

## Electronic Supplementary Information

# Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors

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**Table S1**  $\omega$ B97X-D and B3LYP relative gas-phase free energies (in kJ mol<sup>-1</sup>) of stationary points of motor **1** with different basis sets

Stationary point	$\omega$ B97X-D				B3LYP			
	SVP <sup>a</sup>	TZVP <sup>b</sup>	cc-pVDZ <sup>c</sup>	6-31++G(d,p) <sup>d</sup>	SVP <sup>a</sup>	TZVP <sup>b</sup>	cc-pVDZ <sup>c</sup>	6-31++G(d,p) <sup>d</sup>
( <i>P,P</i> )- <i>trans</i> -1	3.9	3.1	3.4	3.4	0.0	0.0	0.0	0.0
( <i>M,M</i> )- <i>cis</i> -2	54.6	59.5	56.7	55.6	62.0	66.7	63.5	63.3
TS <sub>2</sub>	155.9	156.2	156.0	156.0	145.6	149.2	145.8	147.3
( <i>M,P</i> )- <i>cis</i> -2	68.3	67.5	65.8	68.1	67.7	67.3	66.7	66.5
TS <sub>3</sub>	151.0	151.4	150.9	150.2	143.2	146.7	143.5	143.9
( <i>P,P</i> )- <i>cis</i> -2	0.0	0.0	0.0	0.0	10.6	5.2	3.8	4.0
( <i>M,M</i> )- <i>trans</i> -1	49.4	46.7	47.4	46.0	47.4	51.0	47.5	47.8
TS <sub>5</sub>	173.7	167.4	166.5	172.4	165.6	168.8	153.0	154.4
( <i>M,P</i> )- <i>trans</i> -1	29.6	27.2	28.1	29.2	31.2	32.7	31.1	32.0
TS <sub>6</sub>	165.4	165.7	164.3	164.0	157.1	160.4	156.6	158.4

<sup>a</sup> SVP is the Karlsruhe double- $\zeta$  split valence plus polarization basis set. <sup>b</sup> TZVP is the Karlsruhe triple- $\zeta$  split valence plus polarization basis set. <sup>c</sup> cc-pVDZ is the Dunning-type correlation-consistent polarized valence double- $\zeta$  basis set. <sup>d</sup> 6-31++G(d,p) is the Pople-style 6-31G(d,p) double- $\zeta$  basis set augmented with one set of polarization functions and one set of diffuse functions for both heavy atoms and hydrogens.

**Table S2** Relative gas-phase free energies (in kJ mol<sup>-1</sup>) of stationary points of motor **1** with different density functionals<sup>a</sup>

Stationary point	BP86	BLYP	B3LYP	PBE0	M06	M06-2X	BMK	$\omega$ B97X	$\omega$ B97X-D	B2PLYP	B2PLYP-D
( <i>P,P</i> )- <i>trans</i> -1	0.0	0.0	0.0	0.0	3.4	7.2	0.0	0.5	3.9	3.4	13.3
( <i>M,M</i> )- <i>cis</i> -2	51.3	57.0	62.0	58.5	47.5	50.0	58.4	58.9	54.6	54.0	46.0
TS <sub>2</sub>	133.4	137.9	145.6	143.9	149.6	155.2	154.7	152.1	155.9	146.7	155.0
( <i>M,P</i> )- <i>cis</i> -2	66.4	65.2	67.7	70.2	69.0	73.4	70.1	65.8	68.3	67.7	75.6
TS <sub>3</sub>	130.0	134.8	143.2	141.9	138.1	146.7	142.8	149.6	151.0	144.8	151.4
( <i>P,P</i> )- <i>cis</i> -2	2.1	3.0	10.6	3.2	0.0	0.0	7.9	0.0	0.0	0.0	0.0
( <i>M,M</i> )- <i>trans</i> -1	35.6	42.5	47.4	43.7	39.9	43.1	47.9	46.3	49.4	43.4	44.0
TS <sub>5</sub>	136.9	142.5	165.6	152.6	152.7	160.7	156.8	166.7	173.7	166.4	169.1
( <i>M,P</i> )- <i>trans</i> -1	29.8	30.7	31.2	30.9	31.1	29.8	30.6	27.3	29.6	31.1	36.0
TS <sub>6</sub>	143.7	147.6	157.1	156.6	152.8	162.2	165.6	162.9	165.4	156.4	162.4

<sup>a</sup> All calculations carried out with the SVP basis set.

## Comments on Tables S1 and S2

Based on the observation that the two principal methods of this work,  $\omega$ B97X-D and B3LYP, give opposing free energies for (*P,P*)-*trans*-1 and (*P,P*)-*cis*-2 at the SVP basis-set level, Tables S1 and S2 present key results from an investigation aimed at exploring how sensitive calculated free energies of the ground-state stationary points of motor **1** are to the choice of density functional and basis set. Table S1 focuses on basis-set effects and Table S2 on differences between different functionals. Included in the investigation are, in addition to  $\omega$ B97X-D and B3LYP, also the BP86, BLYP, PBE0, M06-2X and  $\omega$ B97X functionals used elsewhere in the manuscript, as well as M06,<sup>1</sup> BMK,<sup>2</sup> B2PLYP<sup>3</sup> and B2PLYP-D.<sup>4</sup> Of the latter, M06 and BMK are global hybrid meta-GGAs, whereas B2PLYP and B2PLYP-D are so-called double hybrids that contain both exact exchange and an explicit second-order correlation term obtained from Kohn-Sham orbitals and eigenvalues. In analogy with the relationship between  $\omega$ B97X and  $\omega$ B97X-D, B2PLYP-D adds empirical dispersion corrections<sup>5,6</sup> to B2PLYP.<sup>4</sup>

From Table S1, it is observed that all four basis sets considered – SVP and the larger TZVP, cc-pVDZ and 6-31++G(d,p) – consistently give very similar results for all ten stationary points along the rotary cycle. Indeed, the differences in calculated relative free energies between the basis sets are only of the order of a few kJ mol<sup>-1</sup>. Thus, the opposing predictions by  $\omega$ B97X-D and B3LYP as to whether (*P,P*)-*trans*-1 or (*P,P*)-*cis*-2 is the most stable isomer

persist at all basis-set levels.

From Table S2, in turn, it can be inferred that the calculated free energies are not very sensitive to the choice of density functional either, especially considering the number of functionals tested (11) and their different construction. Specifically, for the ten stationary points, the range over which the free-energy estimates vary between the methods is on average  $\sim 18 \text{ kJ mol}^{-1}$ , and a mere  $\sim 6 \text{ kJ mol}^{-1}$  if only the  $\omega\text{B97X-D}$  and B3LYP results are considered. As for the relative free energies of *(P,P)-trans-1* and *(P,P)-cis-2*,  $\omega\text{B97X-D}$  is joined by M06, M06-2X,  $\omega\text{B97X}$ , B2PLYP and B2PLYP-D in predicting that *(P,P)-cis-2* is more stable, and B3LYP is joined by BP86, BLYP, PBE0 and BMK in predicting that *(P,P)-trans-1* is more stable.

**Table S3** Vertical (VEE) and adiabatic (AEE)  $S_0 \rightarrow S_1$  excitation energies (in eV) of the (*P,P*)-*trans*-1 and (*P,P*)-*cis*-2 isomers of motor **1** in the gas phase at different levels of theory

Level of theory <sup>a</sup>	<i>(P,P)</i> - <i>trans</i> -1		<i>(P,P)</i> - <i>cis</i> -2	
	VEE	AEE	VEE	AEE
$\omega$ B97X-D/SVP	4.33	3.26	4.08	3.33
$\omega$ B97X-D/TZVP	4.34	3.31	4.15	3.39
$\omega$ B97X-D/cc-pVDZ	4.32	3.30	4.08	3.33
$\omega$ B97X-D/6-31++G(d,p)	4.29	3.28	4.10	3.35
CC2/SVP	4.24	– <sup>c</sup>	3.70	– <sup>c</sup>
CC2/TZVP	4.15 <sup>b</sup>	– <sup>c</sup>	3.59 <sup>b</sup>	– <sup>c</sup>
CC2/cc-pVDZ	4.17	– <sup>c</sup>	3.66	– <sup>c</sup>

<sup>a</sup> CC2 calculations carried out with the Turbomole 6.3 suite of programs.<sup>7,8</sup> <sup>b</sup> Calculation based on CC2/SVP  $S_0$  geometry. <sup>c</sup> Calculation not performed.

**Table S4**  $\omega$ B97X-D and B3LYP relative free energies (in  $\text{kJ mol}^{-1}$ ) of stationary points of motor **1** in the gas phase and in solution<sup>a</sup>

Stationary point <sup>b</sup>	$\omega$ B97X-D			B3LYP		
	Gas phase	Hexane	Methanol	Gas phase	Hexane	Methanol
<i>(P,P)</i> -trans-1	3.9	9.5	16.8	0.0	0.0	3.6
<i>(M,M)</i> -cis-2	54.6	56.6	54.4	62.0	58.4	55.3
TS <sub>2</sub>	155.9	151.5	156.3	145.6	137.0	139.0
<i>(M,P)</i> -cis-2	68.3	72.8	73.7	67.7	66.0	64.4
TS <sub>3</sub>	151.0	148.0	152.1	143.2	136.1	137.1
<i>(P,P)</i> -cis-2	0.0	0.0	0.0	10.6	3.2	0.0
<i>(M,M)</i> -trans-1	49.4	51.4	58.5	47.4	44.5	47.9
TS <sub>5</sub>	173.7	168.9	175.2	165.6	156.2	158.7
<i>(M,P)</i> -trans-1	29.6	29.7	36.3	31.2	26.1	28.7
TS <sub>6</sub>	165.4	160.7	167.5	157.1	147.6	150.5

<sup>a</sup> All calculations carried out with the SVP basis set. <sup>b</sup> Cartesian coordinates of all stationary points are included in part 10 of this document.

**Table S5**  $\omega$ B97X-D and B3LYP relative free energies (in  $\text{kJ mol}^{-1}$ ) of stationary points of the *i*-propyl-substituted motor in the gas phase and in solution<sup>a</sup>

Stationary point <sup>b</sup>	$\omega$ B97X-D			B3LYP			Exp. <sup>c</sup>
	Gas phase	Hexane	Methanol	Gas phase	Hexane	Methanol	
( <i>P,P</i> )- <i>trans</i> -1	13.0	21.0	29.0	11.0	12.3	16.8	
( <i>M,M</i> )- <i>cis</i> -2	94.3	88.4	86.3	101.9	97.2	95.4	
TS <sub>2</sub>	160.7	159.4	164.0	161.9	155.0	155.9	
( <i>M,P</i> )- <i>cis</i> -2	69.0	75.0	77.1	67.7	68.7	68.8	
TS <sub>3</sub>	171.9	170.3	175.3	162.7	159.6	161.6	
( <i>P,P</i> )- <i>cis</i> -2	0.0	0.0	0.0	0.0	0.0	0.0	
( <i>M,M</i> )- <i>trans</i> -1	106.5	107.8	114.9	106.3	103.0	107.1	
TS <sub>5</sub>	214.7	214.2	222.0	205.7	199.2	203.8	
( <i>M,P</i> )- <i>trans</i> -1	21.2	27.0	34.0	24.0	24.2	27.9	
TS <sub>6</sub>	181.4	178.3	185.5	172.1	168.0	171.8	
<u>Helix inversion barriers</u>							
( <i>M,M</i> )- <i>cis</i> -2 → ( <i>M,P</i> )- <i>cis</i> -2	66.4	71.0	77.7	60.0	57.8	60.5	– <sup>d</sup>
( <i>M,P</i> )- <i>cis</i> -2 → ( <i>P,P</i> )- <i>cis</i> -2	102.9	95.3	98.2	95.1	90.9	92.8	– <sup>d</sup>
( <i>M,M</i> )- <i>trans</i> -1 → ( <i>M,P</i> )- <i>trans</i> -1	108.2	106.4	107.1	99.4	96.2	96.7	124
( <i>M,P</i> )- <i>trans</i> -1 → ( <i>P,P</i> )- <i>trans</i> -1	160.2	151.3	151.5	148.1	143.8	143.9	131

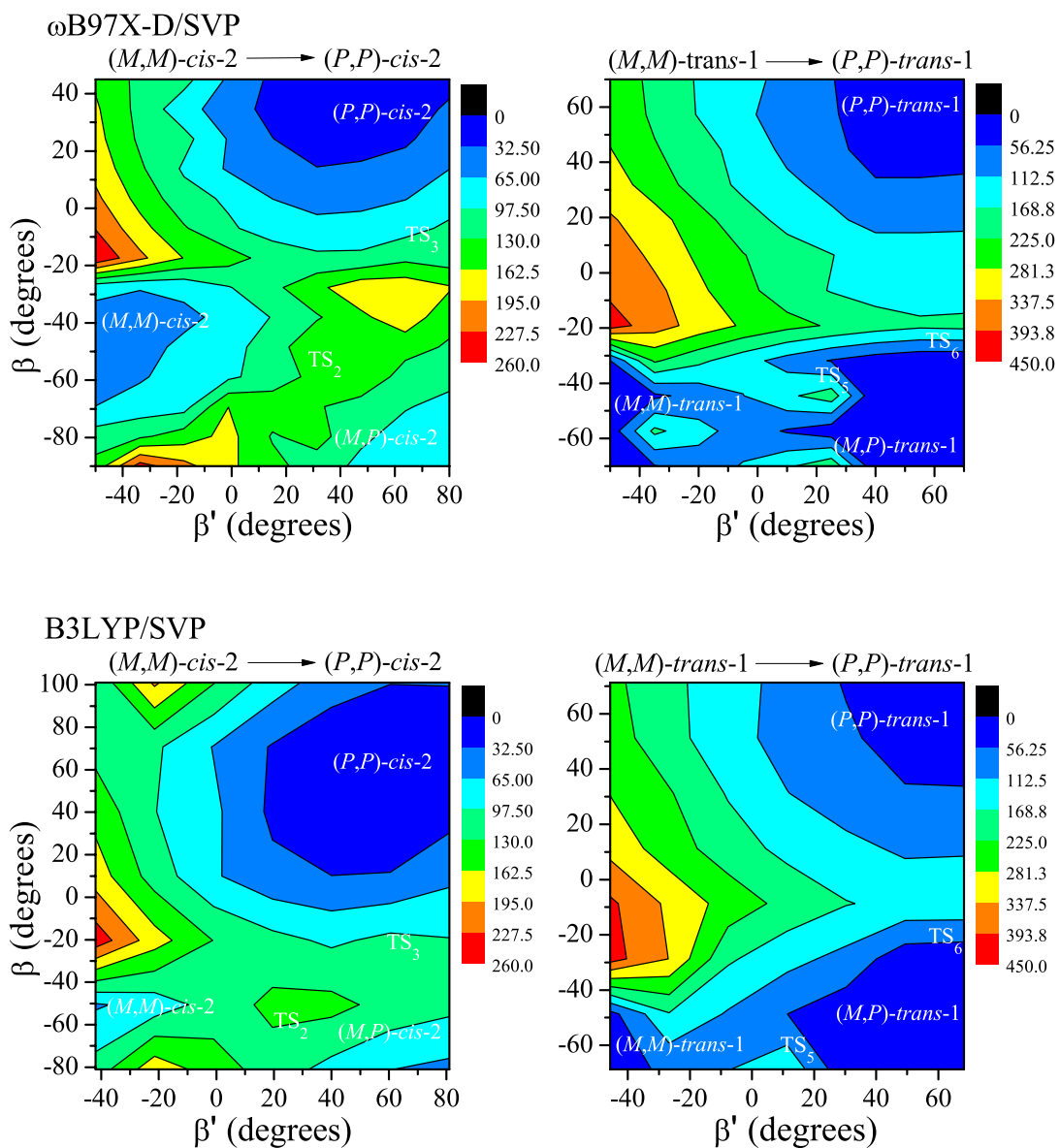
<sup>a</sup> All calculations carried out with the SVP basis set. <sup>b</sup> Stationary points are identified in the same way as for motor **1**.

<sup>c</sup> Experimental free-energy barriers from Ref. 20 of the main text. <sup>d</sup> Not available.

**Table S6** Rate-determining  $\omega$ B97X-D and B3LYP gas-phase free-energy barriers (in  $\text{kJ mol}^{-1}$ ) for the thermal helix inversion steps of motors **2** and **3** with different basis sets

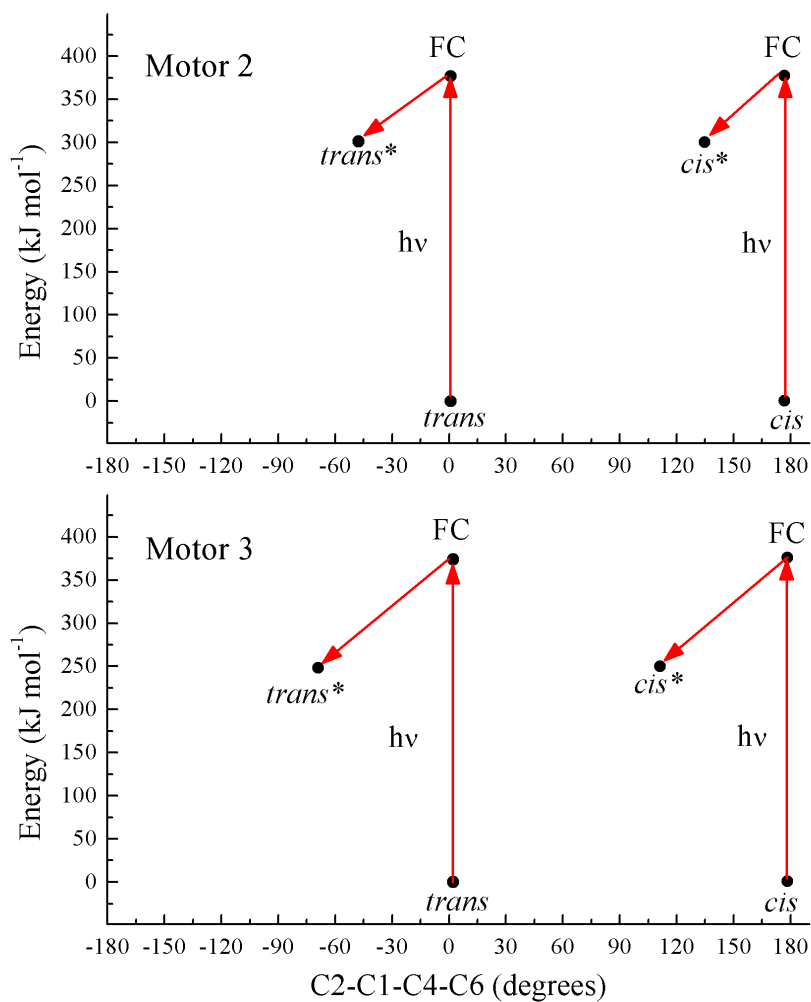
Motor	Half cycle	$\omega$ B97X-D				B3LYP			
		SVP	TZVP	cc-pVDZ	6-31++G(d,p)	SVP	TZVP	cc-pVDZ	6-31++G(d,p)
<b>2</b>	<i>trans</i> $\rightarrow$ <i>cis</i>	41.4	47.4	45.0	47.3	34.8	40.7	36.8	38.0
	<i>cis</i> $\rightarrow$ <i>trans</i>	40.0	45.4	41.6	44.3	35.2	40.6	37.4	39.1
<b>3</b>	<i>trans</i> $\rightarrow$ <i>cis</i>	23.9	33.4	26.6	33.2	19.7	27.1	21.8	25.0
	<i>cis</i> $\rightarrow$ <i>trans</i>	22.9	31.9	24.4	29.3	17.4	25.9	19.2	23.8

**Fig. S1** Two-dimensional  $\omega$ B97X-D/SVP (upper panels) and B3LYP/SVP (lower panels)  $S_0$  PESs (in  $\text{kJ mol}^{-1}$ ) of motor **1** in the gas phase describing torsional motion along the  $\beta$  and  $\beta'$  coordinates. These PESs encompass both stepwise and concerted mechanisms for the  $(M,M)\text{-cis-2} \rightarrow (P,P)\text{-cis-2}$  and  $(M,M)\text{-trans-1} \rightarrow (P,P)\text{-trans-1}$  thermal helix inversion steps, and were obtained by performing a series of constrained geometry optimizations, where for each optimization all other geometric parameters than the  $\beta$  and  $\beta'$  dihedral angles were relaxed. The approximate positions of the relevant stationary points are also indicated in the plots.





**Fig. S2** FC relaxation along the C2–C1–C4–C6 coordinate of the *trans* and *cis* isomers of motors **2** and **3** calculated at the  $\omega$ B97X-D/SVP gas-phase level. These data indicate that the associated photoisomerizations occur in a unidirectional fashion.



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### Cartesian coordinates for stationary points in Table S4

ωB97X-D/SVP in the gas phase

*(P,P)*-trans-1

C	0.094104	-0.492808	-1.971320
C	-0.477461	-1.818807	-2.561913
C	-1.443523	-2.551382	-1.614981
C	-2.420744	-1.581910	-1.006098
C	-1.884092	-0.428467	-0.457960
C	-0.402693	-0.330544	-0.541171
C	-2.739999	0.583257	0.074032
C	-4.146923	0.349942	0.104447
C	-4.659972	-0.863637	-0.427087
C	-3.819602	-1.795788	-0.983149
C	-5.000821	1.347742	0.651527
C	-4.491182	2.530278	1.127068
C	-3.097723	2.776588	1.065943
C	-2.247290	1.828994	0.552214
C	0.402696	-0.330548	0.541181
H	1.189703	-0.565888	-1.949579
C	1.884095	-0.428467	0.457960
C	2.420755	-1.581915	1.006082
C	1.443540	-2.551392	1.614969
C	0.477502	-1.818815	2.561922
C	-0.094094	-0.492827	1.971331
C	3.819614	-1.795786	0.983122
C	4.659977	-0.863625	0.427067
C	4.146919	0.349956	-0.104453
C	2.739994	0.583264	-0.074030
C	-0.290898	0.707184	-2.842892
C	2.247274	1.828999	-0.552205
C	3.097699	2.776602	-1.065930
C	4.491160	2.530302	-1.127060
C	5.000809	1.347766	-0.651529
H	-1.189691	-0.565934	1.949590
C	0.290878	0.707171	2.842908
H	-1.014885	-1.594209	-3.496686
H	0.347142	-2.495489	-2.830918
H	-0.863592	-3.028077	-0.805832
H	-1.966433	-3.359152	-2.148079
H	-5.738662	-1.036890	-0.400191
H	-4.226074	-2.717206	-1.408298
H	-6.076870	1.157970	0.681436
H	-5.158957	3.288292	1.542080
H	-2.699334	3.727664	1.426223
H	-1.175010	2.021074	0.494646
H	1.966456	-3.359167	2.148054
H	0.863594	-3.028077	0.805827
H	1.014954	-1.594202	3.496675
H	-0.347088	-2.495500	2.830962
H	4.226092	-2.717207	1.408259
H	5.738667	-1.036873	0.400163
H	1.174992	2.021068	-0.494636
H	2.699302	3.727677	-1.426205
H	5.158929	3.288323	-1.542070
H	6.076859	1.158001	-0.681443
H	-0.072778	0.568075	3.872663
H	-0.143165	1.641469	2.459709
H	1.385198	0.828354	2.883720
H	-1.385221	0.828336	-2.883711
H	0.072769	0.568106	-3.872646

<i>(P,P)</i> -trans-1*	H	0.143115	1.641490	-2.459682
	C	0.461199	-2.220521	1.480559
	C	1.820243	-2.843134	1.793789
	C	2.811341	-1.763797	2.186833
	C	2.905152	-0.687151	1.138120
	C	1.792316	-0.360281	0.309472
	C	0.579554	-1.105261	0.440512
	C	1.966565	0.748503	-0.637865
	C	3.244267	1.380370	-0.763707
	C	4.318622	0.971666	0.060225
	C	4.132118	-0.023545	0.991271
	C	3.428045	2.432155	-1.703140
	C	2.392110	2.881599	-2.483425
	C	1.119575	2.293652	-2.338487
	C	0.921676	1.265620	-1.441626
	C	-0.575983	-1.104208	-0.444991
	H	-0.177320	-3.005979	1.041925
	C	-1.791167	-0.363938	-0.310849
	C	-2.901092	-0.687207	-1.144804
	C	-2.803056	-1.758195	-2.198998
	C	-1.809800	-2.837142	-1.810362
	C	-0.452791	-2.212766	-1.491736
	C	-4.128770	-0.024678	-0.999227
	C	-4.319275	0.966044	-0.064232
	C	-3.248694	1.369383	0.767217
	C	-1.970658	0.737556	0.644124
	C	-0.278235	-1.742271	2.742378
	C	-0.930520	1.247535	1.458545
	C	-1.132587	2.269345	2.361488
	C	-2.405222	2.858131	2.502206
	C	-3.436795	2.415136	1.712536
	H	0.187255	-2.999402	-1.057329
	C	0.286600	-1.724685	-2.749706
	H	1.716885	-3.593901	2.593309
	H	2.191223	-3.368855	0.898200
	H	3.808903	-2.193964	2.362502
	H	2.505674	-1.309939	3.147401
H	5.289483	1.461265	-0.045681	
H	4.963759	-0.324356	1.634311	
H	4.419411	2.885102	-1.784604	
H	2.547042	3.691983	-3.198975	
H	0.277306	2.656134	-2.931600	
H	-0.074985	0.844238	-1.355631	
H	-2.497475	-1.298822	-3.156960	
H	-3.799330	-2.190012	-2.378009	
H	-1.703333	-3.583300	-2.613781	
H	-2.180675	-3.368708	-0.918175	
H	-4.957642	-0.322336	-1.647316	
H	-5.290371	1.455578	0.039668	
H	0.066081	0.824994	1.376448	
H	-0.293851	2.625989	2.963102	
H	-2.563685	3.663854	3.222238	
H	-4.428214	2.868454	1.791264	
H	1.290118	-1.356000	-2.495205	
H	-0.246219	-0.902765	-3.250023	
H	0.395886	-2.553717	-3.467230	
H	0.253218	-0.922524	3.247731	
H	-0.384744	-2.576335	3.454415	
H	-1.282837	-1.374154	2.491297	
<i>(M,M)</i> -cis-2	C	-2.876352	1.490702	-0.031709

C	-2.682172	2.957196	0.364355
C	-1.437510	3.532918	-0.302380
C	-0.230984	2.765199	0.164784
C	-0.359710	1.427092	0.526513
C	-1.583924	0.671307	0.151540
C	0.728175	0.817187	1.258714
C	1.996756	1.463733	1.287451
C	2.123604	2.769967	0.743999
C	1.019150	3.423034	0.269817
C	3.105316	0.815260	1.896192
C	2.958352	-0.398836	2.517986
C	1.677384	-0.991421	2.592401
C	0.597870	-0.398406	1.984422
C	-1.585102	-0.668614	-0.151546
H	-3.674973	1.078344	0.601686
C	-0.362280	-1.426438	-0.526908
C	-0.235882	-2.764953	-0.165746
C	-1.443744	-3.531311	0.300365
C	-2.687675	-2.952286	-0.364814
C	-2.878613	-1.485918	0.033064
C	1.013324	-3.424645	-0.270379
C	2.119002	-2.773157	-0.743859
C	1.994329	-1.466694	-1.287280
C	0.726711	-0.818258	-1.258929
C	-3.365847	1.424271	-1.491540
C	0.598366	0.397403	-1.984849
C	1.678919	0.988726	-2.592619
C	2.959021	0.394361	-2.517661
C	3.104037	-0.819877	-1.895672
H	-3.677678	-1.071614	-0.598451
C	-3.365499	-1.419773	1.493782
H	-3.579024	3.532588	0.086607
H	-2.566585	3.043155	1.456966
H	-1.309983	4.595598	-0.045639
H	-1.534267	3.498964	-1.401502
H	3.098630	3.262469	0.765572
H	1.095779	4.460032	-0.068140
H	4.077503	1.313912	1.872992
H	3.816306	-0.889432	2.982571
H	1.542557	-1.927374	3.138653
H	-0.384266	-0.860491	2.065708
H	-1.540024	-3.499559	1.399587
H	-1.318103	-4.593685	0.041381
H	-3.585478	-3.526242	-0.087180
H	-2.573009	-3.037101	-1.457618
H	1.088157	-4.461867	0.067301
H	3.093328	-3.267063	-0.765007
H	-0.383110	0.860833	-2.066570
H	1.545584	1.924758	-3.139108
H	3.817812	0.883725	-2.981989
H	4.075517	-1.319895	-1.872092
H	-3.517477	-0.390826	1.841427
H	-2.639561	-1.879070	2.180862
H	-4.318910	-1.959337	1.605679
H	-2.640551	1.882437	-2.180054
H	-4.318881	1.964763	-1.602094
H	-3.519426	0.395355	-1.838498
C	2.152236	-1.764881	1.078091
C	3.314399	-2.140133	0.171764
C	4.036041	-0.868025	-0.230005
C	3.154495	0.364918	-0.288185

TS<sub>2</sub>

C	1.756710	0.377892	-0.171382
C	1.133344	-0.942354	0.287400
C	1.114846	1.670660	-0.416288
C	1.898096	2.869868	-0.430132
C	3.312927	2.788718	-0.417388
C	3.904978	1.565060	-0.429678
C	1.277637	4.143008	-0.537106
C	-0.077194	4.265874	-0.715411
C	-0.843448	3.092137	-0.850133
C	-0.258615	1.854399	-0.715831
C	-0.091336	-1.517616	0.111169
H	1.668638	-2.676985	1.405434
C	-1.378101	-0.899994	-0.329327
C	-1.878205	-1.307307	-1.551276
C	-1.014210	-2.271420	-2.313973
C	-0.568563	-3.424066	-1.387776
C	-0.460281	-3.034051	0.114444
C	-3.144419	-0.853367	-1.991395
C	-3.906211	-0.038417	-1.192416
C	-3.455818	0.336913	0.103404
C	-2.182657	-0.115488	0.557486
C	2.578339	-1.066675	2.378432
C	-1.743299	0.270624	1.852613
C	-2.525493	1.066336	2.653413
C	-3.786383	1.522493	2.200091
C	-4.239330	1.163098	0.954817
H	-1.482539	-3.059200	0.522596
C	0.273239	-4.155945	0.852693
H	4.005141	-2.839356	0.670234
H	2.911486	-2.661109	-0.711867
H	4.532378	-0.980062	-1.208304
H	4.847050	-0.661246	0.487520
H	3.905165	3.706386	-0.447973
H	4.993369	1.484163	-0.493252
H	1.916207	5.029597	-0.502805
H	-0.543889	5.249332	-0.800874
H	-1.909826	3.151503	-1.079113
H	-0.868652	0.989650	-0.911221
H	-0.121539	-1.735305	-2.675007
H	-1.532005	-2.661455	-3.201828
H	0.411511	-3.799692	-1.724050
H	-1.276065	-4.264480	-1.470865
H	-3.512109	-1.160413	-2.973871
H	-4.879401	0.320546	-1.536734
H	-0.763203	-0.063587	2.195891
H	-2.170067	1.356011	3.644642
H	-4.396703	2.159942	2.843450
H	-5.212153	1.510915	0.597576
H	0.324079	-3.987315	1.937587
H	1.287560	-4.340798	0.471344
H	-0.298060	-5.085133	0.697755
H	3.086638	-0.105738	2.217939
H	3.257358	-1.720195	2.949122
H	1.697288	-0.869543	3.007993
C	-2.874185	0.256758	-1.309666
C	-3.778991	1.104617	-0.378914
C	-3.261655	1.123254	1.063530
C	-1.860985	1.682712	1.046261
C	-1.003516	1.225856	0.054305
C	-1.516348	0.015459	-0.664352
C	0.229461	1.906317	-0.178567

(*M,P*)-cis-2

C	0.654151	2.911771	0.740506
C	-0.198533	3.268382	1.817818
C	-1.441958	2.700667	1.936253
C	1.900259	3.563261	0.526269
C	2.664329	3.278468	-0.577976
C	2.202855	2.342035	-1.533381
C	1.018592	1.677883	-1.335890
C	-0.947206	-1.198852	-0.492920
H	-3.364777	-0.707593	-1.456583
C	0.288297	-1.393999	0.328301
C	0.050640	-1.864635	1.607222
C	-1.382143	-2.189024	1.943961
C	-2.095494	-2.945514	0.791798
C	-1.569583	-2.591088	-0.630714
C	1.129849	-2.056526	2.503196
C	2.421079	-1.827163	2.097267
C	2.704291	-1.501863	0.743575
C	1.622892	-1.332076	-0.169886
C	-2.704509	0.912652	-2.683040
C	1.918483	-1.207619	-1.555147
C	3.215338	-1.168349	-2.001932
C	4.289645	-1.233739	-1.081398
C	4.037592	-1.404349	0.257118
H	-0.709576	-3.251485	-0.826373
C	-2.585348	-2.919827	-1.724954
H	-3.811635	2.145524	-0.740254
H	-4.811449	0.723998	-0.419181
H	-3.280669	0.099669	1.474686
H	-3.911247	1.735705	1.706193
H	0.131488	4.033630	2.524655
H	-2.121862	3.024771	2.728605
H	2.231042	4.311177	1.251418
H	3.617598	3.788192	-0.733386
H	2.793071	2.144720	-2.430677
H	0.652495	0.973437	-2.080696
H	-1.913402	-1.243793	2.135633
H	-1.440427	-2.770634	2.875502
H	-3.172360	-2.713055	0.835968
H	-2.003164	-4.032342	0.944609
H	0.924811	-2.384011	3.525791
H	3.251173	-1.948558	2.797598
H	1.088643	-1.162125	-2.263607
H	3.422192	-1.082686	-3.071045
H	5.318372	-1.174291	-1.443503
H	4.862231	-1.495632	0.968777
H	-2.281976	-2.499448	-2.695159
H	-3.600946	-2.566320	-1.498281
H	-2.652182	-4.012641	-1.840949
H	-2.166510	1.870257	-2.592524
H	-3.682875	1.116622	-3.145952
H	-2.131838	0.264097	-3.363116

TS<sub>3</sub>

C	0.669938	-2.930516	-0.211344
C	1.008639	-3.158835	-1.714756
C	1.428060	-1.885974	-2.480300
C	2.078698	-0.890560	-1.563603
C	1.415651	-0.631013	-0.377325
C	0.231479	-1.466519	-0.061494
C	1.980573	0.265836	0.587613
C	3.193030	0.942015	0.264309
C	3.822814	0.683375	-0.983623

C	3.285585	-0.217762	-1.868255
C	3.738692	1.870032	1.193243
C	3.115836	2.117375	2.391085
C	1.918042	1.438297	2.717401
C	1.366414	0.537296	1.840215
C	-1.048843	-1.114971	0.255162
H	-0.173232	-3.588384	0.003619
C	-1.882157	0.109807	-0.101109
C	-3.270196	-0.096950	-0.095314
C	-3.952938	-1.454465	-0.074763
C	-3.038095	-2.626280	0.254831
C	-1.911237	-2.067511	1.112844
C	-4.181817	0.993288	-0.110074
C	-3.753853	2.285436	-0.121025
C	-2.374318	2.554335	-0.305363
C	-1.444176	1.470338	-0.409033
C	1.845609	-3.334314	0.686026
C	-0.160269	1.824610	-0.900375
C	0.230001	3.127969	-1.103417
C	-0.654709	4.192499	-0.841732
C	-1.943411	3.897422	-0.475854
H	-2.389088	-1.364751	1.818148
C	-1.264629	-3.092051	2.048947
H	1.816575	-3.904434	-1.774187
H	0.136695	-3.600952	-2.218948
H	0.526666	-1.416571	-2.909096
H	2.084273	-2.137610	-3.325948
H	4.750401	1.208592	-1.224712
H	3.783452	-0.417949	-2.820471
H	4.666805	2.386206	0.934467
H	3.541908	2.835775	3.094764
H	1.427765	1.635286	3.673099
H	0.436548	0.027420	2.093042
H	-4.457835	-1.591506	-1.045621
H	-4.759963	-1.409907	0.675269
H	-2.615031	-3.086790	-0.653066
H	-3.598693	-3.413906	0.782691
H	-5.251317	0.772120	-0.060409
H	-4.460434	3.116047	-0.054305
H	0.528613	1.046392	-1.188991
H	1.232233	3.326189	-1.489381
H	-0.336060	5.227833	-0.979284
H	-2.680095	4.693908	-0.342503
H	-0.357097	-2.692126	2.521948
H	-1.012664	-4.050951	1.578236
H	-1.983071	-3.319129	2.851625
H	2.764410	-2.794007	0.413643
H	2.047390	-4.411898	0.583055
H	1.640361	-3.128136	1.745817

(*P,P*)-*cis*-2

C	-2.886604	1.465235	-0.295898
C	-2.724679	2.897229	0.264849
C	-1.546178	3.002900	1.235164
C	-0.294145	2.609115	0.498885
C	-0.355654	1.472545	-0.292955
C	-1.595419	0.659648	-0.158734
C	0.764280	1.110944	-1.107041
C	1.987083	1.825708	-0.954001
C	2.032256	2.942748	-0.077582
C	0.908532	3.347563	0.596359
C	3.129961	1.413046	-1.693017
C	3.058790	0.362002	-2.572294



C	1.827144	-0.305968	-2.774891
C	0.711471	0.062970	-2.066023
C	-1.595676	-0.659324	0.158764
H	-3.663798	0.971269	0.303590
C	-0.356163	-1.472581	0.293105
C	-0.294891	-2.609176	-0.498725
C	-1.547025	-3.002843	-1.234922
C	-2.725425	-2.896670	-0.264556
C	-2.887252	-1.464400	0.295390
C	0.907664	-3.347819	-0.596274
C	2.031495	-2.943204	0.077605
C	1.986547	-1.826190	0.954066
C	0.763870	-1.111225	1.107178
C	-3.348979	1.489227	-1.756318
C	0.711265	-0.063315	2.066237
C	1.827020	0.305403	2.775089
C	3.058555	-0.362740	2.572387
C	3.129521	-1.413749	1.693054
H	-3.663725	-0.970423	-0.305051
C	-3.350863	-1.487680	1.755413
H	-2.544210	3.603174	-0.562355
H	-3.662199	3.211872	0.748546
H	-1.713631	2.330554	2.097141
H	-1.455627	4.021687	1.640063
H	2.972736	3.487960	0.033691
H	0.940993	4.229079	1.242175
H	4.069312	1.953227	-1.550407
H	3.944405	0.050721	-3.130522
H	1.764885	-1.118163	-3.502268
H	-0.238094	-0.444996	-2.234053
H	-1.456676	-4.021760	-1.639540
H	-1.714335	-2.330705	-2.097092
H	-2.544813	-3.602153	0.563014
H	-3.663043	-3.211567	-0.747906
H	0.939936	-4.229337	-1.242098
H	2.971884	-3.488559	-0.033742
H	-0.238229	0.444755	2.234363
H	1.764917	1.117548	3.502534
H	3.944249	-0.051624	3.130586
H	4.068782	-1.954065	1.550376
H	-3.554802	-0.472466	2.128310
H	-2.571848	-1.929982	2.396580
H	-4.268011	-2.086603	1.870413
H	-2.569300	1.931509	-2.396688
H	-4.265850	2.088466	-1.871877
H	-3.552925	0.474179	-2.129678

(*P,P*)-*cis*-2\*

C	2.647342	1.942866	0.169096
C	2.238834	3.401658	-0.122276
C	0.968216	3.478771	-0.952664
C	-0.137496	2.761486	-0.233868
C	0.180947	1.521541	0.394424
C	1.471053	0.968761	0.115596
C	-0.883350	0.813670	1.096499
C	-2.240545	1.222018	0.897280
C	-2.506087	2.379492	0.145431
C	-1.459513	3.164934	-0.347585
C	-3.285729	0.436235	1.463097
C	-3.004185	-0.653844	2.253358
C	-1.664787	-0.996121	2.523281
C	-0.629911	-0.253204	1.976306
C	1.693988	-0.406042	-0.192861

H	3.389142	1.640106	-0.587902
C	0.659894	-1.343705	-0.498262
C	0.804350	-2.704265	-0.044472
C	2.160385	-3.273173	0.276665
C	3.141095	-2.209119	0.750315
C	3.105558	-0.981807	-0.166882
C	-0.334886	-3.455820	0.196218
C	-1.621393	-2.971945	-0.079324
C	-1.786728	-1.774826	-0.793262
C	-0.631692	-0.980587	-1.088874
C	3.312596	1.892754	1.558037
C	-0.782251	0.098761	-1.973469
C	-2.034479	0.485879	-2.436186
C	-3.183385	-0.232509	-2.061792
C	-3.061860	-1.342125	-1.255741
H	3.799981	-0.249767	0.256862
C	3.592646	-1.283575	-1.590325
H	2.055360	3.929265	0.827965
H	3.073598	3.923307	-0.615192
H	1.136041	2.997930	-1.935662
H	0.684084	4.522198	-1.155363
H	-3.542904	2.686435	-0.010556
H	-1.688369	4.075990	-0.907158
H	-4.320734	0.729187	1.271016
H	-3.815234	-1.249078	2.678331
H	-1.437449	-1.836240	3.182284
H	0.404817	-0.521526	2.193924
H	2.561222	-3.751155	-0.635726
H	2.066374	-4.077516	1.021882
H	4.161807	-2.621855	0.796485
H	2.878104	-1.889929	1.773283
H	-0.224344	-4.442272	0.654918
H	-2.498879	-3.573752	0.168412
H	0.103704	0.658370	-2.277955
H	-2.119603	1.343416	-3.106444
H	-4.165845	0.085859	-2.417192
H	-3.941444	-1.930500	-0.983451
H	3.635144	-0.359449	-2.186850
H	2.916722	-1.975844	-2.114224
H	4.601394	-1.726683	-1.574837
H	2.579922	2.184091	2.326311
H	4.157193	2.598910	1.604475
H	3.689461	0.895186	1.821872

(*M,M*)-*trans*-1

C	0.338463	-1.918636	-0.880039
C	-0.711520	-2.975264	-1.270820
C	-1.825106	-2.354330	-2.114596
C	-2.567467	-1.407167	-1.216795
C	-1.818111	-0.619393	-0.351443
C	-0.339750	-0.571245	-0.528103
C	-2.497056	0.091414	0.703102
C	-3.924714	0.121910	0.713803
C	-4.645530	-0.597206	-0.274729
C	-3.980301	-1.374990	-1.186272
C	-4.608418	0.843174	1.731902
C	-3.920425	1.480323	2.732469
C	-2.507916	1.408228	2.761121
C	-1.821758	0.739615	1.776711
C	0.340621	0.614201	-0.481575
H	0.874880	-2.302655	0.001601
C	1.818640	0.646992	-0.299681
C	2.570528	1.496889	-1.101691

C	1.831038	2.511419	-1.925279
C	0.716485	3.067247	-1.038430
C	-0.335283	1.985300	-0.730434
C	3.983269	1.458749	-1.072978
C	4.645898	0.610950	-0.224050
C	3.922399	-0.180304	0.705684
C	2.494936	-0.144482	0.697306
C	1.353217	-1.797608	-2.027929
C	1.816956	-0.871261	1.717582
C	2.500621	-1.616790	2.646936
C	3.912850	-1.691725	2.612382
C	4.603419	-0.981028	1.664500
H	-0.871637	2.302433	0.177305
C	-1.349082	1.953014	-1.885005
H	-0.211854	-3.792841	-1.811693
H	-1.168858	-3.420476	-0.372956
H	-2.509170	-3.120701	-2.507847
H	-1.395966	-1.831064	-2.986793
H	-5.737544	-0.556551	-0.268860
H	-4.538952	-1.978595	-1.906228
H	-5.700965	0.866937	1.708343
H	-4.456292	2.025005	3.512634
H	-1.957063	1.883231	3.575900
H	-0.734267	0.695041	1.823522
H	1.402998	2.057001	-2.835774
H	2.516807	3.304661	-2.257463
H	0.218382	3.923755	-1.516845
H	1.172789	3.443034	-0.108843
H	4.544117	2.114121	-1.744322
H	5.737773	0.566594	-0.221205
H	0.729602	-0.826181	1.767800
H	1.947749	-2.151604	3.422340
H	4.446804	-2.297850	3.347192
H	5.695866	-1.006994	1.638973
H	-0.868619	1.628139	-2.821694
H	-1.761856	2.960175	-2.045828
H	-2.193623	1.281710	-1.698600
H	0.874172	-1.399564	-2.936702
H	1.764229	-2.789887	-2.266670
H	2.199085	-1.144838	-1.789188

TS<sub>5</sub>

C	-0.345151	-0.880915	1.499065
C	-0.440397	-2.400440	1.317973
C	0.471749	-2.859263	0.188112
C	1.728302	-2.032737	0.078028
C	1.697625	-0.625874	0.044158
C	0.293251	-0.087192	0.333740
C	2.976217	0.036084	-0.204442
C	4.185286	-0.740013	-0.257940
C	4.139489	-2.147817	-0.143986
C	2.934279	-2.767778	-0.013600
C	5.451301	-0.119983	-0.449970
C	5.571236	1.232012	-0.627683
C	4.395276	2.008276	-0.633368
C	3.165884	1.428184	-0.432088
C	-0.456209	0.967372	-0.145422
H	-1.351737	-0.484058	1.661974
C	-1.950229	0.894694	-0.091322
C	-2.726719	2.015268	0.195700
C	-2.140847	3.394032	0.049249
C	-0.997472	3.327252	-0.958053
C	0.090704	2.356668	-0.485249

C	-4.105065	1.872754	0.501368
C	-4.730886	0.657962	0.436086
C	-4.040388	-0.455139	-0.114621
C	-2.660685	-0.317189	-0.446588
C	0.455406	-0.518579	2.763501
C	-2.076019	-1.340107	-1.239343
C	-2.773916	-2.472981	-1.585427
C	-4.098785	-2.662911	-1.133189
C	-4.719541	-1.664899	-0.422771
H	0.829024	2.282899	-1.295630
C	0.732855	2.942981	0.793011
H	-0.153793	-2.901963	2.255648
H	-1.476284	-2.698498	1.101613
H	-0.066899	-2.788932	-0.766575
H	0.734628	-3.919847	0.305181
H	5.069152	-2.720092	-0.183699
H	2.882043	-3.857627	0.039499
H	6.335852	-0.761839	-0.464272
H	6.548019	1.695809	-0.778142
H	4.451801	3.085454	-0.805999
H	2.313394	2.078559	-0.473847
H	-1.802670	3.814279	1.010312
H	-2.931225	4.071451	-0.309245
H	-0.549554	4.321875	-1.108646
H	-1.399292	3.000416	-1.930724
H	-4.664880	2.763525	0.799673
H	-5.782897	0.552236	0.711429
H	-1.060678	-1.193484	-1.604752
H	-2.300935	-3.228687	-2.216844
H	-4.636550	-3.579927	-1.383165
H	-5.764198	-1.769365	-0.118690
H	-0.032712	3.112911	1.562501
H	1.223702	3.907767	0.585821
H	1.468589	2.268319	1.243786
H	1.478739	-0.922296	2.726443
H	-0.042351	-0.938887	3.651303
H	0.522397	0.571654	2.895476

(*M,P*)-*trans*-1

C	0.258858	1.362928	1.317752
C	0.048779	2.852391	0.910231
C	-0.733484	3.020444	-0.407117
C	-1.940404	2.121607	-0.398026
C	-1.717818	0.800450	-0.047908
C	-0.295071	0.454536	0.224066
C	-2.822015	-0.075804	0.177643
C	-4.140034	0.387290	-0.107871
C	-4.323817	1.723890	-0.552323
C	-3.253796	2.576308	-0.665050
C	-5.239072	-0.496090	0.084485
C	-5.049107	-1.766035	0.568986
C	-3.744596	-2.209565	0.898893
C	-2.663443	-1.385754	0.708266
C	0.446637	-0.452742	-0.442880
H	1.333373	1.178674	1.426161
C	1.852793	-0.798385	-0.065606
C	2.051564	-2.127807	0.273112
C	0.845970	-3.032509	0.235984
C	0.024960	-2.846719	-1.057856
C	0.041755	-1.386616	-1.583821
C	3.343350	-2.588908	0.623660
C	4.418373	-1.736493	0.612140
C	4.264885	-0.386677	0.198534

C	2.971234	0.085776	-0.173908
C	-0.393804	1.038256	2.666010
C	2.855766	1.414425	-0.671747
C	3.948865	2.240976	-0.751373
C	5.224078	1.784537	-0.336768
C	5.375532	0.499521	0.120031
H	0.904076	-1.316704	-2.268959
C	-1.181469	-1.053105	-2.433345
H	-0.502911	3.373678	1.708380
H	1.023502	3.355348	0.821485
H	-0.084476	2.749858	-1.257874
H	-1.022130	4.071673	-0.552576
H	-5.335733	2.073234	-0.772005
H	-3.408615	3.616280	-0.963874
H	-6.244931	-0.138981	-0.151148
H	-5.901947	-2.432271	0.715356
H	-3.601176	-3.209832	1.313682
H	-1.659797	-1.721803	0.968725
H	0.208445	-2.788032	1.103016
H	1.141724	-4.084291	0.360002
H	-1.015250	-3.155420	-0.870967
H	0.411626	-3.514134	-1.843445
H	3.476551	-3.636161	0.907177
H	5.411721	-2.093301	0.895400
H	1.877870	1.765692	-1.002194
H	3.836753	3.254252	-1.143728
H	6.085437	2.453458	-0.394515
H	6.359516	0.131977	0.422581
H	-1.180837	0.003217	-2.739187
H	-2.129146	-1.256380	-1.920633
H	-1.162388	-1.668836	-3.346275
H	-1.483730	1.193639	2.632764
H	0.016186	1.683264	3.458496
H	-0.206535	-0.008863	2.949000

TS<sub>6</sub>

C	0.097449	2.167344	0.232491
C	-0.555505	3.237245	-0.699181
C	-1.531758	2.662938	-1.732012
C	-2.443903	1.689268	-1.046054
C	-1.826694	0.729126	-0.264125
C	-0.339096	0.763189	-0.174951
C	-2.616893	-0.175629	0.517429
C	-4.037805	-0.137322	0.382596
C	-4.628568	0.815197	-0.490004
C	-3.851388	1.720693	-1.167667
C	-4.834100	-1.042814	1.137669
C	-4.259019	-1.931969	2.010064
C	-2.852881	-1.947202	2.174381
C	-2.056253	-1.096000	1.448278
C	0.412486	-0.334798	-0.487249
H	1.170834	2.256175	0.070875
C	1.847363	-0.715918	-0.156581
C	2.138634	-2.080711	-0.313074
C	1.057058	-3.132470	-0.190475
C	-0.233514	-2.788531	-0.938364
C	-0.140208	-1.377491	-1.502127
C	3.467093	-2.531726	-0.513774
C	4.519062	-1.659983	-0.522711
C	4.307654	-0.328398	-0.086173
C	2.981004	0.114789	0.224033
C	-0.234428	2.460492	1.700962
C	2.906500	1.285053	1.030907

C	4.005633	2.060243	1.318329
C	5.279205	1.714207	0.818731
C	5.421918	0.521632	0.156972
H	0.695188	-1.405476	-2.224581
C	-1.356100	-1.064753	-2.374381
H	-1.103873	3.963583	-0.079215
H	0.235881	3.800808	-1.215264
H	-0.964837	2.143936	-2.524531
H	-2.098314	3.469343	-2.220401
H	-5.716160	0.830452	-0.596177
H	-4.315234	2.467951	-1.816653
H	-5.919782	-1.010090	1.015272
H	-4.882076	-2.617392	2.588482
H	-2.399389	-2.638570	2.888220
H	-0.974594	-1.110936	1.585845
H	0.851584	-3.238414	0.888070
H	1.456067	-4.105208	-0.511965
H	-1.112290	-2.875443	-0.282674
H	-0.394109	-3.490945	-1.771166
H	3.631643	-3.594216	-0.709425
H	5.530406	-1.993281	-0.766651
H	1.973451	1.523339	1.522977
H	3.891402	2.932103	1.966455
H	6.144791	2.349059	1.018437
H	6.410955	0.174110	-0.152831
H	-1.357659	-1.784630	-3.208385
H	-1.307489	-0.059385	-2.811193
H	-2.316671	-1.173388	-1.855435
H	-1.324628	2.455390	1.855324
H	0.146430	3.449486	2.000610
H	0.190794	1.707428	2.382334

ωB97X-D/SVP in hexane

(*P,P*)-*trans*-1

C	-0.098620	-0.480036	1.971868
C	0.456292	-1.813270	2.560919
C	1.434027	-2.543540	1.624321
C	2.415658	-1.575939	1.019326
C	1.884354	-0.422402	0.464099
C	0.401829	-0.320302	0.542249
C	2.747325	0.582724	-0.071260
C	4.153706	0.342409	-0.097258
C	4.660599	-0.870147	0.442980
C	3.814165	-1.795416	1.001617
C	5.014047	1.332477	-0.649219
C	4.511035	2.513992	-1.134859
C	3.118532	2.767239	-1.079236
C	2.262076	1.827313	-0.560709
C	-0.401838	-0.320325	-0.542261
H	-1.194570	-0.539909	1.948775
C	-1.884364	-0.422409	-0.464098
C	-2.415685	-1.575963	-1.019273
C	-1.434073	-2.543592	-1.624255
C	-0.456354	-1.813354	-2.560891
C	0.098615	-0.480131	-1.971871
C	-3.814193	-1.795430	-1.001532
C	-4.660612	-0.870136	-0.442914
C	-4.153701	0.342437	0.097270
C	-2.747320	0.582742	0.071241
C	0.296321	0.714442	2.845855
C	-2.262054	1.827344	0.560639
C	-3.118495	2.767293	1.079148
C	-4.510998	2.514058	1.134803
C	-5.014027	1.332530	0.649212
H	1.194563	-0.540056	-1.948760
C	-0.296255	0.714336	-2.845906
H	0.976500	-1.599410	3.507797
H	-0.376058	-2.488844	2.808206
H	0.862523	-3.023443	0.810945
H	1.953883	-3.349336	2.163360
H	5.738714	-1.048109	0.419967
H	4.215489	-2.716313	1.433078
H	6.089228	1.136903	-0.675449
H	5.183439	3.265992	-1.553747
H	2.725476	3.717290	-1.448499
H	1.190618	2.025492	-0.508676
H	-1.953947	-3.349397	-2.163262
H	-0.862558	-3.023480	-0.810877
H	-0.976596	-1.599487	-3.507750
H	0.375971	-2.488949	-2.808208
H	-4.215531	-2.716341	-1.432952
H	-5.738727	-1.048090	-0.419877
H	-1.190595	2.025513	0.508584
H	-2.725425	3.717355	1.448373
H	-5.183390	3.266077	1.553676
H	-6.089209	1.136964	0.675466
H	0.090650	0.588956	-3.869340
H	0.108865	1.658069	-2.452808
H	-1.391455	0.815777	-2.910928
H	1.391527	0.815831	2.910862
H	-0.090581	0.589120	3.869297
H	-0.108755	1.658181	2.452725

*(P,P)*-trans-1\*

C	0.511553	-2.247544	1.455925
C	1.873910	-2.897765	1.690356
C	2.903292	-1.843625	2.049980
C	2.948108	-0.728872	1.038306
C	1.805116	-0.386382	0.251979
C	0.598515	-1.126306	0.418225
C	1.947331	0.752234	-0.669183
C	3.207363	1.422060	-0.785399
C	4.305512	1.004552	0.002796
C	4.158603	-0.037915	0.889373
C	3.350096	2.519445	-1.678980
C	2.293646	2.970788	-2.431142
C	1.042984	2.333887	-2.307192
C	0.884885	1.263277	-1.452056
C	-0.591765	-1.122506	-0.427519
H	-0.162167	-3.017690	1.044498
C	-1.802012	-0.389962	-0.253185
C	-2.941624	-0.727900	-1.046430
C	-2.895004	-1.836678	-2.065237
C	-1.853498	-2.883872	-1.722512
C	-0.497414	-2.221376	-1.487811
C	-4.152244	-0.036325	-0.900564
C	-4.303356	0.999080	-0.006921
C	-3.211319	1.405916	0.795209
C	-1.950953	0.736398	0.682467
C	-0.147659	-1.768663	2.759776
C	-0.895253	1.236037	1.481762
C	-1.060942	2.294630	2.350675
C	-2.312028	2.931480	2.469947
C	-3.361379	2.491660	1.701397
H	0.190417	-2.990556	-1.099263
C	0.143557	-1.704138	-2.786225
H	1.798107	-3.657620	2.484170
H	2.188275	-3.419476	0.771011
H	3.904398	-2.290691	2.146373
H	2.668941	-1.419843	3.044035
H	5.263079	1.521000	-0.097537
H	5.011845	-0.351354	1.497493
H	4.326823	3.005074	-1.748478
H	2.416554	3.818363	-3.109040
H	0.185500	2.689530	-2.882613
H	-0.095836	0.803103	-1.383746
H	-2.673286	-1.404916	-3.058537
H	-3.893113	-2.291725	-2.156087
H	-1.773800	-3.633680	-2.525484
H	-2.156297	-3.418637	-0.806899
H	-5.000269	-0.342612	-1.519399
H	-5.259981	1.518477	0.088396
H	0.086462	0.777028	1.415445
H	-0.210456	2.641171	2.941835
H	-2.440488	3.770896	3.157001
H	-4.337936	2.978532	1.766692
H	1.152017	-1.310191	-2.597094
H	-0.444452	-0.898162	-3.249335
H	0.231757	-2.527560	-3.513510
H	0.427067	-0.966389	3.245631
H	-0.232220	-2.609108	3.467589
H	-1.159058	-1.382674	2.569939

*(M,M)*-cis-2

C	-2.861338	-1.489279	0.066072
C	-2.665498	-2.966517	-0.287861



C	-1.408361	-3.517273	0.377166
C	-0.212352	-2.763840	-0.137157
C	-0.346993	-1.430222	-0.515486
C	-1.569578	-0.672744	-0.138414
C	0.723006	-0.833683	-1.285649
C	1.983687	-1.495079	-1.357832
C	2.121746	-2.792892	-0.797466
C	1.031410	-3.428886	-0.269604
C	3.073730	-0.868132	-2.021922
C	2.914857	0.337603	-2.657008
C	1.639110	0.945709	-2.684281
C	0.579803	0.375970	-2.020560
C	-1.569578	0.672744	0.138414
H	-3.659694	-1.094026	-0.578405
C	-0.346994	1.430222	0.515486
C	-0.212353	2.763840	0.137157
C	-1.408362	3.517273	-0.377166
C	-2.665498	2.966517	0.287862
C	-2.861339	1.489278	-0.066072
C	1.031409	3.428886	0.269604
C	2.121746	2.792892	0.797466
C	1.983686	1.495079	1.357832
C	0.723006	0.833683	1.285649
C	-3.352821	-1.385748	1.522496
C	0.579803	-0.375970	2.020560
C	1.639110	-0.945708	2.684281
C	2.914857	-0.337602	2.657008
C	3.073730	0.868132	2.021922
H	-3.659694	1.094025	0.578405
C	-3.352822	1.385747	-1.522496
H	-3.554778	-3.536399	0.023204
H	-2.568603	-3.088147	-1.378836
H	-1.283817	-4.588087	0.155871
H	-1.486531	-3.443064	1.475788
H	3.091774	-3.293379	-0.847073
H	1.114679	-4.459902	0.084960
H	4.040753	-1.377629	-2.031071
H	3.758358	0.811007	-3.164409
H	1.491623	1.875295	-3.238572
H	-0.398425	0.850558	-2.069219
H	-1.486532	3.443063	-1.475788
H	-1.283818	4.588087	-0.155871
H	-3.554779	3.536399	-0.023204
H	-2.568604	3.088146	1.378836
H	1.114678	4.459903	-0.084959
H	3.091773	3.293379	0.847073
H	-0.398424	-0.850558	2.069220
H	1.491623	-1.875295	3.238572
H	3.758358	-0.811006	3.164408
H	4.040753	1.377629	2.031071
H	-3.502022	0.349148	-1.848776
H	-2.634935	1.835354	-2.224814
H	-4.310812	1.915937	-1.642166
H	-2.634935	-1.835355	2.224814
H	-4.310812	-1.915938	1.642166
H	-3.502022	-0.349149	1.848776
C	2.105119	-1.830540	1.060591
C	3.284297	-2.204461	0.176643
C	4.037429	-0.936594	-0.171689
C	3.174656	0.308601	-0.243272
C	1.773747	0.344373	-0.158229

TS<sub>2</sub>

C	1.115198	-0.970041	0.271860
C	1.160714	1.649028	-0.421750
C	1.966830	2.834344	-0.431464
C	3.379252	2.729802	-0.376385
C	3.949422	1.496068	-0.363523
C	1.376261	4.118260	-0.575482
C	0.029382	4.266235	-0.790526
C	-0.758497	3.106237	-0.917164
C	-0.204178	1.858341	-0.746269
C	-0.123526	-1.512572	0.080359
H	1.599404	-2.741797	1.353995
C	-1.401752	-0.857281	-0.334654
C	-1.929112	-1.235265	-1.555540
C	-1.095081	-2.199042	-2.350655
C	-0.661893	-3.378604	-1.454227
C	-0.527202	-3.021894	0.054237
C	-3.196474	-0.757601	-1.966715
C	-3.935843	0.051090	-1.140830
C	-3.457165	0.400252	0.152266
C	-2.179378	-0.070828	0.576032
C	2.511134	-1.171456	2.386993
C	-1.712988	0.295609	1.868112
C	-2.473804	1.086741	2.694346
C	-3.739890	1.557911	2.271764
C	-4.218450	1.220242	1.030014
H	-1.545122	-3.034383	0.473276
C	0.187919	-4.176482	0.758585
H	3.949053	-2.927057	0.676839
H	2.899760	-2.697052	-0.730808
H	4.571081	-1.037696	-1.131240
H	4.821740	-0.752656	0.581083
H	3.987895	3.637101	-0.396436
H	5.037657	1.395819	-0.395543
H	2.033222	4.991275	-0.539998
H	-0.415049	5.257170	-0.905644
H	-1.818354	3.185933	-1.168928
H	-0.834132	1.004389	-0.927738
H	-0.197485	-1.673452	-2.714881
H	-1.633577	-2.559805	-3.238499
H	0.304314	-3.769398	-1.812036
H	-1.390090	-4.200403	-1.543802
H	-3.584158	-1.043554	-2.947882
H	-4.911658	0.425769	-1.460411
H	-0.730177	-0.051077	2.190647
H	-2.097480	1.360540	3.682593
H	-4.333297	2.190860	2.935367
H	-5.194689	1.580809	0.695183
H	0.242625	-4.041952	1.848316
H	1.197823	-4.371572	0.370342
H	-0.401426	-5.090377	0.579811
H	3.028681	-0.209431	2.265007
H	3.175818	-1.844077	2.952999
H	1.620864	-0.986761	3.007818

(*M,P*)-*cis*-2

C	2.210500	-2.094248	-0.483755
C	2.375141	-2.733886	0.929104
C	1.744623	-1.905685	2.062181
C	0.285131	-1.723267	1.738728
C	-0.005630	-1.380621	0.428841
C	1.172756	-0.979123	-0.394228
C	-1.335525	-1.538403	-0.066869
C	-2.386935	-1.801780	0.860744

C	-2.069750	-1.985012	2.233389
C	-0.761347	-2.000665	2.650108
C	-3.717371	-1.941754	0.375332
C	-3.984344	-1.907089	-0.970458
C	-2.926806	-1.740608	-1.898196
C	-1.641193	-1.550484	-1.456439
C	1.417305	0.308793	-0.727890
H	3.171643	-1.634952	-0.736013
C	0.742221	1.468546	-0.054951
C	1.585971	2.129354	0.831632
C	3.017798	1.662395	0.949463
C	3.669092	1.339287	-0.412879
C	2.639489	0.864001	-1.464684
C	1.095130	3.203342	1.613679
C	-0.205084	3.623354	1.496663
C	-1.061512	3.041736	0.525961
C	-0.569911	1.979214	-0.292131
C	1.882778	-3.146300	-1.542151
C	-1.389607	1.520158	-1.357735
C	-2.651979	2.021983	-1.554360
C	-3.166879	3.019942	-0.692065
C	-2.383578	3.523439	0.316197
H	2.245098	1.774978	-1.943871
C	3.262567	0.060669	-2.605385
H	1.893956	-3.725326	0.937485
H	3.444755	-2.901989	1.128194
H	2.254253	-0.933375	2.150172
H	1.867613	-2.418550	3.027458
H	-2.879314	-2.173407	2.943051
H	-0.518116	-2.224659	3.692150
H	-4.522061	-2.108080	1.096279
H	-5.007606	-2.034101	-1.331177
H	-3.137876	-1.763223	-2.969897
H	-0.825675	-1.427564	-2.172296
H	3.032064	0.750507	1.566642
H	3.614981	2.406572	1.495960
H	4.433103	0.558061	-0.266275
H	4.198520	2.223080	-0.801721
H	1.765948	3.689448	2.327169
H	-0.585343	4.435082	2.121917
H	-0.986993	0.770690	-2.036029
H	-3.262391	1.650755	-2.380558
H	-4.178381	3.402606	-0.845825
H	-2.759319	4.317726	0.966500
H	2.489123	-0.329232	-3.284174
H	3.879072	-0.785070	-2.272001
H	3.918703	0.717621	-3.197921
H	0.897024	-3.601583	-1.353712
H	2.631950	-3.954006	-1.538262
H	1.866974	-2.705731	-2.550316

TS<sub>3</sub>

C	0.731695	-2.906075	-0.248290
C	1.075410	-3.109878	-1.752471
C	1.515906	-1.828434	-2.491030
C	2.129341	-0.834801	-1.547027
C	1.435182	-0.588562	-0.374411
C	0.263912	-1.452505	-0.080164
C	1.967918	0.315787	0.603653
C	3.187412	0.996765	0.315226
C	3.851808	0.745102	-0.916101
C	3.339178	-0.152521	-1.818493
C	3.706414	1.924150	1.260594

C	3.050262	2.169938	2.441025
C	1.843964	1.489690	2.731876
C	1.318746	0.587705	1.839073
C	-1.025820	-1.138542	0.242590
H	-0.100461	-3.580527	-0.043985
C	-1.890996	0.069577	-0.096171
C	-3.276094	-0.159980	-0.062190
C	-3.938078	-1.527178	-0.023702
C	-2.991660	-2.685456	0.253287
C	-1.857399	-2.121328	1.097978
C	-4.206368	0.914974	-0.062501
C	-3.802613	2.214402	-0.094126
C	-2.432294	2.504776	-0.313446
C	-1.484082	1.436144	-0.424208
C	1.912309	-3.303638	0.644900
C	-0.215951	1.809381	-0.942919
C	0.141147	3.117176	-1.179638
C	-0.760136	4.167841	-0.919294
C	-2.032892	3.853352	-0.515269
H	-2.332862	-1.437255	1.822724
C	-1.184202	-3.148665	2.011444
H	1.873693	-3.865229	-1.820445
H	0.200665	-3.530803	-2.269449
H	0.628750	-1.360203	-2.949622
H	2.203299	-2.068447	-3.314760
H	4.783819	1.274363	-1.130084
H	3.861410	-0.346080	-2.759133
H	4.640371	2.442239	1.027443
H	3.455333	2.888303	3.157289
H	1.325532	1.686018	3.673010
H	0.382606	0.077606	2.067166
H	-4.483358	-1.662846	-0.972612
H	-4.711257	-1.502237	0.762070
H	-2.582040	-3.115008	-0.675641
H	-3.522260	-3.497082	0.775558
H	-5.270371	0.675045	0.012960
H	-4.522369	3.033107	-0.019637
H	0.488396	1.041465	-1.223643
H	1.130222	3.330746	-1.590916
H	-0.466808	5.206953	-1.083603
H	-2.782128	4.637295	-0.376995
H	-0.283148	-2.740257	2.489938
H	-0.916870	-4.096636	1.526706
H	-1.893813	-3.401859	2.814752
H	2.833802	-2.773077	0.362080
H	2.109765	-4.383366	0.552650
H	1.717964	-3.087404	1.704999

(*P,P*)-*cis*-2

C	-2.871044	1.480427	-0.217809
C	-2.706796	2.878322	0.425744
C	-1.506975	2.940863	1.373929
C	-0.269383	2.588163	0.594017
C	-0.341116	1.483551	-0.241876
C	-1.580327	0.666056	-0.127932
C	0.759630	1.169473	-1.102048
C	1.974739	1.902316	-0.965147
C	2.032306	2.983923	-0.045896
C	0.926589	3.339079	0.684057
C	3.096063	1.546161	-1.765350
C	3.009575	0.534948	-2.688986
C	1.783895	-0.149187	-2.873428
C	0.690977	0.161831	-2.103153

C	-1.580325	-0.666061	0.127934
H	-3.647986	0.952344	0.351771
C	-0.341111	-1.483552	0.241877
C	-0.269372	-2.588161	-0.594019
C	-1.506964	-2.940865	-1.373932
C	-2.706783	-2.878332	-0.425743
C	-2.871039	-1.480437	0.217807
C	0.926603	-3.339073	-0.684060
C	2.032317	-2.983914	0.045894
C	1.974746	-1.902309	0.965148
C	0.759633	-1.169473	1.102051
C	-3.336935	1.589825	-1.672588
C	0.690975	-0.161835	2.103159
C	1.783891	0.149188	2.873435
C	3.009576	-0.534938	2.688988
C	3.096068	-1.546149	1.765350
H	-3.647980	-0.952358	-0.351780
C	-3.336940	-1.589833	1.672582
H	-2.555902	3.635442	-0.361258
H	-3.634099	3.152538	0.951816
H	-1.653951	2.226590	2.204974
H	-1.412050	3.939164	1.825994
H	2.966962	3.541148	0.055870
H	0.968380	4.192346	1.366306
H	4.029919	2.098991	-1.634708
H	3.877633	0.268150	-3.296173
H	1.708215	-0.929014	-3.634496
H	-0.253740	-0.358577	-2.258436
H	-1.412035	-3.939163	-1.826001
H	-1.653944	-2.226588	-2.204973
H	-2.555880	-3.635450	0.361259
H	-3.634085	-3.152557	-0.951812
H	0.968397	-4.192338	-1.366311
H	2.966976	-3.541135	-0.055873
H	-0.253746	0.358565	2.258446
H	1.708208	0.929012	3.634505
H	3.877634	-0.268137	3.296174
H	4.029928	-2.098973	1.634705
H	-3.533388	-0.598289	2.108709
H	-2.566321	-2.079579	2.289449
H	-4.261150	-2.184796	1.749381
H	-2.566314	2.079575	-2.289448
H	-4.261147	2.184784	-1.749391
H	-3.533377	0.598281	-2.108719

(*P,P*)-*cis*-2\*

C	2.668146	1.896179	0.205027
C	2.284082	3.366719	-0.061018
C	1.006945	3.482997	-0.875915
C	-0.103359	2.769960	-0.160419
C	0.195913	1.506282	0.430280
C	1.476529	0.941021	0.135042
C	-0.876958	0.802580	1.124604
C	-2.226258	1.250382	0.960032
C	-2.475209	2.440751	0.251862
C	-1.417986	3.209562	-0.240018
C	-3.281962	0.478425	1.525148
C	-3.015920	-0.636915	2.285317
C	-1.680939	-1.017372	2.527382
C	-0.637407	-0.291895	1.975424
C	1.681317	-0.433843	-0.201782
H	3.406269	1.593699	-0.554956
C	0.637728	-1.348081	-0.536755

C	0.767103	-2.727396	-0.130996
C	2.116284	-3.322131	0.168765
C	3.106360	-2.287503	0.685113
C	3.087636	-1.024977	-0.183211
C	-0.381063	-3.473865	0.086150
C	-1.661877	-2.969454	-0.175058
C	-1.813669	-1.745672	-0.849226
C	-0.650061	-0.955037	-1.119264
C	3.334230	1.814738	1.592197
C	-0.786524	0.146954	-1.978537
C	-2.031006	0.551470	-2.445988
C	-3.188958	-0.161673	-2.089740
C	-3.082396	-1.289156	-1.305678
H	3.783010	-0.315595	0.275287
C	3.588753	-1.273894	-1.611732
H	2.120867	3.883409	0.898818
H	3.123258	3.879715	-0.555402
H	1.154929	3.021515	-1.871127
H	0.739592	4.535640	-1.052170
H	-3.506236	2.779417	0.124463
H	-1.632009	4.142212	-0.769136
H	-4.312306	0.802818	1.358992
H	-3.835280	-1.219887	2.711871
H	-1.464363	-1.876279	3.165909
H	0.392882	-0.589873	2.174053
H	2.513834	-3.768400	-0.761011
H	2.012428	-4.153385	0.882298
H	4.122159	-2.713104	0.716582
H	2.845319	-2.007216	1.719792
H	-0.280337	-4.476523	0.511092
H	-2.545967	-3.569760	0.052729
H	0.105179	0.706403	-2.265859
H	-2.104204	1.421961	-3.101156
H	-4.166749	0.172919	-2.443757
H	-3.969412	-1.874642	-1.050866
H	3.640382	-0.329317	-2.175309
H	2.921990	-1.946952	-2.171475
H	4.597991	-1.716838	-1.601450
H	2.613029	2.113989	2.368517
H	4.194728	2.501542	1.644304
H	3.692181	0.807595	1.846929

*(M,M)-trans-1*

C	0.341625	-1.955936	-0.786588
C	-0.705416	-3.028499	-1.141868
C	-1.813071	-2.443894	-2.018273
C	-2.561568	-1.459548	-1.166733
C	-1.818771	-0.639931	-0.324752
C	-0.338501	-0.594255	-0.495486
C	-2.506799	0.107376	0.698411
C	-3.934702	0.144062	0.692361
C	-4.647697	-0.607233	-0.278195
C	-3.974986	-1.421093	-1.152348
C	-4.625607	0.904020	1.677324
C	-3.944513	1.570523	2.663912
C	-2.532853	1.490623	2.712354
C	-1.839566	0.786419	1.757823
C	0.338499	0.594785	-0.494871
H	0.869649	-2.301314	0.115737
C	1.818753	0.640344	-0.324037
C	2.561548	1.460967	-1.165045
C	1.813081	2.446324	-2.015443
C	0.705275	3.029791	-1.138470

C	-0.341705	1.956713	-0.784626
C	3.974966	1.422474	-1.150724
C	4.647682	0.607568	-0.277551
C	3.934693	-0.144835	0.692152
C	2.506792	-0.108124	0.698276
C	1.366944	-1.888554	-1.928582
C	1.839573	-0.788339	1.756943
C	2.532869	-1.493648	2.710653
C	3.944524	-1.573544	2.662073
C	4.625608	-0.905935	1.676226
H	-0.870013	2.301011	0.117942
C	-1.366723	1.890442	-1.926955
H	-0.201520	-3.865901	-1.647382
H	-1.167719	-3.440368	-0.230575
H	-2.495072	-3.226243	-2.382391
H	-1.378015	-1.959010	-2.909462
H	-5.739640	-0.562582	-0.286580
H	-4.528387	-2.049312	-1.855273
H	-5.717735	0.934065	1.640081
H	-4.486017	2.144801	3.418803
H	-1.988776	1.988854	3.517950
H	-0.753118	0.734983	1.818242
H	1.378174	1.962520	-2.907293
H	2.495086	3.229160	-2.378506
H	0.201369	3.867757	-1.643041
H	1.167425	3.440598	-0.226619
H	4.528363	2.051515	-1.852917
H	5.739623	0.562897	-0.286022
H	0.753131	-0.736920	1.817474
H	1.988804	-1.992768	3.515707
H	4.486032	-2.148700	3.416293
H	5.717734	-0.935963	1.638919
H	-0.899320	1.538433	-2.860735
H	-1.781345	2.892874	-2.112804
H	-2.212533	1.228647	-1.713556
H	0.899841	-1.535421	-2.862089
H	1.781440	-2.890847	-2.115448
H	2.212818	-1.227148	-1.714232

TS<sub>5</sub>

C	-0.336972	-0.908952	1.472272
C	-0.409365	-2.429861	1.284329
C	0.485932	-2.864694	0.132685
C	1.742650	-2.037704	0.043413
C	1.705512	-0.630556	0.021572
C	0.294667	-0.102426	0.310901
C	2.985655	0.037021	-0.209103
C	4.199678	-0.734080	-0.238439
C	4.158695	-2.142508	-0.124149
C	2.953236	-2.768181	-0.024545
C	5.466293	-0.109069	-0.413077
C	5.582862	1.242838	-0.595729
C	4.403432	2.013591	-0.626218
C	3.173406	1.428784	-0.442004
C	-0.457638	0.954275	-0.159862
H	-1.349245	-0.527636	1.633916
C	-1.953397	0.893272	-0.092188
C	-2.715765	2.022930	0.202156
C	-2.123856	3.398168	0.045810
C	-0.984802	3.322665	-0.964315
C	0.095833	2.342853	-0.494414
C	-4.091810	1.894587	0.526624
C	-4.732573	0.687403	0.469554

C	-4.061461	-0.432997	-0.090916
C	-2.682782	-0.311650	-0.437224
C	0.450627	-0.538939	2.741716
C	-2.119256	-1.344885	-1.232135
C	-2.834874	-2.469445	-1.570333
C	-4.158454	-2.641074	-1.107242
C	-4.759465	-1.634161	-0.392007
H	0.833570	2.267641	-1.304620
C	0.739525	2.917665	0.787804
H	-0.089872	-2.932407	2.210879
H	-1.444248	-2.747214	1.091943
H	-0.059269	-2.763889	-0.815349
H	0.745518	-3.928980	0.219432
H	5.091936	-2.710314	-0.142602
H	2.903900	-3.858543	0.023458
H	6.353697	-0.747231	-0.410582
H	6.559832	1.710891	-0.732756
H	4.457634	3.089881	-0.805939
H	2.317860	2.073615	-0.507233
H	-1.781576	3.823149	1.003309
H	-2.913600	4.075720	-0.313942
H	-0.529002	4.313752	-1.113780
H	-1.390971	3.002459	-1.937332
H	-4.637828	2.791745	0.831612
H	-5.782306	0.593781	0.758336
H	-1.106441	-1.213115	-1.609066
H	-2.377769	-3.232117	-2.205239
H	-4.710724	-3.551301	-1.351391
H	-5.802650	-1.724564	-0.078177
H	-0.024213	3.084714	1.560043
H	1.233421	3.883295	0.590614
H	1.474589	2.239237	1.234570
H	1.483922	-0.917598	2.709961
H	-0.040521	-0.975728	3.625747
H	0.491160	0.551539	2.884573

(*M,P*)-*trans*-1

C	0.261140	1.368671	1.315475
C	0.032687	2.858536	0.920766
C	-0.744821	3.029336	-0.397729
C	-1.947403	2.124488	-0.393987
C	-1.721934	0.802588	-0.045282
C	-0.296900	0.457761	0.224378
C	-2.826881	-0.075303	0.177062
C	-4.145915	0.386710	-0.109076
C	-4.331394	1.724294	-0.550408
C	-3.261959	2.577957	-0.659875
C	-5.244016	-0.500025	0.076373
C	-5.052960	-1.771128	0.557797
C	-3.748744	-2.212749	0.891214
C	-2.668435	-1.386377	0.705533
C	0.445343	-0.452200	-0.440622
H	1.338412	1.194310	1.407986
C	1.853688	-0.796531	-0.063755
C	2.054071	-2.125138	0.280105
C	0.852175	-3.034813	0.242604
C	0.030205	-2.850622	-1.050567
C	0.042899	-1.391440	-1.578984
C	3.346770	-2.583457	0.633134
C	4.422054	-1.731383	0.617234
C	4.268119	-0.383665	0.196036
C	2.973453	0.086884	-0.178120
C	-0.365270	1.033099	2.672904



C	2.858996	1.413440	-0.682559
C	3.952894	2.238742	-0.768782
C	5.228432	1.783947	-0.353444
C	5.379762	0.501352	0.110588
H	0.904133	-1.320985	-2.265193
C	-1.180326	-1.065857	-2.430327
H	-0.530233	3.365095	1.720705
H	1.000516	3.376123	0.842696
H	-0.091581	2.768906	-1.248156
H	-1.039888	4.079580	-0.537081
H	-5.343458	2.072953	-0.771108
H	-3.417693	3.618706	-0.955864
H	-6.249994	-0.144201	-0.161267
H	-5.904948	-2.439809	0.699351
H	-3.604827	-3.213949	1.303995
H	-1.665487	-1.723042	0.967168
H	0.214359	-2.797982	1.111286
H	1.154360	-4.085197	0.362744
H	-1.008936	-3.162069	-0.863227
H	0.417923	-3.517199	-1.836381
H	3.480140	-3.629498	0.921320
H	5.415392	-2.086748	0.902619
H	1.881354	1.766466	-1.011828
H	3.840963	3.250331	-1.165870
H	6.090119	2.452248	-0.416413
H	6.364008	0.134998	0.414114
H	-1.160146	-1.686050	-3.340724
H	-1.183837	-0.012077	-2.745753
H	-2.128566	-1.270339	-1.919191
H	-1.456909	1.180148	2.664124
H	0.053934	1.678907	3.460507
H	-0.163478	-0.012326	2.953313

TS<sub>6</sub>

C	0.092124	2.168992	0.229686
C	-0.567654	3.239441	-0.696118
C	-1.546742	2.666260	-1.726367
C	-2.454013	1.688698	-1.039847
C	-1.832472	0.725660	-0.263856
C	-0.343732	0.764154	-0.177890
C	-2.620416	-0.183173	0.516978
C	-4.042786	-0.140842	0.391751
C	-4.637572	0.814916	-0.474937
C	-3.862534	1.720615	-1.154874
C	-4.837260	-1.045720	1.150280
C	-4.259192	-1.940116	2.015643
C	-2.851866	-1.962247	2.168044
C	-2.057223	-1.111271	1.438970
C	0.413062	-0.329593	-0.494661
H	1.163861	2.258288	0.058547
C	1.849696	-0.708548	-0.161732
C	2.137453	-2.075547	-0.311525
C	1.051592	-3.122699	-0.189499
C	-0.225505	-2.785525	-0.961754
C	-0.134082	-1.370074	-1.515083
C	3.465022	-2.532520	-0.506481
C	4.521305	-1.665875	-0.512114
C	4.313024	-0.331792	-0.080780
C	2.986017	0.119938	0.219170
C	-0.224013	2.461011	1.701097
C	2.913928	1.296049	1.018861
C	4.016423	2.064933	1.311444
C	5.291878	1.707594	0.824782

C	5.431604	0.511524	0.168430
H	0.702371	-1.392168	-2.236275
C	-1.347585	-1.054644	-2.388490
H	-1.113997	3.963587	-0.071844
H	0.220539	3.804828	-1.215074
H	-0.982993	2.150403	-2.523022
H	-2.116988	3.473075	-2.209575
H	-5.725870	0.832337	-0.574602
H	-4.329103	2.470257	-1.799277
H	-5.923794	-1.008182	1.036174
H	-4.880434	-2.625101	2.596899
H	-2.395151	-2.659044	2.874792
H	-0.974998	-1.133796	1.569229
H	0.828337	-3.212029	0.886815
H	1.452588	-4.101153	-0.489690
H	-1.116327	-2.886215	-0.324404
H	-0.361608	-3.483424	-1.802815
H	3.625533	-3.596276	-0.699092
H	5.532443	-2.004001	-0.750652
H	1.979740	1.544955	1.503391
H	3.902242	2.941492	1.953478
H	6.160555	2.336915	1.029643
H	6.420567	0.155813	-0.132460
H	-1.349665	-1.773398	-3.223829
H	-1.296239	-0.049514	-2.826435
H	-2.310223	-1.163234	-1.873171
H	-1.312224	2.471386	1.868958
H	0.171882	3.444323	2.001123
H	0.198071	1.702274	2.378421

ωB97X-D/SVP in methanol

(*P,P*)-*trans*-1

C	0.090314	-0.485669	-1.972997
C	-0.467220	-1.818273	-2.560828
C	-1.442491	-2.549007	-1.621549
C	-2.419668	-1.580260	-1.012208
C	-1.884541	-0.427217	-0.458676
C	-0.402751	-0.327136	-0.541270
C	-2.743174	0.582550	0.075110
C	-4.150893	0.346227	0.104254
C	-4.663160	-0.866831	-0.432152
C	-3.819651	-1.795804	-0.991355
C	-5.008753	1.340588	0.654656
C	-4.500432	2.523252	1.134293
C	-3.106405	2.772891	1.074218
C	-2.252142	1.828610	0.557693
C	0.402677	-0.326623	0.541087
H	1.186779	-0.545010	-1.957470
C	1.884482	-0.426933	0.458814
C	2.419356	-1.579549	1.013476
C	1.441937	-2.547560	1.623589
C	0.466674	-1.815787	2.562075
C	-0.090586	-0.483667	1.972886
C	3.819307	-1.795329	0.993031
C	4.663047	-0.866962	0.433175
C	4.151062	0.345754	-0.104269
C	2.743374	0.582323	-0.075541
C	-0.309244	0.710712	-2.841917
C	2.252649	1.828143	-0.559046
C	3.107151	2.771898	-1.076135
C	4.501139	2.521962	-1.135852
C	5.009179	1.339562	-0.655269
H	-1.187063	-0.542862	1.957246
C	0.309007	0.713555	2.840626
H	-0.989296	-1.603771	-3.506764
H	0.363671	-2.495219	-2.809293
H	-0.868326	-3.031452	-0.811302
H	-1.967057	-3.351944	-2.159859
H	-5.742069	-1.041404	-0.406079
H	-4.224415	-2.716442	-1.420738
H	-6.084574	1.147260	0.683370
H	-5.169684	3.279258	1.552145
H	-2.710848	3.724481	1.437932
H	-1.180555	2.027613	0.501414
H	1.966295	-3.350091	2.162708
H	0.867797	-3.030648	0.813709
H	0.988666	-1.600465	3.507871
H	-0.364350	-2.492371	2.811078
H	4.223861	-2.715649	1.423292
H	5.741936	-1.041713	0.407445
H	1.181099	2.027395	-0.503021
H	2.711817	3.723303	-1.440574
H	5.170586	3.277548	-1.554151
H	6.084972	1.146032	-0.683668
H	-0.083676	0.596993	3.863285
H	-0.084055	1.659091	2.438001
H	1.405061	0.805330	2.913270
H	-1.405297	0.802555	-2.914502
H	0.083273	0.593029	-3.864513
H	0.084002	1.656617	-2.440345

*(P,P)*-trans-1\*

C	-1.561921	-0.398736	-2.062379
C	-1.784461	-1.706461	-2.823410
C	-2.080143	-2.838768	-1.858271
C	-1.023582	-2.959219	-0.793351
C	-0.250137	-1.823764	-0.385368
C	-0.455279	-0.573570	-1.020445
C	0.701285	-2.027177	0.720815
C	0.906729	-3.341953	1.248549
C	0.151080	-4.431355	0.749636
C	-0.798749	-4.220696	-0.228158
C	1.848145	-3.548473	2.295811
C	2.543081	-2.498968	2.847908
C	2.307144	-1.192790	2.373209
C	1.412532	-0.973504	1.344687
C	0.455242	0.573601	-1.020379
H	-1.205329	0.350760	-2.787703
C	0.250096	1.823815	-0.385401
C	1.023699	2.959228	-0.793237
C	2.080307	2.838670	-1.858121
C	1.784455	1.706449	-2.823327
C	1.561829	0.398676	-2.062389
C	0.798899	4.220699	-0.228035
C	-0.151000	4.431475	0.749691
C	-0.906735	3.342099	1.248528
C	-0.701336	2.027310	0.720775
C	-2.865438	0.158295	-1.469620
C	-1.412650	0.973663	1.344617
C	-2.307287	1.192912	2.373122
C	-2.543112	2.499087	2.847892
C	-1.848118	3.548580	2.295840
H	1.205139	-0.350710	-2.787793
C	2.865329	-0.158547	-1.469792
H	-2.606746	-1.583083	-3.545534
H	-0.876937	-1.945274	-3.403226
H	-2.174228	-3.796470	-2.392332
H	-3.059845	-2.668787	-1.374494
H	0.317295	-5.430333	1.160729
H	-1.391017	-5.064724	-0.593473
H	1.995957	-4.567104	2.664872
H	3.259490	-2.670926	3.654913
H	2.828577	-0.343871	2.821668
H	1.263371	0.048974	1.008493
H	3.060009	2.668528	-1.374399
H	2.174519	3.796370	-2.392170
H	2.606681	1.583046	-3.545516
H	0.876919	1.945398	-3.403072
H	1.391294	5.064676	-0.593278
H	-0.317123	5.430450	1.160830
H	-1.263520	-0.048820	1.008418
H	-2.828737	0.343994	2.821564
H	-3.259482	2.671053	3.654933
H	-1.995867	4.567193	2.664983
H	2.717155	-1.166368	-1.058484
H	3.258399	0.477764	-0.662816
H	3.631446	-0.225510	-2.259245
H	-3.258359	-0.478091	-0.662629
H	-3.631613	0.225163	-2.259018
H	-2.717356	1.166124	-1.058305

*(M,M)*-cis-2

C	-2.868596	1.491618	-0.046889
C	-2.670089	2.962934	0.328365

C	-1.416295	3.524655	-0.333112
C	-0.218897	2.762021	0.160927
C	-0.353897	1.423991	0.525861
C	-1.578252	0.671343	0.145626
C	0.721790	0.816933	1.279919
C	1.988903	1.468996	1.337824
C	2.127545	2.772416	0.787632
C	1.031130	3.419728	0.283590
C	3.086379	0.827789	1.978148
C	2.928564	-0.385070	2.602306
C	1.647383	-0.984100	2.645919
C	0.580005	-0.399354	2.006282
C	-1.578336	-0.671154	-0.145750
H	-3.667321	1.087555	0.591327
C	-0.354082	-1.423956	-0.526005
C	-0.219263	-2.762030	-0.161134
C	-1.416757	-3.524627	0.332763
C	-2.670549	-2.962569	-0.328416
C	-2.868723	-1.491276	0.047057
C	1.030721	-3.419851	-0.283676
C	2.127258	-2.772631	-0.787561
C	1.988794	-1.469193	-1.337758
C	0.721741	-0.817006	-1.279976
C	-3.356173	1.408135	-1.505474
C	0.580144	0.399281	-2.006368
C	1.647642	0.983922	-2.645903
C	2.928762	0.384779	-2.602153
C	3.086397	-0.828093	-1.977971
H	-3.667602	-1.087036	-0.590846
C	-3.355866	-1.407791	1.505788
H	-3.560081	3.537664	0.028879
H	-2.570924	3.068679	1.421487
H	-1.286718	4.591413	-0.095564
H	-1.497982	3.466904	-1.432273
H	3.101448	3.266829	0.828341
H	1.114180	4.453956	-0.062222
H	4.056404	1.332230	1.977942
H	3.776474	-0.869997	3.092043
H	1.502669	-1.917262	3.195885
H	-0.401017	-0.868550	2.068945
H	-1.498307	-3.467258	1.431952
H	-1.287333	-4.591326	0.094850
H	-3.560592	-3.537187	-0.028863
H	-2.571591	-3.068171	-1.421571
H	1.113620	-4.454101	0.062107
H	3.101128	-3.267119	-0.828153
H	-0.400829	0.868569	-2.069137
H	1.503059	1.917092	-3.195890
H	3.776766	0.869631	-3.091801
H	4.056375	-1.332626	-1.977665
H	-3.518913	-0.375398	1.840316
H	-2.630377	-1.856960	2.200940
H	-4.308170	-1.949605	1.619942
H	-2.630888	1.857379	-2.200797
H	-4.308536	1.949904	-1.619339
H	-3.519239	0.375752	-1.840009

TS<sub>2</sub>

C	2.120657	-1.794827	1.087931
C	3.288373	-2.181420	0.194428
C	4.028107	-0.918113	-0.198980
C	3.162544	0.324289	-0.270599
C	1.763040	0.358380	-0.158220

C	1.118490	-0.957159	0.290942
C	1.142940	1.662547	-0.408001
C	1.946863	2.849686	-0.436722
C	3.361296	2.747484	-0.420686
C	3.932437	1.513262	-0.417279
C	1.349921	4.134224	-0.558313
C	-0.003675	4.280885	-0.734537
C	-0.793088	3.118951	-0.847589
C	-0.231122	1.870995	-0.697397
C	-0.111162	-1.517678	0.095740
H	1.622569	-2.701509	1.409602
C	-1.390984	-0.879470	-0.337440
C	-1.899393	-1.266334	-1.563635
C	-1.052646	-2.233358	-2.340509
C	-0.615098	-3.398897	-1.427552
C	-0.495108	-3.030584	0.079699
C	-3.162788	-0.793356	-1.995343
C	-3.915888	0.019923	-1.185174
C	-3.457865	0.373006	0.115069
C	-2.187626	-0.098623	0.561555
C	2.539216	-1.104314	2.393992
C	-1.745077	0.266281	1.863356
C	-2.519888	1.060698	2.675033
C	-3.776582	1.536902	2.227483
C	-4.233884	1.197203	0.977137
H	-1.515057	-3.054818	0.494004
C	0.235633	-4.166611	0.796346
H	3.966581	-2.885874	0.702020
H	2.891777	-2.700330	-0.693080
H	4.536497	-1.035016	-1.170589
H	4.832434	-0.715578	0.526760
H	3.967822	3.655876	-0.458128
H	5.019816	1.414054	-0.474066
H	2.006807	5.008075	-0.536565
H	-0.453090	5.271730	-0.833248
H	-1.859027	3.199778	-1.075350
H	-0.861057	1.015124	-0.871660
H	-0.157110	-1.704751	-2.706705
H	-1.583714	-2.608162	-3.226855
H	0.358160	-3.782085	-1.774005
H	-1.334209	-4.228563	-1.515426
H	-3.536256	-1.086323	-2.980293
H	-4.886662	0.393606	-1.521701
H	-0.771817	-0.085995	2.210214
H	-2.163574	1.330835	3.672179
H	-4.380209	2.172480	2.879891
H	-5.202988	1.559485	0.623118
H	0.280256	-4.022977	1.885609
H	1.251168	-4.345203	0.415037
H	-0.337678	-5.091164	0.619074
H	3.070302	-0.152489	2.247389
H	3.198956	-1.769937	2.974010
H	1.653435	-0.894113	3.014343
C	-2.849480	0.584686	-1.190907
C	-3.652775	1.376428	-0.123860
C	-3.064163	1.227322	1.284786
C	-1.633481	1.699210	1.238733
C	-0.862573	1.275118	0.163697
C	-1.494720	0.172543	-0.628445
C	0.379791	1.924645	-0.110882
C	0.909942	2.844395	0.845318

(*M,P*)-cis-2

C	0.152944	3.148679	2.008666
C	-1.106328	2.625610	2.172105
C	2.156319	3.479529	0.580533
C	2.815732	3.269004	-0.606174
C	2.247285	2.424463	-1.591435
C	1.065358	1.768589	-1.346524
C	-1.030733	-1.096413	-0.576301
H	-3.415252	-0.319573	-1.422683
C	0.161149	-1.484849	0.244445
C	-0.155682	-2.111792	1.439882
C	-1.612477	-2.389823	1.708428
C	-2.364544	-2.892123	0.448951
C	-1.757330	-2.406485	-0.895558
C	0.875140	-2.498989	2.332830
C	2.195191	-2.307755	2.006501
C	2.552439	-1.816753	0.721155
C	1.520598	-1.443471	-0.192888
C	-2.687297	1.384335	-2.485099
C	1.883462	-1.148847	-1.536741
C	3.199280	-1.144918	-1.931641
C	4.228467	-1.418539	-0.997035
C	3.910044	-1.753472	0.296884
H	-0.944804	-3.106350	-1.150699
C	-2.750004	-2.514978	-2.052059
H	-3.652593	2.449462	-0.378761
H	-4.704110	1.049933	-0.136619
H	-3.130559	0.174245	1.601836
H	-3.638534	1.817524	2.013629
H	0.564616	3.846640	2.742562
H	-1.716514	2.919268	3.030916
H	2.566652	4.161074	1.330774
H	3.765990	3.771130	-0.803658
H	2.752560	2.296132	-2.551828
H	0.617153	1.139146	-2.114800
H	-2.085558	-1.461702	2.064260
H	-1.713787	-3.115650	2.528144
H	-3.409663	-2.547364	0.506005
H	-2.396052	-3.993098	0.445333
H	0.607078	-2.952787	3.290972
H	2.986804	-2.586252	2.707053
H	1.092912	-0.949441	-2.262018
H	3.454844	-0.928486	-2.971819
H	5.273298	-1.388049	-1.315760
H	4.695461	-2.006486	1.014225
H	-2.368880	-2.024632	-2.960725
H	-3.741102	-2.099315	-1.822905
H	-2.905258	-3.579229	-2.290370
H	-2.079812	2.289428	-2.318151
H	-3.667665	1.707212	-2.871321
H	-2.196535	0.785130	-3.267783

TS<sub>3</sub>

C	0.717080	-2.909118	-0.235694
C	1.050402	-3.122339	-1.742149
C	1.449922	-1.841557	-2.504992
C	2.086404	-0.838842	-1.587288
C	1.428538	-0.597704	-0.393347
C	0.259119	-1.452644	-0.072318
C	1.994625	0.293386	0.577807
C	3.196085	0.989261	0.250231
C	3.817382	0.754002	-1.007664
C	3.282808	-0.146579	-1.895570
C	3.741800	1.913393	1.184964

C	3.129800	2.137446	2.394341
C	1.944428	1.437443	2.726593
C	1.392730	0.540463	1.842996
C	-1.022965	-1.126037	0.265941
H	-0.115829	-3.579049	-0.019940
C	-1.888668	0.080102	-0.083808
C	-3.271775	-0.167162	-0.084516
C	-3.918763	-1.540977	-0.048562
C	-2.972617	-2.687717	0.274861
C	-1.855758	-2.101267	1.126905
C	-4.216217	0.896461	-0.112538
C	-3.830267	2.202296	-0.130843
C	-2.456198	2.511284	-0.301261
C	-1.490196	1.455266	-0.386737
C	1.900690	-3.303232	0.654272
C	-0.207784	1.852252	-0.854173
C	0.141960	3.167910	-1.060804
C	-0.783119	4.204697	-0.822218
C	-2.067525	3.868363	-0.473449
H	-2.346573	-1.414837	1.839103
C	-1.176078	-3.110919	2.054659
H	1.867376	-3.857395	-1.810109
H	0.181000	-3.572119	-2.243738
H	0.541888	-1.384680	-2.933869
H	2.110534	-2.080094	-3.350626
H	4.735561	1.294775	-1.251804
H	3.776227	-0.332484	-2.853442
H	4.660312	2.444534	0.920684
H	3.555379	2.851950	3.103147
H	1.465475	1.612543	3.693033
H	0.475512	0.011795	2.106514
H	-4.435036	-1.693248	-1.011317
H	-4.716149	-1.508596	0.711736
H	-2.544610	-3.139665	-0.635092
H	-3.511524	-3.486541	0.808001
H	-5.278830	0.642319	-0.068358
H	-4.562523	3.011781	-0.077649
H	0.512714	1.094961	-1.122764
H	1.142417	3.400875	-1.434040
H	-0.497397	5.249681	-0.963400
H	-2.832604	4.640586	-0.354860
H	-0.282119	-2.687417	2.534772
H	-0.896023	-4.060177	1.579403
H	-1.888261	-3.362959	2.856253
H	2.824660	-2.781343	0.360808
H	2.092812	-4.384635	0.569735
H	1.710554	-3.078148	1.713976

(*P,P*)-*cis*-2

C	-2.885937	1.468848	-0.284395
C	-2.716674	2.896796	0.284212
C	-1.531994	2.997744	1.247650
C	-0.285411	2.604434	0.503592
C	-0.353645	1.470024	-0.292869
C	-1.595427	0.660158	-0.157231
C	0.761252	1.110818	-1.116588
C	1.988011	1.823085	-0.968289
C	2.042667	2.935091	-0.083807
C	0.921764	3.338478	0.598393
C	3.126541	1.413485	-1.718929
C	3.046675	0.367283	-2.605110
C	1.811239	-0.298345	-2.802774
C	0.700175	0.066880	-2.082021



C	-1.595629	-0.659869	0.157234
H	-3.659475	0.971298	0.315866
C	-0.354058	-1.470040	0.292962
C	-0.286045	-2.604492	-0.503464
C	-1.532705	-2.997618	-1.247496
C	-2.717349	-2.896292	-0.284060
C	-2.886424	-1.468171	0.284108
C	0.920994	-3.338760	-0.598265
C	2.041985	-2.935557	0.083897
C	1.987546	-1.823524	0.968354
C	0.760918	-1.111032	1.116662
C	-3.359816	1.501584	-1.739944
C	0.700055	-0.067062	2.082074
C	1.811200	0.297976	2.802796
C	3.046514	-0.367874	2.605113
C	3.126170	-1.414109	1.718955
H	-3.659518	-0.970545	-0.316674
C	-3.360993	-1.500444	1.739440
H	-2.544991	3.609733	-0.539636
H	-3.648991	3.207811	0.779674
H	-1.692499	2.320570	2.106883
H	-1.436009	4.014872	1.655135
H	2.985454	3.477473	0.025928
H	0.960560	4.216199	1.249514
H	4.067624	1.952651	-1.580533
H	3.927309	0.058795	-3.173812
H	1.742598	-1.103477	-3.538472
H	-0.250986	-0.439596	-2.250206
H	-1.436924	-4.014812	-1.654863
H	-1.693069	-2.320507	-2.106806
H	-2.545704	-3.609002	0.539996
H	-3.649730	-3.207344	-0.779378
H	0.959614	-4.216505	-1.249364
H	2.984675	-3.478108	-0.025848
H	-0.251012	0.439593	2.250259
H	1.742721	1.103136	3.538479
H	3.927221	-0.059526	3.173778
H	4.067154	-1.953443	1.580542
H	-3.562405	-0.487216	2.120610
H	-2.596419	-1.958438	2.388403
H	-4.286015	-2.091201	1.838019
H	-2.594831	1.959550	-2.388442
H	-4.284656	2.092577	-1.838815
H	-3.561289	0.488483	-2.121423

(*P,P*)-*cis*-2\*

C	2.589656	1.977935	0.145988
C	2.171389	3.421845	-0.207731
C	0.858682	3.471286	-0.970348
C	-0.205084	2.762308	-0.186478
C	0.137239	1.514703	0.417227
C	1.429512	0.986250	0.118268
C	-0.903785	0.797565	1.145910
C	-2.262784	1.228324	1.029215
C	-2.555637	2.419057	0.328041
C	-1.529928	3.188102	-0.217460
C	-3.289885	0.449587	1.635954
C	-2.984767	-0.660623	2.391163
C	-1.635818	-1.019192	2.595925
C	-0.622134	-0.290478	1.997542
C	1.682297	-0.399212	-0.170171
H	3.348461	1.650518	-0.580990
C	0.680556	-1.343792	-0.524621

C	0.851278	-2.725406	-0.125114
C	2.209133	-3.270953	0.217934
C	3.137235	-2.203299	0.777151
C	3.106399	-0.939793	-0.087180
C	-0.272217	-3.522880	0.043876
C	-1.562699	-3.075911	-0.261152
C	-1.743504	-1.841553	-0.919424
C	-0.607252	-0.998699	-1.141665
C	3.231521	1.993162	1.547942
C	-0.763866	0.105222	-1.997962
C	-2.007107	0.457236	-2.509325
C	-3.146151	-0.303663	-2.189189
C	-3.015325	-1.436696	-1.413175
H	3.752428	-0.206609	0.403705
C	3.678741	-1.164289	-1.493163
H	2.046750	4.005820	0.718686
H	2.978371	3.906819	-0.777576
H	0.975773	2.968210	-1.949463
H	0.557506	4.508215	-1.180765
H	-3.595317	2.745769	0.242524
H	-1.774083	4.111949	-0.749548
H	-4.329194	0.763054	1.505348
H	-3.782112	-1.249114	2.851467
H	-1.387375	-1.866937	3.238881
H	0.417354	-0.570746	2.174604
H	2.655796	-3.693717	-0.701074
H	2.109436	-4.112162	0.920106
H	4.166594	-2.589429	0.845447
H	2.825816	-1.939404	1.802210
H	-0.141648	-4.525645	0.461274
H	-2.427521	-3.717747	-0.074068
H	0.111149	0.706017	-2.253816
H	-2.096103	1.328806	-3.161997
H	-4.126267	-0.008378	-2.571877
H	-3.884693	-2.062405	-1.193089
H	3.722658	-0.216046	-2.051398
H	3.065480	-1.862640	-2.083488
H	4.702175	-1.569526	-1.434715
H	2.493710	2.334549	2.291342
H	4.082257	2.693805	1.566229
H	3.598426	1.010117	1.874177

(*M,M*)-*trans*-1

C	0.342836	-1.958214	-0.778935
C	-0.703301	-3.028776	-1.143801
C	-1.808955	-2.442601	-2.021027
C	-2.558468	-1.460310	-1.168864
C	-1.817207	-0.642373	-0.323455
C	-0.337041	-0.595609	-0.493147
C	-2.506710	0.104285	0.699293
C	-3.935306	0.141345	0.689960
C	-4.647599	-0.607267	-0.284537
C	-3.972618	-1.420325	-1.158928
C	-4.629748	0.899421	1.675201
C	-3.949608	1.565857	2.663683
C	-2.537005	1.487646	2.713703
C	-1.840687	0.783802	1.760035
C	0.336980	0.594866	-0.493782
H	0.859842	-2.305383	0.129303
C	1.817114	0.642169	-0.324097
C	2.558238	1.459975	-1.169770
C	1.808723	2.442171	-2.022073
C	0.702521	3.027924	-1.145238

C	-0.343333	1.956974	-0.780987
C	3.972405	1.420158	-1.159871
C	4.647567	0.607554	-0.285208
C	3.935402	-0.140643	0.689712
C	2.506812	-0.103763	0.699076
C	1.376970	-1.895770	-1.913071
C	1.840921	-0.782671	1.760272
C	2.537366	-1.485862	2.714342
C	3.949954	-1.564038	2.664234
C	4.629976	-0.898126	1.675304
H	-0.861710	2.304108	0.126499
C	-1.376244	1.893135	-1.916190
H	-0.197319	-3.863524	-1.651572
H	-1.167119	-3.446281	-0.235391
H	-2.491020	-3.223684	-2.387436
H	-1.372069	-1.955527	-2.910425
H	-5.739749	-0.561004	-0.295230
H	-4.524488	-2.046685	-1.865092
H	-5.722134	0.927873	1.635743
H	-4.492092	2.139197	3.419201
H	-1.995299	1.987178	3.520638
H	-0.754161	0.733088	1.824638
H	1.372449	1.955166	-2.911804
H	2.490748	3.223498	-2.388033
H	0.196493	3.862540	-1.653190
H	1.165859	3.445494	-0.236613
H	4.524159	2.046332	-1.866293
H	5.739722	0.561433	-0.295944
H	0.754399	-0.731956	1.824890
H	1.995725	-1.984854	3.521659
H	4.492575	-2.136946	3.419978
H	5.722359	-0.926544	1.635759
H	-0.912910	1.544819	-2.853775
H	-1.789767	2.897212	-2.097001
H	-2.222442	1.231514	-1.700417
H	0.914814	-1.547708	-2.851339
H	1.789906	-2.900270	-2.092841
H	2.223503	-1.234700	-1.696932

TS<sub>5</sub>

C	-0.337130	-0.915194	1.468374
C	-0.407989	-2.435715	1.277361
C	0.487903	-2.868362	0.125368
C	1.743173	-2.039570	0.039557
C	1.703799	-0.631832	0.018020
C	0.292603	-0.105064	0.308547
C	2.984063	0.037395	-0.211607
C	4.199838	-0.732757	-0.232898
C	4.161393	-2.142031	-0.118893
C	2.955277	-2.769351	-0.025452
C	5.467867	-0.106447	-0.400012
C	5.582437	1.245756	-0.588030
C	4.400912	2.014186	-0.634673
C	3.169820	1.428412	-0.455762
C	-0.457471	0.954668	-0.158752
H	-1.349152	-0.534319	1.634343
C	-1.953429	0.894348	-0.089397
C	-2.713973	2.025249	0.207142
C	-2.118768	3.398746	0.056314
C	-0.983718	3.324067	-0.957852
C	0.097581	2.341995	-0.495705
C	-4.091131	1.898653	0.531834
C	-4.734901	0.692356	0.471465

C	-4.064031	-0.428755	-0.089861
C	-2.684491	-0.309582	-0.435994
C	0.450947	-0.548259	2.738198
C	-2.122449	-1.344536	-1.230822
C	-2.840532	-2.468092	-1.569773
C	-4.165559	-2.636990	-1.107325
C	-4.765723	-1.628422	-0.391877
H	0.828487	2.266655	-1.312108
C	0.751343	2.916070	0.781254
H	-0.088144	-2.939645	2.203105
H	-1.442406	-2.755992	1.085201
H	-0.054074	-2.765525	-0.824790
H	0.749799	-3.931971	0.210875
H	5.096066	-2.708093	-0.133123
H	2.906983	-3.860070	0.021005
H	6.356112	-0.743833	-0.388900
H	6.559665	1.715775	-0.719945
H	4.454020	3.089229	-0.823880
H	2.313639	2.071290	-0.537797
H	-1.771750	3.815210	1.015824
H	-2.908175	4.080945	-0.295116
H	-0.526600	4.314603	-1.105718
H	-1.392975	3.007667	-1.931442
H	-4.634960	2.796557	0.839339
H	-5.785013	0.599253	0.760224
H	-1.108770	-1.218500	-1.608035
H	-2.383397	-3.232919	-2.202544
H	-4.719244	-3.546703	-1.352176
H	-5.809313	-1.716065	-0.077549
H	-0.008039	3.099198	1.554550
H	1.255265	3.874123	0.573585
H	1.480443	2.231648	1.229930
H	1.482751	-0.932531	2.709076
H	-0.042840	-0.984084	3.621490
H	0.495629	0.542439	2.882085

(*M,P*)-*trans*-1

C	0.257898	1.363939	1.312853
C	0.033534	2.854343	0.918629
C	-0.743929	3.028245	-0.399363
C	-1.945630	2.123249	-0.397013
C	-1.721280	0.799724	-0.050889
C	-0.296358	0.454316	0.219023
C	-2.827356	-0.076772	0.174308
C	-4.146792	0.388764	-0.107928
C	-4.332037	1.726928	-0.550228
C	-3.260522	2.578899	-0.662075
C	-5.248866	-0.492536	0.085315
C	-5.059898	-1.763547	0.570198
C	-3.754709	-2.209706	0.897564
C	-2.670869	-1.388349	0.704142
C	0.446419	-0.455018	-0.445946
H	1.334601	1.187979	1.411570
C	1.854766	-0.796935	-0.067283
C	2.057274	-2.126205	0.275693
C	0.859457	-3.040063	0.235379
C	0.036489	-2.854464	-1.056315
C	0.046202	-1.395226	-1.583794
C	3.350532	-2.582116	0.633531
C	4.424554	-1.727169	0.623266
C	4.268060	-0.378928	0.201892
C	2.973404	0.089339	-0.177877
C	-0.375014	1.025319	2.666578

C	2.858587	1.416279	-0.683455
C	3.952547	2.243291	-0.764446
C	5.227734	1.790851	-0.342525
C	5.379721	0.507947	0.122904
H	0.905620	-1.322075	-2.272225
C	-1.177561	-1.071880	-2.434660
H	-0.525530	3.363017	1.720220
H	1.002756	3.368963	0.837234
H	-0.089701	2.770272	-1.249728
H	-1.041080	4.078069	-0.535897
H	-5.344687	2.076374	-0.768374
H	-3.414999	3.620341	-0.957236
H	-6.254394	-0.132380	-0.148927
H	-5.913768	-2.428939	0.718819
H	-3.612370	-3.211167	1.311200
H	-1.669540	-1.732729	0.962824
H	0.220969	-2.809282	1.105233
H	1.167937	-4.088924	0.351202
H	-1.001354	-3.168358	-0.865165
H	0.424072	-3.519553	-1.843608
H	3.484933	-3.628476	0.920973
H	5.418076	-2.079505	0.912946
H	1.883975	1.770183	-1.021402
H	3.840600	3.254918	-1.162384
H	6.088242	2.461725	-0.401145
H	6.362872	0.142616	0.432236
H	-1.180516	-0.018792	-2.754575
H	-2.125867	-1.277250	-1.922793
H	-1.156909	-1.694345	-3.343788
H	-1.466224	1.178898	2.655952
H	0.044059	1.666225	3.458535
H	-0.179916	-0.022919	2.943430

TS<sub>6</sub>

C	0.094113	2.167221	0.230293
C	-0.565227	3.237354	-0.695977
C	-1.538551	2.664132	-1.731626
C	-2.447536	1.686397	-1.048759
C	-1.829776	0.725972	-0.265914
C	-0.341507	0.762543	-0.176743
C	-2.620669	-0.178376	0.517092
C	-4.043033	-0.137490	0.384041
C	-4.634796	0.812509	-0.492119
C	-3.856039	1.716347	-1.172049
C	-4.842766	-1.037568	1.144105
C	-4.268325	-1.925674	2.019687
C	-2.860943	-1.946316	2.180080
C	-2.061583	-1.100484	1.448659
C	0.412164	-0.334360	-0.490722
H	1.166064	2.257571	0.061073
C	1.848622	-0.713004	-0.157857
C	2.139788	-2.079594	-0.311081
C	1.060142	-3.133054	-0.193085
C	-0.228090	-2.790511	-0.944094
C	-0.137246	-1.378739	-1.505460
C	3.469513	-2.532639	-0.509280
C	4.524285	-1.662986	-0.515363
C	4.312263	-0.329652	-0.081210
C	2.984057	0.117721	0.223771
C	-0.222197	2.457951	1.701516
C	2.910597	1.293477	1.025104
C	4.012073	2.067193	1.312034
C	5.287541	1.714539	0.819163

C	5.430009	0.517632	0.163034
H	0.696353	-1.406817	-2.230072
C	-1.350416	-1.065265	-2.380227
H	-1.115860	3.959184	-0.072553
H	0.223654	3.805567	-1.210848
H	-0.971873	2.148502	-2.526654
H	-2.108849	3.470204	-2.215708
H	-5.722832	0.827321	-0.598037
H	-4.319674	2.463027	-1.822465
H	-5.928792	-1.000808	1.022311
H	-4.892375	-2.607072	2.602939
H	-2.408305	-2.639612	2.893410
H	-0.979997	-1.126579	1.585894
H	0.851771	-3.240203	0.884770
H	1.463156	-4.103133	-0.516221
H	-1.107784	-2.882938	-0.289875
H	-0.382429	-3.491544	-1.779275
H	3.632280	-3.595584	-0.706035
H	5.536263	-1.996701	-0.757971
H	1.977625	1.540537	1.513981
H	3.897262	2.944688	1.953210
H	6.154335	2.348640	1.019497
H	6.418921	0.164850	-0.142592
H	-1.351409	-1.788171	-3.212173
H	-1.297428	-0.061506	-2.822352
H	-2.314037	-1.172658	-1.865162
H	-1.310991	2.476553	1.868359
H	0.179733	3.438607	2.002142
H	0.196419	1.696419	2.378327

B3LYP/SVP in the gas phase

(*P,P*)-*trans*-1

C	-0.079718	0.509226	-1.979456
C	0.528601	1.822362	-2.582552
C	1.481820	2.562424	-1.622310
C	2.446721	1.589853	-0.991608
C	1.901346	0.426507	-0.447057
C	0.413336	0.330166	-0.539881
C	2.766388	-0.589287	0.080258
C	4.183868	-0.347318	0.116064
C	4.692422	0.875951	-0.399238
C	3.846199	1.810257	-0.955674
C	5.046065	-1.349145	0.646051
C	4.547246	-2.551703	1.098339
C	3.154991	-2.808077	1.030646
C	2.291260	-1.852313	0.536796
C	-0.413392	0.330553	0.539835
H	-1.172097	0.620339	-1.950244
C	-1.901399	0.426707	0.446982
C	-2.446887	1.590296	0.990883
C	-1.482128	2.563414	1.620939
C	-0.528492	1.824221	2.581440
C	0.079737	0.510659	1.979259
C	-3.846381	1.810604	0.954744
C	-4.692511	0.875983	0.398709
C	-4.183843	-0.347514	-0.115954
C	-2.766357	-0.589394	-0.079911
C	0.251665	-0.698590	-2.873365
C	-2.291146	-1.852630	-0.535772
C	-3.154798	-2.808666	-1.029242
C	-4.547052	-2.552379	-1.097212
C	-5.045956	-1.349623	-0.645541
H	1.172115	0.621696	1.949895
C	-0.251624	-0.696537	2.874016
H	1.089323	1.572692	-3.497877
H	-0.282273	2.502344	-2.888836
H	0.887799	3.055565	-0.831815
H	2.020528	3.361925	-2.154648
H	5.770576	1.055268	-0.365568
H	4.249824	2.737618	-1.372225
H	6.120847	-1.149064	0.677655
H	5.222151	-3.312976	1.497767
H	2.764652	-3.771776	1.368002
H	1.222778	-2.060815	0.477491
H	-2.020979	3.363058	2.152929
H	-0.888420	3.056348	0.830066
H	-1.088830	1.575281	3.497197
H	0.282414	2.504550	2.886856
H	-4.250073	2.738152	1.370812
H	-5.770670	1.055227	0.364846
H	-1.222669	-2.061095	-0.476244
H	-2.764383	-3.772519	-1.366077
H	-5.221886	-3.313867	-1.496351
H	-6.120740	-1.149582	-0.677338
H	0.108376	-0.522930	3.901473
H	0.222231	-1.619302	2.508963
H	-1.339364	-0.866663	2.925187
H	1.339410	-0.868758	-2.924359
H	-0.108289	-0.525665	-3.900956
H	-0.222233	-1.621090	-2.507720

*(P,P)*-trans-1\*

C	-0.220770	-1.884286	-1.092210
C	0.504599	-2.146025	-2.431788
C	1.994629	-2.396638	-2.198209
C	2.624746	-1.453956	-1.196323
C	1.824290	-0.624512	-0.341087
C	0.392758	-0.599555	-0.523212
C	2.511620	0.181664	0.669367
C	3.950628	0.238295	0.682065
C	4.683465	-0.531863	-0.254354
C	4.022893	-1.367162	-1.148793
C	4.607620	1.032566	1.662704
C	3.895157	1.710096	2.638729
C	2.492606	1.609661	2.667386
C	1.825251	0.856639	1.702221
C	-0.392765	0.599553	-0.523223
H	-1.279729	-1.689654	-1.313882
C	-1.824303	0.624523	-0.341093
C	-2.624758	1.453990	-1.196277
C	-1.994650	2.396750	-2.198096
C	-0.504649	2.146105	-2.431751
C	0.220769	1.884285	-1.092213
C	-4.022914	1.367181	-1.148755
C	-4.683474	0.531852	-0.254342
C	-3.950625	-0.238316	0.682064
C	-2.511621	-0.181682	0.669354
C	-0.142399	-3.116128	-0.169215
C	-1.825241	-0.856689	1.702175
C	-2.492588	-1.609715	2.667343
C	-3.895142	-1.710133	2.638713
C	-4.607613	-1.032593	1.662704
H	1.279707	1.689643	-1.313978
C	0.142463	3.116078	-0.169144
H	0.050073	-3.009032	-2.947509
H	0.365036	-1.272534	-3.091034
H	2.551079	-2.352568	-3.149704
H	2.133618	-3.430724	-1.829171
H	5.775531	-0.484211	-0.245780
H	4.606966	-1.969103	-1.851676
H	5.699836	1.084658	1.641991
H	4.419809	2.306953	3.389185
H	1.920319	2.118033	3.447428
H	0.738858	0.778709	1.755612
H	-2.133590	3.430801	-1.828941
H	-2.551136	2.352779	-3.149572
H	-0.050105	3.009119	-2.947449
H	-0.365121	1.272630	-3.091024
H	-4.606986	1.969134	-1.851629
H	-5.775539	0.484182	-0.245759
H	-0.738846	-0.778786	1.755538
H	-1.920293	-2.118107	3.447367
H	-4.419784	-2.306985	3.389180
H	-5.699829	-1.084674	1.642001
H	0.796537	2.999889	0.704855
H	-0.878672	3.297224	0.199492
H	0.470076	4.017505	-0.714027
H	0.878734	-3.297213	0.199451
H	-0.469920	-4.017544	-0.714173
H	-0.796518	-3.000038	0.704759

*(M,M)*-cis-2

C	-1.468659	2.805638	0.272701
C	-2.989168	2.624285	0.136811



C	-3.439943	1.345679	0.847132
C	-2.794751	0.166328	0.165601
C	-1.501047	0.295826	-0.365070
C	-0.691395	1.499979	-0.043026
C	-1.048224	-0.732156	-1.290015
C	-1.802741	-1.949788	-1.417576
C	-3.030342	-2.088286	-0.716695
C	-3.533138	-1.031465	0.003176
C	-1.349271	-2.978952	-2.290281
C	-0.230509	-2.806929	-3.074768
C	0.463297	-1.575340	-3.027958
C	0.067857	-0.576822	-2.160324
C	0.691346	1.500044	0.043084
H	-1.164286	3.591306	-0.434977
C	1.501070	0.295962	0.365115
C	2.794764	0.166509	-0.165604
C	3.439866	1.345883	-0.847193
C	2.989029	2.624489	-0.136933
C	1.468498	2.805735	-0.272766
C	3.533201	-1.031250	-0.003185
C	3.030446	-2.088092	0.716695
C	1.802850	-1.949637	1.417601
C	1.048290	-0.732036	1.290050
C	-1.160801	3.330535	1.696116
C	-0.067814	-0.576734	2.160336
C	-0.463192	-1.575237	3.028015
C	0.230693	-2.806782	3.074870
C	1.349449	-2.978784	2.290362
H	1.164095	3.591405	0.434889
C	1.160499	3.330516	-1.696178
H	-3.500391	3.507998	0.552472
H	-3.276171	2.557169	-0.925915
H	-4.535433	1.236218	0.810606
H	-3.176828	1.391562	1.919732
H	-3.592910	-3.021230	-0.808345
H	-4.518672	-1.105525	0.471996
H	-1.928529	-3.904986	-2.344725
H	0.102076	-3.600038	-3.749245
H	1.316365	-1.407244	-3.690414
H	0.605470	0.367548	-2.162023
H	3.176732	1.391693	-1.919793
H	4.535367	1.236507	-0.810676
H	3.500188	3.508199	-0.552671
H	3.276087	2.557443	0.925784
H	4.518725	-1.105272	-0.472034
H	3.593036	-3.021020	0.808339
H	-0.605488	0.367609	2.161983
H	-1.316273	-1.407163	3.690460
H	-0.101847	-3.599888	3.749375
H	1.928756	-3.904785	2.344837
H	0.085519	3.412782	-1.899698
H	1.579390	2.668541	-2.469630
H	1.608882	4.327507	-1.839146
H	-1.579739	2.668606	2.469583
H	-1.609224	4.327521	1.838968
H	-0.085844	3.412835	1.899717

TS<sub>2</sub>

C	1.960911	-1.999529	1.031144
C	3.183845	-2.390048	0.207206
C	4.032458	-1.150590	-0.002551
C	3.241230	0.142670	-0.108617
C	1.830532	0.258611	-0.100476

C	1.065774	-1.023362	0.248305
C	1.312355	1.602582	-0.399109
C	2.200907	2.741094	-0.414541
C	3.599274	2.550368	-0.290555
C	4.090480	1.280099	-0.206254
C	1.701765	4.057236	-0.616811
C	0.369813	4.290422	-0.876358
C	-0.496118	3.182729	-0.969654
C	-0.032909	1.900365	-0.739597
C	-0.213296	-1.472163	0.000801
H	1.387196	-2.897245	1.224574
C	-1.459836	-0.721929	-0.371000
C	-2.020240	-1.004427	-1.614063
C	-1.241616	-1.957800	-2.481675
C	-0.850114	-3.214324	-1.664451
C	-0.706076	-2.961084	-0.129861
C	-3.272181	-0.453124	-1.982632
C	-3.979783	0.332138	-1.098705
C	-3.482553	0.579361	0.211235
C	-2.208004	0.036112	0.595275
C	2.316880	-1.457833	2.432354
C	-1.742970	0.280743	1.918212
C	-2.489586	1.020839	2.812061
C	-3.740452	1.563989	2.428454
C	-4.222254	1.346263	1.155392
H	-1.728792	-2.940228	0.278203
C	-0.076334	-4.211953	0.502823
H	3.766577	-3.184252	0.704787
H	2.844784	-2.801090	-0.758472
H	4.661752	-1.242571	-0.905234
H	4.745779	-1.039099	0.833012
H	4.265162	3.417080	-0.309439
H	5.171289	1.114098	-0.178626
H	2.416179	4.884740	-0.588119
H	-0.001197	5.305509	-1.038658
H	-1.546482	3.326733	-1.234636
H	-0.729192	1.090058	-0.871555
H	-0.322882	-1.456796	-2.830955
H	-1.810365	-2.237263	-3.381642
H	0.102132	-3.617895	-2.047707
H	-1.608157	-4.002759	-1.806071
H	-3.676787	-0.665115	-2.976388
H	-4.945428	0.757638	-1.385307
H	-0.776731	-0.125531	2.218083
H	-2.112258	1.193117	3.823374
H	-4.320599	2.152883	3.143490
H	-5.188646	1.758141	0.850978
H	-0.033863	-4.161061	1.600836
H	0.926471	-4.447515	0.117829
H	-0.721489	-5.070479	0.249905
H	2.872505	-0.509390	2.410839
H	2.929141	-2.197466	2.975967
H	1.402484	-1.288971	3.022817

(*M,P*)-*cis*-2

C	2.007378	2.203963	0.778721
C	2.257606	3.014143	-0.540298
C	1.715732	2.317617	-1.805727
C	0.251556	2.025617	-1.586636
C	-0.094481	1.467818	-0.355864
C	1.072693	1.024749	0.477284
C	-1.464718	1.493011	0.065326
C	-2.477099	1.880711	-0.880695

C	-2.087233	2.290993	-2.184022
C	-0.753596	2.408175	-2.509347
C	-3.839413	1.910483	-0.467241
C	-4.192289	1.647790	0.838746
C	-3.188233	1.349861	1.793466
C	-1.865527	1.265335	1.412791
C	1.411020	-0.278383	0.674779
H	2.974062	1.800969	1.091737
C	0.806791	-1.436852	-0.078470
C	1.671389	-1.971520	-1.038814
C	3.065091	-1.392965	-1.150696
C	3.722892	-1.141533	0.232140
C	2.684039	-0.834214	1.347652
C	1.249995	-3.046507	-1.862160
C	0.005462	-3.613728	-1.704483
C	-0.847712	-3.189345	-0.651563
C	-0.427222	-2.108847	0.201425
C	1.489619	3.115398	1.901942
C	-1.222021	-1.820008	1.345666
C	-2.392270	-2.503151	1.601442
C	-2.843095	-3.511707	0.714656
C	-2.080977	-3.848103	-0.383116
H	2.351153	-1.813028	1.730845
C	3.302927	-0.137666	2.568014
H	1.765637	3.997883	-0.463148
H	3.336889	3.211252	-0.647838
H	2.283498	1.391641	-1.995335
H	1.856362	2.960031	-2.689046
H	-2.861030	2.570128	-2.904450
H	-0.457876	2.803100	-3.485607
H	-4.602449	2.178680	-1.203432
H	-5.240200	1.692468	1.146168
H	-3.465638	1.189541	2.838653
H	-1.095570	1.055619	2.156256
H	3.011701	-0.433761	-1.690946
H	3.699748	-2.049678	-1.765329
H	4.428239	-0.297750	0.144770
H	4.322273	-2.017011	0.532413
H	1.930274	-3.421774	-2.632255
H	-0.320384	-4.429943	-2.355049
H	-0.871813	-1.061584	2.042655
H	-2.976843	-2.264552	2.493531
H	-3.781854	-4.034366	0.915432
H	-2.401122	-4.649300	-1.055255
H	2.529837	0.173661	3.287733
H	3.910858	0.744066	2.320426
H	3.971097	-0.844872	3.086630
H	0.494072	3.520130	1.657677
H	2.169484	3.969841	2.056659
H	1.409776	2.571805	2.856588

TS<sub>3</sub>

C	0.803958	-2.843266	-0.415348
C	1.101529	-2.935799	-1.947036
C	1.547740	-1.602379	-2.597512
C	2.155887	-0.664384	-1.589421
C	1.462291	-0.496221	-0.390309
C	0.312096	-1.405772	-0.131268
C	2.003312	0.361374	0.633754
C	3.224591	1.072384	0.368384
C	3.873728	0.901247	-0.885236
C	3.355177	0.048083	-1.834659
C	3.762551	1.930714	1.368607

C	3.136745	2.083694	2.586798
C	1.939839	1.376059	2.856060
C	1.389913	0.540050	1.905828
C	-0.993011	-1.155930	0.239105
H	-0.010922	-3.546610	-0.233881
C	-1.922546	0.019407	-0.034077
C	-3.307227	-0.258702	0.067707
C	-3.925649	-1.648316	0.136656
C	-2.923324	-2.783832	0.292888
C	-1.751087	-2.213196	1.090956
C	-4.277161	0.780200	0.089315
C	-3.930382	2.098434	-0.007001
C	-2.584391	2.438590	-0.294266
C	-1.585609	1.401607	-0.398904
C	2.025811	-3.297680	0.404903
C	-0.340305	1.823404	-0.936517
C	-0.051903	3.143324	-1.231253
C	-1.002700	4.158933	-1.003224
C	-2.253819	3.796886	-0.556114
H	-2.207267	-1.574572	1.870021
C	-1.001621	-3.262419	1.926066
H	1.883350	-3.698096	-2.096283
H	0.203648	-3.301631	-2.468504
H	0.661294	-1.109407	-3.034671
H	2.241289	-1.785556	-3.432464
H	4.798342	1.451439	-1.080242
H	3.867405	-0.085553	-2.791749
H	4.689914	2.468029	1.150917
H	3.561499	2.745712	3.345685
H	1.447418	1.494105	3.824773
H	0.465798	0.005110	2.123895
H	-4.560454	-1.781951	-0.757267
H	-4.622504	-1.665221	0.993861
H	-2.567231	-3.154506	-0.683392
H	-3.389679	-3.639870	0.808434
H	-5.326815	0.499424	0.216021
H	-4.680405	2.889766	0.071420
H	0.410661	1.085337	-1.171242
H	0.925298	3.391285	-1.653106
H	-0.763518	5.204366	-1.213606
H	-3.037298	4.548834	-0.426604
H	-0.098745	-2.847482	2.396256
H	-0.715352	-4.170134	1.377905
H	-1.672436	-3.588903	2.737838
H	2.926756	-2.719331	0.151595
H	2.244371	-4.358588	0.198357
H	1.858976	-3.194968	1.486743

*(P,P)-cis-2*

C	-1.493316	2.814738	-0.088705
C	-2.731251	2.665614	-1.020079
C	-2.643413	1.422690	-1.917314
C	-2.488342	0.213901	-1.028825
C	-1.534992	0.284852	-0.010305
C	-0.681380	1.509945	-0.003868
C	-1.469171	-0.766086	0.969531
C	-2.303583	-1.925836	0.805444
C	-3.201791	-1.987682	-0.293918
C	-3.309717	-0.931340	-1.170215
C	-2.238865	-2.974754	1.766130
C	-1.416473	-2.881109	2.867446
C	-0.629403	-1.718938	3.059066
C	-0.654568	-0.694891	2.135153

C	0.682868	1.509365	0.003917
H	-0.851463	3.585426	-0.536102
C	1.535354	0.283492	0.010301
C	2.488558	0.211488	1.028875
C	2.644778	1.420134	1.917360
C	2.733989	2.662813	1.019913
C	1.495925	2.813493	0.089094
C	3.308803	-0.934558	1.170207
C	3.199871	-1.990713	0.293794
C	2.301769	-1.927889	-0.805593
C	1.468530	-0.767284	-0.969643
C	-1.916408	3.306152	1.307218
C	0.654040	-0.695204	-2.135290
C	0.627913	-1.719148	-3.059284
C	1.413812	-2.882125	-2.867712
C	2.236049	-2.976678	-1.766363
H	0.854818	3.584356	0.537279
C	1.918979	3.305592	-1.306574
H	-3.646101	2.577546	-0.410672
H	-2.845859	3.578074	-1.627927
H	-1.782285	1.521824	-2.604557
H	-3.540761	1.329852	-2.548799
H	-3.828071	-2.875809	-0.415094
H	-4.031587	-0.969113	-1.991121
H	-2.869903	-3.855795	1.618897
H	-1.380656	-3.691348	3.600183
H	0.001175	-1.632301	3.947711
H	-0.056475	0.199342	2.301635
H	3.541997	1.326445	2.548900
H	1.783689	1.520222	2.604515
H	3.648496	2.573295	0.410184
H	2.850183	3.575233	1.627533
H	4.030606	-0.973116	1.991134
H	3.825270	-2.879470	0.414912
H	0.056861	0.199646	-2.301754
H	-0.002521	-1.631814	-3.947960
H	1.377200	-3.692283	-3.600498
H	2.866193	-3.858366	-1.619159
H	1.047933	3.516412	-1.946605
H	2.534647	2.547433	-1.817327
H	2.516541	4.229599	-1.231522
H	-2.532945	2.548149	1.817156
H	-2.513056	4.230797	1.232793
H	-1.045329	3.515561	1.947691

(*P,P*)-*cis*-2\*

C	2.615139	1.977081	0.146836
C	2.201441	3.429488	-0.200455
C	0.926485	3.476720	-1.034829
C	-0.177223	2.777367	-0.289503
C	0.138347	1.543171	0.364904
C	1.442788	0.981711	0.106192
C	-0.923992	0.875903	1.117055
C	-2.283496	1.325582	0.963473
C	-2.547119	2.477691	0.192230
C	-1.496328	3.217112	-0.367444
C	-3.327531	0.607901	1.616867
C	-3.048522	-0.457403	2.454772
C	-1.711229	-0.836671	2.678149
C	-0.674093	-0.166984	2.029783
C	1.688062	-0.398244	-0.179834
H	3.367344	1.660005	-0.593884
C	0.673619	-1.381144	-0.475180

C	0.864216	-2.736637	-0.010789
C	2.234575	-3.256458	0.351012
C	3.192041	-2.154489	0.795971
C	3.120498	-0.940657	-0.147803
C	-0.244404	-3.560612	0.168861
C	-1.543016	-3.151469	-0.169850
C	-1.746737	-1.943510	-0.866335
C	-0.619298	-1.077393	-1.106554
C	3.286168	1.984591	1.541115
C	-0.800962	-0.006483	-2.000711
C	-2.055514	0.304601	-2.532960
C	-3.177735	-0.476861	-2.204734
C	-3.024427	-1.583400	-1.387311
H	3.792374	-0.183019	0.267211
C	3.632799	-1.257960	-1.566500
H	2.020983	3.996375	0.728350
H	3.036068	3.932221	-0.716030
H	1.100082	2.971473	-2.006036
H	0.636899	4.513336	-1.269032
H	-3.579704	2.817349	0.077748
H	-1.718979	4.125056	-0.935478
H	-4.359427	0.934604	1.462202
H	-3.860750	-0.993131	2.952682
H	-1.480898	-1.651127	3.368928
H	0.357157	-0.466579	2.218180
H	2.657587	-3.760732	-0.539275
H	2.151387	-4.039770	1.121775
H	4.225231	-2.538709	0.843727
H	2.929552	-1.822195	1.815743
H	-0.095780	-4.548373	0.615261
H	-2.394323	-3.809532	0.022200
H	0.061227	0.602267	-2.275407
H	-2.157328	1.152221	-3.214593
H	-4.161315	-0.221201	-2.607337
H	-3.879054	-2.225436	-1.157256
H	3.651849	-0.348772	-2.188397
H	2.992526	-1.988937	-2.083132
H	4.658919	-1.662122	-1.530244
H	2.557302	2.295166	2.306551
H	4.124205	2.702194	1.558569
H	3.679555	1.002099	1.838409

*(M,M)-trans-1*

C	0.292685	-1.962192	-0.867619
C	-0.772025	-3.039404	-1.168958
C	-1.919742	-2.459744	-2.002939
C	-2.623188	-1.449536	-1.137979
C	-1.840619	-0.605690	-0.338361
C	-0.362181	-0.586973	-0.539677
C	-2.503411	0.163402	0.696608
C	-3.941765	0.189076	0.744516
C	-4.685418	-0.587947	-0.182704
C	-4.036384	-1.416982	-1.068557
C	-4.603894	0.959561	1.742739
C	-3.893779	1.649739	2.699754
C	-2.480076	1.579608	2.699892
C	-1.810919	0.863711	1.727279
C	0.362239	0.588188	-0.538490
H	0.865027	-2.310928	0.006272
C	1.840666	0.606498	-0.337063
C	2.623281	1.452066	-1.134814
C	1.919880	2.464057	-1.997729
C	0.772068	3.041943	-1.162654

C	-0.292632	1.964068	-0.863613
C	4.036474	1.419391	-1.065339
C	4.685451	0.588466	-0.181215
C	3.941735	-0.190608	0.744234
C	2.503387	-0.164865	0.696250
C	1.267504	-1.898711	-2.061477
C	1.810804	-0.867550	1.725239
C	2.479885	-1.585589	2.696324
C	3.893593	-1.655631	2.696206
C	4.603786	-0.963288	1.740811
H	-0.865022	2.310976	0.010971
C	-1.267422	1.903009	-2.057624
H	-0.289516	-3.882078	-1.689122
H	-1.194276	-3.443703	-0.234031
H	-2.625187	-3.243495	-2.320470
H	-1.522637	-2.000360	-2.926386
H	-5.777681	-0.552125	-0.149860
H	-4.610699	-2.064745	-1.737023
H	-5.697401	0.976181	1.744307
H	-4.414304	2.230370	3.465454
H	-1.910928	2.090761	3.480692
H	-0.723497	0.818448	1.758533
H	1.522865	2.006589	-2.922165
H	2.625327	3.248489	-2.313565
H	0.289576	3.885677	-1.681111
H	1.194240	3.444326	-0.226865
H	4.610833	2.068594	-1.732369
H	5.777712	0.552588	-0.148360
H	0.723371	-0.822451	1.756435
H	1.910670	-2.098542	3.475894
H	4.414059	-2.237954	3.460659
H	5.697294	-0.979874	1.742457
H	-0.747487	1.601008	-2.981596
H	-1.706980	2.898535	-2.230142
H	-2.094777	1.202200	-1.901795
H	0.747622	-1.594704	-2.984822
H	1.706974	-2.893912	-2.236092
H	2.094920	-1.198316	-1.904145

TS<sub>5</sub>

C	-0.415552	-0.957143	1.631675
C	-0.473996	-2.449257	1.316858
C	0.932755	-2.989702	1.166065
C	1.921324	-2.011141	0.562903
C	1.631107	-0.691944	0.127495
C	0.326470	-0.085654	0.582749
C	2.793249	0.039291	-0.413417
C	4.132394	-0.460875	-0.276768
C	4.335834	-1.769186	0.233243
C	3.247260	-2.532984	0.546296
C	5.237946	0.298647	-0.749546
C	5.055838	1.467647	-1.457162
C	3.739513	1.876630	-1.756742
C	2.658803	1.173428	-1.256267
C	-0.466048	0.979963	0.117908
H	-1.444241	-0.588643	1.705307
C	-1.943276	0.831754	-0.024122
C	-2.791067	1.818670	0.497608
C	-2.166249	3.105202	0.960966
C	-1.098049	3.474078	-0.069020
C	0.045490	2.431044	-0.112971
C	-4.192849	1.628806	0.543999
C	-4.769979	0.473241	0.068604

C	-3.972930	-0.515607	-0.568262
C	-2.547737	-0.336212	-0.635726
C	0.220003	-0.679963	3.015000
C	-1.813265	-1.255318	-1.439948
C	-2.427588	-2.317781	-2.073601
C	-3.817842	-2.537800	-1.925550
C	-4.571034	-1.648102	-1.191117
H	0.488412	2.548502	-1.112076
C	1.100508	2.820683	0.940112
H	-1.014336	-2.989396	2.112671
H	-1.045746	-2.603441	0.393632
H	0.941750	-3.912206	0.558243
H	1.331486	-3.294522	2.149841
H	5.351182	-2.165170	0.317865
H	3.389492	-3.565068	0.879600
H	6.243419	-0.096375	-0.579391
H	5.912815	2.034452	-1.829377
H	3.567857	2.738605	-2.406885
H	1.665417	1.465182	-1.569581
H	-1.707515	2.991926	1.960570
H	-2.930100	3.893376	1.052213
H	-0.659257	4.461388	0.148586
H	-1.584716	3.554394	-1.054978
H	-4.815387	2.412488	0.985221
H	-5.851246	0.323614	0.131648
H	-0.743279	-1.099010	-1.572268
H	-1.834643	-2.991090	-2.698088
H	-4.292506	-3.392280	-2.414589
H	-5.653042	-1.779560	-1.101500
H	0.632564	2.913162	1.934379
H	1.556323	3.792216	0.689377
H	1.906266	2.083557	1.028078
H	1.284598	-0.956977	3.057829
H	-0.311289	-1.250049	3.795833
H	0.149527	0.388423	3.270250

(*M,P*)-*trans*-1

C	0.242235	1.366765	1.330165
C	-0.014659	2.864550	0.953971
C	-0.774540	3.036250	-0.379881
C	-1.971439	2.119645	-0.394602
C	-1.744495	0.787622	-0.046677
C	-0.312977	0.448527	0.231721
C	-2.860678	-0.088867	0.163968
C	-4.186061	0.387129	-0.128722
C	-4.361646	1.725794	-0.572622
C	-3.283261	2.577038	-0.674104
C	-5.296035	-0.485127	0.060623
C	-5.124235	-1.760823	0.552486
C	-3.824580	-2.217039	0.887182
C	-2.726716	-1.404192	0.694918
C	0.455687	-0.453307	-0.432322
H	1.324096	1.210998	1.400299
C	1.872634	-0.783072	-0.048451
C	2.084985	-2.118044	0.299069
C	0.892378	-3.043611	0.250275
C	0.083104	-2.870395	-1.058662
C	0.079420	-1.401525	-1.583373
C	3.379809	-2.569561	0.658917
C	4.456710	-1.711306	0.641568
C	4.300959	-0.367058	0.207991
C	2.995314	0.103049	-0.170919
C	-0.350584	1.017139	2.706689



TS<sub>6</sub>

C	2.889554	1.424118	-0.695942
C	3.992093	2.246483	-0.801251
C	5.268247	1.795293	-0.380779
C	5.414556	0.514987	0.107226
H	0.950747	-1.320106	-2.256740
C	-1.137622	-1.097099	-2.460766
H	-0.606282	3.345455	1.749940
H	0.943229	3.406088	0.905555
H	-0.102501	2.789268	-1.220948
H	-1.079526	4.085119	-0.518989
H	-5.371000	2.078971	-0.800836
H	-3.431370	3.618709	-0.972984
H	-6.296588	-0.115269	-0.180715
H	-5.986409	-2.416336	0.698920
H	-3.693316	-3.218960	1.304323
H	-1.732198	-1.759508	0.963276
H	0.234695	-2.814047	1.107371
H	1.206098	-4.091132	0.377274
H	-0.953080	-3.203207	-0.888511
H	0.496937	-3.525935	-1.842163
H	3.515089	-3.614078	0.953970
H	5.451008	-2.061662	0.931725
H	1.914664	1.775816	-1.033719
H	3.882921	3.251831	-1.216545
H	6.133591	2.458362	-0.458517
H	6.398541	0.148809	0.413591
H	-1.108746	-1.747299	-3.351140
H	-1.132355	-0.053852	-2.810773
H	-2.092213	-1.279608	-1.952810
H	-1.446764	1.128286	2.718115
H	0.062435	1.682581	3.482800
H	-0.110662	-0.019483	2.992064

C	0.084552	2.153874	0.217970
C	-0.554903	3.224882	-0.734301
C	-1.545303	2.648809	-1.759557
C	-2.460687	1.678729	-1.065225
C	-1.847472	0.704883	-0.278038
C	-0.354999	0.738283	-0.177058
C	-2.660256	-0.187956	0.506626
C	-4.092333	-0.119083	0.376909
C	-4.667433	0.845650	-0.494168
C	-3.870198	1.736119	-1.179506
C	-4.906514	-1.004372	1.139772
C	-4.348911	-1.904062	2.021659
C	-2.942244	-1.947454	2.184443
C	-2.124212	-1.116195	1.446447
C	0.425857	-0.357707	-0.477140
H	1.159829	2.231624	0.062513
C	1.868142	-0.715004	-0.136574
C	2.181838	-2.087488	-0.291181
C	1.109066	-3.151413	-0.164061
C	-0.167430	-2.839657	-0.957464
C	-0.099443	-1.414435	-1.506850
C	3.514053	-2.527404	-0.487952
C	4.564720	-1.644433	-0.493118
C	4.342105	-0.312511	-0.062325
C	3.000908	0.128629	0.246137
C	-0.242621	2.483973	1.686645
C	2.926791	1.313769	1.034934
C	4.029904	2.097905	1.316581
C	5.307601	1.749030	0.826575

C	5.453875	0.545751	0.174053
H	0.744498	-1.422084	-2.220595
C	-1.315679	-1.123434	-2.393936
H	-1.086988	3.972824	-0.124825
H	0.247453	3.765200	-1.261465
H	-0.984254	2.129490	-2.557373
H	-2.113798	3.456106	-2.247018
H	-5.755669	0.884843	-0.593533
H	-4.321882	2.492792	-1.827333
H	-5.992058	-0.947407	1.019358
H	-4.986853	-2.572943	2.604892
H	-2.501725	-2.641155	2.905416
H	-1.044523	-1.152433	1.589786
H	0.870211	-3.229682	0.911546
H	1.526564	-4.129966	-0.445216
H	-1.065088	-2.966912	-0.333448
H	-0.274242	-3.536536	-1.805284
H	3.687637	-3.590558	-0.675433
H	5.579718	-1.970362	-0.734356
H	1.993779	1.566813	1.518499
H	3.910588	2.980662	1.950409
H	6.171634	2.389243	1.020609
H	6.444564	0.196291	-0.130143
H	-1.299832	-1.847013	-3.226627
H	-1.282035	-0.119259	-2.836067
H	-2.279105	-1.244587	-1.883002
H	-1.331212	2.481509	1.853465
H	0.136149	3.483646	1.956933
H	0.193978	1.753783	2.386504

B3LYP/SVP in hexane

(*P,P*)-*trans*-1

C	-0.081173	-0.482994	1.980906
C	0.503614	-1.805931	2.584369
C	1.461292	-2.550305	1.631964
C	2.435797	-1.585425	1.004045
C	1.901751	-0.419694	0.451275
C	0.413112	-0.312857	0.540278
C	2.778425	0.585410	-0.078737
C	4.194322	0.330659	-0.107706
C	4.690820	-0.893410	0.417759
C	3.833940	-1.817286	0.975435
C	5.067838	1.321481	-0.640712
C	4.581210	2.524767	-1.104584
C	3.190774	2.793247	-1.045869
C	2.316382	1.848710	-0.548592
C	-0.413123	-0.312908	-0.540301
H	-1.175122	-0.573122	1.954415
C	-1.901761	-0.419718	-0.451264
C	-2.435833	-1.585493	-1.003918
C	-1.461354	-2.550441	-1.631773
C	-0.503709	-1.806151	-2.584273
C	0.081149	-0.483197	-1.980916
C	-3.833979	-1.817329	-0.975263
C	-4.690835	-0.893390	-0.417651
C	-4.194307	0.330712	0.107708
C	-2.778407	0.585437	0.078693
C	0.272617	0.720938	2.870915
C	-2.316330	1.848758	0.548462
C	-3.190697	2.793346	1.045687
C	-4.581138	2.524898	1.104437
C	-5.067796	1.321589	0.640658
H	1.175094	-0.573380	-1.954416
C	-0.272587	0.720669	-2.871037
H	1.051900	-1.568604	3.510419
H	-0.318735	-2.479972	2.872554
H	0.869825	-3.041262	0.838055
H	1.992106	-3.352209	2.168496
H	5.767649	-1.081890	0.390045
H	4.228129	-2.745437	1.399407
H	6.140927	1.111639	-0.666458
H	5.264396	3.277436	-1.506505
H	2.810300	3.757246	-1.393888
H	1.249333	2.066970	-0.498066
H	-1.992189	-3.352389	-2.168218
H	-0.869864	-3.041332	-0.837840
H	-1.052049	-1.568858	-3.510299
H	0.318606	-2.480227	-2.872475
H	-4.228191	-2.745511	-1.399145
H	-5.767665	-1.081852	-0.389901
H	-1.249277	2.066990	0.497911
H	-2.810198	3.757359	1.393638
H	-5.264302	3.277608	1.506318
H	-6.140888	1.111768	0.666437
H	0.103296	0.565444	-3.896059
H	0.171774	1.654754	-2.496113
H	-1.363245	0.866603	-2.936027
H	1.363281	0.866825	2.935904
H	-0.103288	0.565832	3.895947
H	-0.171692	1.655009	2.495893

*(P,P)*-trans-1\*

C	-0.178418	-1.872449	-1.190962
C	0.604461	-2.115044	-2.500650
C	2.081713	-2.368600	-2.204030
C	2.666955	-1.428551	-1.173054
C	1.828439	-0.601603	-0.348260
C	0.406607	-0.594854	-0.572243
C	2.478983	0.216426	0.681205
C	3.917042	0.276007	0.746969
C	4.687001	-0.497633	-0.157041
C	4.061729	-1.336202	-1.073058
C	4.537390	1.075565	1.747330
C	3.789432	1.756343	2.693192
C	2.386393	1.655345	2.669453
C	1.755505	0.898802	1.683603
C	-0.406619	0.595182	-0.571952
H	-1.226634	-1.674705	-1.456074
C	-1.828448	0.601799	-0.347939
C	-2.666999	1.429106	-1.172335
C	-2.081796	2.369651	-2.202880
C	-0.604545	2.116265	-2.499648
C	0.178368	1.873076	-1.190090
C	-4.061769	1.336661	-1.072369
C	-4.687003	0.497640	-0.156740
C	-3.917009	-0.276403	0.746894
C	-2.478952	-0.216742	0.681144
C	-0.143382	-3.119899	-0.286653
C	-1.755435	-0.899585	1.683196
C	-2.386283	-1.656625	2.668689
C	-3.789319	-1.757672	2.692403
C	-4.537315	-1.076461	1.746882
H	1.226583	1.675480	-1.455316
C	0.143316	3.120107	-0.285202
H	0.173595	-2.971212	-3.047033
H	0.494394	-1.233479	-3.154688
H	2.678705	-2.319051	-3.130208
H	2.205114	-3.404674	-1.835159
H	5.777959	-0.447607	-0.107667
H	4.673226	-1.937131	-1.753359
H	5.629721	1.127813	1.766474
H	4.285409	2.356513	3.460531
H	1.785003	2.168231	3.424363
H	0.667894	0.825526	1.697010
H	-2.205214	3.405549	-1.833521
H	-2.678802	2.320519	-3.129072
H	-0.173707	2.972700	-3.045636
H	-0.494466	1.235013	-3.154104
H	-4.673294	1.937881	-1.752388
H	-5.777958	0.447552	-0.107384
H	-0.667826	-0.826290	1.696612
H	-1.784865	-2.169860	3.423339
H	-4.285267	-2.358226	3.459461
H	-5.629643	-1.128759	1.766019
H	0.843069	3.023019	0.555096
H	-0.856574	3.307993	0.134686
H	0.439710	4.013393	-0.861042
H	0.856505	-3.307986	0.133152
H	-0.439783	-4.012915	-0.862907
H	-0.843134	-3.023194	0.553690

*(M,M)*-cis-2

C	-1.459947	2.804360	0.294110
C	-2.982415	2.635060	0.167710

C	-3.439643	1.356642	0.873306
C	-2.803424	0.174275	0.188525
C	-1.511126	0.295871	-0.349859
C	-0.692184	1.495576	-0.033939
C	-1.072482	-0.734743	-1.279835
C	-1.835149	-1.948468	-1.402566
C	-3.058963	-2.079930	-0.693400
C	-3.549683	-1.019793	0.030099
C	-1.392420	-2.980640	-2.277895
C	-0.278038	-2.814396	-3.070309
C	0.421407	-1.585666	-3.030138
C	0.036982	-0.584967	-2.159649
C	0.692467	1.495450	0.033982
H	-1.153957	3.591399	-0.410913
C	1.511190	0.295583	0.349885
C	2.803465	0.173761	-0.188501
C	3.439865	1.356023	-0.873289
C	2.982898	2.634517	-0.167665
C	1.460457	2.804118	-0.294016
C	3.549528	-1.020424	-0.030081
C	3.058662	-2.080475	0.693443
C	1.834845	-1.948829	1.402572
C	1.072358	-0.734989	1.279819
C	-1.137477	3.317783	1.717942
C	-0.037154	-0.585093	2.159551
C	-0.421792	-1.585759	3.029980
C	0.277480	-2.814588	3.070173
C	1.391898	-2.980959	2.277839
H	1.154636	3.591174	0.411064
C	1.138096	3.317683	-1.717819
H	-3.483717	3.519408	0.593823
H	-3.278207	2.579001	-0.893331
H	-4.535726	1.253920	0.837120
H	-3.175898	1.397296	1.945788
H	-3.627522	-3.009721	-0.780513
H	-4.532508	-1.087880	0.505630
H	-1.976494	-3.904011	-2.327605
H	0.046465	-3.610006	-3.746021
H	1.270152	-1.421736	-3.699368
H	0.578553	0.357281	-2.166060
H	3.176062	1.396730	-1.945756
H	4.535936	1.253124	-0.837155
H	3.484367	3.518764	-0.593795
H	3.278710	2.578396	0.893366
H	4.532338	-1.088662	-0.505620
H	3.627092	-3.010343	0.780576
H	-0.578575	0.357239	2.165959
H	-1.270563	-1.421729	3.699151
H	-0.047184	-3.610173	3.745836
H	1.975840	-3.904412	2.327568
H	0.061132	3.378032	-1.920592
H	1.568858	2.664331	-2.492472
H	1.563958	4.324074	-1.865950
H	-1.568321	2.664456	2.492568
H	-1.563138	4.324246	1.866162
H	-0.060492	3.377910	1.920676

TS<sub>2</sub>

C	1.926687	-2.041540	1.016302
C	3.153662	-2.436098	0.200040
C	4.025023	-1.208500	0.026997
C	3.254242	0.095694	-0.087350
C	1.844909	0.234803	-0.089537

C	1.052391	-1.036664	0.244408
C	1.353450	1.589722	-0.387706
C	2.263247	2.712306	-0.405617
C	3.657564	2.497319	-0.273167
C	4.124024	1.218580	-0.180021
C	1.790541	4.036597	-0.619481
C	0.464223	4.294198	-0.884924
C	-0.423933	3.203491	-0.967135
C	0.013324	1.913804	-0.725388
C	-0.235826	-1.458713	-0.008852
H	1.338495	-2.934257	1.185982
C	-1.472222	-0.686936	-0.378338
C	-2.034049	-0.956020	-1.624767
C	-1.265096	-1.912532	-2.497163
C	-0.900350	-3.181542	-1.687563
C	-0.755845	-2.939652	-0.151130
C	-3.284737	-0.397907	-1.988439
C	-3.992820	0.378487	-1.097087
C	-3.494376	0.614280	0.214563
C	-2.218197	0.069014	0.592837
C	2.274966	-1.533729	2.431462
C	-1.749923	0.310753	1.915608
C	-2.495283	1.046014	2.814907
C	-3.749090	1.587068	2.437918
C	-4.233584	1.374622	1.164911
H	-1.779332	-2.901856	0.252765
C	-0.157844	-4.206234	0.479709
H	3.716370	-3.249471	0.689216
H	2.823697	-2.821520	-0.779022
H	4.677080	-1.300138	-0.859248
H	4.716870	-1.114891	0.882583
H	4.339603	3.351422	-0.292507
H	5.201365	1.032884	-0.144466
H	2.521319	4.849851	-0.594767
H	0.114142	5.315074	-1.057898
H	-1.471328	3.367856	-1.232391
H	-0.701833	1.117219	-0.841003
H	-0.336447	-1.423677	-2.837107
H	-1.833489	-2.174986	-3.402271
H	0.043174	-3.602728	-2.072859
H	-1.675185	-3.952191	-1.834980
H	-3.690050	-0.600910	-2.983826
H	-4.959053	0.805690	-1.379314
H	-0.780947	-0.092022	2.211751
H	-2.114638	1.215962	3.825505
H	-4.328626	2.171160	3.157574
H	-5.201055	1.786690	0.864157
H	-0.117389	-4.159618	1.578279
H	0.838484	-4.471516	0.096950
H	-0.825099	-5.047813	0.225900
H	2.837465	-0.588700	2.439880
H	2.877964	-2.288954	2.964562
H	1.357967	-1.372672	3.020575

(*M,P*)-*cis*-2

C	1.997133	-2.197224	-0.812234
C	2.234991	-3.051623	0.478710
C	1.711239	-2.380659	1.764397
C	0.248032	-2.072529	1.562117
C	-0.104270	-1.482564	0.346961
C	1.060896	-1.024642	-0.483112
C	-1.478810	-1.495388	-0.064064
C	-2.485696	-1.909147	0.877767

C	-2.088103	-2.354719	2.167328
C	-0.752217	-2.480089	2.480117
C	-3.850960	-1.929177	0.472500
C	-4.212677	-1.633894	-0.824189
C	-3.214726	-1.311878	-1.777350
C	-1.889547	-1.234071	-1.402667
C	1.403247	0.280570	-0.663841
H	2.966861	-1.782502	-1.099417
C	0.803750	1.435278	0.100440
C	1.667065	1.950812	1.073532
C	3.054141	1.357835	1.188921
C	3.719003	1.113021	-0.192057
C	2.685004	0.839886	-1.320218
C	1.251553	3.024455	1.902263
C	0.018137	3.613241	1.735209
C	-0.829060	3.211530	0.668344
C	-0.417248	2.129054	-0.187314
C	1.498669	-3.070339	-1.973198
C	-1.204246	1.862009	-1.342752
C	-2.356896	2.571088	-1.609590
C	-2.799358	3.582980	-0.722405
C	-2.046047	3.896033	0.388588
H	2.364123	1.830083	-1.682947
C	3.306591	0.170136	-2.553396
H	1.723677	-4.023005	0.374629
H	3.310747	-3.272784	0.574928
H	2.289015	-1.464518	1.970683
H	1.851931	-3.044239	2.631725
H	-2.856974	-2.653408	2.885265
H	-0.449931	-2.901387	3.443317
H	-4.609184	-2.216576	1.206531
H	-5.262668	-1.671996	-1.125851
H	-3.498645	-1.125806	-2.816650
H	-1.125502	-1.006322	-2.146650
H	2.987693	0.395165	1.721148
H	3.690538	2.003576	1.813160
H	4.410077	0.257184	-0.109541
H	4.334660	1.982705	-0.475819
H	1.929019	3.383250	2.682718
H	-0.302082	4.429563	2.388493
H	-0.862444	1.099574	-2.039738
H	-2.934138	2.350585	-2.511312
H	-3.724553	4.126005	-0.932568
H	-2.360200	4.697705	1.063131
H	2.539825	-0.096358	-3.297707
H	3.893567	-0.732651	-2.331605
H	3.996994	0.881089	-3.037480
H	0.503989	-3.494979	-1.760593
H	2.188079	-3.913390	-2.149844
H	1.427977	-2.496463	-2.910826

TS<sub>3</sub>

C	0.824451	-2.832901	-0.420777
C	1.126475	-2.923654	-1.951260
C	1.576881	-1.590631	-2.599127
C	2.172215	-0.648900	-1.586829
C	1.470617	-0.480990	-0.391374
C	0.323968	-1.397793	-0.134987
C	2.005552	0.380606	0.634231
C	3.229376	1.091187	0.375628
C	3.887084	0.917473	-0.873271
C	3.373497	0.063494	-1.824553
C	3.759777	1.953640	1.376821

C	3.124633	2.111940	2.589689
C	1.925883	1.405211	2.852677
C	1.383539	0.564898	1.901543
C	-0.983461	-1.160541	0.239158
H	0.012128	-3.539397	-0.241497
C	-1.926771	0.005454	-0.030669
C	-3.308921	-0.286883	0.075934
C	-3.913292	-1.682636	0.140950
C	-2.899288	-2.807971	0.294764
C	-1.730568	-2.227082	1.090694
C	-4.288347	0.743399	0.104625
C	-3.956735	2.065228	0.001316
C	-2.616281	2.418361	-0.297184
C	-1.607007	1.390717	-0.400600
C	2.045547	-3.285152	0.401098
C	-0.364923	1.824324	-0.936199
C	-0.091515	3.145199	-1.241314
C	-1.055820	4.150825	-1.025459
C	-2.301947	3.778238	-0.572317
H	-2.191681	-1.595346	1.872204
C	-0.970709	-3.270434	1.922971
H	1.908380	-3.686532	-2.097527
H	0.229878	-3.288084	-2.475748
H	0.695366	-1.100601	-3.049284
H	2.280993	-1.773637	-3.425141
H	4.813223	1.466819	-1.063460
H	3.892170	-0.072509	-2.777898
H	4.688535	2.490693	1.163764
H	3.543393	2.777742	3.348773
H	1.425313	1.527618	3.816825
H	0.457788	0.031449	2.116048
H	-4.544211	-1.819398	-0.755274
H	-4.612685	-1.709041	0.995492
H	-2.543254	-3.175930	-0.682408
H	-3.355927	-3.667805	0.812448
H	-5.334218	0.452496	0.239548
H	-4.714925	2.848418	0.083180
H	0.397165	1.093453	-1.157539
H	0.884288	3.402006	-1.661542
H	-0.829424	5.196998	-1.246702
H	-3.093942	4.522331	-0.448819
H	-0.074026	-2.848115	2.398806
H	-0.673807	-4.175171	1.375278
H	-1.638496	-3.606159	2.733915
H	2.952863	-2.720740	0.137974
H	2.255259	-4.350741	0.208498
H	1.886402	-3.168586	1.483001

(*P,P*)-*cis*-2

C	1.485437	2.816693	0.091523
C	2.725328	2.675061	1.020930
C	2.651352	1.428177	1.912892
C	2.504100	0.222219	1.019661
C	1.542599	0.285210	0.006978
C	0.680317	1.505603	0.003313
C	1.478826	-0.768769	-0.970762
C	2.329618	-1.918647	-0.815539
C	3.242842	-1.968091	0.271935
C	3.344272	-0.911320	1.148613
C	2.258122	-2.975614	-1.767264
C	1.414428	-2.898706	-2.853776
C	0.614900	-1.744352	-3.040959
C	0.647094	-0.712692	-2.125459



C	-0.685123	1.503653	-0.003467
H	0.837576	3.578916	0.543354
C	-1.543814	0.280737	-0.006835
C	-2.505212	0.214675	-1.019423
C	-2.656405	1.420121	-1.912696
C	-2.733855	2.666841	-1.020815
C	-1.493949	2.812440	-0.092080
C	-3.341648	-0.921621	-1.148389
C	-3.236654	-1.978127	-0.271814
C	-2.323491	-1.925769	0.815574
C	-1.476622	-0.773015	0.970928
C	1.902611	3.324430	-1.299671
C	-0.645154	-0.714204	2.125676
C	-0.609551	-1.745785	3.041141
C	-1.405098	-2.902858	2.853796
C	-2.248498	-2.982531	1.767259
H	-0.848434	3.576204	-0.544688
C	-1.911905	3.319883	1.298983
H	3.641130	2.599922	0.411154
H	2.830570	3.585716	1.633241
H	1.792229	1.515731	2.604051
H	3.551942	1.340255	2.540256
H	3.882684	-2.847528	0.385897
H	4.075464	-0.940384	1.961701
H	2.898988	-3.850155	-1.623202
H	1.372114	-3.715339	-3.579241
H	-0.031119	-1.669685	-3.919723
H	0.038407	0.174786	-2.289467
H	-3.556931	1.329399	-2.539747
H	-1.797782	1.510196	-2.604151
H	-3.649103	2.588872	-0.410560
H	-2.842265	3.577116	-1.633136
H	-4.072839	-0.953001	-1.961394
H	-3.873570	-2.859684	-0.385799
H	-0.039462	0.175304	2.289789
H	0.036133	-1.668948	3.919961
H	-1.360060	-3.719387	3.579214
H	-2.886390	-3.859232	1.623127
H	-1.040273	3.521152	1.941810
H	-2.544908	2.580810	1.816770
H	-2.490631	4.255624	1.215994
H	2.537835	2.586758	-1.816735
H	2.478779	4.261780	-1.217012
H	1.030704	3.522952	-1.942978

(*P,P*)-*cis*-2\*

C	2.350291	2.238759	-0.000251
C	1.798107	3.596199	-0.512042
C	0.490223	3.435085	-1.279172
C	-0.509267	2.716474	-0.416615
C	-0.060523	1.559323	0.301423
C	1.291142	1.122653	0.050054
C	-1.030193	0.859792	1.145433
C	-2.422036	1.225874	1.073953
C	-2.814893	2.312537	0.259031
C	-1.859884	3.062572	-0.433409
C	-3.371792	0.506572	1.855508
C	-2.973684	-0.488766	2.730177
C	-1.604624	-0.789579	2.864070
C	-0.659349	-0.118504	2.091313
C	1.693614	-0.242545	-0.131817
H	3.152354	1.923559	-0.685842
C	0.810300	-1.346191	-0.415001

C	1.142591	-2.655512	0.106018
C	2.537364	-2.987658	0.578960
C	3.333638	-1.760803	1.010453
C	3.175637	-0.613743	-0.002630
C	0.145128	-3.622043	0.229544
C	-1.161178	-3.412174	-0.226534
C	-1.476996	-2.249555	-0.963583
C	-0.472333	-1.228198	-1.128137
C	2.977854	2.465030	1.395984
C	-0.742394	-0.200877	-2.053442
C	-1.973569	-0.094382	-2.704000
C	-2.988246	-1.036611	-2.459233
C	-2.740363	-2.097505	-1.604794
H	3.732036	0.237521	0.401162
C	3.799791	-0.941403	-1.373238
H	1.610286	4.265713	0.343741
H	2.561946	4.091069	-1.133806
H	0.671788	2.849491	-2.202450
H	0.093102	4.410741	-1.600786
H	-3.872507	2.584072	0.206399
H	-2.180313	3.910723	-1.045440
H	-4.428464	0.773677	1.765844
H	-3.714816	-1.027218	3.326641
H	-1.277736	-1.548085	3.579680
H	0.396715	-0.354954	2.220080
H	3.071999	-3.488081	-0.251613
H	2.493636	-3.733253	1.389597
H	4.399866	-2.017605	1.130292
H	2.979221	-1.412735	1.996509
H	0.394245	-4.569795	0.716354
H	-1.923554	-4.183594	-0.089376
H	0.036299	0.529164	-2.274215
H	-2.142240	0.723822	-3.408461
H	-3.958287	-0.942074	-2.954444
H	-3.504188	-2.861316	-1.434139
H	3.746149	-0.073382	-2.050041
H	3.287021	-1.773898	-1.878841
H	4.864121	-1.211811	-1.262447
H	2.206975	2.796113	2.110119
H	3.751141	3.250803	1.343829
H	3.447059	1.562406	1.813531

(*M,M*)-*trans*-1

C	0.290898	-1.964869	-0.863208
C	-0.772468	-3.044377	-1.161602
C	-1.922183	-2.470020	-1.995526
C	-2.624672	-1.454797	-1.135640
C	-1.842749	-0.606283	-0.339069
C	-0.363089	-0.587180	-0.539641
C	-2.507999	0.164469	0.693982
C	-3.947026	0.189633	0.740547
C	-4.689447	-0.591538	-0.184492
C	-4.038388	-1.422860	-1.066725
C	-4.610696	0.963408	1.735607
C	-3.901759	1.655213	2.692647
C	-2.488149	1.583689	2.695918
C	-1.817417	0.866306	1.725166
C	0.363120	0.587822	-0.539040
H	0.862459	-2.309938	0.012424
C	1.842781	0.606726	-0.338385
C	2.624733	1.456106	-1.134003
C	1.922259	2.472193	-1.992886
C	0.772496	3.045682	-1.158432

C	-0.290869	1.965840	-0.861178
C	4.038447	1.424102	-1.065060
C	4.689470	0.591814	-0.183710
C	3.947013	-0.190405	0.740415
C	2.507988	-0.165203	0.693810
C	1.266791	-1.907590	-2.055402
C	1.817353	-0.868274	1.724120
C	2.488043	-1.586768	2.694077
C	3.901658	-1.658243	2.690815
C	4.610639	-0.965319	1.734618
H	-0.862435	2.310000	0.014806
C	-1.266774	1.909772	-2.053423
H	-0.288962	-3.886403	-1.682034
H	-1.191980	-3.449873	-0.225899
H	-2.628042	-3.256434	-2.305227
H	-1.528137	-2.017975	-2.923809
H	-5.781825	-0.557458	-0.152495
H	-4.611583	-2.073882	-1.733120
H	-5.704276	0.980918	1.734799
H	-4.423350	2.237828	3.456298
H	-1.920084	2.095867	3.476977
H	-0.730169	0.820974	1.759103
H	1.528243	2.021075	-2.921630
H	2.628111	3.258933	-2.301775
H	0.288998	3.888228	-1.678026
H	1.191966	3.450244	-0.222307
H	4.611668	2.075845	-1.730726
H	5.781847	0.557701	-0.151705
H	0.730098	-0.823023	1.758025
H	1.919944	-2.099879	3.474498
H	4.423215	-2.241738	3.453816
H	5.704219	-0.982818	1.733851
H	-0.749395	1.619016	-2.982653
H	-1.713864	2.903890	-2.216504
H	-2.091606	1.204393	-1.903700
H	0.749439	-1.615795	-2.984322
H	1.713817	-2.901563	-2.219554
H	2.091664	-1.202430	-1.904911

TS<sub>5</sub>

C	-0.339980	-0.878547	1.586353
C	-0.324093	-2.418457	1.506798
C	0.533943	-2.885203	0.338529
C	1.774706	-2.041774	0.170718
C	1.716914	-0.625137	0.106231
C	0.306068	-0.098534	0.403520
C	2.984828	0.044680	-0.218027
C	4.207141	-0.729090	-0.316831
C	4.181919	-2.134960	-0.165547
C	2.986382	-2.764694	0.044086
C	5.457354	-0.103224	-0.590664
C	5.558843	1.251441	-0.801618
C	4.378763	2.021532	-0.750660
C	3.159543	1.435790	-0.470369
C	-0.465840	0.957467	-0.083383
H	-1.379021	-0.548104	1.668646
C	-1.962609	0.865364	-0.074056
C	-2.760505	1.989822	0.200000
C	-2.167300	3.372392	0.118320
C	-1.016951	3.339105	-0.887910
C	0.077145	2.359142	-0.430669
C	-4.152971	1.850316	0.434676
C	-4.788797	0.638531	0.311015

C	-4.078606	-0.472290	-0.219696
C	-2.667902	-0.345647	-0.473248
C	0.351135	-0.389468	2.879997
C	-2.056664	-1.381963	-1.232257
C	-2.755113	-2.505937	-1.631202
C	-4.110843	-2.676491	-1.266737
C	-4.757555	-1.669943	-0.581807
H	0.798223	2.279184	-1.256662
C	0.760190	2.972192	0.820908
H	0.077859	-2.835389	2.444898
H	-1.346900	-2.811924	1.400930
H	-0.054983	-2.830367	-0.588078
H	0.816260	-3.942186	0.455017
H	5.114499	-2.700199	-0.239984
H	2.948085	-3.854129	0.122537
H	6.344188	-0.741028	-0.640679
H	6.523469	1.718267	-1.015664
H	4.418666	3.098068	-0.937726
H	2.305711	2.084567	-0.462418
H	-1.822726	3.741386	1.099933
H	-2.951332	4.075872	-0.205320
H	-0.571278	4.340028	-1.008426
H	-1.412115	3.041498	-1.873441
H	-4.721496	2.740453	0.720230
H	-5.855214	0.538804	0.530299
H	-1.020325	-1.257204	-1.539922
H	-2.256234	-3.265750	-2.238707
H	-4.649158	-3.581590	-1.559693
H	-5.820761	-1.757240	-0.340679
H	0.013142	3.224290	1.587316
H	1.293220	3.903210	0.563479
H	1.472445	2.290758	1.298979
H	1.414372	-0.676492	2.912874
H	-0.144071	-0.837870	3.757881
H	0.290610	0.704599	2.985565

(*M,P*)-*trans*-1

C	0.245611	1.369497	1.323792
C	-0.018991	2.866973	0.953913
C	-0.778864	3.041183	-0.378565
C	-1.974094	2.122275	-0.393869
C	-1.746539	0.788703	-0.048429
C	-0.313614	0.448246	0.227915
C	-2.864334	-0.087336	0.161758
C	-4.190697	0.391305	-0.125317
C	-4.366432	1.731719	-0.564272
C	-3.287002	2.581588	-0.666943
C	-5.301219	-0.481336	0.062068
C	-5.129525	-1.759122	0.548739
C	-3.829699	-2.217641	0.879261
C	-2.731306	-1.405124	0.687637
C	0.454367	-0.457714	-0.433457
H	1.328380	1.218090	1.384346
C	1.873222	-0.784608	-0.049103
C	2.088720	-2.117561	0.306463
C	0.899653	-3.047780	0.260364
C	0.090495	-2.880673	-1.048924
C	0.080479	-1.414005	-1.579830
C	3.384946	-2.563075	0.670457
C	4.460422	-1.702891	0.648896
C	4.301946	-0.361255	0.207510
C	2.994927	0.103210	-0.176106
C	-0.328841	1.017659	2.706963

C	2.886684	1.421868	-0.707359
C	3.987088	2.247072	-0.814815
C	5.263958	1.801410	-0.390454
C	5.413514	0.523697	0.103620
H	0.950205	-1.333001	-2.255116
C	-1.137031	-1.122869	-2.459785
H	-0.612802	3.341775	1.751978
H	0.936022	3.413625	0.908290
H	-0.106112	2.800328	-1.220644
H	-1.087142	4.089651	-0.512930
H	-5.376000	2.086834	-0.788781
H	-3.434785	3.624433	-0.962010
H	-6.302056	-0.109733	-0.175750
H	-5.992148	-2.414407	0.694549
H	-3.698642	-3.221548	1.291972
H	-1.737038	-1.764778	0.950441
H	0.240772	-2.820814	1.117014
H	1.218522	-4.093620	0.388351
H	-0.944060	-3.217720	-0.878456
H	0.507405	-3.536265	-1.830739
H	3.522348	-3.605642	0.971494
H	5.454887	-2.049471	0.943132
H	1.911006	1.771685	-1.044906
H	3.875801	3.250583	-1.234211
H	6.127472	2.466854	-0.470028
H	6.398278	0.162116	0.413104
H	-1.111972	-1.790490	-3.337842
H	-1.129981	-0.088205	-2.835043
H	-2.092687	-1.293643	-1.949670
H	-1.424908	1.126910	2.738240
H	0.094338	1.683614	3.477723
H	-0.082163	-0.017659	2.992742

TS<sub>6</sub>

C	0.076198	2.157243	0.231368
C	-0.579087	3.236317	-0.700213
C	-1.559554	2.664933	-1.736767
C	-2.470701	1.683132	-1.053995
C	-1.853925	0.704271	-0.275030
C	-0.360503	0.743097	-0.174016
C	-2.665206	-0.195917	0.504120
C	-4.098310	-0.126647	0.378726
C	-4.676363	0.843093	-0.485075
C	-3.880878	1.738576	-1.165999
C	-4.910636	-1.016945	1.138465
C	-4.350616	-1.922528	2.013043
C	-2.943523	-1.967305	2.171288
C	-2.127426	-1.131048	1.436416
C	0.426602	-0.346235	-0.483402
H	1.148302	2.239622	0.058715
C	1.869757	-0.706064	-0.137824
C	2.172360	-2.082944	-0.280566
C	1.087970	-3.135190	-0.158457
C	-0.163600	-2.826805	-0.990260
C	-0.090877	-1.395822	-1.524714
C	3.501348	-2.537621	-0.467193
C	4.561235	-1.665884	-0.473143
C	4.348988	-0.327394	-0.057196
C	3.010032	0.131761	0.238656
C	-0.225877	2.470104	1.708267
C	2.946379	1.330556	1.008711
C	4.057089	2.105646	1.286049
C	5.333890	1.734825	0.810178

C	5.469628	0.521180	0.174713
H	0.757585	-1.397444	-2.232726
C	-1.299598	-1.095784	-2.418009
H	-1.122712	3.965000	-0.077658
H	0.216006	3.797393	-1.216662
H	-0.992301	2.157000	-2.537254
H	-2.131418	3.473555	-2.217833
H	-5.764882	0.882372	-0.581975
H	-4.334609	2.499627	-1.807298
H	-5.996590	-0.959150	1.021648
H	-4.986847	-2.595467	2.593744
H	-2.500736	-2.666090	2.886117
H	-1.047755	-1.169290	1.577820
H	0.819312	-3.190220	0.911234
H	1.503374	-4.122552	-0.409631
H	-1.079118	-2.969162	-0.396051
H	-0.236342	-3.516214	-1.847796
H	3.664855	-3.603927	-0.645799
H	5.574343	-2.003637	-0.706163
H	2.014963	1.603024	1.484117
H	3.943212	2.999462	1.905415
H	6.204479	2.367256	1.001238
H	6.457724	0.155996	-0.119396
H	-1.278493	-1.811319	-3.257897
H	-1.262348	-0.088039	-2.852648
H	-2.268251	-1.222779	-1.918191
H	-1.311184	2.474739	1.896168
H	0.163931	3.463579	1.986823
H	0.216734	1.729049	2.393095

B3LYP/SVP in methanol

(*P,P*)-*trans*-1

C	-0.075626	-0.496900	1.981049
C	0.525622	-1.812150	2.584995
C	1.471446	-2.559081	1.623193
C	2.440716	-1.592583	0.990751
C	1.901619	-0.425169	0.445763
C	0.413671	-0.322149	0.539664
C	2.772968	0.587156	-0.079455
C	4.190236	0.337242	-0.114443
C	4.693122	-0.889660	0.400486
C	3.840240	-1.819988	0.955761
C	5.059925	1.335098	-0.642657
C	4.566960	2.541340	-1.094405
C	3.175052	2.805208	-1.028351
C	2.304144	1.853670	-0.536175
C	-0.413603	-0.321653	-0.539491
H	-1.168684	-0.601073	1.956369
C	-1.901566	-0.424900	-0.445885
C	-2.440437	-1.591916	-0.991949
C	-1.470956	-2.557701	-1.625147
C	-0.525118	-1.809778	-2.586175
C	0.075875	-0.494989	-1.980967
C	-3.839930	-1.819556	-0.957332
C	-4.693021	-0.889804	-0.401418
C	-4.190390	0.336792	0.114484
C	-2.773152	0.586947	0.079875
C	0.263472	0.712134	2.869087
C	-2.304618	1.853267	0.537431
C	-3.175749	2.804327	1.030137
C	-4.567614	2.540162	1.095888
C	-5.060315	1.334139	0.643270
H	1.168946	-0.599043	-1.956239
C	-0.263215	0.714870	-2.867880
H	1.088179	-1.565080	3.500120
H	-0.288878	-2.487815	2.891098
H	0.871302	-3.047471	0.834089
H	2.007168	-3.361206	2.154044
H	5.770682	-1.074262	0.367523
H	4.238772	-2.749521	1.372957
H	6.133687	1.128368	-0.673251
H	5.246187	3.299906	-1.492861
H	2.790928	3.771686	-1.366241
H	1.236822	2.071018	-0.479952
H	-2.006502	-3.359428	-2.156778
H	-0.870839	-3.046710	-0.836406
H	-1.087569	-1.561978	-3.501168
H	0.289518	-2.485066	-2.892746
H	-4.238272	-2.748799	-1.375354
H	-5.770560	-1.074582	-0.368768
H	-1.237340	2.070866	0.481418
H	-2.791836	3.770658	1.368685
H	-5.247020	3.298346	1.494764
H	-6.134046	1.127210	0.673578
H	0.112148	0.557675	-3.893105
H	0.188364	1.644195	-2.488503
H	-1.352687	0.871433	-2.936023
H	1.352943	0.868683	2.937279
H	-0.111783	0.553939	3.894198
H	-0.188184	1.641799	2.490654

*(P,P)*-trans-1\*

C	-0.178920	-1.868800	-1.195823
C	0.606970	-2.113148	-2.502658
C	2.080073	-2.377316	-2.198742
C	2.664427	-1.443292	-1.162822
C	1.823919	-0.606521	-0.342074
C	0.409435	-0.597347	-0.568741
C	2.478857	0.217838	0.683380
C	3.917630	0.275064	0.746824
C	4.686956	-0.507318	-0.152175
C	4.058345	-1.352780	-1.062062
C	4.542679	1.079934	1.740590
C	3.796661	1.768596	2.683270
C	2.393001	1.667469	2.664328
C	1.758374	0.905254	1.684607
C	-0.409442	0.597340	-0.568717
H	-1.225248	-1.666469	-1.464760
C	-1.823924	0.606517	-0.342036
C	-2.664431	1.443318	-1.162754
C	-2.080076	2.377377	-2.198643
C	-0.606974	2.113220	-2.502573
C	0.178922	1.868810	-1.195752
C	-4.058349	1.352808	-1.061994
C	-4.686960	0.507323	-0.152128
C	-3.917633	-0.275079	0.746853
C	-2.478861	-0.217856	0.683408
C	-0.151664	-3.118579	-0.294467
C	-1.758377	-0.905283	1.684626
C	-2.393005	-1.667513	2.664336
C	-3.796665	-1.768642	2.683275
C	-4.542683	-1.079965	1.740606
H	1.225245	1.666472	-1.464705
C	0.151700	3.118551	-0.294343
H	0.172034	-2.965918	-3.050661
H	0.505055	-1.229301	-3.155065
H	2.683593	-2.327962	-3.120444
H	2.196818	-3.414853	-1.832088
H	5.778301	-0.457434	-0.104614
H	4.669114	-1.957919	-1.739601
H	5.635411	1.129085	1.757459
H	4.294826	2.373530	3.445896
H	1.794411	2.184496	3.418965
H	0.670852	0.832443	1.705399
H	-2.196819	3.414901	-1.831951
H	-2.683599	2.328059	-3.120346
H	-0.172038	2.966012	-3.050541
H	-0.505067	1.229401	-3.155019
H	-4.669118	1.957970	-1.739511
H	-5.778304	0.457442	-0.104563
H	-0.670856	-0.832471	1.705421
H	-1.794415	-2.184551	3.418965
H	-4.294829	-2.373589	3.445890
H	-5.635414	-1.129115	1.757474
H	0.846690	3.019853	0.550114
H	-0.848199	3.318182	0.120495
H	0.456998	4.006389	-0.874005
H	0.848238	-3.318192	0.120372
H	-0.456926	-4.006403	-0.874169
H	-0.846666	-3.019941	0.549987

*(M,M)*-cis-2

C	-1.459985	2.806019	0.281672
C	-2.981092	2.627090	0.153125



C	-3.434242	1.344820	0.854851
C	-2.793282	0.168586	0.166299
C	-1.498381	0.298458	-0.364872
C	-0.686704	1.500074	-0.039762
C	-1.050148	-0.724224	-1.299302
C	-1.806590	-1.941739	-1.432937
C	-3.033441	-2.084533	-0.729067
C	-3.532667	-1.029531	-0.001555
C	-1.355568	-2.966724	-2.314240
C	-0.237998	-2.789200	-3.101219
C	0.456682	-1.556763	-3.049360
C	0.064259	-0.562705	-2.173353
C	0.696615	1.495617	0.039784
H	-1.155434	3.591778	-0.425392
C	1.500514	0.288822	0.365056
C	2.794680	0.150643	-0.165804
C	3.443203	1.322677	-0.854442
C	2.998185	2.607936	-0.152959
C	1.478260	2.796582	-0.281597
C	3.526348	-1.052174	0.002223
C	3.020222	-2.103961	0.729622
C	1.794057	-1.953378	1.433073
C	1.045388	-0.731092	1.299168
C	-1.143158	3.323224	1.704670
C	-0.068500	-0.562650	2.172566
C	-0.467613	-1.554244	3.048341
C	0.219318	-2.790997	3.100548
C	1.336136	-2.975530	2.314116
H	1.178738	3.584252	0.425482
C	1.164807	3.315814	-1.704595
H	-3.487524	3.506814	0.582245
H	-3.276057	2.574879	-0.908912
H	-4.529689	1.236121	0.819788
H	-3.166472	1.381545	1.926255
H	-3.596436	-3.017148	-0.824395
H	-4.516854	-1.105541	0.470267
H	-1.935899	-3.892169	-2.373255
H	0.092560	-3.577940	-3.782511
H	1.306129	-1.383496	-3.715912
H	0.602746	0.382192	-2.174266
H	3.175757	1.360941	-1.925875
H	4.537935	1.207019	-0.819274
H	3.510253	3.484349	-0.582173
H	3.292728	2.554004	0.909106
H	4.510125	-1.134469	-0.469397
H	3.577214	-3.040161	0.825077
H	-0.601052	0.385602	2.173195
H	-1.316316	-1.375674	3.714438
H	-0.116540	-3.577668	3.781638
H	1.910546	-3.904644	2.373368
H	0.088709	3.400814	-1.904927
H	1.583373	2.653566	-2.478719
H	1.610368	4.314148	-1.849852
H	-1.566145	2.663793	2.478795
H	-1.582078	4.324504	1.849877
H	-0.066526	3.401084	1.905039

TS<sub>2</sub>

C	1.939657	-2.012688	1.042855
C	3.162687	-2.415720	0.225527
C	4.021810	-1.185014	0.011315
C	3.244172	0.114324	-0.104324
C	1.833651	0.246764	-0.091476

C	1.055358	-1.029803	0.255498
C	1.331589	1.598729	-0.387461
C	2.235958	2.726272	-0.417150
C	3.633806	2.519046	-0.302350
C	4.107468	1.242021	-0.211765
C	1.754116	4.049549	-0.622594
C	0.422340	4.301416	-0.869867
C	-0.461817	3.205531	-0.944910
C	-0.015002	1.916746	-0.711181
C	-0.225055	-1.469512	-0.005353
H	1.356597	-2.904362	1.237745
C	-1.465889	-0.709265	-0.377950
C	-2.024993	-0.981375	-1.624897
C	-1.252806	-1.935997	-2.495425
C	-0.872080	-3.197848	-1.682471
C	-0.724933	-2.955528	-0.145923
C	-3.274682	-0.422241	-1.993168
C	-3.983505	0.359950	-1.106448
C	-3.488267	0.595702	0.207238
C	-2.215561	0.045238	0.591536
C	2.293575	-1.471998	2.443914
C	-1.754414	0.281831	1.918703
C	-2.502553	1.019785	2.814938
C	-3.751112	1.569747	2.430254
C	-4.229713	1.360418	1.153484
H	-1.746876	-2.936090	0.264265
C	-0.096610	-4.209990	0.476980
H	3.738098	-3.209886	0.730907
H	2.826379	-2.831561	-0.738831
H	4.652514	-1.285642	-0.889444
H	4.735117	-1.071129	0.846133
H	4.310780	3.377053	-0.330389
H	5.186073	1.061865	-0.187567
H	2.481769	4.866008	-0.605874
H	0.064528	5.321055	-1.035709
H	-1.512406	3.367231	-1.201045
H	-0.725641	1.115401	-0.827839
H	-0.330539	-1.439538	-2.843229
H	-1.824110	-2.206596	-3.396067
H	0.075133	-3.608993	-2.069356
H	-1.639455	-3.976430	-1.825339
H	-3.677531	-0.627688	-2.989229
H	-4.947186	0.790888	-1.392339
H	-0.792040	-0.130124	2.225585
H	-2.129377	1.182899	3.829807
H	-4.331831	2.156118	3.147510
H	-5.193703	1.776738	0.846905
H	-0.064311	-4.172283	1.576358
H	0.908646	-4.442457	0.096687
H	-0.740572	-5.066038	0.211096
H	2.865627	-0.532233	2.430703
H	2.892561	-2.219550	2.992145
H	1.378575	-1.291204	3.031247

(*M,P*)-*cis*-2

C	2.444968	-1.719345	-0.797543
C	2.847064	-2.494554	0.502173
C	2.178020	-1.949090	1.779316
C	0.685377	-1.959063	1.563127
C	0.226103	-1.467586	0.338979
C	1.272101	-0.777321	-0.488149
C	-1.115786	-1.763997	-0.075463
C	-2.023195	-2.360266	0.870733

C	-1.549904	-2.701855	2.167293
C	-0.216839	-2.549786	2.484527
C	-3.357533	-2.655565	0.466160
C	-3.768626	-2.446023	-0.833472
C	-2.853013	-1.937758	-1.789640
C	-1.568180	-1.598026	-1.417145
C	1.321031	0.570527	-0.672657
H	3.305021	-1.106107	-1.077793
C	0.477731	1.560769	0.090730
C	1.201082	2.246246	1.074250
C	2.684526	1.975832	1.191559
C	3.391092	1.894565	-0.187953
C	2.450544	1.397259	-1.322007
C	0.551235	3.188404	1.913652
C	-0.784301	3.484547	1.749012
C	-1.515855	2.916336	0.671180
C	-0.866417	1.968231	-0.198098
C	2.159523	-2.685996	-1.955852
C	-1.566934	1.551479	-1.366193
C	-2.850728	1.984958	-1.629227
C	-3.515659	2.853659	-0.727163
C	-2.856567	3.311830	0.394306
H	1.922101	2.291032	-1.693276
C	3.210053	0.870214	-2.546251
H	2.562690	-3.555247	0.399923
H	3.943520	-2.473352	0.611889
H	2.545518	-0.930738	1.987841
H	2.446083	-2.566340	2.650762
H	-2.247332	-3.140502	2.886633
H	0.159901	-2.889191	3.454020
H	-4.043750	-3.082608	1.203365
H	-4.790067	-2.693358	-1.135382
H	-3.168222	-1.815865	-2.829654
H	-0.868257	-1.222989	-2.164688
H	2.830227	1.017706	1.716411
H	3.158171	2.741938	1.824093
H	4.256857	1.216827	-0.103755
H	3.791746	2.883253	-0.466501
H	1.128873	3.680594	2.701758
H	-1.282945	4.197593	2.411686
H	-1.055976	0.904694	-2.077295
H	-3.358922	1.658390	-2.540663
H	-4.539564	3.175510	-0.935954
H	-3.345569	4.011411	1.078559
H	2.522446	0.442594	-3.293507
H	3.973802	0.115358	-2.311856
H	3.735194	1.710749	-3.030771
H	1.276582	-3.313926	-1.749728
H	3.016160	-3.362494	-2.117311
H	1.980242	-2.146699	-2.899905

TS<sub>3</sub>

C	0.800917	-2.847466	-0.394297
C	1.108226	-2.957401	-1.923212
C	1.534873	-1.628803	-2.594575
C	2.145122	-0.676283	-1.602892
C	1.462441	-0.500545	-0.397949
C	0.311945	-1.406187	-0.124376
C	2.016661	0.360168	0.617453
C	3.233484	1.074082	0.333988
C	3.869678	0.898097	-0.926615
C	3.342027	0.036501	-1.864271
C	3.780879	1.941405	1.322916

C	3.168982	2.098873	2.548888
C	1.978640	1.386145	2.837786
C	1.419395	0.542451	1.898005
C	-0.991149	-1.152458	0.251441
H	-0.016453	-3.545951	-0.208542
C	-1.923303	0.020788	-0.031208
C	-3.308211	-0.269511	0.048169
C	-3.915710	-1.663538	0.106220
C	-2.910493	-2.791353	0.297843
C	-1.752328	-2.205891	1.104722
C	-4.287207	0.763022	0.060129
C	-3.952103	2.085815	-0.025612
C	-2.603474	2.438297	-0.289403
C	-1.593494	1.409148	-0.382345
C	2.015459	-3.296600	0.438136
C	-0.340771	1.846826	-0.893524
C	-0.058904	3.171737	-1.176833
C	-1.024240	4.177996	-0.962190
C	-2.280904	3.801913	-0.539717
H	-2.221491	-1.566501	1.874983
C	-1.003363	-3.243510	1.952998
H	1.905226	-3.706941	-2.055735
H	0.219687	-3.346945	-2.443402
H	0.639966	-1.148162	-3.028601
H	2.222604	-1.814837	-3.433319
H	4.790645	1.449690	-1.135312
H	3.845721	-0.104099	-2.825154
H	4.703221	2.481580	1.089976
H	3.600129	2.767207	3.299197
H	1.499702	1.504767	3.813723
H	0.502534	0.002395	2.136125
H	-4.522648	-1.804000	-0.806029
H	-4.638696	-1.678491	0.940540
H	-2.539066	-3.180343	-0.665444
H	-3.382714	-3.637477	0.823716
H	-5.336029	0.472606	0.171389
H	-4.710140	2.870473	0.044993
H	0.419929	1.115362	-1.120481
H	0.922987	3.432745	-1.581106
H	-0.790934	5.226700	-1.164845
H	-3.074331	4.545586	-0.421605
H	-0.110056	-2.819823	2.435047
H	-0.704926	-4.153600	1.414817
H	-1.681397	-3.568665	2.759955
H	2.932056	-2.753327	0.160156
H	2.209260	-4.369266	0.269517
H	1.856762	-3.152998	1.517405

(*P,P*)-*cis*-2

C	1.494267	2.812890	0.103520
C	2.729463	2.656565	1.036723
C	2.645838	1.407868	1.925971
C	2.487853	0.204033	1.032777
C	1.535145	0.281450	0.012392
C	0.682876	1.507920	0.007053
C	1.471943	-0.765122	-0.973797
C	2.300612	-1.930861	-0.811321
C	3.196707	-2.000914	0.290569
C	3.306062	-0.945740	1.170020
C	2.233855	-2.977515	-1.776328
C	1.417481	-2.873765	-2.882532
C	0.639863	-1.703977	-3.075297
C	0.665326	-0.683195	-2.146062

C	-0.682010	1.508308	-0.007020
H	0.848968	3.577709	0.554261
C	-1.534967	0.282318	-0.012373
C	-2.487666	0.205425	-1.032805
C	-2.644973	1.409354	-1.926000
C	-2.727937	2.658078	-1.036731
C	-1.492642	2.813740	-0.103561
C	-3.306508	-0.943895	-1.170078
C	-3.197775	-1.999130	-0.290625
C	-2.301705	-1.929565	0.811317
C	-1.472404	-0.764280	0.973830
C	1.919463	3.320804	-1.284596
C	-0.665825	-0.682774	2.146150
C	-0.640990	-1.703554	3.075405
C	-1.419216	-2.872929	2.882591
C	-2.235571	-2.976250	1.776332
H	-0.846887	3.578132	-0.554377
C	-1.917533	3.321994	1.284521
H	3.647448	2.578686	0.429885
H	2.838068	3.562879	1.654381
H	1.786989	1.499330	2.616527
H	3.546320	1.310172	2.551771
H	3.819477	-2.892015	0.410098
H	4.027946	-0.987739	1.991051
H	2.858909	-3.862992	-1.628289
H	1.380842	-3.680348	-3.619899
H	0.019107	-1.607632	-3.970412
H	0.077781	0.217860	-2.317910
H	-3.545501	1.312150	-2.551811
H	-1.786069	1.500357	-2.616549
H	-3.645948	2.580655	-0.429873
H	-2.836086	3.564469	-1.654355
H	-4.028375	-0.985499	-1.991145
H	-3.821025	-2.889889	-0.410193
H	-0.077792	0.217959	2.318022
H	-0.020247	-1.607534	3.970564
H	-1.383061	-3.679525	3.619968
H	-2.861088	-3.861394	1.628255
H	-1.048258	3.529361	1.928962
H	-2.551104	2.582323	1.802155
H	-2.499246	4.255489	1.195944
H	2.552702	2.580786	-1.802139
H	2.501618	4.254030	-1.196078
H	1.050312	3.528536	-1.929085

(*P,P*)-*cis*-2\*

C	2.355680	2.229314	-0.007728
C	1.807743	3.588578	-0.518323
C	0.483433	3.439345	-1.257662
C	-0.504015	2.721441	-0.382038
C	-0.051321	1.554488	0.321183
C	1.293467	1.120200	0.054024
C	-1.018862	0.843127	1.160319
C	-2.410581	1.212929	1.102139
C	-2.807399	2.316838	0.307777
C	-1.855252	3.071268	-0.382813
C	-3.359044	0.482295	1.875782
C	-2.959201	-0.532088	2.728271
C	-1.588535	-0.837827	2.851369
C	-0.645031	-0.152613	2.089575
C	1.692879	-0.252282	-0.129488
H	3.154367	1.906230	-0.692483
C	0.806823	-1.340899	-0.433375

C	1.126515	-2.661675	0.076092
C	2.514135	-3.009253	0.553626
C	3.309930	-1.793502	1.014522
C	3.170383	-0.629876	0.019174
C	0.117200	-3.617439	0.192820
C	-1.187399	-3.391031	-0.261021
C	-1.490301	-2.217058	-0.991066
C	-0.474261	-1.206242	-1.149140
C	2.986049	2.457270	1.388136
C	-0.731827	-0.168948	-2.068604
C	-1.962419	-0.044059	-2.717171
C	-2.989914	-0.974446	-2.474548
C	-2.752852	-2.046939	-1.629476
H	3.722469	0.213134	0.443811
C	3.812619	-0.935970	-1.348102
H	1.646565	4.267146	0.335847
H	2.563809	4.068135	-1.160717
H	0.640533	2.855581	-2.186258
H	0.084741	4.418490	-1.566094
H	-3.864973	2.592029	0.268413
H	-2.177672	3.927700	-0.982571
H	-4.415343	0.755775	1.798277
H	-3.699046	-1.079760	3.318490
H	-1.260539	-1.607412	3.555168
H	0.411440	-0.391052	2.215864
H	3.051613	-3.495879	-0.283510
H	2.458665	-3.770539	1.348535
H	4.373435	-2.056688	1.141336
H	2.945030	-1.460161	2.001821
H	0.355705	-4.570707	0.674485
H	-1.958814	-4.154818	-0.128824
H	0.054446	0.554418	-2.287212
H	-2.121737	0.779307	-3.418401
H	-3.959702	-0.864224	-2.967715
H	-3.524954	-2.804244	-1.465233
H	3.764640	-0.058121	-2.012792
H	3.313916	-1.767159	-1.870793
H	4.876567	-1.201364	-1.222948
H	2.219020	2.804594	2.099395
H	3.766263	3.235311	1.324834
H	3.447711	1.554599	1.813742

(*M,M*)-*trans*-1

C	0.290992	-1.966599	-0.860099
C	-0.773128	-3.043987	-1.163042
C	-1.921712	-2.468614	-1.997351
C	-2.623529	-1.454202	-1.136909
C	-1.841304	-0.607032	-0.338763
C	-0.362038	-0.588202	-0.539218
C	-2.505714	0.163944	0.694693
C	-3.945275	0.190420	0.740371
C	-4.689085	-0.588034	-0.186987
C	-4.037923	-1.419868	-1.069814
C	-4.610217	0.962471	1.737069
C	-3.900139	1.652810	2.695405
C	-2.485613	1.581701	2.698211
C	-1.813994	0.865123	1.726518
C	0.362034	0.587682	-0.539745
H	0.857797	-2.313544	0.018223
C	1.841323	0.606700	-0.339326
C	2.623513	1.453181	-1.138235
C	1.921625	2.466787	-1.999570
C	0.773109	3.042916	-1.165704

C	-0.291014	1.965808	-0.861715
C	4.037907	1.418944	-1.071126
C	4.689093	0.587924	-0.187548
C	3.945313	-0.189727	0.740508
C	2.505750	-0.163336	0.694810
C	1.269784	-1.911468	-2.049703
C	1.814051	-0.863648	1.727242
C	2.485698	-1.579332	2.699573
C	3.900230	-1.650362	2.696854
C	4.610284	-0.960854	1.737903
H	-0.857703	2.313523	0.016381
C	-1.269944	1.909682	-2.051155
H	-0.289372	-3.885015	-1.684767
H	-1.193150	-3.452228	-0.228333
H	-2.628594	-3.253722	-2.307438
H	-1.526706	-2.014888	-2.924544
H	-5.781610	-0.551649	-0.155831
H	-4.611848	-2.069303	-1.737396
H	-5.703997	0.979715	1.735663
H	-4.421153	2.234456	3.460654
H	-1.918360	2.093850	3.480318
H	-0.726464	0.820251	1.762007
H	1.526544	2.012187	-2.926302
H	2.628461	3.251626	-2.310444
H	0.289326	3.883479	-1.688149
H	1.193195	3.451993	-0.231390
H	4.611813	2.067791	-1.739296
H	5.781619	0.551603	-0.156362
H	0.726516	-0.818819	1.762679
H	1.918463	-2.090827	3.482120
H	4.421265	-2.231293	3.462631
H	5.704064	-0.978047	1.736521
H	-0.754220	1.615504	-2.980494
H	-1.712418	2.905870	-2.215745
H	-2.098262	1.207886	-1.898814
H	0.753976	-1.618034	-2.979231
H	1.712225	-2.907797	-2.213530
H	2.098115	-1.209550	-1.898017

TS<sub>5</sub>

C	-0.343627	-0.874581	1.592532
C	-0.339603	-2.413514	1.508646
C	0.536632	-2.888222	0.356767
C	1.774524	-2.040653	0.188680
C	1.714118	-0.623735	0.115682
C	0.304086	-0.095761	0.410470
C	2.980483	0.045841	-0.217706
C	4.204030	-0.727261	-0.316722
C	4.182661	-2.132711	-0.154949
C	2.987833	-2.762587	0.062852
C	5.452962	-0.101955	-0.601787
C	5.550169	1.251738	-0.825916
C	4.368357	2.020776	-0.775810
C	3.150853	1.435754	-0.483496
C	-0.464816	0.961677	-0.077717
H	-1.379715	-0.535787	1.680978
C	-1.961332	0.864961	-0.070977
C	-2.762280	1.986721	0.206249
C	-2.169293	3.369220	0.138594
C	-1.021675	3.344758	-0.870768
C	0.076236	2.364060	-0.425022
C	-4.156168	1.843456	0.434942
C	-4.790184	0.631030	0.300290

C	-4.074344	-0.476206	-0.232284
C	-2.661691	-0.346856	-0.477312
C	0.355321	-0.394473	2.885325
C	-2.043907	-1.381815	-1.234107
C	-2.739331	-2.505118	-1.642359
C	-4.098797	-2.676657	-1.289524
C	-4.751332	-1.672740	-0.604577
H	0.789747	2.288076	-1.258048
C	0.767787	2.974260	0.822841
H	0.037761	-2.835931	2.454515
H	-1.363592	-2.798816	1.382485
H	-0.038063	-2.848817	-0.580284
H	0.824977	-3.941301	0.490295
H	5.116192	-2.696698	-0.229127
H	2.952049	-3.851693	0.148944
H	6.340453	-0.739241	-0.650479
H	6.512961	1.718756	-1.049282
H	4.404976	3.095656	-0.974056
H	2.296317	2.084142	-0.480476
H	-1.821626	3.725029	1.123890
H	-2.954284	4.076624	-0.173555
H	-0.577772	4.347002	-0.984925
H	-1.418446	3.054186	-1.858309
H	-4.726696	2.731170	0.724668
H	-5.857643	0.527451	0.513715
H	-1.004502	-1.260065	-1.533329
H	-2.234707	-3.263955	-2.246684
H	-4.634516	-3.581158	-1.590290
H	-5.816274	-1.761031	-0.370610
H	0.024311	3.231585	1.591330
H	1.303911	3.901530	0.559275
H	1.478956	2.289474	1.298922
H	1.414267	-0.698276	2.919491
H	-0.146612	-0.835203	3.763416
H	0.311552	0.700836	2.990508

(*M,P*)-*trans*-1

C	0.237843	1.365650	1.325832
C	-0.019071	2.863220	0.951376
C	-0.777816	3.037913	-0.381733
C	-1.972682	2.119338	-0.398489
C	-1.746233	0.785063	-0.053221
C	-0.313960	0.445414	0.226091
C	-2.864432	-0.090304	0.159321
C	-4.191116	0.390132	-0.126096
C	-4.366891	1.730430	-0.567961
C	-3.285917	2.579288	-0.673116
C	-5.304359	-0.478690	0.067909
C	-5.133344	-1.755913	0.558576
C	-3.832409	-2.217146	0.884980
C	-2.731557	-1.408060	0.687196
C	0.456291	-0.457776	-0.435453
H	1.319615	1.210550	1.398836
C	1.874165	-0.783167	-0.047908
C	2.090149	-2.117778	0.303656
C	0.903516	-3.049904	0.251891
C	0.097220	-2.879339	-1.058056
C	0.086685	-1.411621	-1.584558
C	3.386757	-2.563633	0.668879
C	4.462418	-1.702435	0.651404
C	4.302855	-0.359285	0.212601
C	2.995535	0.106371	-0.170824
C	-0.352254	1.014712	2.702600



C	2.887191	1.427330	-0.698413
C	3.989408	2.251544	-0.804485
C	5.266930	1.804084	-0.381303
C	5.416132	0.524980	0.111468
H	0.956299	-1.326815	-2.259712
C	-1.129188	-1.117913	-2.465392
H	-0.608687	3.344079	1.749144
H	0.938719	3.404543	0.901314
H	-0.103244	2.796297	-1.222034
H	-1.087191	4.085839	-0.516115
H	-5.376883	2.085452	-0.791647
H	-3.433090	3.622106	-0.969233
H	-6.304950	-0.104774	-0.168132
H	-5.996889	-2.409225	0.710047
H	-3.702080	-3.221020	1.298750
H	-1.738054	-1.773018	0.946837
H	0.241514	-2.826391	1.107023
H	1.225848	-4.094837	0.376842
H	-0.936874	-3.217847	-0.887254
H	0.516049	-3.532079	-1.841353
H	3.524311	-3.607157	0.967076
H	5.457222	-2.048579	0.945837
H	1.913111	1.781199	-1.037184
H	3.878430	3.256465	-1.221300
H	6.130704	2.469814	-0.459907
H	6.400359	0.161751	0.421443
H	-1.100883	-1.781507	-3.346599
H	-1.121820	-0.081441	-2.837521
H	-2.086139	-1.293697	-1.958279
H	-1.447968	1.133313	2.724995
H	0.068508	1.675792	3.479113
H	-0.117147	-0.023838	2.988386

TS<sub>6</sub>

C	0.079604	2.154324	0.228804
C	-0.572216	3.232171	-0.706147
C	-1.549661	2.660887	-1.745586
C	-2.463232	1.680939	-1.064499
C	-1.850725	0.704329	-0.278714
C	-0.357828	0.740156	-0.174238
C	-2.665332	-0.190450	0.503002
C	-4.098362	-0.120945	0.371067
C	-4.673099	0.843598	-0.501792
C	-3.873487	1.736032	-1.183485
C	-4.916000	-1.005295	1.133316
C	-4.359791	-1.905379	2.017199
C	-2.952544	-1.950680	2.181472
C	-2.131698	-1.120534	1.443633
C	0.425441	-0.353512	-0.478560
H	1.152508	2.236103	0.060693
C	1.868748	-0.711219	-0.134474
C	2.177287	-2.086986	-0.281157
C	1.101055	-3.146773	-0.157148
C	-0.165307	-2.836039	-0.965390
C	-0.094869	-1.409768	-1.511040
C	3.508820	-2.534437	-0.475072
C	4.565178	-1.657187	-0.483017
C	4.347249	-0.320862	-0.060795
C	3.006678	0.130111	0.243277
C	-0.225916	2.468825	1.704196
C	2.939291	1.324550	1.020770
C	4.047404	2.105838	1.294437
C	5.324472	1.744573	0.809185

C	5.465231	0.533096	0.168781
H	0.750235	-1.418199	-2.223357
C	-1.304430	-1.114818	-2.404819
H	-1.116918	3.962369	-0.086172
H	0.225126	3.791386	-1.221124
H	-0.981099	2.151071	-2.544169
H	-2.120789	3.469113	-2.227813
H	-5.761359	0.881565	-0.604032
H	-4.324107	2.494354	-1.830507
H	-6.001420	-0.946932	1.010235
H	-4.998973	-2.573571	2.600745
H	-2.513666	-2.646415	2.902089
H	-1.052545	-1.163692	1.589905
H	0.850394	-3.215895	0.916254
H	1.519494	-4.127059	-0.428975
H	-1.069024	-2.969439	-0.350977
H	-0.257931	-3.530669	-1.816611
H	3.676625	-3.599255	-0.659653
H	5.579117	-1.988191	-0.723025
H	2.008573	1.590239	1.502515
H	3.931674	2.997178	1.917401
H	6.191964	2.382592	0.997649
H	6.453894	0.174446	-0.132165
H	-1.282603	-1.836505	-3.239555
H	-1.266404	-0.109543	-2.845959
H	-2.273438	-1.240102	-1.904000
H	-1.312319	2.483054	1.888153
H	0.170929	3.459509	1.982473
H	0.210303	1.725210	2.390736