-1 carbene fragment

C	1.71097900	1.20191000	0.01415000
N	-0.33135400	-0.11117900	0.47793300
C	-0.78877600	-0.22008600	1.90999600
C	3.07877500	1.24903400	-0.22687500
H	3.56887200	2.20910000	-0.32525700
C	-1.22521800	-0.11070100	-0.48091400
C	1.79459800	-1.19720000	-0.07572100
C	3.80804300	0.08350300	-0.36826500
C	1.05413100	-0.02913000	0.14514300
C	-2.24517500	-0.61745600	1.66813400
H	-2.89966800	-0.15350500	2.40698200

H	-2.34397900	-1.70339800	1.77369400
C	3.16057800	-1.13650800	-0.31973700
H	3.71283100	-2.05243600	-0.48802400
C	-0.64236900	1.11871000	2.62331900
H	0.40599800	1.42175200	2.67459300
H	-1.00400100	1.01385200	3.64770200
H	-1.21314100	1.90648400	2.13523700
C	-0.00785700	-1.26825700	2.68943500
H	-0.12623900	-2.26432000	2.26894400
H	-0.38526900	-1.29048200	3.71329600
H	1.05641800	-1.02220900	2.73926400
C	1.05698200	2.57175500	0.06185800
C	1.24361000	-2.61181300	-0.12622000
C	5.29849400	0.14541900	-0.57046000
F	5.66019200	1.25115400	-1.22425100
F	5.94521500	0.15125300	0.60156700
F	5.74547200	-0.90458000	-1.26179800
F	1.36915600	3.20902200	1.20155900
F	1.53577500	3.32833500	-0.93372100
F	1.74107700	-3.33764300	0.88875900
F	-0.07757400	-2.72960100	-0.08675200
F	1.65491700	-3.20628300	-1.25247800
F	-0.26359800	2.57682200	-0.05203000
C	-2.57033400	-0.22677500	0.20865100
C	-3.30865400	1.13155300	0.07611600
C	-3.43980500	-1.29362100	-0.48849600
H	-2.70793600	1.91245300	0.55364400
C	-4.68221000	1.05782700	0.74750000
C	-3.51469100	1.48283400	-1.40123500
H	-2.92221700	-2.25731000	-0.40889100
C	-4.79898100	-1.37403700	0.20989600
C	-3.65063400	-0.94514600	-1.96214300
H	-5.17877400	2.02797300	0.63524500
H	-4.59482600	0.86769400	1.82111700

C	-5.52442000	-0.03311600	0.08733100
H	-2.55058500	1.57620700	-1.90524500
H	-4.02869800	2.44864400	-1.46568400
C	-4.36096000	0.40256900	-2.07648200
H	-4.67565000	-1.63799900	1.26638600
H	-5.39776800	-2.16503500	-0.25399700
H	-2.68869300	-0.90951600	-2.47587600
H	-4.26201900	-1.72550500	-2.42960800
H	-6.49624300	-0.09610600	0.58567000
C	-5.72236100	0.31207000	-1.38832800
H	-4.49773300	0.65579500	-3.13162400
H	-6.33499900	-0.45609100	-1.87324600
H	-6.25436300	1.26586900	-1.47746900

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m-3-1 carbene-Au fragment

Au	0.47164400	1.07816200	-1.53906800
C	-1.88704000	-1.37272900	-0.12895700
N	0.13797800	-0.43138600	0.93148800
C	0.58565600	-0.95738600	2.26259500
C	-3.24729500	-1.28544500	-0.40191000
H	-3.73335900	-2.08386100	-0.94706500
C	1.07748600	-0.03565300	0.10009300
C	-1.97349100	0.79963700	0.90308500
C	-3.97219200	-0.17824400	-0.00471300
C	-1.24216300	-0.34786600	0.57103000
C	2.02581100	-0.45197500	2.25331400
H	2.68145900	-1.14119100	2.78328100
H	2.06514600	0.51216100	2.77156100
C	-3.33133800	0.87211100	0.62564600
H	-3.88062000	1.76819500	0.88541200
C	0.47659000	-2.47845000	2.28888100
H	-0.56531200	-2.79254100	2.19683400
H	0.84683400	-2.83866100	3.24995500
H	1.05491800	-2.94915100	1.49692500

C	-0.23034000	-0.40430100	3.42180900
H	-0.13517100	0.67372100	3.52030600
H	0.13795700	-0.85887300	4.34293400
H	-1.28711400	-0.66705700	3.32830200
C	-1.22509000	-2.61842700	-0.68914900
C	-1.42096500	2.07102800	1.52663900
C	-5.45715900	-0.11869900	-0.24976200
F	-5.80645700	-0.82056200	-1.32855100
F	-6.13474000	-0.62538000	0.78823500
F	-5.87724300	1.13525500	-0.41991300
F	-1.52719100	-3.69318200	0.05707600
F	-1.69303500	-2.86565700	-1.91510600
F	-1.95560900	2.24644100	2.74827600
F	-0.09963100	2.12783000	1.66726500
F	-1.78760000	3.12392900	0.79723700
F	0.09846800	-2.55912300	-0.78340700
C	2.41942000	-0.21988200	0.77527200
C	3.15027500	-1.42606500	0.11879800
C	3.35622200	1.00306300	0.65148400
H	2.49805100	-2.30310200	0.14614300
C	4.44875700	-1.72409900	0.87270700
C	3.50090600	-1.10895300	-1.33876600
H	2.83876100	1.86984300	1.07988800
C	4.63495200	0.70526900	1.44466600
C	3.75881000	1.30450300	-0.79136000
H	4.94737400	-2.56660300	0.38143700
H	4.25674600	-2.03100600	1.90409300
C	5.36089300	-0.49855000	0.83673200
H	2.59371100	-0.90134500	-1.91438400
H	3.98141400	-1.98845700	-1.78065100
C	4.44772300	0.08972400	-1.40473100
H	4.41080300	0.51649800	2.49957600
H	5.28557100	1.58477900	1.40749300
H	2.88988900	1.59257200	-1.39034700

H	4.44486100	2.15886600	-0.78651800
H	6.26900700	-0.70227100	1.41111300
C	5.72359200	-0.20537200	-0.61837500
H	4.69449600	0.29838900	-2.44893700
H	6.39942600	0.65484600	-0.67226300
H	6.24663800	-1.06623300	-1.04927200

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m-4-1 carbene fragment

C	1.23939900	1.21279500	-0.11960900
N	-0.89241600	-0.00935100	0.16453400
C	-1.50520100	-0.03649300	1.54328000
C	2.62667900	1.20146300	-0.20700000
H	3.16192600	2.13868000	-0.28866200
C	-1.67913000	-0.03363700	-0.88603700
C	1.23737100	-1.18911200	-0.09746800
C	3.31995000	0.00630700	-0.21670500
C	0.52362700	0.01348800	-0.01273000
C	-2.94507400	-0.39980800	1.17039100
H	-3.65690600	0.15169800	1.78816700
H	-3.10871700	-1.46742000	1.34971900
C	2.62296200	-1.18713800	-0.18877400
H	3.15395000	-2.12857100	-0.25386900
C	-1.38840100	1.33085200	2.20620700
H	-0.34165400	1.60846300	2.35023500
H	-1.85443900	1.28495700	3.19199800
H	-1.88236500	2.10885800	1.62722000
C	-0.84876800	-1.06748400	2.45018100
H	-0.95476500	-2.07901000	2.06492800
H	-1.33571100	-1.02864400	3.42617600
H	0.21153000	-0.85003800	2.60545300
C	0.64107300	2.60593600	-0.20009800
C	0.64193700	-2.58593000	-0.14550900
C	4.82493000	0.00106700	-0.25198500
F	5.30746700	1.08777300	-0.85710300

F	5.33688200	-0.02278700	0.98475200
F	5.29728100	-1.06961400	-0.89338300
F	0.87241800	3.28678400	0.93432900
F	1.24332000	3.29315500	-1.17869100
F	1.00641300	-3.27941000	0.94599400
F	-0.67997200	-2.66040000	-0.23710500
F	1.14382800	-3.24471700	-1.19638200
F	-0.66091800	2.65426600	-0.43902300
C	-3.08692700	-0.10581700	-0.33894600
C	-3.76431900	1.24434300	-0.63525800
C	-3.85521700	-1.21079900	-1.07102200
C	-5.24584900	1.23584200	-0.27360900
H	-3.64847900	1.44379200	-1.70614500
H	-3.24413800	2.04923700	-0.10839700
C	-5.32178200	-1.23461400	-0.66073600
H	-3.77479900	-1.02187600	-2.14679800
H	-3.37333400	-2.17409500	-0.87751700
C	-5.97748800	0.10271400	-0.98226500
H	-5.69007900	2.20068300	-0.52882300
H	-5.36595200	1.11527200	0.80948500
H	-5.84087300	-2.05121100	-1.16719700
H	-5.40247400	-1.42872400	0.41663200
H	-7.03361200	0.09573100	-0.70338600
H	-5.93130100	0.26837400	-2.06529500

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m-4-1 carbene-Au fragment

Au	-0.92550000	-1.11737100	-1.63266400
C	1.57860300	1.36154000	-0.16146300
N	-0.52887400	0.50394800	0.80725000
C	-1.05835200	1.07606700	2.09173100
C	2.94738500	1.22496500	-0.36074000
H	3.48700700	1.99510000	-0.89618700
C	-1.42365400	0.12290200	-0.07988300
C	1.54095400	-0.78630700	0.92289100

C	3.61470200	0.10530600	0.09878900
C	0.86529000	0.37603100	0.53002400
C	-2.52593100	0.64477600	1.98970600
H	-3.18492200	1.42035800	2.38360200
H	-2.67851800	-0.25906200	2.58745000
C	2.90888500	-0.90851500	0.71837900
H	3.41485500	-1.81409900	1.02806400
C	-0.88576000	2.59098500	2.08905700
H	0.17158700	2.86198100	2.05267200
H	-1.29947100	2.99253000	3.01534700
H	-1.39702500	3.05883400	1.24997900
C	-0.35603800	0.51558600	3.31920700
H	-0.51679500	-0.55275700	3.43686900
H	-0.75921400	1.01542500	4.20139900
H	0.71781200	0.71820000	3.29137900
C	0.99135900	2.61977000	-0.77527100
C	0.91746000	-2.01972100	1.55605100
C	5.10782600	-0.00446700	-0.06733000
F	5.53087400	0.64670600	-1.15160600
F	5.74683700	0.52234100	0.98478900
F	5.49899100	-1.27489400	-0.17068700
F	1.29753900	3.69563200	-0.03207600
F	1.52936000	2.82709700	-1.98009500
F	1.36953400	-2.16086100	2.81480300
F	-0.41064300	-2.04115300	1.61344600
F	1.30249400	-3.10789500	0.88989900
F	-0.32616100	2.60785800	-0.93509300
C	-2.79471500	0.31828100	0.50467600
C	-3.47845100	1.45877700	-0.27367700
C	-3.63491100	-0.95435500	0.34278000
C	-4.92057300	1.66976800	0.17411500
H	-3.45722200	1.18540600	-1.33503200
H	-2.90282800	2.38278700	-0.17490600
C	-5.05475700	-0.73672400	0.84842400

H	-3.65783200	-1.21642100	-0.72108700
H	-3.14135200	-1.78134300	0.86219600
C	-5.72601400	0.38152900	0.06052400
H	-5.37367600	2.46250600	-0.42490200
H	-4.94225600	2.01578100	1.21410300
H	-5.62418100	-1.66427400	0.76453800
H	-5.03552800	-0.47301100	1.91361900
H	-6.74982900	0.53990900	0.40583600
H	-5.78325700	0.08617800	-0.99359100

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m-5-1 carbene fragment

C	1.18837700	1.20894400	-0.11979300
N	-0.94611800	-0.01316600	0.11500900
C	-1.58734900	-0.04427500	1.48294100
C	2.57706200	1.20040700	-0.17926300
H	3.11254000	2.13871500	-0.24510100
C	-1.71051100	-0.02539700	-0.95207900
C	1.18961300	-1.19346100	-0.11157000
C	3.27211400	0.00611400	-0.18150800
C	0.47314200	0.00765200	-0.03359800
C	-3.02186900	-0.39005900	1.07512700
H	-3.75702800	0.15316200	1.67366300
H	-3.18698300	-1.46150400	1.22970200
C	2.57682500	-1.18864600	-0.17484100
H	3.11074400	-2.12872300	-0.23496400
C	-1.45877500	1.31047300	2.16886600
H	-0.40985900	1.55953300	2.34640000
H	-1.95298800	1.26030500	3.14051100
H	-1.91576800	2.11117100	1.59140300
C	-0.96167900	-1.09643200	2.38778400
H	-1.07608200	-2.10117000	1.98752600
H	-1.46454800	-1.06234700	3.35583000
H	0.09897400	-0.89703600	2.56353500
C	0.58785700	2.60127900	-0.20461400

C	0.59562900	-2.58998600	-0.17922400
C	4.77759300	0.00359000	-0.18589800
F	5.27035700	1.09360100	-0.77660000
F	5.26381600	-0.02428400	1.06104100
F	5.26492000	-1.06363800	-0.82170100
F	0.78880200	3.27453700	0.93973700
F	1.21162900	3.29700500	-1.16333000
F	0.92704600	-3.28590900	0.92098900
F	-0.72319300	-2.66218300	-0.31020000
F	1.12738000	-3.24722400	-1.21626200
F	-0.70855600	2.64834100	-0.47547300
C	-3.12730100	-0.06987100	-0.42949500
C	-3.76384600	1.30147200	-0.69973000
C	-3.93656100	-1.12627200	-1.18367200
C	-5.25366500	1.26692500	-0.52449400
H	-3.50090400	1.62036000	-1.71484200
H	-3.33247200	2.05344000	-0.03186500
C	-5.35141300	-1.21685100	-0.62642800
H	-3.96422700	-0.84139400	-2.23913300
H	-3.42995000	-2.09363600	-1.12078600
C	-5.96309200	0.14304500	-0.46907900
H	-5.75973300	2.22249900	-0.43104100
H	-5.97517600	-1.82825300	-1.28374200
H	-5.35060500	-1.73428900	0.34141900
H	-7.03582800	0.19720100	-0.31399700

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m-5-1 carbene-Au fragment

Au	-0.95661000	-1.15344300	-1.63789300
C	1.54556700	1.36159900	-0.17019000
N	-0.57136400	0.51102900	0.77789600
C	-1.12247200	1.09471100	2.04976000
C	2.91685900	1.22613300	-0.35137700
H	3.46188100	1.99215400	-0.88719300
C	-1.45142000	0.13227400	-0.12652700

C	1.49878900	-0.77615500	0.93448500
C	3.58057800	0.11202400	0.12713100
C	0.82611100	0.38105400	0.52249000
C	-2.58957600	0.66978700	1.91870900
H	-3.26910500	1.43788400	2.29382000
H	-2.74628000	-0.23997400	2.50668700
C	2.86955400	-0.89727300	0.74796500
H	3.37370700	-1.79862300	1.07253100
C	-0.92949600	2.60722200	2.05000100
H	0.13279400	2.86137000	2.05493300
H	-1.37262700	3.01659800	2.95898200
H	-1.39816600	3.08368600	1.19165100
C	-0.45082300	0.53116100	3.29334100
H	-0.62852500	-0.53412000	3.41396100
H	-0.86311200	1.04190900	4.16502200
H	0.62608800	0.71873000	3.28440900
C	0.96224600	2.61449500	-0.79936400
C	0.86870000	-2.00380700	1.57214700
C	5.07584400	0.00398200	-0.02027300
F	5.50959800	0.64193000	-1.10821800
F	5.70140800	0.54632200	1.03193600
F	5.47127900	-1.26666100	-0.10250200
F	1.24675100	3.69451900	-0.05418100
F	1.52204000	2.82126300	-1.99437500
F	1.29658700	-2.12669300	2.84104300
F	-0.46007000	-2.03021200	1.60329500
F	1.27122700	-3.09899300	0.92777300
F	-0.35229100	2.59436200	-0.98544700
C	-2.82914900	0.35197700	0.42944200
C	-3.47885200	1.50975000	-0.34467100
C	-3.70962700	-0.88793000	0.24788300
C	-4.94185400	1.62549600	-0.03169900
H	-3.32297300	1.34227700	-1.41721000
H	-2.97352400	2.45158000	-0.11221800

C	-5.06364900	-0.67326100	0.91178500
H	-3.83657700	-1.06142700	-0.82504500
H	-3.20127800	-1.76566300	0.65705400
C	-5.64702400	0.65946100	0.54992100
H	-5.42764400	2.55901000	-0.29556100
H	-5.75058200	-1.46953400	0.61489900
H	-4.97617700	-0.75389700	2.00260000
H	-6.69677100	0.82408900	0.76931200

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m-6-1 carbene fragment

C	-1.74932500	-1.22870200	-0.21308900
N	0.36357800	-0.03720500	0.27869500
C	0.88503400	-0.12226700	1.69533800
C	-3.13320500	-1.23017600	-0.34466200
H	-3.64707000	-2.16547200	-0.52464900
C	1.22904400	-0.03337200	-0.71346500
C	-1.79153600	1.15486900	0.03180900
C	-3.85071200	-0.05326300	-0.26770300
C	-1.04834400	-0.03557500	0.02799800
C	2.37569800	0.11936300	1.42777500
H	2.99594300	-0.49187600	2.08696300
H	2.59984500	1.16730900	1.63633300
C	-3.17445300	1.13873300	-0.10511000
H	-3.71832000	2.07476200	-0.09686000
C	0.57314200	-1.48465200	2.30503400
H	-0.50654700	-1.63100100	2.39232600
H	0.99015000	-1.52343300	3.31271900
H	0.99036900	-2.30791800	1.73011200
C	0.28382300	0.94366200	2.60030300
H	0.52312200	1.94925500	2.26162700
H	0.70071700	0.81879400	3.60138300
H	-0.80118900	0.83855200	2.68426100
C	-1.15489000	-2.61687800	-0.37746200
C	-1.24565500	2.56538400	0.14256100

C	-5.35363900	-0.06997000	-0.35061200
F	-5.79427800	-1.09225700	-1.08582900
F	-5.90253900	-0.19110400	0.86419800
F	-5.82814800	1.05612100	-0.88643500
F	-1.43261700	-3.37548700	0.69577200
F	-1.72618300	-3.22537600	-1.42479900
F	-1.62430100	3.12415600	1.30319500
F	0.07079800	2.68056000	0.05431200
F	-1.76848900	3.32405500	-0.82876600
F	0.15232500	-2.66440600	-0.57320600
C	2.59864000	-0.17491200	-0.06693400
C	3.02464500	-1.63867200	-0.31082700
C	3.62230100	0.72836600	-0.78080600
C	4.45415000	-1.94484500	0.12629400
H	2.93041300	-1.84591600	-1.38462600
H	2.34446000	-2.32284300	0.19850900
C	5.04437300	0.44602300	-0.30884200
H	3.56366900	0.40396400	-1.83003400
C	5.42556200	-1.00234200	-0.56697300
H	4.53545700	-1.77356700	1.20858900
H	5.73890100	1.12032500	-0.81955400
H	5.13014700	0.66203800	0.76435600
H	6.44823300	-1.20618100	-0.23617900
H	5.39089600	-1.20048000	-1.64673100
C	4.78989600	-3.40025500	-0.16254400
H	5.80671400	-3.64176800	0.15390800
H	4.10275600	-4.07913900	0.34691700
H	4.71722400	-3.59429900	-1.23653300
C	3.26667900	2.23148900	-0.77168500
H	2.19257800	2.30826600	-0.58649200
C	3.99594000	3.07363800	0.27598300
H	3.90884600	2.68492000	1.29153700
H	5.06168000	3.14265500	0.04303400
H	3.59653800	4.08987600	0.27353000

C	3.54426600	2.82443600	-2.14974600
H	4.59830500	2.68265200	-2.41194500
H	2.93576000	2.33736300	-2.91349000
H	3.33763500	3.89673400	-2.17166600

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m-6-1 carbene-Au fragment

Au	-0.63106100	-0.75781900	-1.82456700
C	1.97529600	1.36308100	0.03915600
N	-0.12636600	0.34857400	0.86926600
C	-0.62252600	0.70124900	2.24556600
C	3.34566600	1.28452800	-0.17614200
H	3.87072300	2.14376000	-0.57246300
C	-1.04772500	0.19836000	-0.06156500
C	1.97553100	-0.92931400	0.75427800
C	4.03600000	0.11833100	0.09225000
C	1.26999300	0.26584900	0.55694300
C	-2.12203600	0.42337500	2.06456700
H	-2.72343800	1.14207600	2.62413600
H	-2.33527200	-0.57208800	2.45615500
C	3.34648500	-0.99180800	0.53441200
H	3.86657900	-1.92726500	0.69547600
C	-0.29516700	2.15693600	2.56202500
H	0.78635000	2.30705400	2.60301800
H	-0.69909700	2.40018300	3.54581100
H	-0.71489900	2.85018000	1.83713300
C	-0.00036100	-0.16330600	3.33257400
H	-0.26248900	-1.21284400	3.22656600
H	-0.37463700	0.18216900	4.29774300
H	1.08791600	-0.06219900	3.35003000
C	1.39266700	2.71037300	-0.34903400
C	1.39671800	-2.26590500	1.18008400
C	5.53050100	0.07071800	-0.08866600
F	5.92505500	0.83879700	-1.10529800
F	6.15971000	0.51282900	1.00720600

F	5.95975400	-1.17012600	-0.31848100
F	1.69492300	3.63765100	0.57411800
F	1.93925100	3.12579200	-1.49509300
F	1.84039100	-2.58861000	2.40730700
F	0.07262300	-2.33638700	1.20844500
F	1.82558800	-3.22402600	0.35716500
F	0.07804100	2.73144400	-0.51872900
C	-2.40577700	0.44927700	0.55065500
C	-2.82981400	1.84906400	0.04789900
C	-3.46178700	-0.56154300	0.05498600
C	-4.23388300	2.25828200	0.47996100
H	-2.78582500	1.83716800	-1.04938200
H	-2.11644600	2.60467700	0.37965300
C	-4.85752900	-0.16038900	0.52210400
H	-3.44124600	-0.44664900	-1.03977300
C	-5.24008000	1.21877700	0.01272500
H	-4.26992400	2.29344600	1.57753300
H	-5.57817800	-0.90833500	0.17905800
H	-4.89648400	-0.16967500	1.61949200
H	-6.24622500	1.49410200	0.34135400
H	-5.24946700	1.21260800	-1.08521600
C	-4.56493600	3.64025100	-0.06318900
H	-5.56537900	3.95343900	0.24158000
H	-3.85125900	4.39014100	0.28421200
H	-4.53459000	3.62952300	-1.15630700
C	-3.14792600	-2.04833100	0.33922700
H	-2.06432700	-2.14261900	0.45223600
C	-3.81904600	-2.63904400	1.58085800
H	-3.65388100	-2.06640400	2.49452100
H	-4.89961500	-2.71567200	1.43550600
H	-3.44306900	-3.64970400	1.75055300
C	-3.55751800	-2.88330200	-0.87074100
H	-4.62224100	-2.73927500	-1.08378800
H	-2.98500200	-2.59180500	-1.75484500

H -3.39470300 -3.94765200 -0.68943200

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n-1-1 carbene fragment

C 0.61378100 1.18654100 -0.02858400
N -1.39389700 -0.16451300 -0.14261900
C -2.13608900 -0.69733900 1.05303400
C 1.99310400 1.28566900 -0.03507200
C -2.07770400 0.40072400 -1.11205200
C 0.82908000 -1.20177100 -0.23267000
C 2.82483200 0.18550300 -0.13730400
C 0.03097000 -0.07165500 -0.12509900
C -3.56789500 -0.66006700 0.51253500
H -4.26917400 -0.31308100 1.27476700
H -3.87041600 -1.66871700 0.21748300
C 2.20606700 -1.04505600 -0.23420300
C -1.90245000 0.24538500 2.22823700
H -0.84366000 0.27285400 2.49863700
H -2.46141300 -0.10341800 3.09797500
H -2.22622600 1.25983600 1.99177600
C -1.70180400 -2.10517600 1.43067000
H -1.76158700 -2.77842500 0.57336200
H -2.37238300 -2.48258400 2.20476300
H -0.68755500 -2.12534900 1.83502500
C -3.53389900 0.25860100 -0.72637000
C -4.03471500 1.67348400 -0.41745600
H -3.92815900 2.31063000 -1.29597600
H -5.08984100 1.63511100 -0.13456200
H -3.47853900 2.13408600 0.40184700
C -4.33610500 -0.31187700 -1.89061800
H -5.38942700 -0.40520700 -1.61248200
H -4.25914900 0.34330500 -2.75910600
H -3.96788900 -1.29987800 -2.17474800
H -0.00371600 2.07225400 0.03284100
H 3.89997100 0.28403300 -0.14402400

H	0.40433400	-2.18866400	-0.34266600
N	2.60625700	2.62114800	0.07580200
O	3.81767500	2.68023500	0.03753300
O	1.85684800	3.56759700	0.20145700
N	3.04826700	-2.24813800	-0.35342800
O	4.25003100	-2.08579500	-0.37739200
O	2.48012000	-3.32004500	-0.41578500

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n-1-1 carbene-Au fragment

Au	1.43738700	-1.41855400	-0.79120200
C	-1.21053500	-0.36415400	1.06123800
N	0.58923000	1.13260000	0.40828600
C	0.98129500	2.18103200	1.39621000
C	-2.52630000	-0.77253800	0.92305900
C	1.57713100	0.53385900	-0.23731000
C	-1.60579800	1.31115600	-0.62977900
C	-3.40333200	-0.18643000	0.02903400
C	-0.76158700	0.69514900	0.27956600
C	2.43357300	2.42582500	0.96776900
H	3.07585900	2.61590300	1.82953600
H	2.47061700	3.30629400	0.32049000
C	-2.91174300	0.85615200	-0.73219600
C	0.84962800	1.62730100	2.81057500
H	-0.19467500	1.40931400	3.04594300
H	1.20694600	2.36703500	3.52871800
H	1.43190300	0.71330500	2.93392600
C	0.11302000	3.41858600	1.23790800
H	0.14056300	3.78546300	0.21009900
H	0.48832100	4.20589500	1.89348900
H	-0.92408800	3.21688000	1.51487800
C	2.87974000	1.18208300	0.17193700
C	3.69771500	0.20744400	1.02587900
H	3.97795300	-0.66754600	0.43762100
H	4.60579000	0.70933500	1.36958400

H	3.14193800	-0.14386700	1.89652900
C	3.68708300	1.54694900	-1.07089900
H	4.61899100	2.03856100	-0.78092400
H	3.92786200	0.64454900	-1.63617800
H	3.12673500	2.22111700	-1.72134600
H	-0.54933800	-0.86674600	1.75452600
H	-4.42360800	-0.52693700	-0.06794400
H	-1.26107700	2.12081100	-1.25758500
N	-3.01186000	-1.87965000	1.76206800
O	-4.14812200	-2.26234400	1.57351100
O	-2.24219400	-2.32775600	2.58708500
N	-3.81309900	1.51622700	-1.68974400
O	-4.94188200	1.08156500	-1.78266000
O	-3.36323800	2.45324700	-2.31900700

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o-1-1 carbene fragment

C	1.03745000	1.21702600	-0.02147900
N	-0.96613700	-0.13678300	-0.15682000
C	-1.68578900	-0.68330300	1.04625300
C	2.42448000	1.34940100	-0.03523100
C	-1.66919000	0.42933500	-1.11144400
C	1.25839100	-1.15873200	-0.32131600
C	3.23872600	0.22946800	-0.18918800
C	0.45966900	-0.03749200	-0.15863800
C	-3.12654800	-0.65179900	0.53003500
H	-3.81750900	-0.31462700	1.30601900
H	-3.42766000	-1.66029500	0.23291600
C	2.64797900	-1.02141000	-0.33544100
C	-1.44007000	0.25015400	2.22644100
H	-0.37743900	0.28285400	2.48027400
H	-1.98327100	-0.11034100	3.10142300
H	-1.77516300	1.26422600	2.00417600
C	-1.23455400	-2.09088000	1.40428200
H	-1.31097500	-2.75809800	0.54347700

H	-1.88401900	-2.47829300	2.19134900
H	-0.21054700	-2.10600200	1.78337700
C	-3.11840500	0.27549300	-0.70278700
C	-3.62332300	1.68464700	-0.37588100
H	-3.53419100	2.32881200	-1.25127300
H	-4.67368400	1.63814100	-0.07685600
H	-3.05717800	2.14247200	0.43825500
C	-3.93566800	-0.29219500	-1.85783900
H	-4.98379400	-0.39479800	-1.56365700
H	-3.87696800	0.36946100	-2.72286100
H	-3.56530900	-1.27560900	-2.15491400
H	4.31496500	0.33179200	-0.20101700
H	0.39686100	2.08412700	0.07720500
H	0.81123200	-2.13280200	-0.46398800
C	3.01928000	2.64796100	0.11306500
C	3.47184400	-2.18460900	-0.50898700
N	3.49664400	3.68881500	0.23813500
N	4.12792500	-3.12194700	-0.64345500

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o-1-1 carbene-Au fragment

Au	1.19330800	-1.55002500	-0.39973300
C	-1.56396700	-0.17364200	1.09092900
N	0.21319900	1.18199900	0.13778600
C	0.54689800	2.44800600	0.85559000
C	-2.87190400	-0.65651000	1.05339300
C	1.23717100	0.48365300	-0.32827700
C	-1.95879700	1.04277900	-0.95216500
C	-3.72689700	-0.29652600	0.01434100
C	-1.12268400	0.68341800	0.09113500
C	2.00028600	2.63985700	0.40565800
H	2.61414800	3.05355800	1.20780000
H	2.02433300	3.34240500	-0.43192100
C	-3.26536400	0.55133300	-0.98817800
C	0.39809500	2.24025300	2.35869500

H	-0.64458600	2.04659400	2.62094200
H	0.71415800	3.14128500	2.88681500
H	1.00588300	1.40326100	2.70486000
C	-0.35577800	3.58168600	0.39640200
H	-0.31108900	3.70016400	-0.68796900
H	-0.02301700	4.51331200	0.85673900
H	-1.39312500	3.41157800	0.69276800
C	2.50688600	1.26081300	-0.06326100
C	3.33798900	0.55178700	1.01128300
H	3.66373700	-0.42607100	0.65387100
H	4.21853200	1.15798000	1.23935600
H	2.77357300	0.39577700	1.93183300
C	3.33163200	1.35042300	-1.34444500
H	4.23937800	1.93219200	-1.16587500
H	3.61578200	0.34923200	-1.67426100
H	2.76486600	1.82859600	-2.14558500
H	-4.73946600	-0.67474300	-0.01430900
H	-0.88597100	-0.47197000	1.88068200
H	-1.59469100	1.69170400	-1.73779800
C	-3.34140600	-1.52907100	2.09211800
C	-4.13695200	0.92889100	-2.06435500
N	-3.72320400	-2.22019200	2.93077400
N	-4.83356700	1.24022700	-2.92744600

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p-1-1 carbene fragment

C	0.00679500	1.14244000	-0.01454800
N	-1.98767200	-0.23401800	-0.12057200
C	-2.74485100	-0.64694200	1.11224500
C	1.38834900	1.26669300	0.02361300
C	-2.65846900	0.19917600	-1.16309300
C	0.24551500	-1.24828100	-0.11027700
C	2.22096300	0.15631900	0.00434000
C	-0.56442800	-0.12195200	-0.08017900
C	-4.16538600	-0.69836500	0.54408100

H	-4.88836600	-0.28045600	1.24828600
H	-4.44478800	-1.73947300	0.35967400
C	1.62587200	-1.09378700	-0.07123300
C	-2.55443200	0.42110500	2.18341400
H	-1.50326400	0.50051800	2.47166300
H	-3.12661600	0.15516700	3.07365100
H	-2.89200700	1.39757400	1.83326500
C	-2.28693400	-1.99618800	1.64460300
H	-2.33006000	-2.76050500	0.86622000
H	-2.95380700	-2.29914000	2.45385000
H	-1.27360000	-1.95404800	2.04961000
C	-4.12087700	0.07504700	-0.79017100
C	-4.65035200	1.50606300	-0.65209500
H	-4.53515400	2.04278800	-1.59444800
H	-5.71053500	1.48146200	-0.38680700
H	-4.11814700	2.06480800	0.12071100
C	-4.89000900	-0.63785400	-1.89657400
H	-5.94709900	-0.71952000	-1.62894700
H	-4.80664300	-0.08319200	-2.83206000
H	-4.49942900	-1.64440200	-2.06059200
H	-0.63073300	2.01809800	0.01081500
H	3.29590700	0.26195200	0.07644500
H	-0.18597100	-2.23893800	-0.16781000
S	2.08989000	2.87287600	0.13978900
O	1.22310800	3.67835200	0.91622200
O	3.47642800	2.73608300	0.42841400
S	2.63091600	-2.53325500	-0.09230900
O	3.95535400	-2.16516800	0.27376100
O	1.92027400	-3.57460900	0.55205100
O	2.65568600	-2.91511700	-1.62503900
H	3.45291500	-2.55297000	-2.04264200
O	1.96619000	3.41126800	-1.33908000
H	2.79134700	3.24714900	-1.82196200

p-1-1 carbene-Au fragment

Au	-1.62899500	1.09236000	-1.11663100
C	0.47970800	0.47985500	1.04633800
N	-1.08353500	-1.29514700	0.60289400
C	-1.58863300	-2.31207300	1.57909500
C	1.71591000	1.07102500	0.85374500
C	-1.98569300	-0.69530000	-0.13216400
C	1.30305600	-1.56195900	0.06612900
C	2.77282300	0.35765200	0.30422400
C	0.26757700	-0.82144900	0.60650100
C	-3.02489400	-2.49542000	1.07051800
H	-3.72767200	-2.59054400	1.90005100
H	-3.08314400	-3.41047700	0.47559300
C	2.55331300	-0.96288200	-0.05644400
C	-1.50424900	-1.71364000	2.97807300
H	-0.46757000	-1.48724900	3.23798300
H	-1.88615900	-2.43069900	3.70587600
H	-2.08985200	-0.79649000	3.05414400
C	-0.77789000	-3.59534500	1.50960200
H	-0.74991700	-3.98783900	0.49148900
H	-1.24861000	-4.34278200	2.15001700
H	0.24334600	-3.44648900	1.86539100
C	-3.33777200	-1.27686700	0.17819000
C	-4.14650500	-0.19750500	0.90747600
H	-4.28995700	0.66844500	0.25898500
H	-5.12349400	-0.60417400	1.17796200
H	-3.64944600	0.14334200	1.81749500
C	-4.05812200	-1.65622600	-1.11179300
H	-5.03662900	-2.08216200	-0.87874100
H	-4.19942000	-0.77104900	-1.73500600
H	-3.48749300	-2.39130000	-1.68228200
H	-0.34196100	1.03935700	1.47685500
H	3.73721200	0.82521900	0.14947700
H	1.15003700	-2.57122100	-0.29293000

S	1.90701100	2.79093600	1.19271600
O	2.07074000	3.00250800	2.58373700
O	2.85499600	3.28318100	0.25564100
S	3.86332100	-1.89999100	-0.75738700
O	5.09360500	-1.27020600	-0.42565700
O	3.60676500	-3.26814100	-0.49616400
O	3.63379000	-1.71183500	-2.30692400
H	4.15000700	-0.95773800	-2.63413400
O	0.47469000	3.32487800	0.85729500
H	0.16230700	3.10605900	-0.05022200

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q-1-1 carbene fragment

C	-0.31950200	1.12812800	-0.14253000
N	-2.38023400	-0.17123700	-0.09623300
C	-3.11220100	0.04806600	1.19852200
C	1.07694400	1.18814500	-0.11892500
C	-3.06318300	-0.45508600	-1.17889500
C	-0.21122100	-1.27694200	-0.08655200
C	1.81562900	0.02452900	-0.08428300
C	-0.95158200	-0.09474500	-0.11183400
C	-4.52569100	-0.36863500	0.77953400
H	-5.27885700	0.31337900	1.18076500
H	-4.74086100	-1.36743300	1.16985900
C	1.16725700	-1.21545400	-0.07645100
C	-3.01974400	1.50544100	1.63664200
H	-1.99335900	1.77819500	1.89372100
H	-3.63420700	1.65215400	2.52672000
H	-3.37871100	2.17855500	0.85640000
C	-2.53265700	-0.84997200	2.28219400
H	-2.53329700	-1.89376500	1.96090200
H	-3.14037200	-0.76714000	3.18504700
H	-1.50992000	-0.56044800	2.53484400
C	-4.52013800	-0.40294200	-0.76258500
C	-5.09445600	0.87998800	-1.37096300

H	-4.98832700	0.86359900	-2.45643000
H	-6.15557700	0.96373900	-1.12164500
H	-4.58240500	1.76879700	-0.99582500
C	-5.27619200	-1.60435000	-1.31608200
H	-6.32619400	-1.56507300	-1.01251300
H	-5.22547000	-1.61234900	-2.40568200
H	-4.84840800	-2.53983300	-0.94897500
C	1.70858700	2.56572800	-0.12764900
C	2.04365200	-2.45247300	-0.04815700
H	2.89647300	0.05725600	-0.06670600
H	-0.90427200	2.03779300	-0.20019600
H	-0.73926200	-2.22011500	-0.08866900
Cl	1.12037100	3.48192200	1.27638600
Cl	1.22182800	3.42855800	-1.59521000
Cl	3.46385500	2.52759200	-0.06118000
Cl	3.05746500	-2.41858400	1.40738000
Cl	1.12591100	-3.95230400	-0.04299400
Cl	3.10654900	-2.45572700	-1.46496400

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q-1-1 carbene-Au fragment

Au	-2.36148000	0.59006100	-1.40828500
C	0.27770200	0.76876600	0.71106700
N	-1.36292600	-0.99886400	0.89179800
C	-1.72401800	-1.45945800	2.26610100
C	1.57456100	1.20260000	0.43028400
C	-2.36475500	-0.84648800	0.04472900
C	0.92094800	-1.49498500	0.17874000
C	2.53015100	0.29158000	0.02852800
C	-0.03384300	-0.56877000	0.59144100
C	-3.14276900	-1.98289700	2.01577700
H	-3.79972200	-1.77385100	2.86217700
H	-3.10471900	-3.06738300	1.88021900
C	2.20325700	-1.06166800	-0.09979800
C	-1.67315300	-0.27409800	3.22436600

H	-0.65506000	0.11457000	3.30565200
H	-1.99425500	-0.59147300	4.21789200
H	-2.32561900	0.53306600	2.88862100
C	-0.77850700	-2.55075600	2.74117100
H	-0.74994300	-3.37863800	2.03007500
H	-1.13039300	-2.93437800	3.70029800
H	0.23467600	-2.16826200	2.88136700
C	-3.63609700	-1.31627800	0.71570900
C	-4.55234900	-0.11871300	0.98763400
H	-4.86497800	0.33889800	0.04795300
H	-5.43790100	-0.46219600	1.52885600
H	-4.05755400	0.65152900	1.58122700
C	-4.36544400	-2.29639000	-0.19918200
H	-5.27477800	-2.65775600	0.28779500
H	-4.63945900	-1.79976200	-1.13207300
H	-3.73522300	-3.15506400	-0.43879700
C	1.85355100	2.68496900	0.58088800
C	3.30648000	-2.00045400	-0.54747600
H	3.53810100	0.61508700	-0.19373500
H	-0.49372800	1.47246500	1.00297000
H	0.63990700	-2.53288600	0.07195300
Cl	1.51388900	3.16687900	2.25750900
Cl	0.78051700	3.58991800	-0.49044700
Cl	3.51716800	3.11788000	0.21234200
Cl	4.64327300	-1.92994800	0.61641200
Cl	2.78016700	-3.67481000	-0.67580700
Cl	3.91638300	-1.48688900	-2.12767700

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r-1-1 carbene fragment

C	0.25919900	1.15140400	-0.06179900
N	-1.75193900	-0.20344500	-0.12820500
C	-2.48482500	-0.57595600	1.13088800
C	1.64467300	1.26795700	-0.05846500
C	-2.44434900	0.19209900	-1.17116400

C	0.47107500	-1.24145800	-0.18117100
C	2.44922200	0.14434300	-0.11504200
C	-0.32510500	-0.10235800	-0.11717900
C	-3.91720900	-0.64523900	0.59570700
H	-4.62578900	-0.20458900	1.30084800
H	-4.20053100	-1.69157900	0.45051800
C	1.84920800	-1.10840000	-0.18039000
C	-2.27497100	0.52251200	2.16726300
H	-1.21830300	0.61060300	2.43157700
H	-2.83025300	0.28265800	3.07558400
H	-2.62090400	1.48772000	1.79460100
C	-2.01381100	-1.90801900	1.69436800
H	-2.07695500	-2.69558700	0.94088000
H	-2.65823600	-2.18550200	2.53057600
H	-0.98935000	-1.85053700	2.06834700
C	-3.89926100	0.08452200	-0.76332100
C	-4.42403700	1.51998900	-0.66056200
H	-4.32587700	2.02603100	-1.62165100
H	-5.47895600	1.50692000	-0.37402600
H	-3.87543700	2.10167700	0.08347900
C	-4.69261900	-0.66223200	-1.82944800
H	-5.74404700	-0.73386300	-1.53735500
H	-4.62800500	-0.13835500	-2.78394400
H	-4.30603600	-1.67399800	-1.96930100
C	2.23962200	2.64888600	0.00583900
C	2.74232900	-2.31780200	-0.24648000
H	3.52755700	0.23586700	-0.11500600
H	-0.37439300	2.03054100	-0.03724000
H	0.01366300	-2.21839900	-0.25525100
F	1.88317000	3.38367000	-1.05248700
F	1.81490800	3.30658400	1.09283000
F	3.57229900	2.62236000	0.04819400
F	2.05007400	-3.45057900	-0.38018700
F	3.59380500	-2.24035500	-1.27461000

F 3.48580700 -2.43134600 0.86187500

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r-1-1 carbene-Au fragment

Au	1.80197400	-1.11501100	-1.12628100
C	-0.92649500	-0.62108500	0.92840300
N	0.83573900	1.03328300	0.66951300
C	1.19099800	1.83006400	1.88154500
C	-2.23494400	-1.03333700	0.70593500
C	1.84399600	0.64030500	-0.09013100
C	-1.37534600	1.40879200	-0.28962200
C	-3.11598700	-0.24073100	-0.00950500
C	-0.50641100	0.60491400	0.43604400
C	2.63487100	2.21745200	1.54074100
H	3.26814100	2.21672400	2.42987200
H	2.64407900	3.22795700	1.12282300
C	-2.67527500	0.97969100	-0.50691900
C	1.07316800	0.95272400	3.12291500
H	0.03679600	0.64683900	3.28306500
H	1.39735800	1.51417100	4.00072000
H	1.69042600	0.05776800	3.03506400
C	0.28332900	3.04218900	2.01598900
H	0.30412800	3.64674000	1.10717900
H	0.63172500	3.65890300	2.84608200
H	-0.74779700	2.74824900	2.22330400
C	3.12305700	1.21449700	0.47639000
C	3.97070200	0.09109600	1.08302900
H	4.28209500	-0.60894700	0.30644600
H	4.85951400	0.52549000	1.54815600
H	3.42318900	-0.47562200	1.83769300
C	3.92185300	1.88857800	-0.63552900
H	4.83768400	2.32435400	-0.22826700
H	4.19075800	1.15368700	-1.39687900
H	3.34217200	2.68131400	-1.11233300
C	-2.65854500	-2.37118200	1.25163200

C	-3.64558500	1.85880400	-1.24941600
H	-4.13113500	-0.56963400	-0.18687800
H	-0.22725600	-1.25385400	1.46311600
H	-1.02794000	2.35125800	-0.69230900
F	-1.97183600	-3.36791200	0.68970900
F	-2.43673200	-2.44173300	2.57130100
F	-3.95561600	-2.60747800	1.04943400
F	-3.02038800	2.74473600	-2.02784000
F	-4.46619000	1.14360700	-2.02208700
F	-4.41595100	2.55443200	-0.40121200

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s-1-1 carbene fragment

C	-0.04619200	1.18849000	-0.14336000
N	-2.10456400	-0.12722200	-0.07527200
C	-2.80117000	-0.18777000	1.26281400
C	1.35427900	1.21313000	0.00040700
C	-2.83089700	-0.10998900	-1.16586800
C	0.05245600	-1.25707900	-0.19296500
C	2.11147800	0.04694600	0.18200300
C	-0.67316900	-0.05943100	-0.12415600
C	-4.22654300	-0.50134200	0.80170900
H	-4.96583500	0.05561400	1.38186700
H	-4.42737100	-1.56758500	0.94327100
C	1.44459900	-1.17016600	-0.04940500
C	-2.68366500	1.15089200	1.98279400
H	-1.63913100	1.38537400	2.20173500
H	-3.21834300	1.09015100	2.93218000
H	-3.11217000	1.96527400	1.39940700
C	-2.21941700	-1.27038200	2.16206600
H	-2.32239700	-2.26273400	1.72504100
H	-2.76095600	-1.26373200	3.10966600
H	-1.16491900	-1.08489100	2.38085200
C	-0.86724600	2.43504400	-0.32500600
H	-0.91989900	3.00924000	0.59911300

H	-0.42406800	3.08350600	-1.07578800
H	-1.87066500	2.18000100	-0.65378600
C	-0.67744900	-2.55270400	-0.41802000
H	-0.42197100	-2.95735700	-1.39522700
H	-0.40183500	-3.30611400	0.31965300
H	-1.75062400	-2.39880400	-0.38992700
C	3.53314400	0.07015100	0.68762900
H	3.64552700	0.85379900	1.43112900
H	3.78370000	-0.87483900	1.15859300
H	4.25372800	0.26794700	-0.10298900
C	-4.27260200	-0.16265500	-0.70256100
C	-4.87233400	1.21975600	-0.97517200
H	-4.80086900	1.45841700	-2.03727000
H	-5.92532500	1.23087800	-0.68195700
H	-4.35573400	2.00452300	-0.41746700
C	-5.03755000	-1.21109500	-1.50192100
H	-6.07513800	-1.26626500	-1.16087300
H	-5.02812400	-0.95951000	-2.56325100
H	-4.58522800	-2.19888600	-1.38258500
S	2.13799000	2.80341200	-0.04326800
O	1.47550800	3.67228800	0.85856600
O	3.55557200	2.68236200	-0.03523400
S	2.40385900	-2.66240000	-0.09172900
O	2.80409000	-2.99921300	1.22616400
O	1.77810200	-3.62862200	-0.93019200
O	3.70679300	-2.21693900	-0.87211500
H	3.62308000	-2.50837000	-1.79392900
O	1.76721900	3.30812700	-1.50054600
H	2.50233700	3.10394100	-2.09969000

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s-1-1 carbene-Au fragment

Au	-2.07238200	0.37414400	-1.64015300
C	0.66457900	1.06962800	0.65492600
N	-1.25265000	-0.36898800	1.10715200

C	-1.63515900	-0.55073000	2.54719900
C	2.04713400	1.16587300	0.40992300
C	-2.23057700	-0.43509900	0.23134600
C	0.82284700	-1.35425200	0.30860700
C	2.85832200	0.03453700	0.24042200
C	0.11293200	-0.21220200	0.70335400
C	-3.08023000	-1.04069700	2.38314500
H	-3.73062100	-0.63771100	3.16181500
H	-3.09866300	-2.13201400	2.46118600
C	2.19360500	-1.19369700	0.06588500
C	-1.52683000	0.75740800	3.32230200
H	-0.49647900	1.11866900	3.32939400
H	-1.82435400	0.57393200	4.35610000
H	-2.17014600	1.53575200	2.91454700
C	-0.74081800	-1.58140300	3.22334600
H	-0.78192800	-2.54891300	2.72465500
H	-1.08302400	-1.71629100	4.25063700
H	0.29702900	-1.24278800	3.25718800
C	-0.21528200	2.27434700	0.84020000
H	0.03688600	2.81351200	1.75270800
H	-0.08736800	2.96446500	0.01006300
H	-1.26160500	1.98507400	0.86117400
C	0.10306800	-2.66623200	0.15581900
H	0.02475600	-2.92253200	-0.89997000
H	0.63621900	-3.48064300	0.64430100
H	-0.90332400	-2.60968900	0.55790100
C	4.36321100	0.09317400	0.33026400
H	4.65714100	0.80559700	1.09574200
H	4.76437700	-0.87750000	0.60386500
H	4.82388600	0.41153800	-0.60220800
C	-3.53146000	-0.62594400	0.96934400
C	-4.29401500	0.70343100	0.95585800
H	-4.55368300	0.97631800	-0.06823400
H	-5.21115600	0.60120700	1.54110600

H	-3.70197600	1.51860400	1.37678500
C	-4.37302600	-1.69785400	0.28615600
H	-5.30388800	-1.85498600	0.83655500
H	-4.61341700	-1.38904000	-0.73315400
H	-3.83394500	-2.64692000	0.23815800
S	2.74149300	2.79736200	0.32659000
O	2.37068900	3.51779100	1.48889600
O	4.09476000	2.75289300	-0.10827000
S	3.14408100	-2.60736900	-0.43291900
O	3.91759000	-3.06403800	0.66403600
O	2.32641300	-3.50797700	-1.17280400
O	4.15203500	-1.99418100	-1.48525800
H	3.80275800	-2.15676700	-2.37619000
O	1.92633100	3.44098800	-0.86638500
H	2.39768400	3.29126800	-1.70116500

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t-1-1 carbene fragment

C	0.17157400	1.19524400	-0.12478700
N	-1.89498200	-0.10981400	-0.06930100
C	-2.63404600	-0.14712900	1.24381700
C	1.57198900	1.22259700	-0.09451300
C	-2.58926600	-0.07178400	-1.18033500
C	0.26515700	-1.25116500	-0.12468600
C	2.33736800	0.05322700	-0.16912800
C	-0.45862400	-0.05379900	-0.09140400
C	-4.06273800	-0.38342900	0.74496900
H	-4.78232900	0.22810400	1.29434100
H	-4.33416600	-1.43188400	0.89760600
C	1.66372300	-1.17293100	-0.10589500
C	-2.47076700	1.17580800	1.98216200
H	-1.42036200	1.36247900	2.21921600
H	-3.02488700	1.13096200	2.92126700
H	-2.85499000	2.01110300	1.39672400
C	-2.13840800	-1.27565400	2.13539800

H	-2.29948900	-2.24594300	1.66693600
H	-2.69682400	-1.25597400	3.07307900
H	-1.07757900	-1.16271400	2.37278300
C	-0.64091700	2.44417600	-0.35278300
H	-0.82774800	2.99813500	0.56570400
H	-0.11821000	3.11149700	-1.03590300
H	-1.59386500	2.18279200	-0.80794800
C	-0.45770700	-2.55713900	-0.33207000
H	0.07565200	-3.16960400	-1.05769500
H	-0.53845100	-3.13742300	0.58544700
H	-1.45645400	-2.37086300	-0.72009000
C	3.81874500	0.11349900	-0.46721800
H	4.42700600	0.13030500	0.43551300
H	4.11812200	-0.74629500	-1.06103200
H	4.04905300	1.00349800	-1.04729000
C	-4.04545400	-0.06482500	-0.76354500
C	-4.57572200	1.33988100	-1.06571000
H	-4.45088100	1.57166700	-2.12444500
H	-5.63837600	1.39601600	-0.81531200
H	-4.04928100	2.10329100	-0.48741100
C	-4.82895100	-1.08711200	-1.57811600
H	-5.87930400	-1.09169500	-1.27361700
H	-4.77111400	-0.84866600	-2.64097500
H	-4.42649400	-2.09279900	-1.43277000
C	2.48233100	-2.44800100	-0.05110300
C	2.28364700	2.55863100	-0.01064200
F	3.43867000	2.47848800	0.66052200
F	1.56752400	3.48281000	0.63931900
F	3.62430400	-2.28910300	0.62882400
F	1.84647100	-3.44822200	0.56791900
F	2.81060500	-2.89426100	-1.27491500
F	2.56623200	3.06497100	-1.22227800

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t-1-1 carbene-Au fragment

Au	-1.85751200	-0.80512500	-1.51766400
C	0.96287100	1.38236300	0.07760300
N	-1.08990000	0.46698200	1.03482600
C	-1.49714800	0.90076800	2.41022400
C	2.31512100	1.20610300	-0.24132300
C	-2.06186900	0.34814400	0.15284100
C	0.89474900	-0.94051700	0.86285100
C	2.94836300	-0.03589700	-0.11567600
C	0.28917900	0.30659900	0.66570900
C	-3.02080800	0.75103000	2.31849300
H	-3.53216900	1.57025300	2.82823000
H	-3.32136000	-0.18298900	2.80086500
C	2.24457100	-1.07044600	0.51363500
C	-1.05357000	2.33947300	2.65047300
H	0.03423700	2.42318900	2.58945500
H	-1.36120700	2.64421300	3.65192000
H	-1.50047600	3.02365000	1.92978500
C	-0.89453000	0.01290000	3.48792800
H	-1.24376500	-1.01438200	3.39630800
H	-1.20128500	0.39071800	4.46477700
H	0.19747100	0.02668800	3.44904200
C	0.20823200	2.62237500	-0.32822900
H	0.32926500	3.43650900	0.38499700
H	0.56283900	2.97768900	-1.29402700
H	-0.85144000	2.39891200	-0.43137500
C	0.06385000	-2.12155400	1.29318500
H	0.30623000	-2.98829000	0.67969100
H	0.23844600	-2.39332200	2.33305200
H	-0.99401400	-1.91022400	1.15366600
C	4.28498100	-0.29269000	-0.77373500
H	5.12322900	-0.09863700	-0.10686200
H	4.34775300	-1.32569400	-1.10559600
H	4.39731200	0.33746400	-1.65232400
C	-3.37266400	0.68404000	0.81948600

C	-3.83114900	2.03357200	0.25574700
H	-3.96615500	1.95872600	-0.82486500
H	-4.78349100	2.31629700	0.71088100
H	-3.10750800	2.82681900	0.45465400
C	-4.43911200	-0.36669200	0.53149600
H	-5.35353100	-0.12047200	1.07781500
H	-4.66239400	-0.40310500	-0.53601800
H	-4.10329000	-1.35976100	0.83797800
C	2.96709400	-2.37780200	0.77883500
C	3.11100600	2.38455400	-0.76828200
F	4.39956500	2.32683300	-0.41339400
F	2.67086400	3.55430600	-0.28990500
F	4.25802900	-2.18681600	1.07887500
F	2.46428400	-3.04871000	1.82004600
F	2.92375900	-3.20469500	-0.27619100
F	3.07272200	2.47061400	-2.10698200

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u-1-1 carbene fragment

N	-0.35189800	-0.16576200	-0.14364100
C	-0.95012400	1.04048800	0.52380500
C	-1.17760400	-1.08850900	-0.57692400
C	-2.38479900	0.54812300	0.74742200
H	-3.11222800	1.34978600	0.59721600
H	-2.48708100	0.19626900	1.77882800
C	-0.92183600	2.26465300	-0.39442000
H	0.07873400	2.68224000	-0.49519500
H	-1.56196600	3.03901500	0.03336800
H	-1.29690000	2.02015400	-1.38838200
C	-0.28437300	1.38536600	1.84927400
H	-0.26078600	0.51745000	2.51032300
H	-0.86873500	2.16966700	2.33594200
H	0.73173100	1.76171500	1.71889300
C	-2.57555100	-0.63321700	-0.21717200
C	-3.28287100	-0.23672100	-1.51519700

H	-3.30452200	-1.08475200	-2.20146400
H	-4.31111500	0.06760500	-1.30066100
H	-2.77986300	0.58991200	-2.01982100
C	-3.34120000	-1.78152800	0.43114400
H	-4.34445400	-1.45456000	0.72052000
H	-3.43018300	-2.61649600	-0.26547600
H	-2.82506000	-2.13897800	1.32508900
C	1.09471900	-0.38703000	-0.33249000
C	1.88187600	0.80235100	-0.86632600
C	1.76723600	-0.97103500	0.90725000
H	1.11876100	-1.16862800	-1.09803400
C	3.29985000	0.35293400	-1.20967800
H	1.93800200	1.59507200	-0.11153600
H	1.38582400	1.21666000	-1.74728200
C	3.18242800	-1.41881400	0.55814500
H	1.81928200	-0.22375400	1.70466500
H	1.16438400	-1.80761300	1.26990100
C	3.99112900	-0.25005600	0.00720400
H	3.87436900	1.19464000	-1.60222100
H	3.25137400	-0.39996100	-2.00485600
H	3.67088500	-1.84731400	1.43582800
H	3.13138300	-2.21019900	-0.19860800
H	5.00423800	-0.56864600	-0.24788100
H	4.08392400	0.51901000	0.78411100

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u-1-1 carbene-Au fragment

Au	-1.40607200	-1.33194300	-0.06358300
N	0.57594000	0.94811500	-0.05112700
C	0.82663600	2.39889200	0.23170900
C	-0.68353700	0.60677800	-0.14511300
C	-0.58967800	2.87899400	0.58305500
H	-0.78487000	3.87433400	0.17864800
H	-0.69099200	2.93407800	1.67062000
C	1.36731100	3.12492800	-1.00069100

H	2.40361300	2.86688900	-1.21023300
H	1.32373900	4.19978000	-0.81565700
H	0.76733700	2.90511000	-1.88426100
C	1.76993200	2.60307000	1.40903600
H	1.41469200	2.06394800	2.28846900
H	1.79675300	3.66856200	1.64728800
H	2.78858800	2.28514600	1.18390000
C	-1.55796300	1.81842300	0.03925300
C	-2.13888900	2.17470000	-1.33263100
H	-2.72516300	1.33657400	-1.71416400
H	-2.79083700	3.04652700	-1.23828700
H	-1.35894900	2.40363100	-2.06062500
C	-2.70290500	1.53962000	1.00698400
H	-3.27165500	2.45829900	1.17507200
H	-3.37040900	0.77783000	0.60061700
H	-2.32752700	1.17917400	1.96682100
C	1.61743200	-0.09245400	-0.18174200
C	2.84191100	0.29280500	-0.99844500
C	2.01103600	-0.67593400	1.17212100
H	1.10555000	-0.89455300	-0.72554300
C	3.70048700	-0.95317600	-1.20818500
H	3.43731600	1.04865400	-0.47411100
H	2.54001800	0.71227500	-1.96078100
C	2.86529500	-1.91844800	0.94986900
H	2.57872600	0.05600600	1.75546400
C	4.09971800	-1.57725000	0.12358600
H	3.12718800	-1.68392300	-1.78966900
H	3.14923900	-2.35599200	1.90870200
H	2.26311700	-2.66696700	0.42137200
H	4.70972200	-2.46752300	-0.04262600
H	4.71991000	-0.86488400	0.68192900
H	4.58428400	-0.69922100	-1.79683300
H	1.09799800	-0.92272000	1.72197700

v-1-1 carbene fragment

N	0.73689000	-0.39588600	-0.22377100
C	1.32669400	-0.96621500	1.03608000
C	1.57781500	-0.00900500	-1.15440700
C	2.76469500	-0.45501700	0.91553900
H	3.48305600	-1.17463400	1.31607100
H	2.86200400	0.47080200	1.49310600
C	1.27676100	-2.49567900	1.00928700
H	0.26469600	-2.87413700	1.14782700
H	1.89249800	-2.88454700	1.82316800
H	1.66385000	-2.88397300	0.06719600
C	0.67382600	-0.46798100	2.31855000
H	0.64054500	0.62275700	2.35499600
H	1.27462900	-0.81552200	3.16215400
H	-0.33568700	-0.86103800	2.44873300
C	2.97097500	-0.14806600	-0.57761000
C	3.72290000	-1.24556100	-1.33047100
H	3.73828000	-1.01904700	-2.39780500
H	4.75387900	-1.30561600	-0.97089500
H	3.26048600	-2.22533400	-1.20162300
C	3.69803800	1.17963200	-0.77961500
H	4.68697200	1.14712900	-0.31252200
H	3.81491800	1.39009600	-1.84364600
H	3.13192200	2.00183100	-0.33210700
C	-0.70425700	-0.22847700	-0.46663400
C	-1.53369400	-1.48668800	-0.24279800
C	-1.32805300	0.96442500	0.27969600
H	-0.73952500	0.00774100	-1.53531200
C	-2.95463900	-1.29735900	-0.76540900
H	-1.59452100	-1.72152400	0.82844100
H	-1.06000400	-2.33824800	-0.74068700
C	-2.73095800	1.16399500	-0.29622400
H	-1.45873400	0.68397900	1.33342900
C	-3.58632300	-0.08044800	-0.10013500

H	-2.89067400	-1.09762400	-1.84351100
H	-3.20838700	2.03211900	0.16519800
H	-2.65032500	1.37591000	-1.36882900
H	-4.59520200	0.07637500	-0.49249900
H	-3.69087200	-0.28764000	0.97381900
C	-3.78759700	-2.54901500	-0.53833100
H	-3.86081300	-2.76151200	0.53253000
H	-4.80140800	-2.42578700	-0.92418200
H	-3.34142600	-3.41948300	-1.02344500
C	-0.46895800	2.23810400	0.24537400
H	0.55259900	1.94744200	0.52075500
C	-0.94939200	3.24606600	1.28339000
H	-0.29001400	4.11578300	1.31033200
H	-1.95470500	3.60687900	1.05136500
H	-0.97220300	2.80535000	2.28422000
C	-0.40100600	2.87664200	-1.13725000
H	0.31201300	3.70403300	-1.13452400
H	-0.07287300	2.15968600	-1.89264400
H	-1.37415800	3.28284500	-1.42689500

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v-1-1 carbene-Au fragment

Au	-1.72786900	-1.39555300	0.11164700
N	0.17968400	0.87086300	-0.45429500
C	0.25155900	2.19625800	-1.14872200
C	-1.02518600	0.53728200	-0.05420400
C	-1.02916500	2.85370400	-0.62201300
H	-1.46859600	3.52627200	-1.36144900
H	-0.78192800	3.44349500	0.26696700
C	0.20030800	1.99533700	-2.66440900
H	1.13608000	1.59081100	-3.04846700
H	0.02730000	2.95967800	-3.14635400
H	-0.60615200	1.31673600	-2.94270500
C	1.47466700	3.02512200	-0.78676900
H	1.57335900	3.14655500	0.29349700

H	1.34932700	4.01615100	-1.22839300
H	2.39576300	2.59892000	-1.18606400
C	-1.96751800	1.70234500	-0.22499000
C	-3.04478200	1.40439300	-1.26894100
H	-3.63287600	0.53796000	-0.96123900
H	-3.70810300	2.26852200	-1.35904900
H	-2.62301900	1.18876000	-2.25104300
C	-2.64306700	1.95499500	1.12313100
H	-3.27589100	2.84460800	1.06508300
H	-3.25940400	1.09683600	1.39864400
H	-1.89782400	2.10720200	1.90895400
C	1.31295300	-0.03492500	-0.22072300
C	2.09322900	-0.38304500	-1.48060200
C	2.25416100	0.42862200	0.90276400
H	0.83039000	-0.95838200	0.12397000
C	3.07783300	-1.51465700	-1.19911700
H	2.66224900	0.48655300	-1.83617400
H	1.39927500	-0.67664800	-2.27439400
C	3.19543400	-0.74149300	1.19403000
H	2.87790600	1.24639400	0.51815700
C	3.99391600	-1.12193600	-0.04585900
H	2.49465200	-2.39101200	-0.88672800
H	3.86600100	-0.48808700	2.01892900
H	2.60254900	-1.60550700	1.51604800
H	4.68340400	-1.94134300	0.17528800
H	4.60692500	-0.26728000	-0.36397900
C	3.87325600	-1.86227100	-2.44723700
H	4.45980300	-0.99759600	-2.77235600
H	4.56657800	-2.68374200	-2.25770200
H	3.21749500	-2.15307200	-3.27005600
C	1.52001600	0.94905200	2.14831300
H	0.74887500	1.65043700	1.80311900
C	2.46891800	1.73070900	3.04985500
H	1.93216900	2.15331300	3.90124200

H	3.25602900	1.08567400	3.44819900
H	2.94771900	2.55108800	2.50766800
C	0.81832500	-0.15382200	2.93338000
H	0.19392900	0.27941000	3.71750600
H	0.17257900	-0.76620000	2.29764000
H	1.54815800	-0.80785400	3.41788700

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w-1-1 carbene fragment

N	-0.27374200	-0.12684000	-0.15737400
C	-0.91325700	1.06080800	0.50227700
C	-1.06580400	-1.08089200	-0.58583600
C	-2.32990100	0.52083600	0.73004100
H	-3.08426900	1.29571200	0.57225200
H	-2.42111400	0.17450300	1.76433500
C	-0.93493400	2.27442800	-0.42924000
H	0.05373000	2.70526400	-0.57781800
H	-1.56920400	3.04566900	0.01279300
H	-1.34631500	2.01066800	-1.40363300
C	-0.25397800	1.43085600	1.82437100
H	-0.18969800	0.56145700	2.48109400
H	-0.86668500	2.18792500	2.31886900
H	0.74549700	1.84826500	1.69197200
C	-2.47866700	-0.67494800	-0.22538800
C	-3.21102900	-0.32196900	-1.52187700
H	-3.20549500	-1.17914500	-2.19697400
H	-4.24853300	-0.05489500	-1.30256200
H	-2.74461900	0.51634800	-2.04191800
C	-3.19230400	-1.84749100	0.43969600
H	-4.20539000	-1.55798500	0.73463800
H	-3.25317100	-2.69196000	-0.24836400
H	-2.65502200	-2.17534000	1.33261000
C	1.17953400	-0.31228300	-0.31838500
C	1.95851200	0.89567500	-0.81590800
C	1.85403600	-0.87563900	0.92962600

H	1.24282100	-1.08797800	-1.08619000
C	3.41438000	0.53922300	-0.93831700
H	1.85663700	1.74336300	-0.13033000
H	1.56871100	1.22664200	-1.78277700
C	3.19939600	-1.46786700	0.52664700
H	2.01466800	-0.08318300	1.66640800
H	1.20969300	-1.63484300	1.37852800
C	3.96213100	-0.52422500	-0.35674900
H	4.03138600	1.19330700	-1.54535200
H	3.79337600	-1.70585400	1.41284000
H	3.04514600	-2.41794300	0.00220900
H	5.01536000	-0.73119700	-0.51676000

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w-1-1 carbene-Au fragment

Au	-1.35603800	-1.29842900	-0.06941300
N	0.65017700	0.94650200	-0.07775500
C	0.92441800	2.37959100	0.25658800
C	-0.61554000	0.62880100	-0.19305800
C	-0.48752600	2.87939600	0.59821800
H	-0.65589000	3.88835100	0.21583500
H	-0.60560200	2.90949500	1.68504500
C	1.49591500	3.13226200	-0.94464700
H	2.51153600	2.82478500	-1.18538600
H	1.51800800	4.19774200	-0.70827800
H	0.87163300	2.99146700	-1.82739200
C	1.84774800	2.51685600	1.45992100
H	1.46549400	1.94253500	2.30545400
H	1.88530100	3.56924800	1.74900400
H	2.86655300	2.19306400	1.24502500
C	-1.46908800	1.85273200	0.01261600
C	-2.02684400	2.25784000	-1.35537100
H	-2.63050600	1.44491500	-1.76321500
H	-2.65771200	3.14326800	-1.24546100
H	-1.23467000	2.48426900	-2.07069500

C	-2.63163500	1.57427000	0.95949800
H	-3.18208800	2.50090600	1.14430100
H	-3.31100300	0.83807000	0.52659800
H	-2.27586800	1.18118100	1.91398500
C	1.66821800	-0.11483000	-0.19718500
C	2.94946600	0.25296700	-0.92698200
C	1.99826900	-0.75319100	1.14888800
H	1.16770100	-0.88625400	-0.79133200
C	3.85431100	-0.94982600	-0.95639300
H	3.46923300	1.08314500	-0.43792300
H	2.72780100	0.57718900	-1.94770400
C	2.62381200	-2.11411500	0.87597800
H	2.70056000	-0.12459900	1.70519900
H	1.08108600	-0.86074900	1.73367600
C	3.69338100	-2.01183300	-0.17147100
H	4.66505000	-0.93292700	-1.67662200
H	3.04096600	-2.53685600	1.79298200
H	1.84094700	-2.80873500	0.54609700
H	4.36782200	-2.85469800	-0.28091400

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e-1-0 carbene fragment

C	1.25154800	1.38575600	0.03263000
N	-0.64301200	-0.14319600	0.24727600
C	-1.18767800	-0.27292200	1.61889600
C	2.62639600	1.56260900	-0.10618300
H	3.03305700	2.56478200	-0.16326800
C	-1.49101000	-0.19945400	-0.74979700
C	-0.11613700	2.92209900	-1.37262300
H	-0.58230200	2.06582500	-1.86287500
H	0.76152300	3.21924400	-1.95392300
H	-0.82092600	3.75731300	-1.36750000
C	1.60849300	-1.03998900	0.03984500
C	3.48102300	0.47255700	-0.17084300
H	4.54737100	0.62888600	-0.27742400

C	0.76843100	0.07627000	0.09378300
C	0.70355200	-2.86207300	-1.38487800
H	0.01074900	-2.15757700	-1.84888200
H	0.26074700	-3.86075600	-1.40072200
H	1.62019100	-2.88503600	-1.98097700
C	0.30843800	2.57002700	0.05432900
H	-0.58907200	2.27270000	0.60492800
C	1.03621600	-2.44185600	0.04849900
H	0.09978900	-2.42248600	0.61603000
C	-2.56400500	-0.84604000	1.33544500
H	-3.31904000	-0.53114800	2.05766300
H	-2.51728000	-1.93913400	1.34189800
C	0.89739900	3.79403100	0.74872400
H	1.29535400	3.54993600	1.73534600
H	0.12895500	4.56024700	0.86465200
H	1.70268600	4.23431000	0.15635900
C	2.97599200	-0.81748000	-0.09660400
H	3.65360700	-1.66074400	-0.14757800
C	1.95795300	-3.46686400	0.70067900
H	2.29096700	-3.14412700	1.68883700
H	2.84254200	-3.64905600	0.08619300
H	1.43783200	-4.42053900	0.80488000
C	-2.85533500	-0.35503700	-0.09584700
C	-3.45560200	1.05459100	-0.07819800
C	-3.75306000	-1.30055100	-0.87602700
H	-3.49029400	1.46646900	-1.08846300
H	-2.86063600	1.73209000	0.54186800
H	-3.91630300	-0.92011700	-1.88548900
H	-3.29652400	-2.28984700	-0.95760000
H	-4.47145200	1.02440900	0.32437900
H	-4.72244800	-1.40809600	-0.38097000
H	-0.53925200	-0.91374700	2.21909500
H	-1.21444700	0.71452300	2.09162600

e-1-0 carbene-Au fragment

Au	-1.47525500	0.30984300	-1.17479000
C	1.66557300	1.46252900	0.37598600
N	0.33778700	-0.47025900	1.05630300
C	0.40001800	-0.78693900	2.49195700
C	2.80955300	1.95504600	-0.24906100
H	2.97804800	3.02548500	-0.27569000
C	-0.82831300	-0.68734900	0.49157600
C	0.23187400	3.50670600	0.06197800
H	-0.20292300	3.06794000	-0.83835800
H	1.06623500	4.15024300	-0.22778300
H	-0.52274200	4.13630300	0.53719400
C	2.39799600	-0.81219900	-0.18472400
C	3.72735100	1.09843800	-0.83415900
H	4.60850800	1.50025900	-1.31858800
C	1.48571100	0.07825500	0.39192500
C	1.36320900	-2.67489700	-1.46458800
H	0.43282600	-2.10860500	-1.54738500
H	1.13104100	-3.74220000	-1.47659800
H	1.97456800	-2.44753600	-2.34217400
C	0.68944400	2.41717700	1.02894200
H	-0.19968200	1.85085100	1.32155200
C	2.13392300	-2.30307700	-0.19588600
H	1.50156400	-2.54203700	0.66643700
C	-0.80311700	-1.70337900	2.65054500
H	-1.24425200	-1.66743900	3.64705600
H	-0.50654800	-2.73475100	2.43867800
C	1.31322200	3.03792700	2.27963300
H	1.63622500	2.27532500	2.99223200
H	0.60100100	3.69949600	2.77675400
H	2.19085200	3.63057200	2.00810200
C	3.52155700	-0.27418400	-0.80356000
H	4.24347400	-0.93405600	-1.26849300
C	3.40534900	-3.13878700	-0.08643200

H	4.02425700	-2.82851600	0.75733100
H	4.00621700	-3.06310900	-0.99526700
H	3.14775200	-4.19146500	0.04107700
C	-1.76871600	-1.21182700	1.55753700
C	-2.60329100	-0.03031500	2.06407700
C	-2.67619600	-2.30252800	1.01237600
H	-3.18754900	0.39947200	1.24894800
H	-1.96936200	0.75948800	2.47771700
H	-3.29742900	-1.90188500	0.20859300
H	-2.09017700	-3.13144400	0.60900400
H	-3.28211400	-0.37456700	2.84840600
H	-3.32689300	-2.68690700	1.80182400
H	1.35934400	-1.25111900	2.72533200
H	0.31751900	0.14080900	3.06967600

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e-1-2 carbene fragment

C	1.35352000	1.46025300	-0.32936100
N	-0.49580000	-0.15846500	-0.30932000
C	-1.35714300	-0.18706500	0.93740400
C	2.71007100	1.71019300	-0.12894600
H	3.07592400	2.72840500	-0.19443600
C	-1.04578500	-0.46272900	-1.45833500
C	0.74908000	2.84921600	-2.27958100
H	0.59137500	1.94462300	-2.86946300
H	1.78719400	3.16948600	-2.40506200
H	0.09893600	3.63824200	-2.66437600
C	1.80139900	-0.93132000	-0.07983800
C	3.59934700	0.67624600	0.11667800
H	4.64910700	0.88883300	0.27626500
C	0.90858600	0.13756100	-0.23221300
C	1.77517100	-2.90074900	-1.58521400
H	1.30737800	-2.30189800	-2.36856700
H	1.46869400	-3.94235700	-1.70649200
H	2.86065700	-2.84727900	-1.70726200

C	0.45277600	2.58162400	-0.80228400
H	-0.58077200	2.24200300	-0.74202800
C	1.37280900	-2.37924300	-0.20505500
H	0.28284200	-2.42694700	-0.15270900
C	-2.56675700	-0.94257000	0.38019200
H	-3.50870700	-0.56451500	0.78316400
H	-2.48733600	-1.99729700	0.66623900
C	0.59611200	3.86077100	0.01630900
H	0.45550500	3.67900800	1.08389000
H	-0.14031300	4.59874300	-0.30746500
H	1.58354800	4.30777900	-0.11991000
C	3.14919600	-0.63549400	0.10464900
H	3.85771900	-1.44617400	0.22934600
C	1.94977300	-3.26083600	0.89999900
H	1.75626400	-2.84296200	1.89125400
H	3.03074700	-3.37299100	0.79074900
H	1.51357300	-4.26046000	0.85286300
C	-1.69428000	1.24454600	1.36889800
H	-0.75749900	1.77890700	1.55896900
H	-2.18245300	1.75474500	0.53553300
C	-0.71987600	-0.95647700	2.10454900
H	-0.35899100	-1.91523200	1.72640500
H	-1.54680300	-1.20732500	2.77808400
C	-2.48548400	-0.82275000	-1.15389700
C	-3.37863100	0.27985600	-1.72524200
C	-2.82090400	-2.14464800	-1.83762100
H	-3.22245900	0.36421500	-2.80186800
H	-3.16313900	1.25340700	-1.27985800
H	-2.73245200	-2.04509700	-2.92035400
H	-2.13552300	-2.93252500	-1.51249500
H	-4.43020700	0.04355000	-1.54101900
H	-3.84118000	-2.45352300	-1.59170300
C	-2.59434800	1.33080000	2.59580800
H	-2.12206900	0.91380500	3.48571900

H	-2.83964700	2.37127600	2.81079400
H	-3.53403400	0.79764200	2.44093800
C	0.37320500	-0.26279300	2.91436200
H	1.22285500	0.04568600	2.30464900
H	-0.00305800	0.62357800	3.42757600
H	0.74789500	-0.94445500	3.68030600

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e-1-2 carbene-Au fragment

Au	2.22740800	-0.55284500	0.15859300
C	-1.32400400	-1.54024000	0.94043800
N	-0.52462900	0.59027300	-0.02740600
C	-1.34908300	1.83464300	0.17957000
C	-1.97711000	-2.75437400	0.73108200
H	-2.17044900	-3.39935200	1.58066500
C	0.75126200	0.79694300	-0.26343300
C	0.17545600	-2.22527200	2.82014500
H	1.03505500	-2.25968300	2.14735400
H	-0.26713600	-3.22343100	2.87311600
H	0.52921600	-1.96046300	3.81879000
C	-1.41552000	-1.13635800	-1.47485100
C	-2.36402300	-3.15408100	-0.53612000
H	-2.87461700	-4.09860600	-0.67600800
C	-1.09801300	-0.72251700	-0.17116700
C	0.24907900	-0.97983100	-3.31613700
H	1.06620800	-0.99869500	-2.59100600
H	0.57077400	-0.41587800	-4.19509900
H	0.04234500	-2.00782600	-3.62629400
C	-0.85702200	-1.20390800	2.34010100
H	-0.36314300	-0.23011500	2.31243300
C	-1.00789400	-0.35465400	-2.70903500
H	-0.75298600	0.66570000	-2.41006700
C	-0.40779800	2.87293700	-0.44446400
H	-0.47431000	3.84153500	0.05293800
H	-0.69486700	3.01872600	-1.49188500

C	-2.02940800	-1.15938500	3.32242200
H	-2.85622800	-0.54577400	2.95682900
H	-1.70542000	-0.76928300	4.28916700
H	-2.42069200	-2.16635500	3.48784100
C	-2.06101200	-2.35881900	-1.63144300
H	-2.31835300	-2.69885200	-2.62742000
C	-2.12094000	-0.27349200	-3.75174800
H	-3.06145100	0.07271500	-3.31626900
H	-2.30379100	-1.24712100	-4.21101100
H	-1.83534700	0.41196800	-4.55167600
C	-1.56068600	2.05396300	1.68071500
H	-2.10208500	1.19334700	2.07699000
H	-0.58471200	2.05486100	2.17233300
C	-2.69069300	1.79713800	-0.56314600
H	-2.50370000	1.47992000	-1.59141300
H	-3.01780300	2.84004400	-0.63506300
C	1.01099600	2.27753700	-0.38447000
C	1.84960000	2.79462600	0.78603400
C	1.78386500	2.51551400	-1.68229900
H	2.81794500	2.29130200	0.79860300
H	1.37217200	2.61824800	1.75033700
H	2.76226700	2.03382000	-1.62671800
H	1.24718000	2.09906000	-2.53937600
H	2.01071200	3.86945000	0.66908000
H	1.92311500	3.58753400	-1.84558200
C	-2.31755500	3.32920300	2.02829800
H	-3.32415600	3.33241500	1.60735400
H	-2.41377700	3.42604300	3.10988800
H	-1.80352500	4.22054400	1.66527900
C	-3.81679100	0.96441600	0.04222200
H	-3.55233800	-0.08996300	0.13730000
H	-4.10529700	1.32745200	1.03066500
H	-4.69990800	1.02562500	-0.59537800

e-1-3 carbene fragment

C	-1.88979100	1.40635300	0.18869400
N	-0.31532800	-0.43292700	0.66084200
C	-2.90539400	1.92379800	-0.61103600
H	-3.30015900	2.90912100	-0.39466300
C	-0.67729000	-1.08330100	1.74265400
C	-2.41479200	1.80335400	2.57470700
H	-2.43560500	0.72599400	2.74452600
H	-3.42490900	2.13735700	2.32022500
H	-2.11116700	2.30589800	3.49638500
C	-1.97512500	-0.65923200	-1.11341900
C	-3.43603500	1.18915100	-1.66126800
H	-4.22119900	1.61046000	-2.27663700
C	-1.38710100	0.13602700	-0.12405000
C	-2.76888500	-2.97780400	-0.74477000
H	-2.93655000	-2.75050200	0.30975900
H	-2.53482000	-4.04030900	-0.84436900
H	-3.69422200	-2.77953900	-1.29242800
C	-1.45558400	2.15319100	1.43370300
H	-0.46153600	1.79846600	1.71571100
C	-1.62860000	-2.12227500	-1.29888700
H	-0.74437500	-2.34974300	-0.70070500
C	1.62063900	-1.57078800	1.21504500
H	2.63058300	-1.44612700	1.60248500
H	1.61130500	-2.49813900	0.62861600
C	-1.39460400	3.66772500	1.25271000
H	-0.81554800	3.95693500	0.37352400
H	-0.93858100	4.12723300	2.13147800
H	-2.39635200	4.09203200	1.15337600
C	-2.99187300	-0.10323900	-1.88712800
H	-3.45357300	-0.70236700	-2.66388100
C	-1.33499600	-2.47877100	-2.75379000
H	-0.56693200	-1.82943400	-3.18066800
H	-2.23223100	-2.38448800	-3.36966700

H	-0.99505600	-3.51372300	-2.82909400
C	0.57482500	-1.68530400	2.32871100
C	0.93139000	-0.88941100	3.58591800
C	0.31139200	-3.13828400	2.70806000
H	0.10909400	-0.93756100	4.30204800
H	1.12012300	0.16289200	3.36434300
H	-0.45280500	-3.19490800	3.48459500
H	-0.04353800	-3.70410000	1.84197700
H	1.82665200	-1.30867900	4.05326900
H	1.22691300	-3.61037200	3.07676600
C	1.17107500	-0.42697800	0.29338600
C	1.50153700	-0.75439400	-1.17853400
C	1.85103900	0.92866200	0.60016300
H	1.02015100	-1.69812700	-1.44762800
C	3.02511400	-0.94025500	-1.28545800
C	1.10772100	0.34161000	-2.17479400
H	1.59698900	1.23322500	1.61905000
C	3.37526000	0.79662200	0.48082300
C	1.41961100	2.02010100	-0.38798900
H	3.26689000	-1.22688500	-2.31464400
H	3.36427300	-1.75256700	-0.63749200
C	3.75000600	0.35957000	-0.93487600
H	0.02868900	0.50190100	-2.20091500
H	1.41033800	0.01641400	-3.17750500
C	1.81681200	1.64457800	-1.81436900
H	3.78025900	0.10302600	1.21976800
H	3.82192600	1.77513800	0.68959100
H	0.34247800	2.17826800	-0.35750500
H	1.89750200	2.96219400	-0.09622800
H	4.83061300	0.20279300	-0.99682900
C	3.32680200	1.45287800	-1.91211600
H	1.49689300	2.43528100	-2.49846500
H	3.84345700	2.38851100	-1.67172600
H	3.60239700	1.17340700	-2.93488600

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e-1-3 carbene-Au fragment

Au	2.70328300	-0.56268500	0.01375400
C	0.12769500	1.85133100	-1.27320400
N	-0.29020500	-0.23215700	-0.02391900
C	0.42145200	3.21194000	-1.25486900
H	0.51186600	3.74362100	-2.19450100
C	0.71583100	-1.06233900	-0.19368200
C	1.44793500	0.88766400	-3.15660500
H	2.04420500	0.28446000	-2.46908800
H	1.96345300	1.84065200	-3.30397300
H	1.39328700	0.37713100	-4.12103300
C	0.30330300	1.82816400	1.17054000
C	0.61910200	3.88887700	-0.06195900
H	0.83921400	4.94897200	-0.06831900
C	0.01188200	1.18658800	-0.04237300
C	1.83513600	1.23184500	3.05699100
H	2.57080400	0.85244100	2.34415000
H	1.92353200	0.66420500	3.98590500
H	2.07489600	2.27514900	3.27769600
C	0.04044700	1.14295800	-2.61234900
H	-0.44322500	0.17558500	-2.45888100
C	0.41113500	1.11553200	2.50641000
H	0.20644600	0.05197800	2.35178800
C	-1.16296700	-2.31486700	0.51436900
H	-1.85031500	-3.09527600	0.19494800
H	-1.06516800	-2.39074900	1.60407600
C	-0.75657500	1.92360500	-3.65940500
H	-1.72213300	2.26747400	-3.28675000
H	-0.92923400	1.29483600	-4.53481800
H	-0.19606100	2.79722000	-3.99948800
C	0.57933800	3.19351000	1.13407400
H	0.79189600	3.71048000	2.06277200
C	-0.56305900	1.67382900	3.54543700

H	-1.59984700	1.65653800	3.21001700
H	-0.30769800	2.71017200	3.77998600
H	-0.48928200	1.10143100	4.47248700
C	0.22583800	-2.47853000	-0.10478300
C	0.21731100	-3.05548400	-1.52401300
C	1.12886900	-3.33762300	0.77356200
H	1.23399100	-3.05638800	-1.92256400
H	-0.41029600	-2.47767600	-2.20401800
H	2.11869400	-3.43914000	0.32578900
H	1.25311900	-2.88906600	1.76183600
H	-0.15100200	-4.08416500	-1.50117200
H	0.68587800	-4.33082600	0.89053800
C	-1.65062700	-0.89506700	0.18573400
C	-2.48968300	-0.33285100	1.34967600
C	-2.54433100	-0.82278200	-1.07548200
H	-1.87762000	-0.34306800	2.25558900
C	-3.69081200	-1.27271700	1.55506300
C	-3.04977800	1.07104300	1.09798800
H	-1.97251000	-1.15908700	-1.94343000
C	-3.77077700	-1.72895300	-0.90534900
C	-3.06538900	0.59770100	-1.32035600
H	-4.26668500	-0.91116300	2.41343000
H	-3.35790400	-2.28515800	1.79715900
C	-4.58143100	-1.28492000	0.31164300
H	-2.25614200	1.81127000	0.98454300
H	-3.64323800	1.36397700	1.97217700
C	-3.92731900	1.06416300	-0.14972400
H	-3.49095700	-2.78069800	-0.82434100
H	-4.38773700	-1.63782500	-1.80588800
H	-2.24267600	1.30013500	-1.44428800
H	-3.64494600	0.60161000	-2.25008200
H	-5.41611100	-1.97364200	0.46825800
C	-5.11004000	0.12357900	0.05505200
H	-4.28679000	2.07754500	-0.34698800

H	-5.75340900	0.12492600	-0.83136300
H	-5.71311400	0.46212400	0.90441300

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e-1-4 carbene fragment

C	-1.62665600	1.36314900	-0.22611100
N	0.21187700	-0.05090500	0.57706900
C	-2.88933400	1.45847800	-0.80803100
H	-3.30150500	2.43884800	-1.01787800
C	0.42414800	0.00503500	1.86763900
C	-1.63534100	3.13401300	1.49985700
H	-1.62024000	2.36883100	2.27785500
H	-2.67635300	3.38492000	1.27782200
H	-1.14102100	4.03148100	1.87888200
C	-1.89057400	-1.06605200	-0.15677800
C	-3.63624100	0.32593900	-1.08918600
H	-4.61390700	0.41886800	-1.54557300
C	-1.11726000	0.08547600	0.03866800
C	-2.27498400	-2.72452900	1.63909300
H	-2.11131500	-1.94749200	2.38788400
H	-1.97838500	-3.68763200	2.06066400
H	-3.34347200	-2.76602500	1.41051400
C	-0.93189100	2.62572900	0.23985700
H	0.08800700	2.37210300	0.52679200
C	-1.47229900	-2.42238200	0.37228800
H	-0.42363800	-2.37052300	0.66735100
C	2.49230500	-0.53868600	0.67885700
H	3.42734000	-0.02247200	0.44834000
H	2.70294100	-1.61335800	0.67272600
C	-0.87828600	3.71541200	-0.82628600
H	-0.41947700	3.35756700	-1.75021000
H	-0.30012000	4.56730700	-0.46290600
H	-1.87843400	4.08223400	-1.06789700
C	-3.14798800	-0.92282800	-0.73814100
H	-3.76162300	-1.80269300	-0.89471100

C	-1.63509600	-3.53968000	-0.65366800
H	-1.11043300	-3.31246000	-1.58394400
H	-2.68804000	-3.70431600	-0.89326500
H	-1.24223000	-4.47744400	-0.25556800
C	1.92219900	-0.12546500	2.05196000
C	2.42886500	1.24766200	2.50088100
C	2.22734500	-1.15684200	3.13153600
H	1.93430200	1.54756600	3.42607600
H	2.22945000	2.01531700	1.74880600
H	1.79005000	-0.84962700	4.08264800
H	1.81048500	-2.13168400	2.86529500
H	3.50801000	1.20959000	2.67342800
H	3.30803400	-1.26862700	3.25889400
C	1.39701400	-0.22686400	-0.34469100
C	1.17219200	-1.37184200	-1.33204900
C	1.64674900	1.06208600	-1.13373100
C	2.34163600	-1.51369000	-2.29994700
H	0.25416800	-1.18087900	-1.90184500
H	1.03113000	-2.30415700	-0.78097700
C	2.78312300	0.92575500	-2.14163900
H	0.72263000	1.31780800	-1.66738500
H	1.86314700	1.88081800	-0.44341200
C	2.53601800	-0.23234800	-3.09617400
H	2.16795200	-2.36398600	-2.96274900
H	3.25709100	-1.73206400	-1.73619200
H	2.89725900	1.86491700	-2.68738000
H	3.72712400	0.75515500	-1.61156500
H	3.36278400	-0.33357700	-3.80241400
H	1.63127800	-0.03313500	-3.68282100

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e-1-4 carbene-Au fragment

Au	-2.37766400	-0.48698200	-0.09932600
C	0.42465100	1.62229000	1.52045800
N	0.61710400	-0.23195500	-0.07392100

C	0.36927600	2.99541500	1.74799000
H	0.33417000	3.35794700	2.76884700
C	-0.39821400	-1.05200000	-0.05712200
C	-1.10974600	0.79493000	3.28782400
H	-1.86418900	0.58015100	2.52715100
H	-1.28597400	1.80381600	3.67014700
H	-1.23491300	0.09188600	4.11414800
C	0.33317400	2.06661300	-0.88782100
C	0.32668200	3.89662900	0.69720800
H	0.28797500	4.96048800	0.89489400
C	0.46856000	1.18041600	0.19024300
C	-1.30990000	1.96258900	-2.75302100
H	-2.04669800	1.51253800	-2.08334200
H	-1.49387100	1.60109200	-3.76699100
H	-1.45502400	3.04607100	-2.74799500
C	0.30196900	0.68665800	2.70690500
H	0.42920100	-0.33920100	2.35796300
C	0.11672800	1.61604600	-2.31921100
H	0.21259700	0.52837600	-2.36024000
C	1.57128400	-2.29071900	-0.66511600
H	2.20768800	-3.03693600	-0.18539300
H	1.67757900	-2.41466300	-1.74721300
C	1.33662500	0.96391500	3.79546400
H	2.35863400	0.92830900	3.41477200
H	1.24223200	0.22841400	4.59681300
H	1.17864400	1.94956300	4.23892600
C	0.28135200	3.42956900	-0.60587400
H	0.17784400	4.13174900	-1.42507800
C	1.11309300	2.24563300	-3.29197400
H	2.14951000	2.07752600	-2.99656800
H	0.95484400	3.32478900	-3.35467400
H	0.96839700	1.83725800	-4.29416700
C	0.09214500	-2.45924300	-0.26837400
C	-0.08681100	-3.19720200	1.06207300

C	-0.71860000	-3.16276200	-1.35127100
H	-1.13828800	-3.18315000	1.35604500
H	0.49798900	-2.73692000	1.86202500
H	-1.76271700	-3.25331400	-1.04680700
H	-0.68864500	-2.60153100	-2.28813400
H	0.23705400	-4.23501300	0.95205600
H	-0.30910900	-4.16086800	-1.52802000
C	1.97072600	-0.86267800	-0.27391500
C	2.75181600	-0.15294900	-1.37498400
C	2.76975300	-0.78472100	1.02914500
C	4.14637100	-0.74741900	-1.53708800
H	2.84031000	0.90931200	-1.11696700
H	2.19886500	-0.22247700	-2.31425200
C	4.18470800	-1.33368800	0.87925000
H	2.82346900	0.26981900	1.32466800
H	2.24184800	-1.32000400	1.82212600
C	4.93248800	-0.62534900	-0.24030700
H	4.66375600	-0.24639600	-2.35751800
H	4.06375500	-1.80567500	-1.81378000
H	4.71327900	-1.23029300	1.82906200
H	4.14478200	-2.40656200	0.65971000
H	5.93684400	-1.03807100	-0.35371800
H	5.04509000	0.43541000	0.01280700

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e-1-7 carbene fragment

C	-1.77052400	1.22524800	0.03198700
N	0.29866700	0.00425300	0.54197400
C	-3.12047400	1.18979400	-0.30458700
H	-3.65833500	2.11924400	-0.44640500
C	0.60767400	0.07077300	1.81768100
C	-1.29168200	2.93295000	1.77041600
H	-0.92170700	2.15068700	2.43505600
H	-2.35909100	3.07584100	1.96226600
H	-0.77579500	3.86955400	1.99639300

C	-1.76992500	-1.21893800	0.12140900
C	-3.79070500	-0.01747200	-0.44485600
H	-4.84066400	-0.02638300	-0.70993200
C	-1.10179300	0.00594300	0.19619300
C	-1.58660400	-2.97324400	1.86366800
H	-1.36114800	-2.20915400	2.60998400
H	-1.10532300	-3.90873600	2.15801900
H	-2.66802100	-3.13482900	1.85091900
C	-1.08113500	2.54646900	0.30456600
H	-0.00843600	2.40432700	0.14793700
C	-1.10278600	-2.52915000	0.48269300
H	-0.02656800	-2.36132600	0.55814900
C	2.55484300	-0.51194900	0.52386300
H	3.52646500	-0.12832600	0.20974900
H	2.63155000	-1.60465300	0.58425400
C	-1.55069200	3.67827200	-0.60509800
H	-1.51961700	3.40024700	-1.66075000
H	-0.91795100	4.55584300	-0.46144000
H	-2.57335800	3.97755500	-0.36443000
C	-3.12278700	-1.20864600	-0.21291800
H	-3.66060800	-2.14777500	-0.27608500
C	-1.34850800	-3.61702000	-0.55948900
H	-1.07949800	-3.27965200	-1.56342200
H	-2.39922900	-3.91492800	-0.57745100
H	-0.76169500	-4.50716200	-0.32385500
C	2.11697200	0.03687100	1.88463300
C	2.55795300	1.48900500	2.09204900
C	2.59673300	-0.82096200	3.04564800
H	2.12034900	1.88797500	3.00918500
H	2.23805200	2.12556000	1.26315800
H	2.23636300	-0.41243000	3.99103700
H	2.21975600	-1.84264900	2.95340200
H	3.64715600	1.54337200	2.17039300
H	3.68970500	-0.85820800	3.07203100

C	1.42643400	-0.15630300	-0.44561500
C	1.70174200	1.02583200	-1.41064800
C	1.24549400	-1.16887600	-1.59818000
C	2.90028200	0.48383900	-2.20608400
C	0.50925400	0.99690800	-2.37356000
H	1.88489100	1.99224200	-0.94115000
C	2.61926700	-1.04155600	-2.27061300
C	0.23128100	-0.51725600	-2.54844600
H	1.00705400	-2.18697600	-1.29256100
H	2.93659800	0.94155400	-3.19595500
H	3.85192700	0.69549800	-1.71806000
H	-0.36243500	1.50369400	-1.96560300
H	0.76108900	1.48979100	-3.31415100
H	2.59425200	-1.42434200	-3.29168300
H	3.37905700	-1.60396200	-1.72531000
H	-0.80033900	-0.76032000	-2.29292600
H	0.40300200	-0.85413000	-3.57286000

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e-1-7 carbene-Au fragment

Au	-2.39934700	-0.39029000	-0.06303900
C	0.41975300	1.68728300	1.42526600
N	0.59614900	-0.29442500	-0.00804400
C	0.23424400	3.06091300	1.54503700
H	0.21235200	3.50790900	2.53163200
C	-0.46881200	-1.05523200	0.14548400
C	-0.86553800	0.58840700	3.26190000
H	-1.52413600	0.10149500	2.54000500
H	-1.32103300	1.54136100	3.54528600
H	-0.79556300	-0.03526200	4.15633300
C	0.21280200	1.91400000	-1.00690800
C	0.06344600	3.86061900	0.42507700
H	-0.07688300	4.92837000	0.53735100
C	0.44095700	1.13680300	0.13572900
C	-1.31520600	1.58972400	-2.96526800

H	-2.08457400	1.17001900	-2.31327200
H	-1.40926600	1.13684600	-3.95468300
H	-1.49891100	2.66230600	-3.06822400
C	0.52599200	0.83756900	2.67678200
H	0.95474600	-0.12775100	2.39573500
C	0.08714500	1.34095000	-2.40527400
H	0.23364200	0.25821000	-2.35085100
C	1.29460800	-2.40309500	-0.68611700
H	1.95212400	-3.22933600	-0.41576700
H	1.14479300	-2.43209500	-1.77184900
C	1.41821500	1.45934700	3.75120300
H	2.39361800	1.75927000	3.36456300
H	1.57428800	0.74369500	4.56043900
H	0.94459200	2.34035400	4.18967500
C	0.04312800	3.28653700	-0.83433600
H	-0.12888900	3.90829000	-1.70546500
C	1.11788600	1.94272200	-3.36292000
H	2.14042600	1.85337300	-2.99449300
H	0.91258700	3.00489400	-3.51672000
H	1.05674800	1.45351800	-4.33733600
C	-0.06685700	-2.49801600	0.00597200
C	0.03178100	-3.05618400	1.43040800
C	-1.06952700	-3.31665100	-0.79377300
H	-0.93782700	-2.97834200	1.92687100
H	0.76445700	-2.51099300	2.02905100
H	-2.03235100	-3.35062000	-0.28115000
H	-1.23259200	-2.87913500	-1.78081200
H	0.32554000	-4.10820000	1.39533400
H	-0.69662800	-4.33729800	-0.91702900
C	1.86731600	-1.03486600	-0.31039200
C	2.95650400	-1.03586100	0.79469700
C	2.81385600	-0.43975800	-1.37185600
C	4.05414500	-1.87646000	0.12337700
C	3.46594400	0.40816400	0.79501300

H	2.64926400	-1.40950600	1.77091500
C	3.90376500	-1.51990400	-1.37988100
C	3.42852900	0.79784300	-0.70306300
H	2.36327400	-0.27108100	-2.34861100
H	5.03310100	-1.60237300	0.51908300
H	3.92503100	-2.94491400	0.29777600
H	2.82340400	1.06665600	1.37461000
H	4.46750500	0.46653300	1.22386800
H	4.82719000	-1.14144800	-1.81927700
H	3.59404200	-2.38955900	-1.96182100
H	2.83333300	1.69791100	-0.85286300
H	4.42348100	0.99165500	-1.10885700

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e-1-8 carbene fragment

C	1.22405700	1.88353100	-0.05484600
N	-0.00008200	0.08285000	1.05907600
C	0.00020600	-1.25360500	0.30266400
C	1.20044500	2.96931400	-0.92779800
H	2.13456200	3.42825900	-1.22850600
C	-0.00042300	0.07108100	2.36197400
C	2.75830800	2.40556100	1.80307400
H	1.92939800	2.34141700	2.51039000
H	2.84655200	3.44060600	1.46026300
H	3.68344300	2.13575800	2.31806500
C	-1.22456800	1.88342200	-0.05474300
C	-0.00036900	3.48359800	-1.39461300
H	-0.00043000	4.31891500	-2.08409800
C	-0.00022300	1.30300900	0.29785700
C	-2.75918200	2.40574900	1.80279100
H	-1.93036900	2.34203700	2.51025400
H	-3.68433500	2.13592900	2.31773700
H	-2.84760800	3.44064800	1.45958900
C	2.52119700	1.47694600	0.60933200
H	2.40875100	0.46536700	1.00040200

C	-2.52168400	1.47675000	0.60942600
H	-2.40903400	0.46533800	1.00088100
C	0.00035100	-2.22873100	1.49564300
H	0.86317700	-2.88860900	1.46071600
H	-0.86248200	-2.88860300	1.46083500
C	3.71638100	1.49414800	-0.33549700
H	3.50492600	0.94446000	-1.25379800
H	4.58160900	1.03511400	0.14715600
H	3.99690900	2.51702600	-0.59961800
C	-1.20109100	2.96923400	-0.92768300
H	-2.13527500	3.42811700	-1.22828800
C	-3.71674700	1.49336700	-0.33557900
H	-3.50503600	0.94346100	-1.25368700
H	-3.99747400	2.51610200	-0.60004200
H	-4.58193600	1.03427100	0.14708500
C	0.00034800	-1.37532000	2.78942200
C	1.24888300	-1.61504600	3.63765500
C	-1.24694800	-1.61684300	3.63887300
H	1.22532100	-0.98680000	4.52892000
H	2.15740400	-1.36723900	3.08146000
H	-1.22357000	-0.98831000	4.52994200
H	-2.15640100	-1.37071600	3.08345900
H	1.30455900	-2.66349500	3.94353400
H	-1.30064400	-2.66529000	3.94511000
C	-1.25759900	-1.36626800	-0.56676400
C	-2.46179300	-1.85186100	-0.04762500
C	-1.23858600	-0.98021000	-1.90945600
C	-3.58987900	-2.00875300	-0.83717600
H	-2.53557600	-2.10918100	1.00107000
C	-2.37024400	-1.15507300	-2.70623900
C	-3.54061900	-1.67958100	-2.18612300
H	-4.50118000	-2.39567000	-0.39918700
H	-2.31586000	-0.87559800	-3.75273700
H	-4.40774600	-1.81829400	-2.81929400

C	1.25786700	-1.36602400	-0.56699200
C	2.46221400	-1.85161100	-0.04818500
C	1.23855000	-0.97981500	-1.90964300
C	3.59020200	-2.00813500	-0.83794700
H	2.53621200	-2.10924500	1.00041100
C	2.37012700	-1.15427700	-2.70662800
C	3.54070000	-1.67862600	-2.18680100
H	4.50162200	-2.39503500	-0.40018800
H	2.31550500	-0.87465000	-3.75307400
H	4.40775900	-1.81702400	-2.82013100
C	-0.00015600	-0.38939700	-2.50827900
H	-0.00020600	-0.53472400	-3.59066000
H	-0.00033400	0.69650200	-2.33807300

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e-1-8 carbene-Au fragment

Au	-2.99545400	-0.00002800	-0.08160200
C	0.21738700	-1.22662900	1.78101200
N	0.02693900	0.00004200	-0.33180300
C	1.27349500	0.00005300	-1.21418000
C	0.51739800	-1.19897900	3.14136300
H	0.57777000	-2.13420100	3.68516100
C	-1.11786300	0.00009800	-0.94492500
C	-1.55198400	-2.95799500	1.64941200
H	-2.30365200	-2.19848300	1.42001100
H	-1.52873800	-3.10159900	2.73329300
H	-1.85618900	-3.90006700	1.18795100
C	0.21731900	1.22638500	1.78120100
C	0.70616700	-0.00025900	3.81066500
H	0.94862400	-0.00033300	4.86607200
C	0.15798100	-0.00007000	1.10539400
C	-1.55214700	2.95764800	1.64975100
H	-2.30374600	2.19808900	1.42027800
H	-1.85642300	3.89973500	1.18836800
H	-1.52892400	3.10115800	2.73364600

C	-0.16490600	-2.54825200	1.14793200
H	-0.22384900	-2.41588000	0.06494600
C	-0.16503400	2.54806100	1.14827200
H	-0.22389100	2.41581600	0.06526800
C	0.62331700	0.00004600	-2.61787200
H	0.94477300	-0.86401100	-3.19236500
H	0.94483700	0.86406600	-3.19238300
C	0.83967700	-3.65547400	1.45143100
H	1.86223900	-3.34057600	1.24581800
H	0.62139000	-4.53828200	0.84721100
H	0.77695200	-3.95580200	2.50036800
C	0.51730100	1.19854900	3.14155500
H	0.57755700	2.13368600	3.68551200
C	0.83948400	3.65529500	1.45193000
H	1.86205000	3.34047700	1.24623000
H	0.77679700	3.95546900	2.50091300
H	0.62112500	4.53818500	0.84785200
C	-0.91031500	0.00010900	-2.42980800
C	-1.57738400	-1.24692900	-3.01230100
C	-1.57731900	1.24716000	-3.01231700
H	-2.65372000	-1.21169600	-2.83452400
H	-1.19435300	-2.15889900	-2.54709100
H	-2.65366000	1.21195200	-2.83455000
H	-1.19428500	2.15912700	-2.54710300
H	-1.39183500	-1.29704100	-4.08804200
H	-1.39175800	1.29726100	-4.08805400
C	2.10906400	1.26033600	-0.95678900
C	1.83013600	2.46139500	-1.61523600
C	3.19650500	1.23447800	-0.08035400
C	2.64222700	3.57575900	-1.47687100
H	0.96060800	2.54133700	-2.25488200
C	4.02325600	2.35083300	0.04238400
C	3.76656200	3.51401600	-0.66316000
H	2.40039700	4.48521700	-2.01168700

H	4.88190500	2.29108500	0.70181500
H	4.42398800	4.36857700	-0.56700300
C	2.10915900	-1.26015800	-0.95683800
C	1.83035400	-2.46121000	-1.61534500
C	3.19660400	-1.23422900	-0.08040600
C	2.64252900	-3.57551600	-1.47699500
H	0.96084500	-2.54120400	-2.25500900
C	4.02344600	-2.35052100	0.04230300
C	3.76684000	-3.51371200	-0.66326100
H	2.40077200	-4.48498000	-2.01183500
H	4.88209200	-2.29071600	0.70173300
H	4.42433300	-4.36822300	-0.56712700
C	3.48919900	0.00011800	0.71403400
H	4.52930900	0.00014700	1.04525700
H	2.86823800	0.00006800	1.62127700

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e-1-15 carbene fragment

C	-0.12200500	2.37531500	-0.72359200
N	0.07073300	0.44395400	0.80483900
C	0.42784400	-1.02125400	0.49013500
C	-0.92519100	3.11441800	-1.59232100
H	-0.48984000	3.94868100	-2.12984600
C	0.42922900	0.89575400	1.98388000
C	1.20184000	4.03989700	0.53894000
H	0.70307800	3.73907100	1.46063200
H	0.64092700	4.86026100	0.08193700
H	2.20318800	4.40396200	0.78080800
C	-2.09389200	1.06313100	-0.10818700
C	-2.26991100	2.82222600	-1.75451400
H	-2.87187300	3.40288400	-2.44248600
C	-0.71250800	1.29496800	-0.05528300
C	-3.20960500	0.98770800	2.08734200
H	-2.35329800	1.50149500	2.53150900
H	-3.67838100	0.35848200	2.84778700

H	-3.93523800	1.74227400	1.77125000
C	1.28545900	2.85833700	-0.42976100
H	1.83167000	2.05989800	0.07728900
C	-2.77266700	0.14436000	0.88682000
H	-2.04278500	-0.57960900	1.24990700
C	0.57747800	-1.49136000	1.93529200
H	1.20413100	-2.37312100	2.05760200
H	-0.41758000	-1.73112200	2.32350000
C	2.05974400	3.26222300	-1.68329000
H	2.02020500	2.49633800	-2.46133900
H	3.10654800	3.44268500	-1.43205800
H	1.66448000	4.18753400	-2.10879500
C	-2.85558300	1.82518100	-0.98798400
H	-3.92269300	1.65141300	-1.05558900
C	-3.94468500	-0.63697000	0.30756200
H	-3.65366100	-1.17675600	-0.59529900
H	-4.78252000	0.02124700	0.06487300
H	-4.30498500	-1.36231100	1.03984100
C	1.08002100	-0.26280000	2.70370900
C	2.59616300	-0.05383300	2.63671900
C	0.63288700	-0.29964800	4.15923900
H	2.86436800	0.83931100	3.20361400
H	2.95392600	0.07468000	1.61380900
H	0.95496900	0.60526600	4.67602900
H	-0.45673200	-0.35893800	4.22751600
H	3.11248900	-0.91265100	3.07471200
H	1.05942600	-1.16782400	4.67037000
C	-0.60474300	-1.78742400	-0.33701700
C	-1.16531900	-2.97421700	0.13120000
C	-0.91724100	-1.38338800	-1.63812700
C	-2.02301000	-3.72699400	-0.66487500
H	-0.92515900	-3.33561900	1.12276200
C	-1.77707900	-2.12789200	-2.43174400
H	-0.48085700	-0.47898700	-2.04339300

C	-2.33429900	-3.30702600	-1.94923100
H	-2.43980800	-4.64786700	-0.27653200
H	-2.00582600	-1.78773700	-3.43384700
H	-2.99925900	-3.89270200	-2.57116800
C	1.73632000	-1.13052500	-0.30086800
C	2.57982700	-2.22811200	-0.12819100
C	2.07460100	-0.19740700	-1.27586900
C	3.75096000	-2.35303500	-0.86332700
H	2.32571400	-3.00771900	0.57800300
C	3.24778200	-0.31368900	-2.01045700
H	1.40534100	0.62545600	-1.47774300
C	4.10048300	-1.38808500	-1.79910000
H	4.39139900	-3.21132800	-0.70275500
H	3.48854200	0.43797800	-2.75287400
H	5.01757600	-1.48146700	-2.36649900

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e-1-15 carbene-Au fragment

Au	-2.80624900	-0.13949100	-0.60241600
C	-0.43248100	-0.14437500	2.26638100
N	0.14356900	-0.14762000	-0.14009900
C	1.50052300	-0.23793600	-0.84116300
C	-0.61998700	0.59436000	3.43366000
H	-0.84427100	0.06829700	4.35437300
C	-0.84963300	-0.69280100	-0.82251700
C	-2.17082300	-1.91752500	2.50834700
H	-2.75302200	-1.49993900	1.68438000
H	-2.52738500	-1.47081900	3.44028400
H	-2.35137600	-2.99377900	2.55589500
C	-0.17711700	1.96493800	1.04298700
C	-0.55375900	1.97742900	3.43358500
H	-0.69503700	2.52888300	4.35466900
C	-0.12976600	0.56099800	1.08918000
C	-1.58427500	3.30620100	-0.50940800
H	-2.32685800	2.50650300	-0.55879900

H	-1.60299900	3.86072000	-1.45046600
H	-1.87209400	3.99095800	0.29312500
C	-0.67584000	-1.64264400	2.33300100
H	-0.36240300	-2.09490500	1.38867000
C	-0.17612300	2.76227300	-0.24863900
H	0.08657700	2.09532000	-1.07418800
C	0.98693600	-0.43237100	-2.26612200
H	1.70773100	-0.88688500	-2.94263200
H	0.70899700	0.54593100	-2.67083900
C	0.08161000	-2.31284000	3.48412900
H	1.12361700	-1.99468100	3.55225800
H	0.05861900	-3.39774700	3.36447800
H	-0.39308200	-2.08147400	4.44041000
C	-0.36541700	2.65211600	2.23886100
H	-0.39298200	3.73534600	2.22216000
C	0.80553200	3.93184900	-0.23492600
H	1.80918800	3.62898500	0.05681800
H	0.46674500	4.70680900	0.45738800
H	0.85520500	4.38471200	-1.22731500
C	-0.30624000	-1.24128200	-2.11786200
C	-0.10505800	-2.75177400	-1.93444900
C	-1.23522900	-1.00615500	-3.30119500
H	-1.08211900	-3.23503400	-1.87847600
H	0.44863400	-2.99858600	-1.02817800
H	-2.18019700	-1.53225100	-3.15764500
H	-1.45898200	0.05584600	-3.42122500
H	0.43860600	-3.15969100	-2.79072900
H	-0.76182200	-1.37478000	-4.21588600
C	2.42651100	0.95895300	-0.64030000
C	2.93265900	1.66520100	-1.72814700
C	2.92209900	1.26003500	0.63181800
C	3.90696300	2.64397100	-1.55494300
H	2.58809500	1.44546600	-2.73039900
C	3.88918700	2.23746300	0.80757500

H	2.55942000	0.71678900	1.49563000
C	4.39240100	2.93105600	-0.28841800
H	4.28962600	3.17390600	-2.41807900
H	4.25571000	2.45278300	1.80318400
H	5.15509200	3.68725300	-0.15330200
C	2.31838100	-1.44547800	-0.36494700
C	3.21269800	-2.08168000	-1.22522000
C	2.26312600	-1.87548900	0.95461500
C	3.97524100	-3.15727400	-0.79004600
H	3.33491700	-1.73740000	-2.24403400
C	3.01792700	-2.95466200	1.39523600
H	1.63183100	-1.34690900	1.65093300
C	3.87003000	-3.61166100	0.51850700
H	4.65582100	-3.64083800	-1.47955000
H	2.94021100	-3.27482400	2.42747500
H	4.45823900	-4.45618700	0.85366500

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