Supplementary Materials

Computational Exploration of Dirhodium Complex-Catalyzed Selective Intermolecular Amination of Tertiary *vs.* Benzylic C−H Bonds

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1. Results

1.1 The dirhodium complex Rh₂(S-tfpttl)₄

phthaloyl face   tert-butyl face

Figure S1. The phthaloyl face and *tert*-butyl face of Rh₂(*S*-tfpttl)₄ **1**. The pocket diameters are labeled. The distances are shown in Å.

³1-1
$(\alpha,\alpha,\alpha,\alpha)$
$\Delta\Delta G$ = 10.1

³1-2
$(\alpha,\alpha,\alpha,\beta)$
$\Delta\Delta G$ = 16.6

³1-3
$(\alpha,\alpha,\beta,\beta)$
$\Delta\Delta G$ = 16.3

³1-4
$(\alpha,\beta,\alpha,\beta)$
$\Delta\Delta G$ = 21.0
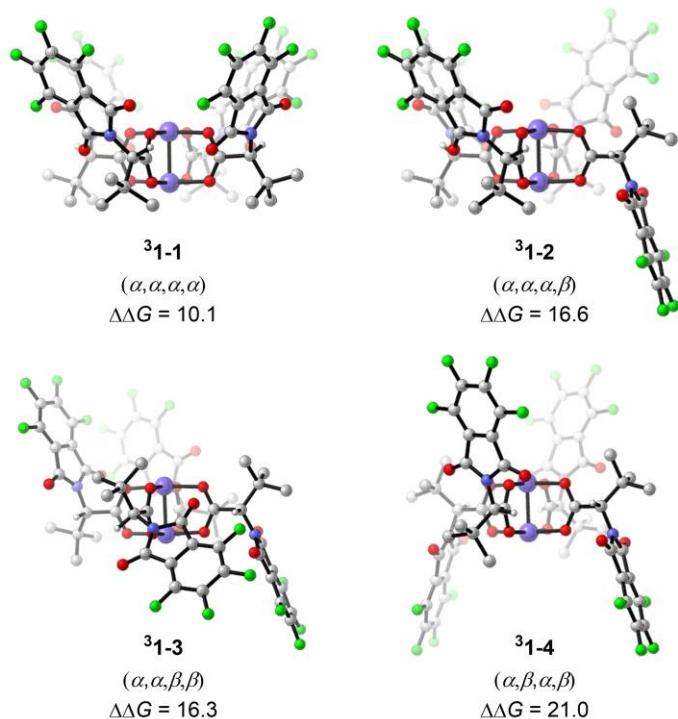
Figure S2. Optimized geometries and energies of triplet state dirhodium catalyst conformers. Free energy obtained at the M06/def2-TZVP//BPW91/6-31G*-LANL2DZ level. Energies are shown in kcal mol⁻¹. The H atoms of ᵗBu groups and aryl groups were omitted for clarity.
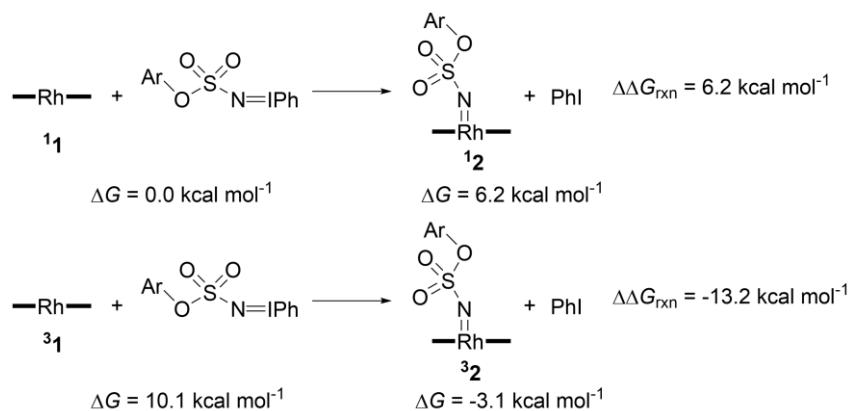
Figure S3. The energetics for the formation of dirhodium–nitrene.

1.2 The Dirhodium–nitrene complex

The singlet $^1\mathbf{2}$ was first optimized by the restricted DFT method. Further analysis performed with the *stable=opt* keyword suggested the instability of the restricted wave function. The reoptimization was conducted with the Gaussian keyword *guess=read* to achieve an unrestricted and symmetry-broken solution accordingly. The resulting structure $^1\mathbf{2}$ was obtained with $\langle S^2 \rangle$ of 0.2728 before annihilation of the spin contamination, and $\langle S^2 \rangle$ of 0.0019 after annihilation. The structure $^1\mathbf{2}$ can be described as closed shell with small spin polarization due to effects of the unrestricted approach. In addition, we have done additional calculations for the high-level (HL) layer of structure $^1\mathbf{2}$ using other functionals (Table S2). The energy ordering of the closed-shell singlet, open-shell singlet and triplet Rh–nitrene intermediate $\mathbf{2}$ obtained from these different functionals (BPW91, M06, MN15 and *w*B97xD) are the same, albeit the numbers of each structure differ. The result at the level of ONIOM(M06:UFF//BPW91:UFF) indicates that the energies of the open-shell and closed-shell are close to a degeneracy. The value of $<S^2>$ in the open-shell singlet state is affected by different functionals.

Table S1. The energies and the $<S^2>$ value of the Rh–nitrene intermediate $\mathbf{2}$ at different levels of theory. The energies are shown in kcal mol^{-1} ($\Delta\Delta E$).

| Computational Level	Triplet	Closed-shell singlet	Open-shell singlet
	$\Delta\Delta E$ $<S^2>$	$\Delta\Delta E$ $<S^2>$	$\Delta\Delta E$ $<S^2>$
ONIOM(M06/def2-TZVP:UFF //BPW91/6-31G*-LANL2DZ:UFF)	0.0 <2.0001>	9.9 <0.0000>	9.6 <0.0019>
ONIOM(M06/def2-TZVP:UFF //M06/6-31G*-LANL2DZ:UFF)	0.0 <2.0005>	7.0 <0.0000>	5.2 <0.2308>
ONIOM(M06/def2-TZVP:UFF //MN15/6-31G*-LANL2DZ:UFF)	0.0 <2.0002>	6.8 <0.0000>	5.1 <0.0431>
ONIOM(M06/def2-TZVP:UFF //*w*B97xD/6-31G*-LANL2DZ:UFF)	0.0 <2.0007>	6.5 <0.0000>	6.0 <0.6409>

Table S2. Calculated spin densities of selected atoms in Rh–nitrene **2** at the level of ONIOM(M06:UFF//BPW91:UFF).
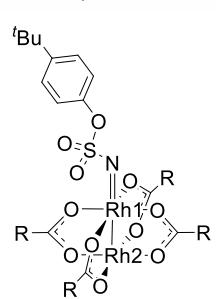
Structure	Rh1–Rh2	N
^{1}**2**	0.040	-0.072
^{3}**2**	0.718	0.960
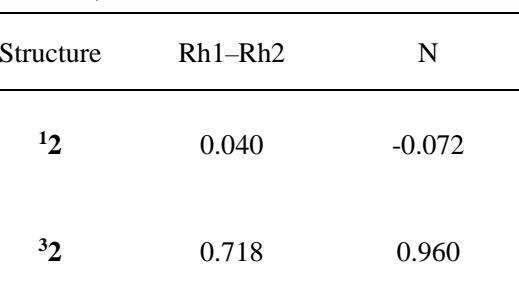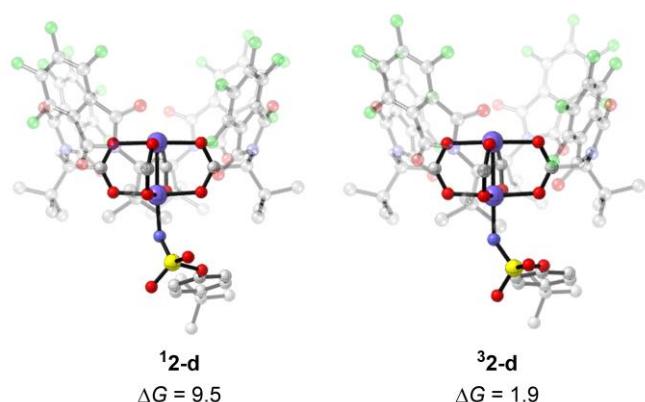
Figure S4. The binding of the nitrene to the *tert*-butyl face of the catalyst. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. Energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.

1.3 Singlet pathway
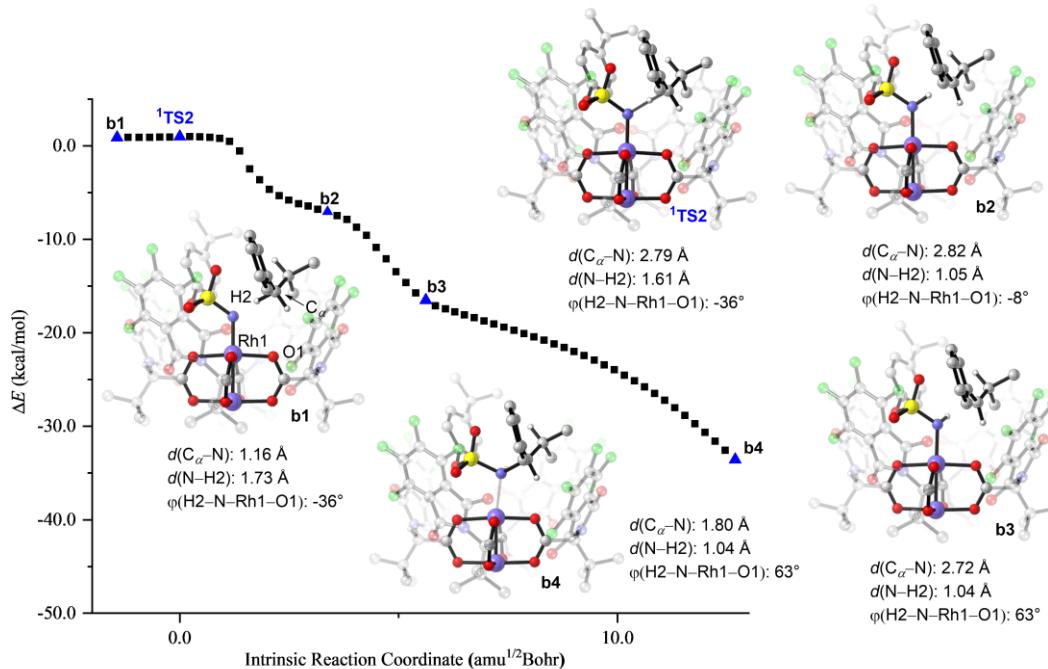
Figure S5. The IRC path for **¹TS2**. The H atoms of *'*Bu groups and aryl groups were omitted for clarity.

1.4 Triplet pathway
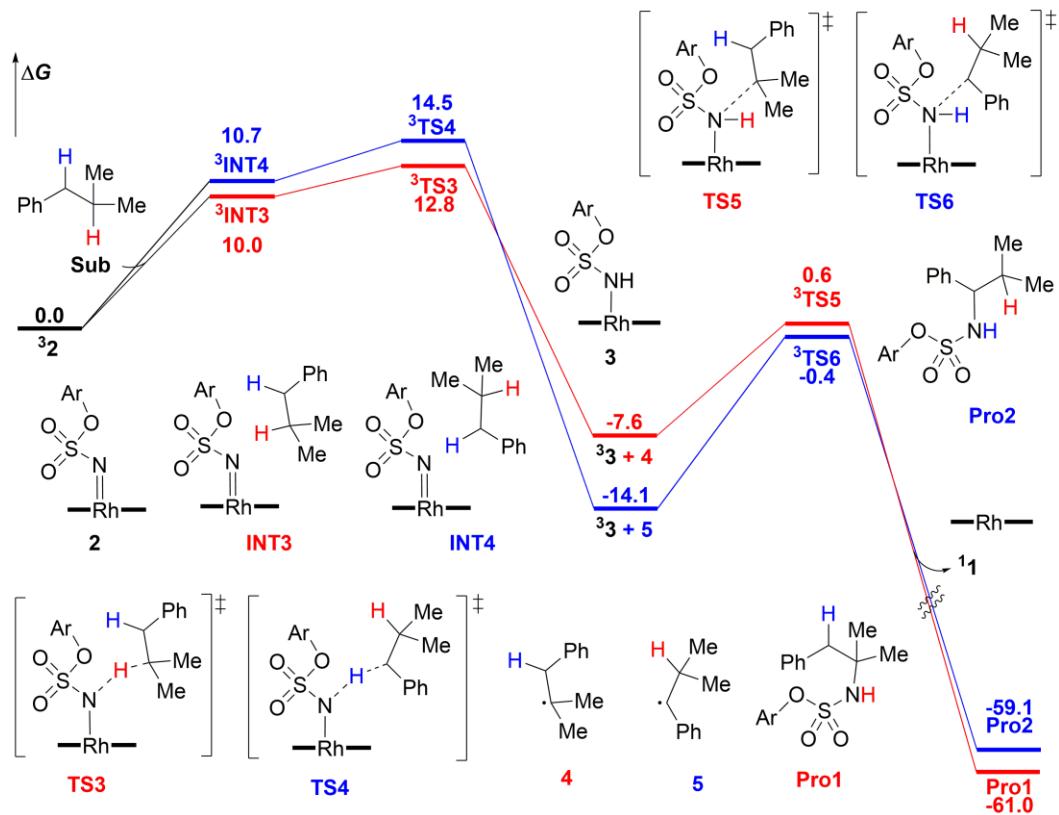
Figure S6. Free energy profiles of the triplet pathway. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. Energies are shown in kcal mol^{-1}. Ar = *p-tert*-butylphenyl.

Table S3. The calculated spin densities on selected atoms in tertiary and benzylic C–H aminations at the level of ONIOM(M06:UFF//BPW91:UFF).

Structures		The Spin Density Distribution					
		N	Rh1–Rh2	C_α	C_β	PhCH$_2$	Ph
Tertiary	^{3}INT3	0.924	0.708	0.001	0.002	0.020	0.019
	^{3}TS3	0.702	0.575	-0.016	0.452	0.036	0.008
	^{3}INT5	0.350	0.596	-0.061	**0.827**	0.023	**0.007**
	^{3}TS5	0.011	1.412	-0.031	0.389	0.002	0.000
Benzylic	^{3}INT4	0.899	0.693	0.028	0.004	0.083	0.059
	^{3}TS4	0.714	0.563	0.320	-0.009	-	0.188
	^{3}INT6	0.366	0.559	**0.678**	-0.047	-	**0.287**
	^{3}TS6	0.052	1.372	0.274	-0.019	-	0.113

³TS3'
ΔΔG‡ = 0.0
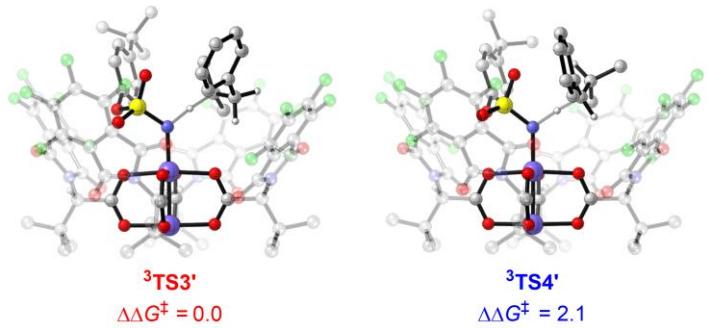
³TS4'
ΔΔG‡ = 2.1

Figure S7. Optimized geometries of selective transition state **³TS3'** and **³TS4'**. Free energy obtained at the M06/def2-TZVP//BPW91/LANL2DZ-6-31G* level. Energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.

1.5 Origins of site-selectivity
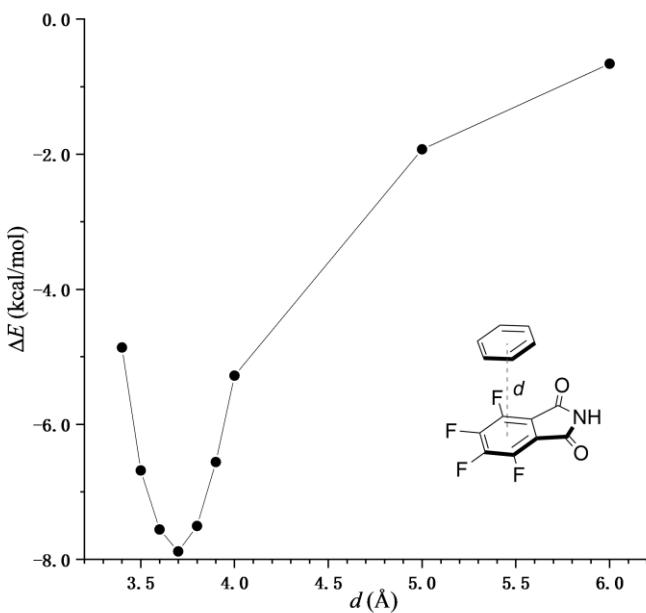
Figure S8. The interaction energy for the C_6H_6-phthalimido complex with the eclipsed face-face orientation at different distances between the centers of mass.
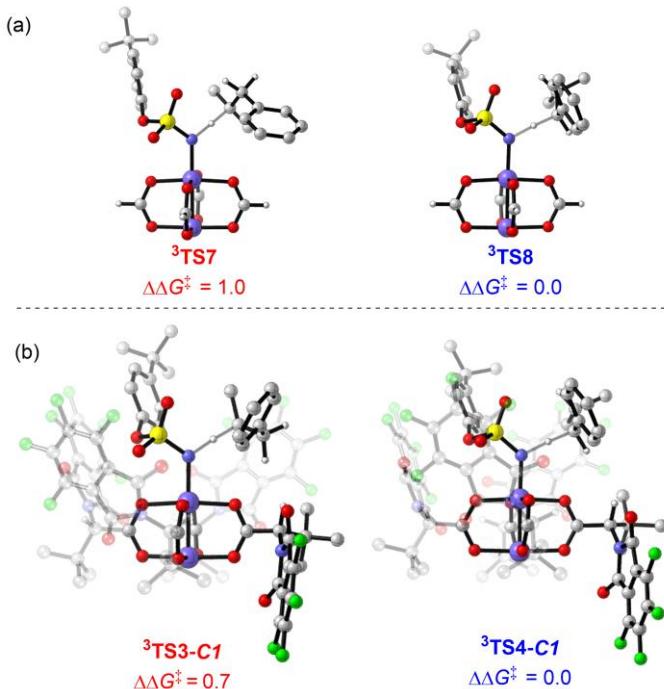
Figure S9. (a) The triplet transition states for $Rh_2(O_2CH)_4$-catalyzed intermolecular amination of tertiary and benzylic C–H bonds. Free energy obtained at the M06/def2-TZVP//BPW91/LANL2DZ-6-31G* level. (b) The triplet transition states for the amination of tertiary and benzylic C–H bonds with the dirhodium catalyst moiety adopting the $\alpha,\alpha,\alpha,\beta$ conformer. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. The H atoms of ^tBu groups and aryl groups were omitted for clarity. The energies are shown in kcal mol^{-1}.

2. Computational detail
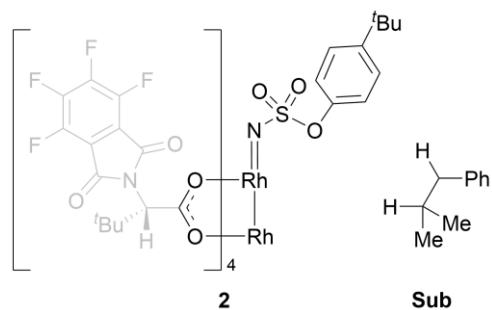
Figure S10. The two-layer ONIOM approach. The ligand part (gray) was calculated by the force field (UFF), and the other parts (black) were calculated by BPW91 or M06 method.
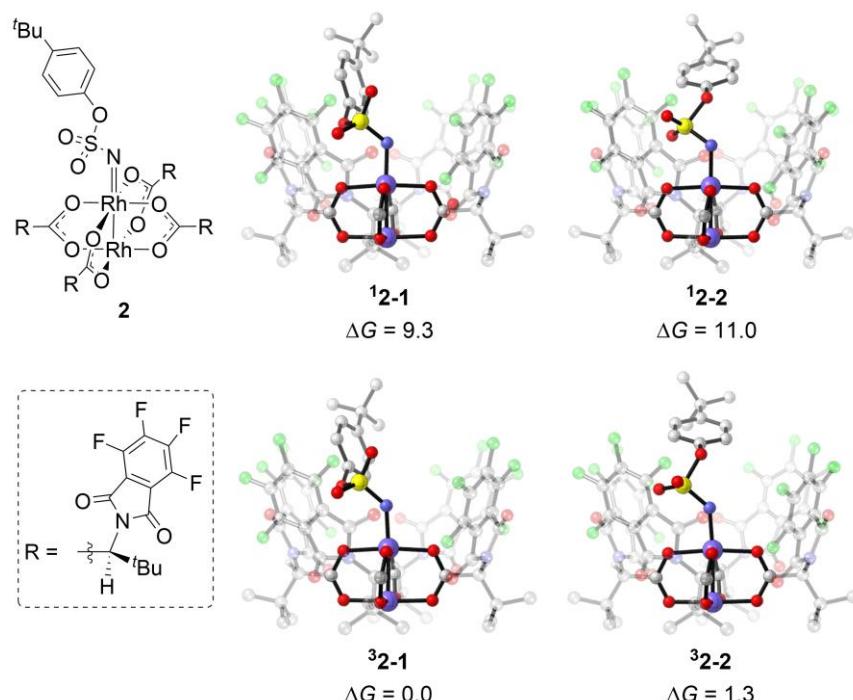
Figure S11. Optimized geometries and energies of conformers for Rh$_2$(*S*-tfpttl)$_4$–nitrene **2**. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. The energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.
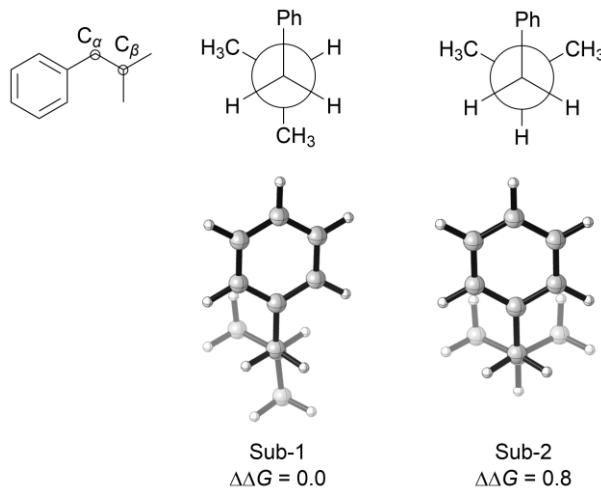
Figure S12. Newman projection along the C −C$_\beta$ bond of the substrate isobutylbenzene. Optimized geometries and energies of conformers for the substrate. The energies are shown in kcal mol^{-1}. Free energy obtained at the M06/def2-TZVP//BPW91/LANL2DZ-6-31G* level.
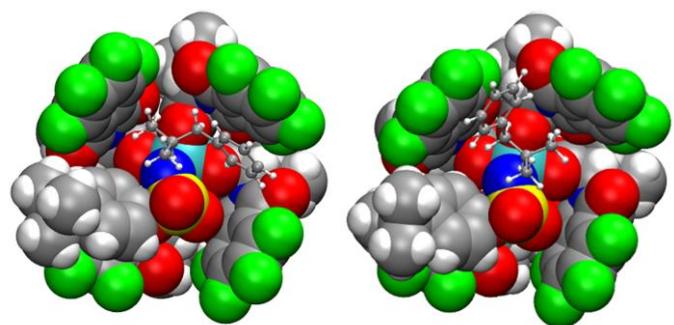
Figure S13. The schematic of the dirhodium−nitrene with substrate adducts displaying the substrate fitting in the catalytic pocket. The dirhodium−nitrene is represented with Van der Waals spheres mimicking the real volume of the molecule.
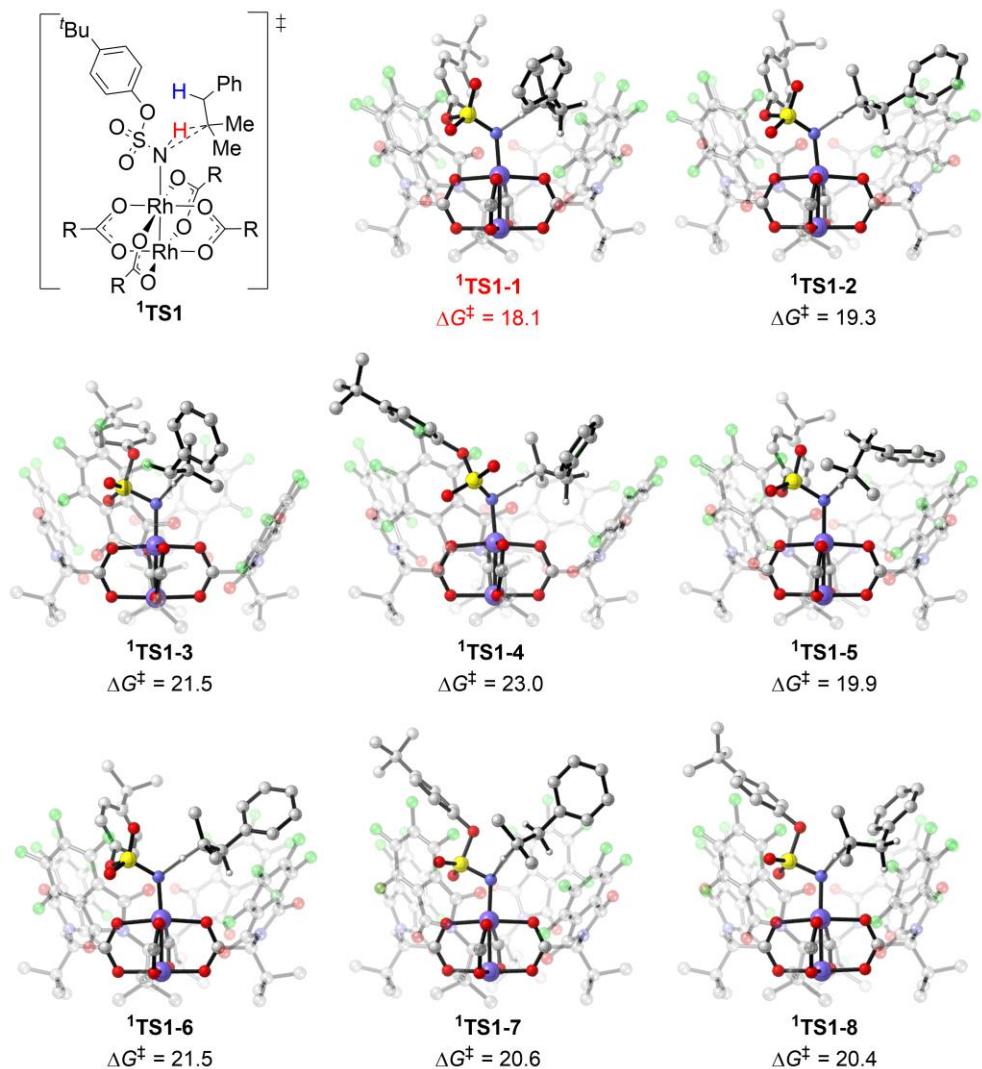
Figure S14. Optimized geometries and energies of conformers for **¹TS1**. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. The energies are shown in kcal mol⁻¹. The H atoms of *t*Bu groups and aryl groups were omitted for clarity.
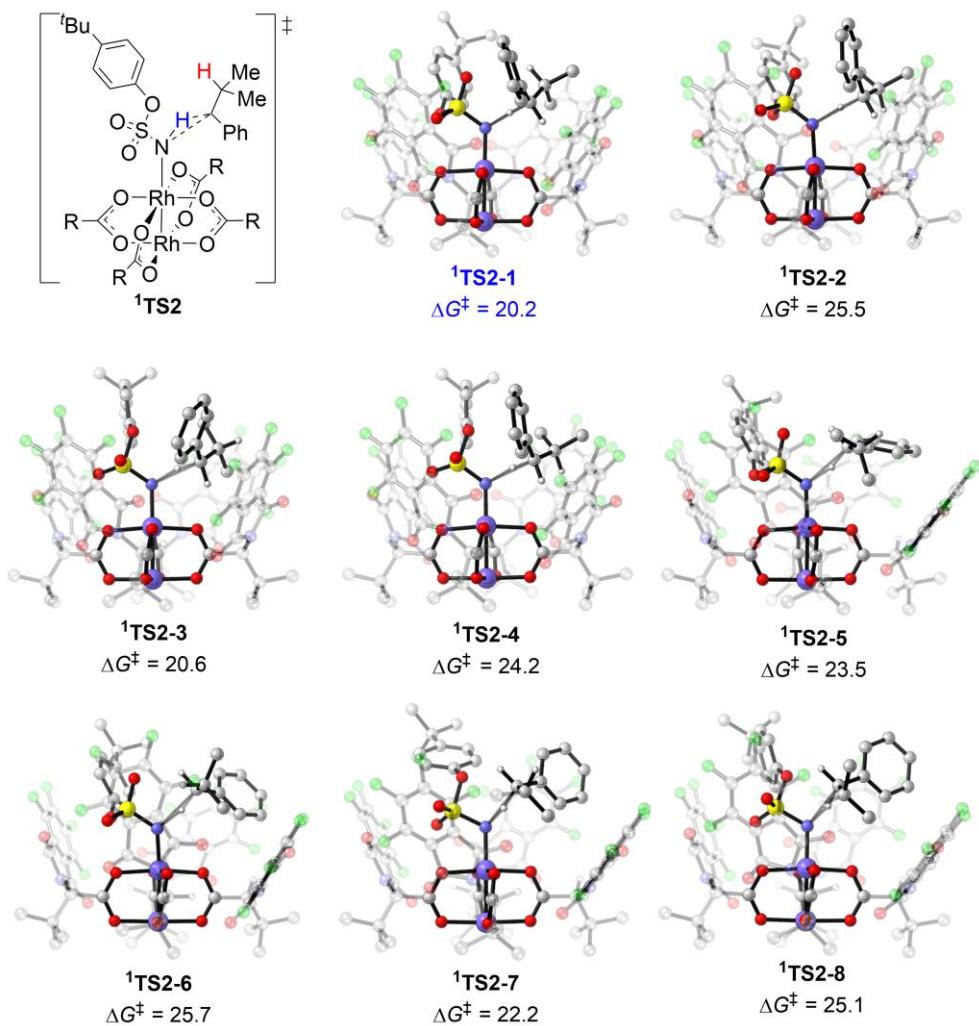
Figure S15. Optimized geometries and energies of conformers for **¹TS2**. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. Energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.
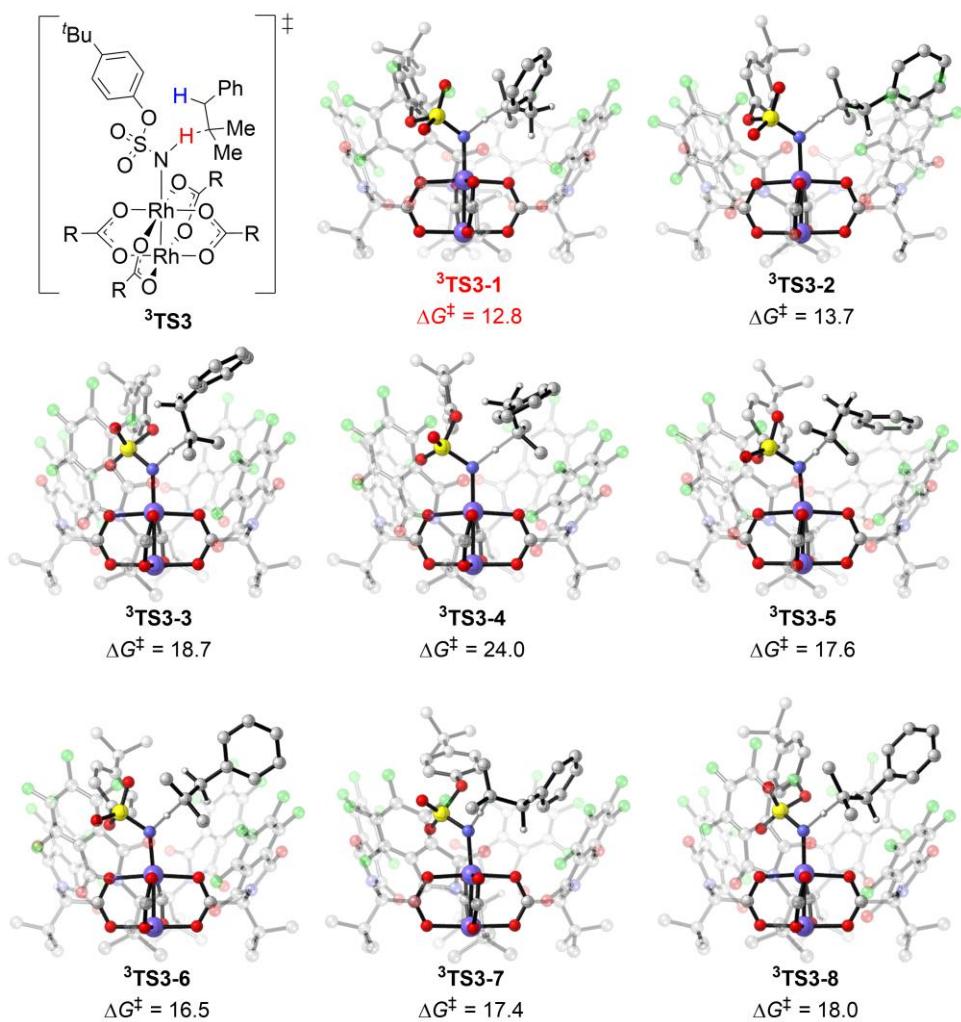
Figure S16. Optimized geometries and energies of conformers for **³TS3**. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. Energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.
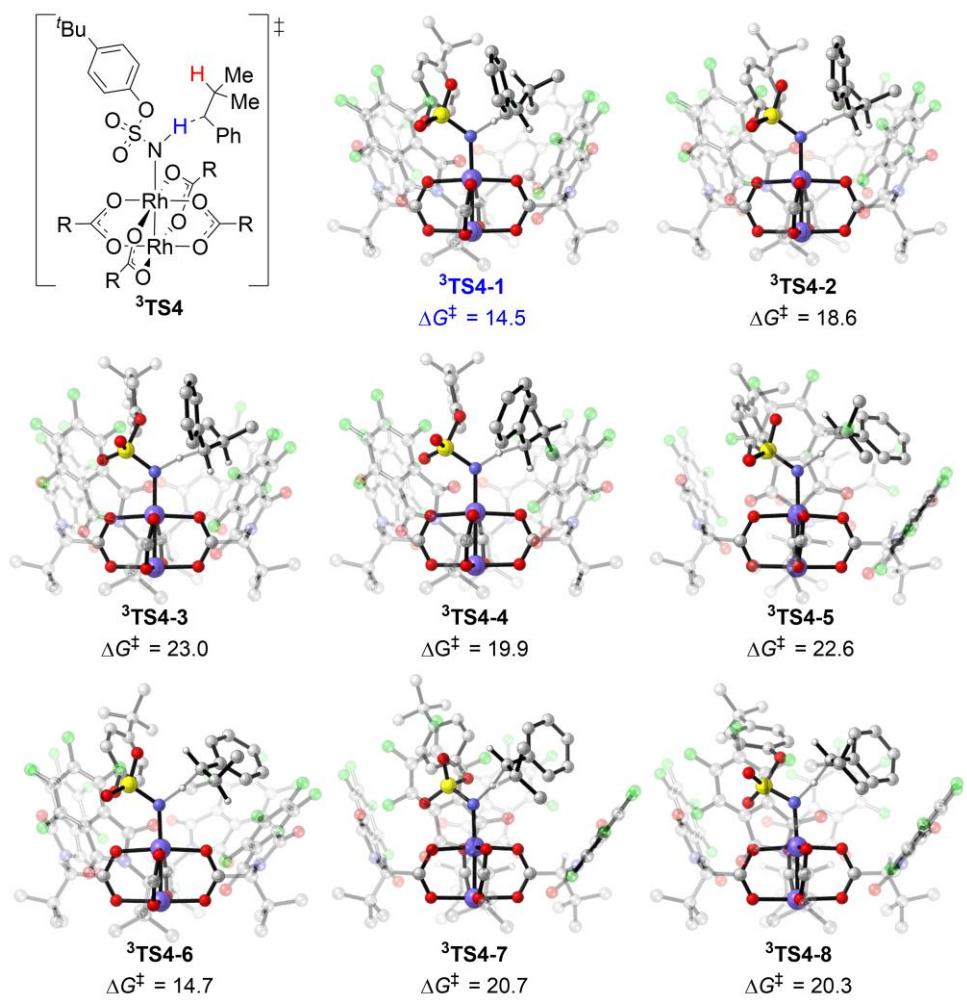
Figure S17. Optimized geometries and energies of conformers for **³TS4**. Free energy obtained at the ONIOM(M06/def2-TZVP:UFF//BPW91/LANL2DZ-6-31G*:UFF) level. Energies are shown in kcal mol⁻¹. The H atoms of ᵗBu groups and aryl groups were omitted for clarity.
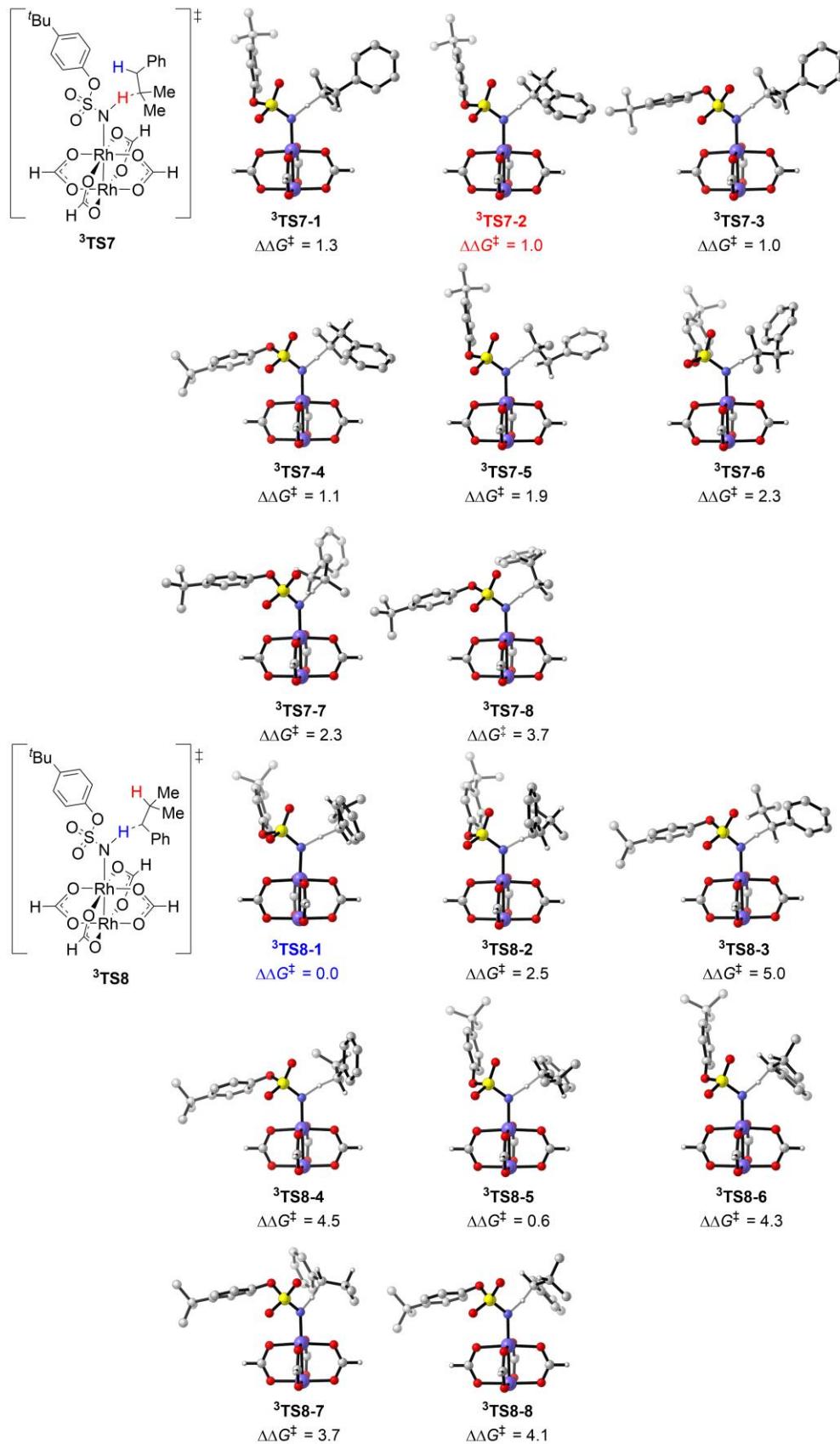
Figure S18. Optimized geometries and energies of conformers for **³TS7** and **³TS8**. Free energy obtained at the M06/def2-TZVP//BPW91/6-31G*-LANL2DZ level. Energies are shown in kcal mol^{-1}. The H atoms of ^{t}Bu groups and aryl groups were omitted for clarity.

Table S4. The energies of the key transition states using different functionals. The energies are shown in kcal mol^{-1} ($\Delta\Delta G^{\ddagger}$).

Methods	$\Delta\Delta G^{\ddagger a}$
ONIOM(M06/def2-TZVP:UFF //BPW91/6-31G*-LANL2DZ:UFF)	1.7
ONIOM(M06/def2-TZVP:UFF //M06/6-31G*-LANL2DZ:UFF)	4.5
ONIOM(M06/def2-TZVP:UFF //M06L-D3/6-31G*-LANL2DZ:UFF)	3.3
ONIOM(M06/def2-TZVP:UFF //MN15/6-31G*-LANL2DZ:UFF)	2.1
ONIOM(M06/def2-TZVP:UFF //wB97xD/6-31G*-LANL2DZ:UFF)	2.3

[a] $\Delta\Delta G^{\ddagger} = \Delta G^{\ddagger}_{TS4} - \Delta G^{\ddagger}_{TS3}$
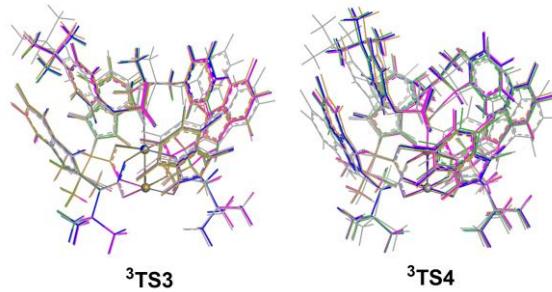
Figure S19. Optimized geometries of **^{3}TS3** and **^{3}TS4**. The geometry optimization of the HL layer was performed using the different functional: BPW91 (in gray), M06 (in green), M06L-D3 (in blue), MN15 (in yellow), and (in pink).

3. Gibbs free energies of calculated structures

Table S5. Electronic energies and free energies (in Hartree) of the structures. Calculated at the ONIOM(M06/def2-TZVP:UFF)//ONIOM(BPW91/LANL2DZ-6-31G*:UFF) Level of Theory.

Structures	ZPVE	TCE	TCH	TCG	E_{gas}	$G_{gas}(E_{gas}+TCG)$	Imaginary Frequency	G_{gas} (kcal/mol)
^{1}**1-1**[a]	0.894214	0.986519	0.987464	0.75623	-5398.797569	-5398.041339	—	—
^{1}**1-2**[a]	0.894181	0.98649	0.987434	0.754601	-5398.786705	-5398.032104	—	—
^{1}**1-3**[a]	0.894187	0.986531	0.987476	0.75545	-5398.786705	-5398.031255	—	—
^{1}**1-4**[a]	0.893878	0.986333	0.987277	0.75197	-5398.775497	-5398.023527	—	—
^{1}**1**	1.002308	1.079837	1.080782	0.888513	-977.8683429	-976.9798299	—	—
sub[a]	0.208972	0.219148	0.220092	0.173041	-389.3207502	-389.1477092	—	—
^{1}**2**	1.208686	1.305487	1.306431	1.068665	-2045.071219	-2044.002554	—	9.3
^{3}**2**	1.209174	1.305688	1.306632	1.069031	-2045.086477	-2044.017446	—	0.0
^{1}**INT1**	1.41776	1.52718	1.52812	1.26272	-2434.400419	-2433.137699	—	17.2
^{1}**TS1**	1.41513	1.522833	1.523777	1.265236	-2434.401473	-2433.136237	219.34i	18.1
^{1}**INT2**	1.418077	1.527185	1.528129	1.265146	-2434.404217	-2433.139071	—	16.4
^{3}**TS2**	1.416598	1.524228	1.525172	1.267428	-2434.400364	-2433.132936	75.61i	20.2
^{3}**INT3**	1.418362	1.527529	1.528473	1.262134	-2434.411415	-2433.149281	—	10.0
^{3}**TS3**	1.413047	1.521227	1.522171	1.261212	-2434.406012	-2433.1448	1161.60i	12.8
^{3}**INT4**	1.418103	1.527187	1.528132	1.263066	-2434.41118	-2433.148114		10.7
^{3}**TS4**	1.41387	1.521866	1.52281	1.262522	-2434.40457	-2433.142048	997.54i	14.5
^{3}**INT5**	1.416554	1.525723	1.526667	1.262432	-2434.427453	-2433.165021	—	0.1
^{3}**TS5**	1.416999	1.525384	1.526328	1.265082	-2434.429218	-2433.164136	206.02i	0.6
^{3}**INT6**	1.417638	1.526616	1.52756	1.262959	-2434.435401	-2433.172442	—	-4.6
^{3}**TS6**	1.417834	1.526425	1.527369	1.265186	-2434.430965	-2433.165779	240.32i	-0.4
Pro1[a]	0.428276	0.454255	0.455200	0.370183	-1456.632071	-1456.261888	—	-59.1
Pro2[a]	0.428359	0.454582	0.455526	0.369437	-1456.62817	-1456.258733	—	-61.0

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy.

[a]Calculated at the M06/def2-TZVP//BPW91/LANL2DZ-6-31G* Level of Theory.

4. Cartesian coordinates of the structures

M06/def2-TZVP//BPW91/LANL2DZ-6-31G*

¹1-1

C	5.63807800	2.54911400	1.50234200
C	-4.30307300	-4.71383900	2.78349300
C	-4.71722900	4.29756400	2.78482700
C	2.55483400	-5.63483700	1.50739200
C	2.12776100	4.55764400	-2.80629900
C	-4.55879700	2.12756300	-2.80565600
C	-2.12839000	-4.55874400	-2.80523600
C	4.55790800	-2.12719100	-2.80659200
C	-4.79135500	0.84431700	-3.64049700
C	2.70242600	5.94251300	-2.41962000
C	5.94272200	-2.70209600	-2.42006600
C	-3.17273500	-3.79829800	-3.64984000
C	3.17307500	3.79758800	-3.65003800
C	3.79740800	-3.17247900	-3.64996400
C	-3.79827100	3.17232900	-3.64965600
C	-2.70435600	-5.94295400	-2.41818800
C	-5.94324200	2.70307100	-2.41870400
C	4.78967500	-0.84401300	-3.64179000
C	-0.84473900	-4.79182000	-3.63931800
C	0.84434200	4.78917700	-3.64115300
C	-1.13502700	-2.39122200	-1.56115400
C	2.39069800	-1.13437400	-1.56159400
C	1.13412300	2.39057900	-1.56166200
C	-2.39144800	1.13407200	-1.56133200
C	-1.73034500	-3.81878400	-1.47820400
C	3.81872100	-1.72856400	-1.47930400
C	1.72956200	3.81808800	-1.47913400
C	-3.81918200	1.72893400	-1.47861800
C	-3.80644200	-2.84104400	-0.34849400
C	4.62997000	-2.70152700	0.70248100
C	2.70530900	4.62702300	0.70236200
C	-2.84218600	3.80403800	-0.34634200
C	-4.52231800	-3.14707600	0.92789100
C	4.22450900	-3.85579700	1.56149700
C	3.86029500	4.22008900	1.55975200
C	-3.14919400	4.51869400	0.93051000
C	-3.86114900	-4.22017100	1.56074400

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C	3.15132500	-4.51853100	0.93037800
C	4.52136500	3.14673300	0.92723700
C	-4.22268400	3.85685100	1.56199200
C	-2.70616500	-4.62732500	0.70345000
C	2.84357900	-3.80437600	-0.34661400
C	3.80534100	2.84022700	-0.34896200
C	-4.62907300	2.70261400	0.70335500
C	-5.63907800	-2.54936600	1.50279800
C	4.71948500	-4.29569900	2.78444000
C	4.30228500	4.71414700	2.78232100
C	-2.55188200	5.63485800	1.50697500
C	-6.09505800	-3.04618700	2.74403200
C	4.12015100	-5.42816500	3.37822300
C	5.43511100	4.11364800	3.37422500
C	-3.04959200	6.08962000	2.74828600
C	-5.43593600	-4.11322900	3.37522000
C	3.05301300	-6.08880300	2.74881600
C	6.09412600	3.04635100	2.74338500
C	-4.11705400	5.42986500	3.37809000
F	-6.29727800	-1.53366300	0.93436700
F	5.73433600	-3.69665700	3.42078600
F	3.70489400	5.72912800	3.42000500
F	-1.53575900	6.29362500	0.93995200
F	-7.16838000	-2.49986200	3.33100000
F	4.57024700	-5.88309000	4.55620600
F	5.89200700	4.56281000	4.55180200
F	-2.50366600	7.16235900	3.33669100
F	-5.89275200	-4.56201500	4.55297200
F	2.50781800	-7.16167900	3.33766600
F	7.16743000	2.50015800	3.33051000
F	-4.56667700	5.88552800	4.55597400
F	-3.70560500	-5.72855500	3.42151500
F	1.53901900	-6.29450100	0.94084400
F	6.29623100	1.53321900	0.93423700
F	-5.73236800	3.69942000	3.42155800
H	6.52648800	-2.89664700	-3.33484700
H	-3.38858900	-4.37558700	-4.56517400
H	-5.40787100	1.08899900	-4.52169500
H	2.89686600	6.52643300	-3.33433000
H	5.85422200	-3.65674200	-1.87611100
H	3.65712000	5.85411200	-1.87572900
H	-2.80739100	-2.80576000	-3.94766100
H	-5.32495900	0.07508000	-3.05792900
H	6.51723000	-2.00170800	-1.79195600

H	2.00198500	6.51682400	-1.79139200
H	-4.12122000	-3.66409800	-3.10804900
H	-3.84572500	0.41126700	-3.99356400
H	4.37417000	-3.38861800	-4.56555900
H	3.38891900	4.37461900	-4.56553700
H	-4.37520100	3.38820300	-4.56521400
H	-2.89885900	-6.52710500	-3.33273700
H	2.80451700	-2.80772900	-3.94738800
H	2.80857600	2.80464700	-3.94756500
H	-2.80551100	2.80728200	-3.94713300
H	-3.65922000	-5.85353300	-1.87476400
H	3.66392000	-4.12063000	-3.10744900
H	4.12138700	3.66431500	-3.10772100
H	-3.66453400	4.12071300	-3.10760200
H	-2.00467300	-6.51754200	-1.78938100
H	1.08856700	5.40563200	-4.52252200
H	5.40560100	-1.08869900	-4.52340200
H	-6.52724000	2.89785400	-3.33329200
H	-1.08902400	-5.40861500	-4.52043100
H	0.07478300	5.32244000	-3.05869300
H	5.32363200	-0.07465300	-3.05968800
H	-0.07594200	-5.32542600	-3.05614100
H	-5.85416700	3.65770800	-1.87482600
H	0.41189400	3.84318100	-3.99398100
H	-6.51783900	2.00296500	-1.79035800
H	-0.41129700	-3.84641900	-3.99250800
H	3.84373700	-0.41114000	-3.99423100
H	-0.92560600	-4.42016600	-1.01493900
H	4.41990800	-0.92288100	-1.01738500
H	0.92483500	4.41969900	-1.01613300
H	-4.42051900	0.92364000	-1.01623900
N	-2.78026200	-3.80370500	-0.44806700
N	3.80543000	-2.77756900	-0.44821500
N	2.77940700	3.80314000	-0.44893900
N	-3.80488100	2.77803300	-0.44765100
O	-0.91064800	-1.85065200	-0.41877400
O	1.85020000	-0.91041400	-0.41908900
O	0.91010500	1.85017500	-0.41911300
O	-1.85084300	0.90992800	-0.41888600
O	-0.86169000	-1.88573400	-2.70337100
O	1.88491800	-0.86098600	-2.70367300
O	0.86048700	1.88486900	-2.70370700
O	-1.88595500	0.86054500	-2.70347900
O	-4.02513300	-1.94342900	-1.15327300

O	5.47765500	−1.84489600	0.91043500
O	1.84977800	5.47547700	0.91165400
O	−1.94376600	4.02337600	−1.15003800
O	−1.85054300	−5.47559800	0.91302100
O	1.94519700	−4.02449600	−1.15011000
O	4.02361600	1.94204800	−1.15321900
O	−5.47738400	1.84667300	0.91154600
Rh	−0.00033200	−0.00022800	−0.37039100
Rh	−0.00058900	−0.00037400	−2.75622500

[1]1-2

C	1.46716400	6.28129500	1.17167800
C	4.94605000	−5.11363500	1.95302100
C	−8.11723600	−0.26409400	0.07246100
C	6.41056900	−0.37175000	−1.54746300
C	−3.75676100	3.99703300	−0.37772300
C	−3.46779300	−3.21454100	2.61281300
C	1.07394400	−4.53265000	−2.57075100
C	1.99916800	2.57735000	−4.05385200
C	−2.35125500	−2.95491200	3.65474300
C	−4.33602400	5.25061500	0.32242600
C	3.14123100	3.53501600	−4.47425000
C	−0.29908700	−5.11476500	−2.17271100
C	−3.22597100	4.39796700	−1.77026000
C	2.03566100	1.32583100	−4.95685900
C	−3.10695600	−4.47409900	1.79847100
C	2.09432100	−5.68859500	−2.71022000
C	−4.79501200	−3.45052400	3.37339000
C	0.65675100	3.32487400	−4.24635700
C	0.97041600	−3.82808700	−3.94645700
C	−4.89949500	2.96263700	−0.52735700
C	0.74364300	−2.31624600	−1.10108900
C	1.17255900	1.31303800	−1.82954500
C	−1.89815200	2.11384800	0.11093700
C	−2.46891300	−1.41524500	0.88096200
C	1.64322100	−3.50453700	−1.51989500
C	2.17858500	2.26337900	−2.52387100
C	−2.65801400	3.38720300	0.56468100
C	−3.65779600	−1.91107300	1.73834200
C	1.48806000	−4.49983700	0.83721200
C	4.41843000	2.72390400	−1.46045100
C	−1.68811100	4.82786800	2.39167800
C	−5.25824900	−2.58432700	−0.20574400
C	2.51585700	−4.94917700	1.82854900

C	5.64459600	1.91585800	−1.18339400
C	−0.45802300	5.66285500	2.53855200
C	−6.57425300	−2.01385000	−0.64295500
C	3.79124900	−4.78092500	1.25266200
C	5.42490500	0.60437500	−1.65448400
C	0.26513100	5.59891700	1.32883700
C	−6.93291100	−0.97547000	0.23810400
C	3.61176800	−4.21538400	−0.11921200
C	4.04291400	0.53568400	−2.22474300
C	−0.48155200	4.71748800	0.38031700
C	−5.85101600	−0.83933400	1.25447400
C	2.37103700	−5.45404200	3.11627400
C	6.84809000	2.27258000	−0.58481200
C	0.01060000	6.40651100	3.61635400
C	−7.39705500	−2.36486100	−1.70822400
C	3.53777500	−5.79558800	3.83458000
C	7.85123500	1.28617900	−0.46436800
C	1.23151500	7.10057600	3.46690800
C	−8.60155100	−1.64930700	−1.88499000
C	4.80818200	−5.62789200	3.26063000
C	7.63635400	−0.01657900	−0.94102700
C	1.94940400	7.03951700	2.26182200
C	−8.95773600	−0.61359600	−1.00600200
F	1.18030300	−5.62941500	3.70370700
F	7.09755500	3.50443900	−0.12187200
F	−0.64113900	6.49411300	4.78238800
F	−7.09947000	−3.34330900	−2.57239400
F	3.43952500	−6.28546100	5.07841600
F	9.02541600	1.59143400	0.10624500
F	1.71549300	7.82886400	4.48263000
F	−9.42002500	−1.95631000	−2.90131000
F	5.89711700	−5.96065500	3.96818300
F	8.61137100	−0.92775800	−0.81931100
F	3.10238500	7.71250100	2.15133800
F	−10.10817400	0.04669300	−1.20143700
F	6.17679500	−4.96791100	1.44525900
F	6.25540200	−1.61965200	−1.99799700
F	2.17898200	6.25454500	0.04074900
F	−8.49232400	0.73126900	0.88635600
H	2.98353900	3.85635200	−5.51699800
H	−0.63209300	−5.82509100	−2.94847000
H	−2.32300100	−3.79903300	4.36404900
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H	4.12776000	3.04557500	−4.42649600

H	−3.58825600	6.05600100	0.40575100
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H	−2.53310600	−2.03322000	4.23329300
H	3.17468400	4.43699700	−3.84142200
H	−4.70755800	5.02183300	1.33470300
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H	−1.36197000	−2.87797700	3.18275000
H	1.88626500	1.63291200	−6.00624400
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H	1.77263200	−6.36121600	−3.52223800
H	1.24385200	0.61164800	−4.69190000
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H	−2.16860000	−4.34404300	1.24197600
H	2.16243500	−6.29254400	−1.79077400
H	3.00141400	0.80187100	−4.89696000
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H	−3.89436400	−4.74893500	1.08446300
H	3.10320400	−5.31823600	−2.95542000
H	−5.73148300	3.41693100	−1.09095800
H	0.56860300	3.65062400	−5.29641400
H	−4.67107500	−4.29549300	4.07044600
H	0.65895200	−4.56151200	−4.70899800
H	−5.29461100	2.64915000	0.45420600
H	0.59923900	4.22167000	−3.60784700
H	1.94368300	−3.41253800	−4.25909300
H	−5.62237500	−3.70429700	2.69129300
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H	−5.09317100	−2.56694700	3.96312700
H	0.23459600	−3.01319800	−3.93418300
H	−0.20376200	2.68305700	−4.01391200
H	2.52039500	−3.02413500	−1.99563700
H	2.04565400	3.22420800	−1.99188900
H	−3.18282100	3.08128300	1.48997800
H	−3.80105800	−1.09618800	2.47202400
N	2.21155900	−4.11870800	−0.31214100
N	3.53599400	1.84962100	−2.14243200
N	−1.66482500	4.35258500	1.05480700
N	−4.90264800	−1.85150600	0.95799200
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O	1.41915100	1.09685800	−0.58770800
O	−0.99361300	1.72270500	0.93245900
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O          0.27395400     -4.44810300      0.97166000
O          4.18235500      3.89032300     -1.17824100
O         -2.55584300      4.57401800      3.21475100
O         -4.63080100     -3.48978400     -0.73063000
O          4.46380900     -3.88733100     -0.93281700
O          3.43979200     -0.43529300     -2.66482700
O         -0.16237500      4.35485400     -0.74583800
O         -5.75328000     -0.02580800      2.16601400
Rh         0.05630900     -0.00882100      0.50369500
Rh        -1.25878900     -0.23480100     -1.47419300
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C         -6.87710000      1.95180900     -0.69164000
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C          6.60358400      2.68791300     -1.31055600
C         -3.21288600      1.44012600      3.89848400
C         -1.18956400     -4.91081500      0.38911100
C          3.20035300     -1.70409200     -3.56744000
C          1.21325800      4.94644500     -1.00767800
C         -0.09780500     -5.12405800      1.46541500
C         -4.49442200      2.14962600      4.39449100
C          1.94369900      6.28488400     -0.73833700
C          2.20171800     -2.85986200     -3.78776000
C         -3.41627800     -0.08865800      3.94779400
C          1.34024100      4.60183300     -2.50718000
C         -0.52904300     -4.89325000     -1.00405800
C          4.59909900     -2.12800500     -4.07713600
C         -2.20336600     -6.07393000      0.48072800
C         -0.27766600      5.12743500     -0.63205200
C          2.75084100     -0.46847200     -4.38769600
C         -2.05055100      1.83691200      4.84308800
C          2.07420100     -0.93692100     -1.24916500
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C         -1.83791300      1.18800800      1.62246100
C         -1.15413600     -2.27223400      0.47065900
C          3.34930300     -1.27123800     -2.05900500
C          1.82565500      3.86555700     -0.04745100
C         -2.87416800      1.98211400      2.44929200
C         -1.95002400     -3.56654600      0.73722700
C          3.86446800     -3.36825800     -0.66526200
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C	5.51781200	3.91617600	0.49770900
C	-5.42694500	3.63481900	0.30637200
C	-5.27515300	-3.17674600	-0.99722900
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C	-5.81044300	2.28949800	0.13377400
C	-5.63074800	-3.16980900	0.36440500
C	5.47148400	-1.66505600	-0.77259300
C	4.01196600	2.97507800	-1.05082800
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C	-4.38774600	-3.33884900	1.16615900
C	5.24887900	-4.90923200	0.94481100
C	6.74041200	4.21890400	1.08752500
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C	-6.23868900	-3.02882300	-1.98931900
C	6.46456900	-5.01666500	1.65537600
C	7.91606100	3.74268500	0.46658500
C	-7.18097700	4.32962700	-1.18484400
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C	7.42759000	-3.99692700	1.58830800
C	7.84893600	2.99095200	-0.71708400
C	-7.56484300	2.98997300	-1.35701100
C	-7.93594700	-2.85457100	-0.23451800
F	4.35962600	-5.90567900	1.03900900
F	6.85180300	4.94081500	2.20970900
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F	-5.95026300	-3.02880800	-3.29769300
F	6.70890200	-6.10081100	2.40430100
F	9.11341800	4.01464300	1.00437500
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F	-8.54127600	-2.71209500	-2.52019400
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F	6.58709200	1.99227700	-2.45084900
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H	1.65962700	4.23671800	0.98054200
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H	−2.10589000	−3.58264800	1.82942500
N	4.21984200	−2.12918300	−1.24280000
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N	−4.02686800	2.31970800	1.60929200
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O	2.21710700	−0.95269500	0.02732400

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O	0.35872000	2.11824500	-0.94209400
O	-2.02552500	1.12804900	0.35538800
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O	2.81205500	-3.96812700	-0.83194700
O	3.73874200	4.91767300	1.86783200
O	-3.61123900	4.62815100	1.62769900
O	-3.13899900	-3.47122000	-2.13624400
O	5.97873700	-0.58658200	-1.05214500
O	3.52172400	2.29945100	-1.94831000
O	-4.92109200	0.20754800	1.06952400
O	-4.25929900	-3.39450700	2.38250500
Rh	0.70965300	-0.15380100	1.17907000
Rh	-0.54748800	0.25685800	-0.80830300

¹1-4

C	2.54649000	4.81578500	4.72452300
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C	3.20156400	1.51157800	-3.79670300
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C	4.60743500	-0.48535700	4.65071600
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C	2.20604600	-1.26253000	4.57811400
C	-2.20694900	0.95994300	4.65527100
C	1.90801100	1.57070900	-4.63512600
C	-4.45136900	-0.96417100	-4.76898900
C	4.41381900	1.27256300	-4.72749800
C	-3.91330500	2.00117800	3.11087900
C	-3.44337300	-2.65804000	-3.22597700
C	3.91126100	-2.20530600	2.97053400
C	-1.93486600	-0.10545800	-1.82989800
C	-1.93102100	-0.23768600	1.77996200
C	1.93102300	0.11826400	1.78841300
C	1.92644400	0.22811400	-1.82467100
C	-3.20435500	-0.18653700	-2.70768700

C	−3.19868800	−0.38877800	2.65184400
C	3.20055500	0.21016400	2.66579400
C	3.18951000	0.36799600	−2.70437900
C	−2.89443300	2.11707300	−3.82864500
C	−4.40154900	−2.57496000	2.52812800
C	4.40749100	2.39718700	2.67438300
C	2.88377700	−1.86570500	−3.96102500
C	−3.71801000	3.36813500	−3.79241100
C	−4.17664800	−3.95722600	3.04365400
C	4.18867000	3.74475700	3.27684400
C	3.71281500	−3.11300100	−4.00322700
C	−4.87193900	3.12435500	−3.02069600
C	−2.99261300	−3.95119100	3.80830400
C	3.00921800	3.69288100	4.04677000
C	4.86970000	−2.91039600	−3.22412900
C	−4.81250600	1.71573000	−2.53224600
C	−2.43416500	−2.56101000	3.81266500
C	2.44772300	2.30613900	3.96742600
C	4.80669900	−1.53377900	−2.65210200
C	−3.49610500	4.61106200	−4.37572300
C	−4.91401000	−5.12351600	2.86595900
C	4.92739600	4.91860000	3.16777600
C	3.49318800	−4.31996600	−4.65850600
C	−4.45753300	5.62523400	−4.17262100
C	−4.44461400	−6.30746700	3.47500000
C	4.46404800	6.06301500	3.85231100
C	4.45995100	−5.34005100	−4.52090800
C	−5.60679000	5.38146700	−3.40359300
C	−3.26511800	−6.30233800	4.23681900
C	3.28913800	6.01224700	4.61951700
C	5.61221100	−5.13727300	−3.74451100
F	−2.41537800	4.88982700	−5.11556600
F	−6.04263200	−5.17252200	2.14742200
F	6.05177100	5.01044500	2.44678600
F	2.40979400	−4.55918000	−5.40823200
F	−4.27786500	6.83696900	−4.71690600
F	−5.12568400	−7.45261900	3.32772500
F	5.14645500	7.21405300	3.77251700
F	4.28257200	−6.51806000	−5.13547400
F	−6.50070700	6.36506600	−3.22948900
F	−2.84426200	−7.44307900	4.80116100
F	2.87393800	7.11625900	5.25644800
F	6.51120600	−6.12541800	−3.63376000
F	−6.93358000	3.92673900	−2.08914100

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F        -1.40452900    -5.15650200     5.14555900
F         1.43171700     4.81511100     5.46640500
F         6.93968400    -3.75735500    -2.35239400
H        -4.89155100     0.96815800     5.38849700
H        -2.04118300    -2.04124300    -5.50878000
H         3.47413000     3.67396300    -3.82582100
H         4.89095200    -1.32241100     5.30969900
H        -4.31710200    -0.70842400     5.26605400
H         4.31800700     0.35909300     5.29623400
H        -1.05957300    -1.52886500    -4.11918100
H         4.35586400     2.87448300    -2.50011500
H        -5.50151900    -0.07991300     4.08340800
H         5.50222200    -0.19248000     4.07549300
H        -1.76462900    -0.30533600    -5.19941700
H         2.58623000     3.09668100    -2.39195400
H        -2.45895800     1.71154400     5.42256000
H         2.45726100    -2.05934000     5.29863500
H         1.99339100     2.37933300    -5.38070600
H        -4.57070000    -1.78158600    -5.49900500
H        -1.37144800     1.35830300     4.06172100
H         1.37155900    -1.62438500     3.96029900
H         1.02690600     1.78565800    -4.01328800
H        -4.32617100    -0.02944500    -5.33832500
H        -1.85546400     0.05208100     5.16492500
H         1.85354900    -0.38724400     5.14115700
H         1.72413900     0.62766600    -5.16823300
H        -5.38609900    -0.89453400    -4.18694700
H         4.14238800    -3.00073000     3.69853200
H        -4.14765800     2.74697200     3.88867500
H         4.52346700     2.13296400    -5.40795400
H        -3.51532500    -3.41835400    -4.02147700
H         4.82540400    -2.01491600     2.38128000
H        -4.82606500     1.84730100     2.50897700
H        -4.37902200    -2.69582600    -2.64097500
H         4.28610700     0.37342600    -5.35099500
H         3.13203000    -2.57845700     2.29185700
H         5.35434800     1.17155000    -4.15955600
H        -2.60953800    -2.93219900    -2.56523000
H        -3.13406400     2.41969300     2.45929000
H        -3.99970500    -0.49134200    -1.99877400
H        -4.03287500    -0.26441900     1.93282600
H         4.03315400     0.12926200     1.93879000
H         3.98867800     0.63445500    -1.98453200
N        -3.62883300     1.16510800    -3.08444000
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N	−3.34849000	−1.78905100	3.05934400
N	3.35544200	1.58144300	3.16089400
N	3.61759000	−0.95661400	−3.16424700
O	−1.61940200	1.05421800	−1.38264500
O	−1.55730500	0.95167600	1.48498300
O	1.41126000	1.23077000	1.41832400
O	1.35102500	1.31015900	−1.45076000
O	−1.35692900	−1.20982400	−1.53304700
O	−1.41324700	−1.32260600	1.33324800
O	1.55734100	−1.04855400	1.41390500
O	1.61281700	−0.95884100	−1.45452400
O	−1.82105300	1.93710500	−4.38461200
O	−5.28909000	−2.15910000	1.79462000
O	5.29022400	2.02642000	1.91148700
O	1.80731900	−1.65802600	−4.50114200
O	−5.59314100	1.11752500	−1.80315300
O	−1.41367500	−2.15924500	4.35182200
O	1.43001200	1.87347800	4.48764600
O	5.58872200	−0.97660700	−1.89263800
Rh	−0.10752800	1.18810600	0.01942100
Rh	0.10439200	−1.18630300	−0.06134900

Sub

C	−0.38664000	−0.12955900	−0.47716800
C	−1.12513700	1.06232500	−0.61374400
C	−2.46861200	1.13306200	−0.21446200
C	−3.10122200	0.00650000	0.33058900
C	−2.38035900	−1.18993700	0.47042400
C	−1.03902800	−1.25455200	0.06910500
H	−0.64060800	1.94506100	−1.04395100
H	−3.02174400	2.06960900	−0.33341000
H	−4.14918200	0.05779200	0.63975200
H	−2.86618000	−2.07717900	0.88764100
H	−0.48809000	−2.19549600	0.17410100
C	1.07091300	−0.21031600	−0.89170000
H	1.31255200	0.63048700	−1.56810000
H	1.23069400	−1.13520500	−1.47659500
C	2.08200400	−0.20358500	0.28977100
H	1.79463800	−1.02605400	0.97339300
C	3.50563000	−0.48630400	−0.22305000
H	3.83766700	0.30149100	−0.92250300
H	4.22928700	−0.51807900	0.60889800
H	3.56078400	−1.45120200	−0.75555800
C	2.03110100	1.11199900	1.08525600

H	2.32472000	1.96725600	0.45025000
H	1.01952500	1.31211000	1.47298300
H	2.72403700	1.08159800	1.94296700

Pro1

N	−2.33485600	−0.86122900	−0.61481100
S	−1.37519500	−2.23152600	−0.47579900
O	−2.19670000	−3.34491800	0.00796500
O	−0.30176000	−1.95670800	0.84136200
O	−0.56808500	−2.28750500	−1.70223700
C	−1.22543700	3.29359900	−1.50442000
C	−2.19289200	2.27896000	−1.43614200
C	−2.90187700	2.02646100	−0.24109300
C	−2.62603500	2.84017900	0.87851900
C	−1.66404400	3.85785700	0.81215900
C	−0.95609300	4.08462100	−0.37870000
H	−0.69133400	3.47068500	−2.44218900
H	−2.41858400	1.68701300	−2.32988300
H	−3.18371800	2.68339800	1.80692100
H	−1.47276700	4.48090200	1.69073800
H	−0.20822500	4.88073800	−0.43113200
C	−3.93436500	0.91649100	−0.17810800
H	−4.75874100	1.21127000	0.49333300
H	−4.37315800	0.77046600	−1.17972400
C	−3.44137200	−0.48708700	0.32541000
H	−1.73530900	−0.06466700	−0.86572600
C	−2.98985600	−0.43214300	1.79785100
H	−2.17084400	0.28755100	1.94609500
H	−3.83453000	−0.13134800	2.44022500
H	−2.64279000	−1.42005900	2.13447900
C	−4.61209000	−1.47618900	0.15796000
H	−4.90328000	−1.55471600	−0.90119000
H	−4.34110400	−2.47813900	0.51606000
H	−5.48088100	−1.12018800	0.73597600
C	0.93865700	−1.36304600	0.57250300
C	1.15348400	−0.03055900	0.94354500
C	1.98509500	−2.11946400	0.02218600
C	2.42228500	0.54328600	0.76675200
H	0.33814200	0.54893900	1.38223000
C	3.23964900	−1.52807600	−0.15109400
H	1.80732900	−3.15736300	−0.26444700
C	3.49351200	−0.18593200	0.21489100
H	2.56293600	1.58226700	1.07070400
H	4.04108700	−2.13510200	−0.58153500

C	4.89829900	0.41643500	0.00618800
C	4.97998700	1.88941700	0.46289800
C	5.93518600	-0.40101900	0.82132900
C	5.26523800	0.35606000	-1.50033300
H	4.28434300	2.53378800	-0.10043500
H	4.76050300	1.99989200	1.53808700
H	5.99903600	2.27445200	0.29235200
H	5.95842400	-1.45854500	0.51302600
H	6.94834600	0.01223000	0.67674000
H	5.70340600	-0.37046100	1.89883900
H	6.27223300	0.77616300	-1.66663900
H	5.26691600	-0.67750900	-1.88186100
H	4.54806300	0.93532300	-2.10511700

Pro2

N	2.09312300	-0.69572500	-0.56578800
S	1.56574600	-2.24745400	-0.16488700
O	2.45296500	-3.23597600	-0.79223000
O	0.16363600	-2.41205500	-1.08537200
O	1.20516400	-2.26586600	1.26175800
C	-0.98335600	-1.69885600	-0.69136600
C	-1.76919000	-2.15062400	0.37841800
C	-1.37950500	-0.59308800	-1.44900600
C	-2.95554200	-1.47509700	0.68176700
H	-1.44844300	-3.01760100	0.95793900
C	-2.57755500	0.06520900	-1.13251800
H	-0.75761500	-0.26125700	-2.28221800
C	-3.39155200	-0.35443700	-0.06186600
H	-3.55731000	-1.84006100	1.51882300
H	-2.86827700	0.92377300	-1.74045500
C	-4.71151800	0.35107300	0.31264700
C	-4.61687300	0.87712100	1.76941800
H	-3.79466800	1.60419800	1.87376100
H	-5.55703500	1.37845900	2.05740200
H	-4.43809100	0.06255900	2.48951300
C	-5.88414500	-0.65945700	0.20524000
H	-6.83609200	-0.17191700	0.47770000
H	-5.97954200	-1.04606000	-0.82291100
H	-5.74642500	-1.52211600	0.87669000
C	-5.02114400	1.54826700	-0.61243600
H	-5.96999000	2.01834000	-0.30497300
H	-4.23662700	2.32164800	-0.56082100
H	-5.13227000	1.23733200	-1.66475100
C	1.83855600	1.67766500	0.13961400

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C            1.56592300      2.08551100     -1.17835300
C            1.08748500      3.37757100     -1.44565700
C            0.87043100      4.28252500     -0.39703300
C            1.13116300      3.88411300      0.92307100
C            1.61036200      2.59373400      1.18582100
H            1.71039500      1.38206400     -2.00230200
H            0.88150000      3.67473200     -2.47823000
H            0.49487500      5.28835700     -0.60518900
H            0.95361500      4.57597200      1.75157500
H            1.80133800      2.28909400      2.22049500
C            2.41156400      0.30107800      0.48250900
H            2.77990900     -0.77341800     -1.31999100
H            1.90397900     -0.05860600      1.39178900
C            3.94390500      0.37146000      0.80248800
C            4.46486600     -0.93778600      1.42117500
H            4.43027100     -1.77041500      0.69903900
H            5.51480500     -0.81964300      1.73660800
H            3.87471500     -1.23548500      2.30270100
C            4.79516200      0.79362200     -0.40931300
H            4.80940700      0.01703500     -1.19610200
H            4.43648500      1.73365500     -0.85776500
H            5.84328300      0.94253300     -0.10311000
H            4.03567700      1.16972300      1.56252500
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ONIOM(M06/def2-TZVP:UFF)//ONIOM(BPW91/LANL2DZ-6-31G*:UFF)

[1]**1**

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C-C_R    0    -4.68140100    -3.58664100     1.16740600 L
C-C_R    0     3.04019700     5.04339800     2.81057400 L
C-C_R    0     5.05221500    -3.03178900     2.81362300 L
C-C_R    0    -3.58709300     4.67536500     1.17401500 L
C-C_3    0    -0.38804000    -4.96640900    -2.68556100 L
C-C_3    0     4.96425800    -0.38348100    -2.68925600 L
C-C_3    0     0.37984900     4.96998700    -2.68084000 L
C-C_3    0    -4.97207500     0.38450800    -2.67775100 L
C-C_3    0     4.72828400     0.91655500    -3.49481400 L
C-C_3    0    -0.45663000    -6.47862900    -2.36309100 L
C-C_3    0    -6.48373300     0.45323700    -2.35269700 L
C-C_3    0     1.59762700     4.61859500    -3.56684300 L
C-C_3    0    -1.60913400    -4.61409600    -3.56661500 L
C-C_3    0    -4.62154800     1.60445700    -3.56110400 L
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C-C_3	0	4.61077400	-1.60228200	-3.57303000	L
C-C_3	0	0.45006500	6.48170900	-2.35642300	L
C-C_3	0	6.47653800	-0.45386500	-2.36747400	L
C-C_3	0	-4.73663000	-0.91460600	-3.48496700	L
C-C_3	0	-0.92114800	4.73494000	-3.48512300	L
C-C_3	0	0.90999400	-4.72985200	-3.49419400	L
C-C_R	0	0.18359000	2.64259100	-1.40671300	H
C-C_R	0	-2.64417500	0.18665500	-1.40490000	H
C-C_R	0	-0.18840300	-2.64068900	-1.40895600	H
C-C_R	0	2.63918200	-0.18508100	-1.41116900	H
C-C_3	0	0.35114600	4.16412200	-1.32740400	L
C-C_3	0	-4.16575200	0.35331400	-1.32466700	L
C-C_3	0	-0.35483200	-4.16244800	-1.33108700	L
C-C_3	0	4.16084600	-0.35268800	-1.33440900	L
C-C_R	0	2.81402400	3.86848700	-0.53715000	L
C-C_R	0	-5.07715100	1.45877300	0.82297100	L
C-C_R	0	-1.45756600	-5.07913500	0.81551700	L
C-C_R	0	3.86712100	-2.81443800	-0.54060800	L
C-C_R	0	3.48541700	4.04852900	0.74599900	L
C-C_R	0	-4.76370600	2.68482500	1.55307000	L
C-C_R	0	-2.68281200	-4.76852000	1.54786000	L
C-C_R	0	4.04995600	-3.48196300	0.74332000	L
C-C_R	0	2.68848500	4.75839000	1.54377000	L
C-C_R	0	-4.05298300	3.48277500	0.75637300	L
C-C_R	0	-3.48402000	-4.05428400	0.75419500	L
C-C_R	0	4.76054400	-2.68597600	1.54139200	L
C-C_R	0	1.46106800	5.07437000	0.81844000	L
C-C_R	0	-3.87086200	2.81401100	-0.52784900	L
C-C_R	0	-2.81428200	-3.86877800	-0.52974900	L
C-C_R	0	5.07423700	-1.45957500	0.81189500	L
C-C_R	0	4.68069100	3.58115100	1.16570600	L
C-C_R	0	-5.05739200	3.02585200	2.82237700	L
C-C_R	0	-3.02088800	-5.06796300	2.81519400	L
C-C_R	0	3.58752400	-4.67110000	1.16972500	L
C-C_R	0	5.08437700	3.85003400	2.43416400	L
C-C_R	0	-4.59966500	4.27139400	3.30489100	L
C-C_R	0	-4.26496700	-4.61035400	3.29080400	L
C-C_R	0	3.88838100	-5.05732000	2.49418600	L
C-C_R	0	4.29074600	4.57270500	3.26851100	L
C-C_R	0	-3.87634500	5.08232100	2.49431000	L
C-C_R	0	-5.09292700	-3.85562900	2.42919300	L
C-C_R	0	4.61553800	-4.22733400	3.28831400	L
F-F_	0	5.46945100	2.85356100	0.33526500	L
F-F_	0	-5.77194900	2.19543800	3.62237400	L

F-F_	0	-2.19182300	-5.78472000	3.61452900	L
F-F_	0	2.85571800	-5.47508600	0.35849300	L
F-F_	0	6.28329100	3.39039100	2.87240200	L
F-F_	0	-4.87850400	4.65065000	4.57695200	L
F-F_	0	-4.65919500	-4.88386300	4.55908400	L
F-F_	0	3.44757000	-6.24802200	2.97131300	L
F-F_	0	4.69280600	4.83596200	4.53688400	L
F-F_	0	-3.42653200	6.27808100	2.94990000	L
F-F_	0	-6.29219600	-3.39836800	2.86785100	L
F-F_	0	4.90141500	-4.59229300	4.56337500	L
F-F_	0	2.22236200	5.75528400	3.62562100	L
F-F_	0	-2.85773900	5.46941300	0.35075000	L
F-F_	0	-5.46494600	-2.85764100	0.33324600	L
F-F_	0	5.76851100	-2.19847300	3.60963000	L
H-H_	0	-7.09149100	0.42394400	-3.28321700	L
H-H_	0	1.54954900	5.17695800	-4.52677800	L
H-H_	0	5.36869200	0.93603500	-4.40325600	L
H-H_	0	-0.42866700	-7.08474900	-3.29472200	L
H-H_	0	-6.73652100	1.39286200	-1.81636400	L
H-H_	0	-1.39560100	-6.73220900	-1.82599200	L
H-H_	0	1.63999500	3.54058400	-3.81482900	L
H-H_	0	4.98343300	1.80764200	-2.88289300	L
H-H_	0	-6.78873900	-0.40394800	-1.71389400	L
H-H_	0	0.40132800	-6.78492100	-1.72594700	L
H-H_	0	2.54768500	4.90614300	-3.07159800	L
H-H_	0	3.67923000	1.01327800	-3.83649000	L
H-H_	0	-5.18055100	1.55852900	-4.52077100	L
H-H_	0	-1.56449900	-5.17119900	-4.52744700	L
H-H_	0	5.16748500	-1.55572600	-4.53399800	L
H-H_	0	0.41913400	7.08917900	-3.28707900	L
H-H_	0	-3.54371100	1.64764400	-3.80971500	L
H-H_	0	-1.65261300	-3.53576100	-3.81301500	L
H-H_	0	3.53231600	-1.64450800	-3.81908500	L
H-H_	0	1.39094700	6.73415500	-1.82213700	L
H-H_	0	-4.90889500	2.55327300	-3.06335800	L
H-H_	0	-2.55729700	-4.90242700	-3.06819000	L
H-H_	0	4.89874300	-2.55182200	-3.07704500	L
H-H_	0	-0.40560600	6.78738400	-1.71591500	L
H-H_	0	0.92801500	-5.37090700	-4.40220900	L
H-H_	0	-5.37928400	-0.93406900	-4.39182100	L
H-H_	0	7.08234300	-0.42429700	-3.29925900	L
H-H_	0	-0.94215400	5.37709800	-4.39229400	L
H-H_	0	1.80267500	-4.98373900	-2.88407800	L
H-H_	0	-4.98918000	-1.80649000	-2.87312800	L

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H-H_        0    -1.81154300     4.98844700    -2.87151600  L
H-H_        0     6.72960500    -1.39418700    -1.83249600  L
H-H_        0     1.00504100    -3.68099600    -3.83692400  L
H-H_        0     6.78367700     0.40247500    -1.72855800  L
H-H_        0    -1.01780500     3.68650100    -3.82870900  L
H-H_        0    -3.68834200    -1.00985700    -3.82939000  L
H-H_        0    -0.55952000     4.51480000    -0.79317000  L
H-H_        0    -4.51573100    -0.55860300    -0.79221000  L
H-H_        0     0.55792500    -4.51336500    -0.80052300  L
H-H_        0     4.51257800     0.55867000    -0.80210700  L
N-N_R       0     1.51853300     4.48494600    -0.48679300  L
N-N_R       0    -4.48699600     1.51873500    -0.48152500  L
N-N_R       0    -1.51908100    -4.48518100    -0.48685200  L
N-N_R       0     4.48307200    -1.51887200    -0.49269300  L
O-O_R       0     0.03005900     2.05848000    -0.27349500  H
O-O_R       0    -2.05947400     0.03126300    -0.27223400  H
O-O_R       0    -0.03223300    -2.05780700    -0.27546700  H
O-O_R       0     2.05706300    -0.03070100    -0.27701200  H
O-O_R       0     0.22280300     2.05561700    -2.54082200  H
O-O_R       0    -2.05778200     0.22834600    -2.53921400  H
O-O_R       0    -0.23062000    -2.05240400    -2.54227700  H
O-O_R       0     2.05023300    -0.22519400    -2.54422100  H
O-O_R       0     3.12414000     2.97628400    -1.36924000  L
O-O_R       0    -5.43328100     0.38218800     1.37290800  L
O-O_R       0    -0.38042600    -5.43747000     1.36293100  L
O-O_R       0     2.97179600    -3.12539300    -1.36901000  L
O-O_R       0     0.38515300     5.42481700     1.37325600  L
O-O_R       0    -2.97874400     3.12689900    -1.35903500  L
O-O_R       0    -3.12886900    -2.97666400    -1.36032400  L
O-O_R       0     5.42913400    -0.38310700     1.36280900  L
Rh-         0    -0.00112900     0.00032600    -0.22198800  H
Rh-         0    -0.00389700     0.00162900    -2.59930900  H

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C-C_R       0     5.52092500     1.65877700     2.60338500  L
C-C_R       0    -4.58103700    -3.79027400     0.61338200  L
C-C_R       0    -4.11437000     4.48406900     0.99372700  L
C-C_R       0     1.69643600    -5.54411000     0.99690800  L
C-C_3       0     3.49918900     4.70953100    -2.07835000  L
C-C_3       0    -2.64129900     2.35041600    -4.52449900  L
C-C_3       0    -0.49972900    -4.23391400    -3.87739400  L
C-C_3       0     5.76228600    -2.00003000    -1.46059300  L
C-C_3       0    -2.50311000     1.10223700    -5.42969000  L
C-C_3       0     3.93306000     6.08883300    -1.52690100  L
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C-C_3   0    6.94092100   -2.63874000   -0.68743700  L
C-C_3   0   -1.20765100   -3.40939200   -4.97744100  L
C-C_3   0    4.76452900    3.98592100   -2.59421800  L
C-C_3   0    5.35472300   -2.97220400   -2.59174400  L
C-C_3   0   -1.63580200    3.43202200   -4.98259700  L
C-C_3   0   -1.16475600   -5.63047800   -3.82700000  L
C-C_3   0   -4.06938800    2.91039700   -4.73075900  L
C-C_3   0    6.28320900   -0.68339000   -2.08472800  L
C-C_3   0    0.98154900   -4.44679000   -4.27332800  L
C-C_3   0    2.54043800    4.96974800   -3.26506400  L
C-C_R   0    0.06505500   -2.20992000   -2.25002800  H
C-C_R   0    3.35566400   -0.97667400   -0.97501900  H
C-C_R   0    2.13842700    2.56595800   -1.29186600  H
C-C_R   0   -1.14957500    1.28584000   -2.60273800  H
C-C_3   0   -0.60306600   -3.57284300   -2.45145900  L
C-C_3   0    4.59325000   -1.70750700   -0.44624900  L
C-C_3   0    2.76210500    3.91859300   -0.93357800  L
C-C_3   0   -2.46410200    1.96380100   -3.00927500  L
C-C_R   0   -2.98252100   -2.51162500   -2.29535400  L
C-C_R   0    4.19061200   -3.09718800    1.68777400  L
C-C_R   0    3.31427300    4.26400400    1.56179300  L
C-C_R   0   -1.74762000    4.05343900   -1.63322700  L
C-C_R   0   -4.05301800   -2.56531400   -1.30317100  L
C-C_R   0    3.22511200   -4.12601800    2.06493600  L
C-C_R   0    4.03027100    3.47837600    2.56358000  L
C-C_R   0   -2.22306800    4.63279700   -0.38196500  L
C-C_R   0   -3.77725600   -3.53841600   -0.43529200  L
C-C_R   0    2.66245000   -4.60649300    0.95656700  L
C-C_R   0    4.77088600    2.56218200    1.93658100  L
C-C_R   0   -3.43450000    4.14357100   -0.12160600  L
C-C_R   0   -2.51831000   -4.16833000   -0.82148500  L
C-C_R   0    3.22916900   -3.90894700   -0.19333600  L
C-C_R   0    4.56725900    2.71093800    0.49858900  L
C-C_R   0   -3.79620100    3.21863000   -1.19256000  L
C-C_R   0   -5.15173100   -1.79025500   -1.17774800  L
C-C_R   0    2.85654300   -4.54732600    3.28985500  L
C-C_R   0    3.98384500    3.55781900    3.90586400  L
C-C_R   0   -1.61517900    5.48683600    0.46078700  L
C-C_R   0   -6.00311500   -2.01634600   -0.14347300  L
C-C_R   0    1.85176200   -5.53457800    3.38506900  L
C-C_R   0    4.75552300    2.64220700    4.64707900  L
C-C_R   0   -2.30911100    5.85925300    1.63308400  L
C-C_R   0   -5.74163300   -2.99933800    0.75836900  L
C-C_R   0    1.28165300   -6.02505700    2.25732400  L
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C-C_R    0     5.53079100     1.68279500     3.95728700  L
C-C_R    0    -3.54630300     5.34908000     1.87344100  L
F-F_     0    -5.40204400    -0.79670700    -2.06738600  L
F-F_     0     3.42796000    -4.03345800     4.40767200  L
F-F_     0     3.21644500     4.48586600     4.53023700  L
F-F_     0    -0.37667200     5.97410200     0.19886100  L
F-F_     0    -7.11191500    -1.24753400    -0.00120000  L
F-F_     0     1.45492500    -5.98422600     4.60160800  L
F-F_     0     4.74902600     2.67629600     6.00263800  L
F-F_     0    -1.74065800     6.71891400     2.51486300  L
F-F_     0    -6.58478800    -3.21661300     1.79784800  L
F-F_     0     0.31076300    -6.96875800     2.33769600  L
F-F_     0     6.27663700     0.78654200     4.65024300  L
F-F_     0    -4.21540900     5.70260100     2.99950800  L
F-F_     0    -4.28870200    -4.76867700     1.50607000  L
F-F_     0     1.13202500    -6.01725300    -0.14205000  L
F-F_     0     6.25712400     0.73882400     1.93058700  L
F-F_     0    -5.34798200     3.97487700     1.23358400  L
H-H_     0     7.80770800    -2.81555500    -1.36086800  L
H-H_     0    -1.05220300    -3.88053100    -5.97211600  L
H-H_     0    -2.75887400     1.35164200    -6.48234700  L
H-H_     0     4.41744400     6.69884000    -2.32020900  L
H-H_     0     6.64971500    -3.61770800    -0.25002600  L
H-H_     0     4.66258600     5.97679600    -0.69639600  L
H-H_     0    -0.82261200    -2.37310900    -5.03843500  L
H-H_     0    -3.19000300     0.29629900    -5.09353700  L
H-H_     0     7.27562500    -1.97520300     0.13934400  L
H-H_     0     3.05564100     6.65415700    -1.14435100  L
H-H_     0    -2.30269800    -3.37069600    -4.80534100  L
H-H_     0    -1.47082600     0.70141300    -5.43787400  L
H-H_     0     6.19215600    -3.09844800    -3.31169500  L
H-H_     0     5.22344300     4.55999700    -3.42812300  L
H-H_     0    -1.78448300     3.66514700    -6.05918700  L
H-H_     0    -1.06567800    -6.15266000    -4.80350500  L
H-H_     0     4.48013200    -2.60729500    -3.16402300  L
H-H_     0     4.54143200     2.97129100    -2.97666400  L
H-H_     0    -0.58473800     3.10706300    -4.85765500  L
H-H_     0    -2.24908000    -5.55080100    -3.59828200  L
H-H_     0     5.12150100    -3.97881200    -2.18827800  L
H-H_     0     5.53041500     3.90386100    -1.79578200  L
H-H_     0    -1.78179000     4.37560900    -4.41705600  L
H-H_     0    -0.69072300    -6.26418100    -3.04623700  L
H-H_     0     3.02432300     5.62201100    -4.02411000  L
H-H_     0     7.17008500    -0.87764100    -2.72620000  L
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H-H_	0	-4.25170000	3.14875800	-5.80125500	L
H-H_	0	1.05486300	-5.01750400	-5.22447900	L
H-H_	0	1.61693300	5.48035100	-2.91799400	L
H-H_	0	6.59017500	0.03107800	-1.29161900	L
H-H_	0	1.51784600	-5.02377400	-3.49008500	L
H-H_	0	-4.22225400	3.84482300	-4.14955600	L
H-H_	0	2.25042400	4.03327800	-3.78083300	L
H-H_	0	-4.83296600	2.17018500	-4.40697000	L
H-H_	0	1.51503900	-3.48921300	-4.43093600	L
H-H_	0	5.52167700	-0.19412200	-2.72326600	L
H-H_	0	-0.05066000	-4.25477000	-1.76860700	L
H-H_	0	5.02493300	-1.00900600	0.30422200	L
H-H_	0	1.89525700	4.55519100	-0.64738400	L
H-H_	0	-3.24579400	1.19965400	-2.79975100	L
N-N_R	0	-1.99919200	-3.50937900	-1.98318600	L
N-N_R	0	4.17297500	-2.92859500	0.26443100	L
N-N_R	0	3.62046300	3.76232500	0.25473300	L
N-N_R	0	-2.71877400	3.12178300	-2.13294500	L
O-O_R	0	0.01842200	-1.77643500	-1.04406400	H
O-O_R	0	2.51747200	-0.62941900	-0.06468400	H
O-O_R	0	1.40559400	2.05902800	-0.36847700	H
O-O_R	0	-1.10954700	0.88128900	-1.38511300	H
O-O_R	0	0.60240100	-1.60262600	-3.23412400	H
O-O_R	0	3.21476900	-0.76990100	-2.22361300	H
O-O_R	0	2.38572100	2.02730900	-2.42124600	H
O-O_R	0	-0.20199600	1.17708400	-3.44710900	H
O-O_R	0	-2.74278000	-1.50402700	-3.01132500	L
O-O_R	0	4.63244000	-2.22376600	2.48172800	L
O-O_R	0	2.29940100	4.96777300	1.81278200	L
O-O_R	0	-0.55197100	4.09503000	-2.02527100	L
O-O_R	0	-1.80862400	-4.85897400	-0.04220700	L
O-O_R	0	2.66652700	-3.85283400	-1.31828400	L
O-O_R	0	4.83366400	1.81138700	-0.34101000	L
O-O_R	0	-4.74543000	2.39222100	-1.13190200	L
Rh-	0	0.67792800	0.12443800	-0.60114400	H
Rh-	0	1.52010700	0.21230200	-2.87384800	H
N-N_R	0	-0.06593000	0.16663100	1.18648200	H
S-S_R	0	-0.31152900	-1.17796900	2.11474900	H
O-O_R	0	0.38140100	-2.42891500	1.76768600	H
O-O_R	0	-1.93325900	-1.39082800	1.40194900	H
O-O_R	0	-0.48028600	-0.78240600	3.52890400	H
C-C_R	0	-3.02956100	-0.87496700	2.03641900	H
C-C_R	0	-3.79932100	0.08260000	1.34810400	H
C-C_R	0	-3.45024500	-1.35337900	3.29686200	H

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C-C_R       0    -4.99694500     0.53245900     1.90454900  H
H-H_        0    -3.42898400     0.45639600     0.39177900  H
C-C_R       0    -4.65638000    -0.89579700     3.82652300  H
H-H_        0    -2.84883400    -2.09779100     3.81999200  H
C-C_R       0    -5.46422100     0.04987900     3.14993900  H
H-H_        0    -5.58097300     1.27004400     1.35292500  H
H-H_        0    -4.98156200    -1.29552700     4.79054100  H
C-C_3       0    -6.79479800     0.50811900     3.77288700  H
C-C_3       0    -7.72989400    -0.72065200     3.93763300  H
H-H_        0    -7.27479200    -1.50597700     4.56174000  H
H-H_        0    -8.67524100    -0.41509400     4.41757500  H
H-H_        0    -7.97298500    -1.16506300     2.95871100  H
C-C_3       0    -7.52611100     1.55410800     2.90398200  H
H-H_        0    -8.47630500     1.83506000     3.38698100  H
H-H_        0    -6.93318400     2.47530600     2.78391400  H
H-H_        0    -7.76890700     1.16224900     1.90217300  H
C-C_3       0    -6.51938400     1.13902600     5.16440600  H
H-H_        0    -7.46592900     1.47176900     5.62344400  H
H-H_        0    -6.04570200     0.42442300     5.85602800  H
H-H_        0    -5.85435800     2.01372800     5.07664500  H
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C-C_R       0     5.65362000     1.52203900     2.51009400  L
C-C_R       0    -4.79723600    -3.69906800     0.55910800  L
C-C_R       0    -3.93669100     4.69342700     1.11775000  L
C-C_R       0     1.61875200    -5.56228600     1.00997500  L
C-C_3       0     3.59367200     4.61706500    -2.12186600  L
C-C_3       0    -2.67955200     2.43864700    -4.39803400  L
C-C_3       0    -0.65420100    -4.21838400    -3.83539200  L
C-C_3       0     5.69439700    -2.12914800    -1.58695800  L
C-C_3       0    -2.61663000     1.18137100    -5.29866200  L
C-C_3       0     4.08493400     5.98199400    -1.58296300  L
C-C_3       0     6.88055400    -2.79208800    -0.84633800  L
C-C_3       0    -1.34086400    -3.38428300    -4.94197500  L
C-C_3       0     4.82175200     3.85380400    -2.66969000  L
C-C_3       0     5.22895400    -3.09758600    -2.69893200  L
C-C_3       0    -1.64827800     3.47856900    -4.89425000  L
C-C_3       0    -1.35676500    -5.59611600    -3.77421000  L
C-C_3       0    -4.09094400     3.05144400    -4.56611400  L
C-C_3       0     6.22739000    -0.82882100    -2.23471000  L
C-C_3       0     0.82044100    -4.47465100    -4.22957700  L
C-C_3       0     2.61359100     4.90749600    -3.28386000  L
C-C_R       0    -0.02858800    -2.20001500    -2.22461200  H
C-C_R       0     3.33028300    -1.04274700    -1.03363100  H
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C-C_R    0     2.18868800     2.51684600    -1.29930100  H
C-C_R    0    -1.16991000     1.33514400    -2.51135800  H
C-C_3    0    -0.74070000    -3.54282300    -2.41492200  L
C-C_3    0     4.56440900    -1.80346400    -0.53903400  L
C-C_3    0     2.86135600     3.84978400    -0.95799200  L
C-C_3    0    -2.47182800     2.05466100    -2.88546700  L
C-C_R    0    -3.07619800    -2.38815200    -2.26263400  L
C-C_R    0     4.20243000    -3.18463700     1.60878800  L
C-C_R    0     3.48622700     4.18085000     1.52254500  L
C-C_R    0    -1.64746900     4.13430200    -1.55337700  L
C-C_R    0    -4.17093900    -2.42943700    -1.29770900  L
C-C_R    0     3.22536300    -4.18900800     2.02098100  L
C-C_R    0     4.20939800     3.37919200     2.50638300  L
C-C_R    0    -2.07419200     4.75282900    -0.30329700  L
C-C_R    0    -3.95511100    -3.44162300    -0.45758400  L
C-C_R    0     2.60742800    -4.65078200     0.93425300  L
C-C_R    0     4.90842900     2.44270400     1.86173800  L
C-C_R    0    -3.29416700     4.30807900    -0.00497300  L
C-C_R    0    -2.70870900    -4.10452300    -0.83187800  L
C-C_R    0     3.14817100    -3.96529300    -0.23510300  L
C-C_R    0     4.66875700     2.59348400     0.42951700  L
C-C_R    0    -3.71063700     3.37453000    -1.04824800  L
C-C_R    0    -5.23958100    -1.61399500    -1.17062600  L
C-C_R    0     2.89429800    -4.60528300     3.25826400  L
C-C_R    0     4.20289800     3.46315100     3.84917200  L
C-C_R    0    -1.42009100     5.60424100     0.50685600  L
C-C_R    0    -6.12521900    -1.84053600    -0.16598100  L
C-C_R    0     1.86851500    -5.56641300     3.39018800  L
C-C_R    0     4.97148200     2.52987100     4.57133000  L
C-C_R    0    -2.07443000     6.02311100     1.68621600  L
C-C_R    0    -5.92925700    -2.86727100     0.70329600  L
C-C_R    0     1.24148500    -6.03717100     2.28443100  L
C-C_R    0     5.70221600     1.54916400     3.86310300  L
C-C_R    0    -3.32124300     5.55808600     1.96542400  L
F-F_     0    -5.42691200    -0.58065400    -2.02990500  L
F-F_     0     3.52263900    -4.11096400     4.35413100  L
F-F_     0     3.47758300     4.41228700     4.49188300  L
F-F_     0    -0.17341600     6.04631700     0.20624500  L
F-F_     0    -7.20464700    -1.03131800    -0.02316400  L
F-F_     0     1.50818200    -6.01025300     4.62014500  L
F-F_     0     5.00414700     2.56754900     5.92641600  L
F-F_     0    -1.45882500     6.88252500     2.53599900  L
F-F_     0    -6.80936200    -3.08873300     1.71081400  L
F-F_     0     0.24953100    -6.95489500     2.40044100  L
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F-F_	0	6.44418800	0.63585100	4.53770000	L
F-F_	0	−3.95255300	5.95672300	3.09821800	L
F-F_	0	−4.56773000	−4.71937300	1.42275400	L
F-F_	0	0.99558000	−6.01375600	−0.10699000	L
F-F_	0	6.34691200	0.58192000	1.81981500	L
F-F_	0	−5.17988900	4.22918700	1.39609700	L
H-H_	0	7.72180300	−2.99334600	−1.54482500	L
H-H_	0	−1.21110600	−3.87522500	−5.93074200	L
H-H_	0	−2.87979200	1.43798100	−6.34776300	L
H-H_	0	4.56743500	6.57647300	−2.38910400	L
H-H_	0	6.57951100	−3.76143600	−0.39441300	L
H-H_	0	4.83196800	5.84704000	−0.77165400	L
H-H_	0	−0.91881700	−2.36403400	−5.02245200	L
H-H_	0	−3.33561600	0.41125000	−4.94659900	L
H-H_	0	7.25634200	−2.13250500	−0.03417700	L
H-H_	0	3.23598300	6.57459800	−1.17810500	L
H-H_	0	−2.43214600	−3.30208100	−4.76107500	L
H-H_	0	−1.60508100	0.73148300	−5.32289000	L
H-H_	0	6.04196100	−3.25112200	−3.44123000	L
H-H_	0	5.27557100	4.41195700	−3.51708200	L
H-H_	0	−1.82140900	3.71129500	−5.96727000	L
H-H_	0	−1.26877900	−6.12999700	−4.74544100	L
H-H_	0	4.34865500	−2.71328400	−3.24927500	L
H-H_	0	4.55721800	2.84584800	−3.04330000	L
H-H_	0	−0.60685600	3.11476900	−4.80009800	L
H-H_	0	−2.43929500	−5.48522800	−3.55016100	L
H-H_	0	4.98001000	−4.09469500	−2.28145100	L
H-H_	0	5.60612900	3.74972400	−1.89208000	L
H-H_	0	−1.74081100	4.43039600	−4.33138200	L
H-H_	0	−0.90241300	−6.23515200	−2.98614000	L
H-H_	0	3.09908400	5.54205200	−4.05676400	L
H-H_	0	7.09004600	−1.04779600	−2.90077300	L
H-H_	0	−4.29705100	3.28719700	−5.63287200	L
H-H_	0	0.87785800	−5.04743900	−5.18056500	L
H-H_	0	1.71721700	5.44954100	−2.91415300	L
H-H_	0	6.57425200	−0.11712900	−1.45567100	L
H-H_	0	1.33791500	−5.06760300	−3.44570800	L
H-H_	0	−4.19001100	3.99619700	−3.98997600	L
H-H_	0	2.27896000	3.98045200	−3.78955000	L
H-H_	0	−4.87192700	2.34412700	−4.21171700	L
H-H_	0	1.38251000	−3.53339000	−4.38611000	L
H-H_	0	5.45916100	−0.32529900	−2.85381300	L
H-H_	0	−0.21521000	−4.23673200	−1.72261200	L
H-H_	0	5.03612700	−1.11447000	0.19594000	L

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H-H_        0     2.02154000     4.51253700    -0.65140100  L
H-H_        0    -3.27304900     1.31971300    -2.64760600  L
N-N_R       0    -2.13705500    -3.42882000    -1.95835600  L
N-N_R       0     4.13480100    -3.01188900     0.18752000  L
N-N_R       0     3.74333300     3.66857500     0.20912200  L
N-N_R       0    -2.66047500     3.22667200    -2.01174300  L
O-O_R       0    -0.03910100    -1.76128900    -1.02035500  H
O-O_R       0     2.53183000    -0.66818100    -0.10051900  H
O-O_R       0     1.46082000     2.02985200    -0.35965500  H
O-O_R       0    -1.10450100     0.93984700    -1.28980200  H
O-O_R       0     0.50577000    -1.60881100    -3.22131600  H
O-O_R       0     3.15699200    -0.84434000    -2.28114300  H
O-O_R       0     2.38687000     1.96950500    -2.43339500  H
O-O_R       0    -0.25335300     1.18803500    -3.38301200  H
O-O_R       0    -2.79402900    -1.38191800    -2.96438700  L
O-O_R       0     4.69850500    -2.32601700     2.38665300  L
O-O_R       0     2.49704600     4.91105400     1.79928200  L
O-O_R       0    -0.46077700     4.12808300    -1.97352800  L
O-O_R       0    -2.04483500    -4.84664000    -0.05957000  L
O-O_R       0     2.54691100    -3.89347500    -1.33887500  L
O-O_R       0     4.88904800     1.68608700    -0.41490400  L
O-O_R       0    -4.68381800     2.58039900    -0.95021100  L
Rh-         0     0.68031400     0.12958700    -0.58160000  H
Rh-         0     1.46401300     0.17719700    -2.86445700  H
N-N_3       0     0.08553000    -0.05469600     1.26764000  H
S-S_3+6     0    -0.43978300    -1.32554900     2.16761500  H
O-O_2       0     0.29380900    -2.56877400     1.87656100  H
O-O_R       0    -1.98573800    -1.58373100     1.45175200  H
O-O_2       0    -0.63925900    -0.86399500     3.55431000  H
C-C_R       0    -3.09473100    -0.99391300     2.05038200  H
C-C_R       0    -3.70353300     0.10080000     1.42141800  H
C-C_R       0    -3.65651500    -1.55739400     3.20880200  H
C-C_R       0    -4.89240300     0.61859600     1.95057700  H
H-H_        0    -3.24136500     0.52590400     0.52802200  H
C-C_R       0    -4.84614000    -1.02914600     3.71344200  H
H-H_        0    -3.17056000    -2.41138700     3.68380400  H
C-C_R       0    -5.49759100     0.06595400     3.09949100  H
H-H_        0    -5.35655100     1.46764600     1.44764600  H
H-H_        0    -5.27868500    -1.48884300     4.60609500  H
C-C_3       0    -6.81445200     0.60435100     3.69177600  H
C-C_3       0    -7.88105800    -0.52293400     3.68627100  H
H-H_        0    -7.55021800    -1.40780200     4.25293000  H
H-H_        0    -8.81794400    -0.16214400     4.14427200  H
H-H_        0    -8.10821300    -0.84691200     2.65756200  H
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C-C_3      0    -7.37607000     1.79942900     2.89202700   H
H-H_       0    -8.32559100     2.13242400     3.34250400   H
H-H_       0    -6.68701300     2.65938200     2.90362000   H
H-H_       0    -7.58389500     1.53288600     1.84222100   H
C-C_3      0    -6.56550200     1.07165900     5.15075500   H
H-H_       0    -7.49957800     1.46071400     5.59115500   H
H-H_       0    -6.21066600     0.24905000     5.79193300   H
H-H_       0    -5.80995300     1.87368600     5.18470900   H
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C-C_R      0     5.84008900    -1.35992700     0.42745800   L
C-C_R      0    -5.82528100     3.56256800    -1.72768000   L
C-C_R      0    -2.88299700    -4.45519900    -3.40543300   L
C-C_R      0     1.11272000     5.78236200     0.73599300   L
C-C_3      0     1.98509600    -4.95104900     3.07632600   L
C-C_3      0    -4.75547400    -3.48794800     2.34515900   L
C-C_3      0    -3.34806400     3.39739300     3.70101200   L
C-C_3      0     3.36619900     1.81009800     4.46560900   L
C-C_3      0    -5.28565900    -2.43880600     3.35212300   L
C-C_3      0     2.79824900    -6.19988300     2.65883800   L
C-C_3      0     4.70353900     2.58794600     4.50963900   L
C-C_3      0    -4.34210000     2.39828600     4.33826000   L
C-C_3      0     2.75243500    -4.24614900     4.21925500   L
C-C_3      0     2.32809700     2.60625400     5.29094700   L
C-C_3      0    -3.93162000    -4.55368200     3.10399900   L
C-C_3      0    -4.07941200     4.75232400     3.54159200   L
C-C_3      0    -5.98717200    -4.19067200     1.72516600   L
C-C_3      0     3.61420100     0.43869700     5.13885300   L
C-C_3      0    -2.16213800     3.63186000     4.66703900   L
C-C_3      0     0.62046800    -5.45005700     3.60979300   L
C-C_R      0    -1.96378100     1.66015900     2.24966000   H
C-C_R      0     1.67394500     0.79682200     2.68772700   H
C-C_R      0     0.91176100    -2.78523000     1.97514500   H
C-C_R      0    -2.71695400    -1.95682100     1.59253600   H
C-C_3      0    -2.83714000     2.92206900     2.28784600   L
C-C_3      0     2.93564400     1.62363000     2.96152100   L
C-C_3      0     1.78406600    -4.03325900     1.81189600   L
C-C_3      0    -3.93879100    -2.79109600     1.19351100   L
C-C_R      0    -4.62873900     1.57317800     0.96023100   L
C-C_R      0     3.69272300     3.37820000     1.22589300   L
C-C_R      0     3.53702100    -4.03873500    -0.09097400   L
C-C_R      0    -2.36882800    -4.56604000     0.11948000   L
C-C_R      0    -5.41541300     1.80516200    -0.24634600   L
C-C_R      0     3.09333300     4.54008900     0.57499300   L
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C-C_R     0     4.64554800    -3.17162900    -0.48208900  L
C-C_R     0    -2.03533100    -4.88799700    -1.26371400  L
C-C_R     0    -5.22730800     3.06792000    -0.62945400  L
C-C_R     0     1.91013900     4.77713300     1.14317700  L
C-C_R     0     4.88319100    -2.30890900     0.50925400  L
C-C_R     0    -2.96047000    -4.35628300    -2.06105800  L
C-C_R     0    -4.32550900     3.71389700     0.32136900  L
C-C_R     0     1.70374000     3.79991800     2.20775300  L
C-C_R     0     3.93829900    -2.57706300     1.59028000  L
C-C_R     0    -3.94327000    -3.66685300    -1.22973900  L
C-C_R     0    -6.20778400     0.96041600    -0.93933000  L
C-C_R     0     3.56021300     5.29431700    -0.43747100  L
C-C_R     0     5.34774400    -3.14745100    -1.62906100  L
C-C_R     0    -0.97715400    -5.55207900    -1.76255100  L
C-C_R     0    -6.83399300     1.41307600    -2.05619100  L
C-C_R     0     2.76195300     6.36332600    -0.89958400  L
C-C_R     0     6.36624300    -2.18401300    -1.75776800  L
C-C_R     0    -0.87935400    -5.67462300    -3.16584600  L
C-C_R     0    -6.66387400     2.69823100    -2.46580900  L
C-C_R     0     1.55907300     6.60394300    -0.32197200  L
C-C_R     0     6.59682700    -1.28334400    -0.69329400  L
C-C_R     0    -1.83627900    -5.12189700    -3.95769400  L
F-F_      0    -6.37441900    -0.32285800    -0.53211400  L
F-F_      0     4.76298700     5.03362200    -1.00681600  L
F-F_      0     5.08578600    -4.02044800    -2.63350800  L
F-F_      0    -0.02982700    -6.08150700    -0.94894500  L
F-F_      0    -7.63014900     0.57733200    -2.76897100  L
F-F_      0     3.19670800     7.14274900    -1.92085300  L
F-F_      0     7.10840800    -2.11748300    -2.89021100  L
F-F_      0     0.16931300    -6.33362000    -3.71869800  L
F-F_      0    -7.28896000     3.14820900    -3.58218700  L
F-F_      0     0.78270900     7.62534100    -0.76187100  L
F-F_      0     7.56413900    -0.33867900    -0.79991600  L
F-F_      0    -1.74213900    -5.23147200    -5.30666800  L
F-F_      0    -5.63188000     4.84730400    -2.11699100  L
F-F_      0    -0.08934400     6.00408500     1.32463700  L
F-F_      0     6.04174900    -0.49118600     1.45022800  L
F-F_      0    -3.83292800    -3.89564900    -4.19624000  L
H-H_      0     5.06952200     2.68962300     5.55451300  L
H-H_      0    -4.69115800     2.77694900     5.32332200  L
H-H_      0    -5.95963300    -2.91590800     4.09636900  L
H-H_      0     2.91706300    -6.90022000     3.51410100  L
H-H_      0     4.58619600     3.61240100     4.09615500  L
H-H_      0     3.81557400    -5.91851800     2.31201900  L
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H-H_	0	-3.88740600	1.40447700	4.51315400	L
H-H_	0	-5.86470200	-1.64935500	2.82726100	L
H-H_	0	5.48505200	2.06108700	3.92022400	L
H-H_	0	2.28849600	-6.74460700	1.83468000	L
H-H_	0	-5.23867200	2.26754500	3.69718900	L
H-H_	0	-4.46901900	-1.95468400	3.92227700	L
H-H_	0	2.66051100	2.69175900	6.34816200	L
H-H_	0	2.82431800	-4.91484600	5.10425100	L
H-H_	0	-4.53066800	-4.98378000	3.93566500	L
H-H_	0	-4.39182400	5.15364100	4.53025000	L
H-H_	0	1.33334100	2.12076900	5.29766000	L
H-H_	0	2.25312700	-3.31515200	4.54975000	L
H-H_	0	-3.00745900	-4.13265700	3.54531400	L
H-H_	0	-4.99583600	4.64438800	2.92349000	L
H-H_	0	2.21353000	3.63790800	4.89947100	L
H-H_	0	3.79000700	-4.00157100	3.91267400	L
H-H_	0	-3.65337400	-5.39335400	2.43440300	L
H-H_	0	-3.41742700	5.50365300	3.05898900	L
H-H_	0	0.76571500	-6.18343900	4.43247000	L
H-H_	0	4.02090000	0.57393700	6.16454900	L
H-H_	0	-6.61886300	-4.65376500	2.51419100	L
H-H_	0	-2.52100800	4.04853200	5.63311600	L
H-H_	0	0.04538700	-5.95420500	2.80422100	L
H-H_	0	4.35152900	-0.15469100	4.55746900	L
H-H_	0	-1.44280300	4.35742600	4.23177800	L
H-H_	0	-5.67947400	-4.99743300	1.02595700	L
H-H_	0	0.00350400	-4.62551700	4.01755100	L
H-H_	0	-6.61335400	-3.46405100	1.16321500	L
H-H_	0	-1.61849900	2.69620900	4.90224700	L
H-H_	0	2.68516400	-0.15571300	5.23754900	L
H-H_	0	-2.17508600	3.73441400	1.91115400	L
H-H_	0	3.75887100	1.05111100	2.47714400	L
H-H_	0	1.23726000	-4.66150100	1.07408700	L
H-H_	0	-4.63715000	-2.05537000	0.73690100	L
N-N_R	0	-3.96058600	2.78139900	1.34527600	L
N-N_R	0	2.83352100	2.92063200	2.27319300	L
N-N_R	0	3.07392100	-3.65563900	1.20857800	L
N-N_R	0	-3.55449600	-3.75634200	0.14718500	L
O-O_R	0	-1.38515500	1.43149800	1.12584200	H
O-O_R	0	1.42922800	0.57526100	1.44572100	H
O-O_R	0	0.65864300	-2.17267500	0.87712100	H
O-O_R	0	-2.15064400	-1.34353800	0.61763400	H
O-O_R	0	-1.88085900	0.92205300	3.28599100	H
O-O_R	0	0.95291900	0.39629800	3.65723200	H

O-O_R	0	0.51090300	-2.43011600	3.13240900	H
O-O_R	0	-2.33073300	-1.92111200	2.80670300	H
O-O_R	0	-4.72208200	0.55786800	1.69846600	L
O-O_R	0	4.90186600	3.04017000	1.12255700	L
O-O_R	0	2.84573500	-4.71089300	-0.90223600	L
O-O_R	0	-1.54208400	-4.61686100	1.06744300	L
O-O_R	0	-3.70959100	4.79194500	0.10645200	L
O-O_R	0	0.58830200	3.54421600	2.73167400	L
O-O_R	0	3.65597500	-1.75107600	2.49739800	L
O-O_R	0	-4.76853500	-2.81969600	-1.66410100	L
Rh-	0	-0.34255300	-0.36859500	0.89905200	H
Rh-	0	-0.69666400	-0.76104200	3.26182800	H
N-N_R	0	-0.15914500	-0.10096200	-1.02594900	H
S-S_R	0	0.57977700	-1.08088000	-2.10634100	H
O-O_R	0	0.63232300	-0.41820500	-3.42603800	H
O-O_R	0	2.22498500	-1.02664900	-1.45155100	H
O-O_R	0	0.19185400	-2.50032200	-2.00711900	H
C-C_R	0	3.17987600	-0.29940000	-2.11298900	H
C-C_R	0	3.83519200	0.72142800	-1.39749600	H
C-C_R	0	3.57966800	-0.60645400	-3.43265700	H
C-C_R	0	4.88584500	1.42013700	-1.99456000	H
H-H_	0	3.49458300	0.94305300	-0.38502600	H
C-C_R	0	4.63524800	0.10112300	-4.00524700	H
H-H_	0	3.07759200	-1.40569400	-3.97879100	H
C-C_R	0	5.31671000	1.13022500	-3.30997500	H
H-H_	0	5.37834700	2.20823900	-1.42395700	H
H-H_	0	4.94082700	-0.16045400	-5.02162900	H
C-C_3	0	6.46935000	1.88732000	-3.99273100	H
C-C_3	0	5.92968000	2.58711500	-5.26967500	H
H-H_	0	5.51378900	1.86533600	-5.99047800	H
H-H_	0	6.74370100	3.13483800	-5.77450300	H
H-H_	0	5.13456300	3.30817600	-5.01891200	H
C-C_3	0	7.09328500	2.96281200	-3.07722100	H
H-H_	0	7.92020800	3.46381900	-3.60662900	H
H-H_	0	7.50856300	2.52719000	-2.15303300	H
H-H_	0	6.36292400	3.73982100	-2.79833900	H
C-C_3	0	7.58585100	0.88387600	-4.38845800	H
H-H_	0	8.39813400	1.41194600	-4.91627900	H
H-H_	0	7.21320800	0.09089200	-5.05596400	H
H-H_	0	8.01742700	0.40070300	-3.49693600	H
C-C_R	0	-3.15760700	2.14525500	-3.43470100	H
C-C_R	0	-3.92485300	2.63573000	-4.51089900	H
C-C_R	0	-4.71910500	1.77728200	-5.28499400	H
C-C_R	0	-4.76205200	0.40505900	-4.99439500	H

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C-C_R    0    -4.00546200    -0.09787700    -3.92495100   H
C-C_R    0    -3.21705800     0.76417500    -3.15134800   H
H-H_     0    -3.90942900     3.70766900    -4.73365600   H
H-H_     0    -5.31162000     2.18239300    -6.11103000   H
H-H_     0    -5.38546700    -0.26603800    -5.59247900   H
H-H_     0    -4.03166300    -1.16509700    -3.68996800   H
H-H_     0    -2.64023700     0.36791600    -2.31014700   H
C-C_3    0    -2.29140600     3.06197800    -2.59469500   H
H-H_     0    -2.72828400     4.07881600    -2.58080000   H
H-H_     0    -2.29346500     2.69593200    -1.55313300   H
C-C_3    0    -0.80722800     3.16824400    -3.04611300   H
H-H_     0    -0.40694400     2.14056400    -3.09832200   H
C-C_3    0    -0.00245500     3.94196400    -1.98800000   H
H-H_     0    -0.38610300     4.97276000    -1.87851800   H
H-H_     0     1.06288800     4.01031300    -2.26726300   H
H-H_     0    -0.06354000     3.45051600    -1.00279500   H
C-C_3    0    -0.66024900     3.81349500    -4.43349400   H
H-H_     0    -1.03917800     4.85225100    -4.43062200   H
H-H_     0    -1.21496300     3.25268600    -5.20265000   H
H-H_     0     0.39915900     3.84664800    -4.73995300   H
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¹TS1
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C-C_R    0    -5.93656300    -1.12559500    -0.58944000   L
C-C_R    0     5.62824700     3.27286000     2.38811500   L
C-C_R    0     2.97638900    -5.22542800     2.67314200   L
C-C_R    0    -0.89074200     5.94065400     0.12878400   L
C-C_3    0    -2.04901200    -4.22339600    -3.76018400   L
C-C_3    0     4.68787100    -2.97252800    -2.69381900   L
C-C_3    0     3.43104600     3.99752300    -3.17298400   L
C-C_3    0    -3.35014800     2.65651600    -4.15668800   L
C-C_3    0     5.23881600    -1.76972600    -3.49661900   L
C-C_3    0    -2.87069800    -5.51778300    -3.54789200   L
C-C_3    0    -4.67725100     3.45091300    -4.09622400   L
C-C_3    0     4.40070000     3.06300800    -3.93432500   L
C-C_3    0    -2.80775700    -3.34260400    -4.78045800   L
C-C_3    0    -2.30691800     3.53160900    -4.89016900   L
C-C_3    0     3.87009700    -3.88640300    -3.63632600   L
C-C_3    0     4.19897400     5.29716600    -2.83025700   L
C-C_3    0     5.90738300    -3.78159300    -2.18998100   L
C-C_3    0    -3.62103400     1.37787900    -4.98573500   L
C-C_3    0     2.26034100     4.39244600    -4.10456000   L
C-C_3    0    -0.68454000    -4.64170000    -4.35984700   L
C-C_R    0     2.00699500     2.11028900    -1.96449900   H
C-C_R    0    -1.66343800     1.41661400    -2.51783300   H
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C-C_R    0    -0.97737400    -2.25618200    -2.33426000  H
C-C_R    0     2.64736400    -1.57568800    -1.71894100  H
C-C_3    0     2.89389400     3.35715200    -1.83715600  L
C-C_3    0    -2.91341000     2.28892900    -2.68853200  L
C-C_3    0    -1.85128700    -3.51461300    -2.36700700  L
C-C_3    0     3.85640300    -2.48054700    -1.44945700  L
C-C_R    0     4.76889900     1.88891300    -0.76920500  L
C-C_R    0    -3.61217600     3.81267500    -0.72518300  L
C-C_R    0    -3.65144500    -3.86881200    -0.54101600  L
C-C_R    0     2.25266100    -4.40090500    -0.71722100  L
C-C_R    0     5.44550500     1.88017900     0.52314500  L
C-C_R    0    -2.92666200     4.78104200     0.12457500  L
C-C_R    0    -4.77457600    -3.09185000    -0.02295000  L
C-C_R    0     1.99038200    -5.07075600     0.55196600  L
C-C_R    0     5.16424400     3.02239400     1.15069800  L
C-C_R    0    -1.76176100     5.08964900    -0.44597500  L
C-C_R    0    -4.97934600    -2.04689900    -0.82953700  L
C-C_R    0     2.95984800    -4.75137100     1.40938900  L
C-C_R    0     4.28143000     3.81944000     0.30051400  L
C-C_R    0    -1.63489200     4.32953200    -1.68656400  L
C-C_R    0    -3.99913200    -2.10074800    -1.91108600  L
C-C_R    0     3.87608900    -3.83026600     0.74201600  L
C-C_R    0     6.20106700     0.91928700     1.09594400  L
C-C_R    0    -3.29780000     5.29833700     1.31073000  L
C-C_R    0    -5.51424900    -3.29253200     1.08221400  L
C-C_R    0     0.97322800    -5.87414300     0.91027700  L
C-C_R    0     6.69866600     1.12886500     2.34198300  L
C-C_R    0    -2.42169400     6.20180200     1.95069300  L
C-C_R    0    -6.53466400    -2.36621400     1.36896500  L
C-C_R    0     0.96918600    -6.38093100     2.22837400  L
C-C_R    0     6.43256600     2.28723200     3.00177400  L
C-C_R    0    -1.23896400     6.51910400     1.36863000  L
C-C_R    0    -6.72842400    -1.26817800     0.50018700  L
C-C_R    0     1.97390500    -6.04630400     3.08140800  L
F-F_     0     6.45450800    -0.24280400     0.44294600  L
F-F_     0    -4.47960400     4.95861300     1.88303800  L
F-F_     0    -5.28573400    -4.35029900     1.89988100  L
F-F_     0    -0.01737700    -6.18843100     0.03841400  L
F-F_     0     7.45625600     0.17276600     2.93556400  L
F-F_     0    -2.76070500     6.74363000     3.14694600  L
F-F_     0    -7.31462200    -2.52375700     2.46639300  L
F-F_     0    -0.03418200    -7.19563800     2.63964100  L
F-F_     0     6.92115300     2.49014000     4.25060300  L
F-F_     0    -0.38612800     7.37853400     1.97980000  L
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F-F_	0	-7.69669600	-0.35583000	0.76341600	L
F-F_	0	1.97158100	-6.52928600	4.34921800	L
F-F_	0	5.32386500	4.42568900	3.03450700	L
F-F_	0	0.29815600	6.22744200	-0.45848900	L
F-F_	0	-6.10280900	-0.06782500	-1.42308000	L
F-F_	0	3.97127300	-4.88048200	3.52869300	L
H-H_	0	-5.04906200	3.68128300	-5.11835000	L
H-H_	0	4.75859800	3.55482000	-4.86469100	L
H-H_	0	5.90625300	-2.11792700	-4.31456100	L
H-H_	0	-2.98299300	-6.07770300	-4.50179500	L
H-H_	0	-4.54346500	4.41674200	-3.56367300	L
H-H_	0	-3.89108900	-5.28875000	-3.17292500	L
H-H_	0	3.92200900	2.11048900	-4.23186800	L
H-H_	0	5.83159300	-1.09931700	-2.83868900	L
H-H_	0	-5.46158800	2.86751800	-3.56677900	L
H-H_	0	-2.37125900	-6.18520300	-2.81242500	L
H-H_	0	5.29493500	2.83059700	-3.31996800	L
H-H_	0	4.43302100	-1.17535400	-3.96958500	L
H-H_	0	-2.64451000	3.74524800	-5.92742800	L
H-H_	0	-2.89106500	-3.86866400	-5.75608400	L
H-H_	0	4.48651700	-4.18830800	-4.51062300	L
H-H_	0	4.53752800	5.81389200	-3.75462500	L
H-H_	0	-1.31874800	3.03775400	-4.96119700	L
H-H_	0	-2.29536200	-2.37965000	-4.96868500	L
H-H_	0	2.96565400	-3.38380600	-4.02977000	L
H-H_	0	5.10162200	5.08154200	-2.21969700	L
H-H_	0	-2.17680700	4.50845500	-4.38063900	L
H-H_	0	-3.84040700	-3.13067800	-4.43518600	L
H-H_	0	3.55926900	-4.81694400	-3.11833000	L
H-H_	0	3.55179300	5.99874200	-2.26043700	L
H-H_	0	-0.83033800	-5.24009300	-5.28526900	L
H-H_	0	-4.03068600	1.63927000	-5.98553200	L
H-H_	0	6.55052600	-4.10038200	-3.03898000	L
H-H_	0	2.63914600	4.92063100	-5.00635800	L
H-H_	0	-0.11452500	-5.26569300	-3.63906400	L
H-H_	0	-4.36425900	0.73012400	-4.47418500	L
H-H_	0	1.55962700	5.07694400	-3.58127500	L
H-H_	0	5.58621600	-4.69862300	-1.65122800	L
H-H_	0	-0.06185900	-3.76875500	-4.63655700	L
H-H_	0	6.52695500	-3.17032600	-1.49840900	L
H-H_	0	1.69088300	3.51231200	-4.46157100	L
H-H_	0	-2.70115200	0.78656300	-5.15998300	L
H-H_	0	2.23313800	4.12522100	-1.37568300	L
H-H_	0	-3.74186500	1.67153800	-2.27397800	L

H-H_	0	-1.30922600	-4.24997100	-1.73174400	L
H-H_	0	4.55080700	-1.84900100	-0.85056900	L
N-N_R	0	4.00127400	3.09249800	-0.90160200	L
N-N_R	0	-2.79093100	3.49635000	-1.85351200	L
N-N_R	0	-3.14501800	-3.23600300	-1.72071600	L
N-N_R	0	3.44597400	-3.61396300	-0.60482600	L
O-O_R	0	1.44591700	1.72039000	-0.87287000	H
O-O_R	0	-1.42571300	1.05212400	-1.30971900	H
O-O_R	0	-0.73886700	-1.80391300	-1.16039800	H
O-O_R	0	2.08602200	-1.09694600	-0.66362000	H
O-O_R	0	1.88841400	1.53395800	-3.09056000	H
O-O_R	0	-0.95496900	1.12599100	-3.53586900	H
O-O_R	0	-0.55624200	-1.74384700	-3.42417800	H
O-O_R	0	2.27137400	-1.36080900	-2.91527800	H
O-O_R	0	4.62006300	0.87860200	-1.50459000	L
O-O_R	0	-4.61255000	3.13157900	-0.37625000	L
O-O_R	0	-2.98999300	-4.69812300	0.13914800	L
O-O_R	0	1.40280800	-4.25550700	-1.63404300	L
O-O_R	0	3.57217000	4.77552000	0.71372900	L
O-O_R	0	-0.54051700	4.12197000	-2.27308500	L
O-O_R	0	-3.69694900	-1.11912500	-2.63901000	L
O-O_R	0	5.02650300	-3.53086700	1.15893100	L
Rh-	0	0.32042100	-0.04140500	-0.86607200	H
Rh-	0	0.66731600	-0.11027400	-3.27157200	H
N-N_3	0	-0.33662600	0.02038900	1.02761000	H
S-S_3+6	0	-0.46125200	-1.42235300	1.91785400	H
O-O_2	0	-0.40589600	-1.12344600	3.36279100	H
O-O_R	0	-2.10823000	-1.70582500	1.48942100	H
O-O_2	0	0.23746300	-2.59702100	1.37843000	H
C-C_R	0	-3.07621900	-0.98076400	2.18400400	H
C-C_R	0	-3.63406000	0.16449100	1.60047300	H
C-C_R	0	-3.54412800	-1.45053400	3.42217700	H
C-C_R	0	-4.66748300	0.83628300	2.26664500	H
H-H_	0	-3.24483600	0.51830200	0.64387400	H
C-C_R	0	-4.58381100	-0.76977300	4.06270400	H
H-H_	0	-3.10033400	-2.34682200	3.85906100	H
C-C_R	0	-5.16855800	0.39117600	3.50787600	H
H-H_	0	-5.09021500	1.72743300	1.80167600	H
H-H_	0	-4.94095400	-1.15529100	5.02172600	H
C-C_3	0	-6.28951500	1.13125000	4.26520400	H
C-C_3	0	-5.74170300	1.61273600	5.63532600	H
H-H_	0	-5.39927100	0.77113100	6.25852600	H
H-H_	0	-6.52755000	2.14807500	6.19569900	H
H-H_	0	-4.88924100	2.29885600	5.50030900	H

C-C_3	0	-6.80661600	2.36401400	3.49190100	H
H-H_	0	-7.61194900	2.85091600	4.06638500	H
H-H_	0	-7.22176800	2.08799200	2.50811800	H
H-H_	0	-6.01368200	3.11392200	3.33505300	H
C-C_3	0	-7.48747500	0.17435200	4.49965100	H
H-H_	0	-8.27045000	0.68156100	5.08922900	H
H-H_	0	-7.19057800	-0.73346100	5.04846500	H
H-H_	0	-7.93448100	-0.14048600	3.54299700	H
C-C_R	0	2.99972900	1.04369800	3.32462700	H
C-C_R	0	3.49170300	1.43142200	4.58752500	H
C-C_R	0	4.25319300	0.55190000	5.36923700	H
C-C_R	0	4.53011700	-0.73978200	4.89907800	H
C-C_R	0	4.04508800	-1.13846600	3.64451500	H
C-C_R	0	3.29350600	-0.25372000	2.85900100	H
H-H_	0	3.28719600	2.44296600	4.95415400	H
H-H_	0	4.63366600	0.87801300	6.34166900	H
H-H_	0	5.12381700	-1.43121000	5.50376400	H
H-H_	0	4.25470600	-2.14476200	3.27661600	H
H-H_	0	2.93905900	-0.57258400	1.87425000	H
C-C_3	0	2.19846300	2.01469100	2.48385400	H
H-H_	0	2.48619700	3.04828600	2.76751300	H
H-H_	0	2.45129800	1.90242600	1.41863600	H
C-C_3	0	0.66118600	1.96188100	2.60108100	H
H-H_	0	0.32255600	0.97769000	1.96494800	H
C-C_3	0	-0.02156000	3.08437100	1.82484500	H
H-H_	0	0.10602000	4.03809900	2.37113300	H
H-H_	0	-1.10196800	2.89407200	1.73032700	H
H-H_	0	0.40267300	3.19765800	0.81742300	H
C-C_3	0	0.10590800	1.78773800	4.00406400	H
H-H_	0	0.33958300	2.69444000	4.59722800	H
H-H_	0	0.54120300	0.92240600	4.52061700	H
H-H_	0	-0.98824600	1.67269800	3.98510200	H

¹INT2

Rh-	0	-0.47798900	-0.43721600	0.86823200	H
Rh-	0	-1.04075800	-1.06949900	3.14246800	H
O-O_R	0	-1.45252000	1.37656300	1.23187100	H
C-C_R	0	-2.08698200	1.52331700	2.33812100	H
F-F_	0	-6.78844900	0.02387700	-0.34522400	L
N-N_R	0	-3.99130100	2.81715200	1.48000200	L
O-O_R	0	-2.11164500	0.67847400	3.29346500	H
C-C_3	0	-2.89168400	2.82292300	2.45940000	L
F-F_	0	-7.69647600	0.91806900	-2.74573000	L
O-O_R	0	-4.83030300	0.60768200	1.72212200	L

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C-C_R      0    -4.87666800    1.73462000    1.16325000   L
F-F_       0    -6.87280300    3.32435100   -3.70431800   L
O-O_R      0    -3.35255300    4.67030500    0.14339700   L
C-C_R      0    -5.10358700    3.17640900   -0.56949200   L
C-C_R      0    -4.16062500    3.73707300    0.39603200   L
C-C_R      0    -6.38149700    1.22632600   -0.82404000   L
C-C_R      0    -6.83444600    1.67610200   -2.02272000   L
C-C_R      0    -6.42404900    2.87933000   -2.50427300   L
C-C_R      0    -5.52051900    3.66233600   -1.75239100   L
C-C_3      0    -3.40856700    3.22289100    3.89336000   L
C-C_3      0    -4.47585700    2.24833500    4.44508000   L
C-C_3      0    -4.05030800    4.62904400    3.81472300   L
C-C_3      0    -2.23217300    3.31054900    4.89425000   L
C-C_R      0    -5.52291700    1.99362400   -0.11923200   L
F-F_       0    -5.08696700    4.86168500   -2.21375800   L
O-O_R      0     0.63259800   -0.07701300    3.80819400   H
C-C_3      0     2.72447300    1.10540100    3.40213600   L
F-F_       0     3.60933400    6.47637500   -1.52759700   L
O-O_R      0     4.83538300    2.28856300    1.62895600   L
C-C_R      0     3.76601800    2.90760900    1.87530400   L
F-F_       0     1.08583800    7.01114300   -0.65842100   L
O-O_R      0     0.51342300    3.14777500    3.02520100   L
C-C_R      0     3.23897100    4.01902800    1.08787700   L
C-C_R      0     1.99939000    4.27481600    1.50510800   L
C-C_R      0     1.67448000    3.34515100    2.58217900   L
C-C_R      0     3.81073900    4.71518700    0.08743000   L
C-C_R      0     3.06424100    5.74721400   -0.52220400   L
C-C_R      0     1.80431600    6.00891600   -0.09475200   L
C-C_R      0     1.24534800    5.24209900    0.94992800   L
C-C_3      0     3.00459400    1.16827300    4.94978500   L
C-C_3      0     4.36860700    1.86219300    5.18230800   L
C-C_3      0     1.92585600    1.97165600    5.71264600   L
C-C_3      0     3.10867800   -0.25487700    5.54957200   L
F-F_       0    -0.01688200    5.48261100    1.38529100   L
O-O_R      0     1.30460300    0.30710200    1.67268900   H
C-C_R      0     1.45065800    0.38150000    2.94539400   H
N-N_R      0     2.77519300    2.45190800    2.80336500   L
F-F_       0     5.07605800    4.44572900   -0.31790400   L
O-O_R      0     0.41956100   -2.28762600    0.71798200   H
C-C_R      0     0.53142600   -3.04406400    1.74662600   H
N-N_R      0     2.71108900   -3.96926400    1.10731800   L
F-F_       0     5.09825600   -3.89246400   -2.53251200   L
O-O_R      0     0.05580800   -2.79831600    2.90391800   H
C-C_3      0     1.33569900   -4.32283700    1.50000700   L
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F-F_	0	7.20337500	-2.07585700	-2.31298400	L
O-O_R	0	2.66553100	-4.70075100	-1.14764400	L
F-F_	0	7.50719200	-0.63893500	0.05077700	L
C-C_R	0	3.29370300	-4.18877200	-0.18258500	L
O-O_R	0	3.23894300	-2.30879300	2.72018700	L
C-C_R	0	4.46896300	-3.33414200	-0.33341600	L
C-C_R	0	4.63384100	-2.63265600	0.79069000	L
C-C_R	0	3.57341200	-3.00267400	1.72396400	L
C-C_R	0	5.28686000	-3.18469700	-1.39094600	L
C-C_R	0	6.34708200	-2.26506600	-1.27907400	L
C-C_R	0	6.49867600	-1.53635200	-0.07748000	L
C-C_R	0	5.62757600	-1.73123300	0.94096600	L
C-C_3	0	1.32066400	-5.41968700	2.62965400	L
C-C_3	0	2.07769000	-6.66846200	2.11767500	L
C-C_3	0	2.00569200	-4.95236800	3.93490100	L
C-C_3	0	-0.13039400	-5.85761400	2.94324200	L
F-F_	0	5.75590300	-1.02902700	2.09493100	L
O-O_R	0	-2.29108300	-1.23699800	0.31321900	H
F-F_	0	-0.42942600	-5.81639600	-1.90259700	L
C-C_R	0	-2.97550800	-1.92123700	1.15919700	H
N-N_R	0	-3.82269400	-3.40578000	-0.60404500	L
O-O_R	0	-2.69479400	-2.05141300	2.39432300	H
F-F_	0	-0.10609700	-5.66238700	-4.66838200	L
C-C_3	0	-4.21444500	-2.60375300	0.56923900	L
O-O_R	0	-1.91812700	-4.53512700	0.25040200	L
F-F_	0	-1.83941700	-4.17302100	-6.14046000	L
C-C_R	0	-2.70065400	-4.29587400	-0.70650000	L
O-O_R	0	-4.86198200	-2.10224600	-2.29336600	L
F-F_	0	-3.87747900	-2.85089600	-4.92023000	L
C-C_R	0	-3.16262800	-3.71083600	-2.85134800	L
C-C_R	0	-4.13194400	-3.07518000	-1.96402300	L
C-C_R	0	-1.29398700	-5.09859600	-2.66263400	L
C-C_R	0	-1.13080000	-5.01229100	-4.06260500	L
C-C_R	0	-1.99855800	-4.26602600	-4.79635700	L
C-C_R	0	-3.01947400	-3.60668200	-4.18975000	L
C-C_3	0	-5.13060800	-3.43025500	1.54825500	L
C-C_3	0	-5.69106200	-2.52439800	2.67119100	L
C-C_3	0	-4.39616200	-4.63398400	2.18245600	L
C-C_3	0	-6.34285000	-3.97517700	0.75499700	L
C-C_R	0	-2.32463700	-4.43392000	-2.10963500	L
H-H_	0	-2.17690000	3.62473100	2.16632600	L
H-H_	0	-4.79550900	2.56333700	5.46203800	L
H-H_	0	-4.09801400	1.21161400	4.52862800	L
H-H_	0	-5.38238600	2.24485400	3.80563900	L

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H-H_      0    -4.37985100     4.97163200     4.81977600  L
H-H_      0    -4.94197200     4.62584300     3.15197500  L
H-H_      0    -3.32515000     5.37243200     3.41817300  L
H-H_      0    -2.58676800     3.66822200     5.88522200  L
H-H_      0    -1.46397900     4.02617600     4.53233200  L
H-H_      0    -1.74829200     2.32723600     5.05677200  L
H-H_      0     3.55529800     0.50824300     2.96414300  L
H-H_      0     4.62921900     1.87401000     6.26302400  L
H-H_      0     4.34830300     2.91670800     4.83330700  L
H-H_      0     5.17841100     1.33004600     4.63744500  L
H-H_      0     2.15541700     1.98947200     6.80004700  L
H-H_      0     0.91606200     1.53271200     5.59607400  L
H-H_      0     1.89318200     3.02452700     5.36350400  L
H-H_      0     3.43154100    -0.20901200     6.61229400  L
H-H_      0     3.85523000    -0.86051300     4.99264900  L
H-H_      0     2.14005200    -0.79088200     5.53369600  L
H-H_      0     0.84286800    -4.79720400     0.62164300  L
H-H_      0     2.04876300    -7.48626300     2.87028200  L
H-H_      0     3.14504100    -6.43500200     1.91592400  L
H-H_      0     1.62149000    -7.04828400     1.17778800  L
H-H_      0     1.93150000    -5.74285600     4.71283900  L
H-H_      0     1.54008500    -4.03783700     4.34978300  L
H-H_      0     3.08547300    -4.75740000     3.77140600  L
H-H_      0    -0.13713400    -6.71059600     3.65604200  L
H-H_      0    -0.65015300    -6.18437300     2.01747800  L
H-H_      0    -0.72106600    -5.04352100     3.40748200  L
H-H_      0    -4.84529300    -1.76246300     0.20729400  L
H-H_      0    -6.42283500    -3.08189900     3.29528200  L
H-H_      0    -6.21548500    -1.64519200     2.24012900  L
H-H_      0    -4.89825400    -2.16167000     3.35367400  L
H-H_      0    -5.06104300    -5.15401300     2.90563400  L
H-H_      0    -3.48523400    -4.32642600     2.73187400  L
H-H_      0    -4.10978000    -5.37794300     1.41111700  L
H-H_      0    -7.04385500    -4.51880600     1.42515300  L
H-H_      0    -6.01949100    -4.68457000    -0.03657800  L
H-H_      0    -6.90106600    -3.14477700     0.27049900  L
N-N_3     0     0.08620100     0.13825100    -0.90548800  H
S-S_3+6   0     0.56309400    -0.89364600    -2.10350500  H
O-O_2     0    -0.01048000    -2.24906900    -2.12027600  H
O-O_R     0     2.19072200    -1.11522600    -1.44678700  H
O-O_2     0     0.70613000    -0.14011700    -3.37055600  H
C-C_R     0     3.22523000    -0.40642900    -2.00470100  H
C-C_R     0     3.65673400    -0.64671900    -3.32395300  H
C-C_R     0     3.91814900     0.50806400    -1.18701900  H
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C-C_R	0	4.79396500	0.01175300	-3.80323800	H
H-H_	0	3.12115000	-1.36612400	-3.94483600	H
C-C_R	0	5.03926800	1.16257200	-1.69152600	H
H-H_	0	3.54432800	0.68562300	-0.17744700	H
C-C_R	0	5.51314000	0.92993200	-3.00844000	H
H-H_	0	5.12319300	-0.20672300	-4.82031600	H
H-H_	0	5.56246600	1.87308000	-1.04752200	H
C-C_3	0	6.74774800	1.69011700	-3.52635800	H
C-C_3	0	6.39875500	3.20099000	-3.61769200	H
H-H_	0	6.11417700	3.61405600	-2.63743500	H
H-H_	0	7.26917600	3.77149200	-3.98464800	H
H-H_	0	5.55967500	3.37124700	-4.31190300	H
C-C_3	0	7.19207900	1.20716300	-4.92426900	H
H-H_	0	8.09285800	1.76016800	-5.23731100	H
H-H_	0	7.44349100	0.13332500	-4.92559300	H
H-H_	0	6.41742500	1.38323100	-5.68874000	H
C-C_3	0	7.93881100	1.49977500	-2.55035200	H
H-H_	0	8.81383700	2.06719000	-2.91005100	H
H-H_	0	7.70795400	1.85753500	-1.53452800	H
H-H_	0	8.22839200	0.43911500	-2.47806300	H
C-C_R	0	-0.87857700	3.71638500	-2.91031500	H
C-C_R	0	-1.33530900	5.05086400	-2.86359100	H
C-C_R	0	-0.49663800	6.11726400	-3.21460200	H
C-C_R	0	0.82889800	5.86969900	-3.60538000	H
C-C_R	0	1.30464300	4.54855100	-3.63940700	H
C-C_R	0	0.46070600	3.48412800	-3.29896600	H
H-H_	0	-2.36555700	5.25128700	-2.55302100	H
H-H_	0	-0.87502700	7.14329900	-3.17636600	H
H-H_	0	1.48929200	6.70095200	-3.86964400	H
H-H_	0	2.34052600	4.34772100	-3.92882000	H
H-H_	0	0.83552300	2.45740000	-3.32733900	H
C-C_3	0	-1.79129400	2.56156400	-2.56637900	H
H-H_	0	-2.66292700	2.93827700	-2.00502000	H
H-H_	0	-1.25271800	1.86561600	-1.89084500	H
C-C_3	0	-2.30689500	1.73552400	-3.77933400	H
H-H_	0	-1.42209000	1.33228700	-4.30410300	H
C-C_3	0	-3.14990000	0.54721000	-3.28642500	H
H-H_	0	-4.05280900	0.89751800	-2.75652500	H
H-H_	0	-3.48062800	-0.08187800	-4.12995900	H
H-H_	0	-2.58616600	-0.09427800	-2.58959300	H
C-C_3	0	-3.10339800	2.60078300	-4.77187200	H
H-H_	0	-4.00066700	3.03114100	-4.29313300	H
H-H_	0	-2.49751900	3.43535000	-5.15953200	H
H-H_	0	-3.44330400	1.99815600	-5.63127700	H

¹TS2

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C-C_R    0    2.24913500   -5.22536200    1.42273500  L
C-C_R    0   -5.02229800    4.10799000    1.15410300  L
C-C_R    0    5.12897700    3.91220300    2.22285200  L
C-C_R    0   -5.50851400   -2.06296200   -1.01596400  L
C-C_3    0    5.25995100   -2.09833400   -2.65791400  L
C-C_3    0    2.36056600    4.64030500   -3.14222600  L
C-C_3    0   -3.65056100    1.91411300   -4.24261200  L
C-C_3    0   -0.92470200   -4.72572200   -3.65890900  L
C-C_3    0    1.04582000    4.73808200   -3.95164600  L
C-C_3    0    6.62156300   -2.62589200   -2.14383400  L
C-C_3    0   -1.46631300   -6.15261000   -3.40396100  L
C-C_3    0   -2.75931100    3.05465000   -4.78714200  L
C-C_3    0    4.59696100   -3.22213000   -3.48783900  L
C-C_3    0   -1.75931200   -4.09968800   -4.80030400  L
C-C_3    0    3.47036300    4.04990200   -4.04343800  L
C-C_3    0   -5.11568800    2.41476900   -4.24251700  L
C-C_3    0    2.77756600    6.08116700   -2.76224400  L
C-C_3    0    0.54577300   -4.86586400   -4.12062500  L
C-C_3    0   -3.58651600    0.70404600   -5.20654100  L
C-C_3    0    5.55901100   -0.88897500   -3.57632500  L
C-C_R    0   -1.84218200    0.92222200   -2.56791400  H
C-C_R    0   -0.38422600   -2.50975400   -2.30092600  H
C-C_R    0    3.00697500   -1.05304700   -1.71148500  H
C-C_R    0    1.55348400    2.40588500   -1.95949300  H
C-C_3    0   -3.25365900    1.48872600   -2.77758700  L
C-C_3    0   -1.00621600   -3.90891800   -2.31529800  L
C-C_3    0    4.38443800   -1.66344600   -1.42286800  L
C-C_3    0    2.13694300    3.81562800   -1.81932300  L
C-C_R    0   -2.61231800    3.63416400   -1.42056000  L
C-C_R    0   -2.84692800   -4.38845100   -0.56489400  L
C-C_R    0    4.78144400   -2.77816400    0.86745600  L
C-C_R    0    4.43344300    2.81399500   -1.09667900  L
C-C_R    0   -3.14541500    4.28511100   -0.22552700  L
C-C_R    0   -4.09470000   -3.73296900   -0.17816900  L
C-C_R    0    4.04228600   -3.72684900    1.69369000  L
C-C_R    0    5.18978300    2.81584100    0.15143400  L
C-C_R    0   -4.30672200    3.70913100    0.08797600  L
C-C_R    0   -4.41704700   -2.84497200   -1.11862700  L
C-C_R    0    3.11971400   -4.31820000    0.93096400  L
C-C_R    0    4.65543000    3.71934200    0.97334300  L
C-C_R    0   -4.57600300    2.65623200   -0.88453700  L
C-C_R    0   -3.39712100   -2.88389700   -2.16190700  L
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C-C_R	0	3.22196900	-3.77333600	-0.42117700	L
C-C_R	0	3.52985100	4.35223500	0.29063100	L
C-C_R	0	-2.62885500	5.29084900	0.51154100	L
C-C_R	0	-4.84269300	-3.89853500	0.92953400	L
C-C_R	0	4.16408200	-4.00029400	3.00487000	L
C-C_R	0	6.23313800	2.05497200	0.52866500	L
C-C_R	0	-3.31139400	5.72557800	1.60260900	L
C-C_R	0	-6.00199200	-3.10688600	1.08044600	L
C-C_R	0	3.28208400	-4.94461800	3.56449200	L
C-C_R	0	6.75102300	2.24683500	1.82831900	L
C-C_R	0	-4.49872800	5.15638200	1.94212200	L
C-C_R	0	-6.32939800	-2.20449000	0.12330600	L
C-C_R	0	2.31364900	-5.55469000	2.73489200	L
C-C_R	0	6.18485200	3.17137800	2.64878100	L
F-F_	0	-1.44435100	5.85916500	0.17159200	L
F-F_	0	-4.49065800	-4.79626200	1.88347900	L
F-F_	0	5.10290400	-3.38775300	3.76816600	L
F-F_	0	6.76848300	1.12869800	-0.30512100	L
F-F_	0	-2.80490300	6.73223200	2.35799800	L
F-F_	0	-6.77878200	-3.24483800	2.18359600	L
F-F_	0	3.35643800	-5.25851400	4.88152900	L
F-F_	0	7.80015100	1.50243900	2.25806400	L
F-F_	0	-5.17982700	5.59268400	3.03086800	L
F-F_	0	-7.43768500	-1.43510400	0.25949700	L
F-F_	0	1.44808000	-6.46058100	3.25427600	L
F-F_	0	6.67228100	3.34967800	3.90217700	L
F-F_	0	-6.21370600	3.53557800	1.45735500	L
F-F_	0	-5.81880500	-1.16338200	-1.98235600	L
F-F_	0	1.31463300	-5.79331400	0.61908000	L
F-F_	0	4.56055300	4.83011500	3.04420600	L
H-H_	0	-1.38473900	-6.77746500	-4.31990900	L
H-H_	0	-3.07349300	3.33123000	-5.81682700	L
H-H_	0	1.17803800	5.39784900	-4.83644800	L
H-H_	0	7.29217200	-2.88676300	-2.99133700	L
H-H_	0	-2.53689200	-6.12706100	-3.10780400	L
H-H_	0	6.49223600	-3.54144400	-1.52796600	L
H-H_	0	-1.69193300	2.76543900	-4.83619900	L
H-H_	0	0.23292200	5.16621500	-3.32773700	L
H-H_	0	-0.89362100	-6.65307300	-2.59321400	L
H-H_	0	7.13168500	-1.85761200	-1.52302400	L
H-H_	0	-2.84724800	3.96418300	-4.15790100	L
H-H_	0	0.71621600	3.74957200	-4.32827200	L
H-H_	0	-1.63599500	-4.68868700	-5.73489300	L
H-H_	0	5.23463300	-3.48531200	-4.35937300	L

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H-H_    0    3.57447700    4.65356100   -4.97100000  L
H-H_    0   -5.45394600    2.65536300   -5.27388000  L
H-H_    0   -1.45208800   -3.06021100   -5.02443400  L
H-H_    0    3.60627200   -2.92333400   -3.88189200  L
H-H_    0    3.25250600    3.01006400   -4.35334100  L
H-H_    0   -5.22619000    3.33842300   -3.63540700  L
H-H_    0   -2.84084500   -4.10508700   -4.55332500  L
H-H_    0    4.47117300   -4.14309500   -2.88207300  L
H-H_    0    4.45390000    4.06896600   -3.53048400  L
H-H_    0   -5.79582700    1.63929100   -3.82802300  L
H-H_    0    6.26948700   -1.17574700   -4.38177300  L
H-H_    0    0.61677100   -5.53344600   -5.00661800  L
H-H_    0    2.90170100    6.71077600   -3.67012400  L
H-H_    0   -3.98789800    0.97841300   -6.20622800  L
H-H_    0    6.02092400   -0.06222600   -2.99588800  L
H-H_    0    1.17011600   -5.30480700   -3.31350000  L
H-H_    0   -4.19466900   -0.13967200   -4.81609500  L
H-H_    0    3.74384900    6.08610400   -2.21385600  L
H-H_    0    4.64952700   -0.50313600   -4.07580100  L
H-H_    0    2.00881100    6.55730400   -2.11569400  L
H-H_    0   -2.55213100    0.34534900   -5.36903600  L
H-H_    0    0.98505100   -3.89140700   -4.41224300  L
H-H_    0   -3.93326700    0.65230900   -2.50478400  L
H-H_    0   -0.40203900   -4.48990900   -1.58229800  L
H-H_    0    4.94852700   -0.84566300   -0.92162000  L
H-H_    0    1.36716700    4.38052000   -1.24573400  L
N-N_R   0   -3.50254200    2.58609100   -1.82736500  L
N-N_R   0   -2.38708700   -3.83848900   -1.80561800  L
N-N_R   0    4.24743000   -2.77048700   -0.45970700  L
N-N_R   0    3.36237300    3.76437000   -1.00408000  L
O-O_R   0   -1.55936600    0.59179600   -1.36021100  H
O-O_R   0   -0.25231100   -2.00615200   -1.13048800  H
O-O_R   0    2.34969100   -0.68481300   -0.66750100  H
O-O_R   0    1.09057800    1.90292200   -0.87093700  H
O-O_R   0   -1.06009800    0.80711300   -3.56688600  H
O-O_R   0   -0.06833100   -1.93907500   -3.39739300  H
O-O_R   0    2.60073700   -0.94234800   -2.91128500  H
O-O_R   0    1.58811000    1.82155300   -3.08965600  H
O-O_R   0   -1.41654400    3.72311900   -1.80369400  L
O-O_R   0   -2.09705700   -5.00544300    0.23829500  L
O-O_R   0    5.58046500   -1.90875100    1.30527700  L
O-O_R   0    4.46163500    1.87663200   -1.93693600  L
O-O_R   0   -5.48603800    1.79047900   -0.78697500  L
O-O_R   0   -3.22049200   -1.96857500   -3.00827600  L
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O-O_R       0     2.32592200    -3.88694100    -1.29810600 L
O-O_R       0     2.65021100     5.05335800     0.85757300 L
Rh-         0     0.39439300    -0.06156300    -0.88268400 H
Rh-         0     0.77306500    -0.06279700    -3.28287000 H
N-N_3       0    -0.15279100     0.01082200     1.02143300 H
S-S_3+6     0    -0.25781100    -1.38518900     1.95655900 H
O-O_2       0     0.55950100    -2.54622600     1.57329000 H
O-O_R       0    -1.85136300    -1.78765500     1.39057400 H
O-O_2       0    -0.36587300    -0.99311700     3.38019200 H
C-C_R       0    -2.92680700    -1.28287500     2.10666500 H
C-C_R       0    -3.29780400    -1.85990000     3.33107000 H
C-C_R       0    -3.69032500    -0.24568500     1.54652500 H
C-C_R       0    -4.44678200    -1.40083500     3.98788600 H
H-H_        0    -2.69949500    -2.67275900     3.74589400 H
C-C_R       0    -4.82167700     0.20572100     2.22768000 H
H-H_        0    -3.36917500     0.19354200     0.60007700 H
C-C_R       0    -5.23234900    -0.35639700     3.46035900 H
H-H_        0    -4.72400000    -1.87441900     4.93132300 H
H-H_        0    -5.40022400     1.02241000     1.79187000 H
C-C_3       0    -6.46891300     0.20777700     4.18662800 H
C-C_3       0    -6.15189100     1.65573000     4.64979700 H
H-H_        0    -5.88951900     2.30673500     3.80113400 H
H-H_        0    -7.02604300     2.09738900     5.15882400 H
H-H_        0    -5.30299000     1.66653300     5.35310400 H
C-C_3       0    -6.85275100    -0.62751900     5.42764400 H
H-H_        0    -7.75761600    -0.20432900     5.89437800 H
H-H_        0    -7.07267600    -1.67527700     5.16246100 H
H-H_        0    -6.05757900    -0.62339600     6.19140100 H
C-C_3       0    -7.68879500     0.22919700     3.22916400 H
H-H_        0    -8.56571900     0.65873000     3.74296800 H
H-H_        0    -7.50361100     0.83588700     2.32865300 H
H-H_        0    -7.95219700    -0.78964200     2.90174000 H
C-C_R       0     2.45493400     0.87309500     3.42707200 H
C-C_R       0     3.75844500     0.56547700     2.96635500 H
C-C_R       0     4.68126900    -0.08742700     3.78713900 H
C-C_R       0     4.30995700    -0.48656100     5.08203900 H
C-C_R       0     3.00793300    -0.22999200     5.54252900 H
C-C_R       0     2.09084800     0.43920700     4.72706200 H
H-H_        0     4.03480600     0.85011300     1.94851800 H
H-H_        0     5.69335700    -0.28520400     3.42461300 H
H-H_        0     5.02829500    -1.00453800     5.72367200 H
H-H_        0     2.70708600    -0.55514600     6.54226000 H
H-H_        0     1.07973900     0.62261600     5.09308200 H
C-C_3       0     1.52613200     1.63980800     2.54913200 H
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H-H_	0	0.85373500	0.87923500	1.93349100	H
C-C_3	0	0.51936200	2.60403900	3.20598900	H
C-C_3	0	1.25440600	3.70314800	4.00647900	H
H-H_	0	1.87830000	4.32354200	3.34175500	H
H-H_	0	0.52363100	4.36942800	4.49528800	H
H-H_	0	1.90840900	3.27799500	4.78376900	H
C-C_3	0	-0.42112800	3.22839700	2.16187800	H
H-H_	0	0.14381400	3.81787200	1.41989200	H
H-H_	0	-0.98568000	2.45600100	1.61944900	H
H-H_	0	-1.13912700	3.90371300	2.65611000	H
H-H_	0	-0.10271900	2.02153500	3.90894200	H
H-H_	0	2.07808000	2.13564600	1.73222200	H

³INT3

C-C_R	0	5.82210200	-1.39413200	0.49133300	L
C-C_R	0	-5.64370700	3.60547100	-1.83309000	L
C-C_R	0	-3.01043600	-4.50021900	-3.34537700	L
C-C_R	0	1.10262800	5.81537100	0.69414800	L
C-C_3	0	1.90786200	-4.93561700	3.12815700	L
C-C_3	0	-4.81009000	-3.36666500	2.39170800	L
C-C_3	0	-3.32067000	3.46962000	3.69922100	L
C-C_3	0	3.39673100	1.85865400	4.40839500	L
C-C_3	0	-5.31254600	-2.29016800	3.38402700	L
C-C_3	0	2.70404700	-6.19841300	2.71998000	L
C-C_3	0	4.73377500	2.63804500	4.42949500	L
C-C_3	0	-4.32203100	2.47371100	4.33042500	L
C-C_3	0	2.67985000	-4.23844300	4.27277900	L
C-C_3	0	2.36933100	2.65894000	5.24313100	L
C-C_3	0	-4.00526600	-4.43784900	3.16334100	L
C-C_3	0	-4.04547400	4.82746400	3.53471300	L
C-C_3	0	-6.05968400	-4.05269500	1.78901000	L
C-C_3	0	3.65552800	0.49213700	5.08716900	L
C-C_3	0	-2.13991900	3.69847600	4.67297700	L
C-C_3	0	0.53270500	-5.41147700	3.65537300	L
C-C_R	0	-1.94919900	1.72052700	2.24921700	H
C-C_R	0	1.67974100	0.83653800	2.65693800	H
C-C_R	0	0.87105500	-2.75983400	2.01429400	H
C-C_R	0	-2.74586600	-1.88769500	1.60556400	H
C-C_3	0	-2.80124600	2.99581100	2.28898700	L
C-C_3	0	2.94656800	1.66194900	2.91110000	L
C-C_3	0	1.72904300	-4.01899800	1.85960600	L
C-C_3	0	-3.98452600	-2.70636000	1.22496800	L
C-C_R	0	-4.69678900	1.72229200	1.02428500	L
C-C_R	0	3.67745100	3.39707100	1.14545100	L

C-C_R	0	3.51536400	-4.07310500	-0.01281000	L
C-C_R	0	-2.44995800	-4.52647900	0.17422600	L
C-C_R	0	-5.41034700	1.92286300	-0.23161100	L
C-C_R	0	3.07210000	4.55972200	0.50072800	L
C-C_R	0	4.63780000	-3.22167100	-0.40031500	L
C-C_R	0	-2.14050900	-4.89027100	-1.20424700	L
C-C_R	0	-5.12463100	3.14519700	-0.68096800	L
C-C_R	0	1.90216800	4.80778600	1.09131600	L
C-C_R	0	4.86125300	-2.33877200	0.57660300	L
C-C_R	0	-3.06787100	-4.36455700	-2.00325700	L
C-C_R	0	-4.20261700	3.78465600	0.25647600	L
C-C_R	0	1.71209900	3.83922200	2.16640100	L
C-C_R	0	3.89527400	-2.57986600	1.64497400	L
C-C_R	0	-4.02805600	-3.63766200	-1.17741800	L
C-C_R	0	-6.21816000	1.08308800	-0.91266100	L
C-C_R	0	3.52352500	5.30608400	-0.52449000	L
C-C_R	0	5.36108100	-3.22471900	-1.53445600	L
C-C_R	0	-1.10000200	-5.58452400	-1.69916900	L
C-C_R	0	-6.76671400	1.50238700	-2.08210800	L
C-C_R	0	2.72295200	6.37778800	-0.97633000	L
C-C_R	0	6.38452500	-2.26667400	-1.66581900	L
C-C_R	0	-1.02366300	-5.74594400	-3.09989900	L
C-C_R	0	-6.50301100	2.74889500	-2.55638100	L
C-C_R	0	1.53300600	6.62864600	-0.37669600	L
C-C_R	0	6.59815300	-1.34316200	-0.61749500	L
C-C_R	0	-1.98236900	-5.19867000	-3.89344800	L
F-F_	0	-6.47997900	-0.16117700	-0.43915900	L
F-F_	0	4.71307700	5.03498300	-1.11606700	L
F-F_	0	5.11319500	-4.11732700	-2.52513200	L
F-F_	0	-0.14877500	-6.10545900	-0.88446300	L
F-F_	0	-7.58002700	0.67217800	-2.78186800	L
F-F_	0	3.14228200	7.14922900	-2.01002600	L
F-F_	0	7.14595800	-2.22523600	-2.78668500	L
F-F_	0	0.00670700	-6.43625300	-3.64892500	L
F-F_	0	-7.05254800	3.16626400	-3.72400200	L
F-F_	0	0.75430100	7.65244700	-0.80674500	L
F-F_	0	7.56884500	-0.40244200	-0.72779700	L
F-F_	0	-1.90847900	-5.34540500	-5.24015000	L
F-F_	0	-5.35010100	4.84773100	-2.29152600	L
F-F_	0	-0.08588700	6.04801600	1.30562400	L
F-F_	0	6.00809600	-0.50387100	1.49842800	L
F-F_	0	-3.96170500	-3.94566600	-4.13813800	L
H-H_	0	5.11381100	2.74641800	5.46867000	L
H-H_	0	-4.66738000	2.84868800	5.31819100	L

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H-H_    0    -5.99503800    -2.74002300     4.13741200  L
H-H_    0     2.80541500    -6.89819800     3.57793500  L
H-H_    0     4.60984100     3.65980300     4.01125200  L
H-H_    0     3.72828800    -5.93428600     2.38008300  L
H-H_    0    -3.87478600     1.47531100     4.49825200  L
H-H_    0    -5.87438200    -1.49519200     2.84872600  L
H-H_    0     5.50774200     2.10839000     3.83266100  L
H-H_    0     2.19174500    -6.73733200     1.89359600  L
H-H_    0    -5.22081300     2.35371900     3.69079800  L
H-H_    0    -4.48309600    -1.81666100     3.94456000  L
H-H_    0     2.71455200     2.74824400     6.29592000  L
H-H_    0     2.74350000    -4.90802500     5.15773800  L
H-H_    0    -4.61095300    -4.84529500     4.00157700  L
H-H_    0    -4.36905700     5.22688200     4.52053000  L
H-H_    0     1.37424200     2.17459200     5.26379900  L
H-H_    0     2.18892000    -3.30295100     4.60294700  L
H-H_    0    -3.07249700    -4.02905700     3.59786800  L
H-H_    0    -4.95354900     4.72440000     2.90327800  L
H-H_    0     2.25141600     3.68941200     4.84970700  L
H-H_    0     3.72013300    -4.00325700     3.96787900  L
H-H_    0    -3.74386800    -5.29121300     2.50430000  L
H-H_    0    -3.37485400     5.57766400     3.06228600  L
H-H_    0     0.66186900    -6.14143100     4.48375600  L
H-H_    0     4.06885900     0.63477800     6.10920900  L
H-H_    0    -6.69706000    -4.48951700     2.58837300  L
H-H_    0    -2.50294800     4.11801800     5.63625500  L
H-H_    0    -0.04374900    -5.91272700     2.84901800  L
H-H_    0     4.39214000    -0.10048300     4.50418800  L
H-H_    0    -1.41313700     4.41941500     4.24227600  L
H-H_    0    -5.77283300    -4.87695100     1.10144900  L
H-H_    0    -0.07526600    -4.57549800     4.05325800  L
H-H_    0    -6.67320600    -3.32193800     1.21852400  L
H-H_    0    -1.60338600     2.75971700     4.91220700  L
H-H_    0     2.72998900    -0.10610200     5.19510200  L
H-H_    0    -2.12167900     3.80049900     1.92808400  L
H-H_    0     3.76253600     1.08421300     2.42062800  L
H-H_    0     1.18107600    -4.64178000     1.11777700  L
H-H_    0    -4.67106800    -1.96658200     0.75673300  L
N-N_R   0    -3.91446700     2.88293200     1.33111700  L
N-N_R   0     2.83790800     2.95389000     2.21459900  L
N-N_R   0     3.02974100    -3.65916400     1.26888500  L
N-N_R   0    -3.62245600    -3.69797700     0.19594900  L
O-O_R   0    -1.38745900     1.46895200     1.12086600  H
O-O_R   0     1.42016800     0.61638300     1.41728500  H
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O-O_R      0     0.62079500   -2.15040700    0.91503400  H
O-O_R      0    -2.18060800   -1.28994400    0.61909300  H
O-O_R      0    -1.85628300    0.98979600    3.28916900  H
O-O_R      0     0.97287500    0.44100500    3.63929500  H
O-O_R      0     0.47812500   -2.38885800    3.17001600  H
O-O_R      0    -2.35138500   -1.84979400    2.81693400  H
O-O_R      0    -4.62382600    0.63367800    1.65165800  L
O-O_R      0     4.88466800    3.05763000    1.02628100  L
O-O_R      0     2.83527800   -4.75820900   -0.82274100  L
O-O_R      0    -1.61275200   -4.56789700    1.11342900  L
O-O_R      0    -3.50407100    4.79949100   -0.00788200  L
O-O_R      0     0.60636500    3.59379500    2.71521600  L
O-O_R      0     3.60872900   -1.74013600    2.53789600  L
O-O_R      0    -4.85042200   -2.79301900   -1.62215800  L
Rh-        0    -0.36449900   -0.33045200    0.90187600  H
Rh-        0    -0.69675800   -0.70532100    3.26473700  H
N-N_3      0    -0.08050900   -0.20452200   -1.03266600  H
S-S_3+6    0     0.60796400   -1.21933000   -2.12255000  H
O-O_2      0     0.61964900   -0.55884400   -3.44209000  H
O-O_R      0     2.23846000   -1.26387400   -1.53612900  H
O-O_2      0     0.13876700   -2.60836400   -1.97810700  H
C-C_R      0     3.19054200   -0.48004100   -2.16973300  H
C-C_R      0     3.77589600    0.57211500   -1.44896100  H
C-C_R      0     3.64163400   -0.79464500   -3.46534500  H
C-C_R      0     4.82656400    1.29605000   -2.02358700  H
H-H_       0     3.39862300    0.80114600   -0.45067400  H
C-C_R      0     4.69320000   -0.06090000   -4.01596400  H
H-H_       0     3.18240600   -1.61884800   -4.01320400  H
C-C_R      0     5.31662300    0.99737900   -3.31347800  H
H-H_       0     5.27306100    2.10854300   -1.44953500  H
H-H_       0     5.04045400   -0.32733300   -5.01770700  H
C-C_3      0     6.47677700    1.77415100   -3.96432000  H
C-C_3      0     5.96657800    2.45411700   -5.26321100  H
H-H_       0     5.58821400    1.71837900   -5.99074700  H
H-H_       0     6.78491500    3.01464900   -5.74682300  H
H-H_       0     5.14927600    3.16068400   -5.04415300  H
C-C_3      0     7.04746000    2.86800800   -3.03607800  H
H-H_       0     7.88438000    3.38002200   -3.53877600  H
H-H_       0     7.43525900    2.44697300   -2.09332800  H
H-H_       0     6.29350700    3.63363200   -2.79096300  H
C-C_3      0     7.62682200    0.79266400   -4.31450100  H
H-H_       0     8.44794900    1.33403500   -4.81467000  H
H-H_       0     7.29482400   -0.01020400   -4.99165700  H
H-H_       0     8.03458200    0.32064700   -3.40588400  H
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C-C_R     0    -3.04350600     2.09568400    -3.49654300  H
C-C_R     0    -3.76470000     2.56637000    -4.61272000  H
C-C_R     0    -4.56976600     1.70427300    -5.37147800  H
C-C_R     0    -4.67042200     0.34837500    -5.02497500  H
C-C_R     0    -3.96067000    -0.13456200    -3.91515100  H
C-C_R     0    -3.16117700     0.73145600    -3.15732600  H
H-H_      0    -3.70467500     3.62655800    -4.87965500  H
H-H_      0    -5.12554400     2.09453500    -6.22956200  H
H-H_      0    -5.30155200    -0.32556000    -5.61164000  H
H-H_      0    -4.03071700    -1.18932700    -3.63721400  H
H-H_      0    -2.62177200     0.34933300    -2.28535800  H
C-C_3     0    -2.16665400     3.01771000    -2.67321000  H
H-H_      0    -2.57306900     4.04660600    -2.70604900  H
H-H_      0    -2.20164600     2.69228300    -1.61859100  H
C-C_3     0    -0.67109600     3.06648000    -3.09578700  H
H-H_      0    -0.29680100     2.02766200    -3.09715800  H
C-C_3     0     0.13177100     3.86464500    -2.05450200  H
H-H_      0    -0.22470500     4.90940000    -2.00148000  H
H-H_      0     1.20450600     3.89002200    -2.31084800  H
H-H_      0     0.03472000     3.42205400    -1.04906300  H
C-C_3     0    -0.47703900     3.64764100    -4.50544300  H
H-H_      0    -0.82978100     4.69439200    -4.55541900  H
H-H_      0    -1.02812500     3.06757600    -5.26269100  H
H-H_      0     0.58946400     3.64177800    -4.78771300  H
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³TS3
```
C-C_R     0    -5.74095900    -1.48056500    -0.57352300  L
C-C_R     0     5.26573400     3.67276000     2.41886600  L
C-C_R     0     3.25684300    -4.86715100     2.84633300  L
C-C_R     0    -1.33110600     5.87653600    -0.16677300  L
C-C_3     0    -1.70707100    -4.52350400    -3.63944000  L
C-C_3     0     4.96946800    -2.75561400    -2.60083700  L
C-C_3     0     3.21599800     4.08102300    -3.23613300  L
C-C_3     0    -3.44924400     2.19559900    -4.29306400  L
C-C_3     0     5.44088700    -1.53849700    -3.43253900  L
C-C_3     0    -2.46056200    -5.85257300    -3.39153300  L
C-C_3     0    -4.82962700     2.89593900    -4.28069800  L
C-C_3     0     4.27093400     3.19465700    -3.93934300  L
C-C_3     0    -2.49809400    -3.72029600    -4.69827200  L
C-C_3     0    -2.46037800     3.11217200    -5.05127900  L
C-C_3     0     4.24043400    -3.75746300    -3.52606600  L
C-C_3     0     3.88054900     5.44170200    -2.91481000  L
C-C_3     0     6.23750300    -3.45249100    -2.05134400  L
C-C_3     0    -3.61835500     0.86894500    -5.07183900  L
```

C-C_3	0	2.04880500	4.36350400	-4.21206800	L
C-C_3	0	-0.31415800	-4.88731900	-4.20819600	L
C-C_R	0	1.89288300	2.13489300	-2.00327100	H
C-C_R	0	-1.70226700	1.14544200	-2.58764300	H
C-C_R	0	-0.76942700	-2.44907000	-2.27052000	H
C-C_R	0	2.81080400	-1.49241200	-1.70286700	H
C-C_3	0	2.68534900	3.44574800	-1.89533300	L
C-C_3	0	-3.00794600	1.91959000	-2.80574500	L
C-C_3	0	-1.56711800	-3.75782000	-2.26985000	L
C-C_3	0	4.08046500	-2.29152600	-1.38689300	L
C-C_R	0	4.62547500	2.14997900	-0.72643200	L
C-C_R	0	-3.85895500	3.49514100	-0.94299500	L
C-C_R	0	-3.34701200	-4.12595400	-0.42770000	L
C-C_R	0	2.61100000	-4.29992600	-0.61324000	L
C-C_R	0	5.25233000	2.22315600	0.58873600	L
C-C_R	0	-3.27613500	4.56985400	-0.14600700	L
C-C_R	0	-4.49422900	-3.36985400	0.06937400	L
C-C_R	0	2.34806200	-4.91198800	0.68565200	L
C-C_R	0	4.86474900	3.35621800	1.17465400	L
C-C_R	0	-2.11752500	4.92437500	-0.70345000	L
C-C_R	0	-4.75271800	-2.37591200	-0.78424000	L
C-C_R	0	3.26002400	-4.47629400	1.55444800	L
C-C_R	0	3.96048800	4.06536600	0.27129200	L
C-C_R	0	-1.89418600	4.09218200	-1.88286800	L
C-C_R	0	-3.78796200	-2.44615400	-1.87794300	L
C-C_R	0	4.13690000	-3.53821500	0.86089800	L
C-C_R	0	6.05858100	1.33780600	1.21187600	L
C-C_R	0	-3.72576100	5.14161300	0.98660600	L
C-C_R	0	-5.20891100	-3.54311400	1.19567100	L
C-C_R	0	1.37239800	-5.75904400	1.05904400	L
C-C_R	0	6.49637600	1.61655400	2.46681300	L
C-C_R	0	-2.94040900	6.15115800	1.58442700	L
C-C_R	0	-6.26038800	-2.64299000	1.45375100	L
C-C_R	0	1.34943600	-6.18232600	2.40618000	L
C-C_R	0	6.12058700	2.76727400	3.08541000	L
C-C_R	0	-1.76365800	6.51352100	1.01658400	L
C-C_R	0	-6.50957700	-1.59791500	0.53533900	L
C-C_R	0	2.29494800	-5.72723700	3.27109600	L
F-F_	0	6.42206600	0.18281900	0.59948900	L
F-F_	0	-4.90050800	4.75793000	1.54507400	L
F-F_	0	-4.92593800	-4.54811700	2.06144400	L
F-F_	0	0.43861600	-6.19198500	0.17543400	L
F-F_	0	7.30436300	0.73712600	3.11038200	L
F-F_	0	-3.36014800	6.75027200	2.72653500	L

F-F_	0	-7.01525300	-2.77251100	2.57230500	L
F-F_	0	0.38573100	-7.03570800	2.83354800	L
F-F_	0	6.55027700	3.03903900	4.34277600	L
F-F_	0	-0.99756900	7.47576200	1.58814600	L
F-F_	0	-7.50794800	-0.71047800	0.76965200	L
F-F_	0	2.27320900	-6.12846700	4.56691600	L
F-F_	0	4.85494400	4.81608900	3.02181800	L
F-F_	0	-0.14672900	6.20983400	-0.73841900	L
F-F_	0	-5.96166600	-0.47358500	-1.45595700	L
F-F_	0	4.19109300	-4.40082000	3.71268500	L
H-H_	0	-5.20375300	3.05444100	-5.31559100	L
H-H_	0	4.61924400	3.68057000	-4.87642500	L
H-H_	0	6.15767600	-1.85675600	-4.22036300	L
H-H_	0	-2.53033400	-6.44978200	-4.32669600	L
H-H_	0	-4.77083900	3.89128100	-3.79066200	L
H-H_	0	-3.49646300	-5.66666800	-3.03562900	L
H-H_	0	3.86997900	2.20084800	-4.21611100	L
H-H_	0	5.95595500	-0.79760500	-2.78465800	L
H-H_	0	-5.57773500	2.28226700	-3.73333600	L
H-H_	0	-1.93530900	-6.46646800	-2.62795100	L
H-H_	0	5.16159800	3.04753400	-3.29421400	L
H-H_	0	4.60197300	-1.03117900	-3.94745300	L
H-H_	0	-2.80018200	3.26194200	-6.09896600	L
H-H_	0	-2.53829400	-4.28189200	-5.65666400	L
H-H_	0	4.89205500	-4.03535100	-4.38261900	L
H-H_	0	4.21103200	5.95195700	-3.84567500	L
H-H_	0	-1.43977200	2.68598700	-5.09517900	L
H-H_	0	-2.03633900	-2.73711100	-4.91176600	L
H-H_	0	3.30569600	-3.33792000	-3.94555700	L
H-H_	0	4.77645100	5.30950200	-2.27140100	L
H-H_	0	-2.40363800	4.11468800	-4.57970600	L
H-H_	0	-3.54571100	-3.55478100	-4.37319300	L
H-H_	0	3.99460100	-4.69382500	-2.98406400	L
H-H_	0	3.16860000	6.11326300	-2.38763900	L
H-H_	0	-0.41510600	-5.52274200	-5.11472400	L
H-H_	0	-4.01847400	1.06184400	-6.09087800	L
H-H_	0	6.91761500	-3.74942600	-2.87918300	L
H-H_	0	2.41584100	4.89309600	-5.11790200	L
H-H_	0	0.27796700	-5.45611500	-3.46007600	L
H-H_	0	-4.33305800	0.19787100	-4.55009800	L
H-H_	0	1.28442900	5.00873900	-3.72949400	L
H-H_	0	5.97700200	-4.37276500	-1.48598300	L
H-H_	0	0.26496100	-3.99178200	-4.50640200	L
H-H_	0	6.79676800	-2.77326200	-1.37187100	L

H-H_	0	1.55590000	3.43470000	-4.55942600	L
H-H_	0	-2.65930100	0.33016200	-5.19889400	L
H-H_	0	1.95811600	4.17877300	-1.47892200	L
H-H_	0	-3.79707100	1.26449700	-2.37327200	L
H-H_	0	-0.98927900	-4.43738400	-1.60448500	L
H-H_	0	4.71312600	-1.58836200	-0.79955300	L
N-N_R	0	3.77924100	3.29108000	-0.92020900	L
N-N_R	0	-2.98043800	3.16631500	-2.02276500	L
N-N_R	0	-2.88304600	-3.53365200	-1.64603900	L
N-N_R	0	3.74371500	-3.42513200	-0.50975300	L
O-O_R	0	1.33603300	1.74158000	-0.91190700	H
O-O_R	0	-1.45287300	0.83127200	-1.36612800	H
O-O_R	0	-0.59458700	-1.93663000	-1.10943000	H
O-O_R	0	2.18803400	-1.04372300	-0.67316400	H
O-O_R	0	1.84398900	1.52237000	-3.11713300	H
O-O_R	0	-0.95538200	0.87614600	-3.58251200	H
O-O_R	0	-0.34922700	-1.95626000	-3.37007700	H
O-O_R	0	2.44495100	-1.32768500	-2.91223500	H
O-O_R	0	4.58167400	1.11493700	-1.44118400	L
O-O_R	0	-4.83057300	2.77703500	-0.58698600	L
O-O_R	0	-2.63988200	-4.88728500	0.28527200	L
O-O_R	0	1.77778500	-4.25381800	-1.55567400	L
O-O_R	0	3.17328000	4.98168500	0.62986500	L
O-O_R	0	-0.77136000	3.93240900	-2.42910700	L
O-O_R	0	-3.53993000	-1.49241500	-2.66082600	L
O-O_R	0	5.22186300	-3.08739100	1.31545400	L
Rh-	0	0.34966200	-0.11378400	-0.89362100	H
Rh-	0	0.75379600	-0.22040500	-3.28040700	H
N-N_3	0	0.03215900	-0.09863400	1.10899400	H
S-S_3+6	0	-0.37927000	-1.45083800	2.01071800	H
O-O_2	0	-0.37680800	-1.11719600	3.44709100	H
O-O_R	0	-2.00775200	-1.70205300	1.53484700	H
O-O_2	0	0.30920600	-2.64731900	1.51044800	H
C-C_R	0	-2.99895700	-0.99673200	2.21963500	H
C-C_R	0	-3.58303000	0.12396900	1.61544300	H
C-C_R	0	-3.46920100	-1.46535600	3.45662500	H
C-C_R	0	-4.64665300	0.77294900	2.26014000	H
H-H_	0	-3.20764700	0.46646700	0.64850000	H
C-C_R	0	-4.53433000	-0.80637000	4.07723500	H
H-H_	0	-3.00526600	-2.34273200	3.91032300	H
C-C_R	0	-5.15026400	0.32683800	3.49912200	H
H-H_	0	-5.09265400	1.64306200	1.77720300	H
H-H_	0	-4.89166500	-1.19077800	5.03660100	H
C-C_3	0	-6.31548500	1.02755400	4.22669800	H

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C-C_3     0    -5.81775500     1.54571700     5.60230800  H
H-H_      0    -5.45054500     0.72613500     6.24056300  H
H-H_      0    -6.63787800     2.05004200     6.14191000  H
H-H_      0    -4.99446100     2.26845800     5.47762000  H
C-C_3     0    -6.86833500     2.22885100     3.42944600  H
H-H_      0    -7.70594600     2.68649100     3.98132200  H
H-H_      0    -7.24971700     1.92585600     2.43991200  H
H-H_      0    -6.10464000     3.01030600     3.28241700  H
C-C_3     0    -7.47539200     0.02134500     4.44683400  H
H-H_      0    -8.29711300     0.50272800     5.00442400  H
H-H_      0    -7.15317800    -0.86126200     5.02191100  H
H-H_      0    -7.87975100    -0.33271400     3.48483000  H
C-C_R     0     2.70358900     1.43424800     3.35211700  H
C-C_R     0     3.12926900     1.86529500     4.62423300  H
C-C_R     0     3.95102100     1.05848900     5.42416300  H
C-C_R     0     4.35948200    -0.20086300     4.96201600  H
C-C_R     0     3.94391100    -0.64104300     3.69666200  H
C-C_R     0     3.12939400     0.17078100     2.89501500  H
H-H_      0     2.82358000     2.85294100     4.98561300  H
H-H_      0     4.27632400     1.41728400     6.40514500  H
H-H_      0     5.00160900    -0.83380300     5.58113700  H
H-H_      0     4.25728300    -1.62127200     3.33087800  H
H-H_      0     2.82811500    -0.17727800     1.90265900  H
C-C_3     0     1.82965300     2.32154000     2.48832600  H
H-H_      0     2.01241700     3.38181300     2.76447900  H
H-H_      0     2.11802100     2.22483100     1.42937700  H
C-C_3     0     0.30896200     2.10853500     2.57054100  H
H-H_      0     0.15465700     0.97212400     1.91215100  H
C-C_3     0    -0.47226700     3.07461900     1.69313700  H
H-H_      0    -0.43264300     4.08912100     2.13685100  H
H-H_      0    -1.53302400     2.78575800     1.62651800  H
H-H_      0    -0.05518300     3.12979200     0.67686000  H
C-C_3     0    -0.27882900     1.91500500     3.95330900  H
H-H_      0    -0.19549500     2.86603400     4.51917700  H
H-H_      0     0.24439500     1.13607000     4.52338600  H
H-H_      0    -1.34699500     1.65459100     3.90193400  H
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³INT4
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C-C_R     0     1.21467100    -5.54027000     1.38848700  L
C-C_R     0    -4.26788100     4.68284000     1.23804200  L
C-C_R     0     6.14137300     3.58206700     1.71730700  L
C-C_R     0    -5.86953800    -1.21286000    -1.01707500  L
C-C_3     0     4.82488800    -2.92726900    -2.51839200  L
C-C_3     0     2.92338900     4.15295500    -3.26331600  L
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C-C_3     0    -3.37608300    2.40383200    -4.26984300  L
C-C_3     0    -1.74209200   -4.59859300    -3.56746300  L
C-C_3     0     1.61961500    4.41644700    -4.05276700  L
C-C_3     0     6.07026500   -3.64347500    -1.94220400  L
C-C_3     0    -2.51545500   -5.90941000    -3.28766500  L
C-C_3     0    -2.30119100    3.36751100    -4.82311500  L
C-C_3     0     4.03078900   -3.95560400    -3.35712500  L
C-C_3     0    -2.45696600   -3.86582300    -4.72659300  L
C-C_3     0     3.91735900    3.38413600    -4.16625000  L
C-C_3     0    -4.73408600    3.14735500    -4.28221900  L
C-C_3     0     3.55128600    5.52947000    -2.93852400  L
C-C_3     0    -0.31492700   -4.99310300    -4.01716600  L
C-C_3     0    -3.51716400    1.18688900    -5.21645400  L
C-C_3     0     5.33703600   -1.79906600    -3.44540400  L
C-C_R     0    -1.76672900    1.13838800    -2.57935900  H
C-C_R     0    -0.85154400   -2.47025600    -2.25405300  H
C-C_R     0     2.73202900   -1.52081100    -1.67199000  H
C-C_R     0     1.81552600    2.09925900    -2.00617200  H
C-C_3     0    -3.05865700    1.94044600    -2.79839300  L
C-C_3     0    -1.68986500   -3.75140100    -2.24094600  L
C-C_3     0     3.98508200   -2.33317000    -1.32494200  L
C-C_3     0     2.61165500    3.40514900    -1.91090000  L
C-C_R     0    -2.01390400    3.87174300    -1.38421300  L
C-C_R     0    -3.59702900   -3.90859600    -0.50089400  L
C-C_R     0     4.05655600   -3.41176300     1.02092400  L
C-C_R     0     4.77469200    2.10600500    -1.22617700  L
C-C_R     0    -2.38704900    4.52727900    -0.13566400  L
C-C_R     0    -4.73741800   -3.06801300    -0.14111900  L
C-C_R     0     3.14400700   -4.25450300     1.78923600  L
C-C_R     0     5.72359400    2.18543400    -0.11995100  L
C-C_R     0    -3.65343200    4.21557700     0.13685800  L
C-C_R     0    -4.90695900   -2.15137800    -1.09429400  L
C-C_R     0     2.22364100   -4.75187200     0.96007900  L
C-C_R     0     5.42520200    3.25460000     0.62075600  L
C-C_R     0    -4.15086000    3.33285400    -0.91488400  L
C-C_R     0    -3.88907600   -2.35595500    -2.12014800  L
C-C_R     0     2.49658100   -4.25359800    -0.38455400  L
C-C_R     0     4.26041900    3.91079200     0.02988100  L
C-C_R     0    -1.65322000    5.31008600     0.68305300  L
C-C_R     0    -5.52055400   -3.10821500     0.95382500  L
C-C_R     0     3.12557200   -4.51376400     3.10897600  L
C-C_R     0     6.75050300    1.37689900     0.19708000  L
C-C_R     0    -2.22567100    5.79778500     1.81413300  L
C-C_R     0    -6.55031100   -2.15019900     1.07737400  L
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C-C_R    0     2.09649700    -5.33713900     3.60458200  L
C-C_R    0     7.51539300     1.70259700     1.33901500  L
C-C_R    0    -3.51981000     5.50367700     2.11065300  L
C-C_R    0    -6.72176900    -1.21824900     0.10794100  L
C-C_R    0     1.13316600    -5.84711300     2.70495600  L
C-C_R    0     7.19353600     2.80028600     2.07453300  L
F-F_     0    -0.36361500     5.60720200     0.38289800  L
F-F_     0    -5.32397500    -4.03918900     1.92051600  L
F-F_     0     4.06841000    -4.00472500     3.93942800  L
F-F_     0     7.04529400     0.28512700    -0.55199500  L
F-F_     0    -1.50326600     6.58455500     2.65061800  L
F-F_     0    -7.35788200    -2.15903100     2.16692900  L
F-F_     0     2.02769000    -5.63101500     4.92653400  L
F-F_     0     8.56090300     0.91877500     1.70232100  L
F-F_     0    -4.09226400     5.99584300     3.23747600  L
F-F_     0    -7.70345700    -0.28933000     0.21868300  L
F-F_     0     0.12760200    -6.63477600     3.16106300  L
F-F_     0     7.92362300     3.11320700     3.17428900  L
F-F_     0    -5.56750100     4.39430500     1.49548300  L
F-F_     0    -6.02346700    -0.28560700    -1.99487000  L
F-F_     0     0.28822100    -6.01286300     0.51668300  L
F-F_     0     5.82278900     4.67848800     2.44992300  L
H-H_     0    -2.53336300    -6.55965100    -4.18929400  L
H-H_     0    -2.57260300     3.70151800    -5.84791200  L
H-H_     0     1.82715300     5.01783300    -4.96431500  L
H-H_     0     6.71989800    -4.02834300    -2.75824600  L
H-H_     0    -3.56876900    -5.69973000    -3.00301000  L
H-H_     0     5.77946100    -4.50952800    -1.30994500  L
H-H_     0    -1.30541200     2.88842700    -4.88755400  L
H-H_     0     0.89367300     4.98242900    -3.43168200  L
H-H_     0    -2.03923000    -6.47964800    -2.46073300  L
H-H_     0     6.67264700    -2.94599300    -1.32043900  L
H-H_     0    -2.21428900     4.27315200    -4.18746300  L
H-H_     0     1.14012900     3.47481000    -4.38555200  L
H-H_     0    -2.43185000    -4.48683800    -5.64816300  L
H-H_     0     4.64423500    -4.31087500    -4.21325900  L
H-H_     0     4.09096900     3.94405100    -5.11070900  L
H-H_     0    -5.02503000     3.42712500    -5.31811600  L
H-H_     0    -1.97941100    -2.89752800    -4.97026500  L
H-H_     0     3.09889400    -3.52689800    -3.77384000  L
H-H_     0     3.54453600     2.38089100    -4.44685500  L
H-H_     0    -4.68591500     4.08497000    -3.68848800  L
H-H_     0    -3.52473000    -3.68469600    -4.48641000  L
H-H_     0     3.76981500    -4.84790500    -2.75202600  L
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H-H_      0     4.90305600     3.26998900    -3.67033300  L
H-H_      0    -5.53720500     2.50539200    -3.85956800  L
H-H_      0     6.01130400    -2.21084500    -4.22744500  L
H-H_      0    -0.35460600    -5.67354900    -4.89530300  L
H-H_      0     3.73157000     6.11251000    -3.86784900  L
H-H_      0    -3.86493700     1.51121200    -6.22124100  L
H-H_      0     5.91325100    -1.04765400    -2.86525100  L
H-H_      0     0.22012500    -5.52375600    -3.20117800  L
H-H_      0    -4.25965400     0.46400600    -4.81583700  L
H-H_      0     4.52778800     5.41197300    -2.42228400  L
H-H_      0     4.51237000    -1.28105900    -3.97221100  L
H-H_      0     2.87978700     6.12573000    -2.28341400  L
H-H_      0    -2.55829900     0.65577000    -5.37001700  L
H-H_      0     0.28654600    -4.11188800    -4.31572700  L
H-H_      0    -3.87206200     1.23848800    -2.51214200  L
H-H_      0    -1.18752200    -4.40587400    -1.49325000  L
H-H_      0     4.65671200    -1.60473400    -0.81719200  L
H-H_      0     1.95844600     4.09590100    -1.33060900  L
N-N_R     0    -3.11112700     3.08517700    -1.86943900  L
N-N_R     0    -3.04178000    -3.44889000    -1.73900000  L
N-N_R     0     3.63444600    -3.37991400    -0.34769300  L
N-N_R     0     3.83592200     3.18293400    -1.12606800  L
O-O_R     0    -1.54665800     0.78226600    -1.36393800  H
O-O_R     0    -0.65317600    -1.95705300    -1.09652100  H
O-O_R     0     2.12598500    -1.02262500    -0.65554600  H
O-O_R     0     1.25241400     1.71656200    -0.91744200  H
O-O_R     0    -1.00814400     0.87732400    -3.56840700  H
O-O_R     0    -0.43344700    -1.98860400    -3.35900100  H
O-O_R     0     2.36512400    -1.39324700    -2.88650200  H
O-O_R     0     1.77585200     1.46971500    -3.11424600  H
O-O_R     0    -0.83981300     3.79324900    -1.82973200  L
O-O_R     0    -2.96132600    -4.62360400     0.31929500  L
O-O_R     0     4.81677900    -2.54619500     1.53142800  L
O-O_R     0     4.60998000     1.09714200    -1.96052600  L
O-O_R     0    -5.20382800     2.64548400    -0.83481200  L
O-O_R     0    -3.56579200    -1.49054700    -2.97573800  L
O-O_R     0     1.64532800    -4.24294400    -1.31197700  L
O-O_R     0     3.57652200     4.81252500     0.58303500  L
Rh-       0     0.27562200    -0.12154900    -0.89394200  H
Rh-       0     0.68313200    -0.26184200    -3.27007400  H
N-N_3     0    -0.04194700    -0.16956200     1.03838200  H
S-S_3+6   0    -0.65779900    -1.32432800     2.02895000  H
O-O_2     0    -0.08618600    -2.65724900     1.77294000  H
O-O_R     0    -2.27865600    -1.44595900     1.44396100  H
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O-O_2	0	-0.71542400	-0.77616300	3.40021500 H
C-C_R	0	-3.27433400	-0.78677300	2.15333400 H
C-C_R	0	-3.73644400	-1.29668000	3.37628800 H
C-C_R	0	-3.87945000	0.34123400	1.57626700 H
C-C_R	0	-4.81512500	-0.67529700	4.01612500 H
H-H_	0	-3.26330500	-2.18184200	3.80495600 H
C-C_R	0	-4.94844300	0.94902600	2.23721800 H
H-H_	0	-3.49969100	0.71825900	0.62461600 H
C-C_R	0	-5.44515400	0.46203800	3.46956100 H
H-H_	0	-5.16534500	-1.09676900	4.95983000 H
H-H_	0	-5.41116200	1.82474000	1.77935300 H
C-C_3	0	-6.60001500	1.19475900	4.17936300 H
C-C_3	0	-6.07942600	2.57337200	4.66961300 H
H-H_	0	-5.70784100	3.18827600	3.83517700 H
H-H_	0	-6.88751000	3.13343700	5.17113900 H
H-H_	0	-5.25120300	2.44903100	5.38635900 H
C-C_3	0	-7.12886700	0.41116300	5.40096500 H
H-H_	0	-7.97492900	0.95536500	5.85212800 H
H-H_	0	-7.48948000	-0.59205500	5.11801400 H
H-H_	0	-6.36074200	0.29546000	6.18328100 H
C-C_3	0	-7.78418900	1.40893700	3.20122300 H
H-H_	0	-8.59915000	1.95230000	3.70889600 H
H-H_	0	-7.49671300	1.99885500	2.31659600 H
H-H_	0	-8.18643200	0.44508200	2.84928800 H
C-C_R	0	3.22753800	0.45861500	3.59003400 H
C-C_R	0	4.61208300	0.33738900	3.35537700 H
C-C_R	0	5.41733500	-0.49808400	4.13997100 H
C-C_R	0	4.84313900	-1.24441300	5.18036700 H
C-C_R	0	3.46049000	-1.15449200	5.41520500 H
C-C_R	0	2.66170200	-0.31465200	4.62959300 H
H-H_	0	5.05393200	0.91000000	2.53822100 H
H-H_	0	6.49027300	-0.56796400	3.93684300 H
H-H_	0	5.46406700	-1.90285800	5.79479200 H
H-H_	0	3.00167500	-1.75055800	6.20965300 H
H-H_	0	1.58350900	-0.27047600	4.80570700 H
C-C_3	0	2.37714200	1.38452100	2.75100900 H
H-H_	0	1.55680500	0.80188200	2.28005200 H
C-C_3	0	1.72851900	2.56799700	3.52089800 H
C-C_3	0	2.79252900	3.52536100	4.08636200 H
H-H_	0	3.35974100	4.00483500	3.26980000 H
H-H_	0	2.32554300	4.32822800	4.68183900 H
H-H_	0	3.51280900	2.99615700	4.73089100 H
C-C_3	0	0.73105500	3.31490300	2.61857700 H
H-H_	0	1.23760900	3.72969300	1.72985400 H

H-H_	0	-0.06740200	2.64461100	2.26157300	H
H-H_	0	0.25938100	4.15385700	3.15844800	H
H-H_	0	1.16373700	2.14156000	4.37124900	H
H-H_	0	2.97942800	1.78715400	1.91622400	H

³TS4

C-C_R	0	2.48815700	-5.16466200	1.47719500	L
C-C_R	0	-5.10592300	4.03760200	1.04391400	L
C-C_R	0	4.81785300	4.15795400	2.20163900	L
C-C_R	0	-5.43446300	-2.23147800	-0.95105100	L
C-C_3	0	5.35210700	-1.96490300	-2.64020200	L
C-C_3	0	2.20986500	4.60923600	-3.27989100	L
C-C_3	0	-3.71860700	1.65343900	-4.26397900	L
C-C_3	0	-0.78884400	-4.87520500	-3.50638800	L
C-C_3	0	0.91514000	4.63155900	-4.12683800	L
C-C_3	0	6.73297300	-2.41817700	-2.10759700	L
C-C_3	0	-1.29838200	-6.30525100	-3.20677600	L
C-C_3	0	-2.85788600	2.79376500	-4.85634800	L
C-C_3	0	4.74309900	-3.13873000	-3.44174600	L
C-C_3	0	-1.63439400	-4.30559800	-4.66909100	L
C-C_3	0	3.36348800	4.02619900	-4.12923800	L
C-C_3	0	-5.19504400	2.11953100	-4.27243700	L
C-C_3	0	2.56638800	6.07676200	-2.94272100	L
C-C_3	0	0.68557900	-4.99663800	-3.96045600	L
C-C_3	0	-3.63195500	0.41072100	-5.18329900	L
C-C_3	0	5.60107600	-0.76784500	-3.58922900	L
C-C_R	0	-1.87877800	0.76312700	-2.56818300	H
C-C_R	0	-0.30649200	-2.60318300	-2.21957800	H
C-C_R	0	3.05473500	-0.98649200	-1.73192700	H
C-C_R	0	1.45313900	2.38989600	-2.03414400	H
C-C_3	0	-3.30302800	1.29164700	-2.78699100	L
C-C_3	0	-0.89261700	-4.01772400	-2.18983200	L
C-C_3	0	4.45258300	-1.53561000	-1.42098700	L
C-C_3	0	1.97748700	3.82584700	-1.93347100	L
C-C_R	0	-2.69418100	3.49721000	-1.51457100	L
C-C_R	0	-2.72232200	-4.48129700	-0.42343400	L
C-C_R	0	4.85392200	-2.55776800	0.90340500	L
C-C_R	0	4.29566600	2.95740200	-1.11451900	L
C-C_R	0	-3.23338400	4.18678000	-0.34462600	L
C-C_R	0	-3.98366600	-3.83966100	-0.05747100	L
C-C_R	0	4.19080700	-3.56085700	1.73143700	L
C-C_R	0	5.00790400	3.02597900	0.15744600	L
C-C_R	0	-4.38513600	3.60589500	-0.00581500	L
C-C_R	0	-4.32639800	-2.99285400	-1.02809000	L

C-C_R	0	3.29116800	-4.20020500	0.98015200	L
C-C_R	0	4.39997600	3.91716600	0.94065800	L
C-C_R	0	-4.63883100	2.50975300	-0.93455000	L
C-C_R	0	-3.30768700	-3.04742300	-2.07173000	L
C-C_R	0	3.35896600	-3.65977100	-0.37465700	L
C-C_R	0	3.26838600	4.47817600	0.20706800	L
C-C_R	0	-2.73058300	5.22862600	0.35069200	L
C-C_R	0	-4.72710300	-3.98247300	1.05652000	L
C-C_R	0	4.36076000	-3.84578900	3.03479500	L
C-C_R	0	6.07483800	2.32786000	0.58646500	L
C-C_R	0	-3.41809600	5.69646000	1.42476400	L
C-C_R	0	-5.90222200	-3.20970800	1.18233800	L
C-C_R	0	3.54838400	-4.84739400	3.60052900	L
C-C_R	0	6.53731700	2.57340400	1.89793300	L
C-C_R	0	-4.59688200	5.12432300	1.78842000	L
C-C_R	0	-6.24963200	-2.34863300	0.19483000	L
C-C_R	0	2.59902700	-5.50340000	2.78385300	L
C-C_R	0	5.89512200	3.48223600	2.67896600	L
F-F_	0	-1.55457400	5.79967400	-0.01338600	L
F-F_	0	-4.35566200	-4.83947900	2.04011000	L
F-F_	0	5.27655500	-3.18607200	3.78669400	L
F-F_	0	6.68353000	1.41163900	-0.20728300	L
F-F_	0	-2.92538100	6.73950400	2.13874000	L
F-F_	0	-6.67472900	-3.32456700	2.29119900	L
F-F_	0	3.67090100	-5.17292100	4.91114300	L
F-F_	0	7.60812300	1.89398100	2.37884200	L
F-F_	0	-5.28333900	5.59416600	2.85969400	L
F-F_	0	-7.37415700	-1.59903800	0.30539300	L
F-F_	0	1.80209300	-6.46723600	3.30879000	L
F-F_	0	6.32796800	3.70993900	3.94434300	L
F-F_	0	-6.28942000	3.46179500	1.37083100	L
F-F_	0	-5.76810700	-1.37698200	-1.94990300	L
F-F_	0	1.57947300	-5.78532700	0.68294300	L
F-F_	0	4.17302300	5.05947600	2.98384500	L
H-H_	0	-1.19917600	-6.95738400	-4.10173600	L
H-H_	0	-3.18423000	3.02409100	-5.89361000	L
H-H_	0	1.04754500	5.26727700	-5.02905700	L
H-H_	0	7.41646300	-2.67683600	-2.94543700	L
H-H_	0	-2.37031300	-6.29495100	-2.91460300	L
H-H_	0	6.64002900	-3.31867600	-1.46357800	L
H-H_	0	-1.78400600	2.52894500	-4.90141900	L
H-H_	0	0.06968400	5.04826700	-3.53940500	L
H-H_	0	-0.71723200	-6.76580900	-2.37857600	L
H-H_	0	7.20876100	-1.60991500	-1.51080100	L

H-H_	0	-2.96459300	3.72395700	-4.26111800	L
H-H_	0	0.63238000	3.62015100	-4.47993000	L
H-H_	0	-1.49489800	-4.92127100	-5.58401000	L
H-H_	0	5.39592900	-3.39686500	-4.30353000	L
H-H_	0	3.46687800	4.59409000	-5.07919800	L
H-H_	0	-5.54502600	2.31327200	-5.30974200	L
H-H_	0	-1.35061500	-3.26704000	-4.92594000	L
H-H_	0	3.74213600	-2.89482900	-3.84740500	L
H-H_	0	3.19403700	2.96622900	-4.39866400	L
H-H_	0	-5.32352200	3.06248600	-3.69952200	L
H-H_	0	-2.71621900	-4.32829600	-4.42444200	L
H-H_	0	4.65493400	-4.04757400	-2.81139500	L
H-H_	0	4.33272800	4.10649400	-3.59551100	L
H-H_	0	-5.85434400	1.34458700	-3.82462500	L
H-H_	0	6.33299700	-1.04101800	-4.38007800	L
H-H_	0	0.77337600	-5.68686500	-4.82739600	L
H-H_	0	2.69518200	6.67684100	-3.86975100	L
H-H_	0	-4.03824500	0.64123300	-6.19203700	L
H-H_	0	6.01474500	0.09685200	-3.02771400	L
H-H_	0	1.31630000	-5.40025200	-3.13997500	L
H-H_	0	-4.22507200	-0.42893800	-4.76233600	L
H-H_	0	3.51568600	6.13569300	-2.36839400	L
H-H_	0	4.67865200	-0.44164500	-4.10730900	L
H-H_	0	1.76348600	6.54873800	-2.33581700	L
H-H_	0	-2.59108800	0.06521100	-5.33251800	L
H-H_	0	1.10521200	-4.02147500	-4.27757100	L
H-H_	0	-3.96285100	0.45277300	-2.47708100	L
H-H_	0	-0.27480700	-4.55914000	-1.43799600	L
H-H_	0	4.98231500	-0.68696500	-0.93188400	L
H-H_	0	1.16872000	4.38126900	-1.40647500	L
N-N_R	0	-3.56715200	2.41947300	-1.87759500	L
N-N_R	0	-2.27586100	-3.96572100	-1.68379200	L
N-N_R	0	4.34804000	-2.62252600	-0.43247700	L
N-N_R	0	3.17622800	3.85450200	-1.07856900	L
O-O_R	0	-1.57834500	0.47225100	-1.35213400	H
O-O_R	0	-0.19583500	-2.05728800	-1.06559300	H
O-O_R	0	2.38392000	-0.61338900	-0.70246000	H
O-O_R	0	0.99243300	1.90789300	-0.93497500	H
O-O_R	0	-1.09517700	0.63911300	-3.56346400	H
O-O_R	0	0.00126800	-2.06132500	-3.33338000	H
O-O_R	0	2.64358400	-0.93659200	-2.93668300	H
O-O_R	0	1.52254100	1.77309400	-3.14564800	H
O-O_R	0	-1.50841900	3.60559600	-1.92221500	L
O-O_R	0	-1.95827600	-5.05308500	0.39960900	L

O-O_R	0	5.92285100	-1.96640600	1.21012300	L
O-O_R	0	4.39017300	1.99597500	-1.92229800	L
O-O_R	0	-5.53998800	1.63877300	-0.80580000	L
O-O_R	0	-3.15296900	-2.15987600	-2.95116700	L
O-O_R	0	2.47649900	-3.83491400	-1.25521100	L
O-O_R	0	2.32658200	5.12744400	0.73474300	L
Rh-	0	0.38171500	-0.08554000	-0.90037800	H
Rh-	0	0.77801600	-0.14932900	-3.28661900	H
N-N_3	0	0.17144100	-0.10797600	1.09661000	H
S-S_3+6	0	-0.22082300	-1.40489900	2.06721300	H
O-O_2	0	0.59465700	-2.59064100	1.76105000	H
O-O_R	0	-1.77876000	-1.82256600	1.49203900	H
O-O_2	0	-0.36167200	-0.92291900	3.45736200	H
C-C_R	0	-2.87672300	-1.29864900	2.17720300	H
C-C_R	0	-3.29206600	-1.87289400	3.38549200	H
C-C_R	0	-3.60899200	-0.25399000	1.59488100	H
C-C_R	0	-4.44964100	-1.39505900	4.01376000	H
H-H_	0	-2.71609000	-2.69292200	3.81804900	H
C-C_R	0	-4.75580800	0.21205700	2.24446400	H
H-H_	0	-3.26997000	0.17165300	0.64816900	H
C-C_R	0	-5.20605800	-0.34024100	3.46490300	H
H-H_	0	-4.75780000	-1.86359200	4.95018000	H
H-H_	0	-5.31463900	1.03163100	1.78920900	H
C-C_3	0	-6.45845500	0.23793900	4.15402700	H
C-C_3	0	-6.15381100	1.69369300	4.59900400	H
H-H_	0	-5.87084400	2.33024700	3.74597500	H
H-H_	0	-7.03973300	2.14432900	5.07910200	H
H-H_	0	-5.32203800	1.71731200	5.32230000	H
C-C_3	0	-6.87001000	-0.57491700	5.40093900	H
H-H_	0	-7.78187500	-0.14041700	5.84321000	H
H-H_	0	-7.08973300	-1.62602300	5.14915200	H
H-H_	0	-6.08916800	-0.56167900	6.17932300	H
C-C_3	0	-7.65592800	0.23895000	3.16869300	H
H-H_	0	-8.54456800	0.68151800	3.65053400	H
H-H_	0	-7.44735500	0.82274800	2.25814300	H
H-H_	0	-7.91256100	-0.78749000	2.85990500	H
C-C_R	0	2.43393300	1.07266400	3.38229700	H
C-C_R	0	3.68051600	0.69359200	2.81734000	H
C-C_R	0	4.66512300	0.07379000	3.58822600	H
C-C_R	0	4.42252600	-0.21501200	4.94206700	H
C-C_R	0	3.17952300	0.11234700	5.51018800	H
C-C_R	0	2.19608800	0.74085600	4.74251800	H
H-H_	0	3.85632700	0.89084800	1.75699200	H
H-H_	0	5.62882700	-0.18205700	3.14125900	H

H-H_	0	5.19243700	-0.70289700	5.54618200	H
H-H_	0	2.97715500	-0.12727500	6.55781000	H
H-H_	0	1.23142800	0.97697300	5.19479300	H
C-C_3	0	1.43842300	1.76272200	2.54048900	H
H-H_	0	0.82390200	0.83673200	1.89159600	H
C-C_3	0	0.33410100	2.61415100	3.17271300	H
C-C_3	0	0.93766700	3.83259800	3.91301400	H
H-H_	0	1.45331900	4.50479400	3.20739600	H
H-H_	0	0.13905100	4.41335400	4.40517700	H
H-H_	0	1.66596400	3.52574400	4.67988300	H
C-C_3	0	-0.68980400	3.07882700	2.12194600	H
H-H_	0	-0.20425600	3.68268400	1.33661600	H
H-H_	0	-1.18297200	2.22599400	1.63145900	H
H-H_	0	-1.46918800	3.69762900	2.59632600	H
H-H_	0	-0.20299700	1.99274800	3.91151400	H
H-H_	0	1.90076900	2.25234400	1.66651300	H

³INT5

C-C_R	0	-5.76942600	-1.46916600	-0.47223400	L
C-C_R	0	5.46598300	3.64475400	2.13643600	L
C-C_R	0	3.06605300	-4.67125800	3.07319800	L
C-C_R	0	-1.18537600	5.92869700	-0.56500400	L
C-C_3	0	-1.82540900	-4.76535200	-3.36956800	L
C-C_3	0	4.88755800	-3.08405800	-2.54998000	L
C-C_3	0	3.26960400	3.75304700	-3.45646600	L
C-C_3	0	-3.46490200	1.99300600	-4.28744000	L
C-C_3	0	5.36786800	-1.92319500	-3.45433100	L
C-C_3	0	-2.60376800	-6.06175700	-3.03962600	L
C-C_3	0	-4.81789400	2.74424200	-4.26519000	L
C-C_3	0	4.28934800	2.80278100	-4.12765600	L
C-C_3	0	-2.61185300	-4.00587000	-4.46356700	L
C-C_3	0	-2.47019600	2.83572900	-5.12032600	L
C-C_3	0	4.11894000	-4.11588100	-3.40729400	L
C-C_3	0	3.97694900	5.10853200	-3.21345400	L
C-C_3	0	6.15085400	-3.77907400	-1.98751800	L
C-C_3	0	-3.70703000	0.63926800	-4.99674300	L
C-C_3	0	2.09735900	4.02104400	-4.43035900	L
C-C_3	0	-0.44761800	-5.18986600	-3.93259800	L
C-C_R	0	1.91509500	1.90486500	-2.11066700	H
C-C_R	0	-1.70059400	0.95752700	-2.59147900	H
C-C_R	0	-0.82124700	-2.64414600	-2.12424800	H
C-C_R	0	2.77626500	-1.72597300	-1.67714800	H
C-C_3	0	2.74166500	3.19951800	-2.07819500	L
C-C_3	0	-2.98505100	1.76696100	-2.80323900	L

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C-C_3    0    -1.65132100    -3.92940500    -2.04566200  L
C-C_3    0     4.03456500    -2.53542800    -1.34577500  L
C-C_R    0     4.64897900     1.90644800    -0.85098700  L
C-C_R    0    -3.70823100     3.45018600    -0.98224000  L
C-C_R    0    -3.40805100    -4.12874000    -0.15570700  L
C-C_R    0     2.54616000    -4.47159000    -0.44723500  L
C-C_R    0     5.32331300     2.05342200     0.43399200  L
C-C_R    0    -3.11933100     4.62337300    -0.34146800  L
C-C_R    0    -4.53704600    -3.31982500     0.29795600  L
C-C_R    0     2.23362800    -4.94019100     0.89869000  L
C-C_R    0     5.00195900     3.24466800     0.93917500  L
C-C_R    0    -1.97132100     4.90878400    -0.95803300  L
C-C_R    0    -4.79356800    -2.38946700    -0.62504100  L
C-C_R    0     3.13662700    -4.44524400     1.74397100  L
C-C_R    0     4.09652200     3.91783700     0.00956800  L
C-C_R    0    -1.78071200     3.95647700    -2.04733900  L
C-C_R    0    -3.84336300    -2.55332500    -1.72147300  L
C-C_R    0     4.08391300    -3.63588300     0.98291900  L
C-C_R    0     6.11977200     1.18881600     1.09720600  L
C-C_R    0    -3.56184700     5.34363800     0.70603100  L
C-C_R    0    -5.23884300    -3.39721200     1.44296100  L
C-C_R    0     1.20584300    -5.69237100     1.33188200  L
C-C_R    0     6.61681200     1.54914600     2.30861300  L
C-C_R    0    -2.77538500     6.42736900     1.15398600  L
C-C_R    0    -6.27641600    -2.46676400     1.64395900  L
C-C_R    0     1.11698100    -5.94941100     2.71748800  L
C-C_R    0     6.31102500     2.76100900     2.84355900  L
C-C_R    0    -1.60676000     6.71483400     0.52927300  L
C-C_R    0    -6.52637600    -1.49309300     0.65041600  L
C-C_R    0     2.05074600    -5.43160600     3.55907000  L
F-F_     0     6.41723400    -0.02409200     0.56679000  L
F-F_     0    -4.72788200     5.03405400     1.32478900  L
F-F_     0    -4.95704300    -4.33720600     2.37924800  L
F-F_     0     0.27844100    -6.18151400     0.47136300  L
F-F_     0     7.41622700     0.69215200     2.99190800  L
F-F_     0    -3.18635200     7.17327500     2.20956700  L
F-F_     0    -7.01756300    -2.49975500     2.77864900  L
F-F_     0     0.09875000    -6.70125100     3.20489800  L
F-F_     0     6.80279100     3.11633600     4.05656100  L
F-F_     0    -0.84128500     7.75001900     0.95578800  L
F-F_     0    -7.51337900    -0.57989600     0.82628700  L
F-F_     0     1.96387000    -5.66927600     4.89194500  L
F-F_     0     5.12716700     4.85087300     2.65605100  L
F-F_     0    -0.01756600     6.19730300    -1.20116700  L
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F-F_     0    -5.98978800   -0.52978900   -1.42641700 L
F-F_     0     3.99049300   -4.14368000    3.91462700 L
H-H_     0    -5.21849700    2.87098900   -5.29452300 L
H-H_     0     4.64485000    3.23535600   -5.08789000 L
H-H_     0     6.06824200   -2.29695200   -4.23249100 L
H-H_     0    -2.69985500   -6.70701600   -3.93988800 L
H-H_     0    -4.70744400    3.75718600   -3.82241300 L
H-H_     0    -3.62994100   -5.83330100   -2.68025100 L
H-H_     0     3.85452400    1.81133700   -4.35769800 L
H-H_     0     5.90358600   -1.15573400   -2.85584700 L
H-H_     0    -5.57014000    2.18349400   -3.66898400 L
H-H_     0    -2.08109200   -6.64509800   -2.25073900 L
H-H_     0     5.18010800    2.65498800   -3.48271200 L
H-H_     0     4.53012300   -1.43141600   -3.98604500 L
H-H_     0    -2.83551400    2.94126300   -6.16480900 L
H-H_     0    -2.66961300   -4.61676500   -5.39039200 L
H-H_     0     4.74208700   -4.44253100   -4.26781600 L
H-H_     0     4.30257700    5.56447400   -4.17375500 L
H-H_     0    -1.46496800    2.37528100   -5.16961500 L
H-H_     0    -2.13570100   -3.04355400   -4.73282500 L
H-H_     0     3.17838900   -3.70114300   -3.81883200 L
H-H_     0     4.88205900    4.98248200   -2.58192500 L
H-H_     0    -2.36935300    3.85977900   -4.70622400 L
H-H_     0    -3.65415500   -3.80637700   -4.14074700 L
H-H_     0     3.87658900   -5.02314200   -2.81650700 L
H-H_     0     3.29397200    5.82412600   -2.70629700 L
H-H_     0    -0.57283800   -5.86594200   -4.80608900 L
H-H_     0    -4.12777100    0.79959100   -6.01312100 L
H-H_     0     6.80657500   -4.13734800   -2.81075200 L
H-H_     0     2.46767100    4.48817200   -5.36864600 L
H-H_     0     0.13824900   -5.73623800   -3.16322600 L
H-H_     0    -4.43270400    0.02307600   -4.42483100 L
H-H_     0     1.36276100    4.71749900   -3.97354400 L
H-H_     0     5.88154600   -4.65997700   -1.36630500 L
H-H_     0     0.14921900   -4.32335000   -4.27827500 L
H-H_     0     6.73912700   -3.07665500   -1.35791300 L
H-H_     0     1.56841300    3.09244800   -4.72012300 L
H-H_     0    -2.77307600    0.05736800   -5.12151300 L
H-H_     0     2.04030200    3.97081400   -1.68732100 L
H-H_     0    -3.78311000    1.16386700   -2.31369500 L
H-H_     0    -1.08321400   -4.58695400   -1.35070700 L
H-H_     0     4.69585200   -1.81301400   -0.81787200 L
N-N_R    0     3.84702200    3.06491900   -1.11348700 L
N-N_R    0    -2.88354200    3.04225100   -2.07647500 L
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N-N_R	0	-2.95300400	-3.63610100	-1.42085800	L
N-N_R	0	3.69362500	-3.60992200	-0.39584200	L
O-O_R	0	1.36926700	1.57283800	-0.99340600	H
O-O_R	0	-1.42651500	0.68673800	-1.36597600	H
O-O_R	0	-0.60367800	-2.08703800	-0.99128000	H
O-O_R	0	2.18124100	-1.21885900	-0.65937900	H
O-O_R	0	1.83163200	1.24561900	-3.19642400	H
O-O_R	0	-0.98802700	0.62262900	-3.59254000	H
O-O_R	0	-0.41996700	-2.20851000	-3.25530600	H
O-O_R	0	2.39085300	-1.60464000	-2.88667000	H
O-O_R	0	4.58572600	0.83945000	-1.51537600	L
O-O_R	0	-4.90129600	3.07388600	-0.83476700	L
O-O_R	0	-2.70099500	-4.84374200	0.60374800	L
O-O_R	0	1.71745800	-4.46560300	-1.39484900	L
O-O_R	0	3.37655600	4.90891000	0.30484600	L
O-O_R	0	-0.67685100	3.73436100	-2.60954600	L
O-O_R	0	-3.58078000	-1.65480200	-2.56280800	L
O-O_R	0	4.87647700	-2.80155400	1.49580400	L
Rh-	0	0.36493000	-0.27028500	-0.89619800	H
Rh-	0	0.71232100	-0.48624200	-3.27672100	H
N-N_3	0	0.06621000	-0.10476700	1.12022000	H
S-S_3+6	0	-0.41146800	-1.32893400	2.14726900	H
O-O_2	0	-0.40062700	-0.83440900	3.53717000	H
O-O_R	0	-2.04339300	-1.56717600	1.68305000	H
O-O_2	0	0.22124600	-2.59194000	1.76340000	H
C-C_R	0	-3.02183900	-0.77269100	2.28108500	H
C-C_R	0	-3.58978700	0.27724900	1.54809400	H
C-C_R	0	-3.50294500	-1.08850900	3.56182700	H
C-C_R	0	-4.65336600	1.00407200	2.10284800	H
H-H_	0	-3.20280200	0.50357400	0.55215200	H
C-C_R	0	-4.56528900	-0.35208200	4.09351700	H
H-H_	0	-3.05081300	-1.91137900	4.11793600	H
C-C_R	0	-5.17158900	0.70688700	3.38031400	H
H-H_	0	-5.08957900	1.81297200	1.51545200	H
H-H_	0	-4.93123500	-0.61776000	5.08911600	H
C-C_3	0	-6.34049400	1.49110000	4.01013600	H
C-C_3	0	-5.83783600	2.20363500	5.29402100	H
H-H_	0	-5.45401300	1.48538600	6.03627300	H
H-H_	0	-6.65938800	2.76948800	5.76633600	H
H-H_	0	-5.02499500	2.91098500	5.06004800	H
C-C_3	0	-6.91298200	2.56027500	3.05459100	H
H-H_	0	-7.75800300	3.07683100	3.53904300	H
H-H_	0	-7.28835000	2.11563400	2.11772200	H
H-H_	0	-6.16305900	3.32620900	2.79848900	H

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C-C_3     0    -7.48875900    0.51626500    4.38112700  H
H-H_      0    -8.31322400    1.06688300    4.86578700  H
H-H_      0    -7.15707000   -0.26898200    5.07871600  H
H-H_      0    -7.89294800    0.02040200    3.48393100  H
C-C_R     0     2.81423500    1.82095400    3.43723300  H
C-C_R     0     3.33717000    2.33887900    4.63817800  H
C-C_R     0     4.15231200    1.55597400    5.46813600  H
C-C_R     0     4.45804600    0.23554500    5.10701700  H
C-C_R     0     3.94508100   -0.29136600    3.91277400  H
C-C_R     0     3.13439900    0.49580200    3.08243700  H
H-H_      0     3.11288000    3.37357200    4.91866600  H
H-H_      0     4.55432800    1.98074900    6.39274300  H
H-H_      0     5.09592200   -0.37782400    5.74980400  H
H-H_      0     4.17698200   -1.31968300    3.62536800  H
H-H_      0     2.75416200    0.07870700    2.14527300  H
C-C_3     0     1.94466500    2.67971800    2.53600600  H
H-H_      0     2.27199400    3.74034600    2.63949800  H
H-H_      0     2.13519300    2.42328100    1.47774400  H
C-C_3     0     0.44696900    2.63750700    2.76603100  H
C-C_3     0    -0.38842900    3.40684700    1.78116500  H
H-H_      0    -0.38517000    4.49123600    2.03077200  H
H-H_      0    -1.44336700    3.08562700    1.79552200  H
H-H_      0    -0.00486500    3.31479100    0.75150700  H
C-C_3     0    -0.11101400    2.40825300    4.13750600  H
H-H_      0    -0.03962300    3.33446600    4.75162200  H
H-H_      0     0.43039300    1.61921700    4.67882900  H
H-H_      0    -1.17744800    2.13501300    4.09774500  H
H-H_      0     0.11764000    0.80308200    1.63709600  H
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³TS5
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C-C_R     0    -6.18347800   -0.91612900   -0.56288400  L
C-C_R     0     5.96185800    2.95052300    2.02149800  L
C-C_R     0     2.73640500   -5.28475000    2.74067900  L
C-C_R     0    -0.25712800    6.04276200    0.05744100  L
C-C_3     0    -2.42543100   -4.24692100   -3.62409400  L
C-C_3     0     4.31154800   -3.36674400   -2.81914300  L
C-C_3     0     3.58808500    3.60653100   -3.49587000  L
C-C_3     0    -3.38380600    2.84874300   -3.80402600  L
C-C_3     0     4.89450000   -2.21889200   -3.67820500  L
C-C_3     0    -3.30324400   -5.50222600   -3.40375100  L
C-C_3     0    -4.60816300    3.78364500   -3.65414800  L
C-C_3     0     4.42052700    2.53717300   -4.24149400  L
C-C_3     0    -3.13983200   -3.34517500   -4.65794000  L
C-C_3     0    -2.32403500    3.59024200   -4.65246700  L
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C-C_3	0	3.37058900	-4.23218600	-3.68969600	L
C-C_3	0	4.49122200	4.84499100	-3.28095300	L
C-C_3	0	5.50033000	-4.25502700	-2.37871200	L
C-C_3	0	-3.86111900	1.59081500	-4.56738800	L
C-C_3	0	2.40502700	4.05226300	-4.38859400	L
C-C_3	0	-1.07694900	-4.72756600	-4.21266700	L
C-C_R	0	2.06324100	1.95165100	-2.08729600	H
C-C_R	0	-1.70388600	1.46126600	-2.27739100	H
C-C_R	0	-1.26294200	-2.32856600	-2.20168200	H
C-C_R	0	2.43978400	-1.81595000	-1.73851700	H
C-C_3	0	3.07254200	3.10669400	-2.09450000	L
C-C_3	0	-2.86150100	2.46398100	-2.36811300	L
C-C_3	0	-2.20194500	-3.53731600	-2.23541800	L
C-C_3	0	3.60024700	-2.79933000	-1.53301600	L
C-C_R	0	4.85314100	1.52205200	-1.03650500	L
C-C_R	0	-3.19157900	4.07443500	-0.38308500	L
C-C_R	0	-3.98879700	-3.72496400	-0.37409800	L
C-C_R	0	1.91387200	-4.57927400	-0.65411500	L
C-C_R	0	5.57173900	1.50208800	0.23274000	L
C-C_R	0	-2.36529000	5.05301800	0.31853200	L
C-C_R	0	-5.07308400	-2.87715600	0.11318900	L
C-C_R	0	1.66300600	-5.15881500	0.66074200	L
C-C_R	0	5.41964000	2.68959800	0.81858300	L
C-C_R	0	-1.23553400	5.22242400	-0.36947300	L
C-C_R	0	-5.25555100	-1.87782900	-0.75389600	L
C-C_R	0	2.70701400	-4.89853000	1.44726200	L
C-C_R	0	4.58264400	3.52970400	-0.03566700	L
C-C_R	0	-1.29123000	4.38571300	-1.56371400	L
C-C_R	0	-4.29053700	-2.02453300	-1.84055800	L
C-C_R	0	3.68325200	-4.13348000	0.67528400	L
C-C_R	0	6.26447100	0.50188400	0.81767800	L
C-C_R	0	-2.59492300	5.69579200	1.47887700	L
C-C_R	0	-5.80032300	-2.98269600	1.23974100	L
C-C_R	0	0.58251600	-5.81331900	1.12240400	L
C-C_R	0	6.83625700	0.71886200	2.03016100	L
C-C_R	0	-1.60083200	6.57164700	1.96714200	L
C-C_R	0	-6.78912300	-2.00956900	1.47889500	L
C-C_R	0	0.59295700	-6.22991000	2.47150300	L
C-C_R	0	6.70633300	1.92453100	2.64459500	L
C-C_R	0	-0.45126800	6.74198000	1.26843500	L
C-C_R	0	-6.96695600	-0.96764200	0.54048100	L
C-C_R	0	1.67232600	-5.95684800	3.25177500	L
F-F_	0	6.38814500	-0.70352200	0.20714400	L
F-F_	0	-3.74272300	5.49650800	2.17378300	L

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F-F_    0    -5.59245600   -3.99355900    2.11985800  L
F-F_    0    -0.48633500   -6.05995800    0.32445200  L
F-F_    0     7.53532000   -0.27466200    2.63407500  L
F-F_    0    -1.79372400    7.23318100    3.13535800  L
F-F_    0    -7.55766100   -2.07208100    2.59395300  L
F-F_    0    -0.47214100   -6.89395000    2.98556900  L
F-F_    0     7.27414800    2.13816600    3.85767900  L
F-F_    0     0.51267600    7.57553100    1.73267900  L
F-F_    0    -7.91461000   -0.02031200    0.74767800  L
F-F_    0     1.68429900   -6.35252200    4.54943800  L
F-F_    0     5.79442100    4.15433900    2.62347700  L
F-F_    0     0.88921500    6.19325700   -0.65230900  L
F-F_    0    -6.33160000    0.08990700   -1.46147300  L
F-F_    0     3.81048600   -5.00784200    3.52166500  L
H-H_    0    -5.04104400    4.03302000   -4.64738300  L
H-H_    0     4.75809300    2.92909500   -5.22536300  L
H-H_    0     5.48253000   -2.62679800   -4.52884400  L
H-H_    0    -3.44203600   -6.06127900   -4.35468000  L
H-H_    0    -4.32573300    4.73909300   -3.16246100  L
H-H_    0    -4.31109300   -5.22533800   -3.02692100  L
H-H_    0     3.84179100    1.61418400   -4.43745000  L
H-H_    0     5.57385400   -1.58294400   -3.07175900  L
H-H_    0    -5.40134100    3.29955800   -3.04393200  L
H-H_    0    -2.83274500   -6.18773900   -2.66585500  L
H-H_    0     5.32942500    2.26675000   -3.66525900  L
H-H_    0     4.10531700   -1.57520200   -4.11281200  L
H-H_    0    -2.72689100    3.81096400   -5.66466300  L
H-H_    0    -3.22818500   -3.87253900   -5.63243600  L
H-H_    0     3.90607900   -4.59269300   -4.59456500  L
H-H_    0     4.82962800    5.26331300   -4.25386300  L
H-H_    0    -1.40128400    2.99463900   -4.78959700  L
H-H_    0    -2.59221200   -2.40142400   -4.84344000  L
H-H_    0     2.48193100   -3.67011600   -4.03581800  L
H-H_    0     5.39885800    4.58339600   -2.69616800  L
H-H_    0    -2.05246900    4.56210200   -4.19180100  L
H-H_    0    -4.16992800   -3.09796100   -4.32926600  L
H-H_    0     3.02611800   -5.12860700   -3.13410300  L
H-H_    0     3.94261100    5.64271800   -2.73463500  L
H-H_    0    -1.24237100   -5.32074900   -5.13813800  L
H-H_    0    -4.30807500    1.87230200   -5.54552100  L
H-H_    0     6.06436300   -4.62950800   -3.26059200  L
H-H_    0     2.77643000    4.50776000   -5.33214600  L
H-H_    0    -0.54081900   -5.37518400   -3.48676400  L
H-H_    0    -4.63788100    1.05263500   -3.98390400  L
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H-H_	0	1.78486900	4.81120200	-3.86553900	L
H-H_	0	5.15017300	-5.14015500	-1.80576500	L
H-H_	0	-0.41431400	-3.88251800	-4.48421700	L
H-H_	0	6.20384000	-3.68135500	-1.73697200	L
H-H_	0	1.75285000	3.20442100	-4.67564500	L
H-H_	0	-3.03085900	0.88931900	-4.78022800	L
H-H_	0	2.51768000	3.96446200	-1.65224300	L
H-H_	0	-3.71356200	1.95395600	-1.86237000	L
H-H_	0	-1.70362000	-4.29660300	-1.59244200	L
H-H_	0	4.37451200	-2.20616600	-0.99756600	L
N-N_R	0	4.19886300	2.78780900	-1.19950900	L
N-N_R	0	-2.53017300	3.66427800	-1.58292300	L
N-N_R	0	-3.48034200	-3.18207400	-1.59702400	L
N-N_R	0	3.17278700	-3.89164500	-0.64095400	L
O-O_R	0	1.53497500	1.67972500	-0.95750200	H
O-O_R	0	-1.42263600	1.07470600	-1.08315400	H
O-O_R	0	-0.97086400	-1.89837600	-1.04171900	H
O-O_R	0	1.96974900	-1.30169300	-0.66167600	H
O-O_R	0	1.81748000	1.31818900	-3.16824600	H
O-O_R	0	-1.09653700	1.10108500	-3.33622700	H
O-O_R	0	-0.84129600	-1.81196500	-3.29613200	H
O-O_R	0	2.01514300	-1.58314800	-2.92080900	H
O-O_R	0	4.57721400	0.49900700	-1.71550100	L
O-O_R	0	-4.42285300	3.90388600	-0.18046900	L
O-O_R	0	-3.34429500	-4.53343600	0.34619700	L
O-O_R	0	1.02385700	-4.38627300	-1.52261600	L
O-O_R	0	3.97888100	4.56305500	0.35882800	L
O-O_R	0	-0.28746500	4.06763100	-2.25369600	L
O-O_R	0	-3.93021700	-1.07602100	-2.58600000	L
O-O_R	0	4.65295900	-3.50190300	1.17302500	L
Rh-	0	0.25236000	-0.13582800	-0.77330700	H
Rh-	0	0.47756700	-0.24301700	-3.19651700	H
N-N_3	0	-0.09144300	0.05028600	1.35920500	H
S-S_3+6	0	-0.41485800	-1.35218700	2.25259900	H
O-O_2	0	-0.44184900	-1.06081500	3.70122800	H
O-O_R	0	-2.03190100	-1.74907900	1.80638300	H
O-O_2	0	0.38495200	-2.46097900	1.73135700	H
C-C_R	0	-3.02121200	-0.88763200	2.28707400	H
C-C_R	0	-3.52626400	0.11089800	1.44264500	H
C-C_R	0	-3.54383900	-1.04777400	3.58057900	H
C-C_R	0	-4.53769400	0.96486800	1.90888800	H
H-H_	0	-3.13732100	0.20456400	0.42651000	H
C-C_R	0	-4.55182000	-0.18555000	4.02379400	H
H-H_	0	-3.14786400	-1.83459200	4.22450900	H

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C-C_R      0    -5.06577300     0.85010400     3.20908900   H
H-H_       0    -4.92466400     1.72263000     1.22677900   H
H-H_       0    -4.93913300    -0.32224700     5.03749700   H
C-C_3      0    -6.13285300     1.81628600     3.76318300   H
C-C_3      0    -5.52563500     2.59545000     4.96088700   H
H-H_       0    -5.20838000     1.91845500     5.77032900   H
H-H_       0    -6.26778700     3.29699600     5.37958100   H
H-H_       0    -4.64423000     3.17843500     4.64520600   H
C-C_3      0    -6.59823000     2.84448300     2.70898300   H
H-H_       0    -7.36690800     3.50274300     3.14651900   H
H-H_       0    -7.04273400     2.35779300     1.82524100   H
H-H_       0    -5.76970100     3.48734300     2.36833700   H
C-C_3      0    -7.37398700     1.02283300     4.24672100   H
H-H_       0    -8.11754800     1.70941200     4.68664300   H
H-H_       0    -7.11495900     0.27624800     5.01412500   H
H-H_       0    -7.85621400     0.49200200     3.41075900   H
C-C_R      0     3.20117300     0.87723200     3.21258800   H
C-C_R      0     3.84223500     1.40842800     4.34922400   H
C-C_R      0     4.61379100     0.59311200     5.18844000   H
C-C_R      0     4.75260500    -0.77223800     4.89949800   H
C-C_R      0     4.11816200    -1.31019800     3.77054100   H
C-C_R      0     3.35083800    -0.49331400     2.92711000   H
H-H_       0     3.75147200     2.47798700     4.56928900   H
H-H_       0     5.11207100     1.02607200     6.06069900   H
H-H_       0     5.35475100    -1.41359900     5.54926600   H
H-H_       0     4.21812500    -2.37408200     3.54672600   H
H-H_       0     2.86492500    -0.92272900     2.04685300   H
C-C_3      0     2.37983200     1.77570300     2.31032000   H
H-H_       0     2.83642300     2.79121500     2.30389900   H
H-H_       0     2.42470000     1.45197600     1.25524300   H
C-C_3      0     0.93652300     2.00235300     2.66601600   H
C-C_3      0     0.20097800     2.97874300     1.80572600   H
H-H_       0     0.50153100     4.00397500     2.11039200   H
H-H_       0    -0.89063300     2.92115400     1.93891200   H
H-H_       0     0.46191200     2.86828000     0.74222800   H
C-C_3      0     0.44382300     1.75989900     4.04760100   H
H-H_       0     0.82861200     2.57603100     4.69874400   H
H-H_       0     0.81297000     0.81435800     4.46478400   H
H-H_       0    -0.65369200     1.78274800     4.10935000   H
H-H_       0    -0.94203500     0.63403300     1.44543300   H
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C-C_R      0     2.62758400    -5.09163100     1.79788600   L
C-C_R      0    -5.23838400     3.94444700     0.58331400   L
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C-C_R      0     4.53631400     4.57496700     1.85455600   L
C-C_R      0    -5.30973400    -2.49374000    -0.61104900   L
C-C_3      0     5.42023100    -2.08529900    -2.51888900   L
C-C_3      0     2.11552800     4.25434000    -3.70347500   L
C-C_3      0    -3.77329400     1.02749500    -4.41805600   L
C-C_3      0    -0.68876100    -5.27034700    -3.07330800   L
C-C_3      0     0.85089700     4.15422800    -4.58991400   L
C-C_3      0     6.81843700    -2.44130900    -1.95851400   L
C-C_3      0    -1.16507800    -6.67881300    -2.64456900   L
C-C_3      0    -2.95840600     2.12873900    -5.13624900   L
C-C_3      0     4.86520300    -3.33495400    -3.24090000   L
C-C_3      0    -1.56874200    -4.81357900    -4.25983600   L
C-C_3      0     3.31206800     3.61333600    -4.44491900   L
C-C_3      0    -5.26596300     1.43600500    -4.46298500   L
C-C_3      0     2.42701000     5.75854700    -3.51511100   L
C-C_3      0     0.77767600    -5.40512600    -3.54911300   L
C-C_3      0    -3.64451600    -0.30163800    -5.20159900   L
C-C_3      0     5.61760400    -0.94324700    -3.54486600   L
C-C_R      0    -1.89725700     0.38535900    -2.65156900   H
C-C_R      0    -0.23468700    -2.88614300    -1.99231600   H
C-C_R      0     3.08393700    -1.14281700    -1.67590300   H
C-C_R      0     1.38405400     2.15398700    -2.25279900   H
C-C_3      0    -3.33901900     0.83758800    -2.91437300   L
C-C_3      0    -0.78008800    -4.30797000    -1.83035000   L
C-C_3      0     4.50056900    -1.61662400    -1.32986000   L
C-C_3      0     1.85630500     3.61203800    -2.28897800   L
C-C_R      0    -2.82534500     3.20687900    -1.92578500   L
C-C_R      0    -2.53428600    -4.63073500     0.03826100   L
C-C_R      0     4.91642200    -2.45730400     1.05990500   L
C-C_R      0     4.14923000     2.90063000    -1.26845200   L
C-C_R      0    -3.39367500     4.01471700    -0.84841800   L
C-C_R      0    -3.79094800    -3.97143300     0.38791700   L
C-C_R      0     4.27048800    -3.41470300     1.95259100   L
C-C_R      0     4.80993100     3.15725400     0.00739000   L
C-C_R      0    -4.50438600     3.41823100    -0.41261700   L
C-C_R      0    -4.19119400    -3.24239900    -0.65330200   L
C-C_R      0     3.40995700    -4.14424500     1.23885100   L
C-C_R      0     4.16963900     4.14885800     0.62713000   L
C-C_R      0    -4.70326900     2.19488200    -1.18178400   L
C-C_R      0    -3.21616700    -3.39421000    -1.72857900   L
C-C_R      0     3.48458500    -3.70869600    -0.15279500   L
C-C_R      0     3.06454400     4.58451300    -0.22285400   L
C-C_R      0    -2.94928500     5.17005400    -0.31044300   L
C-C_R      0    -4.48214300    -3.99953700     1.54371000   L
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C-C_R	0	4.41650400	-3.58214100	3.27897100	L
C-C_R	0	5.85693200	2.53435700	0.57766900	L
C-C_R	0	-3.65313700	5.73825900	0.70295700	L
C-C_R	0	-5.66517900	-3.23404200	1.63658400	L
C-C_R	0	3.62602100	-4.56274400	3.90902300	L
C-C_R	0	6.26472800	2.97122700	1.85727800	L
C-C_R	0	-4.78952200	5.15087100	1.16408800	L
C-C_R	0	-6.07203800	-2.49415000	0.57632500	L
C-C_R	0	2.71972900	-5.31806200	3.13004700	L
C-C_R	0	5.59227100	3.98194800	2.46947200	L
F-F_	0	-1.81529400	5.75597700	-0.77139500	L
F-F_	0	-4.05145500	-4.73566500	2.59845800	L
F-F_	0	5.28218400	-2.82076900	3.99381500	L
F-F_	0	6.49560500	1.51359100	-0.04692700	L
F-F_	0	-3.21817100	6.89644900	1.25963800	L
F-F_	0	-6.38603800	-3.23449000	2.78548600	L
F-F_	0	3.72592800	-4.77218000	5.24498800	L
F-F_	0	7.31166000	2.37242600	2.47762700	L
F-F_	0	-5.49138300	5.71970400	2.17571200	L
F-F_	0	-7.20551400	-1.75400700	0.65345300	L
F-F_	0	1.94293700	-6.26243200	3.71688100	L
F-F_	0	5.97148900	4.39345700	3.70526800	L
F-F_	0	-6.37968100	3.34783900	1.00828400	L
F-F_	0	-5.70362900	-1.76198500	-1.68269700	L
F-F_	0	1.75716300	-5.80549100	1.03998200	L
F-F_	0	3.85904300	5.57634100	2.46994600	L
H-H_	0	-1.07243200	-7.40158100	-3.48426900	L
H-H_	0	-3.28718000	2.22333300	-6.19380800	L
H-H_	0	0.99895400	4.70022100	-5.54680300	L
H-H_	0	7.51384800	-2.72640300	-2.77775000	L
H-H_	0	-2.23066700	-6.66250600	-2.33027400	L
H-H_	0	6.76314300	-3.29908600	-1.25461600	L
H-H_	0	-1.87349600	1.90898100	-5.14776700	L
H-H_	0	-0.02483700	4.60304800	-4.07485400	L
H-H_	0	-0.55819900	-7.05851000	-1.79409200	L
H-H_	0	7.25792200	-1.57469400	-1.41849000	L
H-H_	0	-3.11078000	3.11624000	-4.65439400	L
H-H_	0	0.60499300	3.10600900	-4.85036100	L
H-H_	0	-1.43140200	-5.49626200	-5.12624000	L
H-H_	0	5.52977700	-3.61926400	-4.08529000	L
H-H_	0	3.44586100	4.08725100	-5.44145200	L
H-H_	0	-5.62699200	1.50835600	-5.51200900	L
H-H_	0	-1.31472000	-3.79212300	-4.60247300	L
H-H_	0	3.85465500	-3.16304400	-3.65953100	L

H-H_	0	3.17049800	2.52886000	-4.61470600	L
H-H_	0	-5.42687100	2.42773000	-3.98913900	L
H-H_	0	-2.64505000	-4.84179300	-3.99261300	L
H-H_	0	4.81735700	-4.20373000	-2.55234500	L
H-H_	0	4.25647500	3.76258900	-3.88204700	L
H-H_	0	-5.89428700	0.68825600	-3.93207800	L
H-H_	0	6.36509300	-1.23353100	-4.31476900	L
H-H_	0	0.85939600	-6.16341300	-4.35784200	L
H-H_	0	2.56775300	6.26076300	-4.49695800	L
H-H_	0	-4.06148100	-0.19375400	-6.22642500	L
H-H_	0	5.98731900	-0.02451700	-3.04141700	L
H-H_	0	1.43275800	-5.72955500	-2.71275800	L
H-H_	0	-4.20606900	-1.11265900	-4.69088200	L
H-H_	0	3.35830100	5.90422800	-2.92704800	L
H-H_	0	4.68316700	-0.69590300	-4.08475300	L
H-H_	0	1.59590300	6.26988500	-2.98263200	L
H-H_	0	-2.59209900	-0.62366200	-5.31952200	L
H-H_	0	1.17327600	-4.45330500	-3.95524700	L
H-H_	0	-3.96810400	0.01342100	-2.51470500	L
H-H_	0	-0.12714500	-4.76849600	-1.05483900	L
H-H_	0	4.99546500	-0.71847300	-0.89574800	L
H-H_	0	1.01065500	4.18925900	-1.85114500	L
N-N_R	0	-3.63786100	2.04265600	-2.12352100	L
N-N_R	0	-2.14983500	-4.24794000	-1.28855000	L
N-N_R	0	4.43588400	-2.64168200	-0.27423600	L
N-N_R	0	3.02303500	3.77885400	-1.40558000	L
O-O_R	0	-1.58270800	0.22502800	-1.41605700	H
O-O_R	0	-0.14596000	-2.23296400	-0.89343600	H
O-O_R	0	2.39742900	-0.71579100	-0.67915000	H
O-O_R	0	0.94297900	1.75591000	-1.11173300	H
O-O_R	0	-1.10892000	0.19090700	-3.63261300	H
O-O_R	0	0.06442100	-2.44006100	-3.15082600	H
O-O_R	0	2.66823700	-1.19918700	-2.87975400	H
O-O_R	0	1.47032300	1.44321800	-3.30571400	H
O-O_R	0	-1.64372800	3.31323700	-2.34650600	L
O-O_R	0	-1.72574300	-5.09764000	0.88470100	L
O-O_R	0	5.97329600	-1.82777100	1.33099300	L
O-O_R	0	4.30166600	1.85037100	-1.94614600	L
O-O_R	0	-5.53828100	1.29146100	-0.91010800	L
O-O_R	0	-3.10986000	-2.59518400	-2.69565700	L
O-O_R	0	2.61873700	-3.97535800	-1.02694900	L
O-O_R	0	2.10578200	5.30452600	0.16306200	L
Rh-	0	0.38949100	-0.24828100	-0.92172900	H
Rh-	0	0.78394100	-0.50615300	-3.28655000	H

N-N_3	0	0.14401200	-0.04841300	1.08829600 H
S-S_3+6	0	-0.03847600	-1.26272000	2.22638900 H
O-O_2	0	0.83621500	-2.40033400	1.92746500 H
O-O_R	0	-1.57944400	-1.85461100	1.83202300 H
O-O_2	0	-0.09482400	-0.64476000	3.56387600 H
C-C_R	0	-2.67770000	-1.22157900	2.42827200 H
C-C_R	0	-3.09602100	-1.61826000	3.70321500 H
C-C_R	0	-3.39690600	-0.25970300	1.70541800 H
C-C_R	0	-4.24671100	-1.04379400	4.26055100 H
H-H_	0	-2.52566600	-2.37536300	4.24449100 H
C-C_R	0	-4.53516400	0.30852200	2.28717700 H
H-H_	0	-3.06059600	0.02555800	0.70625800 H
C-C_R	0	-4.98992000	-0.06479100	3.57224400 H
H-H_	0	-4.55734900	-1.37334500	5.25361700 H
H-H_	0	-5.08235600	1.06722400	1.72411500 H
C-C_3	0	-6.23534700	0.61686300	4.17388600 H
C-C_3	0	-5.92523400	2.12239400	4.39011000 H
H-H_	0	-5.63857900	2.62026500	3.45064700 H
H-H_	0	-6.80946100	2.64483400	4.79447400 H
H-H_	0	-5.09387700	2.25299600	5.10241800 H
C-C_3	0	-6.64025000	0.00620500	5.53336800 H
H-H_	0	-7.54497400	0.51022200	5.91193300 H
H-H_	0	-6.86981100	-1.06908800	5.44655500 H
H-H_	0	-5.85164500	0.13133000	6.29379200 H
C-C_3	0	-7.43854100	0.46783500	3.20695500 H
H-H_	0	-8.32295000	0.98583400	3.61585900 H
H-H_	0	-7.23175700	0.89670200	2.21369000 H
H-H_	0	-7.70049100	-0.59372800	3.06741000 H
C-C_R	0	2.28875000	2.06844500	3.34450000 H
C-C_R	0	3.29659800	1.28763000	2.69053300 H
C-C_R	0	4.28069400	0.62355600	3.41704200 H
C-C_R	0	4.30768100	0.70182100	4.82221900 H
C-C_R	0	3.32103500	1.45032400	5.49111500 H
C-C_R	0	2.32854800	2.11684500	4.77520300 H
H-H_	0	3.27656400	1.20819900	1.59977200 H
H-H_	0	5.04199200	0.04357500	2.89157400 H
H-H_	0	5.08356400	0.17958500	5.38820300 H
H-H_	0	3.32951100	1.50929800	6.58348800 H
H-H_	0	1.57115300	2.68948700	5.31541700 H
C-C_R	0	1.30999200	2.75730700	2.57291500 H
C-C_3	0	0.18211900	3.59371300	3.11879700 H
C-C_3	0	0.65414000	5.03264400	3.46274200 H
H-H_	0	0.96887100	5.57318400	2.55541300 H
H-H_	0	-0.16697200	5.60511700	3.92774600 H

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H-H_      0     1.50627700    5.02008100    4.16046600  H
C-C_3     0    -1.00205900    3.63528500    2.13295500  H
H-H_      0    -0.68204400    4.04680100    1.16024200  H
H-H_      0    -1.41876100    2.63137100    1.95459100  H
H-H_      0    -1.81258400    4.27300800    2.52248500  H
H-H_      0    -0.17581800    3.13279800    4.05857000  H
H-H_      0     1.44854800    2.76518700    1.48372700  H
H-H_      0     0.40884800    0.83432800    1.56443800  H
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C-C_R     0     2.94708200   -4.76636500    1.69378300  L
C-C_R     0    -5.31585100    3.81075400    1.05465800  L
C-C_R     0     4.50663600    4.29460200    2.25862600  L
C-C_R     0    -5.39452900   -2.50335700   -1.01845900  L
C-C_3     0     5.39128200   -1.82473000   -2.93313200  L
C-C_3     0     2.02754400    4.65330200   -3.31454600  L
C-C_3     0    -3.81744000    1.46547300   -4.24950400  L
C-C_3     0    -0.53134600   -4.96603800   -3.30443200  L
C-C_3     0     0.73909500    4.61681300   -4.17098700  L
C-C_3     0     6.83608400   -2.23058700   -2.55405200  L
C-C_3     0    -0.96825100   -6.41308500   -2.97391300  L
C-C_3     0    -2.99262700    2.63575800   -4.83423600  L
C-C_3     0     4.72234900   -3.03677400   -3.62178500  L
C-C_3     0    -1.38086500   -4.47874300   -4.50150900  L
C-C_3     0     3.20467400    4.08557700   -4.14109700  L
C-C_3     0    -5.31007900    1.87464900   -4.27961700  L
C-C_3     0     2.33689600    6.13807800   -3.00802600  L
C-C_3     0     0.95642800   -5.01643000   -3.72537900  L
C-C_3     0    -3.66943200    0.22387600   -5.16251800  L
C-C_3     0     5.49559600   -0.65066800   -3.93703200  L
C-C_R     0    -1.97424500    0.64353100   -2.52115100  H
C-C_R     0    -0.17152300   -2.64733700   -2.06258800  H
C-C_R     0     3.19427300   -0.85888400   -1.79727000  H
C-C_R     0     1.33200300    2.44037600   -2.02113600  H
C-C_3     0    -3.41078900    1.12240900   -2.76613900  L
C-C_3     0    -0.70973800   -4.08005600   -2.01444700  L
C-C_3     0     4.62796700   -1.38200600   -1.62971700  L
C-C_3     0     1.80740700    3.89440000   -1.95282100  L
C-C_R     0    -2.90019800    3.36390500   -1.51687600  L
C-C_R     0    -2.58646500   -4.57736100   -0.30499800  L
C-C_R     0     5.35366400   -2.36166100    0.63018700  L
C-C_R     0     4.13832300    3.11537100   -1.08544000  L
C-C_R     0    -3.46253900    4.03741200   -0.34868800  L
C-C_R     0    -3.89805000   -4.00109400   -0.01471100  L
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C-C_R    0    4.76118100   -3.27164000    1.60602200  L
C-C_R    0    4.80068300    3.18838700    0.21298100  L
C-C_R    0   -4.57187000    3.39323100    0.01585300  L
C-C_R    0   -4.23923800   -3.19493800   -1.02022500  L
C-C_R    0    3.72764400   -3.88804200    1.02978800  L
C-C_R    0    4.14172000    4.05563700    0.98082800  L
C-C_R    0   -4.75649400    2.25223600   -0.87392400  L
C-C_R    0   -3.16789200   -3.21081700   -2.01098000  L
C-C_R    0    3.63420900   -3.42314200   -0.35087300  L
C-C_R    0    3.02430400    4.59536000    0.21074600  L
C-C_R    0   -3.02417800    5.12930600    0.31252300  L
C-C_R    0   -4.68954000   -4.16837400    1.06205600  L
C-C_R    0    5.09867600   -3.49543200    2.88848400  L
C-C_R    0    5.86779100    2.51235800    0.67560900  L
C-C_R    0   -3.73482900    5.58326200    1.37751500  L
C-C_R    0   -5.91484900   -3.46830000    1.10889600  L
C-C_R    0    4.31651600   -4.40608400    3.62481000  L
C-C_R    0    6.27479900    2.75595900    2.00565700  L
C-C_R    0   -4.87394300    4.94906500    1.76416900  L
C-C_R    0   -6.26166600   -2.65057200    0.08478300  L
C-C_R    0    3.22258500   -5.03948400    2.99152700  L
C-C_R    0    5.58122600    3.64034500    2.77028800  L
F-F_     0   -1.89118900    5.76570400   -0.07850900  L
F-F_     0   -4.32113900   -4.98460000    2.08084300  L
F-F_     0    6.15036300   -2.85904000    3.46170000  L
F-F_     0    6.52896600    1.62000200   -0.10296200  L
F-F_     0   -3.30681500    6.67643200    2.05740100  L
F-F_     0   -6.73807300   -3.61211100    2.17710000  L
F-F_     0    4.60445400   -4.66576400    4.92414100  L
F-F_     0    7.34307200    2.09767900    2.52046500  L
F-F_     0   -5.58456300    5.40587700    2.82526000  L
F-F_     0   -7.43728800   -1.97576800    0.11570700  L
F-F_     0    2.45181300   -5.91556400    3.68289100  L
F-F_     0    5.96087900    3.86626000    4.05293900  L
F-F_     0   -6.45654700    3.16790000    1.40700300  L
F-F_     0   -5.72750500   -1.69267400   -2.05340800  L
F-F_     0    1.89794800   -5.36480100    1.07494500  L
F-F_     0    3.81363200    5.17513100    3.02314100  L
H-H_     0   -0.81808500   -7.08245300   -3.84882900  L
H-H_     0   -3.29942900    2.83697400   -5.88344500  L
H-H_     0    0.85328100    5.24821400   -5.07870900  L
H-H_     0    7.42413000   -2.49833000   -3.45876600  L
H-H_     0   -2.04414000   -6.45232300   -2.69919200  L
H-H_     0    6.84231100   -3.11423900   -1.88079900  L
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H-H_     0    -1.90691500    2.41995600   -4.84445700   L
H-H_     0    -0.12703600    5.00448300   -3.59345500   L
H-H_     0    -0.37807100   -6.81977800   -2.12421500   L
H-H_     0     7.35698400   -1.39429900   -2.03931500   L
H-H_     0    -3.15928900    3.56842300   -4.25704400   L
H-H_     0     0.49912400    3.59191900   -4.51671900   L
H-H_     0    -1.18852500   -5.11368700   -5.39340600   L
H-H_     0     5.29340900   -3.32818800   -4.52975000   L
H-H_     0     3.29458200    4.62936100   -5.10639900   L
H-H_     0    -5.64914500    2.06492700   -5.32117500   L
H-H_     0    -1.14737600   -3.43531500   -4.78686200   L
H-H_     0     3.68573700   -2.81639100   -3.94185200   L
H-H_     0     3.07185300    3.01296000   -4.37993100   L
H-H_     0    -5.48431500    2.80578500   -3.69933700   L
H-H_     0    -2.46509500   -4.55353600   -4.27912700   L
H-H_     0     4.70028000   -3.91590300   -2.94458300   L
H-H_     0     4.16733200    4.21369500   -3.60468500   L
H-H_     0    -5.94666100    1.07044100   -3.85100200   L
H-H_     0     6.16458000   -0.91733700   -4.78383200   L
H-H_     0     1.10034100   -5.71740700   -4.57602100   L
H-H_     0     2.45881100    6.72011400   -3.94740000   L
H-H_     0    -4.08183800    0.43020700   -6.17401000   L
H-H_     0     5.91308300    0.25224800   -3.44160200   L
H-H_     0     1.58991300   -5.36929200   -2.88404200   L
H-H_     0    -4.22333900   -0.64130400   -4.73938100   L
H-H_     0     3.27725700    6.23830800   -2.42474800   L
H-H_     0     4.51599900   -0.38571200   -4.37963500   L
H-H_     0     1.51342600    6.59979400   -2.42112300   L
H-H_     0    -2.61248500   -0.07212800   -5.30590400   L
H-H_     0     1.32722800   -4.02475700   -4.05258400   L
H-H_     0    -4.04698400    0.26282100   -2.46229900   L
H-H_     0    -0.09835500   -4.58145600   -1.22991800   L
H-H_     0     5.19263800   -0.51441600   -1.22012600   L
H-H_     0     0.97330900    4.43369500   -1.44902300   L
N-N_R    0    -3.72182300    2.24002600   -1.86048700   L
N-N_R    0    -2.10900000   -4.06391600   -1.55421900   L
N-N_R    0     4.65635500   -2.45143200   -0.61565300   L
N-N_R    0     2.99381500    3.98264300   -1.08377000   L
O-O_R    0    -1.67722100    0.37010400   -1.31087700   H
O-O_R    0    -0.02557200   -2.09438000   -0.91965800   H
O-O_R    0     2.61853900   -0.45845600   -0.73413400   H
O-O_R    0     0.90816800    1.96208700   -0.90725700   H
O-O_R    0    -1.16701100    0.54627200   -3.50643500   H
O-O_R    0     0.06066500   -2.09705700   -3.19522200   H
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O-O_R      0    2.65145700   -0.86199400   -2.95666800  H
O-O_R      0    1.40567500    1.80480600   -3.12247100  H
O-O_R      0   -1.72538500    3.52848900   -1.93860500  L
O-O_R      0   -1.83493000   -5.09639600    0.56318600  L
O-O_R      0    6.45416700   -1.76483400    0.77169500  L
O-O_R      0    4.29096800    2.16596200   -1.89905100  L
O-O_R      0   -5.79113100    1.53567600   -0.93301500  L
O-O_R      0   -3.02083200   -2.33634300   -2.90486900  L
O-O_R      0    2.66736200   -3.65542000   -1.12247900  L
O-O_R      0    2.04495800    5.20893600    0.71214600  L
Rh-        0    0.43522500   -0.07521600   -0.80711400  H
Rh-        0    0.74296700   -0.15570100   -3.21036400  H
N-N_3      0    0.01426700    0.09478800    1.26600500  H
S-S_3+6    0   -0.16583000   -1.23808800    2.28219600  H
O-O_2      0    0.90210000   -2.19820600    2.00269800  H
O-O_R      0   -1.59850400   -2.00860300    1.71823800  H
O-O_2      0   -0.44672500   -0.76593400    3.65613500  H
C-C_R      0   -2.79645100   -1.54514500    2.26899600  H
C-C_R      0   -3.26467600   -2.08782200    3.47180300  H
C-C_R      0   -3.55400100   -0.58281000    1.58278900  H
C-C_R      0   -4.48665700   -1.65092200    3.99898300  H
H-H_       0   -2.66828200   -2.84486900    3.98436400  H
C-C_R      0   -4.76469900   -0.14854900    2.13701400  H
H-H_       0   -3.19924300   -0.20018600    0.62161600  H
C-C_R      0   -5.25892900   -0.66124600    3.35710200  H
H-H_       0   -4.82973900   -2.09306200    4.93617100  H
H-H_       0   -5.33744400    0.61029200    1.59960100  H
C-C_3      0   -6.55907200   -0.09934500    3.96907800  H
C-C_3      0   -6.27344800    1.34035900    4.47567100  H
H-H_       0   -5.91483400    1.99169900    3.66336800  H
H-H_       0   -7.18742400    1.79263600    4.89851100  H
H-H_       0   -5.49924700    1.33247100    5.26076800  H
C-C_3      0   -7.05813800   -0.94425800    5.16256200  H
H-H_       0   -8.00992600   -0.53209600    5.53706300  H
H-H_       0   -7.23810700   -1.99289100    4.87203100  H
H-H_       0   -6.34595100   -0.93610400    6.00405400  H
C-C_3      0   -7.69289600   -0.06070800    2.91342300  H
H-H_       0   -8.60250600    0.38428300    3.35161300  H
H-H_       0   -7.42719200    0.53869000    2.02865200  H
H-H_       0   -7.94541500   -1.07678300    2.57014100  H
C-C_R      0    2.23553300    1.14701600    3.19068100  H
C-C_R      0    3.38815300    0.71694800    2.46674900  H
C-C_R      0    4.45362200    0.10833500    3.12554300  H
C-C_R      0    4.39474300   -0.11931200    4.51157500  H
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C-C_R    0     3.24766800     0.25309800     5.23723000 H
C-C_R    0     2.18046100     0.87242400     4.59146100 H
H-H_     0     3.41559400     0.85808800     1.38425900 H
H-H_     0     5.34200500    -0.18669700     2.56495000 H
H-H_     0     5.23412100    -0.59787500     5.02334600 H
H-H_     0     3.19022900     0.05137200     6.31012500 H
H-H_     0     1.28876700     1.13926800     5.16041900 H
C-C_R    0     1.21041600     1.86633100     2.50077900 H
C-C_3    0     0.11474800     2.63694500     3.18928400 H
C-C_3    0     0.75081800     3.87961900     3.88687500 H
H-H_     0     1.15025000     4.58628100     3.14279800 H
H-H_     0    -0.02272000     4.40593900     4.47033400 H
H-H_     0     1.56947600     3.59665700     4.56469700 H
C-C_3    0    -1.00348700     3.11179600     2.24027600 H
H-H_     0    -0.58674000     3.56597900     1.32650000 H
H-H_     0    -1.68145500     2.29843200     1.93679000 H
H-H_     0    -1.62894200     3.86640100     2.74370900 H
H-H_     0    -0.33009000     2.00416600     3.97718800 H
H-H_     0     1.41802300     2.13324600     1.45995200 H
H-H_     0    -0.84174900     0.66174400     1.37238500 H
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