

New Journal of Chemistry

Supporting Information for

Tuning Diastereoisomerism in platinum(II) phosphino- and aminothiolato hydrido complexes

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Figure S1. ^1H NMR (CDCl_3 , 200.13 MHz, 293 K) of ligand **3**.

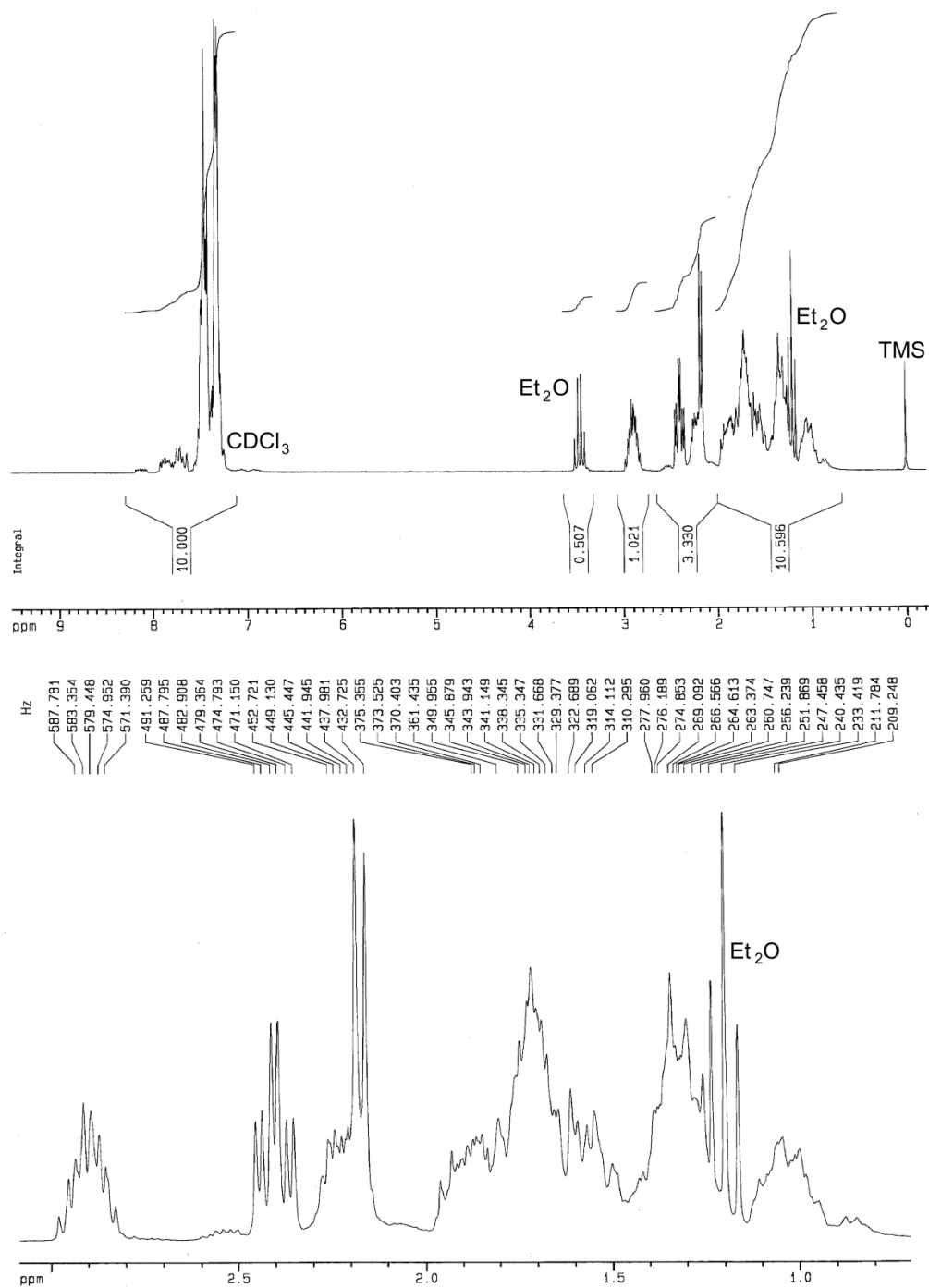
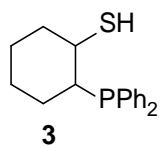


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 50.32 MHz, 293 K) of ligand **3**.

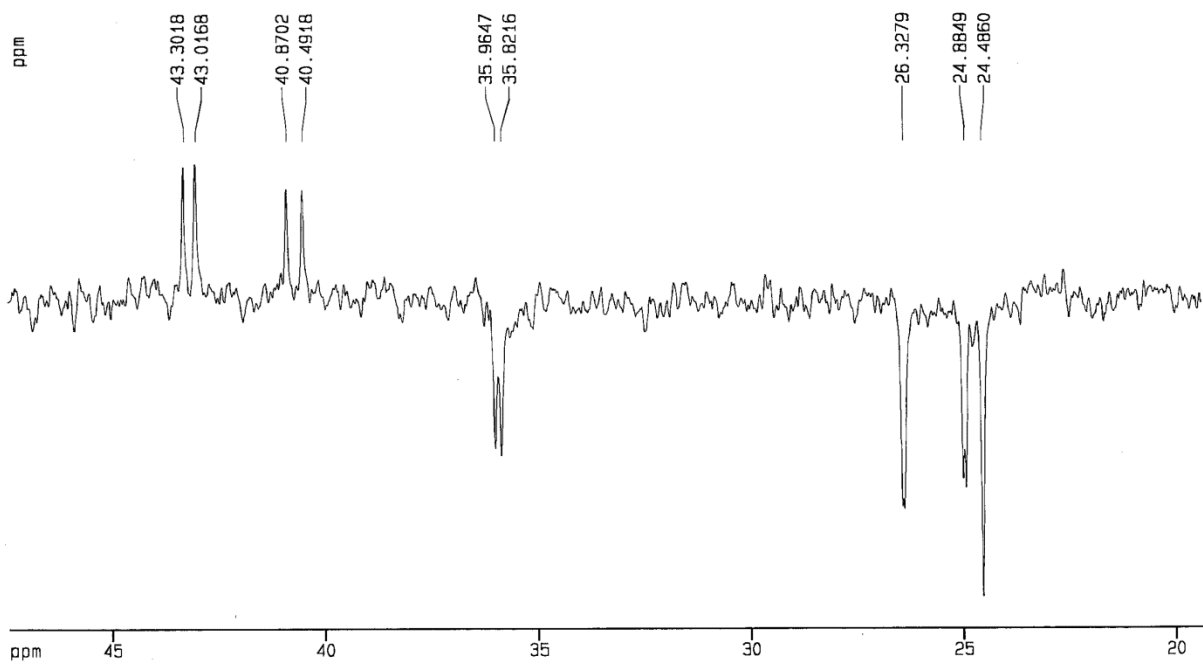
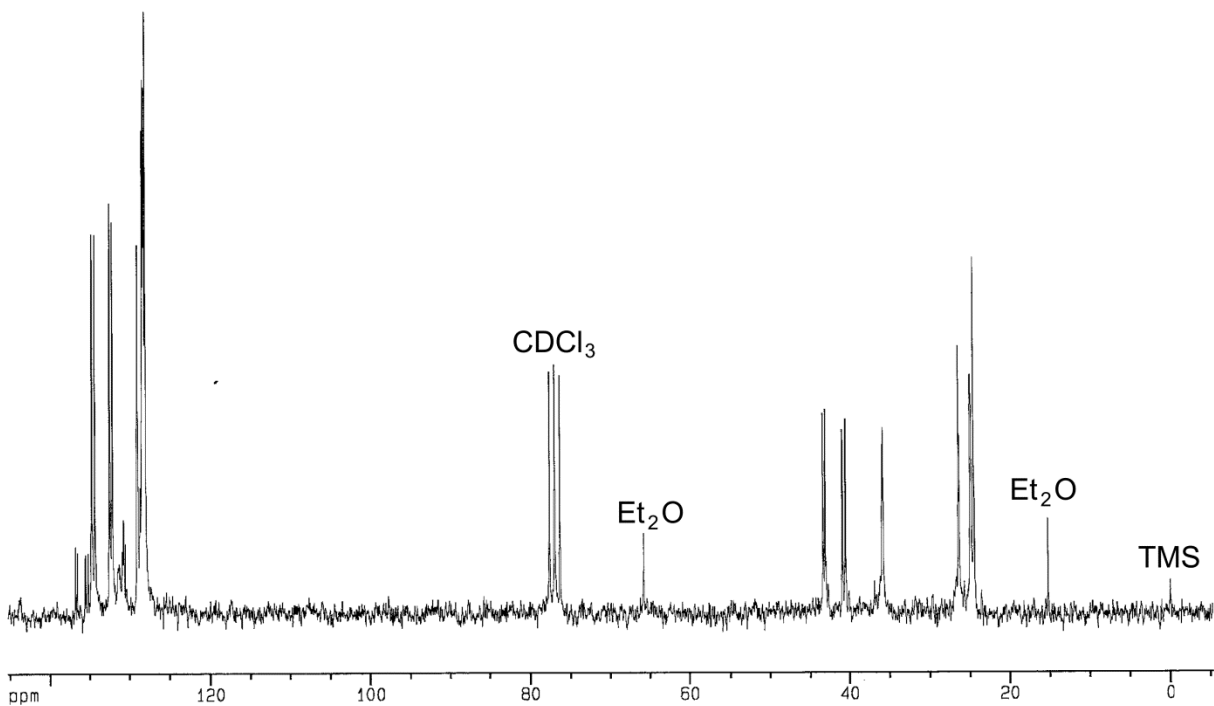
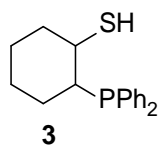


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR (CDCl_3 , 81.01 MHz, 293 K) of ligand **3**.

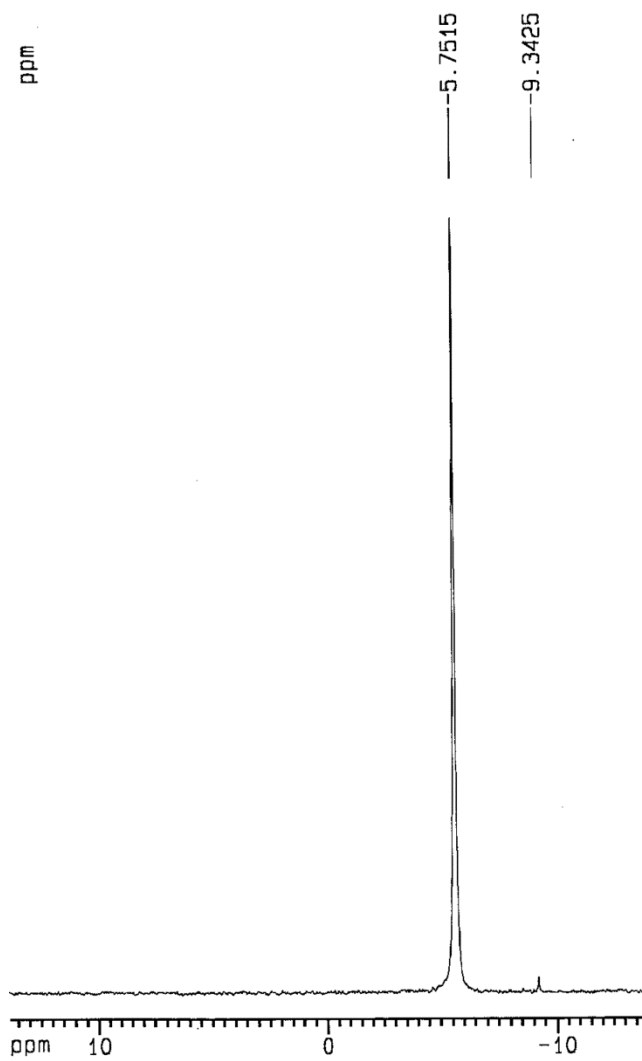
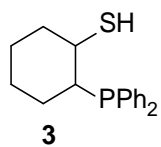
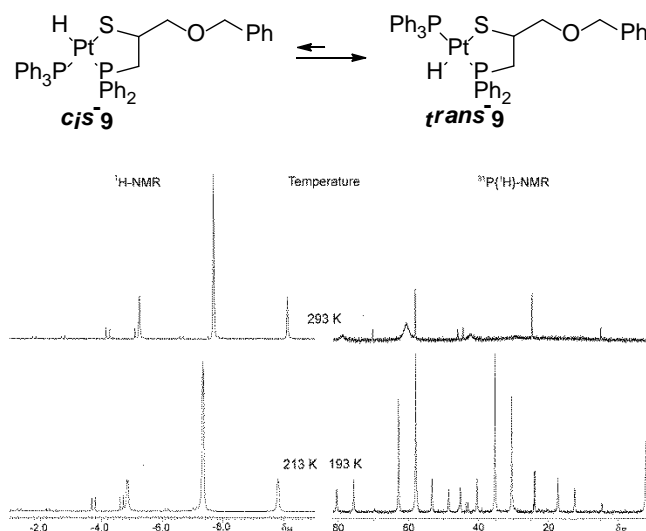
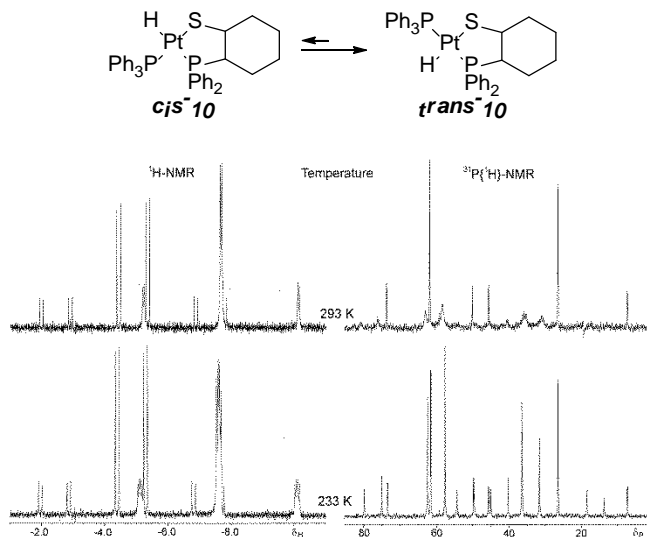


Figure S4. Hydride region of ^1H NMR (left) and $^{31}\text{P}\{^1\text{H}\}$ NMR (right) of a mixture of free triphenylphosphine with hydrido[1-(benzyloxy)-2-(diphenylphosphino- κP)ethanethiolato- κS]triphenylphosphino-platinum(II) (**9**) at room temperature (up) and at low temperature (down).



In solution, complex **9** shows a similar behavior to complex **8** with chemical equilibrium between *cis-9* and *trans-9* isomers (*SP-4-3* and *SP-4-4* configuration respectively) strongly displaced toward the *trans-P,P* form. For complex **9** this equilibrium is slightly more displaced (ca. 90% of *trans-9*). At room temperature, the hydride resonance of the major isomer appears as a singlet with ^{195}Pt satellites that transforms into a broad doublet when the sample is cooled to -60°C . Further cooling just results in a loss of resolution of the spectrum. For isomer *trans-9*, the hydride resonance does not resolve at low temperature because the rapid exchange with the free PPh_3 present in solution. At room temperature, the $^{31}\text{P}\{^1\text{H}\}$ NMR of isomer *trans-9* shows only a broad band with ^{195}Pt satellites for the PPh_2 group. No signal is observed for the free or the coordinated PPh_3 . The expected doublets for the coordinated phosphorous and the singlet for the free PPh_3 appear when the solution is cooled to -80°C . As in complex **8**, the minor isomer *cis-9* shows temperature independent NMR spectra in whole the range studied.

Figure S5. Hydride region of ^1H NMR (left) and $^{31}\text{P}\{^1\text{H}\}$ NMR (right) of hydrido[2-(diphenylphosphino- κP)-cyclohexanethiolato- κS]triphenyl-phosphineplatinum(II) (**10**) at room temperature (up) and at low temperature (down).



The same *cis/trans* equilibrium observed for complexes **8** and **9** in solution is observed for complex **10** (ca. 70% *trans-10*). As for the previous phosphinothiolate complexes, the major isomer of **10** shows temperature dependent NMR spectrums. At room temperature, the hydride resonance of the major isomer appears as a broad doublet with ^{195}Pt satellites that transforms into the predictable doublet of doublets when the sample is cooled to -40°C . At room temperature, the $^{31}\text{P}\{^1\text{H}\}$ NMR of isomer *trans-10* shows only two broad doublets, one for each phosphorous coordinated, with ^{195}Pt satellites. At -40°C , these signals transform in sharp doublets. Once more, the minor isomer *cis-10* has a different behavior showing, in whole temperature range studied, temperature independent NMR spectrums.

Figure S6. Frontier molecular orbitals of **5** and **8**.

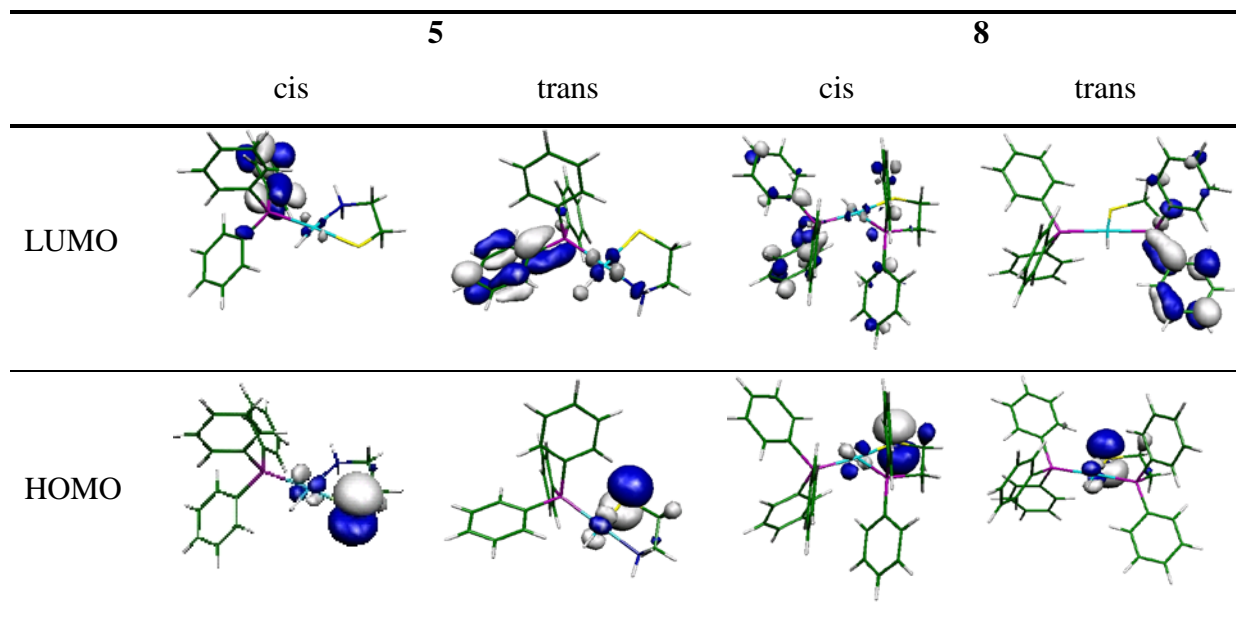


Figure S7. Addition of an extra PPh₃ ligand to *cis*-8 and *trans*-8.

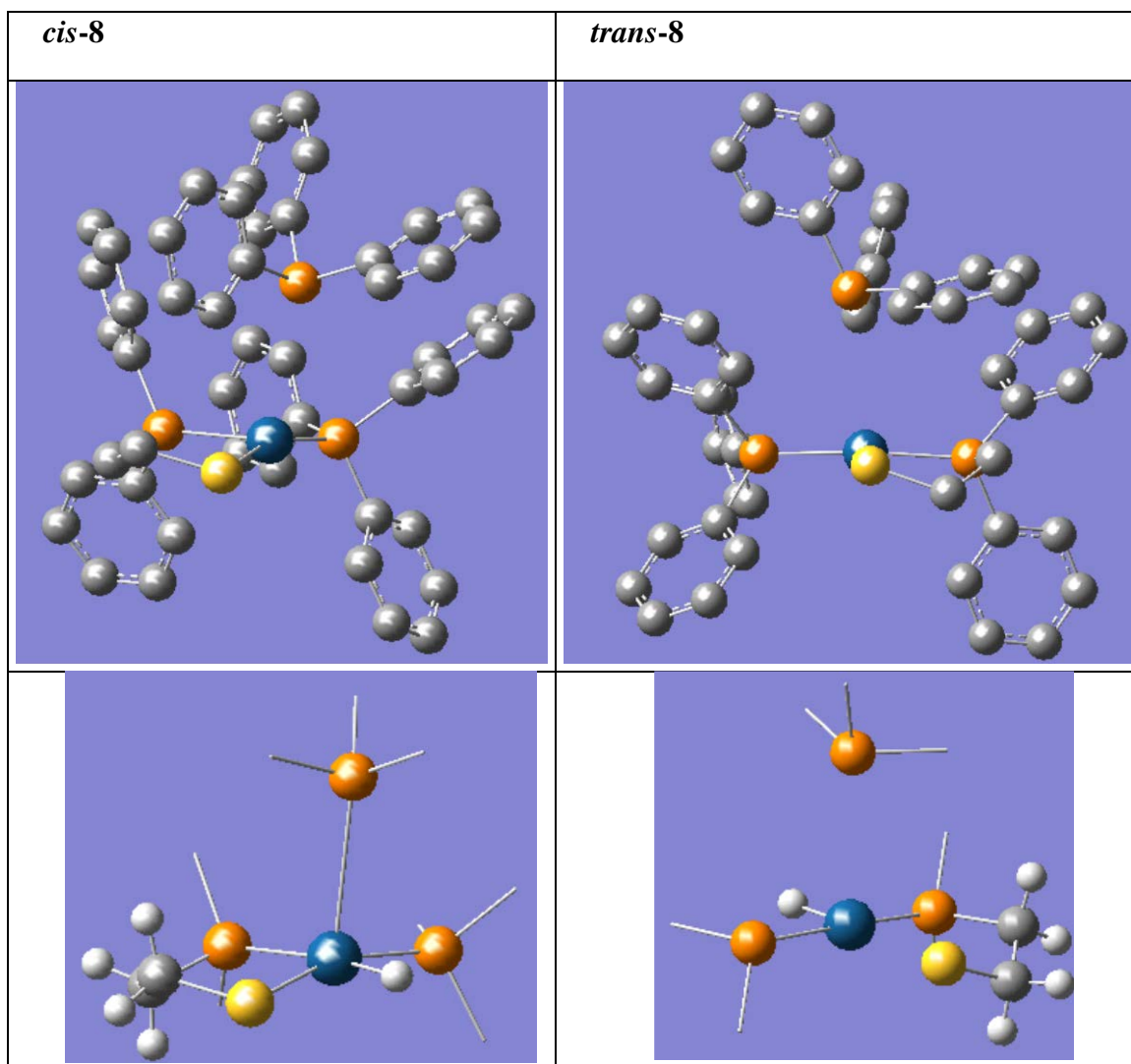


Figure S8. Hydride region of ^1H NMR (400,20 Mhz, left) and $^{31}\text{P}\{^1\text{H}\}$ NMR (162.01 MHz, right) of hydrido[2-(diphenylphosphino- κP)ethanethiolato- κS]triphenylphosphinoplatinum(II) (**8**). Dissolved at $-78\text{ }^\circ\text{C}$, under nitrogen atmosphere, with precooled dichloromethane and recorded directly at $-60\text{ }^\circ\text{C}$ (up) and after leaving temperature raise to room temperature (down).

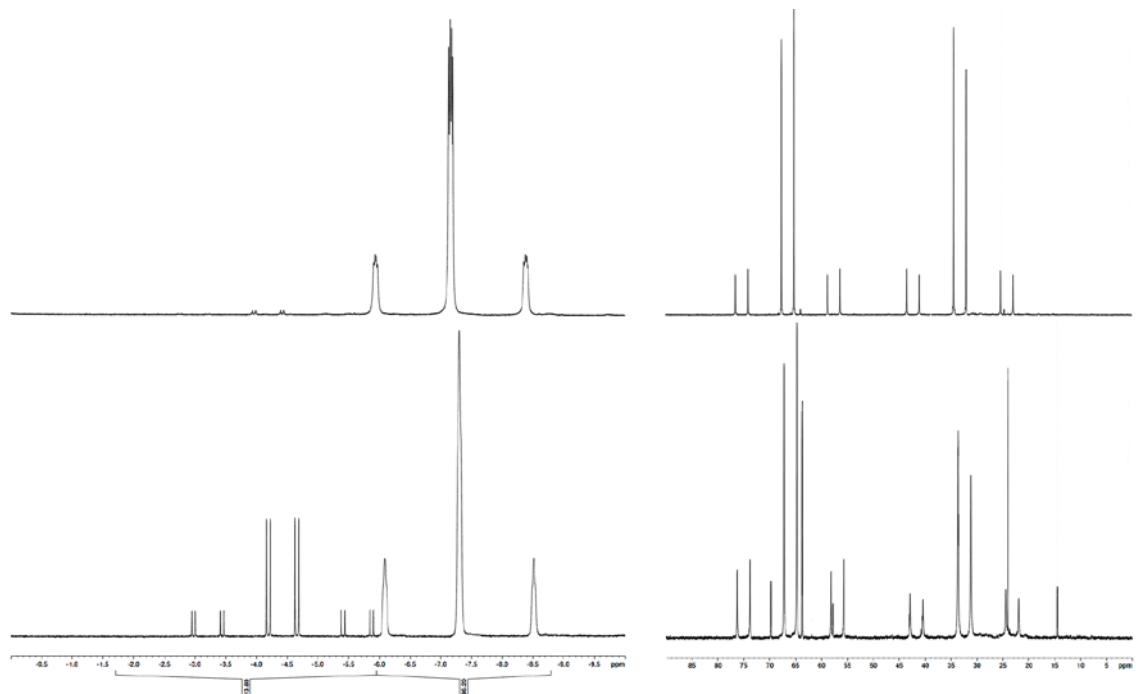


Table S1. Crystallographic data for **5-8**

	5	6	7	8
formula	C ₂₀ H ₂₂ NPPtS	C ₂₂ H ₂₇ NO ₂ PPtS	C ₂₃ H ₂₆ NO ₂ PPtS	C ₃₂ H ₃₀ P ₂ PtS
fw	534.51	595.57	606.57	703.65
crystal size (mm ³)	0.02 x 0.04 x 0.7	0.01 x 0.06 x 0.07	0.04 x 0.04 x 0.08	0.90 x 0.70 x 0.04
crystal color	white	white	white	white
temp (K)	153(2)	153(2)	153(2)	153(2)
cryst syst	monoclinic	triclinic	triclinic	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i> (No. 14)	<i>P</i> $\bar{1}$ (No. 2)	<i>P</i> 1 (No. 1)	<i>P</i> 2 ₁ / <i>n</i> (No. 14)
<i>a</i> (Å)	11.2021(6)	9.2097(15)	9.3040(2)	9.6068(3)
<i>b</i> (Å)	8.9266(5)	9.9559(17)	10.1733(2)	29.7785(11)
<i>c</i> (Å)	19.0001(10)	13.363(2)	13.5601(3)	10.3464(4)
α (deg)	90	75.392(6)	73.6710(10)	90
β (deg)	90.030(2)	87.912(8)	87.5860(10)	111.467(2)
γ (deg)	90	63.361(6)	63.5340(10)	90
<i>V</i> (Å ³)	1899.95(18)	1055.6 (3)	1097.46 (4)	2754.53(17)
<i>Z</i>	4	2	2	4
ρ (g/cm ³)	1.869	1.864	1.836	1.697
μ (mm ⁻¹)	7.580	6.838	6.580	5.306
Theta max (°)	31.54	31.56	31.51	31.53
Completeness 2 θ 25°	99.9 %	97.4 %	99.3 %	99.3 %
no. of rflns measd	28029	15686	17158	42246
no. of unique rflns	6108 [R _{int} = 0.0802]	6372 [R _{int} = 0.1262]	13211 [R _{int} = 0.0333]	8644 [R _{int} = 0.0750]
absorption corr.	Empirical	Empirical	Empirical	Empirical
transm min/max	0.38307/1.00000	0.93412/1.00000	0.67855/1.00000	0.555/1.000
no. of params	238	273	527	431
R1/wR2 (<i>I</i> >2 σ (<i>I</i>))	0.0411/0.0909	0.0601/0.1087	0.0471/0.1190	0.0540/0.1378
R1/wR2 (all data)	0.0583/0.0967	0.1177/0.1232	0.0513/0.1214	0.0798/0.1378
goodness-of-fit on <i>F</i> ²	0.981	0.852	1.039	1.036
Largest diff peak, hole (e/Å ³)	2.064 and -3.139	1.898 and -2.666	1.423 and -3.571	6.202 and -2.872
Abs Struc Flack Para.			-0.001(12)	

Table S2. Comparison between the XRD data (molecule A) and the corresponding BP86 geometry for complex *cis-7*.

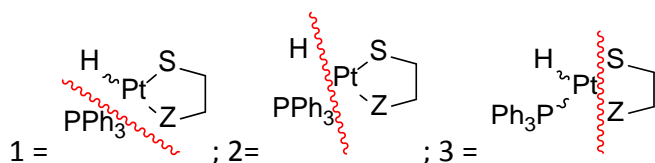
Distances [Å]	BP86	XRD	Angles [deg]	BP86	XRD
Pt-S	2.361	2.291	N-Pt-S	84.565	83.938
Pt-N	2.243	2.176	Pt-P-C1	116.642	118.170
Pt-P	2.264	2.228	Pt-P-C25	115.551	114.399
N-C35	1.475	1.489	Pt-P-C39	110.187	112.680
C35-C44	1.535	1.501	P-C15-C8	117.130	118.402
S-C44	1.845	1.836	C15-C8-C4	119.156	120.533
C35-C26	1.525	1.522	C4-C3-C6	118.220	119.714
C24-C29	1.519	1.331	C6-C12-C15	122.023	120.275
P-C15	1.843	1.830	C12-C15-C8	119.115	119.055
P-C25	1.841	1.811	C35-C44-S	111.830	111.891
P-C39	1.841	1.808	C44-S-Pt	98.102	98.569
C3-C6	1.397	1.404	C35-C26-O32	111.319	111.891
C6-C12	1.400	1.370	C35-C26-O17	124.034	123.912
C12-C15	1.403	1.364	O17-C26-O32	124.614	124.141
C25-C13	1.406	1.429	C26-O32-C24	117.657	118.228
C13-C11	1.397	1.406	P-C25-C31	122.507	123.174
C11-C18	1.399	1.366	C25-C31-C11	120.344	121.376
C18-C30	1.398	1.387	C13-C11-C18	120.103	118.322
C30-C33	1.398	1.393	C11-C18-C30	119.832	120.484
C33-C25	1.405	1.372	C18-C30-C33	120.250	122.996
C39-C41	1.405	1.395	C30-C33-C25	120.227	118.094
C41-C48	1.396	1.411	C33-C25-P	118.254	118.116
C48-C53	1.400	1.411	P-C39-C41	122.205	121.863
C53-C52	1.397	1.381	C39-C41-C48	120.274	119.889
C52-C46	1.399	1.408	C41-C48-C53	120.118	121.841
C46-C39	1.404	1.374	C48-C53-C52	119.884	118.974
C26-O17	1.211	1.337	C53-C52-C46	120.161	120.477
C26-O32	1.337	1.387	C52-C46-C39	120.198	119.184
O32-C24	1.444	1.405	C46-C39-P	118.415	118.622

Standard deviations for the distances and for the angles, $s_{n-1} = \sqrt{\frac{\sum_{i=1}^N (CV - EV)^2}{N - 1}}$, where

CV means calculated value, EV experimental value (X-ray data), and N is the number of distances or angles taken into account.

Table S3. Three different methods to analyze the BE (kcal·mol⁻¹) by the energy decomposition analysis (EDA) for **5** (Z = NH₂) and **8** (Z = PPh₂). Frag2 is the fragment containing the metal species in all cases.

Method	Complex	ΔE_{Pauli}	ΔE_{oi}	ΔE_{elstat}	ΔE_{int}	$\Delta E_{\text{def fr.1}}$	$\Delta E_{\text{def fr. 2}}$	ΔE_{def}	BE
1	<i>cis</i> - 5	153.5	-66.4	-136.9	-49.9	0.6	0.8	1.4	-48.5
1	<i>trans</i> - 5	169.0	-77.9	-153.1	-62.0	0.8	0.7	1.4	-60.6
1	<i>cis</i> - 8	161.3	-72.0	-143.2	-53.9	2.3	1.7	4.0	-49.9
1	<i>trans</i> - 8	140.9	-67.6	-126.4	-53.1	2.3	1.5	3.8	-49.3
2	<i>cis</i> - 5	183.1	-124.5	-255.7	-197.1	8.9	13.7	22.5	-174.6
2	<i>trans</i> - 5	176.5	-119.4	-251.3	-194.2	8.5	13.9	22.3	-171.9
2	<i>cis</i> - 8	224.8	-147.7	-271.4	-194.3	7.0	9.3	16.3	-177.9
2	<i>trans</i> - 8	222.7	-148.6	-273.9	-199.8	10.3	8.7	19.0	-180.8
3	<i>cis</i> - 5	287.6	-202.7	-341.3	-256.5	3.2	23.3	26.5	-230.0
3	<i>trans</i> - 5	295.3	-207.6	-346.6	-258.9	4.4	27.2	31.5	-227.4
3	<i>cis</i> - 8	286.0	-189.8	-326.8	-230.6	6.8	24.2	31.0	-199.6
3	<i>trans</i> - 8	290.4	-206.1	-331.9	-247.6	6.4	39.0	45.5	-202.1



The EDA of the molecule has been done for three different fragmentation schemes (Table S3). The first one takes in account the dissociation of the triphenylphosphine ligand and reflects that BE is similar for all the compounds except for *trans*-**5**, which has the highest value, according to the smaller *trans* influence of the amine group compared with thiolate and phosphine ligands. For 2-phosphinothiolate complex **8**, the Pauli repulsion is higher in the *cis* isomer than the *trans* one, opposite to what happens for 2-aminothiolato complex **5**, because of the entrance of the phosphine in *cis* places the phenyl groups close to each other. Nevertheless, the electrostatic and the orbital interaction terms compensate the higher Pauli repulsions and makes *trans*-**5** and *cis*-**8** the most favorable isomers. The second decomposition method analyzes the BE of the two monodentate ligands that bind the platinum atom with the chelate ligand. The split of the interaction energy confirms that the repulsion is higher in all the *cis* conformations according to the Pauli repulsion term. Furthermore, the values are much higher complex **8** because of the two extra phenyls of the 2-phosphinothiolato ligand. Nevertheless, the energetic difference between both isomers is only 2.1 kcal·mol⁻¹ because the higher steric repulsions caused by phenyls in *cis* conformation is compensated by the ΔE_{elstat} and ΔE_{orb} terms. The deformation energy is higher because the metal, now, presents one more free position with respect to the extraction of a phosphine ligand. The ΔE_{orb} term is higher for complex **8** due to the higher *trans* influence of the phosphines with respect to the amines. The third method reflects the

BE presented for the fragmentation of the chelate ligand. The results also support the experimental observations. Thus, *cis*-**5** and *trans*-**8** present the higher BE values. In this case the deformation energies are even higher because the position of the ligands in free metal fragment has to change significantly to achieve the geometry that the ligands have in the final complex. The second and the third methods used to describe the binding energies reflect that there is an increase of the electrostatic term, surely due to the charged fragments that appear in these two methods.

The differences found between the behavior of the 2-aminothiolato and 2-phosphinothiolato complexes has been studied from an electronic point of view also. The frontier molecular orbitals for **5** and **8** are depicted in Figure S6 and the relative energies for molecular frontier orbitals of **5-8** are presented in Table S4. For all complexes, the LUMO is more stable energetically for the *cis* isomer, and the gap defined by the difference between the energies of HOMO and LUMO is lower for the same isomer. On the other hand, the HOMO is more stabilized for the *cis* isomer of the 2-aminothiolate complexes **5-7** and for the *trans* isomer of the 2-phosphinothiolate complex **8**, thus the most stable HOMO agrees with the most stable isomer. Moreover, the charge over the metal is lower for the 2-phosphinothiolate complex **8** than for the 2-aminothioalate complexes **5-7** (Table S5), due to major σ -donor power of the phosphine ligand relative to the amine one. The metal is less positively charged when it has the anionic ligands in *cis* position, nevertheless the difference is not quantitatively important.

Table S4. Calculated relative energies (kcal·mol⁻¹) for frontier molecular orbitals of **5-8**.

	5		6		7		8	
	<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>
LUMO	-53,8	-49,2	-53,5	-49,8	-52,9	-49,7	-56,1	-52,7
HOMO	-99.0	-98.5	-101.6	-100.4	-101.0	-99.7	-101.8	-103.4
GAP	45.2	49.3	48.1	50.6	48.1	50.0	45.7	50.7

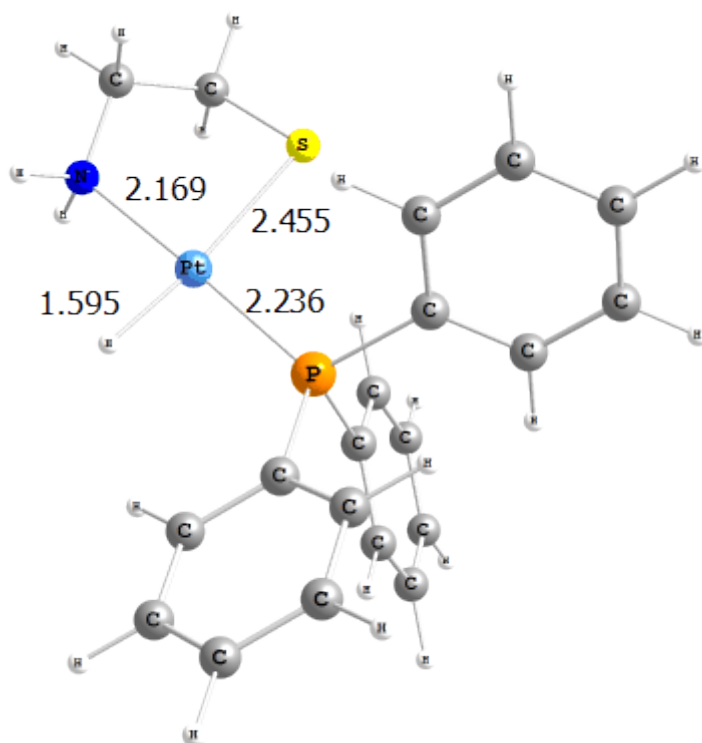
Table S5. Calculated charges (e⁻) of some atoms of **5-8**.

Method	Atom	5		6		7		8	
		<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>	<i>cis</i>	<i>trans</i>
Mulliken	Pt	0.291	0.306	0.276	0.307	0.283	0.312	0.016	0.046
Voronoi	Pt	0.067	0.080	0.067	0.080	0.066	0.081	0.046	0.055
Mulliken	S	-0.219	-0.209	-0.213	-0.211	-0.213	-0.213	-0.187	-0.225
Voronoi	S	-0.266	-0.275	-0.264	-0.277	-0.266	-0.278	-0.262	-0.278
Mulliken	P(2)	-0.219	-0.209	-0.213	-0.211	-0.213	-0.213	-0.187	-0.225
Voronoi	P(2)	-0.266	-0.275	-0.264	-0.277	-0.266	-0.278	-0.262	-0.278

Table S6. Coordinate data sets and absolute energy (in a.u.), 3D structure for DFT optimized complexes with selected distances (in Å).

<i>cis-5</i>					
		H	-4.494997	3.246631	-4.471568
		H	-3.117080	1.164439	-4.414016
		C	-4.463912	2.634331	-3.566905
		C	-3.690218	1.467313	-3.533797
		H	-5.804914	3.918708	-2.457242
		C	-5.197251	3.010348	-2.438230
		H	-6.169443	-3.605408	-2.367230
		C	-3.648663	0.686403	-2.376952
		H	-5.798709	-1.222393	-1.804642
		H	-3.039612	-0.221759	-2.355322
		C	-5.495596	-3.341072	-1.548099
		C	-5.162371	2.225949	-1.278912
		C	-5.290648	-1.997031	-1.225307
		H	-4.997343	-5.394702	-1.082435
		C	-4.389382	1.055382	-1.238065
	C	-4.837768	-4.343689	-0.828001	
	H	-5.740472	2.527780	-0.402650	
	H	-1.039499	1.474510	-1.112703	
	H	-2.182730	2.575281	-0.738432	
	C	-4.423490	-1.641914	-0.176732	
	N	-1.412054	2.034630	-0.341347	
	C	-3.968076	-3.997227	0.210523	
	P	-4.135803	0.106942	0.323035	
	C	-3.755447	-2.653742	0.532503	
	H	-3.442800	-4.775842	0.769301	
	C	-0.354610	2.925268	0.198408	
	H	1.226868	1.455701	0.232531	
	H	-7.071628	-0.520285	0.178115	
	C	-5.594477	0.548590	1.357686	
	Pt	-2.120925	0.592955	1.232813	
	C	-6.896511	0.124922	1.041294	
	H	-3.058189	-2.381074	1.327553	
	H	-0.841613	3.625885	0.893755	
	C	0.686500	2.105414	0.944968	
	H	-4.374486	1.676666	2.738248	
	C	-5.390343	1.362812	2.483305	
	H	1.430758	2.779894	1.397275	
	C	-7.976904	0.517106	1.834294	
	H	-8.985584	0.179767	1.582171	
	H	-2.466914	-0.386312	2.401710	
	S	-0.069294	1.082468	2.288268	
	C	-6.475327	1.755061	3.274437	
	C	-7.768249	1.334573	2.951348	
	H	-6.305260	2.386020	4.150460	
	H	-8.614985	1.637675	3.572756	
	H	0.113413	3.510371	-0.616702	
Zero-point correction=	0.371639 (Hartree/Particle)				
Thermal correction to Energy=	0.395111				
Thermal correction to Enthalpy=	0.396055				
Thermal correction to Gibbs Free Energy=	0.314782				
Sum of electronic and zero-point Energies=	-1688.058843				
Sum of electronic and thermal Energies=	-1688.035371				
Sum of electronic and thermal Enthalpies=	-1688.034427				
Sum of electronic and thermal Free Energies=	-1688.115700				

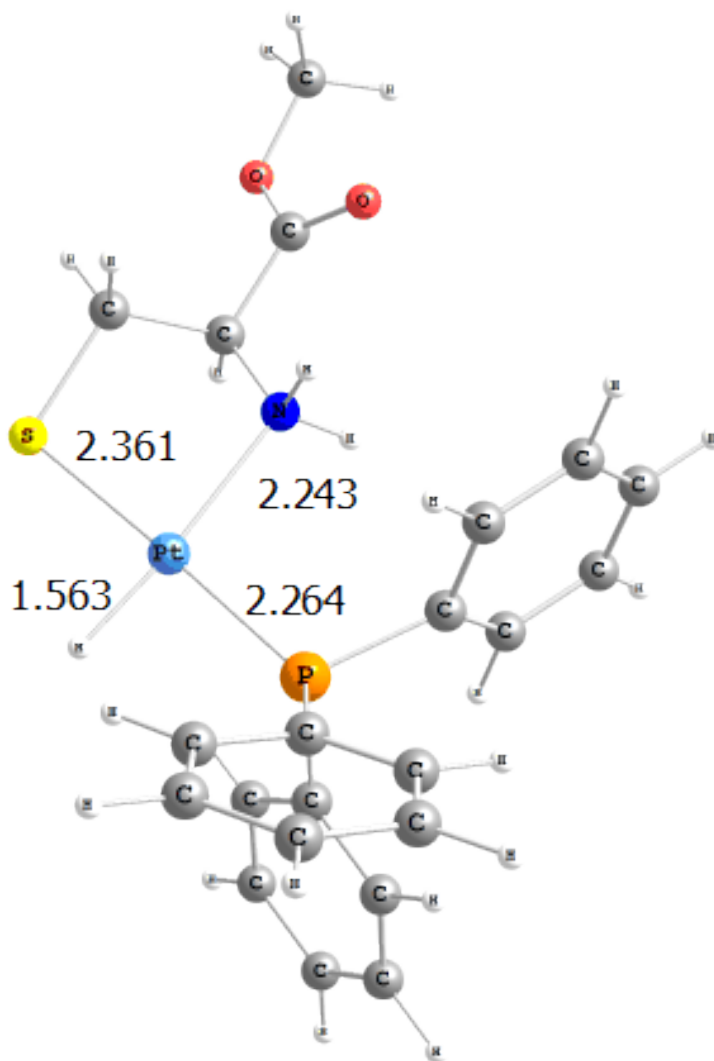
trans-5



Zero-point correction=	0.371411 (Hartree/Particle)
Thermal correction to Energy=	0.394787
Thermal correction to Enthalpy=	0.395731
Thermal correction to Gibbs Free Energy=	0.315228
Sum of electronic and zero-point Energies=	-1688.055062
Sum of electronic and thermal Energies=	-1688.031686
Sum of electronic and thermal Enthalpies=	-1688.030741
Sum of electronic and thermal Free Energies=	-1688.111245

H	-8.219258	-2.726137	2.491255
H	-6.722181	-2.714647	0.492538
C	-7.196700	-2.348677	2.573688
C	-6.357506	-2.342014	1.453228
H	-7.374355	-1.861452	4.674097
C	-6.723778	-1.865148	3.795761
H	-2.141683	-5.731284	3.465488
C	-5.055837	-1.849085	1.554395
H	-3.538604	-3.692171	3.273882
H	-4.409572	-1.822501	0.674511
C	-1.663578	-4.760687	3.309584
C	-5.414577	-1.382384	3.903727
C	-2.452342	-3.610055	3.200134
H	0.342567	-5.569055	3.305759
C	-4.570287	-1.369907	2.782809
C	-0.272082	-4.668989	3.220575
H	-5.056404	-1.012872	4.866127
H	-0.849410	1.009798	-1.039342
H	-2.067154	2.098305	-0.952083
C	-1.849294	-2.359678	2.994645
N	-1.298004	1.689641	-0.418682
C	0.331828	-3.422170	3.019741
P	-2.820859	-0.798455	2.878265
C	-0.448595	-2.270439	2.901817
H	1.419987	-3.344957	2.949822
C	-0.315779	2.732992	-0.010221
H	1.279627	1.371489	0.504780
H	-2.266159	-1.925063	5.587991
C	-2.673867	-0.061464	4.555443
Pt	-2.082819	0.524388	1.233382
C	-2.416608	-0.848028	5.690204
H	0.021764	-1.295639	2.739783
H	-0.884891	3.548388	0.461075
C	0.671045	2.154838	0.992760
H	-3.010313	1.942723	3.814378
C	-2.847063	1.324315	4.699302
H	1.364017	2.948054	1.315772
C	-2.344024	-0.255373	6.953642
H	-2.137543	-0.873387	7.831230
H	-3.281112	0.031075	0.304016
S	-0.193503	1.481258	2.474143
C	-2.778092	1.911621	5.965062
C	-2.527460	1.124304	7.092984
H	-2.906758	2.992002	6.067038
H	-2.465213	1.587191	8.081357
H	0.200997	3.134460	-0.902685

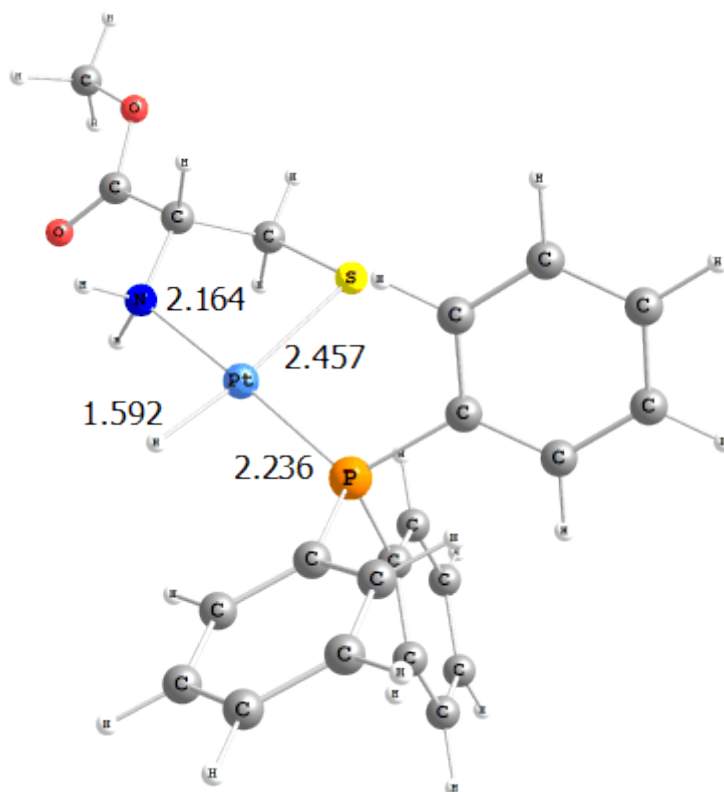
cis-6



H	-4.386313	3.620458	-4.127767
H	-2.932182	1.590948	-4.131266
C	-4.394248	2.939126	-3.273495
C	-3.579413	1.800396	-3.276092
H	-5.854935	4.087202	-2.165543
C	-5.214890	3.201171	-2.173106
H	-5.920955	-3.455370	-2.591478
C	-3.584552	0.933465	-2.182007
H	-5.677024	-1.100090	-1.863994
H	-2.939867	0.050020	-2.186213
C	-5.307423	-3.219214	-1.718170
C	-5.223161	2.333024	-1.074660
C	-5.174582	-1.891586	-1.302870
H	-4.756907	-5.278907	-1.348350
C	-4.408229	1.190571	-1.069753
H	2.422997	4.909079	-1.595442
O	0.128902	3.540716	-1.747784
C	-4.654032	-4.240967	-1.021399
H	-5.865566	2.548451	-0.217886
H	-1.163883	1.708086	-0.844029
H	-2.295000	2.758243	-0.363528
C	1.726149	5.559735	-1.045191
C	-4.384916	-1.572904	-0.184003
C	0.223255	3.809649	-0.572361
H	2.278450	6.314907	-0.472991
N	-1.528525	2.181203	-0.010936
C	-3.860748	-3.929858	0.087194
P	-4.197887	0.149872	0.436448
O	0.977490	4.803126	-0.088569
C	-3.720231	-2.602644	0.502282
H	-3.338819	-4.722930	0.628488
C	-0.460952	3.032953	0.546013
H	1.088083	1.526185	0.586619
H	-7.092906	-0.560043	0.090292
C	-5.719469	0.465367	1.423522
Pt	-2.244391	0.651732	1.465885
C	-6.986874	0.023545	1.007029
H	-3.081863	-2.356081	1.353331
H	-0.913597	3.740462	1.257300
C	0.558682	2.174187	1.307819
H	-4.614567	1.527341	2.946193
C	-5.603385	1.199163	2.614859
H	1.305578	2.833779	1.773305
C	-8.120235	0.319045	1.767181
H	-9.101535	-0.031308	1.436937
H	-2.611136	-0.393634	2.568933
S	-0.246117	1.156050	2.618344
C	-6.741332	1.494473	3.373074
C	-7.999432	1.056755	2.950787
H	-6.640107	2.063462	4.300667
H	-8.887581	1.284291	3.546083
H	1.053972	6.042827	-1.770874

Zero-point correction= 0.414361 (Hartree/Particle)
 Thermal correction to Energy= 0.442463
 Thermal correction to Enthalpy= 0.443407
 Thermal correction to Gibbs Free Energy= 0.350559
 Sum of electronic and zero-point Energies= -1915.733121
 Sum of electronic and thermal Energies= -1915.705018
 Sum of electronic and thermal Enthalpies= -1915.704074
 Sum of electronic and thermal Free Energies= -1915.796922

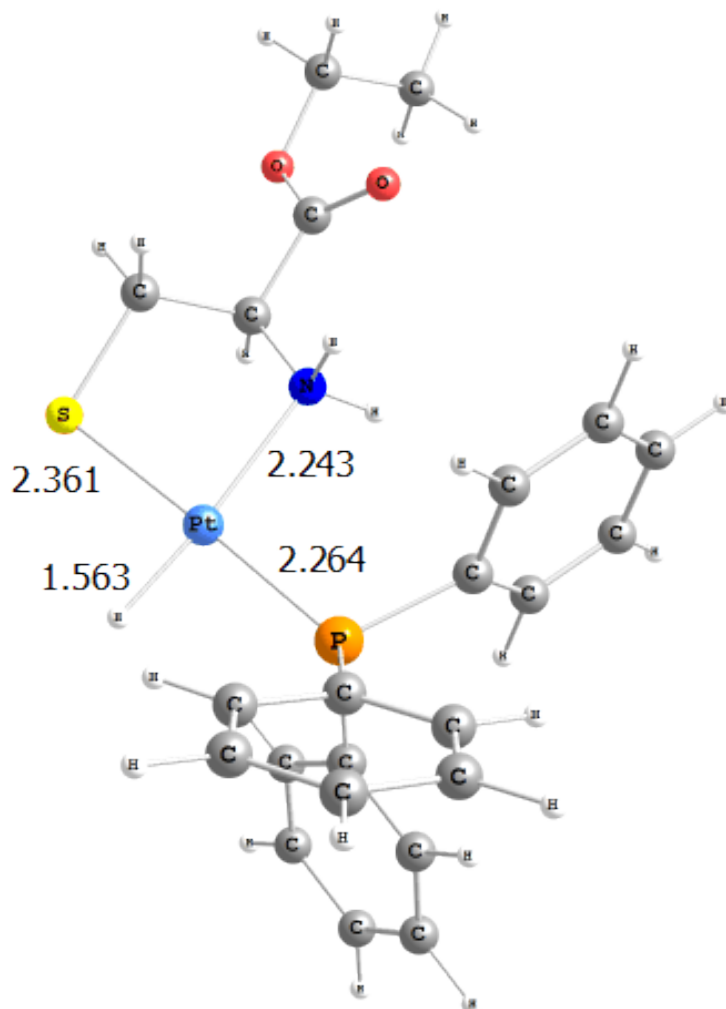
trans-6



Zero-point correction= 0.414122 (Hartree/Particle)
Thermal correction to Energy= 0.442133
Thermal correction to Enthalpy= 0.443077
Thermal correction to Gibbs Free Energy= 0.351064
Sum of electronic and zero-point Energies= -1915.728808
Sum of electronic and thermal Energies= -1915.700797
Sum of electronic and thermal Enthalpies= -1915.699853
Sum of electronic and thermal Free Energies= -1915.791866

H	-8.188667	-2.829053	2.264713
H	-6.671999	-2.516690	0.305577
C	-7.183438	-2.424268	2.408018
C	-6.333365	-2.248957	1.309740
H	-7.403651	-2.202523	4.548870
C	-6.744049	-2.073988	3.686827
H	-2.010796	-5.689798	2.997939
C	-5.054126	-1.720927	1.489830
H	-3.485769	-3.697238	3.010965
H	-4.399977	-1.563363	0.629704
C	-1.569769	-4.690096	2.966415
C	-5.457192	-1.556321	3.872609
C	-2.402569	-3.565616	2.972583
H	0.467239	-5.415218	2.914418
C	-4.602341	-1.374887	2.774486
H	2.534779	4.813814	-1.681961
O	0.315870	3.321675	-1.784184
C	-0.181785	-4.535528	2.920200
H	-5.124590	-1.291971	4.877891
H	-0.965556	1.601641	-0.733327
H	-2.190447	2.629327	-0.454918
C	1.772336	5.504566	-1.290718
C	-1.847046	-2.277784	2.926844
C	0.306588	3.772457	-0.661861
H	2.247837	6.364031	-0.803091
N	-1.413937	2.152385	0.007371
C	0.374645	-3.251697	2.878450
P	-2.879079	-0.752434	2.967064
O	0.979836	4.863989	-0.284842
C	-0.449669	-2.124844	2.876821
H	1.459815	-3.125385	2.842009
C	-0.431915	3.140517	0.510978
H	1.154324	1.729578	0.916446
H	-2.300503	-2.146309	5.545178
C	-2.785488	-0.200855	4.717657
Pt	-2.167850	0.777179	1.498917
C	-2.502476	-1.095162	5.762831
H	-0.016302	-1.120728	2.839147
H	-0.975738	3.920397	1.065024
C	0.550818	2.464719	1.478678
H	-3.210854	1.854985	4.196055
C	-3.025460	1.151218	5.010155
H	1.238018	3.228427	1.871340
C	-2.469846	-0.642488	7.084563
H	-2.242983	-1.343361	7.892044
H	-3.329945	0.347096	0.498752
S	-0.334977	1.662843	2.874198
C	-2.995974	1.598205	6.333391
C	-2.719067	0.703576	7.371681
H	-3.176590	2.653674	6.551387
H	-2.687881	1.057055	8.405635
H	1.141025	5.838130	-2.128418

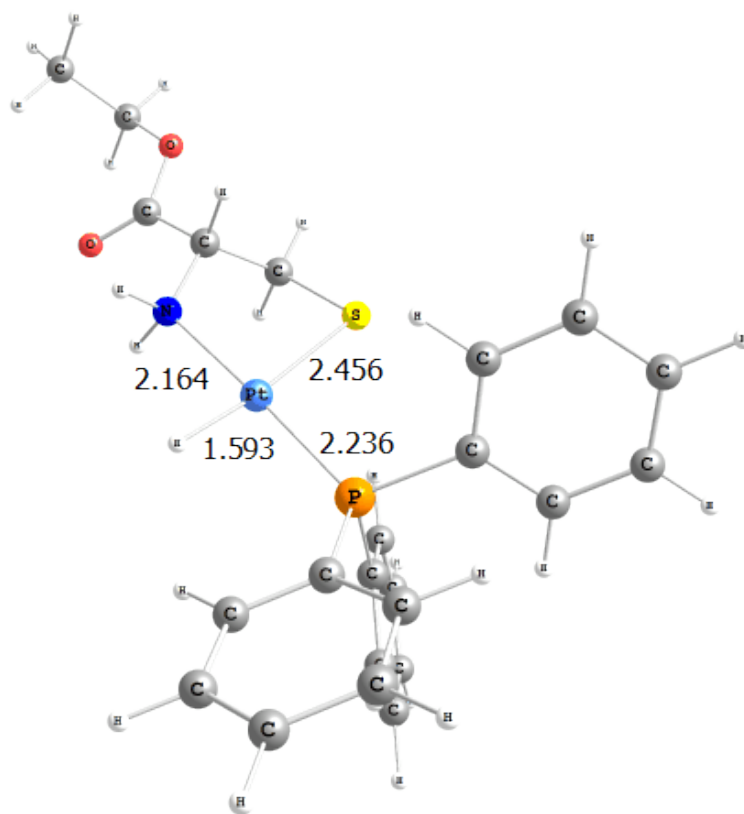
cis-7



Zero-point correction= 0.442917 (Hartree/Particle)
 Thermal correction to Energy= 0.472165
 Thermal correction to Enthalpy= 0.473109
 Thermal correction to Gibbs Free Energy= 0.377390
 Sum of electronic and zero-point Energies= -1954.998156
 Sum of electronic and thermal Energies= -1954.968907
 Sum of electronic and thermal Enthalpies= -1954.967963
 Sum of electronic and thermal Free Energies= -1955.063683

H	-4.367812	3.838756	-3.915730
H	-2.888649	1.828824	-3.992274
C	-4.380406	3.117467	-3.094948
C	-3.551598	1.989672	-3.138610
H	-5.872216	4.194245	-1.957241
C	-5.221130	3.317134	-1.996661
H	-5.850926	-3.315990	-2.738243
C	-3.562871	1.071574	-2.087169
H	-5.641239	-0.995835	-1.896066
H	-2.906961	0.197130	-2.122830
C	-5.251685	-3.115844	-1.846204
C	-5.235472	2.397591	-0.940889
C	-5.138208	-1.808336	-1.366349
H	-4.684748	-5.185391	-1.567339
C	-4.406550	1.265829	-0.977111
H	2.142483	5.080660	-1.435123
O	0.109310	3.680169	-1.485299
C	-4.597097	-4.163305	-1.189875
H	-5.893577	2.564517	-0.085210
H	-1.168547	1.797275	-0.682141
H	-2.315531	2.815430	-0.172506
H	1.457808	7.477879	-1.865059
H	0.055331	6.375046	-1.891008
C	1.697661	5.709610	-0.648731
C	-4.367014	-1.535823	-0.222655
C	0.193520	3.899194	-0.297723
H	2.500224	6.121674	-0.020854
N	-1.549412	2.229426	0.165751
C	0.836937	6.807650	-1.249509
C	-3.822065	-3.897810	-0.056776
P	-4.205654	0.157218	0.481190
O	0.934170	4.871229	0.244638
C	-3.700951	-2.590626	0.422997
H	-3.299220	-4.710725	0.453311
C	-0.497492	3.064821	0.774939
H	1.066454	1.573205	0.770412
H	-7.087830	-0.570404	0.066430
H	0.360130	7.406464	-0.458013
C	-5.743570	0.411627	1.460666
Pt	-2.271440	0.628157	1.560184
C	-7.000265	-0.026026	1.008877
H	-3.076618	-2.378691	1.293580
H	-0.966664	3.736116	1.510276
C	0.519290	2.182102	1.512156
H	-4.670554	1.418615	3.042316
C	-5.651233	1.094149	2.684155
H	1.252072	2.826905	2.018806
C	-8.146544	0.223155	1.766299
H	-9.119358	-0.123713	1.408398
H	-2.643262	-0.470277	2.608836
S	-0.293958	1.096563	2.762309
C	-6.802041	1.343210	3.439531
C	-8.049444	0.909969	2.982255
H	-6.719282	1.872329	4.392225
H	-8.947650	1.101184	3.575248

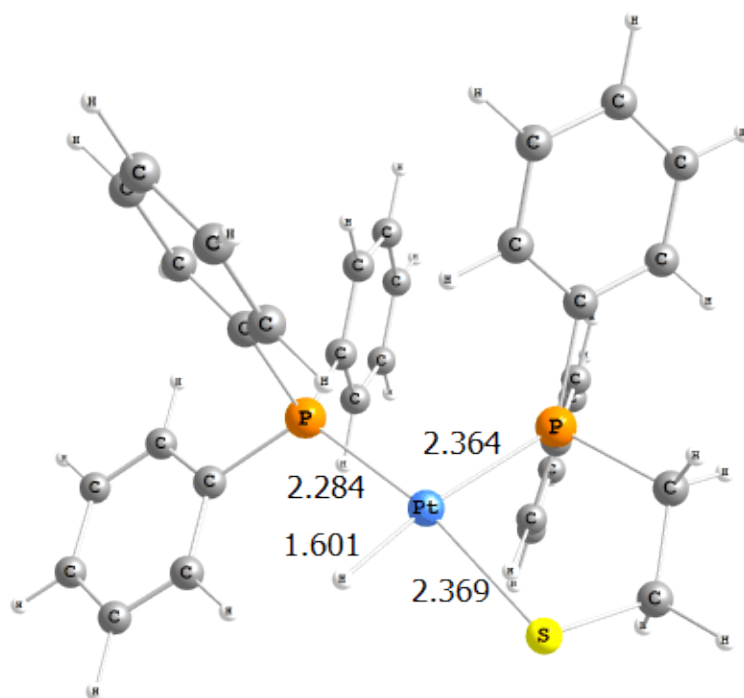
trans-7



Zero-point correction= 0.442612 (Hartree/Particle)
Thermal correction to Energy= 0.471797
Thermal correction to Enthalpy= 0.472741
Thermal correction to Gibbs Free Energy= 0.377659
Sum of electronic and zero-point Energies= -1954.993861
Sum of electronic and thermal Energies= -1954.964677
Sum of electronic and thermal Enthalpies= -1954.963732
Sum of electronic and thermal Free Energies= -1955.058814

H	-8.193505	-2.786165	2.205842
H	-6.672029	-2.370931	0.269660
C	-7.189579	-2.387163	2.372604
C	-6.336788	-2.154178	1.287176
H	-7.416323	-2.275616	4.521310
C	-6.754569	-2.101842	3.668898
H	-2.004941	-5.664124	2.787296
C	-5.059276	-1.633401	1.497760
H	-3.486716	-3.680699	2.914562
H	-4.403067	-1.430640	0.648712
C	-1.567552	-4.662530	2.807621
C	-5.469297	-1.591791	3.884687
C	-2.404171	-3.543134	2.878235
H	0.471699	-5.376196	2.707089
C	-4.611823	-1.352740	2.799800
H	2.262407	5.079439	-1.512653
O	0.271764	3.617701	-1.486236
C	-0.180337	-4.500514	2.763298
H	-5.140101	-1.378532	4.903150
H	-0.991227	1.833988	-0.532673
H	-2.216683	2.841652	-0.192889
H	1.552851	7.374807	-2.305011
H	0.179789	6.236795	-2.263677
C	1.755819	5.795334	-0.847408
C	-1.853384	-2.252573	2.899360
C	0.276873	4.001675	-0.338184
H	2.508064	6.312361	-0.235198
N	-1.438848	2.339788	0.239791
C	0.909614	6.775179	-1.641570
C	0.371388	-3.214245	2.788174
P	-2.890916	-0.735766	3.027715
O	0.956936	5.061781	0.106734
C	-0.456817	-2.091972	2.851150
H	1.455923	-3.082082	2.753551
C	-0.457100	3.298773	0.797592
H	1.133352	1.870972	1.118533
H	-2.311125	-2.275086	5.521289
H	0.371092	7.460438	-0.968742
C	-2.798921	-0.285854	4.807321
Pt	-2.187062	0.878699	1.649625
C	-2.514766	-1.238588	5.799214
H	-0.027183	-1.085652	2.866000
H	-1.001300	4.044521	1.396545
C	0.528322	2.570449	1.723054
H	-3.227517	1.796041	4.405371
C	-3.041059	1.046669	5.177423
H	1.213811	3.311976	2.158573
C	-2.483021	-0.863014	7.144885
H	-2.255218	-1.609038	7.910572
H	-3.350648	0.504864	0.628503
S	-0.353234	1.685989	3.070744
C	-3.012422	1.416516	6.524304
C	-2.734286	0.463855	7.509254
H	-3.194694	2.457366	6.802834
H	-2.703760	0.757065	8.561912

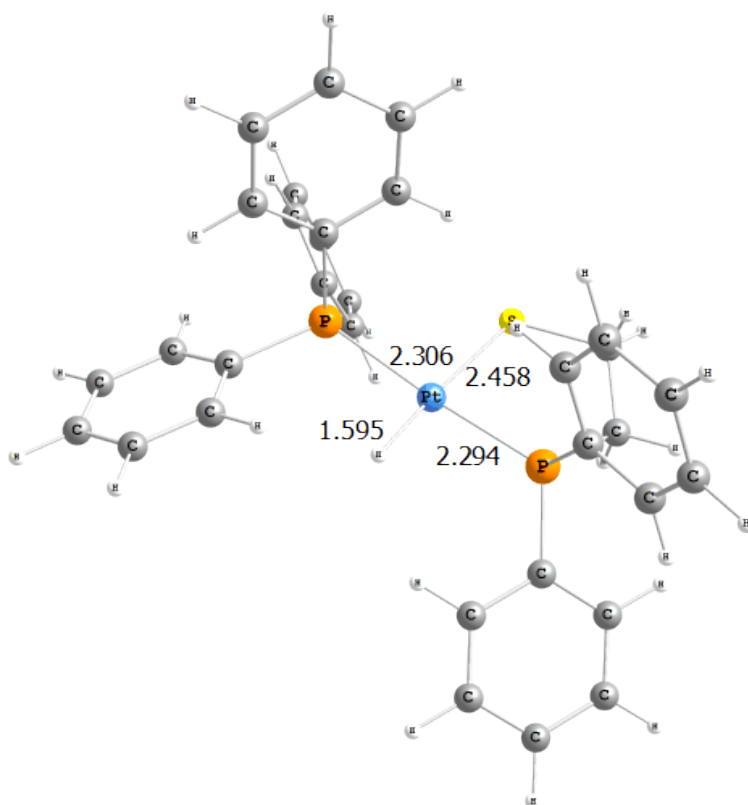
cis-8



Zero-point correction= 0.526825 (Hartree/Particle)
Thermal correction to Energy= 0.560289
Thermal correction to Enthalpy= 0.561233
Thermal correction to Gibbs Free Energy= 0.458695
Sum of electronic and zero-point Energies= -2436.273147
Sum of electronic and thermal Energies= -2436.239683
Sum of electronic and thermal Enthalpies= -2436.238739
Sum of electronic and thermal Free Energies= -2436.341277

H	-6.523438	0.136822	-4.092588
H	-5.026084	2.101602	-3.725661
C	-5.523493	-0.005383	-3.675038
C	-4.682976	1.095463	-3.476425
H	-5.736445	-2.148879	-3.467699
C	-5.083980	-1.283721	-3.325213
H	-7.649406	1.952706	-1.262901
C	-3.412333	0.916983	-2.931450
H	-2.770710	1.784952	-2.764829
H	-6.624608	4.219295	-1.454669
C	-3.803954	-1.467470	-2.790548
C	-6.642123	2.133750	-0.878890
C	-6.066005	3.401227	-0.992475
C	-2.953480	-0.369668	-2.593928
H	-3.474551	-2.473339	-2.529133
H	-6.387016	0.095020	-0.239066
H	-3.883539	-4.787992	-0.177353
H	-1.328950	-0.053417	-4.724711
C	-5.930970	1.084132	-0.288639
H	0.200831	1.141835	-6.250528
H	-6.189316	-5.090262	0.741607
H	-1.242395	-2.335030	-4.163676
C	-4.417259	-3.942889	0.264955
C	-4.763830	3.614452	-0.525879
H	-4.298016	4.598169	-0.625751
H	0.296631	0.305729	0.260927
C	-5.704561	-4.111390	0.781983
H	-2.788164	-2.567474	-0.068068
C	-0.456051	0.457062	-4.312759
C	-3.799873	-2.689965	0.317697
C	0.402139	1.140685	-5.176110
C	-4.632829	1.293912	0.197662
C	-6.366488	-3.025681	1.366796
C	-4.047499	2.567435	0.056757
C	-0.852605	-2.880240	-3.302004
H	-7.366644	-3.155775	1.788140
H	-0.501421	-4.678976	-4.441983
P	-1.308117	-0.507960	-1.777083
C	-4.463126	-1.589286	0.879815
C	-0.216172	0.446711	-2.926001
C	-5.748309	-1.774065	1.421993
Pt	-1.291474	0.165208	0.405774
C	-0.436649	-4.203469	-3.459911
H	-3.015574	2.726131	0.382822
C	1.510609	1.826316	-4.667384
H	2.180541	2.363916	-5.343470
C	-0.779760	-2.256852	-2.044082
P	-3.577649	0.012907	0.988442
H	-6.270729	-0.940070	1.896851
C	0.891971	1.145208	-2.423680
C	1.750870	1.827843	-3.291258
C	0.063629	-4.918194	-2.364871
C	-0.270310	-2.977610	-0.952096
H	1.073469	1.159694	-1.347753
H	2.608676	2.368621	-2.883569
H	-0.204389	-2.491348	0.025017
C	-3.659333	0.396148	2.810254
H	-4.683859	0.700529	3.083629
C	0.148308	-4.302815	-1.113336
S	-0.920272	1.047703	2.572429
H	-2.930167	2.439468	2.810728
H	-3.429226	-0.556867	3.312977
C	-2.622682	1.448784	3.184815
H	0.543634	-4.852384	-0.255369
H	-2.553451	1.527466	4.281803
H	0.389950	-5.953861	-2.490634

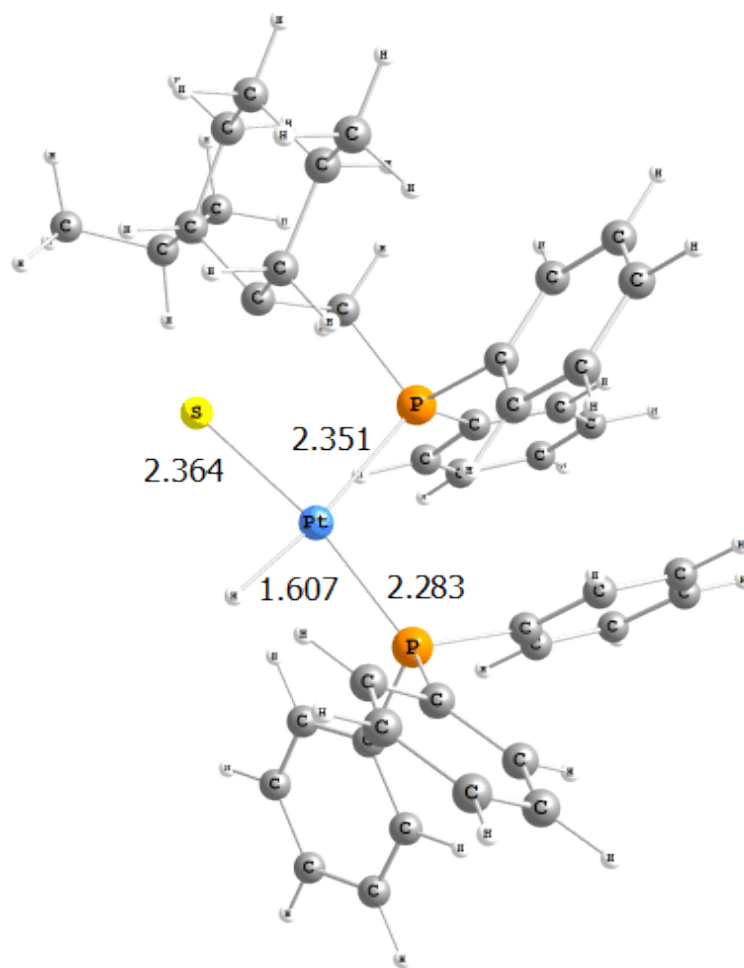
trans-8



Zero-point correction= 0.525963 (Hartree/Particle)
Thermal correction to Energy= 0.559942
Thermal correction to Enthalpy= 0.560886
Thermal correction to Gibbs Free Energy= 0.453876
Sum of electronic and zero-point Energies= -2436.271847
Sum of electronic and thermal Energies= -2436.237869
Sum of electronic and thermal Enthalpies= -2436.236924
Sum of electronic and thermal Free Energies= -2436.343934

H	2.616789	-2.290589	-5.242008
H	0.585132	-0.859870	-4.992358
C	2.314827	-1.933795	-4.253879
C	1.175851	-1.132177	-4.113897
H	3.947877	-2.911110	-3.224799
C	3.060330	-2.281041	-3.124629
H	-6.901427	3.452335	-0.065328
C	0.782341	-0.686515	-2.851104
H	-0.119343	-0.080430	-2.739206
H	-5.207264	5.280869	-0.165122
C	2.676346	-1.824698	-1.858707
C	-5.840701	3.224960	0.069164
C	-4.890381	4.249812	0.012155
C	1.533232	-1.023636	-1.712032
H	3.270622	-2.099008	-0.985269
H	-6.189398	1.112945	0.327060
H	-5.086215	-3.020991	-2.842077
H	2.790947	1.238515	-1.902675
C	-5.438205	1.905542	0.293492
H	3.573431	3.589197	-1.806389
H	-7.230137	-3.629613	-1.719094
H	3.754129	0.121591	0.983031
C	-5.322932	-2.615055	-1.855343
C	-3.534218	3.950343	0.173963
H	-2.785283	4.744754	0.122540
H	-1.560540	-0.457125	-1.172419
C	-6.523433	-2.957764	-1.225194
H	-3.464294	-1.512690	-1.699025
C	2.474958	1.878399	-1.076289
C	-4.414442	-1.763065	-1.222438
C	2.916514	3.205330	-1.021493
C	-4.077762	1.598598	0.459398
C	-6.813531	-2.446560	0.043488
C	-3.126292	2.631243	0.390838
C	3.356854	-0.781580	1.452063
H	-7.746475	-2.717342	0.544456
H	5.144184	-1.136270	2.610883
P	1.001289	-0.356691	-0.079975
C	-4.704136	-1.235007	0.046700
C	1.627291	1.376451	-0.077321
C	-5.909679	-1.589264	0.677680
Pt	-1.256591	-0.370076	0.390569
C	4.138510	-1.489479	2.368709
H	-2.064185	2.393516	0.496037
C	2.520247	4.034969	0.030678
H	2.865379	5.071500	0.070760
C	2.060937	-1.224297	1.140787
P	-3.492970	-0.107376	0.829188
H	-6.151002	-1.202057	1.669958
C	1.228799	2.214290	0.980726
C	1.679527	3.534685	1.032197
C	3.632554	-2.642059	2.979316
C	1.553434	-2.375113	1.764375
H	0.568225	1.822233	1.760416
H	4.243495	-3.191748	3.700150
H	1.368277	4.178190	1.859330
H	0.531795	-2.698708	1.553230
C	-3.744265	-0.271170	2.661469
H	-4.710052	0.174404	2.955266
C	2.340585	-3.082432	2.676517
S	-0.928434	-0.260901	2.824026
H	-2.608955	1.481684	3.244094
H	-3.767319	-1.351954	2.875484
C	-2.567986	0.387663	3.381615
H	1.935206	-3.972664	3.163561
H	-2.643488	0.195208	4.463682

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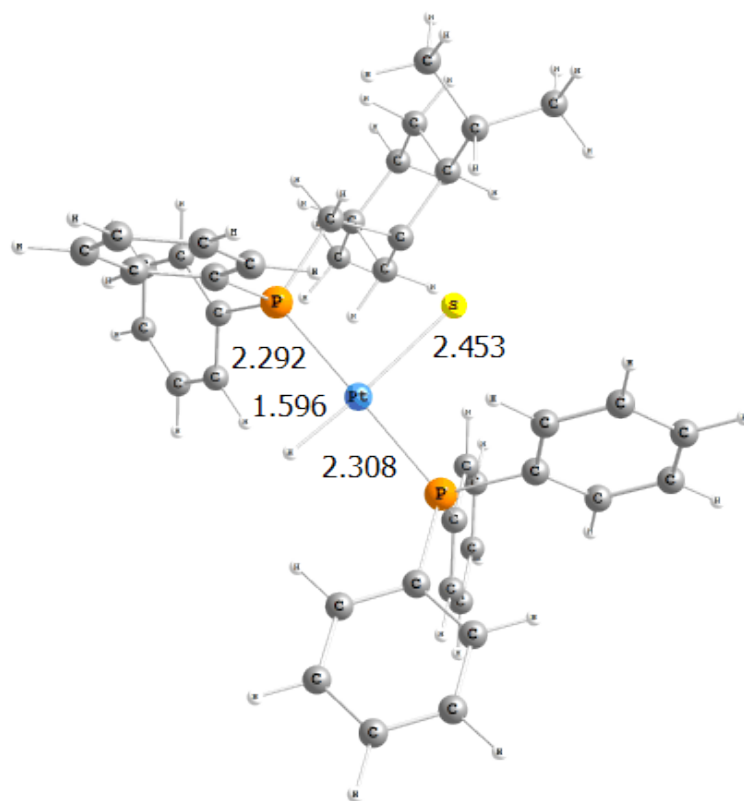


Zero-point correction= 0.761561 (Hartree/Particle)
 Thermal correction to Energy= 0.805028
 Thermal correction to Enthalpy= 0.805972
 Thermal correction to Gibbs Free Energy= 0.682578
 Sum of electronic and zero-point Energies= -2788.441544
 Sum of electronic and thermal Energies= -2788.398076
 Sum of electronic and thermal Enthalpies= -2788.397132
 Sum of electronic and thermal Free Energies= -2788.520527

H	2.630534	-3.916791	-5.203511
H	2.158852	-1.524830	-4.664645
C	2.264933	-3.638719	-4.211600
H	-5.842807	1.393875	-4.008099
H	-4.218775	2.056840	-4.319522
H	2.251229	-5.673503	-3.471554
H	-4.416175	0.326993	-3.936527
C	2.000924	-2.299555	-3.910119
C	-4.784927	1.338708	-3.701721
H	-2.801765	-2.992693	-4.196184
C	2.053179	-4.623512	-3.241000
H	-5.280350	-3.302663	-4.173131
C	-3.385303	-2.696459	-3.320908
C	-4.773159	-2.867605	-3.308242
H	-6.251793	3.088639	-2.083453
H	-4.667112	3.797398	-2.433465
C	1.527833	-1.942236	-2.643886
C	-4.617889	1.650885	-2.213749
C	-5.179124	3.025172	-1.829262
C	1.582567	-4.270150	-1.973891
H	1.311095	-0.896697	-2.412843
H	-2.584907	2.353478	-2.353084
H	-5.181367	0.883961	-1.650676
H	-1.658607	-1.970188	-2.238305
C	-2.739073	-2.133041	-2.217531
C	-5.513544	-2.467996	-2.190533
H	-6.599843	-2.587746	-2.180986
H	-2.696658	0.625536	-2.099319
C	1.318858	-2.924386	-1.660244
H	1.401763	-5.052666	-1.234004
C	-3.143016	1.582861	-1.794654
C	-4.970806	3.317429	-0.341082
H	-5.342179	4.327814	-0.101004
C	-3.471813	-1.740172	-1.085752
C	-4.867518	-1.903898	-1.087169
H	-2.934378	3.925256	-0.525900
H	-5.591941	2.620313	0.246592
C	-2.886793	1.821780	-0.289238
C	-3.495700	3.209026	0.099904
P	0.709343	-2.384094	-0.004057
H	-5.459420	-1.583467	-0.226257
H	-4.535481	0.549617	0.461418
Pt	-0.321404	-0.347664	-0.033590
S	-1.019935	1.911273	-0.041148
P	-2.576575	-0.923876	0.293834
C	-3.449806	0.686104	0.583511
H	-3.791699	5.750365	1.231699
H	-2.052237	5.394756	1.067353
H	-4.283596	-3.365114	1.014399
C	-2.959237	5.152765	1.643304
C	-3.269603	3.650679	1.578966
H	-5.315407	3.918291	2.341803
H	-3.261352	0.907840	1.641942
H	-2.367097	3.121890	1.927126
C	-3.794548	-2.977091	1.908534
C	-2.942508	-1.868476	1.825808
C	-4.415236	3.316850	2.548882
H	-4.712362	2.258275	2.514840
H	-2.798080	5.484475	2.682462
H	-4.667450	-4.481030	3.186275
H	-4.108779	3.538868	3.584205
C	-4.005536	-3.612716	3.136910
C	-2.281113	-1.424172	2.987164
H	-1.583924	-0.583644	2.921033
C	-3.366777	-3.152595	4.289844
C	-2.497899	-2.057706	4.210911
H	-3.535210	-3.651835	5.247504
H	-1.981025	-1.700237	5.105188
H	1.155512	0.255094	-0.228149
C	-0.291105	-3.816596	0.587987
C	-1.165320	-4.490209	-0.281856
C	-0.264109	-4.187163	1.942542
C	-1.974910	-5.527318	0.187354
H	-1.209904	-4.217295	-1.336499
C	-1.076793	-5.222533	2.409352
H	0.396438	-3.666859	2.638678
C	-1.928622	-5.900437	1.533245
H	-2.645155	-6.042526	-0.505439
H	-1.049019	-5.493249	3.467213
H	-2.563764	-6.709904	1.901645
C	2.182686	-2.440442	1.105410
C	3.120448	-3.484661	1.044831
C	2.338185	-1.435300	2.072749
C	4.194606	-3.521505	1.936329

	H	3.021643	-4.272848	0.296566
	C	3.410817	-1.478926	2.969478
	H	1.620293	-0.612715	2.111502
	C	4.340588	-2.519808	2.902700
	H	4.921910	-4.335160	1.875054
	H	3.521964	-0.689329	3.716923
	H	5.182511	-2.549647	3.599267

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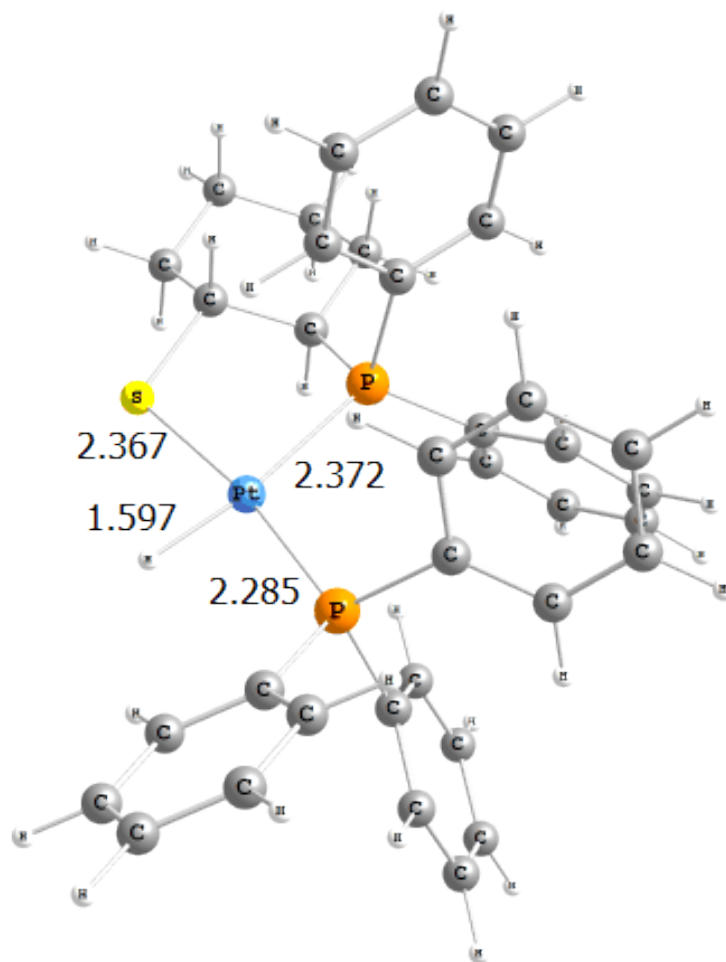


Zero-point correction= 0.760758 (Hartree/Particle)
Thermal correction to Energy= 0.804734
Thermal correction to Enthalpy= 0.805678
Thermal correction to Gibbs Free Energy= 0.678415
Sum of electronic and zero-point Energies= -2788.439120
Sum of electronic and thermal Energies= -2788.395144
Sum of electronic and thermal Enthalpies= -2788.394200
Sum of electronic and thermal Free Energies= -2788.521463

H	2.672172	1.074894	-5.513242
H	0.822771	2.150132	-4.223207
C	2.533074	0.840513	-4.454541
H	-4.989353	1.607271	-4.231407
H	-3.314255	2.213252	-4.218846
H	4.199374	-0.537943	-4.378531
H	-3.637671	0.482639	-3.937578
C	1.496136	1.443034	-3.731677
C	-4.008337	1.501484	-3.739268
H	-2.452043	-3.170401	-3.977335
C	3.388451	-0.063663	-3.819579
H	-4.925980	-3.196429	-4.303080
C	-3.111889	-2.774976	-3.201107
C	-4.497811	-2.789510	-3.383429
H	-5.687434	3.261548	-2.356352
H	-4.043140	3.918713	-2.382250
C	1.309010	1.139651	-2.382364
C	-4.106458	1.765708	-2.236042
C	-4.683117	3.148801	-1.911608
C	3.212012	-0.367283	-2.464573
H	0.494141	1.600898	-1.816782
H	-2.059342	2.387674	-1.982319
H	-4.788618	1.006181	-1.812106
H	-1.478847	-2.217368	-1.887655
C	-2.561758	-2.246651	-2.029306
C	-5.337192	-2.279253	-2.386964
H	-6.421340	-2.287817	-2.524697
H	-2.278579	0.657011	-1.812963
C	2.171447	0.232012	-1.739717
H	3.886161	-1.074522	-1.977150
C	-2.736202	1.625272	-1.559238
C	-4.743543	3.386521	-0.400562
H	-5.122154	4.401730	-0.194390
C	-3.397150	-1.726907	-1.027735
C	-4.790322	-1.750060	-1.215759
H	-2.689284	3.922386	-0.193272
H	-5.482853	2.694321	0.037080
C	-2.747319	1.815075	-0.024732
C	-3.377628	3.210297	0.294972
P	1.856297	-0.125435	0.038761
H	-5.456729	-1.352301	-0.446353
H	-4.549983	0.592809	0.393832
Pt	-0.390765	-0.555133	0.343896
S	-0.966662	1.818324	0.573653
P	-2.643949	-0.960323	0.458023
C	-3.493217	0.671937	0.692557
H	-3.793022	5.726493	1.444153
H	-2.064651	5.310395	1.584074
H	-4.350301	-3.445073	0.838354
C	-3.068530	5.086363	1.977907
C	-3.408711	3.599487	1.805148
H	-5.549916	3.916884	2.197004
H	-3.470188	0.842975	1.776521
H	-2.600158	3.027796	2.289635
C	-3.987344	-3.101909	1.808946
C	-3.183152	-1.957095	1.899709
C	-4.720069	3.277969	2.540664
H	-5.036737	2.232022	2.415383
H	-3.088731	5.381493	3.040208
H	-4.949688	-4.709765	2.882864
H	-4.599870	3.457396	3.621640
C	-4.323592	-3.817422	2.963998
C	-2.705422	-1.547879	3.158467
H	-2.046686	-0.677378	3.229092
C	-3.861733	-3.396545	4.213290
C	-3.050284	-2.259355	4.307941
H	-4.126608	-3.957253	5.113340
H	-2.675499	-1.931799	5.280980
H	-0.123912	-2.125471	0.238109
C	3.072181	-1.441531	0.464576
C	2.709235	-2.788037	0.301444
C	4.370399	-1.131035	0.903666
C	3.631148	-3.804848	0.561496
H	1.693817	-3.032302	-0.017016
C	5.287985	-2.151464	1.170925
H	4.669041	-0.090171	1.042132
C	4.922021	-3.489642	0.997977
H	3.335190	-4.848951	0.431394
H	6.292944	-1.897320	1.517707
H	5.640086	-4.286302	1.209315
C	2.473785	1.362189	0.920161
C	3.398169	2.248566	0.345721
C	1.997383	1.605142	2.218425
C	3.847148	3.358838	1.066775

	H	3.762020	2.077516	-0.669989
	C	2.452313	2.712503	2.937203
	H	1.248466	0.938667	2.652470
	C	3.377514	3.590462	2.363457
	H	4.562350	4.048255	0.610717
	H	2.069845	2.898571	3.943812
	H	3.725432	4.462277	2.923644

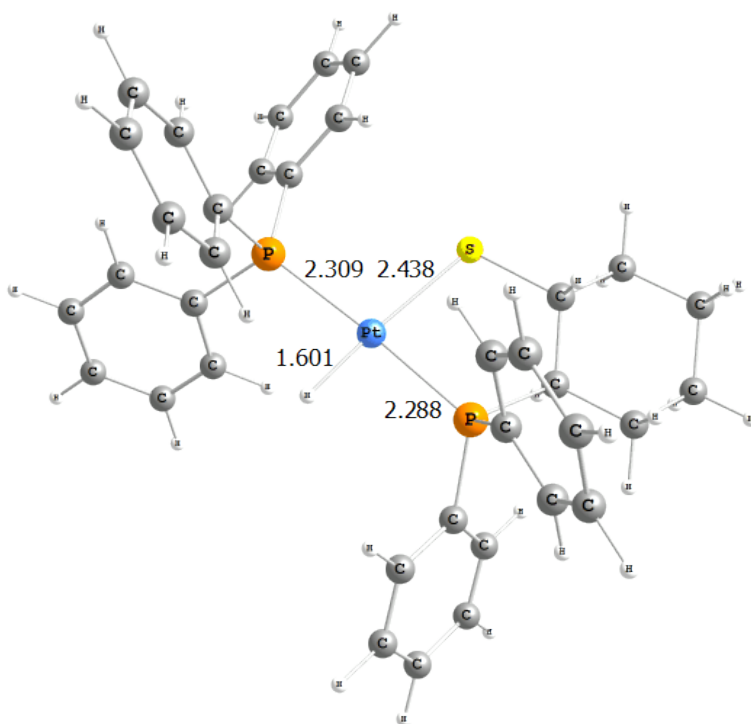
cis-10



Zero-point correction= 0.621087 (Hartree/Particle)
Thermal correction to Energy= 0.657905
Thermal correction to Enthalpy= 0.658850
Thermal correction to Gibbs Free Energy= 0.549554
Sum of electronic and zero-point Energies= -2592.140331
Sum of electronic and thermal Energies= -2592.103513
Sum of electronic and thermal Enthalpies= -2592.102569
Sum of electronic and thermal Free Energies= -2592.211864

H	4.577687	-3.940591	-4.340232
H	4.377442	-1.579291	-3.552007
C	3.808336	-3.667961	-3.613199
H	3.006130	-5.672255	-3.469043
C	3.696378	-2.344604	-3.171313
H	-4.819941	-2.336179	-3.835627
C	2.928458	-4.637291	-3.125962
H	-6.684381	-3.539982	-2.689480
C	-4.869463	-2.360574	-2.744072
C	-5.914878	-3.032710	-2.101756
C	2.706705	-1.991930	-2.252641
C	1.942422	-4.289321	-2.195782
H	2.607768	-0.953768	-1.928584
H	-3.052698	-1.208337	-2.493452
C	-3.878798	-1.722395	-1.993425
C	-5.975631	-3.048261	-0.704541
H	-6.794875	-3.564019	-0.196899
C	1.822838	-2.962658	-1.752430
H	1.265329	-5.058120	-1.818760
C	-5.075223	3.139475	-0.086959
H	-5.369974	4.195952	0.028950
C	-3.926892	-1.744993	-0.587992
C	-4.992276	-2.401153	0.049255
H	-3.630273	3.544362	-1.672253
C	-3.204705	1.592069	-0.834612
C	-3.665718	3.049187	-0.688517
P	0.579018	-2.456754	-0.487785
H	-5.054507	-2.415326	1.139161
Pt	-0.594076	-0.544007	-0.917280
S	-1.500655	1.542533	-1.571202
P	-2.599647	-0.846667	0.312399
C	-3.291040	0.872033	0.521844
H	-2.754474	-3.621971	1.318652
H	-2.567189	1.372971	1.189042
C	-2.564153	-2.967377	2.169350
C	-2.532720	-1.572570	1.995052
H	-2.360708	-4.618472	3.536156
C	-2.342019	-3.531362	3.427457
C	-2.276684	-0.758695	3.113817
H	-2.231418	0.326850	3.009156
C	-2.085549	-2.714946	4.532542
C	-2.057112	-1.326368	4.371528
H	-1.906503	-3.158251	5.515211
H	-1.859477	-0.677926	5.228950
H	0.646190	-0.088138	-1.813822
C	-0.476419	-3.958538	-0.313522
C	-1.546183	-4.095667	-1.213448
C	-0.291717	-4.928412	0.683216
C	-2.432009	-5.169061	-1.106142
H	-1.700142	-3.338144	-1.983523
C	-1.175117	-6.008356	0.785206
H	0.527806	-4.832541	1.397411
C	-2.250138	-6.126832	-0.101537
H	-3.275773	-5.242646	-1.796364
H	-1.028485	-6.753697	1.571295
H	-2.948171	-6.962726	-0.008244
C	1.559454	-2.428647	1.071819
C	2.719509	-3.202419	1.244515
C	1.099149	-1.635532	2.134379
C	3.396800	-3.191728	2.467332
H	3.098308	-3.813333	0.421952
C	1.772002	-1.634932	3.358406
H	0.212778	-1.015508	1.998655
C	2.921666	-2.412652	3.527743
H	4.300845	-3.793643	2.591028
H	1.395453	-1.019622	4.179193
H	3.452712	-2.406778	4.483219
C	-5.154510	2.411845	1.259576
C	-4.699373	0.951409	1.129820
H	-5.801293	2.685981	-0.786638
H	-6.180196	2.450856	1.663504
H	-4.507610	2.929676	1.991515
H	-5.406117	0.406223	0.480963
H	-4.722044	0.450882	2.112104
H	-2.946225	3.581443	-0.041100
H	-3.895752	1.086869	-1.533657

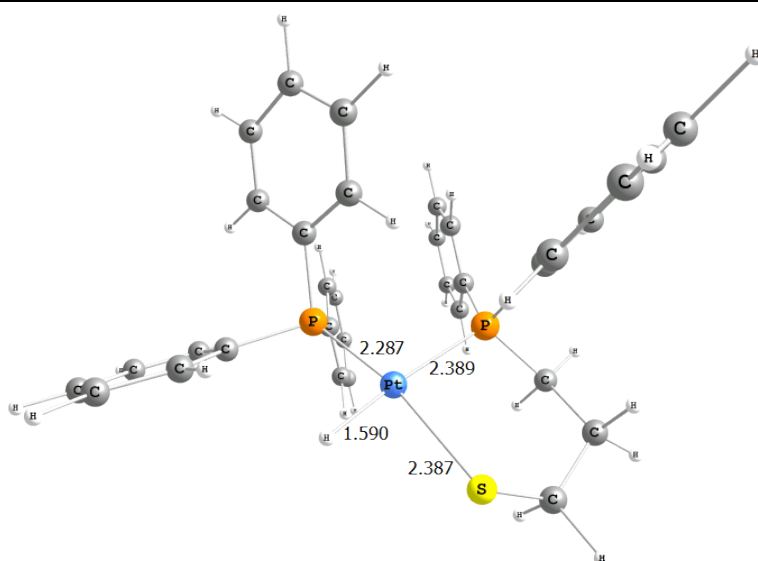
trans-10



Zero-point correction= 0.619861 (Hartree/Particle)
Thermal correction to Energy= 0.657190
Thermal correction to Enthalpy= 0.658134
Thermal correction to Gibbs Free Energy= 0.543890
Sum of electronic and zero-point Energies= -2592.133163
Sum of electronic and thermal Energies= -2592.095834
Sum of electronic and thermal Enthalpies= -2592.094890
Sum of electronic and thermal Free Energies= -2592.209134

H	3.280567	-1.112976	-5.611940
H	1.315262	-2.256718	-4.582037
C	3.014689	-0.915901	-4.570092
H	4.627979	0.493212	-4.259018
C	1.913786	-1.557176	-3.992739
H	-3.212939	-0.123356	-4.385340
C	3.769985	-0.015884	-3.812322
H	-5.408836	-1.303613	-4.507836
C	-3.656660	-0.52437	-3.483361
C	-4.886947	-1.213769	-3.551541
C	1.567013	-1.301057	-2.663788
C	3.428839	0.241067	-2.481042
H	0.699280	-1.789293	-2.215008
H	-2.013701	0.057965	-2.207552
C	-2.983361	-0.444419	-2.263237
C	-5.446823	-1.765236	-2.394088
H	-6.406842	-2.285598	-2.443245
C	2.326196	-0.402669	-1.894564
H	4.018101	0.954726	-1.901085
C	-4.856341	3.355568	1.211478
H	-5.197921	4.276191	1.713892
C	-3.543787	-0.991334	-1.096090
C	-4.781295	-1.652261	-1.170619
H	-2.897752	4.165430	0.689016
C	-2.800204	2.007136	0.555501
C	-3.322725	3.293360	1.211330
P	1.853117	-0.127384	-0.134824
H	-5.224489	-2.086321	-0.271427
Pt	-0.416731	-0.361167	0.217181
S	-0.946132	1.990577	0.584729
P	-2.655484	-0.745028	0.492316
C	-3.423313	0.775824	1.243532
H	-2.517854	-3.591109	0.011700
H	-3.052480	0.774045	2.284548
C	-2.917001	-3.468299	1.021703
C	-3.130729	-2.175609	1.532869
H	-3.031762	-5.590911	1.386219
C	-3.201137	-4.592423	1.797149
C	-3.615876	-2.032738	2.841837
H	-3.774436	-1.042099	3.270820
C	-3.692079	-4.442383	3.099858
C	-3.894769	-3.162155	3.619771
H	-3.911019	-5.323214	3.708725
H	-4.272113	-3.036108	4.637755
H	-0.166900	-1.928761	0.006229
C	2.867893	-1.333706	0.813170
C	4.178734	-1.661887	0.430346
C	2.322974	-1.910957	1.970940
C	4.934134	-2.552082	1.197679
H	4.611844	-1.226808	-0.473030
C	3.084281	-2.795893	2.740300
H	1.295526	-1.671750	2.256413
C	4.389094	-3.118376	2.355278
H	5.951428	-2.806153	0.888871
H	2.651483	-3.240167	3.640220
H	4.980989	-3.815645	2.954054
C	2.592191	1.503477	0.272554
C	2.138523	2.628793	-0.438964
C	3.534667	1.672540	1.298539
C	2.634962	3.897428	-0.137387
H	1.383448	2.512798	-1.218697
C	4.023603	2.947575	1.601158
H	3.890941	0.810482	1.865457
C	3.578260	4.060373	0.882929
H	2.271927	4.764817	-0.694107
H	4.756486	3.068497	2.403064
H	3.960998	5.056057	1.121708
C	-5.464640	2.121554	1.886432
C	-4.959527	0.828081	1.232297
H	-5.220534	3.413293	0.169119
H	-6.566295	2.157571	1.844012
H	-5.189973	2.118906	2.957391
H	-5.314665	0.787372	0.188576
H	-5.383937	-0.053396	1.740610
H	-2.945338	3.333220	2.248787
H	-3.128325	2.004938	-0.500337

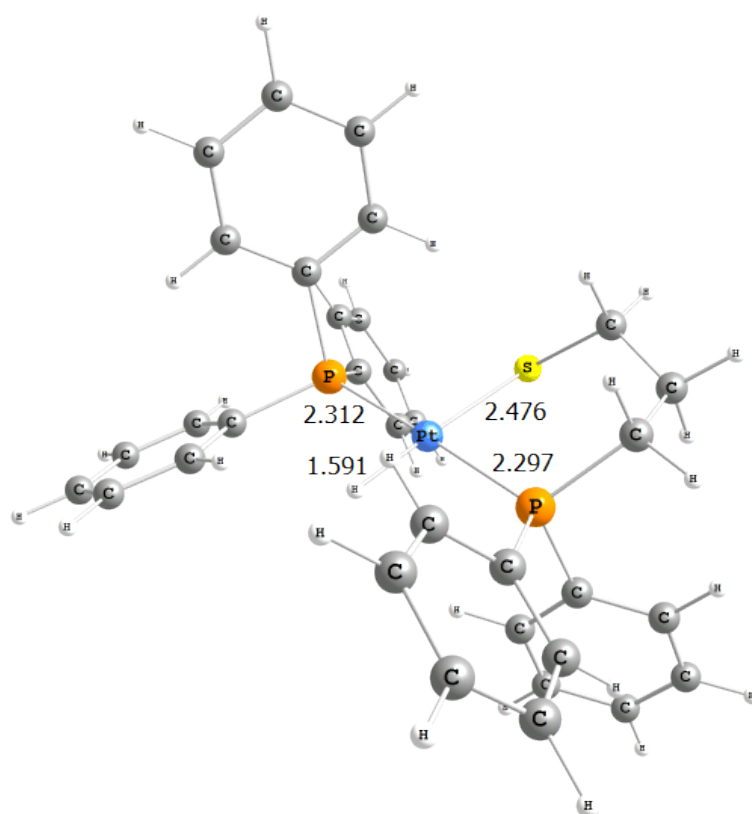
cis-11-chair



Zero-point correction= 0.555401 (Hartree/Particle)
 Thermal correction to Energy= 0.590186
 Thermal correction to Enthalpy= 0.591130
 Thermal correction to Gibbs Free Energy= 0.486276
 Sum of electronic and zero-point Energies= -2475.529151
 Sum of electronic and thermal Energies= -2475.494366
 Sum of electronic and thermal Enthalpies= -2475.493422
 Sum of electronic and thermal Free Energies= -2475.598276

H	2.703086	0.371822	-5.277847
H	1.039956	1.903219	-4.217354
C	2.425146	0.238421	-4.229176
C	1.493302	1.097342	-3.634672
H	3.715375	-1.473711	-3.938357
C	2.992128	-0.794655	-3.479305
H	3.607921	-0.431243	5.164941
C	1.127698	0.920842	-2.299414
H	0.382053	1.577729	-1.845575
H	3.758399	-2.920396	5.340158
C	2.635359	-0.968575	-2.137126
C	2.781953	-1.059115	4.821010
C	2.866180	-2.450438	4.918792
C	1.699843	-0.111488	-1.537762
H	3.085180	-1.780723	-1.562466
H	1.589029	0.628660	4.229313
H	-2.186173	4.311696	3.660408
H	4.129576	0.444618	-0.086826
C	1.639481	-0.458950	4.286317
H	5.565486	2.177346	0.950705
H	-1.798217	4.332877	6.126772
H	3.746991	-1.236182	1.687630
C	-1.837267	3.409909	4.169861
C	1.806708	-3.237847	4.460431
H	1.870269	-4.327236	4.510866
H	-1.210704	0.230072	-0.823036
C	-1.623588	3.420243	5.550883
H	-1.807630	2.226719	2.355927
C	3.700922	1.133619	0.644752
C	-1.614464	2.243314	3.430600
C	4.508054	2.116941	1.220834
C	0.559499	-1.240828	3.839979
C	-1.191096	2.256195	6.196862
C	0.666188	-2.640160	3.920011
C	3.139202	-2.085360	1.374419
H	-1.028232	2.256455	7.277801
H	4.533630	-3.528810	2.165675
P	1.236702	-0.237871	0.244702
C	-1.166680	1.075783	4.069960
C	2.340320	1.039032	0.988074
C	-0.965776	1.090504	5.461633
Pt	-0.993650	-0.074414	0.722872
C	3.581911	-3.383647	1.648808
H	-0.138335	-3.279364	3.552760
C	3.962468	3.030611	2.130623
H	4.595033	3.802512	2.576604
C	1.914559	-1.881221	0.725963
P	-0.926150	-0.460281	3.079919
H	-0.619248	0.189803	5.974617
C	1.796785	1.975924	1.878837
C	2.603943	2.964133	2.450819
C	2.808889	-4.486405	1.279929
C	1.127301	-2.995027	0.378096
H	0.734391	1.937710	2.119787
H	3.159664	-5.499150	1.494663
H	2.162320	3.684227	3.144441
H	0.157724	-2.839015	-0.103077
C	-2.311585	-1.529830	3.685524
C	1.575535	-4.288694	0.648406
S	-3.365255	0.199754	0.739813
H	-3.935951	-2.045983	1.500808
C	-4.107741	-1.029665	1.895398
H	0.958129	-5.145711	0.367266
H	-5.190634	-0.842049	1.815360
C	-3.710065	-0.979765	3.371822
H	-2.189105	-2.517653	3.211542
H	-2.175440	-1.663640	4.771137
H	-4.432454	-1.592834	3.942182
H	-3.810027	0.050444	3.753421

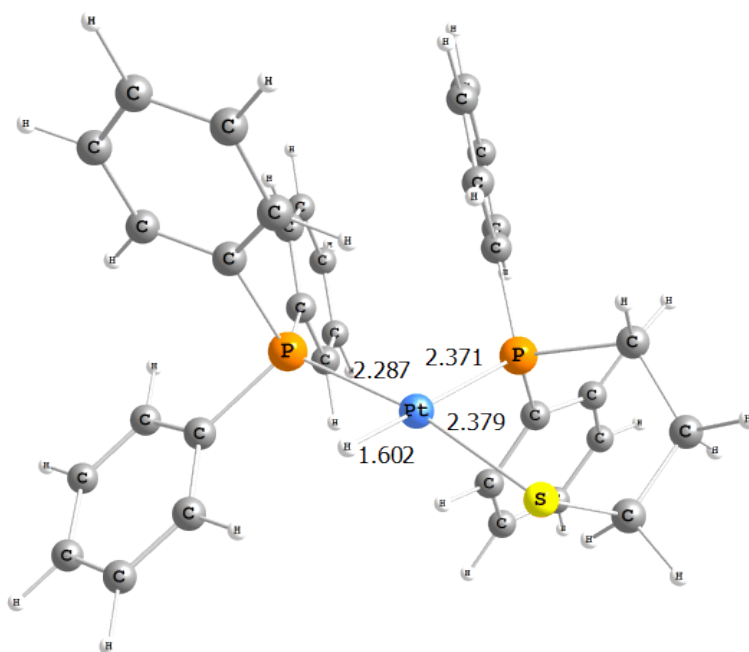
trans-11-chair



Zero-point correction= 0.554762 (Hartree/Particle)
 Thermal correction to Energy= 0.589935
 Thermal correction to Enthalpy= 0.590879
 Thermal correction to Gibbs Free Energy= 0.481227
 Sum of electronic and zero-point Energies= -2475.529625
 Sum of electronic and thermal Energies= -2475.494452
 Sum of electronic and thermal Enthalpies= -2475.493508
 Sum of electronic and thermal Free Energies= -2475.603160

H	2.711791	-0.591053	-5.230165
H	0.818715	0.892278	-4.557683
C	2.413968	-0.522438	-4.180634
C	1.353548	0.308828	-3.803831
H	3.912066	-1.926393	-3.496787
C	3.086237	-1.270198	-3.210044
H	-7.363824	1.938383	-1.466908
C	0.964835	0.387966	-2.464871
H	0.121603	1.018048	-2.174674
H	-6.126626	3.800969	-2.573187
C	2.706466	-1.184417	-1.866651
C	-6.300720	2.088705	-1.261630
C	-5.606698	3.131875	-1.882601
C	1.641142	-0.353825	-1.482235
H	3.242745	-1.771101	-1.118613
H	-6.1888631	0.415677	0.095322
H	-4.044040	-4.282886	-0.459413
H	3.207140	1.636291	-0.987142
C	-5.637406	1.230871	-0.379230
H	4.448767	3.596101	-0.112832
H	-6.033773	-4.717770	0.983884
H	3.830693	-0.651969	1.510915
C	-4.420640	-3.501495	0.205518
C	-4.244135	3.311709	-1.623239
H	-3.695181	4.121863	-2.110207
H	-1.354163	0.465411	-0.795786
C	-5.535432	-3.745431	1.014648
H	-2.892817	-2.078156	-0.363530
C	3.035296	1.969571	0.038190
C	-3.776831	-2.263279	0.251925
C	3.736690	3.075237	0.532636
C	-4.268946	1.404914	-0.117111
C	-6.005808	-2.744338	1.868979
C	-3.575735	2.448974	-0.750363
C	3.232708	-1.560556	1.612677
H	-6.872023	-2.930984	2.508902
H	4.806170	-2.654435	2.608581
P	1.145800	-0.158344	0.282118
C	-4.248662	-1.248338	1.102241
C	2.116339	1.296331	0.857083
C	-5.367384	-1.500836	1.912270
Pt	-1.108669	0.092414	0.731042
C	3.780445	-2.687437	2.232235
H	-2.505149	2.570589	-0.566753
C	3.529594	3.509806	1.844275
H	4.078953	4.373492	2.228247
C	1.914333	-1.591665	1.132371
P	-3.361393	0.357182	1.094930
H	-5.748233	-0.733769	2.589372
C	1.906585	1.737909	2.176534
C	2.616043	2.836469	2.664407
C	3.016395	-3.849824	2.377073
C	1.148044	-2.757503	1.289506
H	1.188927	1.206112	2.809462
H	3.444341	-4.728045	2.867511
H	2.451280	3.171417	3.691884
H	0.108976	-2.772161	0.951394
C	-3.797267	1.198036	2.681602
C	1.699961	-3.882226	1.906155
S	-0.780854	-0.602692	3.084263
H	-1.360303	1.613027	3.942780
C	-1.733112	0.587941	4.116343
H	1.092887	-4.781903	2.033301
H	-1.477809	0.331631	5.157077
C	-3.256491	0.559761	3.967795
H	-3.398116	2.220025	2.564872
H	-4.894493	1.299854	2.716303
H	-3.701087	1.116642	4.814156
H	-3.611635	-0.480651	4.056056

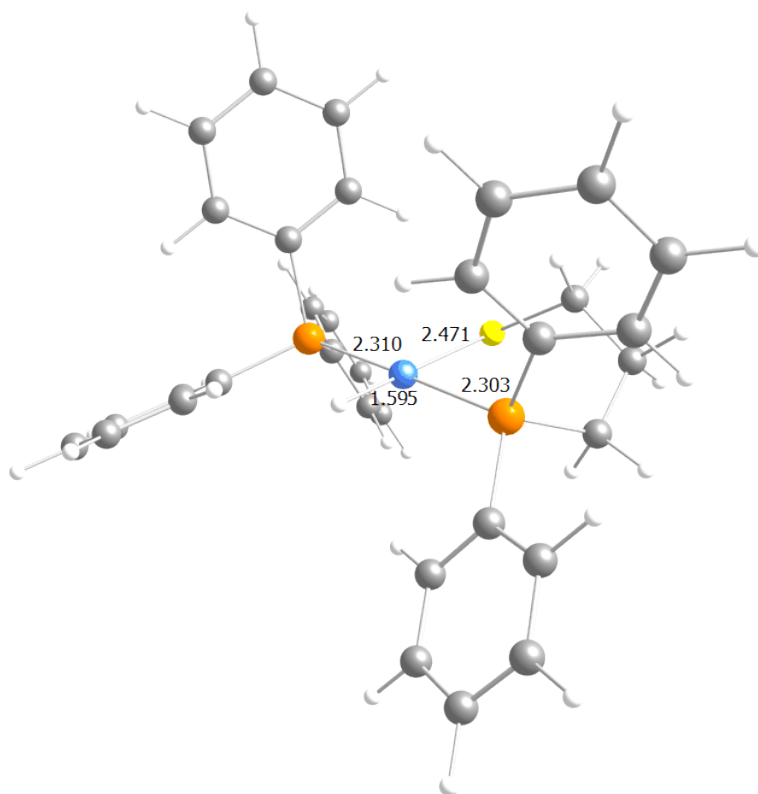
cis-11-skew-boat



Zero-point correction= 0.555412 (Hartree/Particle)
 Thermal correction to Energy= 0.590126
 Thermal correction to Enthalpy= 0.591070
 Thermal correction to Gibbs Free Energy= 0.486070
 Sum of electronic and zero-point Energies= -2475.530524
 Sum of electronic and thermal Energies= -2475.495810
 Sum of electronic and thermal Enthalpies= -2475.494866
 Sum of electronic and thermal Free Energies= -2475.599867

H	-6.456841	-0.310277	-4.132503
H	-5.619162	1.757134	-3.000346
C	-5.515066	-0.329822	-3.578176
C	-5.046874	0.827656	-2.946199
H	-5.147805	-2.426405	-3.959255
C	-4.779545	-1.513259	-3.485810
H	-8.312162	2.557545	1.695676
C	-3.845136	0.798177	-2.238989
H	-3.482434	1.707490	-1.756873
H	-7.282646	4.631906	0.770194
C	-3.575940	-1.545802	-2.773779
C	-7.258723	2.563072	1.404114
C	-6.680101	3.727394	0.886596
C	-3.093693	-0.386750	-2.150929
H	-3.021588	-2.482044	-2.698787
H	-6.948519	0.506077	1.971804
H	-7.461344	-2.467497	-1.419722
H	-1.531961	0.588240	-4.015498
C	-6.489219	1.406772	1.556803
H	-0.134078	2.209737	-5.250689
H	-6.229135	-4.632872	-1.302698
H	-0.436402	-1.591292	-3.648889
C	-6.526180	-2.536661	-0.858347
C	-5.327349	3.735719	0.532806
H	-4.866252	4.647867	0.145717
H	-0.116221	0.108462	1.026486
C	-5.833165	-3.747565	-0.798600
H	-6.563871	-0.455798	-0.300303
C	-0.747473	1.131501	-3.484387
C	-6.022629	-1.399072	-0.218653
C	0.036739	2.053451	-4.182340
C	-5.134429	1.399925	1.182102
C	-4.620406	-3.817134	-0.103813
C	-4.557417	2.578881	0.683429
C	-0.291072	-2.284972	-2.818358
H	-4.059385	-4.754339	-0.066023
H	0.629795	-3.785208	-4.067613
P	-1.537455	-0.326840	-1.165519
C	-4.818176	-1.465520	0.493886
C	-0.544440	0.917347	-2.108649
C	-4.115576	-2.684208	0.535137
Pt	-1.717152	0.138392	1.066744
C	0.311684	-3.522061	-3.055525
H	-3.492509	2.585197	0.434749
C	1.030768	2.776896	-3.515906
H	1.641542	3.500821	-4.061633
C	-0.703785	-1.932044	-1.521997
P	-4.054211	-0.064706	1.408630
H	-3.158064	-2.738012	1.058671
C	0.449325	1.655873	-1.445106
C	1.232711	2.576441	-2.147429
C	0.512949	-4.419168	-2.000123
C	-0.486351	-2.831230	-0.466550
H	0.599813	1.514526	-0.373506
H	2.000652	3.144620	-1.616432
H	-0.774866	-2.543942	0.547309
C	-4.355150	-0.591080	3.162568
C	0.116261	-4.070314	-0.706431
S	-1.334690	0.704421	3.345960
H	-3.229483	2.214448	3.208553
C	-2.914779	1.449668	3.934632
H	0.283957	-4.759883	0.124814
H	-2.667790	1.990755	4.861914
H	0.987555	-5.386030	-2.186832
C	-4.076308	0.486598	4.223483
H	-3.893690	-0.032485	5.179429
H	-4.988002	1.094697	4.365130
H	-5.380642	-0.981143	3.257758
H	-3.666005	-1.440130	3.287642

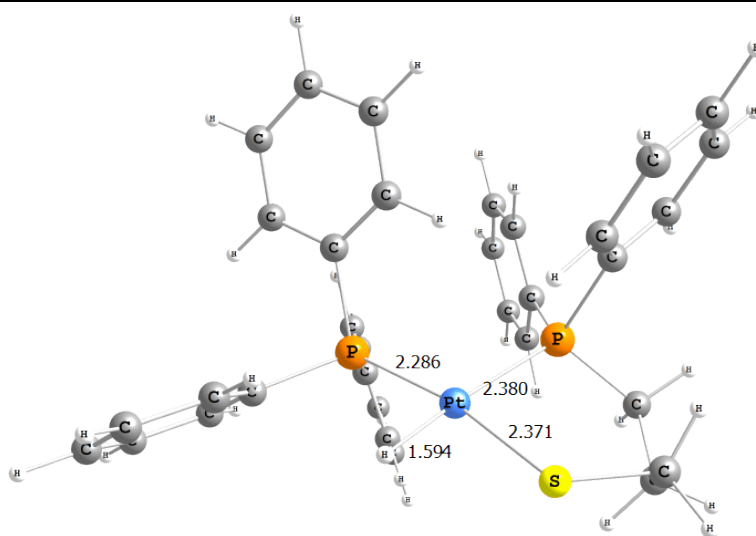
trans-11-skew-boat



Zero-point correction= 0.554957 (Hartree/Particle)
Thermal correction to Energy= 0.590061
Thermal correction to Enthalpy= 0.591005
Thermal correction to Gibbs Free Energy= 0.482319
Sum of electronic and zero-point Energies= -2475.528670
Sum of electronic and thermal Energies= -2475.493567
Sum of electronic and thermal Enthalpies= -2475.492622
Sum of electronic and thermal Free Energies= -2475.601309

H	-6.895023	0.632642	-3.460704
H	-6.056747	2.217574	-1.725155
C	-5.905048	0.489313	-3.019836
C	-5.434377	1.380229	-2.050138
H	-5.481758	-1.298248	-4.165127
C	-5.113086	-0.593493	-3.415318
H	-0.073263	-1.373915	7.497690
C	-4.174606	1.192217	-1.477510
H	-3.820396	1.867870	-0.695379
H	1.614528	-2.791428	6.330185
C	-3.849923	-0.782880	-2.847781
C	0.098501	-1.251267	6.425251
C	1.044309	-2.045872	5.770041
C	-3.371303	0.113196	-1.879132
H	-3.238800	-1.634741	-3.154681
H	-1.374074	0.307671	6.235222
H	1.104215	4.549555	5.965803
H	-1.983851	0.930695	-3.931113
C	-0.634844	-0.300493	5.709424
H	-0.407490	2.080197	-5.454686
H	1.015374	6.241531	4.134366
H	0.138363	-1.528889	-2.989852
C	0.622562	4.304503	5.015624
C	1.252435	-1.890144	4.395809
H	1.984608	-2.514503	3.877611
H	-0.130076	1.054480	0.903431
C	0.573797	5.252316	3.988108
H	0.113480	2.304887	5.637544
C	-0.980328	1.176788	-3.579316
C	0.059915	3.038781	4.830338
C	-0.088760	1.824167	-4.440949
C	-0.428571	-0.135265	4.328774
C	-0.033806	4.927946	2.771325
C	0.518137	-0.943854	3.676463
C	-0.351950	-2.255240	-2.338581
H	-0.068193	5.661715	1.961963
H	0.662097	-3.941000	-3.231253
P	-1.709150	-0.057903	-1.120216
C	-0.552004	2.707155	3.610521
C	-0.590254	0.848863	-2.270427
C	-0.589209	3.659683	2.578984
Pt	-1.611487	0.504449	1.117709
C	-0.057428	-3.616643	-2.474897
H	0.662147	-0.833602	2.598823
C	1.201656	2.142571	-4.009073
H	1.896987	2.648892	-4.683673
C	-1.270724	-1.828363	-1.368103
P	-1.370181	1.083871	3.333294
H	-1.042312	3.394244	1.620559
C	0.705577	1.179973	-1.841028
C	1.597067	1.816420	-2.707203
C	-0.680740	-4.556248	-1.649615
C	-1.894538	-2.775650	-0.535331
H	1.005836	0.946954	-0.817410
H	2.602643	2.067009	-2.359674
H	-2.610537	-2.437678	0.220727
C	-2.995801	1.305062	4.185511
C	-1.601120	-4.132404	-0.683344
S	-3.887943	-0.370541	1.516949
H	-2.804851	-1.580249	3.328650
C	-3.747398	-1.016573	3.238525
H	-2.091955	-4.863472	-0.035572
H	-4.559746	-1.747813	3.375662
H	-0.449078	-5.619188	-1.757776
C	-3.845326	0.031807	4.357373
H	-4.895220	0.353491	4.461966
H	-3.573469	-0.462360	5.307308
H	-2.840990	1.814170	5.150219
H	-3.509572	2.018129	3.522432

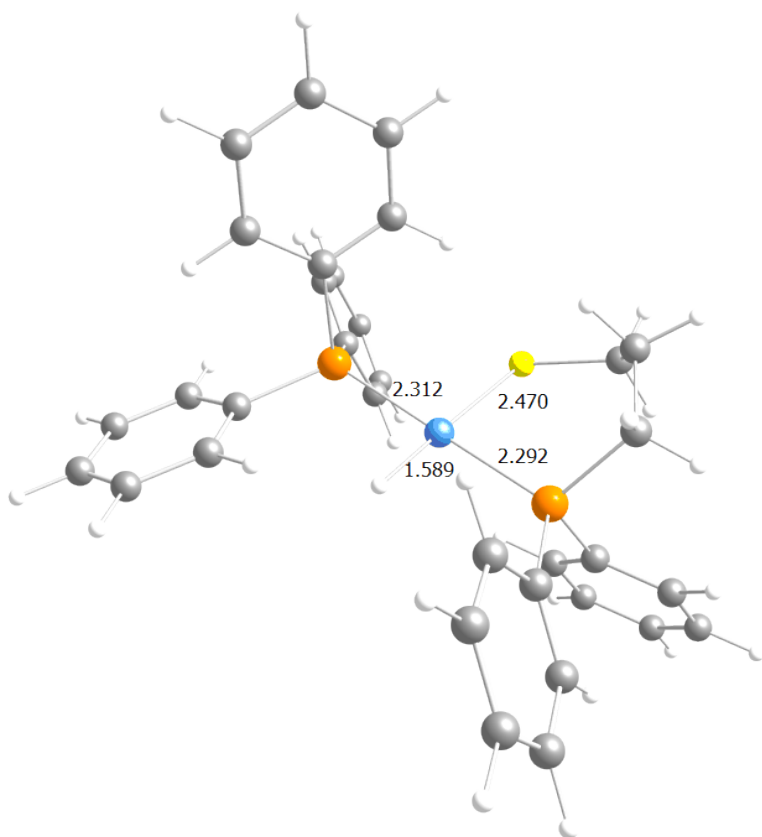
cis-11-boat



Zero-point correction= 0.555600 (Hartree/Particle)
 Thermal correction to Energy= 0.590243
 Thermal correction to Enthalpy= 0.591187
 Thermal correction to Gibbs Free Energy= 0.487145
 Sum of electronic and zero-point Energies= -2475.528041
 Sum of electronic and thermal Energies= -2475.493398
 Sum of electronic and thermal Enthalpies= -2475.492454
 Sum of electronic and thermal Free Energies= -2475.596496

H	3.051582	0.438883	-5.031366
H	1.206114	1.882084	-4.165747
C	2.660913	0.283761	-4.022377
C	1.626677	1.093142	-3.537107
H	3.989307	-1.367387	-3.588083
C	3.185916	-0.727104	-3.214540
H	2.553497	-0.034821	5.574447
C	1.118350	0.888531	-2.253984
H	0.295679	1.507099	-1.887840
H	3.124435	-2.465615	5.692319
C	2.685434	-0.928550	-1.922641
C	1.912763	-0.775873	5.089759
C	2.232336	-2.134308	5.154865
C	1.646887	-0.122213	-1.433528
H	3.106333	-1.721830	-1.301975
H	0.530034	0.709975	4.382641
H	-3.289406	3.926096	3.130586
H	3.789189	0.725155	0.229198
C	0.767879	-0.353441	4.09257
H	4.915739	2.595546	1.400525
H	-3.424615	3.912611	5.623749
H	3.436834	-1.000118	1.956826
C	-2.980385	3.041601	3.693347
C	1.410463	-3.065621	4.514507
H	1.662703	-4.127941	4.535525
H	-1.323414	0.030905	-1.097713
C	-3.059453	3.032401	5.088166
H	-2.472021	1.918449	1.912851
C	3.218398	1.352173	0.918262
C	-2.511204	1.917373	3.004718
C	3.851355	2.413086	1.569555
C	-0.075240	-1.282818	3.775415
C	-2.673722	1.889415	5.798749
C	0.274791	-2.643410	3.821422
C	2.943941	-1.911984	1.618505
H	-2.736528	1.873818	6.889959
H	4.408643	-3.193219	2.550712
P	0.977981	-0.285122	0.280288
C	-2.116230	0.769980	3.710740
C	1.850723	1.100954	1.129906
C	-2.207670	0.765394	5.114577
Pt	-1.300471	-0.290724	0.462882
C	3.491350	-3.153593	1.958028
H	-0.327714	-3.389261	3.299975
C	3.122703	3.248596	2.424397
H	3.618621	4.081974	2.928805
C	1.761210	-1.844132	0.870741
P	-1.532175	-0.722881	2.792286
H	-1.900641	-0.118454	5.679999
C	1.123655	1.959721	1.966691
C	1.756457	3.025331	2.613960
C	2.864776	-4.335256	1.555972
C	1.120439	-3.037278	0.488956
H	0.053747	1.801828	2.102048
H	3.297220	-5.303524	1.821169
H	1.172803	3.683883	3.262389
H	0.181861	-2.986888	-0.070326
C	-2.843743	-1.987509	3.196387
C	1.672774	-4.274386	0.824720
S	-3.641858	-0.150220	0.119114
H	-5.545766	-1.020461	1.222051
C	-4.521287	-0.843334	1.584254
H	1.169384	-5.194303	0.516354
H	-4.597691	-0.091432	2.389911
C	-3.938989	-2.154668	2.133269
H	-2.339296	-2.949337	3.365049
H	-3.280083	-1.685513	4.162304
H	-3.553319	-2.745792	1.286716
H	-4.746526	-2.750581	2.595250

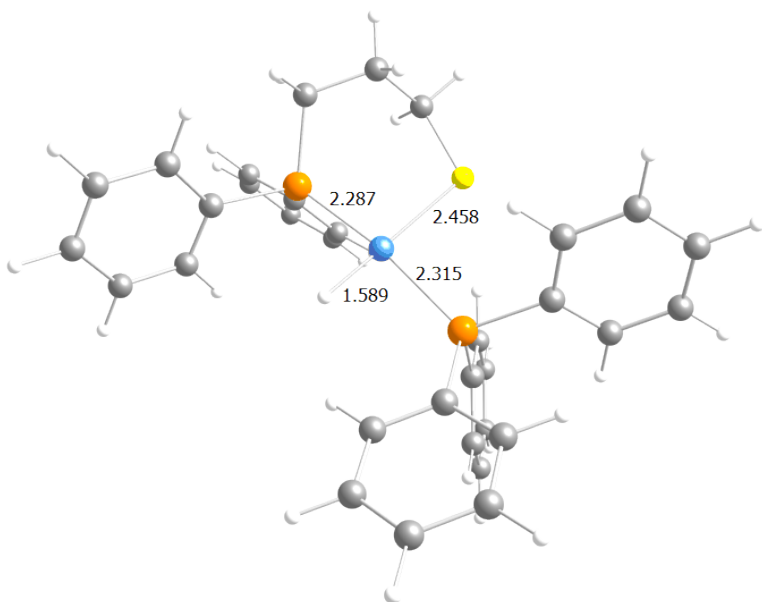
trans-11-boat



Zero-point correction= 0.554674 (Hartree/Particle)
 Thermal correction to Energy= 0.589883
 Thermal correction to Enthalpy= 0.590827
 Thermal correction to Gibbs Free Energy= 0.481567
 Sum of electronic and zero-point Energies= -2475.526610
 Sum of electronic and thermal Energies= -2475.491402
 Sum of electronic and thermal Enthalpies= -2475.490457
 Sum of electronic and thermal Free Energies= -2475.599717

H	2.842866	-0.140345	-5.260250
H	0.885499	1.227143	-4.528958
C	2.518060	-0.160413	-4.216679
C	1.421786	0.606004	-3.806949
H	4.045901	-1.563872	-3.600473
C	3.191850	-0.957789	-3.287319
H	-7.021078	1.291480	-2.280973
C	0.998777	0.572077	-2.476421
H	0.128798	1.151768	-2.161361
H	-6.020310	3.457420	-3.008015
C	2.777140	-0.986038	-1.952024
C	-6.092660	1.647077	-1.826596
C	-5.531686	2.858724	-2.235042
C	1.675720	-0.220377	-1.534980
H	3.314518	-1.610485	-1.235904
H	-5.919117	-0.069244	-0.532332
H	-3.967148	-4.537312	1.082803
C	3.222206	1.726006	-0.825218
C	-5.470467	0.878041	-0.835620
H	4.405162	3.628358	0.238096
H	-6.280914	-4.458737	2.012991
H	3.779708	-0.690453	-1.544589
C	-4.438439	-3.575805	1.300918
C	-4.333729	3.298084	-1.657993
H	-3.881043	4.238867	-1.981683
H	-1.323783	0.608208	-0.810695
C	-5.733517	-3.531691	1.823661
H	-2.713430	-2.423648	0.677987
C	3.005632	1.982952	0.213586
C	-3.733342	-2.392044	1.064033
C	3.673843	3.055859	0.814637
C	-4.275150	1.316411	-0.248622
C	-6.327867	-2.297282	2.108634
C	-3.704943	2.527905	-0.679625
C	3.214948	-1.625280	1.526637
H	-7.340199	-2.256176	2.518697
H	4.780504	-2.754168	2.495371
P	1.137221	-0.176769	0.226517
C	-4.321608	-1.149197	1.347509
C	2.061932	1.244673	0.943225
C	-5.625789	-1.113231	1.872759
Pt	-1.127301	0.019839	0.651751
C	3.777268	-2.787255	2.062690
H	-2.748410	2.853554	-0.261095
C	3.409042	3.392421	2.144646
H	3.932472	4.230705	2.612075
C	1.924640	-1.656448	0.975115
P	-3.355914	0.383146	1.043049
H	-6.105844	-0.157247	2.096793
C	1.793433	1.587949	2.281128
C	2.470665	2.653897	2.875786
C	3.056442	-3.985646	2.051702
C	1.201256	-2.859667	0.976589
H	1.054370	1.010403	2.845711
H	3.495744	-4.892132	2.476239
H	2.260355	2.912411	3.916989
H	0.183235	-2.877637	0.581187
C	-3.603961	1.426577	2.565152
C	1.768201	-4.019483	1.508666
S	-0.866472	-0.960228	2.904191
H	-1.806420	-0.319805	4.997916
C	-2.193087	-0.243827	3.969997
H	1.194739	-4.949692	1.512975
H	-3.098866	-0.874593	3.928137
C	-2.557555	1.219313	3.672650
H	-3.592448	2.470784	2.217097
H	-4.620390	1.229400	2.941631
H	-1.635392	1.764481	3.414058
H	-2.958792	1.689741	4.588405

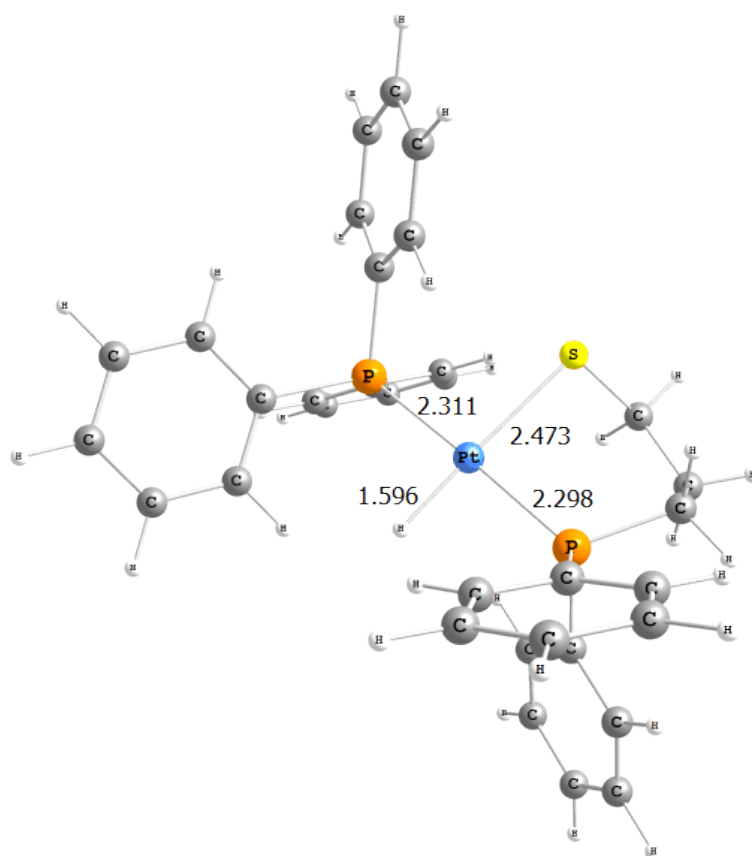
TS[*trans*-11-boat→skew-boat]



Zero-point correction= 0.554465 (Hartree/Particle)
 Thermal correction to Energy= 0.588880
 Thermal correction to Enthalpy= 0.589824
 Thermal correction to Gibbs Free Energy= 0.483135
 Sum of electronic and zero-point Energies= -2475.524323
 Sum of electronic and thermal Energies= -2475.489907
 Sum of electronic and thermal Enthalpies= -2475.488963
 Sum of electronic and thermal Free Energies= -2475.595652

H	2.813526	-4.295733	-3.707598
H	0.568831	-3.226571	-3.943641
C	2.464416	-3.580503	-2.958269
C	1.206802	-2.981331	-3.090670
H	4.250365	-3.733517	-1.746064
C	3.269013	-3.265839	-1.860098
H	-7.010419	3.201102	0.217897
C	0.754676	-2.077105	-2.127828
H	-0.236290	-1.627797	-2.219935
H	-5.344097	5.040423	-0.049190
C	2.823962	-2.351304	-0.899621
C	-5.940488	2.984948	0.275857
C	-5.005209	4.015817	0.124978
C	1.561705	-1.749063	-1.025592
H	3.464472	-2.111475	-0.049051
H	-6.245294	0.875384	0.597477
H	-5.243484	-1.199162	-3.685936
H	2.485326	0.317347	-2.282261
C	-5.507472	1.676413	0.496698
H	2.991184	2.541313	-3.254639
H	-6.425739	-3.325441	-3.115470
H	3.594619	0.761370	0.833806
C	-5.241588	-1.569543	-2.657576
C	-3.639258	3.730289	0.193571
H	-2.903397	4.529464	0.073651
H	-1.545556	-1.330650	-0.640110
C	-5.903820	-2.761290	-2.338402
H	-4.053817	0.074272	-1.926214
C	2.126340	1.218797	-1.781712
C	-4.574404	-0.850787	-1.666218
C	2.412396	2.474613	-2.329700
C	-4.134243	1.384034	0.572623
C	-5.890502	-3.226038	-1.022179
C	-3.201637	2.420069	0.413935
C	3.327525	0.078308	1.643384
H	-6.400584	-4.157364	-0.763097
H	5.130677	0.476400	2.763771
P	0.956169	-0.495697	0.181654
C	-4.562199	-1.307317	-0.335515
C	1.379469	1.119975	-0.598446
C	-5.222726	-2.504375	-0.025508
Pt	-1.298648	-0.524623	0.706970
C	4.192054	-0.082703	2.729865
H	-2.135230	2.197066	0.474705
C	1.961725	3.636512	-1.698168
H	2.185552	4.616205	-2.128470
C	2.116733	-0.630563	1.595345
P	-3.572214	-0.346148	0.883254
H	-5.220711	-2.896484	0.992958
C	0.925614	2.292058	0.034538
C	1.221946	3.541255	-0.513282
C	3.854227	-0.952757	3.771520
C	1.775157	-1.491117	2.650705
H	0.340805	2.220748	0.956789
H	4.529686	-1.074956	4.622347
H	0.868424	4.446399	-0.012382
H	0.814712	-2.009749	2.633223
C	-4.287878	-0.749444	2.549438
H	-5.215925	-0.163009	2.646498
C	2.646254	-1.656226	3.729733
S	-0.915536	0.667978	2.822323
H	-3.139855	1.624991	3.274293
H	-4.578997	-1.809404	2.538162
C	-2.532017	0.804831	3.695191
H	2.371446	-2.324279	4.549729
H	-2.272089	1.103825	4.722226
C	-3.347492	-0.497552	3.741783
H	-2.643173	-1.339339	3.839522
H	-3.976191	-0.504093	4.650086

TS[*trans*-11-skew-boat→chair]



Zero-point correction= 0.554283 (Hartree/Particle)
 Thermal correction to Energy= 0.588875
 Thermal correction to Enthalpy= 0.589820
 Thermal correction to Gibbs Free Energy= 0.481878
 Sum of electronic and zero-point Energies= -2475.524967
 Sum of electronic and thermal Energies= -2475.490374
 Sum of electronic and thermal Enthalpies= -2475.489430
 Sum of electronic and thermal Free Energies= -2475.597371

H	1.900650	-1.163559	-5.507240
H	-0.138573	-2.020852	-4.348195
C	1.749276	-0.964533	-4.443101
C	0.606695	-1.444653	-3.793760
H	3.585607	0.159814	-4.227582
C	2.693036	-0.223658	-3.726528
H	-4.326190	2.642314	-2.942003
C	0.406708	-1.180193	-2.437165
H	-0.496689	-1.534060	-1.936061
H	-5.907257	4.332706	-2.005093
C	2.501596	0.032241	-2.364805
C	-4.525740	2.670747	-1.867774
C	-5.410383	3.619102	-1.342794
C	1.355241	-0.443887	-1.707987
H	3.248825	0.608991	-1.816819
H	-3.172453	1.041753	-1.428051
H	-4.055095	-4.349662	1.343933
H	3.968076	-0.117038	0.894228
C	-3.882911	1.764909	-1.022011
H	5.488464	1.766928	1.448376
H	-6.542586	-4.161662	1.387316
H	1.273860	-0.979426	2.848905
C	-4.530912	-3.365725	1.355310
C	-5.649362	3.656518	0.033286
H	-6.332951	4.399630	0.451928
H	-1.640659	-0.431714	-0.563380
C	-5.924633	-3.259980	1.379558
H	-2.649103	-2.289016	1.300575
C	3.591348	0.908294	0.875224
C	-3.739211	-2.212932	1.337345
C	4.445972	1.968983	1.189092
C	-4.127758	1.787087	0.362652
C	-6.528706	-1.997462	1.387244
C	-5.013320	2.745345	0.883125
C	1.725630	-1.796142	2.276700
H	-7.618339	-1.911049	1.398530
H	2.186480	-2.992721	4.009628
P	1.084048	-0.184819	0.096442
C	-4.339727	-0.944125	1.353063
C	2.249678	1.158106	0.547984
C	-5.740672	-0.844231	1.376249
Pt	-1.085541	0.189378	0.798566
C	2.238459	-2.923556	2.919895
H	-5.212175	2.796807	1.954815
C	3.966914	3.282793	1.178881
H	4.635116	4.110518	1.430480
C	1.793110	-1.695204	0.874739
P	-3.269754	0.549561	1.414315
H	-6.219812	0.138566	1.372713
C	1.770982	2.477853	0.548353
C	2.628810	3.534956	0.859205
C	2.812077	-3.962426	2.176434
C	2.373187	-2.734354	0.132169
H	0.717796	2.671167	0.328743
H	3.207443	-4.846702	2.683283
H	2.245797	4.558359	0.865979
H	2.433394	-2.667331	-0.955824
C	-3.479044	1.145770	3.146238
C	2.877782	-3.865527	0.784251
S	-0.320679	1.147802	2.946697
H	-0.869563	0.406035	5.143812
C	-1.261396	0.117276	4.156440
H	3.325658	-4.672098	0.197882
H	-0.968740	-0.933104	4.004459
C	-2.817041	0.221665	4.178494
H	-3.034330	2.151881	3.183126
H	-4.556880	1.223934	3.360261
H	-3.134873	0.578138	5.172363
H	-3.250216	-0.788119	4.075261

ADF xyz coordinates for EDA:

<i>cis-5</i>				<i>trans-5</i>			
-10.12399				-10.11940868			
H	-5.034959	2.995798	-4.687181	H	-8.215198	-2.714741	2.519652
H	-2.958607	1.656723	-4.376854	H	-6.875580	-2.386295	0.447011
C	-4.871371	2.446792	-3.760690	C	-7.187484	-2.358605	2.583033
C	-3.705165	1.697899	-3.584725	C	-6.437109	-2.172771	1.420975
H	-6.741567	3.060657	-2.878491	H	-7.206133	-2.195019	4.734763
C	-5.825835	2.485903	-2.746189	C	-6.622693	-2.068184	3.823940
H	-6.224428	-3.437928	-2.568854	H	-2.194493	-5.696253	3.896145
C	-3.495089	1.002531	-2.396534	C	-5.131018	-1.694795	1.498621
H	-5.728968	-1.088456	-1.989992	H	-3.549290	-3.647210	3.644870
H	-2.592276	0.403490	-2.271646	H	-4.558173	-1.513113	0.589960
C	-5.591600	-3.217732	-1.709884	C	-1.714835	-4.770391	3.581274
C	-5.618398	1.787890	-1.554757	C	-5.309713	-1.604237	3.907034
C	-5.313061	-1.891120	-1.382275	C	-2.479502	-3.611526	3.444924
H	-5.273646	-5.291886	-1.209031	H	0.244329	-5.655246	3.408568
C	-4.450678	1.039454	-1.367702	C	-4.552054	-1.418362	2.743707
C	-5.057011	-4.256640	-0.947509	C	-0.347461	-4.746003	3.307645
H	-6.372935	1.827951	-0.770276	H	-4.883557	-1.371069	4.881462
H	-0.676018	1.667286	-0.918943	H	-0.709558	1.159489	-1.063708
H	-1.833869	2.782001	-0.575069	H	-1.981183	2.207429	-0.939743
C	-4.485247	-1.595716	-0.291152	C	-1.873403	-2.418380	3.034662
N	-1.141374	2.159416	-0.148346	N	-1.199579	1.794936	-0.425972
C	-4.233164	-3.966932	0.141120	C	0.257906	-3.558246	2.893724
P	-4.075869	0.129987	0.191083	P	-2.803135	-0.846786	2.828127
C	-3.936030	-2.643485	0.460726	C	-0.500932	-2.398846	2.749022
H	-3.805709	-4.774320	0.733426	H	1.324329	-3.536300	2.671563
C	-0.125013	2.923977	0.624547	C	-0.268144	2.826205	0.103858
H	1.376781	1.381743	0.551940	H	1.328466	1.436442	0.503048
H	-6.819327	-1.021112	0.768350	H	-1.960356	-1.823136	5.543090
C	-5.487850	0.611077	1.264731	C	-2.713825	-0.086055	4.495873
Pt	-2.019644	0.564190	1.185484	Pt	-1.966218	0.500102	1.189911
C	-6.679054	-0.116299	1.357890	C	-2.270383	-0.782276	5.625120
H	-3.263625	-2.409115	1.284828	H	-0.041599	-1.462371	2.422830
H	-0.660509	3.514502	1.379274	H	-0.871710	3.558817	0.655263
C	0.822831	1.962998	1.309122	C	0.724470	2.181837	1.048395
H	-4.353681	2.270711	2.035801	H	-3.367538	1.819040	3.723201
C	-5.307969	1.744061	2.070093	C	-3.066168	1.265753	4.611718
H	1.566572	2.536933	1.879416	H	1.419892	2.952747	1.409114
C	-7.681090	0.296600	2.237778	C	-2.198817	-0.136113	6.859840
H	-8.595129	-0.289027	2.324891	H	-1.838436	-0.680789	7.731366
H	-2.441969	-0.579031	2.243196	H	-3.186023	-0.055844	0.239821
S	-0.030616	0.835920	2.491979	S	-0.094905	1.432463	2.515464
C	-6.320645	2.170577	2.924577	C	-3.008422	1.901610	5.848343
C	-7.508760	1.442534	3.013431	C	-2.572454	1.201969	6.974783
H	-6.172323	3.056630	3.540286	H	-3.283248	2.952227	5.929076
H	-8.291199	1.758023	3.702801	H	-2.508826	1.704276	7.939397
H	0.429059	3.611893	-0.039206	H	0.248334	3.338744	-0.727592

<i>cis</i> -6				<i>trans</i> -6			
-11.51524246				-11.50788			
H	-4.998615	3.031569	-4.630970	H	-8.214975	-2.787848	2.405099
H	-3.043321	1.507311	-4.400342	H	-6.933188	-2.203386	0.351675
C	-4.855771	2.460481	-3.714496	C	-7.191905	-2.422054	2.484122
C	-3.758013	1.605838	-3.584444	C	-6.473584	-2.093916	1.333221
H	-6.626131	3.241001	-2.760350	H	-7.161574	-2.497790	4.640283
C	-5.765017	2.580703	-2.665712	C	-6.601769	-2.260336	3.736860
H	-6.385605	-3.506887	-2.406557	H	-2.250271	-5.771071	3.797241
C	-3.570181	0.884237	-2.408934	C	-5.170501	-1.608875	1.432739
H	-5.859957	-1.148231	-1.874670	H	-3.583482	-3.710759	3.569643
H	-2.716488	0.211461	-2.318162	H	-4.621833	-1.321409	0.536515
C	-5.685416	-3.277728	-1.604444	C	-1.759516	-4.845279	3.500271
C	-5.580028	1.857891	-1.484941	C	-5.295077	-1.784920	3.839964
C	-5.393637	-1.948497	-1.301034	C	-2.512499	-3.677993	3.377885
H	-5.310405	-5.347757	-1.126377	H	0.193492	-5.745275	3.326948
C	-4.481902	1.001080	-1.345944	C	-4.565649	-1.463642	2.686977
H	2.148912	5.631460	-1.112258	H	1.804698	5.540947	-1.787369
O	0.250837	4.158069	-1.406694	O	-0.108673	4.069095	-1.679942
C	-5.080135	-4.310203	-0.887059	C	-0.390034	-4.830151	3.236277
H	-6.297250	1.966829	-0.672407	H	-4.847234	-1.650613	4.823561
H	-0.873215	1.933555	-0.939422	H	-0.698533	1.527386	-0.863294
H	-2.056664	2.914162	-0.400635	H	-1.966144	2.546931	-0.645909
C	1.758838	6.014180	-0.165023	C	1.628559	5.923523	-0.778337
C	-4.490436	-1.644091	-0.273733	C	-1.895043	-2.482868	2.988427
C	0.356457	4.100547	-0.194450	C	0.233222	4.023392	-0.511364
H	2.563928	6.349227	0.492248	H	2.558295	6.247072	-0.306044
N	-1.314812	2.283041	-0.079869	N	-1.215078	2.057563	-0.152683
C	-4.168690	-4.011395	0.126327	C	0.227813	-3.643177	2.841124
P	-4.107634	0.085673	0.208419	P	-2.817986	-0.903252	2.814564
O	1.078424	4.958995	0.566254	O	1.106896	4.872722	0.078820
C	-3.866516	-2.684441	0.426555	C	-0.521561	-2.474439	2.705223
H	-3.682172	-4.813086	0.679731	H	1.294679	-3.628523	2.621569
C	-0.294877	3.032045	0.685054	C	-0.301586	3.012764	0.506906
H	1.248900	1.550770	0.400182	H	1.344859	1.618858	0.539891
H	-6.976219	-0.852025	0.509297	H	-1.825776	-1.861772	5.493964
C	-5.522086	0.551799	1.284348	C	-2.769228	-0.186237	4.503548
Pt	-2.037222	0.550724	1.168320	Pt	-1.964567	0.584819	1.308935
C	-6.786794	-0.043010	1.212724	C	-2.227861	-0.855501	5.604426
H	-3.136964	-2.440489	1.197684	H	-0.051016	-1.539584	2.388712
H	-0.791215	3.524229	1.533843	H	-0.887259	3.571344	1.254378
C	0.742492	2.056053	1.240769	C	0.777661	2.237198	1.258197
H	-4.275897	1.962938	2.321217	H	-3.635120	1.658895	3.791956
C	-5.282373	1.549508	2.237072	C	-3.246670	1.123844	4.658123
H	1.503317	2.620471	1.793805	H	1.480939	2.950578	1.702021
C	-7.803933	0.377415	2.069181	C	-2.180578	-0.225912	6.850141
H	-8.781217	-0.100595	2.020368	H	-1.741329	-0.746261	7.699997
H	-2.366953	-0.674136	2.164022	H	-3.274905	0.230649	0.392401
S	-0.000042	0.831557	2.394893	S	0.056709	1.226467	2.610437
C	-6.305574	1.980720	3.078922	C	-3.212538	1.741182	5.903757
C	-7.568957	1.394693	2.995091	C	-2.677138	1.066618	7.004135
H	-6.109458	2.759731	3.814016	H	-3.585064	2.758791	6.012452
H	-8.365573	1.716455	3.664916	H	-2.630548	1.557220	7.975722
H	1.055052	6.831681	-0.357510	H	0.908931	6.748975	-0.814091

<i>cis</i> -7				<i>trans</i> -7			
-12.10888253				-12.10313			
H	-5.059447	2.974198	-4.657110	H	-8.242372	-2.741353	2.393837
H	-3.023438	1.568346	-4.378452	H	-6.954437	-2.168336	0.340796
C	-4.899283	2.421080	-3.732440	C	-7.214090	-2.390051	2.472771
C	-3.756216	1.633233	-3.575205	C	-6.492165	-2.068995	1.322113
H	-6.729421	3.104287	-2.816555	H	-7.181147	-2.479533	4.628259
C	-5.832620	2.496935	-2.700601	C	-6.619133	-2.244993	3.725415
H	-6.311113	-3.479030	-2.479926	H	-2.233527	-5.770214	3.854491
C	-3.547535	0.934526	-2.388995	C	-5.181967	-1.603319	1.421802
H	-5.818815	-1.125425	-1.907312	H	-3.575980	-3.716179	3.613062
H	-2.660179	0.310038	-2.278484	H	-4.631182	-1.318525	0.525997
C	-5.645090	-3.255143	-1.647695	C	-1.749893	-4.847091	3.537119
C	-5.626920	1.796375	-1.510274	C	-5.304889	-1.790204	3.828491
C	-5.370061	-1.927416	-1.322520	C	-2.507495	-3.683624	3.406918
H	-5.281721	-5.328150	-1.173232	H	0.203013	-5.744803	3.354861
C	-4.482619	1.007585	-1.342893	C	-4.573825	-1.471126	2.675827
H	1.814763	5.845350	-1.137589	H	1.525983	5.718867	-1.731077
O	0.116754	4.262875	-1.365137	O	-0.199453	4.155890	-1.605242
C	-5.065265	-4.291850	-0.915704	C	-0.383696	-4.832270	3.255870
H	-6.364480	1.868325	-0.712146	H	-4.852460	-1.667569	4.811681
H	-0.761066	1.812800	-0.930220	H	-0.691520	1.531114	-0.850697
H	-1.964649	2.831709	-0.522059	H	-1.958843	2.551780	-0.633182
H	1.266934	8.170591	-0.272466	H	1.205263	8.094758	-0.884418
H	-0.174344	7.129784	-0.332278	H	-0.258403	7.107957	-0.663633
C	1.692038	6.071199	-0.072529	C	1.592822	5.990965	-0.671895
C	-4.503044	-1.628464	-0.262988	C	-1.897782	-2.493497	2.990650
C	0.333070	4.107166	-0.175562	C	0.203549	4.054058	-0.458854
H	2.672612	6.195081	0.400080	H	2.642713	6.098911	-0.377592
N	-1.253455	2.211055	-0.121546	N	-1.213101	2.055057	-0.139086
C	0.799499	7.272113	0.153474	C	0.786351	7.230356	-0.350831
C	-4.196088	-3.998674	0.135897	C	0.224925	-3.649718	2.834073
P	-4.104297	0.099498	0.216079	P	-2.823075	-0.916381	2.806724
O	1.120404	4.896871	0.591980	O	1.113076	4.862304	0.132065
C	-3.904970	-2.673434	0.453732	C	-0.528828	-2.485520	2.689195
H	-3.730103	-4.803961	0.701756	H	1.289953	-3.633506	2.605293
C	-0.277918	2.987469	0.671698	C	-0.303380	3.004293	0.535526
H	1.308511	1.544461	0.429720	H	1.354605	1.624116	0.525976
H	-6.881982	-0.993417	0.730662	H	-1.691557	-1.785880	5.463596
H	0.640732	7.440202	1.226704	H	0.813101	7.442288	0.725959
C	-5.514237	0.587068	1.290549	C	-2.781286	-0.188967	4.493510
Pt	-2.029133	0.533451	1.165772	Pt	-1.959321	0.572490	1.310293
C	-6.731264	-0.101402	1.336904	C	-2.149299	-0.804181	5.577564
H	-3.200307	-2.434381	1.248975	H	-0.063362	-1.555185	2.353240
H	-0.815725	3.453202	1.511452	H	-0.890576	3.537256	1.300974
C	0.766884	2.039446	1.254939	C	0.787068	2.222557	1.260770
H	-4.348775	2.193130	2.124185	H	-3.809765	1.581990	3.803470
C	-5.321706	1.700346	2.119694	C	-3.341019	1.087863	4.654409
H	1.499164	2.621117	1.827024	H	1.487653	2.931496	1.715353
C	-7.748914	0.336336	2.185997	C	-2.085862	-0.152014	6.811925
H	-8.686055	-0.216514	2.232550	H	-1.579336	-0.632230	7.647942
H	-2.399342	-0.646755	2.200949	H	-3.283420	0.245543	0.401348
S	0.018353	0.798113	2.388688	S	0.082479	1.176951	2.596615
C	-6.349034	2.152277	2.944466	C	-3.290938	1.725105	5.888867
C	-7.565645	1.468790	2.979314	C	-2.656695	1.108330	6.970700
H	-6.191400	3.024614	3.577392	H	-3.728781	2.715581	6.003170
H	-8.363399	1.807949	3.638929	H	-2.600257	1.618017	7.931469

<i>cis</i> -8				<i>trans</i> -8			
-14.90249165				-14.90419974			
H	-6.634827	-0.831816	-3.945327	H	1.896856	-1.062992	-5.608961
H	-5.459658	1.346771	-3.632499	H	1.060523	1.148351	-4.822370
C	-5.610762	-0.808950	-3.573811	C	1.776156	-0.871438	-4.543397
C	-4.954060	0.410668	-3.400430	C	1.309366	0.369496	-4.102651
H	-5.459354	-2.952965	-3.387994	H	2.432719	-2.837517	-3.948313
C	-4.951938	-1.997306	-3.265558	C	2.076354	-1.864394	-3.613361
H	-7.255219	2.813153	-1.161650	H	-7.116257	2.515422	-1.646408
C	-3.651771	0.441766	-2.911544	C	1.144815	0.611652	-2.742652
H	-3.158910	1.402533	-2.760744	H	0.760759	1.575924	-2.410731
H	-5.828278	4.849774	-1.160249	H	-5.894786	4.675627	-1.487310
C	-3.640519	-1.971748	-2.790087	C	1.917257	-1.623104	-2.246525
C	-6.249019	2.774335	-0.745583	C	-6.153869	2.563359	-1.138800
C	-5.447802	3.914942	-0.749755	C	-5.466132	3.772671	-1.054393
C	-2.976607	-0.752351	-2.610392	C	1.459681	-0.379105	-1.799705
H	-3.140865	-2.909923	-2.556033	H	2.142626	-2.414813	-1.534020
H	-6.396177	0.688093	-0.271097	H	-6.146292	0.464024	-0.676833
H	-4.147627	-4.737107	-0.074527	H	-4.273846	-4.436295	-1.190395
H	-1.563825	-0.110979	-4.755870	H	3.523828	1.194463	-1.283937
C	-5.768686	1.573916	-0.220262	C	-5.607816	1.405150	-0.585301
H	-0.319506	1.378104	-6.279311	H	4.853089	3.183897	-0.670017
H	-6.618768	-4.809207	0.238575	H	-6.602259	-4.665146	-0.344256
H	-0.966977	-2.485180	-4.166095	H	3.930080	-0.973821	-0.011942
C	-4.693733	-3.836426	0.203170	C	-4.730011	-3.630620	-0.617299
C	-4.148448	3.849278	-0.243556	C	-4.211349	3.818343	-0.447590
H	-3.506271	4.728860	-0.263046	H	-3.657677	4.755335	-0.408078
H	0.336376	0.155079	0.276511	H	-1.441176	-0.507797	-1.033940
C	-6.074691	-3.876748	0.385647	C	-6.034028	-3.758393	-0.140999
H	-2.925609	-2.596599	0.225233	H	-2.971534	-2.368193	-0.701492
C	-0.745774	0.492408	-4.366048	C	3.218462	1.804014	-0.434601
C	-4.006411	-2.635957	0.368397	C	-3.996987	-2.475086	-0.348385
C	-0.050148	1.341132	-5.224896	C	3.965911	2.929512	-0.091497
C	-4.474985	1.504282	0.308368	C	-4.358284	1.450461	0.042924
C	-6.757431	-2.723164	0.775568	C	-6.607533	-2.728480	0.606907
C	-3.659581	2.650203	0.268047	C	-3.647054	2.659315	0.077336
C	-0.554716	-2.956361	-0.3275781	C	3.363962	-1.556904	0.712218
H	-7.833383	-2.757627	0.941133	H	-7.624980	-2.827432	0.982153
H	0.026937	-4.742477	-4.324972	H	5.072151	-2.712341	1.326018
P	-1.327470	-0.626227	-1.814887	P	1.078595	-0.036852	-0.035092
C	-4.685175	-1.466111	0.735982	C	-4.566076	-1.440201	0.401880
C	-0.423549	0.451063	-3.002586	C	2.068436	1.477826	0.296866
C	-6.066516	-1.527673	0.969084	C	-5.876243	-1.576017	0.883457
Pt	-1.302559	0.041257	0.434718	Pt	-1.230057	0.003785	0.511650
C	0.006225	-4.227713	-3.365813	C	4.007514	-2.532684	1.467920
H	-2.622919	2.575611	0.607500	H	-2.638714	2.672503	0.494496
C	0.976860	2.149293	-4.734457	C	3.578557	3.728213	0.986023
H	1.513003	2.819052	-5.405993	H	4.165317	4.606297	1.251815
C	-0.593095	-2.293824	-2.042561	C	1.993342	-1.327841	0.888913
P	-3.642169	0.015878	0.992114	P	-3.540727	0.007491	0.820700
H	-6.608695	-0.650988	1.316356	H	-6.328148	-0.782623	1.476255
C	0.603097	1.268223	-2.514640	C	1.669045	2.294205	1.362151
C	1.305350	2.106316	-3.379766	C	2.431779	3.407013	1.711462
C	0.546096	-4.840219	-2.231916	C	3.293832	-3.270644	2.416226
C	-0.042041	-2.907348	-0.911988	C	1.282095	-2.067778	1.837956
H	0.828219	1.248788	-1.448749	H	0.759088	2.056748	1.920839
H	2.100593	2.739236	-2.988707	H	3.805084	-4.023608	3.015052
H	-0.054243	-2.365685	0.035485	H	2.117597	4.030038	2.548119
C	-3.708058	0.249879	2.834482	H	0.221276	-1.858955	1.984301
H	-4.717150	0.576761	3.133785	C	-3.879965	0.264350	2.628214
C	0.527374	-4.177089	-1.006401	H	-4.906883	0.643239	2.756636
S	-0.931730	0.795382	2.693878	C	1.933708	-3.034401	2.604397
H	-2.890674	2.245449	2.967566	S	-1.108286	0.670763	2.915636
H	-3.515499	-0.748664	3.256271	H	-3.003368	2.229211	2.852964
C	-2.631197	1.224590	3.282960	H	-3.796160	-0.730070	3.092233
H	0.960355	-4.643074	-0.122440	C	-2.846739	1.207405	3.226490
H	-2.574269	1.230186	4.380962	H	1.376126	-3.593285	3.354234
H	0.987857	-5.833200	-2.308369	H	-2.974165	1.240031	4.317783

Benchmark, alternative structures, M06L/TZVP(SMD):

<i>cis-5</i>				<i>trans-5</i>			
H	-4.663273	3.178523	-4.497888	H	-8.186006	-2.637363	2.484438
H	-3.205023	1.177921	-4.432617	H	-6.664890	-2.781468	0.534774
C	-4.585870	2.592711	-3.590304	C	-7.165172	-2.284271	2.564371
C	-3.767882	1.469636	-3.554310	C	-6.312586	-2.363422	1.469837
H	-5.941596	3.834490	-2.483836	H	-7.364757	-1.683616	4.614598
C	-5.302975	2.959870	-2.461365	C	-6.705604	-1.748989	3.757607
H	-6.084854	-3.554925	-2.392591	H	-2.225855	-5.714683	3.633776
C	-3.668049	0.720107	-2.393123	C	-5.010636	-1.901513	1.568226
H	-5.692332	-1.188602	-1.855351	H	-3.554957	-3.656701	3.424666
H	-3.021693	-0.151438	-2.367563	H	-4.350629	-1.955690	0.709711
C	-5.447787	-3.294137	-1.556191	C	-1.730467	-4.778152	3.408052
C	-5.209134	2.208162	-1.297035	C	-5.396716	-1.295602	3.862870
C	-5.226690	-1.958889	-1.251486	C	-2.480876	-3.616589	3.286925
H	-5.025553	-5.332952	-1.035825	H	0.229401	-5.647633	3.338615
C	-4.395863	1.077528	-1.254544	C	-4.539711	-1.363327	2.766660
C	-4.853783	-4.291065	-0.794543	C	-0.353364	-4.739412	3.243875
H	-5.773739	2.504161	-0.420584	H	-5.048111	-0.888279	4.804038
H	-0.971278	1.478312	-1.083279	H	-0.761528	1.088197	-1.024666
H	-2.095505	2.584683	-0.719636	H	-2.016644	2.108391	-0.946295
C	-4.404406	-1.607570	-0.179638	C	-1.855107	-2.406770	2.991490
N	-1.352699	2.023366	-0.313476	N	-1.258170	1.716977	-0.398022
C	-4.034474	-3.949385	0.272371	C	0.275744	-3.535148	2.955116
P	-4.112527	0.144640	0.301197	P	-2.782932	-0.825382	2.866291
C	-3.806187	-2.615660	0.575847	C	-0.469931	-2.374017	2.824291
H	-3.563499	-4.722973	0.866458	H	1.350746	-3.500566	2.826044
C	-0.294722	2.905379	0.226460	C	-0.340572	2.794174	0.043154
H	1.254483	1.427063	0.262634	H	1.301513	1.504505	0.517225
H	-7.019814	-0.442349	0.106758	H	-1.940801	-1.861937	5.539936
C	-5.568825	0.561812	1.343470	C	-2.647041	-0.090147	4.542035
Pt	-2.097569	0.611791	1.241607	Pt	-2.022625	0.507040	1.229125
C	-6.857732	0.155762	0.996496	C	-2.226843	-0.822394	5.649833
H	-3.153295	-2.347253	1.398539	H	0.014285	-1.429114	2.594016
H	-0.773653	3.610569	0.906965	H	-0.948243	3.562509	0.522190
C	0.730282	2.085417	0.960343	C	0.665937	2.242220	1.015127
H	-4.373910	1.633104	2.761035	H	-3.318680	1.824031	3.836561
C	-5.379772	1.327523	2.491408	C	-3.008209	1.248255	4.701992
H	1.477508	2.739502	1.410041	H	1.317544	3.044386	1.362883
C	-7.938665	0.514416	1.786512	C	-2.170783	-0.222616	6.900871
H	-8.936182	0.194352	1.511028	H	-1.837452	-0.797286	7.756405
H	-2.502902	-0.372158	2.405790	H	-3.212548	-0.014870	0.288936
S	-0.035838	1.078112	2.302715	S	-0.161359	1.483741	2.474166
C	-6.464058	1.685873	3.280862	C	-2.960078	1.840791	5.953630
C	-7.742955	1.279941	2.929474	C	-2.540301	1.105719	7.054948
H	-6.306611	2.279162	4.173325	H	-3.242842	2.880065	6.068238
H	-8.588981	1.556110	3.547063	H	-2.495166	1.571232	8.031977
H	0.173845	3.476703	-0.581746	H	0.151591	3.239852	-0.827361

<i>cis</i> -6				<i>trans</i> -6			
H	-4.462703	3.552129	-4.154165	H	-8.194848	-2.655192	2.280348
H	-3.059241	1.512235	-4.191734	H	-6.634830	-2.619930	0.356566
C	-4.442928	2.891027	-3.296611	C	-7.180628	-2.297661	2.409626
C	-3.655306	1.746351	-3.318197	C	-6.306392	-2.275975	1.329700
H	-5.816358	4.076899	-2.150663	H	-7.428615	-1.870708	4.497778
C	-5.201474	3.185425	-2.173020	C	-6.752050	-1.856887	3.652033
H	-5.901727	-3.432311	-2.563602	H	-2.189185	-5.734491	3.345132
C	-3.625407	0.902136	-2.219505	C	-5.012983	-1.808142	1.492225
H	-5.623873	-1.091452	-1.868315	H	-3.550197	-3.686151	3.294950
H	-2.998156	0.016758	-2.237504	H	-4.336019	-1.783201	0.645693
C	-5.304459	-3.200441	-1.690158	C	-1.710897	-4.777771	3.173991
C	-5.177311	2.339951	-1.071461	C	-5.451649	-1.398678	3.821249
C	-5.148507	-1.879659	-1.295998	C	-2.479071	-3.622099	3.142865
H	-4.815075	-5.249909	-1.282361	H	0.259012	-5.611658	3.012298
C	-4.393132	1.187745	-1.086899	C	-4.573253	-1.365782	2.740554
H	2.391944	5.005280	-1.542250	H	2.460388	5.131349	-1.478394
O	0.134665	3.571783	-1.727970	O	0.448961	3.400619	-1.717804
C	-4.694846	-4.219418	-0.971129	C	-0.337484	-4.707763	2.989181
H	-5.769759	2.580888	-0.196289	H	-5.126360	-1.067250	4.799826
H	-1.098749	1.674951	-0.824116	H	-0.716040	1.522574	-0.719955
H	-2.235864	2.730137	-0.374110	H	-2.020205	2.467314	-0.583160
C	1.666129	5.617169	-1.008308	C	1.610046	5.716890	-1.131474
C	-4.378050	-1.565370	-0.175281	C	-1.874502	-2.386472	2.918560
C	0.228605	3.823002	-0.548544	C	0.325473	3.830018	-0.593858
H	2.173494	6.390256	-0.440102	H	1.954302	6.610138	-0.620179
N	-1.482095	2.153163	-0.009194	N	-1.266403	2.051670	-0.044217
C	-3.925951	-3.914388	0.143295	C	0.270288	-3.478229	2.770097
P	-4.172869	0.162648	0.419283	P	-2.827618	-0.817309	2.921176
O	0.951701	4.825558	-0.043909	O	0.848562	4.978937	-0.160489
C	-3.763348	-2.594610	0.537089	C	-0.493252	-2.321839	2.731594
H	-3.442874	-4.705116	0.704100	H	1.342084	-3.419464	2.624710
C	-0.433557	3.019032	0.554009	C	-0.413282	3.116164	0.520345
H	1.118926	1.536384	0.565500	H	1.246474	1.839686	0.989002
H	-7.053483	-0.418983	-0.000810	H	-1.893701	-2.029816	5.488367
C	-5.690332	0.479970	1.405911	C	-2.724815	-0.227539	4.655553
Pt	-2.211449	0.645283	1.461323	Pt	-2.054352	0.671849	1.434567
C	-6.951419	0.097786	0.946874	C	-2.240115	-1.023237	5.690560
H	-3.149845	-2.353178	1.397619	H	-0.025874	-1.356647	2.559531
H	-0.902909	3.701490	1.265050	H	-1.059421	3.826889	1.038490
C	0.594000	2.170685	1.285445	C	0.565166	2.514543	1.516168
H	-4.594564	1.432688	2.979569	H	-3.522848	1.696306	4.126004
C	-5.578602	1.143123	2.625420	C	-3.161121	1.068843	4.933679
H	1.335061	2.815146	1.756870	H	1.167285	3.308732	1.956117
C	-8.081109	0.377550	1.699103	C	-2.194756	-0.528187	6.987253
H	-9.056581	0.075995	1.337507	H	-1.810539	-1.151228	7.785642
H	-2.617543	-0.405372	2.563583	H	-3.164803	0.169995	0.393859
S	-0.188071	1.133359	2.586635	S	-0.315207	1.627274	2.858056
C	-6.712144	1.422864	3.376645	C	-3.124098	1.555314	6.230339
C	-7.962713	1.040149	2.914907	C	-2.639045	0.757321	7.258985
H	-6.615382	1.937382	4.324858	H	-3.465397	2.562124	6.437454
H	-8.847311	1.255037	3.501968	H	-2.602155	1.141165	8.271151
H	0.976341	6.066322	-1.721532	H	0.985430	5.987584	-1.981665

<i>cis-7</i>				<i>trans-7</i>			
H	-4.496724	3.728642	-3.988234	H	-8.194906	-2.611214	2.212942
H	-3.023075	1.739551	-4.069435	H	-6.612342	-2.500863	0.310474
C	-4.469098	3.038969	-3.153648	C	-7.183200	-2.256639	2.367642
C	-3.641878	1.923184	-3.199635	C	-6.296261	-2.192945	1.299648
H	-5.902863	4.136634	-1.993895	H	-7.457114	-1.908001	4.466988
C	-5.256864	3.268069	-2.035113	C	-6.770452	-1.861609	3.630555
H	-5.827192	-3.289258	-2.721521	H	-2.164945	-5.711610	3.202593
C	-3.602803	1.042813	-2.130414	C	-5.006103	-1.729186	1.494922
H	-5.584801	-0.981850	-1.909574	H	-3.534505	-3.669347	3.275893
H	-2.946093	0.179534	-2.167753	H	-4.319073	-1.671072	0.658058
C	-5.246555	-3.094027	-1.828110	C	-1.697471	-4.747147	3.045695
C	-5.224073	2.385393	-0.963120	C	-5.473003	-1.407850	3.832442
C	-5.109509	-1.792244	-1.369102	C	-2.470329	-3.595072	3.083959
H	-4.744767	-5.156445	-1.509968	H	0.267828	-5.564907	2.778258
C	-4.400842	1.261610	-1.003880	C	-4.581944	-1.333934	2.764452
H	2.095927	5.121823	-1.433019	H	2.265249	5.294320	-1.302555
O	0.112598	3.712973	-1.468395	O	0.497658	3.621940	-1.399090
C	-4.639528	-4.140967	-1.148053	C	-0.332530	-4.663825	2.809310
H	-5.841172	2.574908	-0.092276	H	-5.160053	-1.112589	4.826554
H	-1.104376	1.779717	-0.664625	H	-0.731032	1.753917	-0.518121
H	-2.255843	2.803821	-0.183750	H	-2.029353	2.697281	-0.326497
H	1.417097	7.506560	-1.773907	H	1.384099	7.463347	-2.195247
H	-0.000387	6.459819	-1.745659	H	0.124716	6.230691	-2.205822
C	1.689863	5.732690	-0.626221	C	1.645194	5.962814	-0.704688
C	-4.360987	-1.525416	-0.221215	C	-1.879536	-2.348966	2.879678
C	0.210702	3.910897	-0.278175	C	0.345863	4.026985	-0.268411
H	2.513900	6.107261	-0.021987	H	2.289687	6.551144	-0.054369
N	-1.503791	2.215436	0.166264	N	-1.277459	2.247556	0.187182
C	0.823120	6.843986	-1.144606	C	0.765960	6.829403	-1.559770
C	-3.892608	-3.883021	-0.007070	C	0.261336	-3.424733	2.608179
P	-4.180757	0.174019	0.457861	P	-2.839772	-0.787358	2.980966
O	0.951639	4.867927	0.281321	O	0.854947	5.159589	0.215913
C	-3.748935	-2.582231	0.451814	C	-0.507463	-2.271366	2.639758
H	-3.411687	-4.695528	0.523664	H	1.326114	-3.355708	2.421652
C	-0.467885	3.061587	0.781478	C	-0.415478	3.274574	0.806378
H	1.094060	1.589556	0.758678	H	1.226385	1.957747	1.224851
H	-7.037125	-0.534063	0.048354	H	-1.926160	-2.161326	5.475315
H	0.411364	7.436470	-0.327805	H	0.137614	7.477232	-0.948879
C	-5.709449	0.429044	1.445351	C	-2.741188	-0.305939	4.748825
Pt	-2.239709	0.629439	1.548550	Pt	-2.072415	0.790001	1.584975
C	-6.955009	-0.004823	0.990855	C	-2.268453	-1.166918	5.736184
H	-3.152484	-2.376922	1.333434	H	-0.051217	-1.298651	2.482191
H	-0.951644	3.714645	1.510458	H	-1.055857	3.969336	1.352133
C	0.551087	2.188542	1.495329	C	0.549037	2.614819	1.778986
H	-4.649185	1.428693	3.014873	H	-3.522388	1.652106	4.333286
C	-5.622102	1.102071	2.661828	C	-3.170912	0.973805	5.103544
H	1.278664	2.817098	2.007378	H	1.157536	3.379837	2.260169
C	-8.094217	0.236094	1.742534	C	-2.229395	-0.752717	7.061067
H	-9.057405	-0.105981	1.384094	H	-1.854154	-1.426108	7.822016
H	-2.647758	-0.485745	2.584595	H	-3.173202	0.340123	0.508608
S	-0.245605	1.089338	2.735216	S	-0.349134	1.673229	3.071077
C	-6.764832	1.343252	3.412122	C	-3.140481	1.379445	6.427903
C	-8.000506	0.910661	2.953635	C	-2.668156	0.516431	7.408689
H	-6.687048	1.865538	4.357836	H	-3.477084	2.373889	6.694059
H	-8.892206	1.095233	3.540282	H	-2.636263	0.836670	8.442961

<i>cis</i> -8				<i>trans</i> -8			
H	-6.419311	0.120591	-4.230116	H	2.714959	-2.615463	-5.057851
H	-4.995362	2.089773	-3.744319	H	0.765158	-1.091279	-4.976911
C	-5.444307	-0.012263	-3.777095	C	2.396854	-2.190276	-4.113816
C	-4.645613	1.092514	-3.506735	C	1.302750	-1.335245	-4.068772
H	-5.607018	-2.150411	-3.669792	H	3.931855	-3.166621	-2.975076
C	-4.990284	-1.284136	-3.462539	C	3.078858	-2.499601	-2.946775
H	-7.732034	1.849203	-1.130927	H	-7.055737	3.340667	0.461963
C	-3.402608	0.924205	-2.919672	C	0.888128	-0.800057	-2.860084
H	-2.790150	1.792597	-2.700297	H	0.026515	-0.142624	-2.824825
H	-6.804036	4.133855	-1.344492	H	-5.469284	5.210875	0.140529
C	-3.736399	-1.457538	-2.889021	C	2.673939	-1.954783	-1.735290
C	-6.729167	2.064040	-0.781546	C	-5.989482	3.150695	0.443499
C	-6.207894	3.343722	-0.904493	C	-5.097784	4.200802	0.263205
C	-2.930151	-0.355737	-2.614637	C	1.573288	-1.101714	-1.682637
H	-3.388930	-2.457825	-2.660828	H	3.220377	-2.196023	-0.831497
H	-6.386646	0.051996	-0.141677	H	-6.218232	1.039435	0.734761
H	-3.968466	-4.690342	-0.303539	H	-5.710133	-1.907622	-3.171107
H	-1.401097	0.063458	-4.684537	H	3.001305	1.047003	-1.913045
C	-5.968633	1.047986	-0.217833	C	-5.517519	1.856369	0.598145
H	0.136044	1.187963	-6.228395	H	3.890038	3.340572	-1.940587
H	-6.174436	-5.025248	0.777113	H	-7.248966	-3.386239	-1.915177
H	-1.053181	-2.237597	-4.169724	H	3.571773	0.367691	1.320014
C	-4.460070	-3.868569	0.204316	C	-5.675913	-1.934589	-2.088922
C	-4.912837	3.604679	-0.474978	C	-3.732643	3.954712	0.235704
H	-4.492925	4.597541	-0.580586	H	-3.034552	4.770368	0.092018
H	0.316015	0.327616	0.252452	H	-1.550896	-0.393404	-1.220034
C	-5.693042	-4.055520	0.811410	C	-6.539295	-2.764246	-1.383649
H	-2.873439	-2.480420	-0.202173	H	-4.081811	-0.507165	-1.963490
C	-0.487712	0.501433	-4.299840	C	2.659035	1.763231	-1.175433
C	-3.846072	-2.625123	0.253876	C	-4.762019	-1.146006	-1.410435
C	0.380400	1.137443	-5.174269	C	3.162396	3.057160	-1.189841
C	-4.673896	1.303820	0.227371	C	-4.145934	1.602153	0.569413
C	-6.305705	-2.999275	1.474782	C	-6.488240	-2.796296	0.001463
C	-4.147293	2.590342	0.077936	C	-3.257214	2.659448	0.384663
C	-0.746867	-2.814030	-3.303923	C	3.218573	-0.592696	1.677035
H	-7.262498	-3.145064	1.961150	H	-7.158866	-3.441155	0.556083
H	-0.320892	-4.568256	-4.455073	H	4.853325	-0.841612	3.039739
P	-1.301565	-0.492339	-1.776212	P	1.031949	-0.310302	-0.115400
C	-4.459158	-1.554996	0.898340	C	-4.708306	-1.169519	-0.015458
C	-0.193423	0.428516	-2.935828	C	1.719486	1.389469	-0.216746
C	-5.692723	-1.756788	1.523002	C	-5.579280	-2.000354	0.686576
Pt	-1.284333	0.196490	0.415107	Pt	-1.247285	-0.271960	0.350150
C	-0.335107	-4.127265	-3.465860	C	3.942716	-1.275936	2.645331
H	-3.122739	2.787284	0.379891	H	-2.191087	2.454598	0.352573
C	1.553933	1.708148	-4.701162	C	2.738217	3.982169	-0.246909
H	2.229515	2.207777	-5.384705	H	3.132160	4.991074	-0.261572
C	-0.774148	-2.237355	-2.033137	C	2.042289	-1.139223	1.170104
P	-3.579369	0.047028	0.996793	P	-3.493495	-0.094426	0.825901
H	-6.174869	-0.942383	2.051474	H	-5.556421	-2.033039	1.768622
C	0.986122	1.006188	-2.471347	C	1.293055	2.325233	0.727592
C	1.854427	1.639519	-3.348883	C	1.805365	3.612975	0.713905
C	0.058963	-4.875603	-2.363014	C	3.502858	-2.508560	3.105705
C	-0.370937	-2.991811	-0.933502	C	1.600142	-2.375336	1.644003
H	1.220698	0.963801	-1.414850	H	0.562056	2.029627	1.475146
H	2.765980	2.085395	-2.969899	H	4.069053	-3.038434	3.862013
H	-0.388372	-2.536519	0.052283	H	1.471130	4.331451	1.452522
C	-3.657907	0.428360	2.811585	H	0.674968	-2.794809	1.263260
H	-4.672243	0.734263	3.081609	C	-3.696286	-0.381257	2.634472
C	0.043043	-4.306731	-1.098151	H	-4.690192	-0.059313	2.959458
S	-0.938254	1.054364	2.600407	C	2.331351	-3.059061	2.601569
H	-2.925044	2.452173	2.800510	S	-0.914237	-0.131146	2.773670
H	-3.443343	-0.514535	3.319935	H	-2.725319	1.433319	3.262107
C	-2.638243	1.472445	3.188413	H	-3.609238	-1.457322	2.801656
H	0.353638	-4.884531	-0.236313	C	-2.593716	0.353042	3.364641
H	-2.580051	1.564942	4.274179	H	1.980750	-4.018151	2.962596
H	0.381020	-5.901706	-2.492613	H	-2.638705	0.126032	4.430509

<i>cis-9</i>				<i>trans-9</i>			
H	2.608026	-3.954859	-5.175923	H	2.836402	1.077203	-5.499039
H	2.058628	-1.589448	-4.692744	H	0.701430	1.718989	-4.419154
C	2.246172	-3.669796	-4.195508	C	2.661495	0.839241	-4.456880
H	-5.760221	1.410254	-4.007376	H	-4.955589	1.640530	-4.202075
H	-4.171784	2.115770	-4.296060	H	-3.298859	2.239958	-4.187254
H	2.316095	-5.670291	-3.416570	H	4.568432	-0.110984	-4.193267
H	-4.319134	0.396625	-3.943025	H	-3.617739	0.528067	-3.915911
C	1.939096	-2.344161	-3.925112	C	1.464162	1.198609	-3.852090
C	-4.714911	1.383326	-3.692759	C	-3.986149	1.535548	-3.710466
H	-2.899245	-3.135434	-4.073478	H	-2.652652	-3.291225	-3.875505
C	2.081912	-4.633319	-3.208931	C	3.633219	0.170838	-3.725034
H	-5.355090	-3.436230	-3.978551	H	-5.118061	-3.331769	-4.085199
C	-3.458034	-2.789168	-3.212385	C	-3.271904	-2.857904	-3.099703
C	-4.834966	-2.954979	-3.159342	C	-4.654199	-2.880083	-3.216792
H	-6.171878	3.130637	-2.113237	H	-5.606663	3.324741	-2.353203
H	-4.588901	3.813992	-2.437079	H	-3.960848	3.931950	-2.367726
C	1.468590	-1.980718	-2.671497	C	1.236553	0.887181	-2.520575
C	-4.566676	1.683475	-2.213058	C	-4.081001	1.797248	-2.219204
C	-5.114460	3.055705	-1.842610	C	-4.619156	3.186477	-1.903389
C	1.612603	-4.273199	-1.954784	C	3.412569	-0.138582	-2.390072
H	1.214645	-0.947849	-2.458371	H	0.303061	1.163530	-2.039438
H	-2.542051	2.364891	-2.340324	H	-2.033430	2.374762	-1.979374
H	-5.135737	0.928180	-1.652980	H	-4.773230	1.061174	-1.786651
H	-1.719172	-2.021315	-2.203880	H	-1.596680	-2.241852	-1.895908
C	-2.794694	-2.169383	-2.163215	C	-2.677305	-2.274689	-1.989319
C	-5.548225	-2.494128	-2.059719	C	-5.444352	-2.319781	-2.220806
H	-6.623971	-2.614086	-2.020605	H	-6.523766	-2.335909	-2.309044
H	-2.665550	0.647446	-2.070763	H	-2.284073	0.658425	-1.790749
C	1.305531	-2.939970	-1.672396	C	2.211220	0.217378	-1.779158
H	1.477472	-5.035003	-1.195695	H	4.178356	-0.658016	-1.825490
C	-3.105536	1.607754	-1.783386	C	-2.720029	1.634960	-1.550151
C	-4.926495	3.342027	-0.363861	C	-4.682973	3.418768	-0.404706
H	-5.295683	4.342823	-0.120394	H	-5.046628	4.428392	-0.191243
C	-3.498639	-1.718226	-1.047942	C	-3.462779	-1.711821	-0.985464
C	-4.885369	-1.876648	-1.009298	C	-4.853399	-1.740046	-1.108632
H	-2.896834	3.948847	-0.513210	H	-2.635008	3.929972	-0.178484
H	-5.546654	2.647288	0.213289	H	-5.423933	2.736693	0.027164
C	-2.870000	1.851988	-0.289690	C	-2.730080	1.830622	-0.030045
C	-3.467461	3.230143	0.091167	C	-3.332037	3.221961	0.290309
P	0.692883	-2.399873	-0.024687	P	1.869637	-0.132146	-0.009020
H	-5.449268	-1.516050	-0.155756	H	-5.477535	-1.311605	-0.331736
H	-4.512085	0.599772	0.442150	H	-4.529679	0.638950	0.372170
Pt	-0.309450	-0.335109	-0.041264	Pt	-0.391910	-0.562284	0.306412
S	-1.007587	1.929955	-0.024743	S	-0.949150	1.804704	0.562995
P	-2.576448	-0.880830	0.295697	P	-2.663327	-0.927640	0.463370
C	-3.433967	0.731954	0.576329	C	-3.483631	0.711285	0.685732
H	-3.729624	5.736535	1.234896	H	-3.682031	5.704044	1.467399
H	-2.012172	5.354709	1.131824	H	-1.990487	5.240141	1.640953
H	-4.145737	-3.378831	0.982181	H	-4.017726	-3.568698	0.806442
C	-2.934556	5.121410	1.666932	C	-2.999958	5.037477	2.003620
C	-3.275337	3.640679	1.572343	C	-3.382717	3.578689	1.796718
H	-5.320891	3.958136	2.255898	H	-5.500372	3.976712	2.131193
H	-3.261911	0.961092	1.629367	H	-3.478982	0.896268	1.760545
H	-2.409531	3.080004	1.942304	H	-2.618432	2.965904	2.288116
C	-3.727382	-2.959591	1.888926	C	-3.819986	-3.154458	1.787710
C	-2.962226	-1.798299	1.837762	C	-3.218433	-1.904225	1.912032
C	-4.456824	3.330209	2.485591	C	-4.717336	3.299350	2.480253
H	-4.785540	2.292083	2.425990	H	-5.075762	2.281253	2.323794
H	-2.806915	5.439671	2.703737	H	-3.036630	5.317925	3.058435
H	-4.549296	-4.500453	3.128824	H	-4.637695	-4.848485	2.811444
H	-4.189631	3.525993	3.525929	H	-4.626513	3.448159	3.558016
C	-3.954831	-3.594894	3.103746	C	-4.167777	-3.878573	2.920298
C	-2.405833	-1.298663	3.020082	C	-2.951846	-1.399933	3.187294
H	-1.784511	-0.408268	2.986601	H	-2.454880	-0.441402	3.298305
C	-3.417520	-3.082322	4.274256	C	-3.916104	-3.364440	4.183361
C	-2.637566	-1.932675	4.229509	C	-3.304758	-2.123735	4.314394
H	-3.596936	-3.581053	5.218881	H	-4.188825	-3.930896	5.065262
H	-2.205001	-1.531463	5.137949	H	-3.096121	-1.720908	5.297924
H	1.199913	0.227354	-0.238637	H	-0.108426	-2.140127	0.187582

C	-0.282739	-3.848565	0.558096	C	3.079486	-1.446890	0.418220
C	-1.140638	-4.515477	-0.318339	C	2.834743	-2.747679	-0.023228
C	-0.227976	-4.257676	1.890522	C	4.249148	-1.177096	1.125680
C	-1.910825	-5.581075	0.123028	C	3.747605	-3.757733	0.231965
H	-1.190399	-4.217811	-1.358454	H	1.922968	-2.965646	-0.568470
C	-0.998488	-5.325538	2.328752	C	5.156419	-2.194847	1.390363
H	0.425512	-3.747897	2.589260	H	4.457895	-0.171461	1.470256
C	-1.837828	-5.992102	1.447094	C	4.909418	-3.483853	0.943248
H	-2.564772	-6.092831	-0.573355	H	3.548155	-4.763119	-0.118176
H	-0.942811	-5.634315	3.365664	H	6.059941	-1.974947	1.945950
H	-2.436809	-6.826314	1.791604	H	5.618666	-4.275946	1.150047
C	2.161504	-2.443399	1.085704	C	2.480589	1.345538	0.887682
C	3.200804	-3.356007	0.915235	C	3.219108	2.351617	0.270646
C	2.199056	-1.562078	2.165469	C	2.166469	1.458170	2.243151
C	4.262063	-3.381337	1.808212	C	3.639533	3.454858	1.002052
H	3.192841	-4.044563	0.079038	H	3.463551	2.280534	-0.782674
C	3.256534	-1.596096	3.062670	C	2.597481	2.554488	2.971919
H	1.394888	-0.843166	2.290036	H	1.575743	0.684569	2.722803
C	4.289669	-2.505492	2.885011	C	3.332686	3.556557	2.350914
H	5.069287	-4.088548	1.661155	H	4.207439	4.237088	0.513228
H	3.275405	-0.906557	3.897806	H	2.349594	2.632547	4.023377
H	5.119491	-2.527843	3.580927	H	3.660167	4.419217	2.918254

<i>cis</i> -10				<i>trans</i> -10			
H	3.674006	-4.195803	-4.734777	H	3.329890	-1.192215	-5.595783
H	3.290349	-1.774074	-4.389198	H	1.291821	-2.204283	-4.621121
C	3.090257	-3.852504	-3.889362	C	3.058002	-0.984452	-4.568026
H	2.711313	-5.830509	-3.143975	H	4.738322	0.306731	-4.219671
C	2.876073	-2.495325	-3.695309	C	1.916000	-1.552839	-4.021664
H	-3.884760	-2.426045	-4.240021	H	-3.204873	-0.122784	-4.366860
C	2.549645	-4.769282	-2.998627	C	3.848456	-0.143285	-3.796609
H	-6.120590	-3.271617	-3.593504	H	-5.419172	-1.223510	-4.486673
C	-4.218129	-2.354017	-3.212056	C	-3.657417	-0.534432	-3.473046
C	-5.471834	-2.825355	-2.849607	C	-4.898839	-1.151232	-3.539370
C	2.122058	-2.054945	-2.617642	C	1.563801	-1.282591	-2.707626
C	1.797930	-4.331963	-1.917890	C	3.500465	0.128200	-2.481769
H	1.944706	-0.995843	-2.474748	H	0.666464	-1.716165	-2.279907
H	-2.399397	-1.429094	-2.531190	H	-2.008107	0.015616	-2.205606
C	-3.385795	-1.791176	-2.255663	C	-2.986878	-0.451789	-2.261447
C	-5.895909	-2.720766	-1.531271	C	-5.471159	-1.682336	-2.390859
H	-6.877184	-3.079307	-1.245264	H	-6.438700	-2.166886	-2.439494
C	1.578361	-2.967464	-1.714828	C	2.356090	-0.444143	-1.923574
H	1.381621	-5.058818	-1.230221	H	4.119136	0.792658	-1.889707
C	-5.115484	3.106219	0.161745	C	-4.781693	3.304172	1.336972
H	-5.443343	4.118537	0.408357	H	-5.100776	4.206177	1.863958
C	-3.796471	-1.690036	-0.925275	C	-3.557492	-0.977619	-1.101928
C	-5.068577	-2.150902	-0.575277	C	-4.807458	-1.594108	-1.176474
H	-3.463226	3.774712	-1.069161	H	-2.838390	4.105592	0.815738
C	-3.128236	1.717137	-0.532269	C	-2.770516	1.964280	0.614549
C	-3.639959	3.116868	-0.215289	C	-3.260538	3.227983	1.310340
P	0.629344	-2.353919	-0.256107	P	1.875178	-0.146713	-0.174933
H	-5.416231	-2.066965	0.446754	H	-5.262342	-2.009986	-0.284722
Pt	-0.482962	-0.373274	-0.552502	Pt	-0.405173	-0.418061	0.199516
S	-1.322353	1.806552	-0.943148	S	-0.918008	1.924340	0.607523
P	-2.646635	-0.888231	0.255748	P	-2.660668	-0.779965	0.485253
C	-3.406139	0.772809	0.630526	C	-3.383118	0.732922	1.278651
H	-3.803666	-3.536329	1.157867	H	-2.774930	-3.618110	-0.076852
H	-2.825688	1.128925	1.491882	H	-3.009748	0.700830	2.310565
C	-3.355455	-3.035506	2.006015	C	-3.099884	-3.491456	0.950221
C	-2.768654	-1.781849	1.851884	C	-3.181924	-2.209770	1.499590
H	-3.814841	-4.640247	3.345943	H	-3.365567	-5.590248	1.269087
C	-3.353980	-3.664849	3.244168	C	-3.429643	-4.602374	1.708437
C	-2.152535	-1.185673	2.957377	C	-3.580706	-2.065637	2.827302
H	-1.663018	-0.223231	2.849502	H	-3.637925	-1.083203	3.279852
C	-2.756489	-3.058788	4.338483	C	-3.835785	-4.450091	3.028495
C	-2.149426	-1.817786	4.190044	C	-3.907348	-3.182280	3.585343
H	-2.755149	-3.553120	5.302179	H	-4.091407	-5.319464	3.621679
H	-1.669428	-1.340874	5.036009	H	-4.218153	-3.056813	4.615320
H	0.941681	0.196126	-1.074609	H	-0.142779	-1.990829	-0.033439
C	-0.389612	-3.821435	0.172008	C	2.919836	-1.292180	0.809681
C	-1.349500	-4.229135	-0.757226	C	4.249153	-1.545444	0.472911
C	-0.247004	-4.533900	1.359077	C	2.377989	-1.884634	1.948388
C	-2.138748	-5.340894	-0.512097	C	5.021759	-2.381613	1.264312
H	-1.465507	-3.680153	-1.685504	H	4.683901	-1.092521	-0.410764
C	-1.039747	-5.649256	1.602034	C	3.155950	-2.714994	2.742824
H	0.483553	-4.223926	2.097072	H	1.340191	-1.693370	2.201586
C	-1.980827	-6.057542	0.668777	C	4.477108	-2.965030	2.401146
H	-2.876826	-5.647526	-1.244297	H	6.051698	-2.578298	0.992478
H	-0.921220	-6.195934	2.529948	H	2.726251	-3.169834	3.626973
H	-2.594616	-6.928899	0.862498	H	5.082870	-3.617928	3.017724
C	1.881973	-2.278397	1.087221	C	2.571051	1.508305	0.197499
C	2.944724	-3.178252	1.162457	C	2.268512	2.574616	-0.652313
C	1.733289	-1.313630	2.081736	C	3.298438	1.750602	1.360847
C	3.839058	-3.114969	2.220311	C	2.707520	3.853965	-0.352745
H	3.076621	-3.931057	0.393715	H	1.687229	2.401451	-1.551038
C	2.625149	-1.256783	3.143044	C	3.730275	3.035635	1.660806
H	0.916997	-0.602073	2.007155	H	3.531885	0.935786	2.036156
C	3.678803	-2.157057	3.213204	C	3.437737	4.087784	0.805581
H	4.663904	-3.815406	2.269107	H	2.471101	4.672445	-1.021660
H	2.501273	-0.502000	3.910054	H	4.296765	3.212222	2.567079
H	4.380077	-2.108546	4.037370	H	3.775589	5.089586	1.041089
C	-5.377199	2.160984	1.323017	C	-5.385413	2.066968	1.981893
C	-4.885575	0.755882	1.000102	C	-4.907716	0.800638	1.283821
H	-5.710320	2.790756	-0.702859	H	-5.158389	3.395964	0.312101
H	-6.441653	2.134966	1.566686	H	-6.476448	2.114452	1.960110
H	-4.862276	2.529922	2.217001	H	-5.096965	2.027896	3.038546

H	-5.465606	0.363305	0.158726	H	-5.269987	0.800315	0.250044
H	-5.056572	0.080122	1.843028	H	-5.329297	-0.088186	1.761009
H	-3.050974	3.521025	0.615837	H	-2.872330	3.231818	2.335172
H	-3.657184	1.341387	-1.417325	H	-3.107240	1.990400	-0.429744

<i>cis-11-chair</i>				<i>trans-11-chair</i>			
H	2.743851	-0.767926	-5.262819	H	2.681342	-0.531160	-5.208310
H	1.290861	1.064502	-4.445518	H	1.251816	1.337438	-4.433953
C	2.462062	-0.723124	-4.217950	C	2.395818	-0.461837	-4.165786
C	1.646089	0.304877	-3.759913	C	1.593085	0.586608	-3.731795
H	3.546424	-2.495628	-3.683932	H	3.451759	-2.239736	-3.592907
C	2.910692	-1.691385	-3.333886	C	2.826704	-1.419582	-3.261140
H	3.361094	0.432658	5.228063	H	-7.346907	1.630437	-1.625352
C	1.277085	0.356748	-2.426417	C	1.219191	0.670421	-2.401035
H	0.628950	1.152879	-2.075526	H	0.583731	1.484100	-2.068022
H	3.685131	-1.932774	5.895346	H	-6.277112	3.669930	-2.529869
C	2.550747	-1.636099	-1.992470	C	2.464130	-1.331329	-1.922702
C	2.614166	-0.311968	4.979536	C	-6.333991	1.886018	-1.338643
C	2.795015	-1.636364	5.353924	C	-5.733589	3.029117	-1.846307
C	1.727472	-0.613546	-1.529599	C	1.655925	-0.286045	-1.482576
H	2.916318	-2.395314	-1.311680	H	2.815758	-2.080520	-1.223653
H	1.329360	1.108606	4.027798	H	-6.118424	0.171289	-0.073778
H	-2.353305	4.405669	2.891898	H	-3.896237	-4.332808	-0.272359
H	4.057975	0.361296	-0.220613	H	3.684136	1.158194	-0.677062
C	1.470006	0.067807	4.293588	C	-5.639472	1.061808	-0.463763
H	5.350565	2.339774	0.468353	H	5.011440	3.052001	0.162543
H	-2.306396	4.692346	5.349893	H	-5.922844	-4.740365	1.089450
H	3.762272	-0.993242	1.825250	H	3.727150	-0.602148	1.727775
C	-2.079941	3.575501	3.531690	C	-4.310282	-3.539489	0.337852
C	1.830087	-2.579403	5.028383	C	-4.431876	3.346544	-1.480638
H	1.966154	-3.616653	5.310499	H	-3.956728	4.235342	-1.877694
H	-1.188065	-0.233666	-0.962536	H	-1.331886	0.588959	-0.813017
C	-2.054930	3.735236	4.909267	C	-5.446622	-3.767561	1.101931
H	-1.788346	2.211424	1.891713	H	-2.798468	-2.116727	-0.222136
C	3.584068	1.133963	0.375120	C	3.348036	1.704088	0.197087
C	-1.758608	2.347624	2.967840	C	-3.696091	-2.296885	0.361053
C	4.310562	2.250523	0.757523	C	4.096997	2.771511	0.670792
C	0.489634	-0.871392	3.968234	C	-4.331633	1.371769	-0.097057
C	-1.707479	2.665194	5.725285	C	-5.968523	-2.749070	1.887174
C	0.688747	-2.203704	4.334132	C	-3.731969	2.518914	-0.616305
C	3.217057	-1.918723	1.686774	C	3.152407	-1.520754	1.713752
H	-1.688728	2.786111	6.801565	H	-6.853053	-2.924272	2.487365
H	4.686580	-3.086839	2.717596	H	4.639022	-2.629673	2.786406
P	1.237409	-0.444403	0.240346	P	1.162471	-0.093839	0.277542
C	-1.401614	1.271916	3.777912	C	-4.217902	-1.265014	1.141718
C	2.244152	1.005682	0.748494	C	2.168115	1.334317	0.842392
C	-1.382235	1.440620	5.163951	C	-5.360251	-1.501940	1.906449
Pt	-1.020595	-0.321925	0.633867	Pt	-1.109274	0.152736	0.712012
C	3.739598	-3.102857	2.191452	C	3.666884	-2.664146	2.309875
H	-0.050413	-2.955903	4.086168	H	-2.707349	2.753774	-0.345910
C	3.704518	3.257204	1.500221	C	3.676347	3.475490	1.790701
H	4.274011	4.131343	1.791602	H	4.261858	4.309848	2.157253
C	1.996161	-1.923642	1.018113	C	1.900036	-1.553181	1.106027
P	-1.007131	-0.361827	3.030481	P	-3.377956	0.361447	1.106392
H	-1.102627	0.612467	5.806465	H	-5.781653	-0.715100	2.520936
C	1.641101	2.027583	1.475704	C	1.748906	2.047151	1.965889
C	2.368051	3.147596	1.854608	C	2.503208	3.111013	2.437815
C	3.052953	-4.297171	2.030144	C	2.938821	-3.845051	2.298067
C	1.297602	-3.126291	0.880017	C	1.166888	-2.740638	1.107623
H	0.592853	1.939305	1.740358	H	0.832171	1.751640	2.466155
H	3.466403	-5.218269	2.422613	H	3.342400	-4.735379	2.764706
H	1.885279	3.935274	2.421143	H	2.171371	3.659858	3.310715
H	0.337165	-3.129374	0.373602	H	0.180461	-2.761391	0.654017
C	-2.312348	-1.444389	3.758489	C	-3.817486	1.183484	2.693997
C	1.826722	-4.306459	1.377291	C	1.687873	-3.882408	1.695197
S	-3.418688	-0.208651	0.632525	S	-0.791812	-0.578553	3.055944
H	-3.819653	-2.367798	1.668282	H	-1.402902	1.604623	3.940063
C	-4.088250	-1.339272	1.922665	C	-1.761306	0.583873	4.104020
H	1.280333	-5.233860	1.256155	H	1.112229	-4.799837	1.691914
H	-5.170054	-1.263735	1.799687	H	-1.498038	0.326064	5.131327
C	-3.731774	-1.058890	3.368246	C	-3.270299	0.536535	3.957908
H	-2.104441	-2.467662	3.433823	H	-3.444710	2.207684	2.597595
H	-2.189093	-1.419117	4.844170	H	-4.907058	1.260167	2.734160
H	-4.411534	-1.638864	4.001589	H	-3.714195	1.067264	4.807423
H	-3.920976	-0.007407	3.606070	H	-3.615192	-0.498824	4.033474

<i>cis-11-skew-boat</i>				<i>trans-11-skew-boat</i>			
H	-6.353986	-0.404863	-4.208598	H	-6.757157	0.339611	-3.656556
H	-5.581542	1.654461	-3.060785	H	-5.936229	2.133005	-2.159826
C	-5.436083	-0.414018	-3.633555	C	-5.784494	0.252368	-3.187898
C	-5.004620	0.739725	-2.990178	C	-5.324450	1.259481	-2.349161
H	-5.028987	-2.485589	-4.018905	H	-5.358746	-1.658697	-4.067625
C	-4.691618	-1.579773	-3.529446	C	-5.000527	-0.868890	-3.418588
H	-8.247484	2.610709	1.682731	H	0.176035	-0.667349	7.610488
C	-3.829568	0.724808	-2.256681	C	-4.084716	1.143350	-1.741048
H	-3.488695	1.632108	-1.770489	H	-3.731038	1.920325	-1.071139
H	-7.233132	4.630021	0.676748	H	1.157589	-2.692949	6.584840
C	-3.514142	-1.598450	-2.791815	C	-3.754082	-0.984654	-2.818206
C	-7.207818	2.602037	1.379005	C	0.099674	-0.825955	6.541702
C	-6.636893	3.736386	0.815710	C	0.650865	-1.963676	5.964521
C	-3.069244	-0.442406	-2.155915	C	-3.287695	0.022548	-1.977052
H	-2.943230	-2.516427	-2.718931	H	-3.147532	-1.863192	-3.005103
H	-6.896793	0.577495	2.007173	H	-0.969679	1.000766	6.205050
H	-7.506462	-2.377731	-1.340608	H	2.530253	3.909813	3.828699
H	-1.505356	0.549888	-3.982823	H	-2.019487	1.216567	-3.838522
C	-6.446965	1.456820	1.559347	C	-0.547438	0.110473	5.750870
H	-0.159405	2.210856	-5.187354	H	-0.477599	2.419534	-5.326625
H	-6.369328	-4.568016	-1.161563	H	1.295084	6.000489	4.315085
H	-0.265083	-1.495838	-3.603852	H	-0.000215	-1.498854	-3.192329
C	-6.582604	-2.466820	-0.781363	C	1.447541	3.906683	3.861561
C	-5.300289	3.728672	0.442051	C	0.553206	-2.164851	4.595341
H	-4.848025	4.616340	0.017140	H	0.983220	-3.049969	4.142734
H	-0.076525	-0.027789	1.037825	H	-0.140423	1.101562	0.897434
C	-5.943096	-3.693633	-0.685041	C	0.754219	5.079645	4.134384
H	-6.546448	-0.388284	-0.269557	H	1.304540	1.818678	3.407805
C	-0.752828	1.115879	-3.446357	C	-0.991684	1.368777	-3.532256
C	-6.040246	-1.341060	-0.173631	C	0.757106	2.729059	3.628011
C	0.005056	2.056330	-4.127883	C	-0.119422	2.045485	-4.375217
C	-5.106844	1.433382	1.167354	C	-0.650505	-0.086995	4.373064
C	-4.748284	-3.794271	0.016899	C	-0.631676	5.067574	4.171793
C	-4.538336	2.583299	0.621401	C	-0.095899	-1.229591	3.800890
C	-0.177935	-2.231135	-2.812138	C	-0.323370	-2.211655	-2.442544
H	-4.236157	-4.746386	0.089905	H	-1.178674	5.979097	4.380003
H	0.819958	-3.653110	-4.063748	H	0.650595	-3.862894	-3.398063
P	-1.527786	-0.368984	-1.157250	P	-1.646081	-0.048942	-1.165041
C	-4.848434	-1.435958	0.538819	C	-0.637858	2.707039	3.675322
C	-0.556196	0.902527	-2.079613	C	-0.547693	0.887826	-2.302254
C	-4.203109	-2.672908	0.621584	C	-1.327640	3.887499	3.943141
Pt	-1.688439	0.070577	1.090611	Pt	-1.638037	0.556504	1.077608
C	0.433569	-3.447482	-3.072896	C	0.042513	-3.545705	-2.559579
H	-3.486297	2.574642	0.351519	H	-0.180946	-1.377611	2.727991
C	0.965465	2.798728	-3.454541	C	1.202239	2.237556	-4.003561
H	1.553091	3.536853	-3.986717	H	1.881234	2.764270	-4.662906
C	-0.674989	-1.952557	-1.538712	C	-1.102530	-1.791556	-1.366036
P	-4.047155	-0.038081	1.420676	P	-1.514330	1.137392	3.317119
H	-3.262824	-2.750393	1.159286	H	-2.410108	3.895078	3.974409
C	0.407143	1.657415	-1.411612	C	0.782601	1.091162	-1.932079
C	1.164003	2.597148	-2.096424	C	1.652734	1.755360	-2.780631
C	0.551876	-4.398280	-2.066966	C	-0.369811	-4.468523	-1.608880
C	-0.547439	-2.908806	-0.533611	C	-1.512362	-2.723900	-0.411022
H	0.555317	1.509406	-0.348708	H	1.134007	0.726833	-0.973020
H	1.906523	3.177790	-1.562737	H	2.683966	1.903390	-2.484064
H	-0.918719	-2.682099	0.460819	H	-2.122725	-2.392635	0.424474
C	-4.376564	-0.539622	3.171776	C	-3.171110	1.357890	4.082515
C	0.061136	-4.127966	-0.797908	C	-1.149971	-4.056084	-0.536347
S	-1.349530	0.630967	3.389273	S	-3.938551	-0.289007	1.409003
H	-3.187336	2.172621	3.144243	H	-2.899425	-1.499114	3.221897
C	-2.913138	1.447903	3.913526	C	-3.840775	-0.952543	3.124953
H	0.157503	-4.863425	-0.008530	H	-1.474610	-4.773090	0.207917
H	-2.672148	2.028593	4.805276	H	-4.633371	-1.695045	3.230087
H	1.033145	-5.346763	-2.272444	H	-0.081708	-5.508577	-1.702182
C	-4.087218	0.531900	4.215248	C	-3.972890	0.070188	4.244908
H	-3.931488	0.033802	5.175671	H	-5.022401	0.351458	4.363293
H	-4.973627	1.162943	4.339427	H	-3.681512	-0.418965	5.180244
H	-5.406116	-0.893653	3.253691	H	-3.061170	1.863471	5.044160
H	-3.730777	-1.408316	3.318674	H	-3.691939	2.044758	3.412372

cis-11-boat				trans-11-boat			
H	2.978539	0.263050	-5.104495	H	2.601324	-0.338855	-5.267165
H	1.547774	2.025109	-4.111892	H	1.101965	1.444962	-4.428443
C	2.610420	0.157203	-4.091343	C	2.328400	-0.306934	-4.219459
C	1.806512	1.145538	-3.535068	C	1.486237	0.693611	-3.749457
H	3.561022	-1.739729	-3.773573	H	3.472330	-2.047709	-3.703997
C	2.935869	-0.965007	-3.346366	C	2.815395	-1.265261	-3.344101
H	2.393604	0.229117	5.658328	H	-6.610872	1.002538	-2.581893
C	1.327847	1.006078	-2.243601	C	1.127814	0.728838	-2.412104
H	0.689843	1.773758	-1.818501	H	0.460513	1.503350	-2.050136
H	3.060994	-2.145244	5.919978	H	-6.180633	3.429452	-2.807947
C	2.465501	-1.103220	-2.045671	C	2.468785	-1.225137	-1.999476
C	1.820145	-0.555733	5.179571	C	-5.903148	1.493439	-1.924954
C	2.192882	-1.884749	5.326902	C	-5.661169	2.852754	-2.052573
C	1.654660	-0.120247	-1.485784	C	1.619007	-0.229069	-1.523679
H	2.734089	-1.982693	-1.473143	H	2.865300	-1.972695	-1.323186
H	0.408820	0.814146	4.343235	H	-5.436155	-0.309671	-0.869135
H	-3.038410	3.939855	3.429346	H	-3.789261	-4.491969	0.885259
H	3.815822	0.747418	0.074489	H	3.641158	1.221038	-0.722893
C	0.702302	-0.225292	4.428640	C	-5.240379	0.752191	-0.955585
H	5.006523	2.578494	1.209184	H	4.990448	3.073077	0.174041
H	-3.624144	3.604994	5.811158	H	-6.133475	-4.529855	1.677371
H	3.487732	-0.979119	1.793864	H	3.634452	-0.585363	1.867251
C	-2.892017	2.973237	3.895737	C	-4.296044	-3.566543	1.130092
C	1.444888	-2.877640	4.710760	C	-4.743723	3.470937	-1.212311
H	1.728859	-3.917847	4.815847	H	-4.541809	4.530460	-1.311935
H	-1.298700	0.342893	-1.094162	H	-1.295170	0.780421	-0.726017
C	-3.220502	2.785026	5.229670	C	-5.609682	-3.587250	1.574294
H	-2.133263	2.058357	2.101565	H	-2.593078	-2.335087	0.664372
C	3.288311	1.373343	0.786023	C	3.331452	1.719109	0.188703
C	-2.375997	1.921027	3.149670	C	-3.623774	-2.358929	1.000726
C	3.958047	2.407806	1.420623	C	4.093214	2.762193	0.695103
C	-0.055280	-1.216040	3.799255	C	-4.327854	1.367392	-0.101840
C	-3.029587	1.541528	5.820850	C	-6.255553	-2.396980	1.885990
C	0.336018	-2.547570	3.944304	C	-4.076140	2.733072	-0.248400
C	2.935569	-1.876251	1.542050	C	3.112130	-1.526046	1.739532
H	-3.282719	1.390481	6.863209	H	-7.282863	-2.408929	2.229052
H	4.374512	-3.171375	2.457854	H	4.557909	-2.636361	2.865166
P	1.008635	-0.217240	0.238186	P	1.159781	-0.095141	0.251259
C	-2.185372	0.670503	3.732768	C	-4.261122	-1.161847	1.319245
C	1.937462	1.141055	1.054946	C	2.173269	1.312428	0.850281
C	-2.513131	0.491784	5.078596	C	-5.586108	-1.190126	1.759566
Pt	-1.271354	-0.125020	0.447324	Pt	-1.106604	0.144015	0.730218
C	3.437409	-3.115634	1.916967	C	3.633773	-2.683827	2.302137
H	-0.218155	-3.341144	3.459378	H	-3.343131	3.220816	0.385374
C	3.284977	3.229256	2.317262	C	3.708185	3.402729	1.864809
H	3.810390	4.039462	2.807936	H	4.304124	4.217709	2.257215
C	1.726313	-1.789894	0.857547	C	1.921558	-1.574777	1.019552
P	-1.487982	-0.724294	2.749762	P	-3.359824	0.425865	1.142506
H	-2.357624	-0.471707	5.552621	H	-6.101940	-0.265759	1.996281
C	1.267024	1.982309	1.938329	C	1.789021	1.961701	2.023630
C	1.937692	3.019254	2.571373	C	2.557046	3.000174	2.528797
C	2.742047	-4.275630	1.607730	C	2.975564	-3.894541	2.144700
C	1.020493	-2.960212	0.567652	C	1.256327	-2.793893	0.876961
H	0.210055	1.818998	2.121905	H	0.887768	1.639198	2.536463
H	3.138366	-5.240380	1.900404	H	3.385153	-4.795685	2.584578
H	1.402732	3.665012	3.257888	H	2.253056	3.499084	3.440897
H	0.067774	-2.892222	0.050356	H	0.317684	-2.832006	0.333312
C	-2.698867	-2.098164	3.017316	C	-3.689769	1.340743	2.717884
C	1.529629	-4.196169	0.934495	C	1.785895	-3.948646	1.429316
S	-3.642016	0.049828	0.237339	S	-0.808676	-0.861550	2.960494
H	-5.480919	-0.973453	1.306173	H	-1.840047	-0.401061	5.049537
C	-4.452667	-0.826950	1.638673	C	-2.195940	-0.281606	4.025651
H	0.976787	-5.097435	0.698954	H	1.263941	-4.890157	1.310235
H	-4.501264	-0.178824	2.519214	H	-3.054752	-0.952602	3.917956
C	-3.823715	-2.166832	1.993015	C	-2.625799	1.160838	3.790643
H	-2.135335	-3.031199	3.003485	H	-3.788419	2.394298	2.452963
H	-3.094640	-1.986716	4.029953	H	-4.668348	1.016140	3.080183
H	-3.457509	-2.635991	1.076303	H	-1.745625	1.758277	3.537051
H	-4.591272	-2.834191	2.395460	H	-3.026230	1.576682	4.720186

TS[<i>trans</i> -11-boat→skew-boat]				TS[<i>trans</i> -11-skew-boat→chair]			
H	2.889627	-4.330047	-3.647614	H	1.968294	-0.818399	-5.504080
H	0.789455	-3.087389	-4.071706	H	0.231795	-2.137670	-4.328842
C	2.530683	-3.606428	-2.925948	C	1.811267	-0.684616	-4.440779
C	1.352281	-2.910504	-3.163296	C	0.836204	-1.424310	-3.781949
H	4.165264	-3.912648	-1.568690	H	3.340559	0.806999	-4.240774
C	3.245119	-3.374055	-1.760276	C	2.579575	0.226755	-3.733258
H	-6.918346	3.434168	1.097701	H	-5.341588	1.776874	-2.922720
C	0.887007	-1.993507	-2.234677	C	0.628658	-1.246285	-2.424614
H	-0.038849	-1.459675	-2.416927	H	-0.140705	-1.816850	-1.915667
H	-5.419869	5.112138	0.067904	H	-6.078653	4.028839	-2.204552
C	2.788064	-2.447199	-0.832922	C	2.382937	0.398287	-2.368403
C	-5.920803	3.151661	0.784093	C	-5.139358	2.119081	-1.915110
C	-5.079639	4.092773	0.203991	C	-5.553083	3.383200	-1.511683
C	1.601459	-1.751865	-1.061040	C	1.403923	-0.335962	-1.704002
H	3.361011	-2.267234	0.068651	H	2.997119	1.106294	-1.825073
H	-6.155339	1.119986	1.411140	H	-4.130210	0.313879	-1.355073
H	-6.822651	-1.069806	-2.907769	H	-3.919054	-4.284251	1.612450
H	2.865837	0.256297	-2.111372	H	3.876439	-0.263157	1.227294
C	-5.486763	1.847311	0.964344	C	-4.460866	1.295549	-1.032669
H	3.553840	2.430571	-3.033363	H	5.423601	1.527072	1.905568
H	-6.560744	-3.528010	-2.804578	H	-6.386778	-4.158946	1.734744
H	3.324744	1.041332	1.217481	H	0.506240	-1.643730	2.516960
C	-6.156743	-1.515876	-2.179005	C	-4.416575	-3.322389	1.590021
C	-3.804215	3.725735	-0.200360	C	-5.287767	3.816506	-0.221988
H	-3.145003	4.455631	-0.654373	H	-5.605028	4.801758	0.097332
H	-1.536622	-0.994030	-0.924835	H	-1.618808	-0.343931	-0.621205
C	-6.009623	-2.893174	-2.121678	C	-5.800479	-3.251215	1.659412
H	-5.574459	0.375868	-1.361123	H	-2.582584	-2.203434	1.423481
C	2.452098	1.168694	-1.698215	C	3.571907	0.772880	1.136549
C	-5.451943	-0.698815	-1.304095	C	-3.666471	-2.159309	1.486327
C	2.841961	2.396007	-2.217574	C	4.444412	1.782731	1.519266
C	-4.202373	1.472441	0.566954	C	-4.199388	1.721150	0.271545
C	-5.146653	-3.456432	-1.189560	C	-6.435521	-2.015702	1.628987
C	-3.367089	2.421308	-0.020645	C	-4.614933	2.990178	0.669125
C	3.113443	0.201466	1.868729	C	1.261411	-2.224046	1.996506
H	-5.020414	-4.531268	-1.144250	H	-7.516058	-1.959048	1.680716
H	4.701720	0.680773	3.224993	H	1.366971	-3.752961	3.493081
P	0.989364	-0.469528	0.105124	P	1.104173	-0.180280	0.102908
C	-4.589520	-1.256868	-0.364192	C	-4.296750	-0.916816	1.455847
C	1.534052	1.112734	-0.651692	C	2.308427	1.090683	0.645422
C	-4.436121	-2.644467	-0.321138	C	-5.688413	-0.851960	1.530838
Pt	-1.299596	-0.397622	0.544125	Pt	-1.082740	0.233593	0.781359
C	3.892088	-0.003067	3.000889	C	1.747530	-3.403533	2.540966
H	-2.367187	2.127633	-0.325011	H	-4.416443	3.343370	1.673243
C	2.324898	3.572275	-1.694284	C	4.064060	3.112467	1.409268
H	2.631126	4.527871	-2.102161	H	4.745969	3.898416	1.710301
C	2.066784	-0.668064	1.574546	C	1.744914	-1.765687	0.770706
P	-3.585667	-0.240136	0.789547	P	-3.276276	0.604997	1.390880
H	-3.746007	-3.090363	0.387413	H	-6.189137	0.110118	1.503953
C	1.013699	2.299501	-0.131599	C	1.927218	2.429422	0.547036
C	1.413508	3.522280	-0.647159	C	2.803908	3.434889	0.921799
C	3.635993	-1.077639	3.839337	C	2.714056	-4.136628	1.865804
C	1.806081	-1.740439	2.429684	C	2.715739	-2.506896	0.097151
H	0.298132	2.253294	0.684495	H	0.934871	2.677827	0.183843
H	4.244519	-1.235063	4.721547	H	3.089463	-5.060061	2.289796
H	1.007324	4.437758	-0.234217	H	2.499732	4.471336	0.842240
H	0.979956	-2.409765	2.214754	H	3.097943	-2.161711	-0.856836
C	-4.227392	-0.800609	2.426304	C	-3.474371	1.324674	3.067979
H	-5.293453	-0.564703	2.440542	C	3.196929	-3.687174	0.644281
C	2.592451	-1.948522	3.550533	S	-0.322063	1.175876	2.925667
S	-0.938991	0.502316	2.793224	H	-1.005689	0.808725	5.155736
H	-3.053002	1.712911	2.949307	C	-1.339398	0.352207	4.222966
H	-4.169201	-1.889266	2.381060	H	3.951021	-4.256147	0.114249
C	-2.578989	0.908195	3.517354	H	-1.032448	-0.693701	4.276795
H	2.383875	-2.785310	4.205826	C	-2.878710	0.426480	4.142001
H	-2.361151	1.320247	4.503672	H	-2.983577	2.299582	3.063799
C	-3.524899	-0.271355	3.684960	H	-4.540604	1.480898	3.248161
H	-2.970118	-1.085598	4.154841	H	-3.260593	0.770429	5.105663
H	-4.300398	0.017028	4.399946	H	-3.281706	-0.582806	4.017630

M06L/TZVP(PCM):

<i>cis-5</i>				<i>trans-5</i>			
H	-4.626795	3.187848	-4.466010	H	-8.189651	-2.672683	2.510513
H	-3.185395	1.175200	-4.415855	H	-6.685921	-2.795774	0.547349
C	-4.556141	2.593384	-3.563983	C	-7.172152	-2.309435	2.582434
C	-3.746852	1.464036	-3.536194	C	-6.328813	-2.377400	1.480082
H	-5.904776	3.835186	-2.450028	H	-7.360943	-1.714283	4.634887
C	-5.272784	2.956089	-2.433565	C	-6.708196	-1.771862	3.772831
H	-6.130919	-3.538980	-2.398217	H	-2.215404	-5.699372	3.670174
C	-3.653850	0.704860	-2.380990	C	-5.030927	-1.902949	1.568430
H	-5.709276	-1.180685	-1.842803	H	-3.558277	-3.648840	3.447108
H	-3.015211	-0.172388	-2.362122	H	-4.378102	-1.942023	0.703745
C	-5.482128	-3.291816	-1.567214	C	-1.728447	-4.763697	3.425134
C	-5.186746	2.193640	-1.275729	C	-5.402582	-1.307354	3.868225
C	-5.245688	-1.962070	-1.251671	C	-2.485813	-3.607410	3.297265
H	-5.072122	-5.338544	-1.071253	H	0.234578	-5.623935	3.342933
C	-4.380607	1.057835	-1.240487	C	-4.554324	-1.365922	2.764789
C	-4.888124	-4.300980	-0.822070	C	-0.353796	-4.720318	3.243085
H	-5.751572	2.483874	-0.397626	H	-5.047874	-0.898095	4.806242
H	-0.996122	1.522396	-1.086406	H	-0.701262	1.067933	-1.003968
H	-2.129928	2.605386	-0.689556	H	-1.966018	2.077044	-0.984913
C	-4.409007	-1.628874	-0.185254	C	-1.869158	-2.399135	2.978081
N	-1.375682	2.046727	-0.302148	N	-1.224524	1.700994	-0.405095
C	-4.052156	-3.977538	0.237526	C	0.265873	-3.517512	2.929106
P	-4.103163	0.114338	0.310163	P	-2.800676	-0.821163	2.851572
C	-3.809119	-2.649057	0.551806	C	-0.486508	-2.361657	2.792375
H	-3.580573	-4.761424	0.816823	H	1.338654	-3.480563	2.785653
C	-0.324461	2.928107	0.253701	C	-0.331235	2.792474	0.055657
H	1.246742	1.469637	0.242080	H	1.312990	1.523482	0.579355
H	-6.993622	-0.590467	0.210624	H	-1.993723	-1.875557	5.525011
C	-5.558568	0.544986	1.346408	C	-2.654937	-0.087957	4.526876
Pt	-2.088213	0.580598	1.237951	Pt	-2.033636	0.502611	1.221237
C	-6.838955	0.078821	1.049065	C	-2.254705	-0.829644	5.635975
H	-3.142599	-2.391463	1.366830	H	-0.013327	-1.416150	2.542600
H	-0.809182	3.604454	0.958521	H	-0.962015	3.552172	0.517832
C	0.719864	2.104409	0.958735	C	0.657976	2.257393	1.056421
H	-4.375830	1.747473	2.663256	H	-3.273631	1.840947	3.817607
C	-5.377228	1.397997	2.432807	C	-2.982964	1.258668	4.685627
H	1.461262	2.759796	1.415045	H	1.291524	3.069430	1.412513
C	-7.919526	0.463766	1.827164	C	-2.184303	-0.231042	6.886354
H	-8.910165	0.095118	1.591944	H	-1.865785	-0.812553	7.742471
H	-2.461277	-0.435852	2.381488	H	-3.204457	-0.036168	0.271117
S	-0.017019	1.057312	2.285839	S	-0.195736	1.502160	2.499809
C	-6.460976	1.784002	3.208954	C	-2.920794	1.850721	5.936804
C	-7.732021	1.317734	2.906727	C	-2.519598	1.106592	7.038651
H	-6.310515	2.445975	4.052537	H	-3.176644	2.896639	6.050706
H	-8.577546	1.615042	3.514432	H	-2.462453	1.571602	8.014912
H	0.128535	3.531457	-0.539776	H	0.176288	3.244720	-0.802395

<i>cis-6</i>				<i>trans-6</i>			
H	-4.461872	3.526940	-4.150126	H	-8.194213	-2.757050	2.352729
H	-3.022773	1.512106	-4.168674	H	-6.705162	-2.565763	0.384140
C	-4.440014	2.867904	-3.291580	C	-7.188735	-2.372138	2.467931
C	-3.632342	1.737176	-3.302633	C	-6.353813	-2.263643	1.362786
H	-5.850197	4.028279	-2.165848	H	-7.378814	-2.063111	4.582505
C	-5.218015	3.149269	-2.178456	C	-6.732401	-1.982490	3.717573
H	-5.940476	-3.407379	-2.578255	H	-2.101177	-5.703378	3.124017
C	-3.600163	0.896580	-2.201783	C	-5.071514	-1.760710	1.507635
H	-5.636022	-1.074610	-1.861840	H	-3.527237	-3.697010	3.106012
H	-2.960722	0.019845	-2.211974	H	-4.425591	-1.662233	0.642666
C	-5.334927	-3.188832	-1.707590	C	-1.647613	-4.724321	3.032734
C	-5.191245	2.306782	-1.074499	C	-5.442827	-1.489622	3.868157
C	-5.165218	-1.873795	-1.300963	C	-2.452138	-3.592635	3.020325
H	-4.859657	-5.245476	-1.323908	H	0.354944	-5.486183	2.941813
C	-4.384280	1.170741	-1.077574	C	-4.603023	-1.371052	2.762561
H	2.345641	5.041513	-1.543211	H	2.568889	4.954085	-1.481225
O	0.105516	3.619994	-1.708680	O	0.510428	3.291329	-1.703666
C	-4.728567	-4.219640	-1.003041	C	-0.269650	-4.601653	2.932123
H	-5.800333	2.535584	-0.207746	H	-5.093857	-1.196529	4.850680
H	-1.120884	1.712918	-0.841140	H	-0.814115	1.583664	-0.737836
H	-2.250083	2.745882	-0.337565	H	-2.084199	2.558209	-0.536516
C	1.653859	5.644690	-0.958187	C	1.735514	5.592854	-1.194724
C	-4.383986	-1.577724	-0.182788	C	-1.878085	-2.329215	2.898062
C	0.219702	3.841456	-0.525210	C	0.367093	3.783241	-0.607884
H	2.193895	6.382141	-0.375021	H	2.097164	6.496836	-0.717743
N	-1.488614	2.161441	-0.002870	N	-1.326124	2.110858	-0.031588
C	-3.947420	-3.932680	0.107606	C	0.307506	-3.343431	2.815281
P	-4.163036	0.140946	0.426008	P	-2.869294	-0.784149	2.922781
O	0.956518	4.825252	-0.004880	O	0.913557	4.935063	-0.215343
C	-3.771392	-2.618605	0.513714	C	-0.491060	-2.211440	2.793098
H	-3.466057	-4.733149	0.655271	H	1.382946	-3.244310	2.735954
C	-0.429109	3.011086	0.566131	C	-0.419336	3.140546	0.517587
H	1.120800	1.522750	0.526436	H	1.172182	1.791751	1.029221
H	-7.022093	-0.622519	0.136109	H	-1.987685	-2.052097	5.477148
C	-5.676541	0.472787	1.412458	C	-2.757798	-0.215474	4.663089
Pt	-2.195789	0.610966	1.452045	Pt	-2.122253	0.721042	1.450338
C	-6.927569	-0.003298	1.020606	C	-2.307291	-1.039223	5.692117
H	-3.146984	-2.387831	1.369125	H	-0.050269	-1.223184	2.696815
H	-0.886845	3.675306	1.301620	H	-1.027411	3.895023	1.018739
C	0.608028	2.144985	1.265049	C	0.524310	2.514052	1.534254
H	-4.595044	1.619837	2.860903	H	-3.494186	1.735080	4.151216
C	-5.572833	1.260571	2.556740	C	-3.162628	1.087117	4.955591
H	1.356872	2.781688	1.733990	H	1.163937	3.289767	1.953636
C	-8.055796	0.307533	1.763214	C	-2.261827	-0.564054	6.995674
H	-9.023166	-0.068374	1.454285	H	-1.904075	-1.208155	7.789170
H	-2.577287	-0.463498	2.536352	H	-3.214962	0.201697	0.403703
S	-0.154102	1.086895	2.559073	S	-0.405765	1.707537	2.890271
C	-6.704371	1.572215	3.297354	C	-3.124898	1.554950	6.259142
C	-7.945750	1.096683	2.901150	C	-2.672482	0.729968	7.280742
H	-6.614209	2.183849	4.186274	H	-3.439999	2.567672	6.476886
H	-8.828579	1.336076	3.480696	H	-2.634659	1.098570	8.298205
H	0.947321	6.132272	-1.627342	H	1.149159	5.837334	-2.078502

<i>cis-7</i>				<i>trans-7</i>			
H	-4.413249	3.684580	-4.005728	H	-8.189493	-2.709673	2.279048
H	-2.964048	1.677994	-4.069776	H	-6.670245	-2.446149	0.341889
C	-4.399689	2.998218	-3.168691	C	-7.185905	-2.329893	2.423923
C	-3.586406	1.871986	-3.205326	C	-6.334028	-2.180891	1.336411
H	-5.830056	4.115739	-2.025163	H	-7.408609	-2.097947	4.545032
C	-5.193872	3.240133	-2.057733	C	-6.748787	-1.986762	3.693709
H	-5.892106	-3.290522	-2.695558	H	-2.055591	-5.665752	2.828145
C	-3.565000	0.996557	-2.131969	C	-5.054346	-1.684162	1.519443
H	-5.589280	-0.984055	-1.899369	H	-3.505270	-3.679208	2.937500
H	-2.920983	0.123618	-2.161307	H	-4.395784	-1.553196	0.668350
C	-5.302597	-3.103618	-1.806697	C	-1.612121	-4.677860	2.823961
C	-5.178430	2.362110	-0.981510	C	-5.461345	-1.500911	3.882318
C	-5.133704	-1.803226	-1.355039	C	-2.430016	-3.557125	2.882997
H	-4.846769	-5.174386	-1.479495	H	0.401067	-5.409044	2.717480
C	-4.366445	1.230072	-1.010879	C	-4.604435	-1.342642	2.795365
H	2.023938	5.203396	-1.437986	H	2.299934	5.143874	-1.369005
O	0.068973	3.767855	-1.466048	O	0.456752	3.562789	-1.409552
C	-4.716146	-4.160064	-1.123746	C	-0.234045	-4.533209	2.763689
H	-5.800394	2.559622	-0.116202	H	-5.128422	-1.243679	4.880238
H	-1.139693	1.828657	-0.700901	H	-0.878564	1.847352	-0.529702
H	-2.276802	2.820535	-0.138389	H	-2.143829	2.806582	-0.244417
H	1.303526	7.594345	-1.683950	H	1.535971	7.330897	-2.331760
H	-0.090083	6.516929	-1.658660	H	0.218505	6.161636	-2.305286
C	1.635997	5.785865	-0.602380	C	1.720533	5.865506	-0.793234
C	-4.373024	-1.547423	-0.213094	C	-1.869103	-2.282121	2.873453
C	0.191087	3.935685	-0.273484	C	0.327950	4.013674	-0.293297
H	2.471005	6.151620	-0.008836	H	2.396577	6.437902	-0.161875
N	-1.510691	2.223806	0.162576	N	-1.376590	2.329603	0.217647
C	0.738136	6.899632	-1.064355	C	0.886966	6.749516	-1.678322
C	-3.955399	-3.913160	0.010453	C	0.329946	-3.263494	2.759397
P	-4.159757	0.149637	0.457915	P	-2.876264	-0.751855	2.999074
O	0.932274	4.885411	0.297015	O	0.889241	5.136721	0.152175
C	-3.780007	-2.613776	0.461478	C	-0.481618	-2.141795	2.809069
H	-3.489408	-4.733491	0.541800	H	1.405555	-3.147121	2.712155
C	-0.455724	3.048752	0.775682	C	-0.456305	3.324651	0.807828
H	1.101445	1.572001	0.663598	H	1.131434	1.942713	1.236214
H	-7.021377	-0.540742	0.063069	H	-2.160773	-2.251456	5.468752
H	0.333960	7.454557	-0.218905	H	0.291395	7.445516	-1.089315
C	-5.685006	0.437762	1.440144	C	-2.770765	-0.307771	4.775889
Pt	-2.206305	0.585944	1.521555	Pt	-2.147489	0.849623	1.621218
C	-6.934696	0.007644	0.994005	C	-2.415825	-1.236862	5.752027
H	-3.171423	-2.414429	1.335889	H	-0.050791	-1.144451	2.800701
H	-0.917199	3.674218	1.542222	H	-1.052947	4.059352	1.350286
C	0.583250	2.152345	1.431924	C	0.491845	2.641558	1.783071
H	-4.614673	1.458923	2.987409	H	-3.350324	1.721951	4.392324
C	-5.591259	1.135147	2.642294	C	-3.095002	0.994471	5.155187
H	1.327505	2.767317	1.935734	H	1.139266	3.391136	2.236608
C	-8.071279	0.273533	1.740861	C	-2.384495	-0.865729	7.088687
H	-9.037543	-0.065976	1.389314	H	-2.101902	-1.591587	7.840852
H	-2.583895	-0.554143	2.537461	H	-3.242893	0.383631	0.551081
S	-0.176797	1.023244	2.665951	S	-0.430804	1.770078	3.103329
C	-6.731250	1.401143	3.388028	C	-3.069683	1.359894	6.491948
C	-7.970841	0.971090	2.938209	C	-2.713497	0.430393	7.459904
H	-6.649030	1.941549	4.322709	H	-3.320212	2.373846	6.777388
H	-8.860120	1.174815	3.521520	H	-2.686380	0.718110	8.503484

<i>cis</i> -8				<i>trans</i> -8			
H	-6.433628	0.181558	-4.147876	H	2.894912	-2.749208	-4.973312
H	-5.011491	2.142271	-3.628065	H	0.788023	-1.449848	-4.933185
C	-5.450262	0.040102	-3.716860	C	2.540144	-2.318377	-4.045429
C	-4.652328	1.140507	-3.428300	C	1.357579	-1.590260	-4.023034
H	-5.603107	-2.100039	-3.669066	H	4.183882	-3.065083	-2.885682
C	-4.986364	-1.237955	-3.446753	C	3.262392	-2.496509	-2.875136
H	-7.747511	1.818046	-1.104689	H	-6.858052	3.469958	0.590745
C	-3.401502	0.960717	-2.864082	C	0.897300	-1.048530	-2.833964
H	-2.789641	1.824375	-2.625540	H	-0.033461	-0.493146	-2.812627
H	-6.826514	4.103131	-1.326943	H	-5.164926	5.268149	0.467500
C	-3.723795	-1.422044	-2.896079	C	2.810369	-1.944574	-1.684168
C	-6.744209	2.035655	-0.759289	C	-5.803681	3.223226	0.587501
C	-6.226598	3.315918	-0.887588	C	-4.852077	4.232736	0.518510
C	-2.920195	-0.324737	-2.599119	C	1.621914	-1.216925	-1.653980
H	-3.368247	-2.426489	-2.701352	H	3.386255	-2.083038	-0.777280
H	-6.392479	0.025723	-0.118278	H	-6.155003	1.112131	0.699356
H	-3.961126	-4.681394	-0.396900	H	-5.665447	-1.796540	-3.308136
H	-1.458104	0.161256	-4.666286	H	2.760643	1.063877	-2.052538
C	-5.978613	1.023041	-0.197266	C	-5.407044	1.896329	0.649984
H	0.097429	1.216803	-6.241046	H	3.463516	3.420318	-2.156470
H	-6.159160	-5.042958	0.690552	H	-7.452984	-3.041890	-2.133760
H	-1.030232	-2.226351	-4.146202	H	3.577614	0.444244	1.141634
C	-4.449144	-3.872671	0.134147	C	-5.700686	-1.805067	-2.226032
C	-4.930400	3.581567	-0.464962	C	-3.501974	3.913159	0.510123
H	-4.514000	4.575041	-0.575622	H	-2.756849	4.697042	0.452994
H	0.297187	0.513171	0.229993	H	-1.549806	-0.521101	-1.237768
C	-5.677817	-4.074574	0.744760	C	-6.703668	-2.504449	-1.566362
H	-2.866967	-2.474905	-0.249741	H	-3.944166	-0.591784	-2.014645
C	-0.507043	0.533635	-4.305149	C	2.417210	1.760307	-1.296986
C	-3.836309	-2.630414	0.208698	C	-4.736824	-1.124770	-1.500993
C	0.370923	1.131806	-5.196716	C	2.815309	3.089669	-1.354504
C	-4.682370	1.282688	0.239834	C	-4.051174	1.568241	0.640295
C	-6.285978	-3.035119	1.437697	C	-6.740891	-2.516868	-0.180413
C	-4.159555	2.570287	0.085276	C	-3.101802	2.585978	0.567493
C	-0.738712	-2.800519	-3.273630	C	3.275049	-0.492908	1.594036
H	-7.239260	-3.192815	1.926221	H	-7.519445	-3.062020	0.338210
H	-0.316387	-4.566229	-4.408049	H	4.984012	-0.584445	2.882026
P	-1.287449	-0.463451	-1.770882	P	1.016510	-0.414995	-0.116550
C	-4.445009	-1.575815	0.881542	C	-4.771997	-1.126158	-0.105825
C	-0.175746	0.419982	-2.953263	C	1.580010	1.325634	-0.272590
C	-5.673692	-1.793690	1.510250	C	-5.781834	-1.827882	0.549946
Pt	-1.288492	0.273510	0.399674	Pt	-1.260151	-0.439001	0.336283
C	-0.335944	-4.117746	-3.422716	C	4.068541	-1.073449	2.573276
H	-3.131356	2.766132	0.375986	H	-2.048035	2.325627	0.549954
C	1.591269	1.620565	-4.752743	C	2.388025	3.988755	-0.389073
H	2.274296	2.090524	-5.449220	H	2.699643	5.024674	-0.437141
C	-0.773421	-2.214742	-2.007272	C	2.092107	-1.111265	1.194061
P	-3.573396	0.028743	0.991905	P	-3.498947	-0.176434	0.795901
H	-6.155370	-0.993315	2.060116	H	-5.827647	-1.841890	1.631699
C	1.051959	0.914238	-2.517824	C	1.150174	2.235622	0.695941
C	1.929822	1.508388	-3.412033	C	1.557856	3.558373	0.638936
C	0.045046	-4.859796	-2.311128	C	3.690688	-2.275638	3.153913
C	-0.382784	-2.963054	-0.899127	C	1.714054	-2.315808	1.787232
H	1.313511	0.839530	-1.469464	H	0.496642	1.892081	1.493084
H	2.878841	1.890098	-3.056708	H	4.310493	-2.726178	3.919034
H	-0.406149	-2.498852	0.082444	H	1.222899	4.256871	1.395857
C	-3.653009	0.398013	2.808619	H	0.782130	-2.786311	1.492780
H	-4.682579	0.625896	3.096808	C	-3.746935	-0.537523	2.587683
C	0.023871	-4.281585	-1.050718	H	-4.731389	-0.187696	2.912483
S	-0.992385	1.225148	2.557082	C	2.513227	-2.896960	2.758959
H	-3.075460	2.470286	2.774594	S	-0.958538	-0.386843	2.775081
H	-3.357081	-0.525854	3.310444	H	-2.724004	1.211511	3.307028
C	-2.710074	1.518950	3.166852	H	-3.706367	-1.622411	2.708233
H	0.325033	-4.854932	-0.183045	C	-2.629677	0.124217	3.365707
H	-2.643416	1.624683	4.250220	H	2.211406	-3.831179	3.215478
H	0.361671	-5.888383	-2.430719	H	-2.696464	-0.146467	4.419601

<i>cis-9</i>				<i>trans-9</i>			
H	2.635163	-4.010148	-5.147564	H	2.715631	1.076406	-5.510779
H	2.123152	-1.632566	-4.692536	H	0.637960	1.788634	-4.366333
C	2.268377	-3.710157	-4.173865	C	2.564727	0.843191	-4.464119
H	-5.742480	1.321691	-3.991185	H	-4.893134	1.542978	-4.192096
H	-4.153905	2.021903	-4.293430	H	-3.248048	2.174203	-4.162777
H	2.294875	-5.704060	-3.376362	H	4.445630	-0.170179	-4.258678
H	-4.299839	0.310402	-3.897323	H	-3.538549	0.460170	-3.868431
C	1.982204	-2.376871	-3.918907	C	1.399151	1.242013	-3.822700
C	-4.697806	1.302668	-3.675879	C	-3.928999	1.463575	-3.686969
H	-2.952487	-3.003374	-4.131901	H	-2.593505	-3.087232	-3.944364
C	2.077510	-4.661531	-3.180529	C	3.534994	0.141818	-3.762636
H	-5.400143	-3.345257	-3.989714	H	-5.056665	-3.207469	-4.138118
C	-3.494826	-2.696160	-3.246377	C	-3.220460	-2.719055	-3.142050
C	-4.867577	-2.884977	-3.166948	C	-4.601953	-2.785615	-3.250562
H	-6.171758	3.071145	-2.132566	H	-5.602124	3.242783	-2.373979
H	-4.594392	3.764571	-2.458852	H	-3.968020	3.879878	-2.373309
C	1.506211	-1.992873	-2.673604	C	1.200701	0.936660	-2.485345
C	-4.552223	1.637844	-2.203038	C	-4.050036	1.745647	-2.200733
C	-5.115370	3.009859	-1.856076	C	-4.618794	3.127816	-1.909174
C	1.602460	-4.280802	-1.935070	C	3.343562	-0.162879	-2.421957
H	1.269068	-0.953974	-2.471228	H	0.290862	1.242275	-1.977218
H	-2.540239	2.355793	-2.333095	H	-2.019111	2.371638	-1.933471
H	-5.112430	0.887185	-1.628037	H	-4.734164	1.000923	-1.769567
H	-1.744885	-1.930400	-2.254319	H	-1.558632	-2.102697	-1.916373
C	-2.816361	-2.102042	-2.192684	C	-2.637862	-2.173547	-2.006814
C	-5.560796	-2.472555	-2.036306	C	-5.403345	-2.308556	-2.220984
H	-6.633202	-2.609171	-1.976289	H	-6.481769	-2.359501	-2.302709
H	-2.630266	0.638904	-2.053330	H	-2.233474	0.652747	-1.739224
C	1.317044	-2.939823	-1.667713	C	2.173897	0.231473	-1.774632
H	1.443202	-5.032130	-1.170166	H	4.106503	-0.710443	-1.880739
C	-3.090491	1.591247	-1.772775	C	-2.696268	1.619218	-1.510883
C	-4.936997	3.317292	-0.380036	C	-4.707088	3.376470	-0.414019
H	-5.317559	4.317081	-0.150904	H	-5.091483	4.381808	-0.217741
C	-3.499300	-1.700531	-1.045588	C	-3.434192	-1.693199	-0.969488
C	-4.881852	-1.881452	-0.981130	C	-4.823673	-1.765935	-1.084780
H	-2.912003	3.943237	-0.521313	H	-2.670766	3.923831	-0.161298
H	-5.555445	2.625130	0.202171	H	-5.444659	2.689186	0.015354
C	-2.864531	1.850265	-0.280795	C	-2.735105	1.825660	0.006943
C	-3.479556	3.223743	0.085125	C	-3.363948	3.209558	0.303911
P	0.701074	-2.379277	-0.029630	P	1.869635	-0.113213	0.003449
H	-5.433185	-1.558586	-0.104644	H	-5.456646	-1.400792	-0.283089
H	-4.499432	0.597707	0.465514	H	-4.529787	0.622470	0.400839
Pt	-0.294647	-0.319281	-0.051161	Pt	-0.382613	-0.545065	0.355796
S	-1.007021	1.947585	-0.005630	S	-0.967278	1.823252	0.632494
P	-2.558069	-0.880474	0.296022	P	-2.649025	-0.931263	0.498611
C	-3.420123	0.729407	0.591321	C	-3.485383	0.701540	0.719524
H	-3.754641	5.737378	1.214624	H	-3.767581	5.695378	1.453611
H	-2.037030	5.353675	1.112754	H	-2.072110	5.254896	1.652313
H	-4.144198	-3.368342	1.002604	H	-4.033206	-3.564695	0.813937
C	-2.958798	5.126706	1.650530	C	-3.082869	5.044619	2.005110
C	-3.298588	3.644921	1.564523	C	-3.443673	3.578915	1.805774
H	-5.353118	3.954483	2.220408	H	-5.572857	3.944016	2.091858
H	-3.240118	0.961154	1.642502	H	-3.486930	0.890317	1.793800
H	-2.434318	3.088394	1.944395	H	-2.679197	2.981238	2.314963
C	-3.700033	-2.958403	1.900855	C	-3.838882	-3.157469	1.798599
C	-2.918708	-1.809494	1.835341	C	-3.225783	-1.914218	1.932134
C	-4.487009	3.338021	2.470514	C	-4.786117	3.287337	2.469565
H	-4.805479	2.296382	2.421132	H	-5.122957	2.260790	2.322470
H	-2.832156	5.449979	2.685190	H	-3.138561	5.332684	3.056343
H	-4.510036	-4.493566	3.154284	H	-4.683509	-4.844879	2.810942
H	-4.231573	3.551560	3.509510	H	-4.717577	3.456716	3.545240
C	-3.903813	-3.596604	3.117775	C	-4.204701	-3.880460	2.926067
C	-2.322352	-1.325150	3.004212	C	-2.964266	-1.416809	3.211005
H	-1.685709	-0.446120	2.955192	H	-2.455856	-0.464833	3.326915
C	-3.326158	-3.099885	4.275328	C	-3.959463	-3.371938	4.192528
C	-2.529003	-1.962966	4.215598	C	-3.335920	-2.138401	4.332999
H	-3.486853	-3.601255	5.221566	H	-4.247634	-3.937047	5.069935
H	-2.064465	-1.575247	5.113696	H	-3.132507	-1.740535	5.319235
H	1.211196	0.246872	-0.255048	H	-0.087314	-2.117016	0.222318

C	-0.300239	-3.811483	0.548309	C	3.083912	-1.430647	0.407019
C	-1.180842	-4.442738	-0.331521	C	2.838554	-2.725040	-0.053188
C	-0.248418	-4.239949	1.874047	C	4.247297	-1.174986	1.129320
C	-1.978180	-5.491714	0.099811	C	3.745215	-3.741511	0.195988
H	-1.226572	-4.130523	-1.367622	H	1.927103	-2.931802	-0.603081
C	-1.045416	-5.291617	2.302187	C	5.148184	-2.199801	1.389086
H	0.424856	-3.759145	2.574071	H	4.453791	-0.175680	1.492549
C	-1.908858	-5.921525	1.417640	C	4.901581	-3.481174	0.921309
H	-2.650682	-5.975160	-0.598683	H	3.545921	-4.741155	-0.169384
H	-0.993633	-5.615363	3.334393	H	6.046265	-1.991485	1.957110
H	-2.530020	-6.741599	1.755825	H	5.605902	-4.278201	1.124041
C	2.159120	-2.440402	1.091291	C	2.517620	1.363068	0.873826
C	3.231285	-3.305104	0.883178	C	3.433739	2.235513	0.290389
C	2.154015	-1.620526	2.219528	C	2.087553	1.592843	2.180368
C	4.281631	-3.346044	1.788762	C	3.913962	3.322100	1.007676
H	3.257313	-3.942088	0.007634	H	3.770308	2.068757	-0.726327
C	3.199497	-1.671631	3.129097	C	2.575227	2.674262	2.896684
H	1.325328	-0.935947	2.372077	H	1.356312	0.925764	2.624933
C	4.265907	-2.533497	2.913764	C	3.488572	3.540479	2.310499
H	5.115369	-4.014308	1.612756	H	4.621445	3.999710	0.546271
H	3.184474	-1.031381	4.002202	H	2.234488	2.846798	3.909816
H	5.087271	-2.567480	3.618566	H	3.863613	4.390230	2.867144

<i>cis</i> -10				<i>trans</i> -10			
H	4.617555	-3.953430	-4.253722	H	3.351950	-1.075229	-5.604951
H	4.605957	-1.693259	-3.242338	H	1.332701	-2.140304	-4.649990
C	3.846378	-3.680089	-3.544510	C	3.077074	-0.891634	-4.573796
H	2.860618	-5.583046	-3.639297	H	4.733532	0.422963	-4.202661
C	3.839645	-2.411063	-2.977707	C	1.945200	-1.489821	-4.038178
H	-4.931874	-2.317781	-3.767510	H	-3.250378	-0.201111	-4.376015
C	2.861638	-4.592736	-3.201190	C	3.852698	-0.050722	-3.787626
H	-6.770994	-3.459576	-2.566418	H	-5.475247	-1.281392	-4.451588
C	-4.945050	-2.337862	-2.685008	C	-3.694612	-0.595333	-3.470659
C	-5.977265	-2.975998	-2.010784	C	-4.942449	-1.200797	-3.512335
C	2.847526	-2.056656	-2.079489	C	1.588600	-1.249492	-2.719801
C	1.871899	-4.244030	-2.290611	C	3.500314	0.190631	-2.468205
H	2.835406	-1.060383	-1.651733	H	0.698138	-1.703459	-2.298987
H	-3.103483	-1.241096	-2.492110	H	-2.024892	-0.040173	-2.233625
C	-3.922863	-1.730065	-1.972151	C	-3.007468	-0.500983	-2.269370
C	-5.991316	-2.992437	-0.622668	C	-5.505606	-1.708524	-2.349080
H	-6.798882	-3.482430	-0.093138	H	-6.478715	-2.182569	-2.378135
C	1.854805	-2.971506	-1.725427	C	2.366441	-0.411655	-1.920755
H	1.112947	-4.969020	-2.023424	H	4.104292	0.858876	-1.865283
C	-5.081315	3.075973	-0.079651	C	-4.790914	3.300516	1.244741
H	-5.385120	4.118967	0.029853	H	-5.111713	4.216712	1.744711
C	-3.924698	-1.748058	-0.576200	C	-3.567255	-1.005901	-1.095337
C	-4.975386	-2.375722	0.092786	C	-4.824800	-1.609497	-1.145393
H	-3.687682	3.486787	-1.687297	H	-2.858023	4.098064	0.677329
C	-3.227681	1.557855	-0.851308	C	-2.778193	1.953449	0.540549
C	-3.696699	3.000063	-0.709871	C	-3.269728	3.234216	1.203062
P	0.588476	-2.457466	-0.492770	P	1.879761	-0.159682	-0.167663
H	-5.001334	-2.383899	1.176005	H	-5.271234	-2.007185	-0.241185
Pt	-0.574297	-0.542485	-0.966238	Pt	-0.400870	-0.437250	0.192639
S	-1.542402	1.525130	-1.620245	S	-0.926951	1.923917	0.519272
P	-2.572011	-0.859361	0.286859	P	-2.654519	-0.792074	0.480502
C	-3.261369	0.855202	0.500849	C	-3.375156	0.737567	1.246044
H	-2.740261	-3.604006	1.302771	H	-2.834412	-3.635534	-0.036608
H	-2.537808	1.367559	1.148392	H	-2.986013	0.738197	2.272935
C	-2.554238	-2.954188	2.150787	C	-3.141555	-3.486935	0.992777
C	-2.510907	-1.570332	1.970839	C	-3.192413	-2.195298	1.521430
H	-2.399276	-4.583509	3.527571	H	-3.439921	-5.574876	1.350031
C	-2.364873	-3.507503	3.408004	C	-3.480074	-4.579200	1.773488
C	-2.271731	-0.755226	3.079582	C	-3.571446	-2.022971	2.851522
H	-2.220254	0.321170	2.966710	H	-3.606125	-1.032804	3.289031
C	-2.129983	-2.688646	4.503521	C	-3.865055	-4.398095	3.096080
C	-2.087564	-1.311573	4.336244	C	-3.907410	-3.120407	3.632514
H	-1.981072	-3.121790	5.484552	H	-4.128119	-5.252515	3.706761
H	-1.906319	-0.665304	5.185977	H	-4.203142	-2.972435	4.663502
H	0.689994	-0.104843	-1.867192	H	-0.132956	-2.011775	0.004053
C	-0.472658	-3.947975	-0.334739	C	2.936164	-1.318454	0.786409
C	-1.531106	-4.071092	-1.235210	C	4.268320	-1.546072	0.442777
C	-0.287764	-4.929169	0.636809	C	2.404620	-1.940924	1.913394
C	-2.402010	-5.146185	-1.157383	C	5.053965	-2.386547	1.216025
H	-1.677240	-3.304727	-1.989026	H	4.693634	-1.069905	-0.433142
C	-1.160475	-6.006431	0.713059	C	3.195220	-2.776156	2.689819
H	0.523664	-4.843848	1.349630	H	1.364031	-1.769061	2.167818
C	-2.219954	-6.114180	-0.177452	C	4.519235	-3.000153	2.341614
H	-3.227428	-5.220850	-1.854687	H	6.085902	-2.563034	0.939473
H	-1.016613	-6.758761	1.478696	H	2.774137	-3.255018	3.564941
H	-2.903838	-6.950730	-0.107212	H	5.135106	-3.656120	2.944136
C	1.544120	-2.418586	1.075227	C	2.571991	1.487262	0.244232
C	2.650099	-3.243331	1.284539	C	2.249128	2.575317	-0.569709
C	1.124806	-1.568264	2.096309	C	3.324220	1.700112	1.397287
C	3.316910	-3.221509	2.500196	C	2.689880	3.847497	-0.244624
H	2.991698	-3.902363	0.494027	H	1.649230	2.423787	-1.459786
C	1.789175	-1.553385	3.313680	C	3.757465	2.977973	1.723622
H	0.279436	-0.910492	1.925679	H	3.575960	0.867149	2.042847
C	2.885283	-2.379735	3.516970	C	3.444384	4.051690	0.903429
H	4.175879	-3.862815	2.653369	H	2.437727	4.682679	-0.885927
H	1.454223	-0.888591	4.100387	H	4.343382	3.131798	2.621198
H	3.408879	-2.363469	4.464679	H	3.785171	5.047307	1.158513
C	-5.113025	2.365385	1.264120	C	-5.376613	2.080264	1.937178
C	-4.650998	0.920355	1.127523	C	-4.899942	0.796655	1.270652
H	-5.811727	2.611162	-0.751197	H	-5.180118	3.355624	0.221919
H	-6.116403	2.396594	1.693542	H	-6.467755	2.119724	1.931648
H	-4.457807	2.889440	1.968905	H	-5.071606	2.075754	2.989659

H	-5.356641	0.374058	0.492258	H	-5.275962	0.762556	0.242421
H	-4.654744	0.416941	2.098085	H	-5.310268	-0.080734	1.777930
H	-2.975406	3.540387	-0.086622	H	-2.869077	3.271720	2.222358
H	-3.914915	1.033812	-1.527892	H	-3.125334	1.946485	-0.501116

<i>cis-11-chair</i>				<i>trans-11-chair</i>			
H	2.730412	0.321758	-5.257917	H	2.744467	-0.473139	-5.199019
H	1.241251	1.975818	-4.172218	H	1.286032	1.373347	-4.428085
C	2.445339	0.197119	-4.220796	C	2.445866	-0.415108	-4.159854
C	1.609044	1.125301	-3.611948	C	1.626816	0.621259	-3.727532
H	3.559910	-1.617997	-3.966314	H	3.511448	-2.187231	-3.589083
C	2.909589	-0.889987	-3.497483	C	2.875298	-1.375886	-3.257961
H	3.504108	-0.407586	5.279734	H	-7.403481	1.638969	-1.568213
C	1.236517	0.961112	-2.288598	C	1.236297	0.690221	-2.401047
H	0.570565	1.677422	-1.819993	H	0.584433	1.490690	-2.068537
H	3.695917	-2.876617	5.368275	H	-6.329591	3.639073	-2.550022
C	2.545483	-1.051918	-2.166259	C	2.496561	-1.301481	-1.923326
C	2.710287	-1.031161	4.886725	C	-6.378095	1.882496	-1.319148
C	2.816744	-2.413398	4.937995	C	-5.775198	3.003862	-1.870564
C	1.702581	-0.128930	-1.552816	C	1.672896	-0.267811	-1.484614
H	2.920713	-1.902399	-1.609878	H	2.845970	-2.052241	-1.225092
H	1.500302	0.641115	4.327489	H	-6.150091	0.192276	-0.024157
H	-1.998483	4.343250	3.729162	H	-3.838719	-4.378782	-0.131792
H	4.072421	0.509620	-0.200238	H	3.656999	1.214372	-0.692729
C	1.581009	-0.438966	4.340465	C	-5.669895	1.066165	-0.448365
H	5.506177	2.232661	0.815483	H	4.987774	3.087375	0.190762
H	-1.842000	4.233307	6.195878	H	-5.900061	-4.740875	1.188637
H	3.777176	-1.172588	1.571677	H	3.796334	-0.670326	1.541605
C	-1.745809	3.410275	4.217145	C	-4.272295	-3.563501	0.433642
C	1.792302	-3.200477	4.430724	C	-4.457574	3.306475	-1.553994
H	1.871847	-4.280243	4.456834	H	-3.980902	4.177929	-1.985303
H	-1.202459	0.257484	-0.868586	H	-1.311110	0.639364	-0.820366
C	-1.659496	3.347773	5.599886	C	-5.428156	-3.766407	1.174896
H	-1.594902	2.314723	2.372048	H	-2.748429	-2.158623	-0.137913
C	3.666363	1.168847	0.559273	C	3.335196	1.725032	0.207567
C	-1.513041	2.274513	3.453137	C	-3.663358	-2.318302	0.423715
C	4.472535	2.143666	1.125368	C	4.085429	2.780896	0.705001
C	0.542401	-1.220943	3.833781	C	-4.345897	1.361429	-0.130227
C	-1.339708	2.146684	6.221053	C	-5.974635	-2.720242	1.904546
C	0.667940	-2.610875	3.874058	C	-3.744316	2.485620	-0.694255
C	3.172192	-2.033472	1.315902	C	3.188100	-1.565782	1.596057
H	-1.273207	2.093613	7.300580	H	-6.873138	-2.875166	2.488538
H	4.615348	-3.431043	2.056609	H	4.711418	-2.712035	2.572752
P	1.232315	-0.238633	0.225952	P	1.160684	-0.091547	0.270830
C	-1.184438	1.067458	4.066808	C	-4.209876	-1.257773	1.146866
C	2.333392	1.039460	0.956089	C	2.170850	1.323078	0.861168
C	-1.103632	1.013221	5.459798	C	-5.371055	-1.471145	1.889922
Pt	-1.003428	-0.059461	0.693988	Pt	-1.108674	0.168773	0.693822
C	3.646064	-3.309761	1.588772	C	3.703656	-2.715958	2.176525
H	-0.114254	-3.242764	3.470629	H	-2.706887	2.704195	-0.463016
C	3.954117	3.010553	2.080004	C	3.681318	3.440598	1.857066
H	4.585384	3.774239	2.516766	H	4.267229	4.265687	2.242572
C	1.924138	-1.863571	0.724182	C	1.890498	-1.559385	1.089895
P	-0.931229	-0.447819	3.056027	P	-3.375852	0.370981	1.075925
H	-0.845111	0.081528	5.951389	H	-5.810831	-0.664609	2.464764
C	1.818539	1.926991	1.895950	C	1.767310	1.992371	2.017100
C	2.624556	2.905541	2.460101	C	2.523015	3.044140	2.512320
C	2.881654	-4.422784	1.272973	C	2.930835	-3.866128	2.250140
C	1.148757	-2.987810	0.430063	C	1.115272	-2.715690	1.175723
H	0.774895	1.850568	2.179474	H	0.860986	1.671789	2.521225
H	3.256321	-5.416359	1.485448	H	3.334778	-4.761853	2.705198
H	2.208549	3.587705	3.191940	H	2.203909	3.558715	3.410202
H	0.165845	-2.853604	-0.011364	H	0.094893	-2.701641	0.804527
C	-2.300599	-1.527965	3.667285	C	-3.821974	1.208796	2.656834
C	1.627817	-4.259829	0.697771	C	1.635622	-3.864890	1.749408
S	-3.386862	0.222859	0.791659	S	-0.828066	-0.591944	3.047287
H	-3.942108	-2.020792	1.532052	H	-1.412193	1.603301	3.914809
C	-4.115023	-1.020974	1.937485	C	-1.784510	0.588880	4.085430
H	1.021211	-5.124639	0.459500	H	1.026071	-4.757354	1.814614
H	-5.188845	-0.840819	1.870654	H	-1.531161	0.334808	5.115508
C	-3.692404	-0.976340	3.392650	C	-3.293630	0.558823	3.927630
H	-2.187130	-2.505201	3.190928	H	-3.437735	2.228450	2.560525
H	-2.146408	-1.674162	4.739137	H	-4.910773	1.298295	2.687470
H	-4.402193	-1.577870	3.969875	H	-3.740284	1.093406	4.772943
H	-3.778436	0.044116	3.778514	H	-3.650420	-0.472886	3.998964

cis-11-skew-boat				trans-11-skew-boat			
H	-6.353986	-0.404863	-4.208598	H	-6.725474	0.358184	-3.762599
H	-5.581542	1.654461	-3.060785	H	-6.037909	2.041576	-2.084455
C	-5.436083	-0.414018	-3.633555	C	-5.766176	0.270379	-3.268018
C	-5.004620	0.739725	-2.990178	C	-5.380546	1.216281	-2.327511
H	-5.028987	-2.485589	-4.018905	H	-5.227125	-1.535438	-4.295504
C	-4.691618	-1.579773	-3.529446	C	-4.925882	-0.792906	-3.567155
H	-8.247484	2.610709	1.682731	H	0.268605	-0.705661	7.549616
C	-3.829568	0.724808	-2.256681	C	-4.156332	1.099315	-1.688348
H	-3.488695	1.632108	-1.770489	H	-3.858415	1.822932	-0.936414
H	-7.233132	4.630021	0.676748	H	1.196809	-2.736180	6.486423
C	-3.514142	-1.598450	-2.791815	C	-3.696791	-0.909161	-2.933863
C	-7.207818	2.602037	1.379005	C	0.168105	-0.853004	6.481626
C	-6.636893	3.736386	0.815710	C	0.689332	-1.993757	5.883254
C	-3.069244	-0.442406	-2.155915	C	-3.303458	0.038901	-1.991904
H	-2.943230	-2.516427	-2.718931	H	-3.043743	-1.740703	-3.172439
H	-6.896793	0.577495	2.007173	H	-0.877925	0.992101	6.183989
H	-7.506462	-2.377731	-1.340608	H	2.498267	3.946727	4.103670
H	-1.505356	0.549888	-3.982823	H	-2.038792	1.268544	-3.827499
C	-6.446965	1.456820	1.559347	C	-0.480356	0.099761	5.712393
H	-0.159405	2.210856	-5.187354	H	-0.473288	2.427877	-5.328089
H	-6.369328	-4.568016	-1.161563	H	1.225626	6.051684	4.381296
H	-0.265083	-1.495838	-3.603852	H	-0.072437	-1.534480	-3.175072
C	-6.582604	-2.466820	-0.781363	C	1.417643	3.941626	4.034781
C	-5.300289	3.728672	0.442051	C	0.560814	-2.180683	4.514891
H	-4.848025	4.616340	0.017140	H	0.967277	-3.068028	4.046019
H	-0.076525	-0.027789	1.037825	H	-0.160070	1.163087	0.873764
C	-5.943096	-3.693633	-0.685041	C	0.703356	5.122657	4.190607
H	-6.546448	-0.388284	-0.269557	H	1.313275	1.833521	3.667371
C	-0.752828	1.115879	-3.446357	C	-1.001715	1.380228	-3.535979
C	-6.040246	-1.341060	-0.173631	C	0.750492	2.752396	3.790677
C	0.005056	2.056330	-4.127883	C	-0.116642	2.032289	-4.385268
C	-5.106844	1.433382	1.167354	C	-0.614548	-0.082388	4.335046
C	-4.748284	-3.794271	0.016899	C	-0.680457	5.108418	4.099848
C	-4.538336	2.583299	0.621401	C	-0.089315	-1.228281	3.742224
C	-0.177935	-2.231135	-2.812138	C	-0.384044	-2.226807	-2.401545
H	-4.236157	-4.746386	0.089905	H	-1.242893	6.026070	4.218379
H	0.819958	-3.653110	-4.063748	H	0.562789	-3.907745	-3.331844
P	-1.527786	-0.368984	-1.157250	P	-1.671629	-0.023014	-1.161876
C	-4.848434	-1.435958	0.538819	C	-0.642007	2.728812	3.707034
C	-0.556196	0.902527	-2.079613	C	-0.558879	0.873132	-2.316629
C	-4.203109	-2.672908	0.621584	C	-1.352405	3.918294	3.857390
Pt	-1.688439	0.070577	1.090611	Pt	-1.653885	0.617376	1.067791
C	0.433569	-3.447482	-3.072896	C	-0.025883	-3.564775	-2.490135
H	-3.486297	2.574642	0.351519	H	-0.198670	-1.365519	2.670396
C	0.965465	2.798728	-3.454541	C	1.215868	2.172611	-4.030629
H	1.553091	3.536853	-3.986717	H	1.904524	2.679195	-4.695110
C	-0.674989	-1.952557	-1.538712	C	-1.139498	-1.773495	-1.321300
P	-4.047155	-0.038081	1.420676	P	-1.495831	1.157427	3.313567
H	-3.262824	-2.750393	1.159286	H	-2.433141	3.923773	3.786053
C	0.407143	1.657415	-1.411612	C	0.782362	1.027279	-1.962231
C	1.164003	2.597148	-2.096424	C	1.664895	1.665364	-2.817166
C	0.551876	-4.398280	-2.066966	C	-0.420838	-4.458753	-1.505326
C	-0.547439	-2.908806	-0.533611	C	-1.532642	-2.677155	-0.332275
H	0.555317	1.509406	-0.348708	H	1.130190	0.646371	-1.008351
H	1.906523	3.177790	-1.562737	H	2.704180	1.774300	-2.533370
H	-0.918719	-2.682099	0.460819	H	-2.122935	-2.319569	0.506474
C	-4.376564	-0.539622	3.171776	C	-3.147278	1.336746	4.109079
C	0.061136	-4.127966	-0.797908	C	-1.176356	-4.013401	-0.428470
S	-1.349530	0.630967	3.389273	S	-3.961333	-0.228695	1.429975
H	-3.187336	2.172621	3.144243	H	-2.856838	-1.496150	3.159051
C	-2.913138	1.447903	3.913526	C	-3.806358	-0.957296	3.115025
H	0.157503	-4.863425	-0.008530	H	-1.485858	-4.708343	0.342339
H	-2.672148	2.028593	4.805276	H	-4.589006	-1.709557	3.218737
H	1.033145	-5.346763	-2.272444	H	-0.138137	-5.501721	-1.575518
C	-4.087218	0.531900	4.215248	C	-3.908654	0.025827	4.274705
H	-3.931488	0.033802	5.175671	H	-4.957275	0.276715	4.452212
H	-4.973627	1.162943	4.339427	H	-3.559595	-0.481870	5.179985
H	-5.406116	-0.893653	3.253691	H	-3.037175	1.843307	5.070211
H	-3.730777	-1.408316	3.318674	H	-3.701043	2.004548	3.446326

cis-11-boat				trans-11-boat			
H	3.060075	0.392516	-5.031463	H	2.803372	-0.270510	-5.253818
H	1.404095	1.983855	-4.104336	H	1.104525	1.365832	-4.502492
C	2.667240	0.247190	-4.032989	C	2.487885	-0.252265	-4.218156
C	1.737496	1.140118	-3.513161	C	1.534079	0.665633	-3.797029
H	3.810167	-1.531251	-3.669838	H	3.775721	-1.865484	-3.632134
C	3.087189	-0.830926	-3.270390	C	3.032101	-1.147422	-3.309705
H	2.421566	0.037659	5.671875	H	-6.768273	0.947954	-2.481931
C	1.228450	0.948830	-2.240294	C	1.122527	0.682918	-2.474382
H	0.491193	1.637654	-1.842571	H	0.367170	1.389071	-2.148824
H	3.051921	-2.356451	5.786850	H	-6.323732	3.360885	-2.800279
C	2.585776	-1.019453	-1.987847	C	2.630007	-1.125197	-1.980985
C	1.827262	-0.708630	5.158861	C	-6.024631	1.448763	-1.874620
C	2.179311	-2.048853	5.224268	C	-5.774939	2.800552	-2.053901
C	1.649355	-0.132315	-1.464698	C	1.668868	-0.210767	-1.553361
H	2.928049	-1.861832	-1.398978	H	3.068308	-1.821722	-1.276535
H	0.426383	0.729749	4.425478	H	-5.527992	-0.327127	-0.786202
H	-3.084683	3.961202	3.232356	H	-3.792796	-4.478252	0.982110
H	3.752343	0.759356	0.118393	H	3.593616	1.326444	-0.758735
C	0.702935	-0.317216	4.447195	C	-5.324352	0.728576	-0.915955
H	4.893844	2.599739	1.287187	H	4.932661	3.149134	0.213002
H	-3.461866	3.795224	5.672189	H	-6.113204	-4.493182	1.838031
H	3.443798	-0.958751	1.860489	H	3.594498	-0.636266	1.856993
C	-2.878008	3.034663	3.753188	C	-4.291169	-3.546248	1.217530
C	1.408425	-2.993358	4.561603	C	-4.812365	3.432547	-1.276880
H	1.680418	-4.040898	4.597597	H	-4.605586	4.486143	-1.416980
H	-1.326064	0.117368	-1.137676	H	-1.293892	0.829080	-0.772800
C	-3.090689	2.940830	5.120032	C	-5.592099	-3.554362	1.697621
H	-2.250218	2.000757	1.972524	H	-2.598902	-2.329873	0.679477
C	3.205750	1.363960	0.833990	C	3.301873	1.760620	0.190325
C	-2.400865	1.939106	3.045266	C	-3.621003	-2.343632	1.040317
C	3.847701	2.404386	1.486638	C	4.057597	2.787485	0.738426
C	-0.081273	-1.258777	3.778766	C	-4.365162	1.357172	-0.125805
C	-2.828079	1.747172	5.781844	C	-6.228393	-2.356094	1.996987
C	0.295199	-2.601715	3.834400	C	-4.107603	2.714968	-0.324588
C	2.945032	-1.874392	1.568305	C	3.061879	-1.568773	1.712918
H	-2.992940	1.669360	6.849238	H	-7.245407	-2.357713	2.368481
H	4.421457	-3.123216	2.487704	H	4.468596	-2.711612	2.855145
P	0.976993	-0.278591	0.245152	P	1.157734	-0.093614	0.206949
C	-2.134095	0.739034	3.700192	C	-4.249018	-1.137952	1.344197
C	1.858149	1.097756	1.087355	C	2.172120	1.290431	0.857443
C	-2.352922	0.653619	5.077037	C	-5.561521	-1.154408	1.820721
Pt	-1.305230	-0.251384	0.428454	Pt	-1.107382	0.165451	0.669345
C	3.497945	-3.097679	1.922396	C	3.554863	-2.739072	2.274705
H	-0.273676	-3.354246	3.302092	H	-3.340333	3.212410	0.259109
C	3.149339	3.200073	2.386957	C	3.694925	3.346915	1.955227
H	3.652537	4.015051	2.892015	H	4.285769	4.148638	2.380444
C	1.752989	-1.827456	0.851408	C	1.883556	-1.592419	0.972000
P	-1.518300	-0.722193	2.762458	P	-3.353813	0.444658	1.104446
H	-2.140345	-0.270715	5.603742	H	-6.072304	-0.224562	2.046052
C	1.162763	1.914801	1.973385	C	1.808360	1.859887	2.078625
C	1.804723	2.958315	2.624800	C	2.571250	2.880409	2.624917
C	2.868489	-4.280329	1.564058	C	2.880510	-3.937557	2.094456
C	1.112612	-3.021667	0.512719	C	1.203719	-2.799942	0.803963
H	0.107251	1.732985	2.143887	H	0.927978	1.486233	2.593604
H	3.303925	-5.232347	1.841112	H	3.266875	-4.848315	2.534641
H	1.249007	3.583970	3.313098	H	2.284730	3.315992	3.574134
H	0.170563	-2.984289	-0.026214	H	0.271893	-2.816099	0.247647
C	-2.792331	-2.017663	3.145546	C	-3.647569	1.390486	2.670506
C	1.670679	-4.240846	0.861876	C	1.704434	-3.967296	1.355735
S	-3.673621	-0.075602	0.193948	S	-0.822292	-0.877345	2.895898
H	-5.536187	-0.946639	1.353642	H	-1.814147	-0.375101	4.995985
C	-4.500306	-0.810606	1.664326	C	-2.179106	-0.255302	3.976045
H	1.168645	-5.160624	0.588766	H	1.170719	-4.899443	1.219608
H	-4.513152	-0.092531	2.489971	H	-3.056236	-0.904131	3.881818
C	-3.909527	-2.138940	2.119404	C	-2.572840	1.196664	3.731093
H	-2.272202	-2.969894	3.245032	H	-3.726504	2.442211	2.392274
H	-3.195378	-1.776751	4.132420	H	-4.627658	1.092392	3.050825
H	-3.548212	-2.682064	1.242974	H	-1.679971	1.764474	3.455380
H	-4.696422	-2.756344	2.561822	H	-2.945665	1.635690	4.661090

TS[<i>trans</i> -11-boat→skew-boat]				TS[<i>trans</i> -11-skew-boat→chair]			
H	3.188284	-4.459548	-3.395142	H	1.983453	-0.806251	-5.500968
H	0.852349	-3.696768	-3.686060	H	0.216354	-2.098020	-4.343125
C	2.769088	-3.723939	-2.720115	C	1.824990	-0.677042	-4.437672
C	1.458863	-3.296327	-2.883351	C	0.832576	-1.401668	-3.788227
H	4.562126	-3.539675	-1.553761	H	3.380927	0.783804	-4.221511
C	3.539308	-3.209979	-1.686441	C	2.607776	0.214288	-3.721001
H	-6.417752	3.744634	1.594693	H	-5.177071	1.863106	-2.977108
C	0.917781	-2.360777	-2.014489	C	0.622026	-1.228145	-2.430964
H	-0.109037	-2.034857	-2.132198	H	-0.163890	-1.781995	-1.929288
H	-5.049624	5.222871	0.159026	H	-6.147842	4.000826	-2.191014
C	3.003058	-2.269577	-0.819388	C	2.408481	0.379910	-2.355977
C	-5.553957	3.349718	1.074876	C	-5.059672	2.165962	-1.944194
C	-4.785728	4.178551	0.269323	C	-5.604300	3.366038	-1.502596
C	1.685148	-1.837208	-0.975812	C	1.412431	-0.339258	-1.700371
H	3.613150	-1.869367	-0.018185	H	3.032091	1.072672	-1.804257
H	-5.821767	1.382555	1.862755	H	-3.920142	0.428853	-1.414607
H	-7.608015	-1.023589	-2.126931	H	-3.937225	-4.256601	1.780156
H	2.848274	0.198361	-2.112483	H	3.938350	-0.279321	1.046330
C	-5.215291	2.012482	1.222890	C	-4.357637	1.358324	-1.066268
H	3.434591	2.371067	-3.109693	H	5.515330	1.499923	1.692452
H	-6.844414	-3.244432	-2.902217	H	-6.407241	-4.127835	1.746821
H	3.117997	1.201686	1.307093	H	0.626366	-1.541031	2.592782
C	-6.657534	-1.419051	-1.790964	C	-4.430318	-3.297524	1.682710
C	-3.675682	3.667479	-0.388693	C	-5.446903	3.749841	-0.180106
H	-3.069140	4.310598	-1.014237	H	-5.867213	4.684766	0.168752
H	-1.517061	-1.030320	-0.984769	H	-1.606441	-0.308983	-0.634876
C	-6.228571	-2.664612	-2.226178	C	-5.815836	-3.224447	1.664820
H	-6.213535	0.299822	-0.591821	H	-2.588006	-2.185991	1.572129
C	2.393566	1.104695	-1.730770	C	3.619781	0.756443	1.026771
C	-5.870085	-0.672528	-0.925277	C	-3.673439	-2.140245	1.569180
C	2.724754	2.330560	-2.292897	C	4.508257	1.758774	1.390100
C	-4.101055	1.490240	0.565877	C	-4.203845	1.732766	0.270113
C	-5.006032	-3.163824	-1.796948	C	-6.445246	-1.992717	1.537561
C	-3.333025	2.332455	-0.238968	C	-4.751993	2.936711	0.706201
C	2.977125	0.339142	1.947245	C	1.329845	-2.164498	2.050218
H	-4.664786	-4.133629	-2.137014	H	-7.526433	-1.934681	1.521011
H	4.454904	0.974850	3.362216	H	1.487991	-3.640070	3.593686
P	0.984871	-0.536056	0.115766	P	1.107139	-0.183128	0.104813
C	-4.640303	-1.165809	-0.495253	C	-4.298015	-0.900735	1.442672
C	1.476225	1.041029	-0.684987	C	2.320684	1.079970	0.643147
C	-4.212929	-2.415989	-0.940982	C	-5.691064	-0.834321	1.430110
Pt	-1.309158	-0.495585	0.509988	Pt	-1.077042	0.243218	0.777310
C	3.732610	0.209847	3.105962	C	1.817064	-3.336800	2.607531
H	-2.455699	1.932133	-0.736173	H	-4.641940	3.249631	1.736565
C	2.149785	3.497582	-1.812004	C	4.107884	3.087243	1.367371
H	2.409364	4.451532	-2.253814	H	4.802656	3.867215	1.652841
C	2.043287	-0.635942	1.609958	C	1.748022	-1.764958	0.780148
P	-3.588558	-0.265753	0.711554	P	-3.270515	0.617324	1.379802
H	-3.246970	-2.791622	-0.619977	H	-6.186824	0.125158	1.327676
C	0.896045	2.218774	-0.208154	C	1.921473	2.416234	0.630790
C	1.237257	3.440280	-0.765899	C	2.813283	3.415316	0.986810
C	3.564945	-0.893198	3.928939	C	2.718988	-4.122224	1.902065
C	1.870303	-1.737349	2.450173	C	2.655243	-2.556802	0.077229
H	0.176003	2.162874	0.603422	H	0.902272	2.664426	0.351855
H	4.155614	-0.991543	4.831129	H	3.094225	-5.040440	2.336464
H	0.785168	4.348788	-0.387420	H	2.494790	4.450097	0.976326
H	1.127803	-2.488963	2.203908	H	2.986029	-2.257361	-0.910593
C	-4.298532	-0.880125	2.300750	C	-3.476001	1.321753	3.064962
H	-5.352784	-0.594060	2.308761	C	3.136773	-3.731092	0.637841
C	2.633173	-1.869342	3.597619	S	-0.326087	1.168203	2.942086
S	-0.982817	0.319750	2.804777	H	-1.019570	0.767521	5.164661
H	-3.077437	1.552685	3.013209	C	-1.348917	0.327976	4.222843
H	-4.297471	-1.965095	2.184192	H	3.840254	-4.340779	0.084681
C	-2.626879	0.703436	3.532002	H	-1.047597	-0.720177	4.259681
H	2.493390	-2.728785	4.241182	C	-2.887896	0.409844	4.132745
H	-2.416297	1.041366	4.547014	H	-2.984600	2.296431	3.073962
C	-3.593165	-0.470649	3.601925	H	-4.543157	1.472484	3.244330
H	-3.051146	-1.329893	4.000622	H	-3.275005	0.742449	5.097951
H	-4.366348	-0.234222	4.338283	H	-3.294441	-0.595951	3.994037

BP86-D3/SVP:

<i>cis-5</i>				<i>trans-5</i>			
H	-4.703521	3.196528	-4.597269	H	-8.251089	-2.705108	2.470850
H	-3.225659	1.164033	-4.530745	H	-6.747907	-2.670504	0.455998
C	-4.618302	2.604602	-3.672175	C	-7.216684	-2.335886	2.558300
C	-3.789344	1.467527	-3.633797	C	-6.375157	-2.316235	1.430451
H	-5.991462	3.865358	-2.546489	H	-7.387637	-1.879512	4.680880
C	-5.338468	2.978156	-2.524520	C	-6.733785	-1.875064	3.794083
H	-6.207243	-3.609208	-2.381785	H	-2.121473	-5.757438	3.449772
C	-3.680522	0.711808	-2.454197	C	-5.061760	-1.832387	1.537342
H	-5.822102	-1.206963	-1.835392	H	-3.527069	-3.701440	3.268975
H	-3.032715	-0.180552	-2.434097	H	-4.412425	-1.787671	0.648327
C	-5.517386	-3.339741	-1.565870	C	-1.638292	-4.777953	3.303698
C	-5.236839	2.220043	-1.342995	C	-5.413075	-1.402301	3.907984
C	-5.304459	-1.985729	-1.252692	C	-2.431125	-3.619818	3.201322
H	-5.017376	-5.405849	-1.092156	H	0.380012	-5.594355	3.298291
C	-4.409200	1.076327	-1.295361	C	-4.565431	-1.376494	2.779461
C	-4.850521	-4.345429	-0.844004	C	-0.238728	-4.685930	3.219439
H	-5.810287	2.517606	-0.451011	H	-5.045350	-1.045883	4.882268
H	-0.868445	1.430207	-1.038414	H	-0.915629	1.005225	-1.063555
H	-2.036235	2.557299	-0.756563	H	-2.113509	2.130956	-0.917287
C	-4.418283	-1.624403	-0.211454	C	-1.823705	-2.360358	3.007163
N	-1.291008	2.012948	-0.298361	N	-1.324455	1.698645	-0.416367
C	-3.962377	-3.992644	0.187426	C	0.369057	-3.430786	3.029771
P	-4.113393	0.139860	0.281562	P	-2.804954	-0.789649	2.882200
C	-3.741053	-2.640366	0.499264	C	-0.414926	-2.271149	2.917177
H	-3.427982	-4.775095	0.749407	H	1.466100	-3.352654	2.961559
C	-0.256470	2.908727	0.293147	C	-0.299409	2.722012	-0.041679
H	1.338873	1.438691	0.440906	H	1.306142	1.331214	0.423846
H	-7.066145	-0.578498	0.226946	H	-2.250545	-1.928653	5.614060
C	-5.578709	0.576413	1.337081	C	-2.683104	-0.056051	4.578333
Pt	-2.109230	0.615680	1.230118	Pt	-2.072101	0.544783	1.243634
C	-6.883134	0.102291	1.072821	C	-2.420415	-0.845498	5.719745
H	-3.026482	-2.355736	1.288471	H	0.055472	-1.284078	2.754035
H	-0.783661	3.628478	0.952973	H	-0.838057	3.558598	0.449165
C	0.733675	2.090196	1.112231	C	0.705668	2.120181	0.932525
H	-4.334664	1.767243	2.656742	H	-3.042625	1.954028	3.829024
C	-5.363061	1.426366	2.444269	C	-2.875659	1.335428	4.725411
H	1.442612	2.770409	1.629254	H	1.417144	2.908531	1.257181
C	-7.954805	0.483338	1.897683	C	-2.363226	-0.250284	6.992051
H	-8.967661	0.104492	1.686371	H	-2.150660	-0.872244	7.876336
H	-2.516650	-0.357743	2.395440	H	-3.319611	0.096923	0.342720
S	-0.123144	1.062877	2.396488	S	-0.141264	1.443995	2.428500
C	-6.438755	1.807508	3.266025	C	-2.823359	1.924210	6.000061
C	-7.735256	1.338083	2.993724	C	-2.568076	1.133696	7.134439
H	-6.258040	2.467401	4.129513	H	-2.969312	3.011083	6.104355
H	-8.577135	1.631174	3.641375	H	-2.518148	1.598770	8.132097
H	0.265988	3.483631	-0.508423	H	0.198713	3.112233	-0.960765

<i>cis-6</i>				<i>trans-6</i>			
H	-4.243311	3.693534	-4.066536	H	-8.197658	-2.909262	2.292017
H	-2.867853	1.591707	-4.117892	H	-6.730043	-2.479660	0.297566
C	-4.285214	2.985765	-3.223807	C	-7.192274	-2.479701	2.427877
C	-3.515064	1.807470	-3.253299	C	-6.370619	-2.238721	1.310687
H	-5.711629	4.175611	-2.086835	H	-7.369395	-2.344065	4.594520
C	-5.104652	3.256575	-2.113875	C	-6.728911	-2.164181	3.716398
H	-5.935903	-3.464284	-2.621177	H	-1.989844	-5.677067	2.924477
C	-3.561327	0.908632	-2.175834	C	-5.094537	-1.679672	1.481028
H	-5.675761	-1.094319	-1.872719	H	-3.496183	-3.680597	2.938103
H	-2.947680	-0.007371	-2.193755	H	-4.455259	-1.466412	0.609361
C	-5.319260	-3.234656	-1.737506	C	-1.554989	-4.664767	2.917775
C	-5.154369	2.358392	-1.031305	C	-5.445394	-1.616139	3.893094
C	-5.178997	-1.902625	-1.312153	C	-2.403736	-3.542587	2.923326
H	-4.779852	-5.313293	-1.376388	H	0.502443	-5.375622	2.898776
C	-4.382521	1.177284	-1.054820	C	-4.621162	-1.369732	2.774565
H	2.382298	4.920213	-1.616620	H	2.606876	4.722715	-1.668416
O	0.125806	3.476567	-1.765177	O	0.372924	3.240757	-1.773439
C	-4.670625	-4.269834	-1.040301	C	-0.159937	-4.495118	2.904180
H	-5.792308	2.577749	-0.160238	H	-5.087246	-1.376857	4.906266
H	-1.205034	1.710252	-0.847597	H	-1.000761	1.627896	-0.735364
H	-2.352600	2.748232	-0.334497	H	-2.219834	2.680320	-0.434054
C	1.649478	5.579755	-1.107594	C	1.835279	5.442773	-1.326329
C	-4.385452	-1.597328	-0.182958	C	-1.853015	-2.244084	2.908259
C	0.183987	3.798939	-0.588989	C	0.334693	3.742121	-0.660528
H	2.169832	6.384388	-0.557360	H	2.308592	6.327685	-0.864098
N	-1.567116	2.171829	0.005693	N	-1.442212	2.180676	0.021991
C	-3.872925	-3.969128	0.078459	C	0.388856	-3.198544	2.894238
P	-4.185373	0.124707	0.449016	P	-2.900473	-0.722821	2.954299
O	0.900741	4.843534	-0.120304	O	1.008480	4.854727	-0.301489
C	-3.723464	-2.638332	0.503659	C	-0.449739	-2.072937	2.890626
H	-3.353004	-4.775402	0.619689	H	1.482030	-3.061391	2.883600
C	-0.494491	3.037857	0.551033	C	-0.431918	3.153879	0.524073
H	1.072994	1.532492	0.581310	H	1.124137	1.696177	0.944929
H	-7.092746	-0.602675	0.095729	H	-2.269777	-2.142417	5.516597
C	-5.717385	0.448521	1.428488	C	-2.800263	-0.184143	4.714550
Pt	-2.247905	0.635338	1.470634	Pt	-2.205041	0.810592	1.504668
C	-6.990185	0.002067	1.010227	C	-2.488985	-1.088922	5.752415
H	-3.078177	-2.391541	1.361886	H	-0.029023	-1.051278	2.876004
H	-0.948576	3.753290	1.267532	H	-0.961665	3.959122	1.073627
C	0.537149	2.181971	1.310086	C	0.529900	2.454166	1.504387
H	-4.594630	1.533407	2.937622	H	-3.269079	1.877274	4.200420
C	-5.597507	1.205884	2.613581	C	-3.061746	1.169238	5.018641
H	1.286708	2.849214	1.781938	H	1.237645	3.207246	1.906704
C	-8.130514	0.318945	1.766183	C	-2.449682	-0.642888	7.084424
H	-9.120585	-0.034580	1.436727	H	-2.200017	-1.351067	7.890549
H	-2.598653	-0.430085	2.571322	H	-3.372463	0.392520	0.492962
S	-0.267602	1.155862	2.623528	S	-0.397187	1.680011	2.895630
C	-6.742485	1.521437	3.366543	C	-3.023619	1.608238	6.352258
C	-8.008593	1.080595	2.943737	C	-2.719025	0.704465	7.385796
H	-6.641392	2.109744	4.292345	H	-3.220375	2.667053	6.583157
H	-8.904751	1.324791	3.536343	H	-2.681438	1.053174	8.430252
H	0.972270	6.008432	-1.874947	H	1.222126	5.741819	-2.201275

<i>cis-7</i>				<i>trans-7</i>			
H	-4.201908	3.919130	-3.840011	H	-8.200578	-2.880686	2.231546
H	-2.809393	1.832036	-3.972200	H	-6.738016	-2.321479	0.265719
C	-4.252178	3.170074	-3.034218	C	-7.197920	-2.453396	2.392444
C	-3.472591	2.000004	-3.109119	C	-6.379084	-2.139811	1.291306
H	-5.706327	4.292032	-1.863818	H	-7.373606	-2.450079	4.563443
C	-5.091896	3.379683	-1.926210	C	-6.735268	-2.213213	3.697355
H	-5.868848	-3.312352	-2.775598	H	-1.976524	-5.641364	2.694837
C	-3.529770	1.048386	-2.078545	C	-5.106567	-1.583574	1.494236
H	-5.637477	-0.980996	-1.906740	H	-3.494681	-3.658717	2.832590
H	-2.908560	0.138859	-2.131379	H	-4.469617	-1.313684	0.636659
C	-5.266652	-3.122784	-1.872668	C	-1.547771	-4.627718	2.745816
C	-5.152546	2.428422	-0.890529	C	-5.455184	-1.668346	3.905966
C	-5.142568	-1.812655	-1.379674	C	-2.403173	-3.513150	2.821094
H	-4.716576	-5.213043	-1.607486	H	0.513775	-5.323337	2.676019
C	-4.371381	1.255228	-0.959554	C	-4.633788	-1.349339	2.803822
H	2.094339	5.079006	-1.450771	H	2.307607	4.996336	-1.506822
O	0.112293	3.624098	-1.485979	O	0.314734	3.555235	-1.466163
C	-4.620146	-4.186891	-1.218371	C	-0.153837	-4.448833	2.736110
H	-5.806366	2.599889	-0.020485	H	-5.097520	-1.488476	4.931534
H	-1.206870	1.805469	-0.676888	H	-1.037451	1.876250	-0.522276
H	-2.367623	2.808265	-0.126318	H	-2.258680	2.904148	-0.154853
H	1.362892	7.463966	-1.965580	H	1.646043	7.291048	-2.393490
H	-0.023158	6.321111	-1.966678	H	0.247199	6.166535	-2.330957
C	1.630050	5.733488	-0.683447	C	1.804289	5.754251	-0.870619
C	-4.367539	-1.558432	-0.225224	C	-1.860368	-2.212522	2.880038
C	0.162857	3.888951	-0.293995	C	0.292122	3.987610	-0.323014
H	2.426348	6.182344	-0.057327	H	2.564464	6.281457	-0.260988
N	-1.583043	2.219607	0.194434	N	-1.478594	2.380218	0.268510
C	0.748126	6.795438	-1.327925	C	0.981109	6.720446	-1.712577
C	-3.840854	-3.936751	-0.074469	C	0.387073	-3.150507	2.800024
P	-4.188932	0.131623	0.493686	P	-2.916986	-0.703279	3.020538
O	0.869977	4.906341	0.241344	O	0.974065	5.067517	0.108836
C	-3.707600	-2.627772	0.418460	C	-0.458241	-2.031878	2.866262
H	-3.322568	-4.765365	0.433569	H	1.479343	-3.006087	2.792678
C	-0.523584	3.063894	0.796699	C	-0.469866	3.324608	0.825723
H	1.056036	1.571326	0.771655	H	1.093157	1.851300	1.156817
H	-7.085694	-0.596042	0.060829	H	-2.275757	-2.273798	5.490296
H	0.246865	7.414560	-0.556288	H	0.439111	7.443096	-1.069202
C	-5.737803	0.397235	1.464159	C	-2.817134	-0.272819	4.810449
Pt	-2.270556	0.603854	1.567671	Pt	-2.233049	0.919714	1.665964
C	-7.001011	-0.036467	1.005407	C	-2.499623	-1.237843	5.790539
H	-3.076456	-2.419504	1.297171	H	-0.043866	-1.008435	2.910101
H	-0.992010	3.739358	1.542216	H	-1.001076	4.094246	1.422920
C	0.504264	2.177929	1.525068	C	0.495666	2.571297	1.761214
H	-4.645190	1.414248	3.040972	H	-3.296661	1.813920	4.424323
C	-5.640871	1.096257	2.686597	C	-3.084445	1.058110	5.197279
H	1.241324	2.825677	2.041478	H	1.200216	3.302078	2.207566
C	-8.154589	0.235090	1.758874	C	-2.459880	-0.874045	7.147279
H	-9.137098	-0.108344	1.397638	H	-2.205321	-1.629039	7.908120
H	-2.626461	-0.520133	2.606892	H	-3.400815	0.558889	0.632568
S	-0.309674	1.078552	2.772227	S	-0.426024	1.709867	3.104126
C	-6.799021	1.366527	3.437025	C	-3.045766	1.414858	6.555208
C	-8.055502	0.938449	2.974235	C	-2.734906	0.451046	7.531013
H	-6.715853	1.909138	4.392061	H	-3.247015	2.456621	6.850770
H	-8.961981	1.146967	3.564768	H	-2.696875	0.735384	8.594787

<i>cis</i> -8				<i>trans</i> -8			
H	-6.391503	-1.588149	-4.591321	H	2.498778	-2.148348	-5.314430
H	-5.841603	0.605497	-3.489279	H	0.552265	-0.585646	-5.014547
C	-5.424034	-1.451091	-4.082505	C	2.222984	-1.794514	-4.308121
C	-5.116796	-0.223518	-3.466449	C	1.133269	-0.920051	-4.140140
H	-4.724498	-3.465650	-4.522834	H	3.802329	-2.910752	-3.306784
C	-4.491995	-2.501240	-4.043199	C	2.952298	-2.220302	-3.185643
H	-7.414998	2.990545	-0.700731	H	-7.206200	3.293684	0.010742
C	-3.887186	-0.049791	-2.812077	C	0.771789	-0.480286	-2.856767
H	-3.660940	0.911760	-2.323602	H	-0.100083	0.179834	-2.721602
H	-5.939586	5.010115	-0.929892	H	-5.633157	5.172792	-0.535538
C	-3.253991	-2.328299	-3.395960	C	2.601877	-1.770186	-1.899217
C	-6.348748	2.929981	-0.428867	C	-6.117459	3.125080	0.027024
C	-5.523042	4.060056	-0.558829	C	-5.235482	4.177408	-0.280420
C	-2.940474	-1.100166	-2.774537	C	1.507701	-0.895579	-1.723873
H	-2.528763	-3.156303	-3.376582	H	3.182087	-2.108802	-1.027280
H	-6.478609	0.836172	0.132152	H	-6.314547	1.033139	0.575829
H	-5.307673	-4.350145	-0.550633	H	-5.054281	-3.061901	-2.780217
H	-1.632460	-0.052612	-4.766084	H	2.932757	1.262537	-1.837325
C	-5.821440	1.714931	0.045985	C	-5.614332	1.853682	0.349960
H	-0.433496	1.593473	-6.203573	H	3.938871	3.539962	-1.647775
H	-7.447785	-4.259388	0.764364	H	-7.063104	-3.893600	-1.520141
H	0.169446	-1.957127	-4.220887	H	3.813401	-0.006548	1.036105
C	-5.538840	-3.471392	0.071779	C	-5.265380	-2.686696	-1.766188
C	-4.159623	3.968344	-0.224853	C	-3.847821	3.953809	-0.269568
H	-3.501522	4.844754	-0.336795	H	-3.152846	4.772166	-0.516652
H	0.205729	-0.291334	0.162272	H	-1.552280	-0.343591	-1.147147
C	-6.734610	-3.420709	0.807613	C	-6.388598	-3.153833	-1.060256
H	-3.682706	-2.447166	-0.431674	H	-3.501246	-1.404211	-1.713996
C	-0.837548	0.571598	-4.328619	C	2.682009	1.898882	-0.974525
C	-4.627206	-2.402797	0.131153	C	-4.398877	-1.751311	-1.177648
C	-0.164789	1.503496	-5.138733	C	3.249043	3.182266	-0.866511
C	-4.456354	1.617740	0.393583	C	-4.220363	1.624748	0.367098
C	-7.014376	-2.298874	1.608809	C	-6.642021	-2.681738	0.238878
C	-3.625541	2.754084	0.238069	C	-3.339901	2.681752	0.048168
C	0.227986	-2.669476	-3.382930	C	3.356077	-0.915286	1.458434
H	-7.945094	-2.257323	2.197067	H	-7.514932	-3.049940	0.801302
H	1.414257	-4.100077	-4.509670	H	5.128911	-1.448284	2.597312
P	-1.350093	-0.802879	-1.862207	P	1.014923	-0.252027	-0.052763
C	-4.902838	-1.266900	0.921187	C	-4.653247	-1.261786	0.123313
C	-0.508623	0.444762	-2.959194	C	1.792256	1.431919	0.017047
C	-6.104802	-1.229611	1.668575	C	-5.780681	-1.739859	0.829647
Pt	-1.387822	-0.187728	0.346485	Pt	-1.249660	-0.190697	0.420007
C	0.931975	-3.875475	-3.544779	C	4.094842	-1.726119	2.337503
H	-2.547634	2.668782	0.459537	H	-2.253651	2.484353	0.044002
C	0.840938	2.319497	-4.592435	C	2.938155	4.002533	0.231197
H	1.364650	3.051749	-5.227660	H	3.382885	5.007411	0.313088
C	-0.386524	-2.365191	-2.148032	C	2.026711	-1.257684	1.125803
P	-3.639371	0.079434	1.035505	P	-3.498859	-0.014106	0.843139
H	-6.334673	-0.365414	2.311837	H	-5.992771	-1.386775	1.850775
C	0.496094	1.276367	-2.415420	C	1.476205	2.261763	1.118226
C	1.168155	2.203444	-3.229875	C	2.054533	3.537310	1.222893
C	1.028439	-4.787498	-2.478229	C	3.514270	-2.882392	2.888736
C	-0.274208	-3.279054	-1.077075	C	1.443841	-2.412839	1.692539
H	0.735869	1.198864	-1.342959	H	0.770111	1.896619	1.886975
H	1.948305	2.845763	-2.791060	H	4.093879	-3.513946	3.581026
H	-0.722112	-3.015904	-0.103290	H	1.806036	4.176084	2.085739
C	-3.554377	0.363893	2.890612	H	0.394421	-2.657941	1.462338
H	-4.494229	0.842855	3.242908	C	-3.742646	-0.107255	2.693965
C	0.425046	-4.486936	-1.244445	H	-4.730806	0.320016	2.975881
S	-0.760268	0.523270	2.503982	C	2.189137	-3.223242	2.565450
H	-2.459282	2.248362	2.967658	S	-0.925921	-0.008883	2.830563
H	-3.486898	-0.652612	3.334523	H	-2.654824	1.710896	3.218100
C	-2.322510	1.183828	3.257144	H	-3.728892	-1.187437	2.954940
H	0.509678	-5.189593	-0.400195	C	-2.582228	0.613988	3.384435
H	-2.168528	1.165236	4.357314	H	1.724347	-4.119070	3.006799
H	1.585052	-5.729676	-2.606741	H	-2.637319	0.446137	4.481074

<i>cis-9</i>				<i>trans-9</i>			
H	3.136301	-4.053697	-5.048499	H	3.155801	1.245680	-5.506828
H	2.506024	-1.658492	-4.617494	H	1.226660	2.344914	-4.328846
C	2.667189	-3.767380	-4.093545	C	2.921926	0.981362	-4.462974
H	-6.183395	1.917792	-3.960712	H	-5.336257	1.914495	-4.269919
H	-4.508891	2.441051	-4.330022	H	-3.644910	2.507336	-4.303929
H	2.675802	-5.796082	-3.298635	H	4.545073	-0.462082	-4.298489
H	-4.863967	0.705283	-4.058058	H	-3.974859	0.753851	-4.130240
C	2.315352	-2.427793	-3.852291	C	1.841349	1.596566	-3.803294
C	-5.114121	1.733375	-3.722232	C	-4.325718	1.764410	-3.833532
H	-3.195432	-3.183568	-4.218915	H	-2.573696	-3.623589	-3.857093
C	2.409974	-4.742774	-3.113999	C	3.699159	0.025340	-3.787610
H	-5.685046	-3.482228	-4.048915	H	-5.073301	-3.744089	-4.079275
C	-3.732986	-2.849733	-3.317094	C	-3.219803	-3.145019	-3.104053
C	-5.125986	-3.014086	-3.223017	C	-4.618375	-3.212081	-3.228472
H	-6.301083	3.513613	-1.909929	H	-5.908616	3.458564	-2.256375
H	-4.664602	4.079845	-2.332810	H	-4.246001	4.094956	-2.345666
C	1.710899	-2.061965	-2.637244	C	1.531856	1.254800	-2.477052
C	-4.832293	1.918975	-2.224035	C	-4.342966	1.927034	-2.306541
C	-5.219446	3.323917	-1.728788	C	-4.875261	3.304638	-1.872648
C	1.808949	-4.380805	-1.895641	C	3.402936	-0.314715	-2.454494
H	1.417805	-1.016162	-2.448711	H	0.674052	1.720344	-1.959270
H	-2.723321	2.365078	-2.477782	H	-2.244762	2.456673	-2.143855
H	-5.457292	1.178479	-1.668991	H	-5.031718	1.151234	-1.893659
H	-1.931855	-2.092191	-2.335397	H	-1.543037	-2.391020	-1.916262
C	-3.021547	-2.249897	-2.262800	C	-2.638390	-2.461746	-2.021444
C	-5.806928	-2.571139	-2.074110	C	-5.437758	-2.596008	-2.264805
H	-6.899621	-2.690860	-1.999058	H	-6.534416	-2.645801	-2.357812
H	-3.049042	0.641097	-2.250204	H	-2.536285	0.715164	-2.008402
C	1.458481	-3.033839	-1.642707	C	2.318109	0.298574	-1.792292
H	1.598588	-5.158434	-1.144572	H	4.018906	-1.062537	-1.931510
C	-3.348229	1.650677	-1.896439	C	-2.939594	1.706206	-1.704341
C	-4.886804	3.513956	-0.242703	C	-4.842564	3.470665	-0.347088
H	-5.141476	4.550145	0.071152	H	-5.194591	4.488969	-0.070981
C	-3.694669	-1.809846	-1.102162	C	-3.453876	-1.841086	-1.050058
C	-5.097536	-1.969541	-1.020432	C	-4.860391	-1.913976	-1.180288
H	-2.808754	3.922793	-0.575497	H	-2.756251	3.962688	-0.262096
H	-5.538186	2.845804	0.364422	H	-5.572190	2.765362	0.110894
C	-2.959982	1.809011	-0.402373	C	-2.849691	1.843885	-0.161283
C	-3.398623	3.241010	0.080625	C	-3.435061	3.244004	0.252929
P	0.697016	-2.479545	-0.037634	P	1.858906	-0.097893	-0.040282
H	-5.644335	-1.626150	-0.127279	H	-5.514701	-1.444321	-0.428045
H	-4.636489	0.569688	0.358167	H	-4.615445	0.556207	0.263175
Pt	-0.439003	-0.491765	-0.176836	Pt	-0.410403	-0.507147	0.170394
S	-1.068471	1.766688	-0.301703	S	-1.023235	1.840789	0.324819
P	-2.710660	-0.972844	0.225408	P	-2.651738	-0.948239	0.353858
C	-3.537893	0.688689	0.482162	C	-3.552267	0.677275	0.566440
H	-3.292475	5.784204	1.301865	H	-3.690648	5.753254	1.523953
H	-1.620928	5.218168	0.970229	H	-1.960590	5.271988	1.507437
H	-4.185432	-3.562741	0.899316	H	-4.092425	-3.577944	0.838551
C	-2.505176	5.066164	1.623154	C	-2.944577	5.061537	1.975236
C	-3.006171	3.610885	1.551663	C	-3.350028	3.588174	1.778928
H	-4.955861	4.090531	2.482199	H	-5.462487	3.953922	2.327698
H	-3.351116	0.923709	1.548645	H	-3.541678	0.859206	1.659284
H	-2.138885	2.960745	1.807427	H	-2.516765	2.969249	2.182560
C	-3.837227	-3.093907	1.831622	C	-3.792531	-3.153372	1.808758
C	-3.137145	-1.869603	1.791162	C	-3.121542	-1.913544	1.862386
C	-4.105276	3.387413	2.610690	C	-4.619166	3.284154	2.601182
H	-4.523322	2.359860	2.597970	H	-4.976395	2.240477	2.484197
H	-2.212078	5.342280	2.658654	H	-2.868744	5.319659	3.053295
H	-4.639185	-4.683737	3.075321	H	-4.601554	-4.824642	2.937675
H	-3.694583	3.560761	3.628137	H	-4.419924	3.441873	3.682560
C	-4.089358	-3.729157	3.061434	C	-4.077840	-3.856846	2.993550
C	-2.666402	-1.311852	3.004615	C	-2.724743	-1.398809	3.119290
H	-2.079683	-0.378403	2.988214	H	-2.164060	-0.450730	3.169724
C	-3.644206	-3.154500	4.262984	C	-3.698127	-3.331368	4.239505
C	-2.926439	-1.944758	4.230203	C	-3.019408	-2.099967	4.298833
H	-3.848140	-3.651657	5.224737	H	-3.923928	-3.883796	5.165495
H	-2.559808	-1.492358	5.165510	H	-2.707255	-1.686341	5.271056
H	1.033517	0.105930	-0.444273	H	-0.112753	-2.082523	0.118752

C	-0.182346	-4.006657	0.550769	C	3.029800	-1.460760	0.433890
C	-1.063236	-4.689626	-0.320031	C	2.669775	-2.802593	0.179762
C	-0.038180	-4.471704	1.876172	C	4.286663	-1.186872	1.018413
C	-1.763133	-5.825405	0.119165	C	3.554057	-3.848401	0.491301
H	-1.195138	-4.341829	-1.356297	H	1.677093	-3.019501	-0.246558
C	-0.747253	-5.603901	2.315272	C	5.165334	-2.237306	1.338720
H	0.639191	-3.951154	2.570288	H	4.580718	-0.147850	1.232414
C	-1.605214	-6.288065	1.438072	C	4.803498	-3.569146	1.073672
H	-2.435338	-6.352516	-0.576737	H	3.258307	-4.890096	0.288182
H	-0.621327	-5.954366	3.351984	H	6.138687	-2.009593	1.802082
H	-2.151948	-7.180870	1.781171	H	5.492097	-4.390803	1.328002
C	2.140225	-2.367225	1.131490	C	2.481004	1.356625	0.922291
C	3.221579	-3.274926	1.090388	C	3.465203	2.233873	0.416675
C	2.136445	-1.343632	2.103824	C	1.955607	1.574813	2.215345
C	4.277298	-3.161575	2.010766	C	3.923159	3.308505	1.199471
H	3.251369	-4.069478	0.328984	H	3.870198	2.082623	-0.596278
C	3.190709	-1.237379	3.028153	C	2.421991	2.645190	2.996223
H	1.302962	-0.620873	2.110989	H	1.162985	0.911267	2.596797
C	4.262835	-2.145028	2.983126	C	3.405719	3.513503	2.490519
H	5.119888	-3.869975	1.963678	H	4.686319	3.992068	0.794094
H	3.177193	-0.432048	3.779797	H	2.002781	2.809621	4.001546
H	5.093771	-2.056438	3.701280	H	3.763359	4.358410	3.100618

<i>cis</i> -10				<i>trans</i> -10			
H	3.546164	-4.002988	-5.015853	H	3.708213	-1.576834	-5.468436
H	3.003082	-1.588334	-4.572290	H	1.702767	-2.702766	-4.455409
C	2.990178	-3.717220	-4.108552	C	3.355698	-1.283002	-4.466704
H	2.796562	-5.764266	-3.387638	H	4.896213	0.233342	-4.195383
C	2.687617	-2.367184	-3.859814	C	2.233691	-1.913547	-3.899274
H	-3.999688	-2.216745	-4.192870	H	-3.340195	0.075164	-4.476038
C	2.570960	-4.702530	-3.197794	C	4.020716	-0.269903	-3.754537
H	-6.250816	-3.129940	-3.546330	H	-5.622084	-0.972345	-4.574272
C	-4.319648	-2.207138	-3.138668	C	-3.789978	-0.358056	-3.568465
C	-5.579164	-2.716312	-2.777017	C	-5.066526	-0.944629	-3.623148
C	1.971584	-2.001302	-2.707224	C	1.776602	-1.533734	-2.626399
C	1.856811	-4.340173	-2.042207	C	3.570319	0.110453	-2.477576
H	1.716312	-0.946038	-2.520451	H	0.885689	-2.006654	-2.182412
H	-2.465366	-1.290250	-2.424542	H	-2.064961	0.107033	-2.303051
C	-3.460291	-1.686689	-2.155049	C	-3.076615	-0.331038	-2.357485
C	-5.980455	-2.695723	-1.428840	C	-5.630996	-1.503529	-2.462118
H	-6.967690	-3.091163	-1.140361	H	-6.628829	-1.969170	-2.501621
C	1.554422	-2.982793	-1.781206	C	2.445780	-0.522316	-1.901460
H	1.522955	-5.125149	-1.345765	H	4.092055	0.911182	-1.930359
C	-4.969389	3.283165	0.026356	C	-4.835271	3.289344	1.615820
H	-5.259977	4.337390	0.226113	H	-5.142954	4.163345	2.230082
C	-3.855484	-1.661799	-0.797500	C	-3.641000	-0.883643	-1.185728
C	-5.128267	-2.166958	-0.443875	C	-4.925130	-1.471990	-1.247212
H	-3.196020	3.819057	-1.152709	H	-2.887679	4.142193	1.067138
C	-3.002246	1.748158	-0.508966	C	-2.821402	1.995277	0.724567
C	-3.460341	3.199767	-0.269177	C	-3.299222	3.219630	1.528843
P	0.647727	-2.465375	-0.235544	P	1.836513	-0.079364	-0.204839
H	-5.456570	-2.153942	0.606939	H	-5.372403	-1.918948	-0.345381
Pt	-0.494236	-0.487954	-0.410480	Pt	-0.446990	-0.325736	0.089335
S	-1.167145	1.730286	-0.817488	S	-0.961960	1.968370	0.674933
P	-2.686694	-0.870849	0.402672	P	-2.680076	-0.754017	0.389330
C	-3.402079	0.853917	0.678806	C	-3.421272	0.701765	1.318565
H	-3.407233	-3.689600	1.158669	H	-2.795259	-3.579642	-0.384671
H	-2.828784	1.229344	1.558451	H	-2.991314	0.597900	2.343020
C	-3.270243	-3.109547	2.083884	C	-3.057519	-3.530976	0.684308
C	-2.957056	-1.732541	2.018858	C	-3.125379	-2.276631	1.334591
H	-3.647324	-4.828538	3.352457	H	-3.256379	-5.684542	0.870652
C	-3.399375	-3.755671	3.325613	C	-3.313104	-4.715717	1.392078
C	-2.745706	-1.030041	3.229635	C	-3.437650	-2.238539	2.711368
H	-2.471066	0.036101	3.212117	H	-3.476244	-1.278324	3.247892
C	-3.207981	-3.044086	4.521846	C	-3.632540	-4.668267	2.761638
C	-2.874065	-1.679506	4.468524	C	-3.691163	-3.427969	3.418266
H	-3.311690	-3.552306	5.493725	H	-3.830625	-5.598879	3.316794
H	-2.711038	-1.112028	5.398724	H	-3.934681	-3.380477	4.491668
H	0.918635	0.061746	-0.949291	H	-0.191391	-1.877845	-0.248725
C	-0.282512	-4.020123	0.172743	C	2.793501	-1.189378	0.928416
C	-1.261486	-4.468851	-0.745245	C	4.055276	-1.721611	0.585662
C	-0.061577	-4.758941	1.353761	C	2.228825	-1.497177	2.186380
C	-1.986040	-5.645272	-0.495787	C	4.744424	-2.545668	1.493262
H	-1.453038	-3.896423	-1.667008	H	4.499638	-1.500696	-0.397606
C	-0.794414	-5.934456	1.604262	C	2.925120	-2.313581	3.093295
H	0.690900	-4.419496	2.081839	H	1.229692	-1.101192	2.435002
C	-1.751998	-6.384116	0.679979	C	4.182977	-2.840155	2.748257
H	-2.738093	-5.986574	-1.224862	H	5.725433	-2.962720	1.214434
H	-0.608688	-6.502823	2.529657	H	2.476113	-2.548218	4.071578
H	-2.317522	-7.309708	0.873504	H	4.724127	-3.488056	3.456419
C	1.984068	-2.395895	1.054250	C	2.569490	1.595658	0.084258
C	3.107705	-3.252032	1.043345	C	2.028707	2.689411	-0.631862
C	1.858703	-1.434957	2.081445	C	3.617911	1.821019	1.002550
C	4.081735	-3.154342	2.051893	C	2.547209	3.980850	-0.444715
H	3.233669	-3.991724	0.237351	H	1.186646	2.530264	-1.323199
C	2.832257	-1.343382	3.091321	C	4.126495	3.118646	1.191862
H	0.995920	-0.747169	2.061578	H	4.040551	0.980783	1.574361
C	3.944625	-2.202755	3.078825	C	3.596042	4.199045	0.466496
H	4.957771	-3.822316	2.030396	H	2.116701	4.825296	-1.005924
H	2.725332	-0.586839	3.884984	H	4.943222	3.282963	1.912937
H	4.712634	-2.125223	3.865117	H	3.995304	5.214916	0.616898
C	-5.356331	2.385289	1.212397	C	-5.423692	1.993244	2.196020
C	-4.910927	0.927213	0.982666	C	-4.959932	0.758109	1.398360
H	-5.542276	2.967493	-0.875895	H	-5.256811	3.459931	0.598379
H	-6.453393	2.419410	1.389219	H	-6.534498	2.036934	2.208124
H	-4.877406	2.774342	2.140315	H	-5.102930	1.886419	3.257925

H	-5.481278	0.503290	0.126694	H	-5.378362	0.808723	0.368627
H	-5.156035	0.303792	1.870019	H	-5.362310	-0.171475	1.856658
H	-2.882061	3.612789	0.588643	H	-2.861202	3.158825	2.551222
H	-3.509866	1.367527	-1.425724	H	-3.193598	2.099568	-0.321520

<i>cis-11-chair</i>				<i>trans-11-chair</i>			
H	2.766426	0.359968	-5.257056	H	2.920322	-0.352102	-5.253402
H	1.078892	1.906762	-4.219642	H	0.896590	0.996176	-4.618393
C	2.469400	0.227789	-4.204474	C	2.576211	-0.330274	-4.207010
C	1.524364	1.094564	-3.623575	C	1.443759	0.424821	-3.851696
H	3.760400	-1.498034	-3.891169	H	4.146116	-1.663440	-3.496481
C	3.026059	-0.811468	-3.440337	C	3.262836	-1.064168	-3.223641
H	3.663134	-0.443343	5.056154	H	-7.400073	1.706110	-1.650810
C	1.134767	0.920263	-2.286711	C	0.997261	0.443803	-2.520148
H	0.377360	1.582413	-1.836999	H	0.096140	1.011683	-2.237423
H	3.805286	-2.948626	5.248665	H	-6.228790	3.639320	-2.743439
C	2.646146	-0.984373	-2.096478	C	2.825675	-1.039432	-1.887850
C	2.821756	-1.074831	4.729470	C	-6.345857	1.919774	-1.412375
C	2.901055	-2.473450	4.836709	C	-5.689147	3.001223	-2.025539
C	1.697246	-0.118485	-1.513534	C	1.688406	-0.283423	-1.527497
H	3.085489	-1.802499	-1.504405	H	3.370064	-1.615587	-1.123654
H	1.618300	0.627059	4.140084	H	-6.180364	0.253492	-0.025350
H	-2.262966	4.297067	3.637705	H	-3.947190	-4.445898	0.048681
H	4.114385	0.445748	-0.042899	H	3.133697	1.769469	-0.950274
C	1.667247	-0.469300	4.207140	C	-5.660089	1.102516	-0.496194
H	5.546232	2.189965	1.031281	H	4.372830	3.690610	0.065070
H	-1.753011	4.356152	6.098403	H	-6.031378	-4.704738	1.427329
H	3.744328	-1.218953	1.702694	H	3.770780	-0.727541	1.533846
C	-1.868398	3.401573	4.143548	C	-4.363567	-3.580835	0.588731
C	1.825920	-3.264363	4.396014	C	-4.338700	3.260416	-1.727569
H	1.888415	-4.362264	4.448496	H	-3.817153	4.101834	-2.211058
H	-1.232088	0.232303	-0.837788	H	-1.353635	0.535643	-0.887783
C	-1.586629	3.432977	5.520438	C	-5.530242	-3.725888	1.361334
H	-1.898389	2.183449	2.328552	H	-2.789232	-2.216125	-0.069397
C	3.674371	1.140097	0.690936	C	2.985577	2.017258	0.112399
C	-1.654998	2.225242	3.403190	C	-3.718041	-2.336443	0.512808
C	4.475692	2.129380	1.284380	C	3.682967	3.096762	0.685844
C	0.570978	-1.255596	3.784928	C	-4.305178	1.358291	-0.196862
C	-1.097328	2.279596	6.161772	C	-6.051478	-2.620903	2.056872
C	0.672753	-2.662718	3.868007	C	-3.645846	2.437937	-0.824050
C	3.134046	-2.079732	1.393066	C	3.158685	-1.642594	1.575782
H	-0.882063	2.296634	7.242196	H	-6.960514	-2.731331	2.669297
H	4.549406	-3.528441	2.174263	H	4.691858	-2.804901	2.587612
P	1.205673	-0.239019	0.266528	P	1.126121	-0.159242	0.227132
C	-1.148868	1.070372	4.039073	C	-4.241008	-1.220612	1.202652
C	2.301800	1.048228	1.015800	C	2.098564	1.256483	0.901452
C	-0.881735	1.102474	5.426436	C	-5.411414	-1.371606	1.977934
Pt	-1.016407	-0.087259	0.718048	Pt	-1.118018	0.103852	0.633483
C	3.584289	-3.384151	1.663796	C	3.672309	-2.808205	2.170117
H	-0.146952	-3.303518	3.510220	H	-2.578024	2.613651	-0.610797
C	3.910763	3.049712	2.187678	C	3.503362	3.414082	2.043037
H	4.541184	3.827183	2.648014	H	4.052017	4.259254	2.488882
C	1.892924	-1.880825	0.758838	C	1.851358	-1.639531	1.045651
P	-0.927108	-0.473660	3.045992	P	-3.351508	0.379555	1.044552
H	-0.490727	0.205912	5.934160	H	-5.830095	-0.516883	2.532075
C	1.736045	1.994377	1.894491	C	1.913594	1.577834	2.266355
C	2.537678	2.987959	2.482303	C	2.620693	2.650178	2.831044
C	2.803462	-4.494969	1.304405	C	2.884457	-3.971011	2.240506
C	1.095517	-3.000288	0.422318	C	1.059732	-2.805411	1.125625
H	0.657993	1.952974	2.111320	H	1.210834	0.969294	2.865915
H	3.162247	-5.514572	1.517250	H	3.286645	-4.880990	2.713746
H	2.079995	3.716688	3.169945	H	2.478149	2.894571	3.895968
H	0.110103	-2.837394	-0.046089	H	0.025395	-2.785551	0.744650
C	-2.316566	-1.528634	3.687635	C	-3.720340	1.322468	2.601158
C	1.552974	-4.299814	0.689100	C	1.577720	-3.966923	1.719640
S	-3.377394	0.173692	0.714510	S	-0.834991	-0.670040	2.960769
H	-3.991149	-2.050467	1.531323	H	-1.199628	1.614824	3.784385
C	-4.132382	-1.015306	1.914389	C	-1.652818	0.621131	4.001859
H	0.927811	-5.165191	0.417245	H	0.950940	-4.869831	1.789930
H	-5.219334	-0.797510	1.841282	H	-1.375389	0.364899	5.046577
C	-3.710211	-0.948233	3.387522	C	-3.181785	0.706540	3.903129
H	-2.214369	-2.527966	3.211577	H	-3.271381	2.324694	2.423940
H	-2.159015	-1.657171	4.780094	H	-4.820171	1.476911	2.647732
H	-4.445413	-1.535266	3.985397	H	-3.557742	1.337237	4.742881
H	-3.777986	0.099658	3.755115	H	-3.615479	-0.306942	4.051030

<i>cis-11-skew-boat</i>				<i>trans-11-skew-boat</i>			
H	-6.937751	0.493194	-3.438483	H	-6.937751	0.493194	-3.438483
H	-6.111560	2.166806	-1.758195	H	-6.111560	2.166806	-1.758195
C	-5.932839	0.385148	-2.999940	C	-5.932839	0.385148	-2.999940
C	-5.469428	1.325109	-2.061878	C	-5.469428	1.325109	-2.061878
H	-5.483513	-1.445318	-4.093396	H	-5.483513	-1.445318	-4.093396
C	-5.118538	-0.701140	-3.367617	C	-5.118538	-0.701140	-3.367617
H	-0.152989	-1.397026	7.512682	H	-0.152989	-1.397026	7.512682
C	-4.193504	1.183725	-1.493380	C	-4.193504	1.183725	-1.493380
H	-3.837114	1.896899	-0.732433	H	-3.837114	1.896899	-0.732433
H	1.407855	-2.958164	6.318572	H	1.407855	-2.958164	6.318572
C	-3.839443	-0.846513	-2.803650	C	-3.839443	-0.846513	-2.803650
C	0.003898	-1.297871	6.426791	C	0.003898	-1.297871	6.426791
C	0.877974	-2.172509	5.756751	C	0.877974	-2.172509	5.756751
C	-3.370418	0.100022	-1.868349	C	-3.370418	0.100022	-1.868349
H	-3.205847	-1.703185	-3.083474	H	-3.205847	-1.703185	-3.083474
H	-1.365732	0.375690	6.246245	H	-1.365732	0.375690	6.246245
H	1.352148	4.429442	5.943833	H	1.352148	4.429442	5.943833
H	-1.970476	0.755404	-3.992453	H	-1.970476	0.755404	-3.992453
C	-0.677945	-0.298295	5.711491	C	-0.677945	-0.298295	5.711491
H	-0.423663	1.912372	-5.575728	H	-0.423663	1.912372	-5.575728
H	1.162885	6.205360	4.179324	H	1.162885	6.205360	4.179324
H	0.251741	-1.447597	-2.921506	H	0.251741	-1.447597	-2.921506
C	0.796922	4.227470	5.013915	C	0.796922	4.227470	5.013915
C	1.066884	-2.048894	4.368322	C	1.066884	-2.048894	4.368322
H	1.743289	-2.738171	3.838565	H	1.743289	-2.738171	3.838565
H	-0.122361	1.130624	0.900991	H	-0.122361	1.130624	0.900991
C	0.692285	5.221334	4.024325	C	0.692285	5.221334	4.024325
H	0.295443	2.194789	5.595416	H	0.295443	2.194789	5.595416
C	-0.988215	1.105577	-3.638910	C	-0.988215	1.105577	-3.638910
C	0.198822	2.970317	4.819326	C	0.198822	2.970317	4.819326
C	-0.115908	1.755161	-4.529636	C	-0.115908	1.755161	-4.529636
C	-0.487616	-0.166293	4.317275	C	-0.487616	-0.166293	4.317275
C	-0.005028	4.952823	2.832571	C	-0.005028	4.952823	2.832571
C	0.385381	-1.053440	3.648631	C	0.385381	-1.053440	3.648631
C	-0.247765	-2.189483	-2.278967	C	-0.247765	-2.189483	-2.278967
H	-0.081493	5.724552	2.050158	H	-0.081493	5.724552	2.050158
H	0.837888	-3.871294	-3.127865	H	0.837888	-3.871294	-3.127865
P	-1.695617	-0.009214	-1.113340	P	-1.695617	-0.009214	-1.113340
C	-0.502161	2.698091	3.625243	C	-0.502161	2.698091	3.625243
C	-0.608760	0.906284	-2.292928	C	-0.608760	0.906284	-2.292928
C	-0.594251	3.693939	2.627917	C	-0.594251	3.693939	2.627917
Pt	-1.604763	0.555840	1.107549	Pt	-1.604763	0.555840	1.107549
C	0.079589	-3.553241	-2.394530	C	0.079589	-3.553241	-2.394530
H	0.505138	-0.962164	2.556034	H	0.505138	-0.962164	2.556034
C	1.141490	2.203641	-4.088318	C	1.141490	2.203641	-4.088318
H	1.822838	2.713599	-4.788005	H	1.822838	2.713599	-4.788005
C	-1.213768	-1.776569	-1.338444	C	-1.213768	-1.776569	-1.338444
P	-1.369479	1.101082	3.320124	P	-1.369479	1.101082	3.320124
H	-1.115973	3.461652	1.684203	H	-1.115973	3.461652	1.684203
C	0.650854	1.366168	-1.853047	C	0.650854	1.366168	-1.853047
C	1.523114	2.005993	-2.748741	C	1.523114	2.005993	-2.748741
C	-0.558543	-4.504675	-1.580427	C	-0.558543	-4.504675	-1.580427
C	-1.852822	-2.732476	-0.514746	C	-1.852822	-2.732476	-0.514746
H	0.930739	1.228035	-0.796011	H	0.930739	1.228035	-0.796011
H	2.504112	2.360675	-2.394463	H	2.504112	2.360675	-2.394463
H	-2.604495	-2.391745	0.221196	H	-2.604495	-2.391745	0.221196
C	-3.005831	1.359425	4.158667	C	-3.005831	1.359425	4.158667
C	-1.526558	-4.091262	-0.644832	C	-1.526558	-4.091262	-0.644832
S	-3.861449	-0.340137	1.479870	S	-3.861449	-0.340137	1.479870
H	-2.794706	-1.538608	3.322758	H	-2.794706	-1.538608	3.322758
C	-3.745541	-0.973556	3.215065	C	-3.745541	-0.973556	3.215065
H	-2.029272	-4.834092	-0.004869	H	-2.029272	-4.834092	-0.004869
H	-4.564708	-1.712426	3.341941	H	-4.564708	-1.712426	3.341941
H	-0.300240	-5.571806	-1.673541	H	-0.300240	-5.571806	-1.673541
C	-3.863898	0.087057	4.327055	C	-3.863898	0.087057	4.327055
H	-4.923599	0.411953	4.415266	H	-4.923599	0.411953	4.415266
H	-3.603442	-0.404963	5.291733	H	-3.603442	-0.404963	5.291733
H	-2.850963	1.879616	5.127582	H	-2.850963	1.879616	5.127582
H	-3.504379	2.078350	3.475044	H	-3.504379	2.078350	3.475044

cis-11-boat				trans-11-boat			
H	3.111409	0.416579	-5.006209	H	2.970566	-0.090967	-5.263105
H	1.242436	1.875544	-4.171278	H	0.902948	1.172051	-4.595031
C	2.700765	0.264312	-3.995367	C	2.615352	-0.123153	-4.220695
C	1.653935	1.081654	-3.527978	C	1.458286	0.584297	-3.846854
H	4.029289	-1.398036	-3.532871	H	4.215525	-1.440502	-3.549078
C	3.214539	-0.750514	-3.171234	C	3.312554	-0.878667	-3.261473
H	2.637308	-0.043366	5.440111	H	-7.128195	1.310188	-2.202437
C	1.120895	0.881339	-2.245742	C	0.997787	0.534743	-2.521001
H	0.286680	1.505642	-1.887087	H	0.078843	1.065692	-2.224158
H	3.181397	-2.495618	5.595106	H	-6.096102	3.444818	-3.027534
C	2.690319	-0.948693	-1.880102	C	2.860659	-0.923410	-1.931090
C	1.970197	-0.791098	4.982750	C	-6.166659	1.655110	-1.789821
C	2.273913	-2.159963	5.068844	C	-5.588180	2.848291	-2.253117
C	1.638731	-0.133817	-1.411817	C	1.698718	-0.215096	-1.552597
H	3.100032	-1.745811	-1.240494	H	3.412964	-1.515633	-1.184904
H	0.577743	0.710063	4.277127	H	-5.981718	-0.046621	-0.449595
H	-3.328040	3.921821	3.140758	H	-3.981587	-4.541117	1.113923
H	3.764971	0.724723	0.262427	H	3.170737	1.777639	-0.833663
C	0.808529	-0.363917	4.318570	C	-5.522160	0.890373	-0.799422
H	4.884664	2.614577	1.454734	H	4.343626	3.686100	0.280109
H	-3.354769	3.924467	5.654392	H	-6.277534	-4.441270	2.126647
H	3.412287	-0.966779	1.994832	H	3.738082	-0.684060	1.593832
C	-2.985905	3.036313	3.699633	C	-4.443716	-3.567519	1.341079
C	1.421263	-3.098261	4.462078	C	-4.350124	3.272677	-1.733568
H	1.663635	-4.171356	4.496219	H	-3.883614	4.199941	-2.102639
H	-1.346093	0.047026	-1.113436	H	-1.328122	0.610218	-0.864345
C	-3.004584	3.035970	5.105003	C	-5.727920	-3.511436	1.909522
H	-2.536719	1.892424	1.891747	H	-2.720481	-2.415378	0.647301
C	3.183276	1.361149	0.948700	C	2.962318	2.007992	0.222846
C	-2.534129	1.905962	2.995187	C	-3.737158	-2.383466	1.069006
C	3.809146	2.431726	1.608356	C	3.622470	3.080058	0.851580
C	-0.064613	-1.300991	3.720953	C	-4.286511	1.316111	-0.271226
C	-2.578296	1.894616	5.810155	C	-6.310474	-2.265189	2.205553
C	0.269814	-2.672466	3.782210	C	-3.697349	2.506198	-0.756579
C	2.928106	-1.892963	1.652369	C	3.180604	-1.633148	1.550023
H	-2.594445	1.886492	6.911788	H	-7.315999	-2.215727	2.652799
H	4.415439	-3.170171	2.585706	H	4.733808	-2.768599	2.561461
P	0.941394	-0.286315	0.296805	P	1.119929	-0.185755	0.200211
C	-2.099081	0.761483	3.697538	C	-4.315047	-1.129976	1.364969
C	1.805353	1.113238	1.144239	C	2.034338	1.232562	0.947933
C	-2.130918	0.762139	5.111038	C	-5.607012	-1.079512	1.936390
Pt	-1.324116	-0.291824	0.456008	Pt	-1.131951	0.009839	0.602766
C	3.489872	-3.137175	1.989604	C	3.736695	-2.803565	2.094264
H	-0.358922	-3.423901	3.280682	H	-2.706600	2.812768	-0.380709
C	3.062378	3.277630	2.450078	C	3.365375	3.374914	2.201419
H	3.554836	4.119922	2.961789	H	3.884445	4.214652	2.690838
C	1.735252	-1.838168	0.906206	C	1.901033	-1.670857	0.956893
P	-1.535417	-0.733740	2.758272	P	-3.341952	0.394374	1.016138
H	-1.789695	-0.124336	5.670507	H	-6.075039	-0.109975	2.172491
C	1.057646	1.984006	1.962438	C	1.770823	1.531723	2.304887
C	1.683912	3.058625	2.616708	C	2.442283	2.596138	2.925812
C	2.868410	-4.330582	1.585779	C	3.019439	-4.012625	2.050479
C	1.095568	-3.041024	0.525831	C	1.179469	-2.883698	0.923077
H	-0.025006	1.821644	2.074250	H	1.036533	0.916515	2.857380
H	3.314606	-5.302602	1.849933	H	3.454900	-4.927264	2.483633
H	1.085089	3.728584	3.253984	H	2.238604	2.823288	3.984656
H	0.143930	-2.989549	-0.030109	H	0.165919	-2.898490	0.491089
C	-2.854803	-1.994094	3.183142	C	-3.553664	1.462973	2.534570
C	1.664142	-4.280131	0.859045	C	1.740844	-4.050411	1.465719
S	-3.653689	-0.136125	0.112272	S	-0.869683	-0.996191	2.828861
H	-5.573396	-0.971467	1.232710	H	-1.784355	-0.369425	4.947217
C	-4.534072	-0.816404	1.590214	C	-2.178715	-0.262992	3.915311
H	1.162698	-5.211703	0.551838	H	1.169559	-4.991821	1.444859
H	-4.586839	-0.057496	2.404227	H	-3.107681	-0.876018	3.865610
C	-3.964390	-2.143742	2.127803	C	-2.504440	1.217993	3.636602
H	-2.347799	-2.966558	3.343943	H	-3.507307	2.510194	2.170602
H	-3.275230	-1.685152	4.164307	H	-4.584978	1.300333	2.914597
H	-3.590230	-2.737078	1.265584	H	-1.560410	1.741528	3.372293
H	-4.782159	-2.737819	2.595022	H	-2.886731	1.694908	4.567539

TS[<i>trans</i> -11-boat→skew-boat]				TS[<i>trans</i> -11-skew-boat→chair]			
H	2.939806	-3.924181	-3.946096	H	2.012440	-1.170980	-5.531297
H	0.462798	-3.754945	-3.561328	H	-0.166145	-1.830115	-4.465301
C	2.548329	-3.295264	-3.130537	C	1.833322	-0.962881	-4.464319
C	1.162379	-3.200090	-2.916146	C	0.613852	-1.331675	-3.867882
H	4.523753	-2.667677	-2.455197	H	3.774950	-0.023056	-4.158498
C	3.436348	-2.591594	-2.295685	C	2.820380	-0.320651	-3.695937
H	-6.311180	3.846231	-0.378262	H	-4.360386	2.697283	-2.952915
C	0.660993	-2.402103	-1.872858	C	0.380021	-1.055930	-2.510549
H	-0.423178	-2.324007	-1.689895	H	-0.581405	-1.318801	-2.040074
H	-4.331686	5.189259	-1.139192	H	-6.035505	4.310980	-2.000750
C	2.940221	-1.794230	-1.251814	C	2.595045	-0.053272	-2.334422
C	-5.300211	3.410107	-0.338919	C	-4.573699	2.699414	-1.872188
C	-4.189255	4.161997	-0.767076	C	-5.510209	3.604008	-1.339028
C	1.546457	-1.690181	-1.038349	C	1.371068	-0.419955	-1.732577
H	3.640118	-1.252971	-0.595651	H	3.374165	0.448111	-1.739523
H	-5.999879	1.517254	0.465834	H	-3.141252	1.112317	-1.435421
H	-6.174104	-1.423502	-3.291359	H	-3.936918	-4.357486	1.469868
H	1.752607	0.582253	-2.344317	H	3.933028	-0.146741	0.963561
C	-5.123290	2.101725	0.140675	C	-3.895904	1.804679	-1.029208
H	1.840883	2.953430	-3.138738	H	5.482769	1.732885	1.547514
H	-6.518089	-3.795282	-2.541790	H	-6.444973	-4.224803	1.474070
H	3.380602	0.893491	1.111638	H	1.330114	-0.878427	2.836849
C	-5.780699	-1.758265	-2.318196	C	-4.438964	-3.377269	1.443608
C	-2.901640	3.600158	-0.718649	C	-5.766612	3.609814	0.042686
H	-2.022482	4.177095	-1.047223	H	-6.492442	4.321183	0.467894
H	-1.626102	-1.149610	-0.675156	H	-1.668423	-0.393976	-0.605546
C	-5.972782	-3.085816	-1.899375	C	-5.843222	-3.302331	1.445995
H	-4.933511	0.187921	-1.839714	H	-2.567336	-2.245285	1.374800
C	1.511513	1.402909	-1.650697	C	3.577440	0.895089	0.920074
C	-5.085265	-0.848605	-1.500818	C	-3.669784	-2.201400	1.397917
C	1.559287	2.737407	-2.095755	C	4.444381	1.950978	1.250880
C	-3.829751	1.532814	0.190792	C	-4.158435	1.796483	0.359774
C	-5.458504	-3.508154	-0.658905	C	-6.480659	-2.048245	1.404751
C	-2.721510	2.289359	-0.245545	C	-5.095917	2.710081	0.890456
C	3.228925	0.054416	1.809137	C	1.724730	-1.743356	2.271305
H	-5.594748	-4.550448	-0.329216	H	-7.580715	-1.987591	1.397787
H	5.007963	0.505161	2.974054	H	2.198681	-2.928525	4.025866
P	0.889130	-0.602734	0.299162	P	1.063382	-0.157595	0.069758
C	-4.578560	-1.265110	-0.253042	C	-4.306467	-0.941864	1.365396
C	1.141535	1.118587	-0.321017	C	2.244919	1.169123	0.546954
C	-4.759223	-2.605571	0.157192	C	-5.716149	-0.870171	1.367686
Pt	-1.340271	-0.675688	0.831601	Pt	-1.091709	0.227281	0.758251
C	4.139745	-0.162920	2.857252	C	2.207473	-2.887244	2.924834
H	-1.715715	1.840580	-0.200616	H	-5.307172	2.733633	1.970208
C	1.247664	3.788808	-1.216831	C	3.985439	3.279717	1.212372
H	1.283840	4.832021	-1.569599	H	4.664953	4.104929	1.478965
C	2.112433	-0.795368	1.658339	C	1.740252	-1.682609	0.858321
P	-3.563225	-0.175430	0.832132	P	-3.259098	0.574188	1.401881
H	-4.331740	-2.949835	1.113790	H	-6.218426	0.110427	1.325965
C	0.825036	2.177267	0.563946	C	1.784259	2.502973	0.516609
C	0.886838	3.505126	0.115287	C	2.654798	3.553542	0.846665
C	3.939762	-1.225462	3.756834	C	2.695449	-3.978923	2.180522
C	1.906268	-1.852493	2.571378	C	2.234319	-2.772040	0.112108
H	0.497746	1.943742	1.592807	H	0.731663	2.707064	0.258996
H	4.652612	-1.390883	4.580456	H	3.067583	-4.878152	2.697239
H	0.635926	4.324199	0.807967	H	2.287178	4.591632	0.831816
H	1.010391	-2.485930	2.474493	H	2.250973	-2.728227	-0.988085
C	-4.484950	-0.210014	2.467687	C	-3.447724	1.166106	3.145144
H	-4.909388	0.805855	2.616783	C	2.707104	-3.919097	0.776551
C	2.822858	-2.067907	3.612827	S	-0.295105	1.168610	2.886914
S	-0.858928	-0.076137	3.126757	H	-0.797974	0.403500	5.094860
H	-2.739130	1.388198	3.743377	C	-1.213581	0.118196	4.106087
H	-5.341528	-0.903987	2.341229	H	3.089428	-4.769420	0.189438
C	-2.448730	0.337121	3.970218	H	-0.915021	-0.937027	3.934776
H	2.653868	-2.889656	4.326400	C	-2.773486	0.219314	4.154201
H	-2.204310	0.303342	5.052567	H	-2.987056	2.175928	3.179590
C	-3.633318	-0.606024	3.684062	H	-4.531255	1.250519	3.373848
H	-3.250312	-1.644075	3.568604	H	-3.081256	0.555953	5.167582
H	-4.313814	-0.613830	4.565957	H	-3.210738	-0.796412	4.032703

B3LYP-D3/SVP(PCM):

<i>cis-5</i>				<i>trans-5</i>			
H	-4.731357	3.154958	-4.587317	H	-8.224044	-2.669800	2.462386
H	-3.133590	1.238465	-4.470120	H	-6.727319	-2.639074	0.462633
C	-4.636514	2.575311	-3.665820	C	-7.195936	-2.309871	2.551379
C	-3.740314	1.501487	-3.600001	C	-6.357369	-2.291973	1.430688
H	-6.109988	3.738369	-2.590510	H	-7.360274	-1.869316	4.663481
C	-5.408187	2.901699	-2.547745	C	-6.712802	-1.861607	3.783069
H	-6.155127	-3.559345	-2.442950	H	-2.189996	-5.749288	3.556523
C	-3.617390	0.761621	-2.421766	C	-5.047191	-1.821585	1.541341
H	-5.733323	-1.187636	-1.893436	H	-3.538711	-3.683070	3.393449
H	-2.913443	-0.074432	-2.384505	H	-4.406570	-1.793501	0.657441
C	-5.501708	-3.308662	-1.603498	C	-1.692998	-4.794860	3.365245
C	-5.291820	2.157856	-1.367038	C	-5.396110	-1.400161	3.898603
C	-5.264334	-1.966884	-1.289182	C	-2.455690	-3.625222	3.271727
H	-5.090129	-5.372321	-1.097803	H	0.289257	-5.658383	3.285375
C	-4.398082	1.077435	-1.292578	C	-4.549978	-1.372735	2.777793
C	-4.905141	-4.324170	-0.849540	C	-0.304420	-4.743420	3.214200
H	-5.905420	2.423297	-0.504093	H	-5.034358	-1.060326	4.870275
H	-0.930100	1.538177	-1.048926	H	-0.870422	1.057589	-1.059716
H	-2.061709	2.637956	-0.647006	H	-2.063026	2.155746	-0.897770
C	-4.424075	-1.623986	-0.214329	C	-1.833676	-2.390679	3.020956
N	-1.312097	2.063546	-0.257611	N	-1.284575	1.721419	-0.398481
C	-4.065701	-3.992551	0.218656	C	0.321720	-3.516150	2.968643
P	-4.114737	0.133778	0.272312	P	-2.788922	-0.811034	2.897181
C	-3.822346	-2.652067	0.532179	C	-0.435658	-2.346310	2.867281
H	-3.590194	-4.780139	0.808499	H	1.407162	-3.468403	2.849037
C	-0.255347	2.925210	0.327534	C	-0.278040	2.749905	-0.020078
H	1.344475	1.470468	0.345981	H	1.365500	1.406342	0.385489
H	-7.028901	-0.635600	0.293475	H	-1.954216	-1.834620	5.603568
C	-5.557564	0.572933	1.341558	C	-2.683622	-0.064808	4.582015
Pt	-2.075438	0.577916	1.223363	Pt	-2.023772	0.541181	1.251706
C	-6.847958	0.064468	1.111446	C	-2.257141	-0.790740	5.705485
H	-3.153647	-2.398168	1.357023	H	0.054793	-1.389032	2.668361
H	-0.744325	3.619667	1.027336	H	-0.816375	3.568217	0.480932
C	0.772266	2.082605	1.063933	C	0.758291	2.157838	0.919397
H	-4.347814	1.839738	2.604568	H	-3.375704	1.859757	3.866294
C	-5.354688	1.459940	2.412000	C	-3.062755	1.280355	4.738753
H	1.491152	2.740174	1.576397	H	1.445025	2.953095	1.248433
C	-7.913150	0.443571	1.932929	C	-2.214180	-0.181742	6.964742
H	-8.910923	0.038750	1.745824	H	-1.874953	-0.755388	7.830929
H	-2.468171	-0.453186	2.338980	H	-3.278938	0.117006	0.369029
S	-0.017396	0.982123	2.326762	S	-0.030866	1.400869	2.407053
C	-6.422941	1.840949	3.230762	C	-3.027781	1.882748	5.998472
C	-7.703565	1.333549	2.992529	C	-2.601461	1.153015	7.114117
H	-6.250165	2.530419	4.060890	H	-3.325105	2.928699	6.107409
H	-8.538040	1.626020	3.634940	H	-2.566184	1.627052	8.098282
H	0.232930	3.524039	-0.462632	H	0.197956	3.157393	-0.929950

<i>cis-6</i>				<i>trans-6</i>			
H	-4.709492	3.375213	-4.385626	H	-8.214689	-2.718830	2.242269
H	-3.014465	1.544064	-4.273883	H	-6.682710	-2.437000	0.289398
C	-4.628407	2.756930	-3.488272	C	-7.198416	-2.345320	2.391005
C	-3.677904	1.730638	-3.425820	C	-6.340236	-2.186655	1.296595
H	-6.215581	3.786087	-2.438707	H	-7.413586	-2.137950	4.534076
C	-5.471105	2.987043	-2.398008	C	-6.750398	-2.019910	3.673490
H	-6.023892	-3.444493	-2.612322	H	-2.062660	-5.730944	3.042401
C	-3.571880	0.942089	-2.278235	C	-5.045667	-1.698043	1.484434
H	-5.677414	-1.094836	-1.930222	H	-3.492497	-3.712753	3.087995
H	-2.824351	0.144558	-2.242965	H	-4.390258	-1.559237	0.622136
C	-5.406500	-3.222544	-1.738251	C	-1.600759	-4.741670	2.992791
C	-5.371315	2.194370	-1.247853	C	-5.449199	-1.540625	3.865619
C	-5.211616	-1.893522	-1.349346	C	-2.409294	-3.599507	3.017388
H	-4.964462	-5.299698	-1.321485	H	0.418074	-5.511682	2.884301
C	-4.422940	1.161555	-1.177341	C	-4.583827	-1.371970	2.772113
H	2.490894	5.131802	-1.360364	H	2.524555	4.877649	-1.750355
O	0.225982	3.695464	-1.618899	O	0.342100	3.296542	-1.795371
C	-4.813211	-4.261715	-1.014619	C	-0.211359	-4.618382	2.905172
H	-6.040359	2.384334	-0.406489	H	-5.115028	-1.297477	4.875378
H	-1.096152	1.820970	-0.841457	H	-0.953373	1.626440	-0.727365
H	-2.212012	2.839753	-0.252568	H	-2.170095	2.648166	-0.392447
C	1.773858	5.719660	-0.769378	C	1.742852	5.548618	-1.366045
C	-4.417744	-1.587578	-0.229080	C	-1.831802	-2.321013	2.949352
C	0.313102	3.894878	-0.427980	C	0.333664	3.779965	-0.685041
H	2.302850	6.438926	-0.134000	H	2.194069	6.427210	-0.891390
N	-1.444068	2.228668	0.032508	N	-1.376461	2.166684	0.035653
C	-4.019928	-3.966550	0.098593	C	0.370403	-3.346902	2.841563
P	-4.166620	0.150998	0.349095	P	-2.844749	-0.775076	2.988758
O	1.038652	4.868370	0.121926	O	0.976974	4.894753	-0.342962
C	-3.819047	-2.638782	0.487015	C	-0.432328	-2.203599	2.858494
H	-3.546939	-4.772421	0.665285	H	1.456313	-3.243452	2.772625
C	-0.364479	3.033298	0.637247	C	-0.383944	3.157540	0.511397
H	1.209566	1.545618	0.560217	H	1.242231	1.782531	0.906763
H	-7.044903	-0.742081	0.302625	H	-2.052300	-2.090750	5.575793
C	-5.645504	0.509001	1.397782	C	-2.784901	-0.223114	4.748400
Pt	-2.163146	0.594505	1.374127	Pt	-2.098396	0.776686	1.523160
C	-6.908555	-0.049924	1.135818	C	-2.372704	-1.069410	5.790338
H	-3.185162	-2.413308	1.346699	H	0.023001	-1.210710	2.802516
H	-0.808543	3.695877	1.395147	H	-0.919398	3.949240	1.055924
C	0.664537	2.125865	1.323792	C	0.619210	2.499560	1.468190
H	-4.513963	1.805169	2.705252	H	-3.493123	1.760952	4.243643
C	-5.499348	1.385016	2.486726	C	-3.187889	1.089706	5.050092
H	1.399115	2.747909	1.854616	H	1.288004	3.274621	1.869159
C	-8.003042	0.268369	1.944749	C	-2.366858	-0.609844	7.111917
H	-8.978949	-0.175692	1.733055	H	-2.038962	-1.275724	7.914074
H	-2.535884	-0.537809	2.391114	H	-3.267501	0.347596	0.532801
S	-0.132540	0.983152	2.533906	S	-0.236600	1.657926	2.863017
C	-6.596985	1.705432	3.292156	C	-3.189260	1.542782	6.371523
C	-7.850276	1.147546	3.022674	C	-2.776852	0.694146	7.405008
H	-6.468536	2.386948	4.136745	H	-3.504814	2.565253	6.593395
H	-8.707307	1.392344	3.655219	H	-2.770442	1.051476	8.437864
H	1.089760	6.244063	-1.452092	H	1.091347	5.855497	-2.196924

<i>cis-7</i>				<i>trans-7</i>			
H	-4.720908	3.542505	-4.234521	H	-8.194197	-2.671597	2.127901
H	-3.001026	1.732459	-4.167012	H	-6.601597	-2.375272	0.226199
C	-4.640936	2.894303	-3.358428	C	-7.180574	-2.306979	2.312479
C	-3.676506	1.879887	-3.320750	C	-6.288254	-2.140190	1.246487
H	-6.254829	3.863319	-2.292372	H	-7.459906	-2.126160	4.450276
C	-5.499200	3.074053	-2.270803	C	-6.769879	-2.001551	3.611999
H	-5.957961	-3.354487	-2.713592	H	-2.084170	-5.729959	3.029816
C	-3.571934	1.053147	-2.200177	C	-4.997100	-1.663422	1.480157
H	-5.661202	-1.026030	-1.941590	H	-3.493020	-3.701540	3.161760
H	-2.813730	0.265096	-2.184042	H	-4.314988	-1.518562	0.639560
C	-5.350231	-3.153800	-1.827690	C	-1.618009	-4.744027	2.958355
C	-5.400779	2.243078	-1.147938	C	-5.471372	-1.534523	3.850258
C	-5.183323	-1.836890	-1.388004	C	-2.414389	-3.596037	3.032315
H	-4.870418	-5.236305	-1.486230	H	0.385647	-5.528911	2.733071
C	-4.438129	1.222116	-1.102272	C	-4.572813	-1.358061	2.785946
H	2.137077	5.256046	-1.350987	H	2.122563	5.142620	-1.694377
O	0.206145	3.778255	-1.429161	O	0.225449	3.625904	-1.517608
C	-4.741270	-4.207931	-1.139497	C	-0.234512	-4.630888	2.792995
H	-6.081928	2.393854	-0.308371	H	-5.165931	-1.307517	4.872840
H	-1.100789	1.871342	-0.714729	H	-1.049953	1.897596	-0.534232
H	-2.234392	2.870243	-0.126410	H	-2.223854	2.908584	-0.049433
H	1.560597	7.714336	-1.465796	H	1.478568	7.515398	-2.276688
H	0.094235	6.704583	-1.544307	H	0.042338	6.464914	-2.178811
C	1.763611	5.811787	-0.479373	C	1.718947	5.840314	-0.947153
C	-4.402196	-1.558248	-0.251719	C	-1.831552	-2.320784	2.938347
C	0.283605	3.950957	-0.232721	C	0.285804	4.017046	-0.372261
H	2.614755	6.112789	0.146476	H	2.550471	6.279549	-0.379464
N	-1.467593	2.258747	0.160715	N	-1.421880	2.375908	0.294025
C	0.931665	7.009794	-0.899112	C	0.860289	6.911553	-1.593929
C	-3.960852	-3.939837	-0.010476	C	0.352329	-3.363935	2.701570
P	-4.185075	0.162038	0.390971	P	-2.836814	-0.773134	3.053075
O	1.001919	4.906431	0.356608	O	0.970115	5.083746	0.036330
C	-3.788069	-2.624006	0.428878	C	-0.438941	-2.213995	2.769321
H	-3.475957	-4.757332	0.528840	H	1.433353	-3.268338	2.571487
C	-0.404795	3.058371	0.801046	C	-0.383128	3.301679	0.801447
H	1.181346	1.584197	0.718899	H	1.233698	1.872402	0.973824
H	-7.042604	-0.791757	0.292487	H	-2.072243	-2.219444	5.581080
H	0.529480	7.537881	-0.020853	H	0.429503	7.583147	-0.835445
C	-5.682237	0.462455	1.432046	C	-2.794520	-0.312354	4.839187
Pt	-2.200575	0.595008	1.457017	Pt	-2.099963	0.873273	1.686596
C	-6.929970	-0.117152	1.143365	C	-2.393970	-1.209438	5.842215
H	-3.164382	-2.418647	1.301006	H	0.020957	-1.224563	2.694478
H	-0.867104	3.700769	1.565480	H	-0.870296	4.049910	1.443994
C	0.618796	2.143586	1.485343	C	0.655986	2.540542	1.635228
H	-4.593245	1.751492	2.782811	H	-3.493855	1.695935	4.425175
C	-5.566586	1.315114	2.543111	C	-3.198367	0.985155	5.201081
H	1.339248	2.758895	2.042521	H	1.360514	3.263937	2.069904
C	-8.039404	0.157509	1.948028	C	-2.401300	-0.815316	7.184877
H	-9.002977	-0.302729	1.715406	H	-2.082312	-1.520331	7.956592
H	-2.584241	-0.560385	2.444141	H	-3.334676	0.570319	0.731480
S	-0.190229	0.968388	2.656101	S	-0.136687	1.579529	2.989694
C	-6.679180	1.592135	3.344006	C	-3.213207	1.372641	6.543062
C	-7.917092	1.013586	3.048087	C	-2.812915	0.473218	7.537721
H	-6.574371	2.255784	4.205912	H	-3.529870	2.383493	6.811722
H	-8.785610	1.224175	3.677269	H	-2.817076	0.779150	8.586961

<i>cis</i> -8				<i>trans</i> -8			
H	-6.392651	-1.598262	-4.536490	H	2.406349	-2.175860	-5.274568
H	-5.826862	0.593480	-3.478655	H	0.576654	-0.501410	-4.976539
C	-5.428396	-1.460370	-4.041004	C	2.154662	-1.809497	-4.276118
C	-5.111653	-0.232051	-3.448605	C	1.128860	-0.871619	-4.109087
H	-4.744201	-3.470529	-4.455623	H	3.652093	-3.012217	-3.279823
C	-4.505944	-2.508417	-3.995129	C	2.851622	-2.277878	-3.159743
H	-7.386691	2.943419	-0.730690	H	-7.344953	3.169558	0.195671
C	-3.881945	-0.056771	-2.811119	C	0.799015	-0.412137	-2.832388
H	-3.651351	0.905942	-2.349088	H	-0.016104	0.304419	-2.710142
H	-5.933994	4.957601	-0.981012	H	-5.907380	5.076283	-0.529747
C	-3.268826	-2.332980	-3.363187	C	2.530835	-1.809387	-1.879934
C	-6.329600	2.895155	-0.456966	C	-6.260678	3.046673	0.135030
C	-5.516011	4.023052	-0.598532	C	-5.453833	4.115802	-0.272225
C	-2.944973	-1.105268	-2.764271	C	1.499616	-0.872726	-1.703212
H	-2.558411	-3.160929	-3.341443	H	3.090386	-2.181102	-1.020062
H	-6.450072	0.827027	0.128346	H	-6.327656	0.989762	0.770700
H	-5.298322	-4.346912	-0.465933	H	-5.157590	-2.733286	-2.900084
H	-1.637739	-0.037531	-4.765511	H	3.176825	1.114714	-1.719904
C	-5.798489	1.696741	0.033430	C	-5.683740	1.817262	0.462217
H	-0.489305	1.629221	-6.179837	H	4.276672	3.325598	-1.582133
H	-7.412519	-4.243135	0.858478	H	-6.893121	-3.921496	-1.553521
H	0.288878	-1.865781	-4.189719	H	3.763298	0.027802	1.268921
C	-5.522565	-3.468559	0.144145	C	-5.280786	-2.504335	-1.838648
C	-4.161242	3.945987	-0.257641	C	-4.068433	3.950292	-0.352846
H	-3.514080	4.818798	-0.374916	H	-3.433649	4.780087	-0.673528
H	0.234240	-0.349700	0.145402	H	-1.519193	-0.309149	-1.090017
C	-6.704999	-3.410606	0.886213	C	-6.252777	-3.170798	-1.083729
H	-3.689938	-2.460040	-0.388587	H	-3.687205	-1.049104	-1.828024
C	-0.862641	0.591751	-4.324212	C	2.889470	1.806429	-0.926049
C	-4.616491	-2.403392	0.183036	C	-4.456455	-1.551263	-1.236937
C	-0.214926	1.536818	-5.125960	C	3.512743	3.056778	-0.848182
C	-4.441693	1.611476	0.386530	C	-4.289993	1.643315	0.386395
C	-6.976798	-2.285155	1.672320	C	-6.397397	-2.876384	0.274426
C	-3.625778	2.747649	0.222117	C	-3.487754	2.719301	-0.027464
C	0.293641	-2.610793	-3.391892	C	3.298857	-0.906602	1.590093
H	-7.895558	-2.236289	2.262100	H	-7.151769	-3.394374	0.871794
H	1.518100	-3.984080	-4.521253	H	4.985350	-1.472693	2.814775
P	-1.343517	-0.811267	-1.885612	P	1.057621	-0.198469	-0.037042
C	-4.882890	-1.264146	0.958475	C	-4.599661	-1.242253	0.128075
C	-0.526392	0.456311	-2.964693	C	1.902603	1.446066	0.007140
C	-6.072698	-1.220658	1.711637	C	-5.577894	-1.916323	0.879165
Pt	-1.346684	-0.216621	0.352541	Pt	-1.230158	-0.081546	0.457930
C	0.989734	-3.809022	-3.580703	C	3.990248	-1.755052	2.461935
H	-2.559174	2.686898	0.454402	H	-2.404993	2.586554	-0.097406
C	0.775387	2.360790	-4.582421	C	3.160978	3.956809	0.161936
H	1.278146	3.101620	-5.209245	H	3.647910	4.933635	0.220057
C	-0.384706	-2.364993	-2.186182	C	2.016970	-1.252924	1.133749
P	-3.632902	0.086549	1.049982	P	-3.505686	0.041653	0.863484
H	-6.301669	-0.357007	2.339763	H	-5.712920	-1.703101	1.940804
C	0.466632	1.293920	-2.426749	C	1.550309	2.358170	1.018915
C	1.113986	2.236313	-3.231471	C	2.181040	3.602880	1.095969
C	1.013138	-4.776545	-2.571061	C	3.411700	-2.956986	2.880344
C	-0.347730	-3.339010	-1.173088	C	1.437261	-2.458620	1.567387
H	0.726195	1.211664	-1.369887	H	0.779785	2.087259	1.746528
H	1.882174	2.880271	-2.796034	H	3.953318	-3.617845	3.561857
H	-0.850927	-3.147035	-0.221533	H	1.900087	4.301851	1.887980
C	-3.535459	0.390242	2.893431	H	0.431031	-2.726042	1.234290
H	-4.448567	0.903794	3.236286	C	-3.743949	-0.063035	2.702833
C	0.341918	-4.539589	-1.367167	H	-4.752196	0.287374	2.980415
S	-0.738640	0.444643	2.556668	C	2.134079	-3.308222	2.429914
H	-2.372738	2.222679	2.961981	S	-0.947025	0.245294	2.881233
H	-3.511828	-0.610754	3.353598	H	-2.798589	1.818995	3.228526
C	-2.284735	1.169187	3.271588	H	-3.657447	-1.127642	2.973243
H	0.362495	-5.286815	-0.569972	C	-2.652008	0.740882	3.404973
H	-2.159384	1.164816	4.365968	H	1.673153	-4.242781	2.759108
H	1.559641	-5.711250	-2.719944	H	-2.719825	0.579969	4.492268

<i>cis-9</i>				<i>trans-9</i>			
H	3.091379	-4.109982	-5.030217	H	3.340485	1.376877	-5.444965
H	2.413693	-1.737464	-4.644720	H	1.279863	2.297755	-4.376555
C	2.639970	-3.814675	-4.079671	C	3.078021	1.092304	-4.422806
H	-6.214142	1.901161	-3.919090	H	-5.484874	1.795860	-4.234947
H	-4.560724	2.433909	-4.308765	H	-3.817726	2.412455	-4.333692
H	2.719940	-5.807968	-3.238090	H	4.797333	-0.197889	-4.169846
H	-4.896649	0.707460	-4.032456	H	-4.109735	0.670343	-4.111033
C	2.261408	-2.486456	-3.863592	C	1.922745	1.607634	-3.824141
C	-5.148134	1.726938	-3.697809	C	-4.466368	1.674755	-3.830419
H	-3.179679	-3.204301	-4.194323	H	-2.606255	-3.643004	-3.781007
C	2.431775	-4.766286	-3.075829	C	3.893719	0.209483	-3.709301
H	-5.664575	-3.414428	-4.072377	H	-5.091741	-3.769592	-3.970825
C	-3.719371	-2.843068	-3.315463	C	-3.239477	-3.157669	-3.034250
C	-5.110835	-2.958463	-3.247846	C	-4.631514	-3.228262	-3.140417
H	-6.323076	3.485525	-1.870639	H	-6.028122	3.365144	-2.245711
H	-4.712395	4.068132	-2.316220	H	-4.395500	4.030200	-2.403062
C	1.679261	-2.109100	-2.649229	C	1.579695	1.238257	-2.520893
C	-4.852129	1.914926	-2.207036	C	-4.443913	1.871887	-2.311816
C	-5.244802	3.311358	-1.709645	C	-4.987600	3.244509	-1.896783
C	1.850956	-4.391663	-1.860722	C	3.559133	-0.157864	-2.401067
H	1.374247	-1.073097	-2.488790	H	0.672742	1.636351	-2.056871
H	-2.769845	2.385225	-2.484502	H	-2.369809	2.444252	-2.227176
H	-5.458477	1.175119	-1.651244	H	-5.100547	1.100743	-1.867003
H	-1.927189	-2.149018	-2.320783	H	-1.563128	-2.397738	-1.890228
C	-3.012747	-2.258422	-2.259007	C	-2.650563	-2.461704	-1.973169
C	-5.794347	-2.482795	-2.122736	C	-5.435789	-2.603341	-2.180278
H	-6.882613	-2.565455	-2.066581	H	-6.524548	-2.656760	-2.257309
H	-3.067327	0.667381	-2.262026	H	-2.617012	0.713369	-2.048098
C	1.472146	-3.055632	-1.630569	C	2.399005	0.353376	-1.795805
H	1.686167	-5.151868	-1.094723	H	4.207696	-0.846286	-1.856465
C	-3.365801	1.663220	-1.900025	C	-3.023044	1.693700	-1.749889
C	-4.895570	3.502528	-0.232638	C	-4.912922	3.444870	-0.381889
H	-5.150676	4.529241	0.079275	H	-5.271087	4.455454	-0.122875
C	-3.687246	-1.784629	-1.121718	C	-3.449429	-1.830358	-1.005618
C	-5.089119	-1.897154	-1.067863	C	-4.849946	-1.908686	-1.118838
H	-2.836892	3.929420	-0.578971	H	-2.849697	3.978218	-0.363663
H	-5.530257	2.835599	0.375490	H	-5.610155	2.743343	0.107397
C	-2.956675	1.819494	-0.413952	C	-2.883427	1.866395	-0.216409
C	-3.404892	3.243466	0.074610	C	-3.487750	3.260134	0.181336
P	0.732906	-2.506139	-0.023089	P	1.908057	-0.085182	-0.068376
H	-5.641544	-1.530923	-0.199144	H	-5.494610	-1.435046	-0.374470
H	-4.606331	0.591181	0.378868	H	-4.601879	0.573800	0.303349
Pt	-0.409446	-0.496303	-0.170561	Pt	-0.393048	-0.468015	0.155115
S	-1.066730	1.774203	-0.345050	S	-1.041734	1.899641	0.196273
P	-2.716570	-0.971363	0.219200	P	-2.647232	-0.916259	0.375129
C	-3.514372	0.696460	0.476934	C	-3.539464	0.707741	0.561697
H	-3.325554	5.779642	1.283246	H	-3.760610	5.786318	1.385379
H	-1.659160	5.243391	0.954082	H	-2.035215	5.344726	1.349054
H	-4.291079	-3.488396	0.894584	H	-3.988304	-3.566683	0.913559
C	-2.533358	5.080838	1.604510	C	-2.998185	5.128711	1.838668
C	-3.012837	3.622019	1.539635	C	-3.376975	3.646599	1.691664
H	-4.949752	4.082518	2.480442	H	-5.469875	3.991273	2.283403
H	-3.308595	0.930206	1.529677	H	-3.496975	0.920282	1.637866
H	-2.147162	2.992736	1.803496	H	-2.536012	3.062596	2.100071
C	-3.916474	-3.042635	1.816655	C	-3.715536	-3.112138	1.867280
C	-3.162892	-1.859125	1.778343	C	-3.097398	-1.852174	1.901322
C	-4.100488	3.390992	2.603476	C	-4.617763	3.345237	2.550479
H	-4.505282	2.367897	2.592912	H	-4.957444	2.301969	2.467674
H	-2.245421	5.360650	2.631473	H	-2.907735	5.414161	2.899962
H	-4.781750	-4.590021	3.047846	H	-4.470297	-4.779662	3.012229
H	-3.683647	3.567199	3.608744	H	-4.391935	3.531887	3.613310
C	-4.192167	-3.669814	3.037484	C	-3.987796	-3.799958	3.055771
C	-2.670154	-1.332304	2.988466	C	-2.742844	-1.302033	3.147958
H	-2.053677	-0.429391	2.983350	H	-2.233714	-0.336004	3.197437
C	-3.718775	-3.126667	4.234089	C	-3.647246	-3.239449	4.289226
C	-2.952427	-1.955819	4.205580	C	-3.022512	-1.987455	4.331957
H	-3.939017	-3.616335	5.185970	H	-3.862707	-3.777390	5.215765
H	-2.567035	-1.527912	5.134478	H	-2.744744	-1.544337	5.291567
H	1.068860	0.073971	-0.423705	H	-0.089621	-2.032540	0.174851

C	-0.142221	-4.027132	0.571133	C	3.029247	-1.492912	0.366807
C	-1.035765	-4.695621	-0.285727	C	2.702506	-2.789455	-0.068674
C	0.035010	-4.515534	1.875947	C	4.214566	-1.301414	1.096041
C	-1.718785	-5.834719	0.146225	C	3.545388	-3.867101	0.212149
H	-1.192421	-4.337757	-1.305147	H	1.776076	-2.957433	-0.621837
C	-0.655758	-5.653050	2.308985	C	5.052001	-2.384817	1.386367
H	0.721135	-4.015799	2.561779	H	4.491712	-0.305145	1.444338
C	-1.529092	-6.318881	1.445355	C	4.721586	-3.668378	0.944250
H	-2.400679	-6.346877	-0.537328	H	3.277179	-4.868074	-0.135086
H	-0.502711	-6.020777	3.326666	H	5.966780	-2.220029	1.961246
H	-2.061693	-7.211714	1.782317	H	5.376004	-4.513501	1.172260
C	2.169639	-2.374020	1.139966	C	2.537701	1.307668	0.965536
C	3.322567	-3.166868	1.013070	C	3.466822	2.246635	0.490042
C	2.087947	-1.459310	2.203745	C	2.071451	1.414305	2.288059
C	4.369197	-3.047090	1.932657	C	3.923868	3.272460	1.325029
H	3.417927	-3.878101	0.191097	H	3.837234	2.183113	-0.534962
C	3.131200	-1.347722	3.128093	C	2.537051	2.433395	3.122243
H	1.203595	-0.824146	2.296791	H	1.334269	0.699335	2.662353
C	4.275339	-2.140206	2.993354	C	3.463032	3.366177	2.641454
H	5.263108	-3.665018	1.816125	H	4.643286	4.000628	0.942060
H	3.051684	-0.631640	3.949859	H	2.167828	2.504733	4.148346
H	5.095339	-2.047494	3.709987	H	3.820795	4.168507	3.291688

<i>cis</i> -10				<i>trans</i> -10			
H	4.341667	-3.931222	-4.592409	H	3.874772	-1.766751	-5.371365
H	4.249933	-1.600108	-3.696285	H	1.784270	-2.768955	-4.443696
C	3.629141	-3.672435	-3.805146	C	3.493637	-1.441552	-4.400021
H	2.794803	-5.664519	-3.676907	H	5.085133	-0.010522	-4.074471
C	3.577032	-2.366637	-3.303785	C	2.323238	-2.003190	-3.880166
H	-4.688824	-2.419854	-3.932616	H	-3.442557	0.160283	-4.486132
C	2.763028	-4.641334	-3.293969	C	4.171456	-0.457022	-3.674139
H	-6.779943	-3.314787	-2.901288	H	-5.743905	-0.805286	-4.541863
C	-4.835458	-2.365308	-2.851029	C	-3.881872	-0.265459	-3.580600
C	-6.006250	-2.865642	-2.273462	C	-5.170295	-0.806826	-3.611544
C	2.658956	-2.032719	-2.306280	C	1.831050	-1.582681	-2.641017
C	1.849308	-4.310958	-2.285536	C	3.683429	-0.036337	-2.433103
H	2.618568	-1.006166	-1.936432	H	0.910282	-2.012866	-2.242639
H	-2.923657	-1.416545	-2.497523	H	-2.131683	0.134874	-2.371301
C	-3.842770	-1.798377	-2.045194	C	-3.145178	-0.274075	-2.391599
C	-6.183648	-2.789814	-0.887634	C	-5.721698	-1.357336	-2.449112
H	-7.097328	-3.177102	-0.429681	H	-6.726710	-1.786217	-2.468440
C	1.783114	-3.000987	-1.782384	C	2.508157	-0.597653	-1.901449
H	1.189087	-5.086276	-1.895107	H	4.222376	0.736728	-1.882028
C	-4.983153	3.266874	-0.022502	C	-4.795539	3.233693	1.821021
H	-5.229872	4.329389	0.140298	H	-5.077141	4.066013	2.487663
C	-4.010866	-1.716873	-0.651226	C	-3.693186	-0.818690	-1.217093
C	-5.196626	-2.215522	-0.081383	C	-4.990168	-1.362855	-1.258464
H	-3.420893	3.681476	-1.487039	H	-2.872464	4.102950	1.271131
C	-3.128187	1.672586	-0.727512	C	-2.814433	1.986645	0.812949
C	-3.541767	3.139849	-0.534573	C	-3.267669	3.163578	1.690908
P	0.611725	-2.520329	-0.421774	P	1.858278	-0.093900	-0.244440
H	-5.355252	-2.162103	0.997239	H	-5.432220	-1.802642	-0.362104
Pt	-0.580803	-0.570040	-0.787316	Pt	-0.454089	-0.335195	0.032108
S	-1.371408	1.600962	-1.328308	S	-0.959340	1.962301	0.696961
P	-2.692968	-0.874975	0.330163	P	-2.709238	-0.753407	0.340140
C	-3.339398	0.874211	0.569380	C	-3.401947	0.665500	1.346847
H	-3.124829	-3.654210	1.300024	H	-2.918100	-3.539379	-0.535248
H	-2.654322	1.306637	1.320013	H	-2.963501	0.506812	2.348749
C	-2.942145	-3.020458	2.169414	C	-3.117961	-3.525676	0.538913
C	-2.749067	-1.636042	2.009991	C	-3.133389	-2.304235	1.237800
H	-3.057019	-4.681248	3.539902	H	-3.340010	-5.668468	0.646673
C	-2.900696	-3.604489	3.438940	C	-3.353865	-4.729543	1.205711
C	-2.490609	-0.858580	3.154801	C	-3.376637	-2.319909	2.621471
H	-2.316942	0.215599	3.070241	H	-3.380526	-1.393367	3.197861
C	-2.656854	-2.820310	4.570248	C	-3.602904	-4.734559	2.583025
C	-2.448165	-1.445873	4.422824	C	-3.611761	-3.528180	3.287474
H	-2.626045	-3.278445	5.561895	H	-3.786624	-5.677061	3.104659
H	-2.252116	-0.822207	5.298588	H	-3.802146	-3.521270	4.363532
H	0.733420	-0.097633	-1.563335	H	-0.221151	-1.865954	-0.365432
C	-0.357426	-4.071602	-0.157264	C	2.788258	-1.134868	0.966020
C	-1.394677	-4.363577	-1.061177	C	4.052811	-1.676724	0.681907
C	-0.094724	-4.969353	0.889150	C	2.207593	-1.378073	2.223403
C	-2.146646	-5.533031	-0.926741	C	4.723734	-2.444552	1.639297
H	-1.617990	-3.670806	-1.875442	H	4.519879	-1.507628	-0.290144
C	-0.853654	-6.137412	1.026534	C	2.883986	-2.139128	3.181095
H	0.702338	-4.762698	1.605028	H	1.216110	-0.974770	2.445326
C	-1.878465	-6.423101	0.120114	C	4.142727	-2.675453	2.890265
H	-2.947708	-5.746233	-1.638721	H	5.704605	-2.865039	1.403627
H	-0.639837	-6.825730	1.848086	H	2.421076	-2.319538	4.154476
H	-2.468907	-7.336364	0.228646	H	4.668318	-3.277132	3.636118
C	1.719820	-2.407480	1.054522	C	2.551598	1.602063	-0.014903
C	2.921702	-3.131401	1.143053	C	2.128030	2.619951	-0.889385
C	1.343655	-1.577366	2.124326	C	3.450025	1.919638	1.015738
C	3.726817	-3.029361	2.281723	C	2.609706	3.922351	-0.745433
H	3.237395	-3.775989	0.320108	H	1.418579	2.394667	-1.689010
C	2.148053	-1.480797	3.263791	C	3.922861	3.229052	1.163854
H	0.419488	-0.998702	2.058550	H	3.788871	1.147023	1.707992
C	3.341560	-2.205236	3.344298	C	3.507762	4.230956	0.283146
H	4.660596	-3.594676	2.336068	H	2.276097	4.701708	-1.435112
H	1.843004	-0.830850	4.087661	H	4.621623	3.461841	1.971340
H	3.974099	-2.123991	4.231908	H	3.879927	5.252108	0.398311
C	-5.186768	2.465990	1.267220	C	-5.371686	1.913598	2.342242
C	-4.785366	0.994896	1.081551	C	-4.934932	0.728556	1.468027
H	-5.681853	2.898569	-0.795795	H	-5.238278	3.460794	0.833900
H	-6.237552	2.524142	1.597038	H	-6.472938	1.959436	2.379722
H	-4.579082	2.912124	2.075516	H	-5.028997	1.748039	3.379921

H	-5.472149	0.523741	0.358659	H	-5.377009	0.839574	0.463645
H	-4.900616	0.447279	2.030909	H	-5.327749	-0.213874	1.883043
H	-2.848565	3.609233	0.186294	H	-2.813510	3.049718	2.691640
H	-3.768189	1.236306	-1.514372	H	-3.209722	2.149995	-0.205455

<i>cis-11-chair</i>				<i>trans-11-chair</i>			
H	2.404429	0.408339	-5.415950	H	2.581372	-0.957071	-5.203201
H	1.114211	2.133440	-4.149364	H	0.721095	0.585297	-4.570396
C	2.206170	0.272694	-4.349797	C	2.315349	-0.819353	-4.152127
C	1.482610	1.239422	-3.639983	C	1.273061	0.044299	-3.797673
H	3.233865	-1.626997	-4.232847	H	3.824988	-2.187212	-3.421729
C	2.669560	-0.865861	-3.688026	C	3.011092	-1.508310	-3.155066
H	3.398002	-0.449553	5.639839	H	-7.272061	2.166710	-1.420479
C	1.220899	1.061780	-2.280768	C	0.925199	0.211898	-2.455035
H	0.642217	1.816535	-1.742465	H	0.097533	0.872602	-2.189356
H	3.507589	-2.934188	5.880686	H	-5.967888	4.075162	-2.361369
C	2.416309	-1.041441	-2.320964	C	2.671244	-1.333775	-1.808883
C	2.602162	-1.077332	5.230963	C	-6.213211	2.281686	-1.175146
C	2.664069	-2.467771	5.365657	C	-5.482077	3.350819	-1.702671
C	1.687003	-0.080706	-1.604883	C	1.622688	-0.472126	-1.443775
H	2.791491	-1.935676	-1.821001	H	3.229648	-1.875812	-1.044051
H	1.485347	0.607607	4.498192	H	-6.178563	0.522206	0.068346
H	-1.868792	4.399760	3.697356	H	-4.231747	-4.119162	-0.877133
H	4.167137	0.531878	-0.396473	H	3.224465	1.528660	-1.068347
C	1.519262	-0.480152	4.579566	C	-5.593472	1.352489	-0.333324
H	5.663641	2.280482	0.502158	H	4.417342	3.582225	-0.375965
H	-1.971333	4.315749	6.190439	H	-6.212756	-4.649353	0.548395
H	3.955825	-1.190898	1.457079	H	3.843462	-0.463287	1.694141
C	-1.708778	3.454944	4.222783	C	-4.574099	-3.404290	-0.124760
C	1.639169	-3.256574	4.835605	C	-4.125667	3.486193	-1.388984
H	1.678047	-4.344580	4.930701	H	-3.546924	4.316800	-1.800901
H	-1.091526	0.223564	-0.789470	H	-1.355526	0.369337	-0.701362
C	-1.767483	3.407329	5.617892	C	-5.683653	-3.701376	0.674055
H	-1.421660	2.325961	2.399270	H	-3.014825	-1.977012	-0.570100
C	3.802425	1.194097	0.391821	C	3.032047	1.951815	-0.080995
C	-1.449715	2.290322	3.490350	C	-3.892378	-2.196441	0.042665
C	4.647024	2.187789	0.892325	C	3.708000	3.113449	0.310808
C	0.476647	-1.262669	4.050867	C	-4.230439	1.479455	-0.016342
C	-1.565801	2.190698	6.281044	C	-6.109154	-2.783110	1.637942
C	0.557122	-2.660875	4.179818	C	-3.501803	2.553111	-0.555366
C	3.333683	-2.051421	1.207698	C	3.314796	-1.415802	1.767073
H	-1.612092	2.146386	7.372123	H	-6.972129	-3.009383	2.269083
H	4.811051	-3.465184	1.900184	H	4.926668	-2.375405	2.837377
P	1.339358	-0.226543	0.214055	P	1.172975	-0.185408	0.329783
C	-1.240308	1.066194	4.145781	C	-4.317375	-1.261300	1.004263
C	2.490983	1.056515	0.885475	C	2.114292	1.339095	0.787456
C	-1.303422	1.029009	5.551343	C	-5.432802	-1.569110	1.801990
Pt	-0.912585	-0.088073	0.756530	Pt	-1.105112	0.035012	0.831134
C	3.818699	-3.340164	1.459812	C	3.927220	-2.495957	2.411841
H	-0.224742	-3.303281	3.771201	H	-2.436832	2.648133	-0.328514
C	4.190375	3.068234	1.880252	C	3.478881	3.669880	1.572027
H	4.850628	3.849345	2.265406	H	4.007445	4.577158	1.875576
C	2.060466	-1.871166	0.646146	C	2.028969	-1.554157	1.220653
P	-0.944493	-0.473584	3.162781	P	-3.385782	0.322401	1.152205
H	-1.139610	0.090232	6.086374	H	-5.787082	-0.869468	2.560939
C	2.039132	1.953643	1.864810	C	1.884914	1.906677	2.055330
C	2.883670	2.952992	2.361078	C	2.568500	3.061164	2.444100
C	3.041487	-4.459803	1.151781	C	3.264446	-3.722920	2.512352
C	1.275328	-3.003806	0.358389	C	1.365321	-2.788275	1.333089
H	1.013772	1.880925	2.229111	H	1.170112	1.431379	2.733318
H	3.425353	-5.464594	1.345456	H	3.744051	-4.565009	3.017731
H	2.512859	3.645592	3.120689	H	2.385032	3.490587	3.432405
H	0.272842	-2.873953	-0.058605	H	0.355994	-2.900653	0.929055
C	-2.365270	-1.555471	3.684196	C	-3.863165	1.055660	2.784469
C	1.765805	-4.288551	0.601936	C	1.982472	-3.867455	1.970447
S	-3.303769	0.108596	0.689445	S	-0.742148	-0.582368	3.202022
H	-3.928383	-2.123459	1.452289	H	-1.509013	1.517395	4.193407
C	-4.106790	-1.102283	1.828730	C	-1.825425	0.462868	4.269208
H	1.147637	-5.158281	0.365621	H	1.455636	-4.821347	2.052710
H	-5.183502	-0.905054	1.703788	H	-1.600814	0.142484	5.298919
C	-3.760020	-1.033749	3.314158	C	-3.335246	0.360527	4.047295
H	-2.207469	-2.541766	3.217910	H	-3.489905	2.093018	2.741341
H	-2.287657	-1.698497	4.773620	H	-4.962218	1.130901	2.808023
H	-4.491239	-1.659662	3.857613	H	-3.839245	0.838455	4.907429
H	-3.900100	-0.005892	3.689143	H	-3.640375	-0.699109	4.063365

<i>cis-11-skew-boat</i>				<i>trans-11-skew-boat</i>			
H	-6.190175	-0.723450	-4.641901	H	-6.839851	0.725931	-3.568792
H	-5.629867	1.397215	-3.444904	H	-5.903758	2.386134	-1.955939
C	-5.310361	-0.673586	-3.995475	C	-5.863360	0.553629	-3.109114
C	-4.996368	0.514673	-3.325399	C	-5.338518	1.484949	-2.206154
H	-4.733692	-2.728780	-4.347217	H	-5.544425	-1.334913	-4.116986
C	-4.494407	-1.795362	-3.831575	C	-5.137868	-0.601266	-3.416306
H	-8.188330	2.777333	2.013553	H	-0.004316	-1.154540	7.667966
C	-3.870838	0.578567	-2.502140	C	-4.094805	1.260008	-1.611161
H	-3.635759	1.515488	-1.992205	H	-3.698089	1.981256	-0.892227
H	-7.157146	4.761615	0.906926	H	1.623316	-2.690816	6.565444
C	-3.361584	-1.731393	-3.011224	C	-3.887962	-0.824847	-2.828400
C	-7.167172	2.720856	1.628293	C	0.136834	-1.118649	6.584911
C	-6.588006	3.834104	1.008137	C	1.049446	-1.979513	5.966169
C	-3.034374	-0.541391	-2.343240	C	-3.354916	0.105700	-1.922202
H	-2.730036	-2.614629	-2.902938	H	-3.330662	-1.729642	-3.078762
H	-6.909032	0.676269	2.250179	H	-1.305025	0.456583	6.323842
H	-7.784247	-2.174956	-1.259740	H	1.682606	4.392384	5.511525
H	-1.409674	0.541688	-4.117195	H	-1.965592	1.013822	-3.899916
C	-6.441303	1.534149	1.761164	C	-0.600368	-0.209033	5.820697
H	-0.099593	2.290536	-5.262297	H	-0.393973	2.221403	-5.375313
H	-6.911892	-4.491238	-0.938825	H	0.967085	6.239610	3.994224
H	0.262145	-1.300688	-3.518263	H	0.083123	-1.531985	-3.103033
C	-6.875938	-2.343452	-0.675666	C	0.934616	4.207407	4.736360
C	-5.278316	3.758464	0.525729	C	1.221390	-1.931045	4.579154
H	-4.816982	4.626786	0.048881	H	1.929235	-2.604423	4.089607
H	-0.139692	-0.047947	0.906511	H	-0.145503	0.963598	0.927845
C	-6.386607	-3.639943	-0.498594	C	0.534253	5.241873	3.886289
H	-6.606204	-0.246605	-0.262695	H	0.705648	2.132471	5.274397
C	-0.722944	1.158070	-3.534205	C	-0.958467	1.232224	-3.541265
C	-6.208623	-1.250821	-0.109508	C	0.381914	2.928419	4.601283
C	0.015173	2.151418	-4.184345	C	-0.068038	1.913503	-4.378605
C	-5.125704	1.443773	1.269232	C	-0.432936	-0.152074	4.424882
C	-5.215611	-3.841420	0.240691	C	-0.417954	4.993067	2.891077
C	-4.550929	2.570701	0.657982	C	0.482324	-1.025713	3.811869
C	0.191924	-2.099452	-2.778093	C	-0.375070	-2.275202	-2.448234
H	-4.819770	-4.850666	0.379692	H	-0.731085	5.794794	2.217538
H	1.484472	-3.410743	-3.904504	H	0.624435	-3.925392	-3.418892
P	-1.534998	-0.379713	-1.269700	P	-1.700315	-0.106328	-1.134251
C	-5.040697	-1.443811	0.643725	C	-0.573848	2.671437	3.606000
C	-0.591590	0.958510	-2.146665	C	-0.562778	0.833971	-2.252769
C	-4.545534	-2.752406	0.802427	C	-0.962768	3.715013	2.746396
Pt	-1.733699	0.017657	1.005746	Pt	-1.624960	0.417743	1.146341
C	0.885361	-3.293658	-2.997962	C	-0.069326	-3.629335	-2.627932
H	-3.519770	2.517451	0.298758	H	0.603331	-0.997923	2.726178
C	0.891978	2.964998	-3.459631	C	1.229349	2.198240	-3.944280
H	1.465467	3.744054	-3.968265	H	1.923500	2.731147	-4.599000
C	-0.577234	-1.926762	-1.614658	C	-1.261088	-1.877357	-1.433901
P	-4.106668	-0.078693	1.469243	P	-1.380051	1.026317	3.378729
H	-3.627918	-2.926314	1.370447	H	-1.687321	3.520256	1.950833
C	0.287789	1.786803	-1.427803	C	0.742723	1.130495	-1.823194
C	1.024704	2.780351	-2.080476	C	1.633292	1.801634	-2.664672
C	0.816904	-4.331107	-2.062315	C	-0.647736	-4.597122	-1.802180
C	-0.632501	-2.971430	-0.676206	C	-1.837474	-2.856605	-0.602653
H	0.388493	1.656109	-0.349275	H	1.059513	0.842415	-0.818816
H	1.701396	3.415658	-1.503520	H	2.644767	2.022655	-2.314694
H	-1.208895	-2.836740	0.241986	H	-2.526754	-2.551537	0.190175
C	-4.347889	-0.563334	3.253441	C	-3.012435	1.285486	4.221463
C	0.055249	-4.167848	-0.901115	C	-1.534859	-4.207264	-0.791931
S	-1.249962	0.521151	3.295571	S	-3.906373	-0.447075	1.558615
H	-3.031977	2.163554	3.278461	H	-2.915441	-1.631265	3.434476
C	-2.740778	1.366979	3.978887	C	-3.831785	-1.033796	3.307625
H	0.002475	-4.969928	-0.160675	H	-1.990902	-4.958922	-0.142455
H	-2.406836	1.871295	4.899327	H	-4.674452	-1.729032	3.447327
H	1.361800	-5.262602	-2.235356	H	-0.406909	-5.653836	-1.943726
C	-3.947662	0.480798	4.308633	C	-3.912782	0.047465	4.393999
H	-3.760852	-0.060753	5.251506	H	-4.951841	0.410141	4.470800
H	-4.805548	1.148397	4.502660	H	-3.684554	-0.435365	5.360520
H	-5.393464	-0.874454	3.401235	H	-2.843930	1.781281	5.190246
H	-3.729276	-1.467254	3.360271	H	-3.502553	2.028445	3.573284

cis-11-boat				trans-11-boat			
H	2.725386	0.498401	-5.224694	H	2.438860	-0.684017	-5.284464
H	1.250234	2.156147	-4.075376	H	0.652409	0.888500	-4.524616
C	2.422217	0.336986	-4.187180	C	2.197200	-0.598936	-4.221992
C	1.594869	1.265977	-3.543123	C	1.196214	0.281502	-3.796441
H	3.498946	-1.528557	-3.990601	H	3.665189	-2.063630	-3.603414
C	2.854321	-0.796870	-3.496964	C	2.883051	-1.371585	-3.281264
H	2.063468	0.069095	6.303950	H	-6.523661	1.418721	-2.557109
C	1.199509	1.055096	-2.221644	C	0.879081	0.382188	-2.439844
H	0.541476	1.780024	-1.735971	H	0.083809	1.058470	-2.119976
H	2.860026	-2.298164	6.267227	H	-5.801854	3.802577	-2.718325
C	2.466664	-1.005406	-2.166377	C	2.574539	-1.264318	-1.920385
C	1.580468	-0.663622	5.652456	C	-5.761981	1.809253	-1.877468
C	2.027018	-1.987754	5.631532	C	-5.357923	3.143166	-1.968383
C	1.633160	-0.083047	-1.517159	C	1.566921	-0.387085	-1.484528
H	2.819472	-1.895015	-1.642483	H	3.125511	-1.870999	-1.200127
H	0.169331	0.768665	4.889332	H	-5.525326	-0.076244	-0.860390
H	-3.043668	4.062941	3.145619	H	-4.072848	-4.476350	0.321912
H	3.866872	0.761344	-0.099052	H	3.276890	1.512818	-0.995854
C	0.508062	-0.267545	4.846714	C	-5.196671	0.962800	-0.915703
H	5.123071	2.584401	0.998863	H	4.498237	3.521838	-0.224789
H	-3.764682	3.920685	5.531698	H	-6.420323	-4.513158	1.170047
H	3.643536	-1.054111	1.713944	H	3.829549	-0.492782	1.668725
C	-2.933190	3.126834	3.698635	C	-4.532162	-3.562749	0.707349
C	1.402871	-2.911095	4.787148	C	-4.376593	3.629845	-1.096302
H	1.748902	-3.946825	4.753030	H	-4.048659	4.670217	-1.163608
H	-1.227296	0.015539	-1.046515	H	-1.344224	0.540060	-0.621618
C	-3.337650	3.046753	5.033255	C	-5.846354	-3.583153	1.182075
H	-2.087892	2.067956	2.012247	H	-2.767191	-2.361355	0.359675
C	3.383777	1.345559	0.687192	C	3.066566	1.919898	-0.005290
C	-2.388207	2.006363	3.060029	C	-3.795946	-2.373296	0.726842
C	4.092830	2.380727	1.301319	C	3.758517	3.055681	0.431011
C	-0.136614	-1.190304	4.004062	C	-4.216676	1.443906	-0.034081
C	-3.194234	1.841206	5.730970	C	-6.426132	-2.407622	1.672421
C	0.337136	-2.514590	3.975167	C	-3.806106	2.785801	-0.141589
C	3.107795	-1.958750	1.423085	C	3.325526	-1.461067	1.673918
H	-3.507322	1.770862	6.775720	H	-7.454697	-2.414895	2.041568
H	4.615042	-3.259032	2.258542	H	4.959847	-2.448194	2.683202
P	1.088114	-0.281415	0.246904	P	1.158852	-0.189444	0.311246
C	-2.240424	0.791852	3.749454	C	-4.366374	-1.188549	1.222379
C	2.056480	1.066471	1.065144	C	2.109693	1.311441	0.823188
C	-2.649801	0.723620	5.094911	C	-5.692891	-1.218474	1.691239
Pt	-1.215461	-0.283677	0.515750	Pt	-1.112743	0.017140	0.860347
C	3.658182	-3.207607	1.733050	C	3.965451	-2.566368	2.245398
H	-0.117030	-3.252366	3.310474	H	-3.024636	3.176737	0.515911
C	3.483684	3.160380	2.291438	C	3.506488	3.590284	1.697552
H	4.037697	3.974229	2.765946	H	4.047508	4.477701	2.035837
C	1.878065	-1.873003	0.753019	C	2.045761	-1.595206	1.112064
P	-1.529505	-0.687344	2.888057	P	-3.377023	0.369289	1.214441
H	-2.537021	-0.204456	5.660959	H	-6.170873	-0.310853	2.067401
C	1.452162	1.862212	2.049907	C	1.857411	1.857160	2.095793
C	2.161325	2.901904	2.661113	C	2.556953	2.985998	2.529671
C	2.990206	-4.381706	1.374935	C	3.336809	-3.814960	2.256642
C	1.202626	-3.059873	0.411885	C	1.415927	-2.852010	1.136829
H	0.414247	1.677680	2.328460	H	1.111148	1.389105	2.743669
H	3.424797	-5.355529	1.614424	H	3.838079	-4.677156	2.703755
H	1.672949	3.514229	3.423183	H	2.354795	3.398754	3.521412
H	0.233268	-3.003943	-0.091272	H	0.412599	-2.965524	0.719661
C	-2.790467	-2.027676	3.227974	C	-3.771618	1.223969	2.829198
C	1.758610	-4.305140	0.714112	C	2.061061	-3.955946	1.699303
S	-3.571304	-0.254206	0.134111	S	-0.761252	-0.823781	3.152943
H	-5.484507	-1.201839	1.158339	H	-1.810914	-0.365731	5.242808
C	-4.488252	-0.972114	1.566596	C	-2.186107	-0.307766	4.209482
H	1.226015	-5.218153	0.436234	H	1.560800	-4.927477	1.711188
H	-4.635497	-0.210923	2.351116	H	-3.003078	-1.045815	4.132272
C	-3.871816	-2.245001	2.158542	C	-2.726568	1.103873	3.948403
H	-2.230212	-2.961506	3.376668	H	-3.932438	2.284002	2.583610
H	-3.251591	-1.785281	4.198187	H	-4.742900	0.834540	3.171399
H	-3.468448	-2.856142	1.334962	H	-1.878472	1.777699	3.744534
H	-4.670349	-2.845690	2.628647	H	-3.207173	1.479227	4.869386

TS[<i>trans</i> -11-boat→skew-boat]				TS[<i>trans</i> -11-skew-boat→chair]			
H	2.366338	-3.909748	-4.143913	H	1.844106	-0.941550	-5.521095
H	0.513535	-2.256821	-4.419717	H	-0.086832	-2.000159	-4.341757
C	2.118825	-3.221995	-3.331401	C	1.711382	-0.797699	-4.445836
C	1.079788	-2.296019	-3.485770	C	0.629314	-1.390350	-3.785206
H	3.645932	-3.984631	-2.002263	H	3.464557	0.452658	-4.231794
C	2.834428	-3.264278	-2.132807	C	2.618239	-0.017045	-3.724262
H	-7.557478	2.721380	0.339538	H	-5.006282	2.004500	-2.970378
C	0.755761	-1.425046	-2.444055	C	0.452520	-1.196528	-2.413199
H	-0.068159	-0.718577	-2.568766	H	-0.406626	-1.645081	-1.910139
H	-6.248654	4.684526	-0.477182	H	-5.789850	4.237033	-2.168146
C	2.518850	-2.383277	-1.090640	C	2.449561	0.168663	-2.347309
C	-6.470445	2.656116	0.247024	C	-4.883892	2.284851	-1.921189
C	-5.735981	3.756416	-0.211906	C	-5.322925	3.536280	-1.471553
C	1.474192	-1.457117	-1.235192	C	1.363173	-0.418156	-1.676939
H	3.093086	-2.425680	-0.163736	H	3.171103	0.776704	-1.799254
H	-6.407118	0.615740	0.928191	H	-3.930423	0.424107	-1.397717
H	-5.248832	-1.928848	-3.405145	H	-4.216377	-4.371847	1.306803
H	3.254962	0.389944	-1.800576	H	3.971393	-0.098424	1.118714
C	-5.816611	1.469291	0.584560	C	-4.281525	1.392658	-1.033015
H	4.242477	2.524331	-2.563084	H	5.448346	1.815078	1.662364
H	-6.307417	-3.984684	-2.455578	H	-6.695324	-4.113658	1.429752
H	3.664272	0.681972	1.229583	H	1.197872	-1.282282	2.851349
C	-5.206013	-2.122629	-2.330415	C	-4.663113	-3.375530	1.352996
C	-4.347255	3.662271	-0.332653	C	-5.158478	3.885233	-0.129319
H	-3.768033	4.516189	-0.692883	H	-5.496449	4.860276	0.230476
H	-1.482309	-1.109597	-0.633422	H	-1.603228	-0.373728	-0.535480
C	-5.799262	-3.274480	-1.798595	C	-6.051571	-3.230420	1.422024
H	-4.091681	-0.326767	-1.921870	H	-2.753598	-2.352483	1.274620
C	2.850766	1.331115	-1.423074	C	3.589138	0.919986	1.024255
C	-4.555291	-1.217941	-1.491088	C	-3.839586	-2.244145	1.337904
C	3.409821	2.537727	-1.855241	C	4.423785	2.000537	1.330123
C	-4.417511	1.368480	0.473056	C	-4.119019	1.731692	0.323273
C	-5.736008	-3.509322	-0.424107	C	-6.617245	-1.950836	1.477247
C	-3.689631	2.473885	0.006595	C	-4.562045	2.988707	0.766103
C	3.293584	-0.145890	1.836725	C	1.753947	-1.995506	2.235474
H	-6.194910	-4.404695	0.002629	H	-7.702625	-1.832916	1.527443
H	4.993881	-0.096179	3.167672	H	2.212412	-3.309758	3.883942
P	1.025877	-0.248089	0.094164	P	1.121271	-0.227843	0.148848
C	-4.488435	-1.443250	-0.102882	C	-4.398856	-0.957512	1.396083
C	1.776887	1.329190	-0.514813	C	2.269027	1.142983	0.601619
C	-5.085645	-2.599951	0.420384	C	-5.796881	-0.820122	1.465448
Pt	-1.268060	-0.143574	0.605904	Pt	-1.077971	0.125043	0.883430
C	4.046306	-0.586877	2.931527	C	2.325819	-3.132694	2.811269
H	-2.604126	2.401376	-0.082315	H	-4.447391	3.286481	1.809178
C	2.904907	3.754837	-1.386530	C	3.950043	3.310725	1.213008
H	3.341030	4.697169	-1.727802	H	4.603287	4.153249	1.453797
C	2.071344	-0.760804	1.524960	C	1.895727	-1.751090	0.856326
P	-3.559869	-0.210087	0.917878	P	-3.294174	0.518298	1.439223
H	-5.054704	-2.814858	1.489166	H	-6.252024	0.173148	1.501473
C	1.272474	2.556714	-0.051073	C	1.796909	2.463079	0.494079
C	1.837459	3.760617	-0.483138	C	2.635050	3.540105	0.792981
C	3.589630	-1.647473	3.718535	C	3.035651	-4.043977	2.020681
C	1.612373	-1.820200	2.328845	C	2.612319	-2.667450	0.069021
H	0.434930	2.570338	0.651412	H	0.764900	2.646460	0.182866
H	4.179075	-1.989972	4.572798	H	3.476928	-4.936061	2.472521
H	1.435697	4.707648	-0.113890	H	2.256407	4.561534	0.705984
H	0.650293	-2.290409	2.108259	H	2.734407	-2.497755	-1.001989
C	-4.076064	-0.540121	2.674963	C	-3.523882	1.195922	3.143131
H	-5.086339	-0.117592	2.794888	C	3.176636	-3.808863	0.650355
C	2.370866	-2.265217	3.413540	S	-0.348186	0.959804	3.097679
S	-0.959095	1.361226	2.544626	H	-1.076830	0.471056	5.307811
H	-3.247938	2.053839	3.120437	C	-1.425993	0.102396	4.331311
H	-4.174144	-1.629219	2.783101	H	3.729608	-4.514905	0.025611
C	-2.506419	1.360342	3.552286	H	-1.182153	-0.970177	4.305807
H	2.004313	-3.090477	4.029106	C	-2.970580	0.282362	4.245757
H	-2.211895	1.783154	4.525016	H	-3.015366	2.171386	3.167038
C	-3.132620	-0.021780	3.777057	H	-4.600036	1.365741	3.305994
H	-2.320739	-0.748699	3.940036	H	-3.328961	0.691699	5.204498
H	-3.721644	-0.001102	4.710734	H	-3.444100	-0.709472	4.156261