

# Excited-State Decay Paths in Tetraphenylethene Derivatives

## Supporting Information

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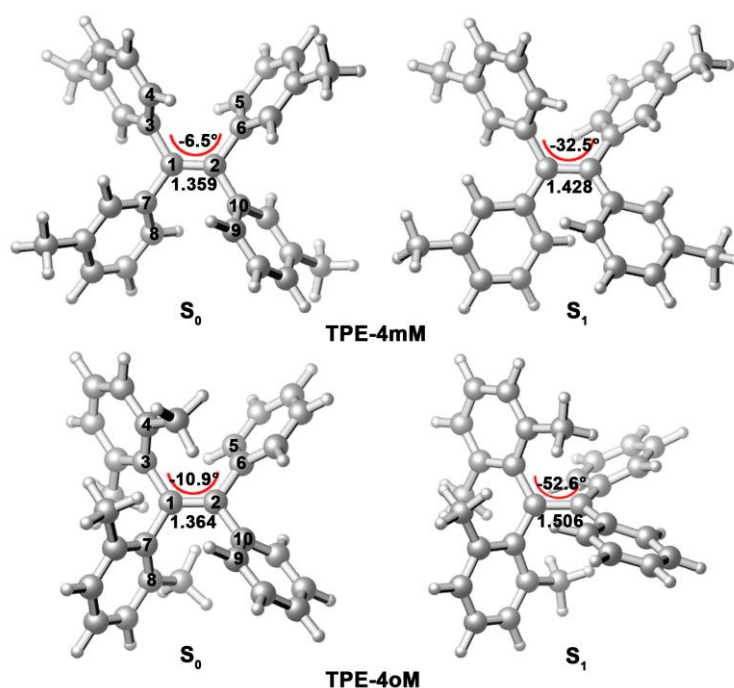
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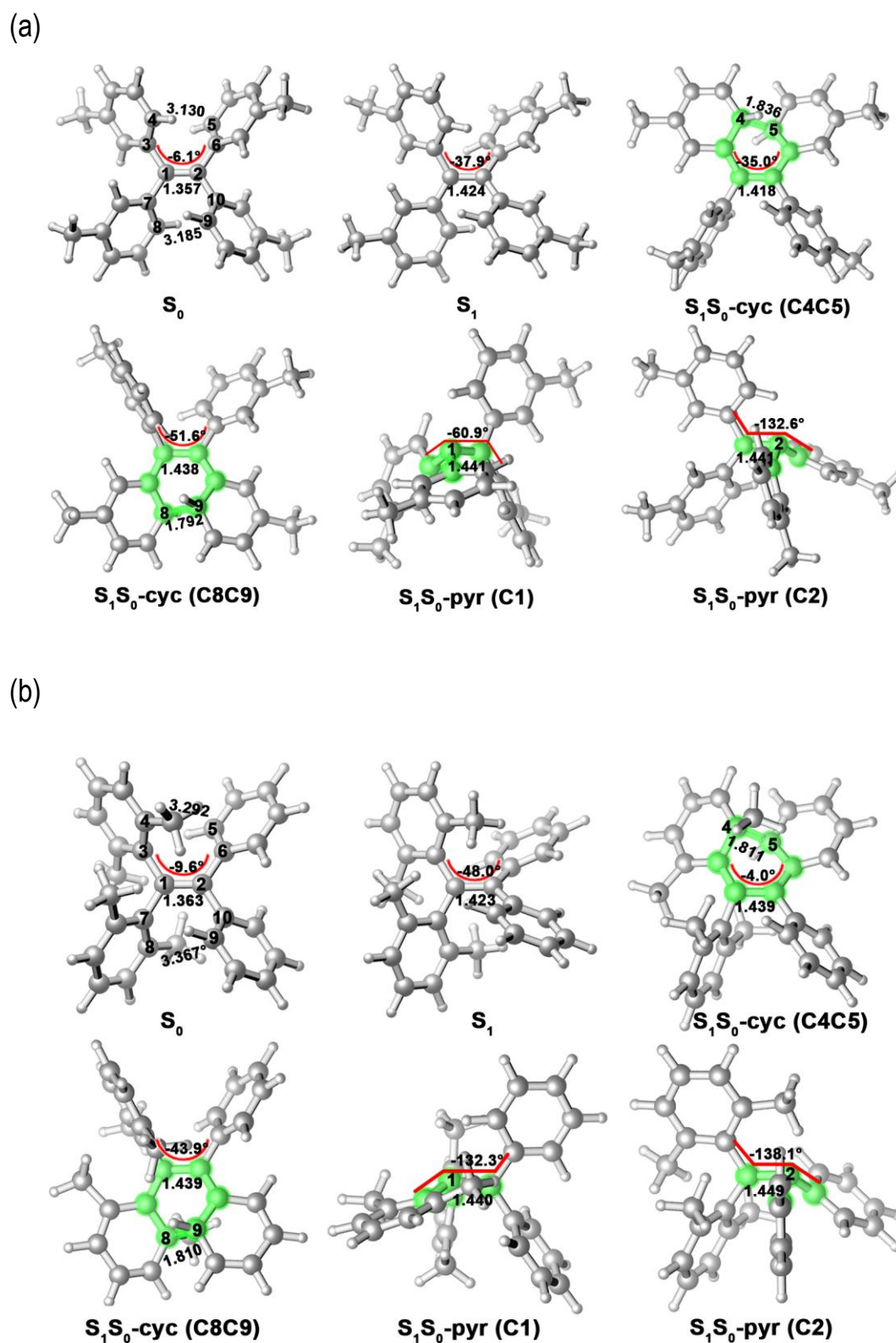
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## 1. Optimized Structures

Figures S1 and S2 show the ground- and excited-state minima of TPE-4mM and TPE-4oM optimized by the CASSCF and OM2/MRCI methods, respectively. In the present nonadiabatic dynamics simulations, we use OM2/MRCI calculations with an active space of twelve electrons distributed over twelve orbitals. This approach provides accurate structures for the  $S_0$  and  $S_1$  minima and the  $S_1/S_0$  conical intersections of TPE-4mM and TPE-4oM, which are close to those obtained by the CASSCF method, as is evident from overlays of the corresponding optimized geometries (Fig. S3). It also gives reasonably accurate energies compared with those computed at the CASPT2(10,8)/6-31G\* level.

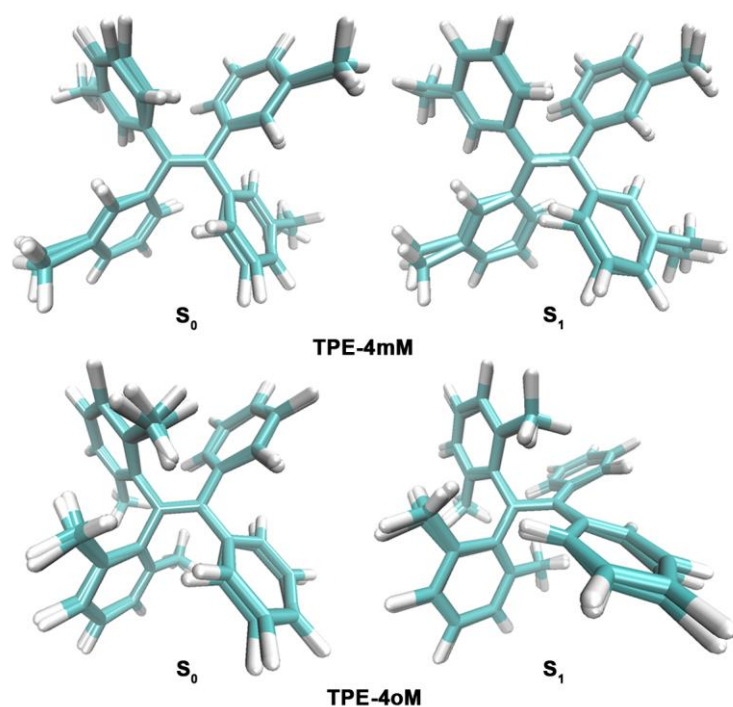


**Figure S1:** Geometric structures of TPE-4mM and TPE-4oM optimized at the CASSCF/6-31G\* level (carbon atoms in gray and hydrogen atoms in white). Selected bond lengths are given in Å and dihedral angles are given in degree. Also shown is the atomic numbering.

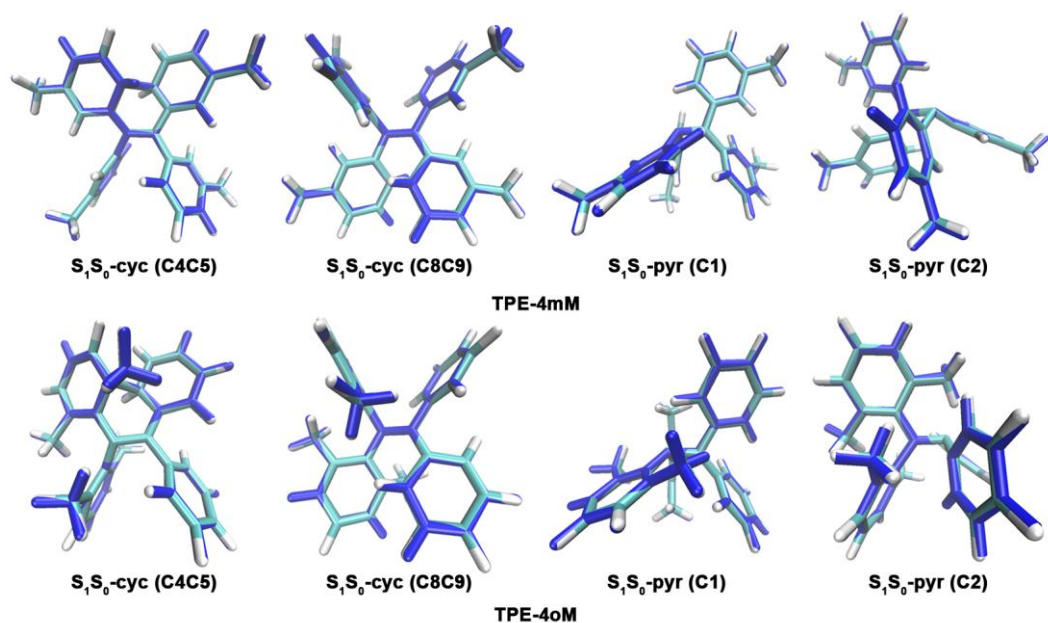


**Figure S2:** Geometric structures of TPE-4mM (a) and TPE-4oM (b) optimized at the OM2/MRCI level. Selected bond lengths are given in Å and dihedral angles are given in degree. Also shown is the atomic numbering.

(a)



(b)

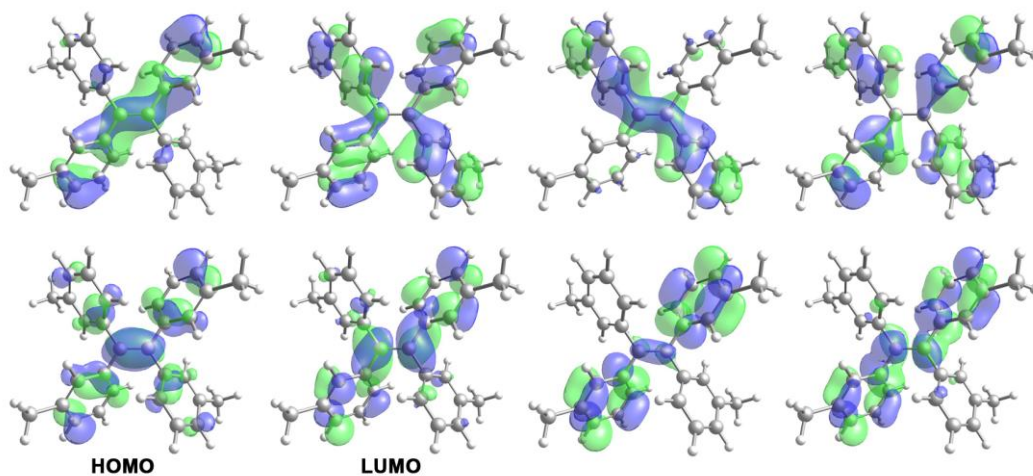


**Figure S3:** (a) Overlays of the OM2/MRCI and CASSCF optimized  $S_0$  and  $S_1$  structures of TPE-4mM (top) and TPE-4oM (bottom), respectively. (b) Overlays of the OM2/MRCI and CASSCF optimized  $S_1S_0$  conical intersection structures of TPE-4mM (top) and TPE-4oM (bottom), respectively.

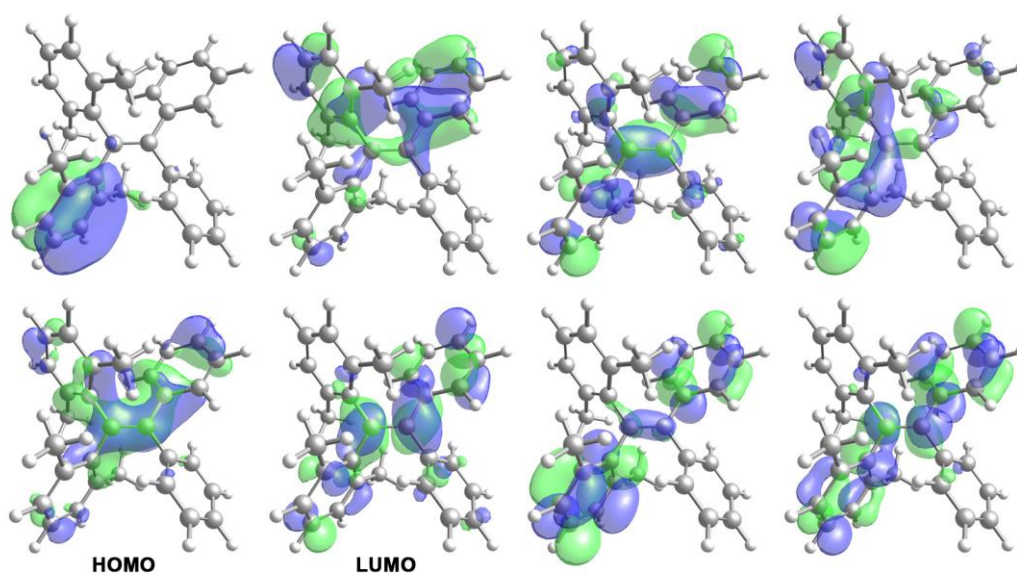


## 2. Active Orbitals

(a)



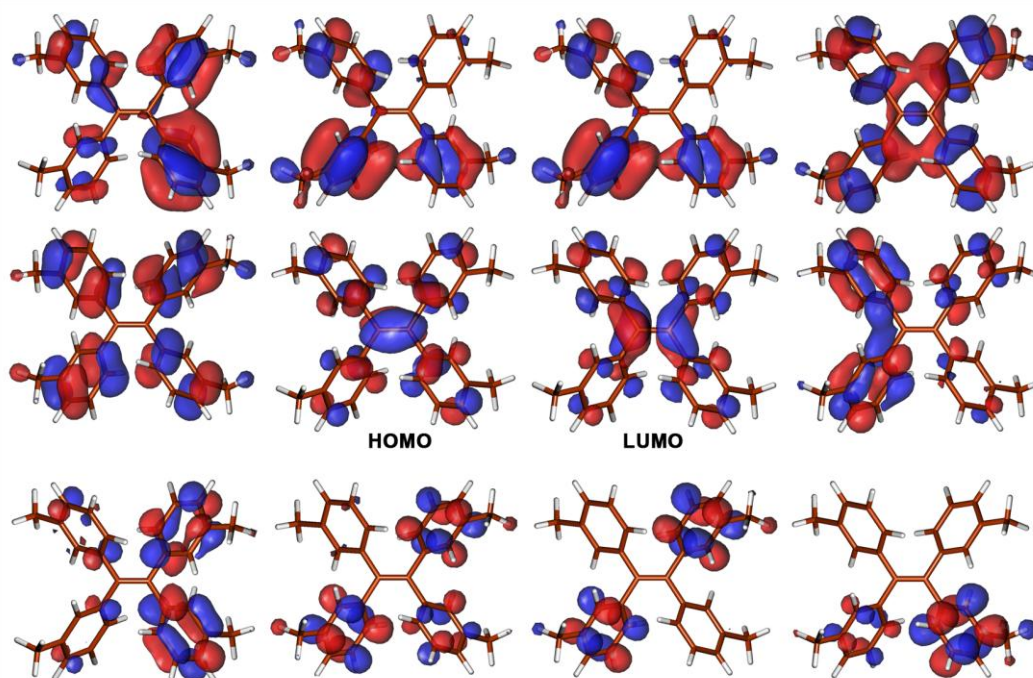
(b)



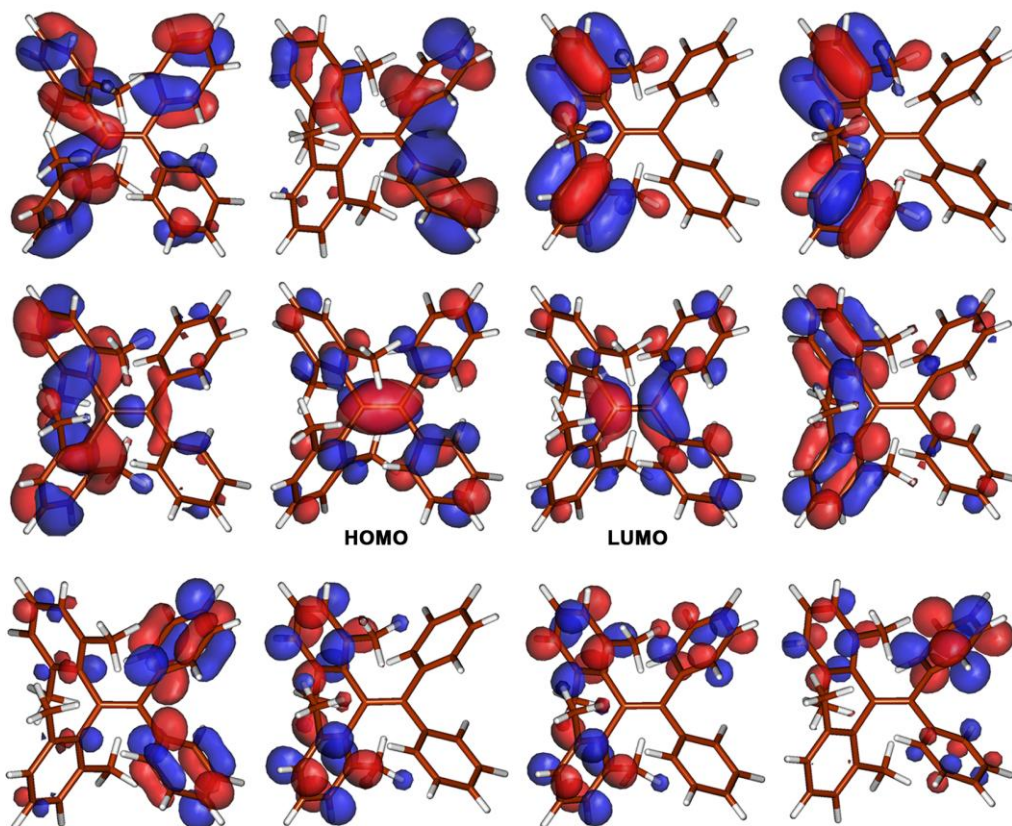
**Figure S4:** Active-space orbitals in the CASPT2 calculations for (a) TPE-4mM, (b) TPE-4oM.



(a)



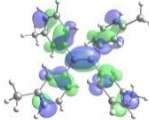
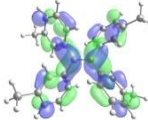
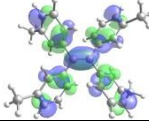
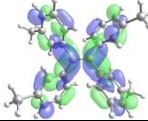
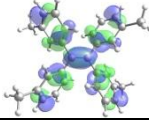
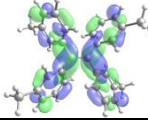
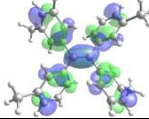
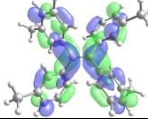
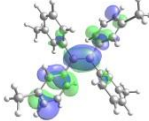
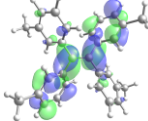
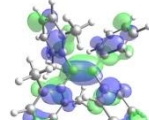
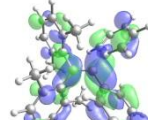
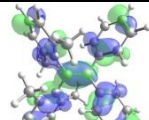
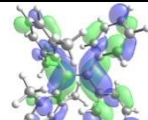
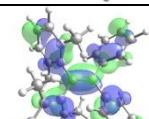
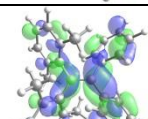
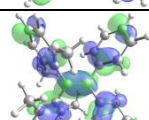
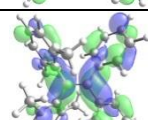
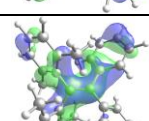
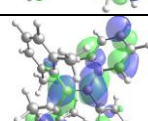
(b)



**Figure S5:** Active-space orbitals in the OM2/MRCI calculations for (a) TPE-4mM, (b) TPE-4oM.

### 3. Tables

**Table S1.** Vertical Excitation Energies ( $E_{\perp}$ , kcal/mol ), Oscillator Strengths ( $f$ ), and Singly Occupied Orbitals Involved in the  $S_0 \rightarrow S_1$  ( ${}^1\pi\pi^*$ ) Electronic Transitions of TPE-4mM and TPE-4oM in the Gas Phase, Computed by TD-B3LYP, TD-CAM-B3LYP, TD- $\omega$ B97XD, OM2/MRCI, and CASPT2 Methods, respectively.

<b>S<sub>0</sub>-TPE-4mM</b>	<b>E<sub>⊥</sub></b>	<b>f</b>	<b>Singly occupied orbitals</b>	
<b>TD-B3LYP</b>	84.5 (3.7 eV)	0.4006		
<b>TD-CAM-B3LYP</b>	97.9 (4.2 eV)	0.4912		
<b>TD-<math>\omega</math>B97XD</b>	99.2 (4.2 eV)	0.4896		
<b>OM2/MRCI</b>	101.1 (4.4 eV)	0.3852		
<b>CASPT2</b>	96.9 (4.2 eV)	0.7444		
<b>S<sub>0</sub>-TPE-4oM</b>	<b>E<sub>⊥</sub></b>	<b>f</b>	<b>Singly occupied orbitals</b>	
<b>TD-B3LYP</b>	85.6 (3.7 eV)	0.3055		
<b>TD-CAM-B3LYP</b>	98.9 (4.3 eV)	0.3929		
<b>TD-<math>\omega</math>B97XD</b>	98.9 (4.3 eV)	0.3830		
<b>OM2/MRCI</b>	101.6 (4.4 eV)	0.3774		
<b>CASPT2</b>	101.7 (4.4 eV)	0.4569		

**Table S2.** Selected Geometric Parameters of the Optimized OM2/MRCI Structures of TPE-4mM and TPE-4oM (see Fig. S1 for Atom Numbering).

Structures		Distance (Å)			Dihedral angle (°)	
		C1C2	C4C5	C8C9	Pyramidalization	
					C2C3C7C 1	C1C10C6C 2
TPE-4mM	S <sub>0</sub>	1.357	3.130	3.185	-0.2	-0.3
	S <sub>1</sub>	1.426	3.096	3.094	-0.2	-0.1
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	1.418	1.836	4.175	-11.1	-0.4
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	1.438	4.201	1.794	-27.1	-0.2
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	1.441	4.561	4.284	43.5	-4.3
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	1.441	4.297	4.550	-4.2	43.2
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	1.444	1.532	4.323	-0.1	0.2
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	1.444	4.405	1.532	0.4	-0.2
TPE-4oM	S <sub>0</sub>	1.363	3.292	3.337	-0.1	-0.3
	S <sub>1</sub>	1.423	3.571	3.576	-0.1	-0.2
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	1.439	1.811	3.959	28.3	1.8
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	1.439	3.961	1.810	-28.3	-1.8
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	1.440	4.104	4.953	-42.0	3.5
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	1.449	4.453	4.989	-5.7	40.5
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	1.455	1.542	4.741	2.4	-0.7
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	1.455	4.734	1.542	-2.3	0.6

Structures		Dihedral angle (°)				
		EZ <sup>a</sup>	IR <sup>b</sup>			
		C3C1C2C6	C2C1C3C4	C2C1C7C8	C1C2C6C5	C1C2C10C9
TPE-4mM	S <sub>0</sub>	-6.1	-47.3	-48.9	-49.6	-51.3
	S <sub>1</sub>	-37.9	-25.9	-25.9	-26.0	-26.0
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	-35.0	19.7	-87.4	-13.4	-57.7
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	-51.6	-65.7	-31.7	-38.5	-11.8
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	-60.9	-84.9	43.1	-54.0	-0.2
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	-132.6	-0.7	-53.3	43.0	-84.2
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	-10.5	-5.3	-84.8	-4.9	-85.7
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	-10.1	-87.9	-5.7	-88.3	-5.9
TPE-4oM	S <sub>0</sub>	-9.6	-60.5	-60.5	-39.5	-46.2
	S <sub>1</sub>	-48.0	-39.9	-40.0	-22.1	-21.8
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	-4.0	-36.8	-58.9	-7.7	-44.4
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	-43.9	-59.0	-36.8	-44.4	-7.7
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	-132.3	46.8	-99.0	23.2	-77.3
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	-138.1	-1.8	-72.6	69.2	-102.2
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	-11.4	-3.2	-92.7	-5.7	-105.8
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	-16.1	-92.6	-3.0	-105.5	-5.6

Notes: <sup>a</sup>: E-Z isomerization; <sup>b</sup>: Intramolecular rotation

**Table S3.** OM2/MRCI and CASPT2 Refined Relative Energies (kcal/mol) of the OM2/MRCI and CASSCF Optimized Structures for TPE-4mM and TPE-4oM.

	Structure	OM2/MRCI	CASPT2 // OM2/MRCI	CASPT2 // CASSCF
TPE-4mM	S <sub>0</sub>	0.0	0.0	0.0
	S <sub>1</sub>	79.7	76.0	79.3
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	79.4/79.4	75.1/89.0	72.0/81.7
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	79.9/79.9	76.8/88.0	71.5/82.7
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	80.7/80.7	89.5/91.5	89.5/90.9
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	80.7/80.7	89.6/91.5	89.5/91.5
TPE-4oM	S <sub>0</sub>	0.0	0.0	0.0
	S <sub>1</sub>	80.6	84.8	86.6
	S <sub>1</sub> S <sub>0</sub> <sup>C4C5</sup>	88.0/88.0	89.4/99.4	78.9/86.3
	S <sub>1</sub> S <sub>0</sub> <sup>C8C9</sup>	87.9/87.9	89.3/99.4	79.0/86.3
	S <sub>1</sub> S <sub>0</sub> <sup>C1</sup>	88.6/88.6	96.4/97.8	95.0/95.4
	S <sub>1</sub> S <sub>0</sub> <sup>C2</sup>	92.0/92.0	111.3/121.2	114.6/122.1

Note: There is generally reasonable agreement between the results from the different approaches. The discrepancies in the bottom line are not relevant mechanistically because they concern the highest-energy conical intersection.

**Table S4.** Relative Energies (kcal/mol) of OM2/MRCI and B3LYP Optimized Ground-State Structures for TPE-4mM and TPE-4oM.

	Structure	OM2/MRCI	B3LYP
TPE-4mM	S <sub>0</sub>	0.0	0.0
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	30.4	39.3
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	30.6	39.4
TPE-4oM	S <sub>0</sub>	0.0	0.0
	S <sub>0</sub> -cyclic <sup>C4C5</sup>	33.8	42.6
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	33.8	42.6

**Table S5.** Vertical Excitation Energies (kcal/mol) of S<sub>0</sub>-cyclic for TPE-4mM and TPE-4oM, Computed by TD-B3LYP, TD-CAM-B3LYP and OM2/MRCI Methods, respectively.

	Structure	TD-B3LYP	TD-CAM-B3LYP	OM2/MRCI
TPE-4mM	S <sub>0</sub> -cyclic <sup>C4C5</sup>	49.8	56.5	62.1
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	49.8	56.5	60.4
TPE-4oM	S <sub>0</sub> -cyclic <sup>C4C5</sup>	57.5	65.2	63.0
	S <sub>0</sub> -cyclic <sup>C8C9</sup>	55.8	62.9	63.3

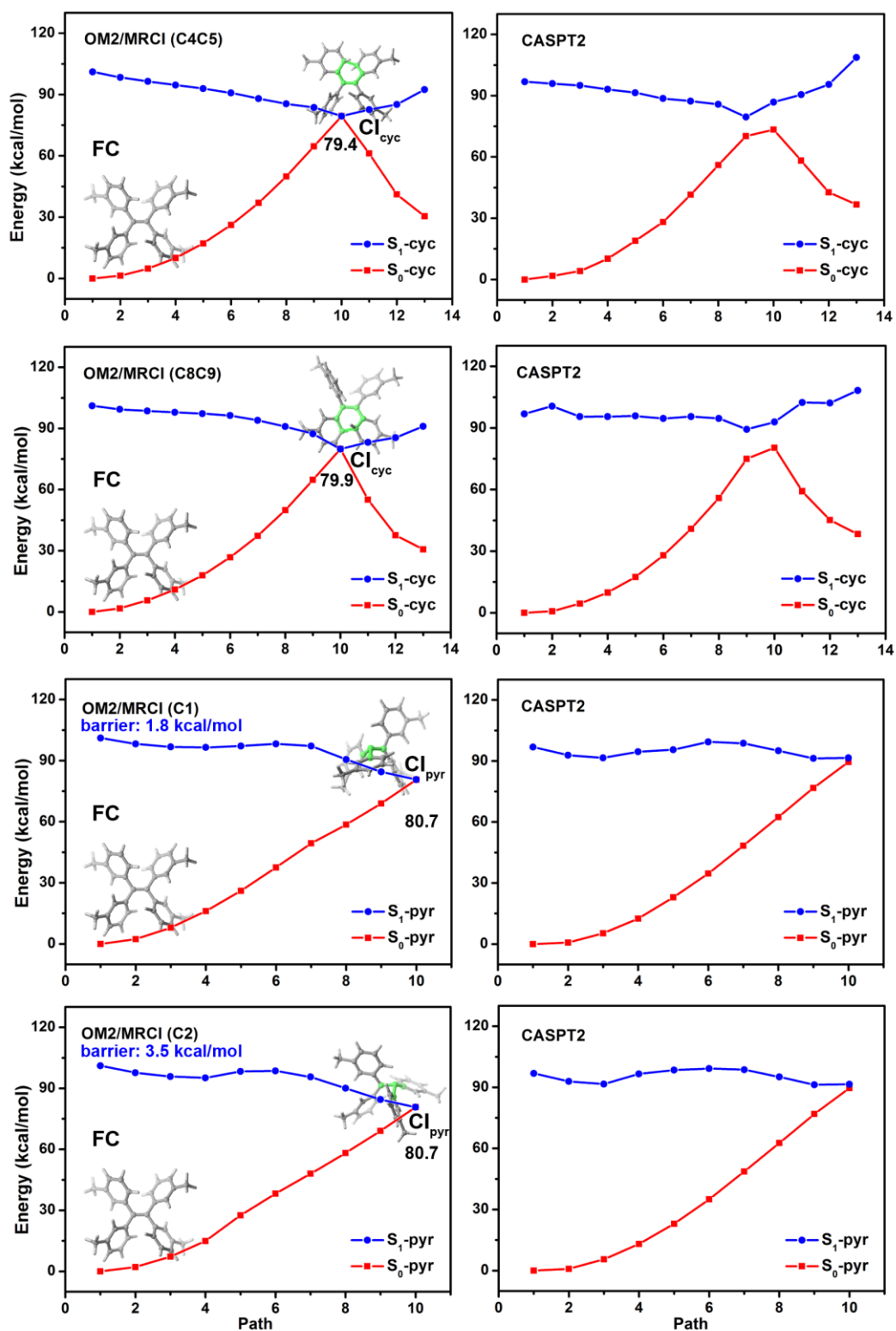
#### **4. LIIC Paths**

Hundreds of trajectories are needed to gain statistically meaningful results in surface hopping dynamics simulations. For molecules of the size of TPE-4oM and TPE-4mM (58 atoms), this can be achieved by using the semi-empirical OM2/MRCI electronic structure method, which is efficient and normally provides results close to those from the high-level CASSCF (structures) and CASPT2 (energies) methods, as demonstrated in many previous applications. [29-38]

In the present case, the data in Figs. S1-S3 and Tables S1-S3 clearly show that the OM2/MRCI and CASSCF (CASPT2) methods predict similar optimized geometries (energies) for all relevant minima and conical intersections. In addition, OM2/MRCI and first-principles methods give similar vertical excitation energies for the lowest  $S_0 \rightarrow S_1$  electronic transition at the Franck-Condon points (see 1).

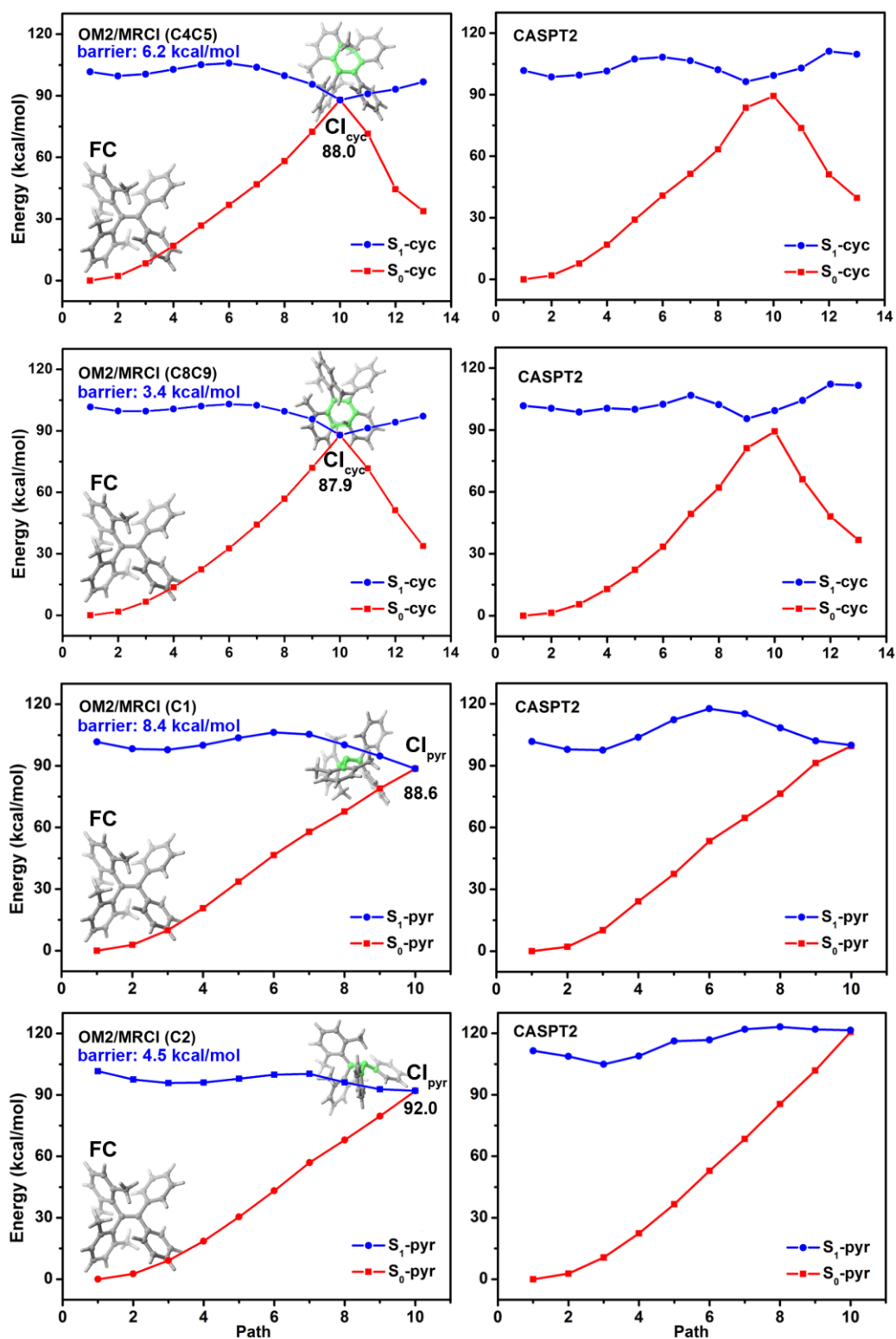
For further validation, we present OM2/MRCI and CASPT2 profiles along linearly interpolated internal coordinate (LIIC) paths that connect the OM2/MRCI optimized geometries of the  $S_0$  minima (i.e. Franck-Condon points) and of the relevant conical intersections in TPE-4mM and TPE-4oM (see Fig. 6). Evidently, the computed profiles are generally similar, indicating that OM2/MRCI and CASPT2//OM2/MRCI give similar topological structures for the  $S_1$  and  $S_0$  potential energy surfaces. We conclude that the OM2/MRCI method is suitable for simulating the photodynamics of TPE-4oM and TPE-4mM.

(a)





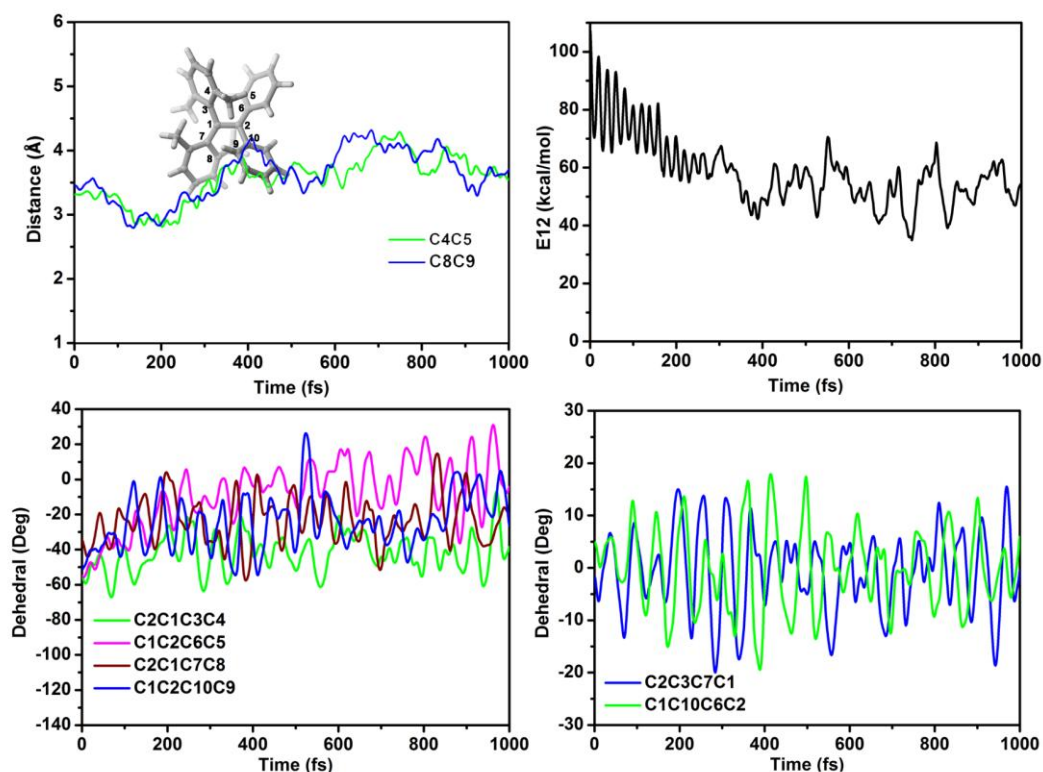
(b)



**Figure S6:** (left) OM2/MRCI and (right) CASPT2 re-computed reaction profiles along linearly interpolated internal coordinate (LIIC) paths connecting the optimized OM2/MRCI structures of the  $S_0$  minimum (i.e. Franck-Condon points) and of the relevant conical intersections: (a) TPE-4mM, (b) TPE-4oM.

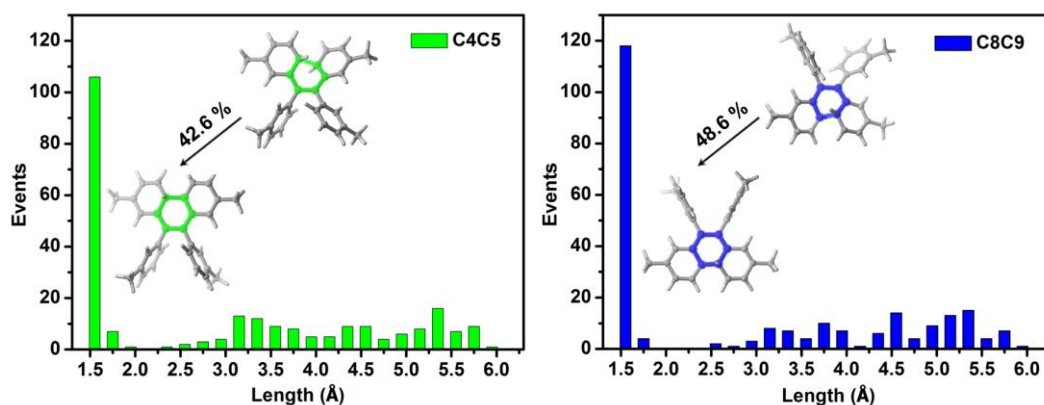


## 5. Typical Trajectory of TPE-4oM



**Figure S7:** Time-dependent physical variables obtained from typical OM2/MRCI trajectory of TPE-4oM: two key bond lengths (top-left);  $S_1$ - $S_0$  energy gap (top-right); six key dihedral angles (bottom).

## 6. Product Analysis

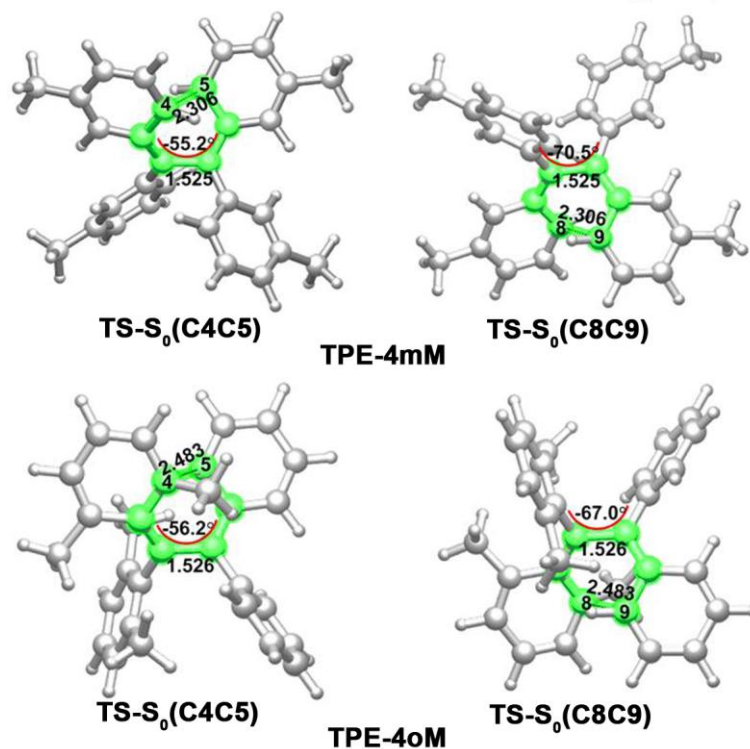


**Figure S8:** Distribution of the key C4C5 (left) and C8C9 (right) distances for TPE-4mM at the end of 1 ps simulations. Hops via  $S_1$ - $S_0$ -cyc (C4C5) [ $S_1$ - $S_0$ -cyc (C8C9)] are shown in green [blue].

## 7. Transition states

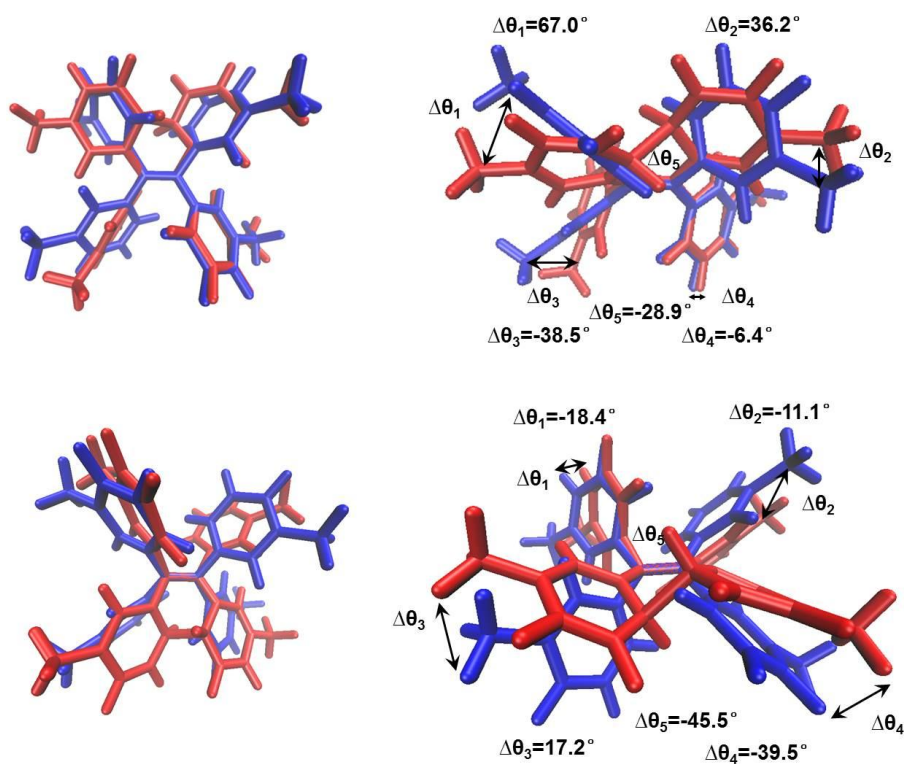
**Table S6.** Relative Energies (kcal/mol) of B3LYP Optimized Ground-State Structures for TPE-4mM and TPE-4oM.

TPE-4mM	S <sub>0</sub>	TS-S <sub>0</sub> <sup>C4C5</sup>	S <sub>0</sub> -cyclic <sup>C4C5</sup>
B3LYP	0.0	77.3	39.3
M06-2X	0.0	83.1	36.6
M06L	0.0	72.5	37.0
TPE-4mM	S <sub>0</sub>	TS-S <sub>0</sub> <sup>C8C9</sup>	S <sub>0</sub> -cyclic <sup>C8C9</sup>
B3LYP	0.0	77.3	39.4
M06-2X	0.0	83.1	37.3
M06L	0.0	72.5	36.8
TPE-4oM	S <sub>0</sub>	TS-S <sub>0</sub> <sup>C4C5</sup>	S <sub>0</sub> -cyclic <sup>C4C5</sup>
B3LYP	0.0	86.1	42.6
M06-2X	0.0	93.7	39.8
M06L	0.0	82.5	43.1
TPE-4oM	S <sub>0</sub>	TS-S <sub>0</sub> <sup>C8C9</sup>	S <sub>0</sub> -cyclic <sup>C8C9</sup>
B3LYP	0.0	86.1	42.6
M06-2X	0.0	93.7	40.7
M06L	0.0	82.5	43.1

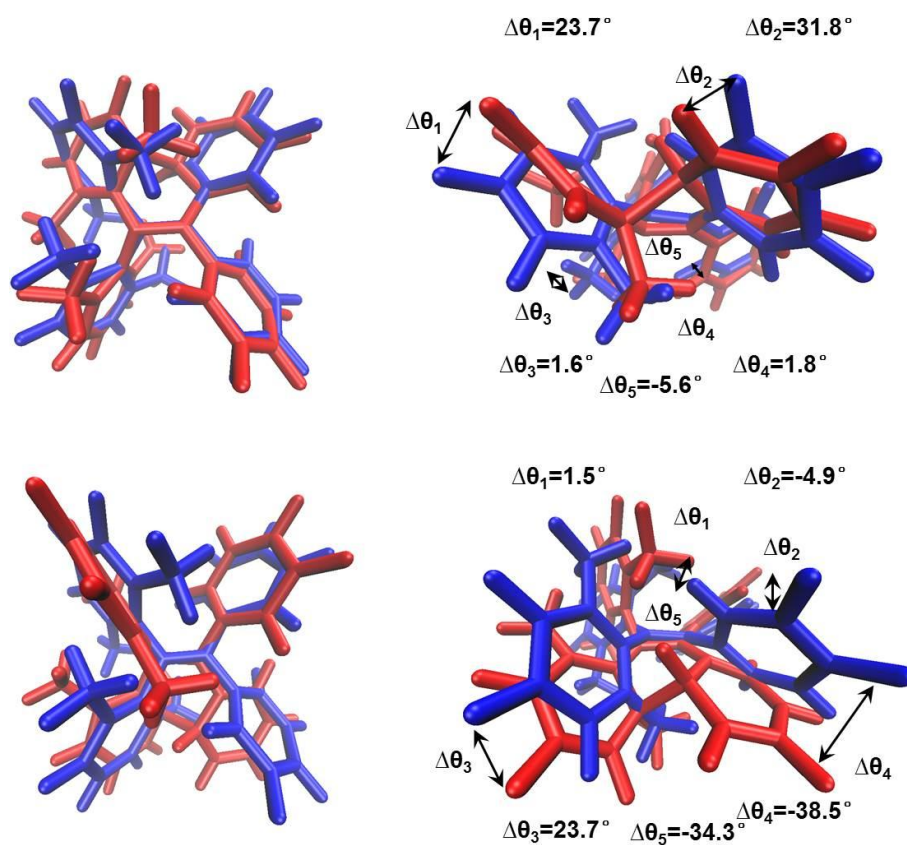


**Figure S9:** Transition-state structures of TPE-4mM and TPE-4oM optimized at the B3LYP level.

## 8. Overlaps between $S_0$ minima and cyclic $S_1/S_0$ conical intersections



**Figure S10:** Overlays of OM2/MRCI optimized  $S_0$  and (top)  $S_1/S_0$ -cyc (C4C5) and (bottom)  $S_1/S_0$ -cyc (C8C9) conical intersection structures of TPE-4mM from different angles (left and right panels). Also shown are the differences of five key dihedral angles i.e.  $\theta_1$ (C2C1C3C4);  $\theta_2$ (C1C2C6C5);  $\theta_3$ (C2C1C7C8);  $\theta_4$ (C1C2C10C9);  $\theta_5$ (C3C1C2C6). See Figure S1 for atomic numbering and Table S2 for specific numbers of these dihedral angles.



**Figure S11:** Overlays of OM2/MRCI optimized  $S_0$  and (top)  $S_1/S_0$ -cyc (C4C5) and (bottom)  $S_1/S_0$ -cyc (C8C9) conical intersection structures of TPE-4oM from different angles (left and right panels). Also shown are the differences of five key dihedral angles i.e.  $\theta_1$ (C2C1C3C4);  $\theta_2$ (C1C2C6C5);  $\theta_3$ (C2C1C7C8);  $\theta_4$ (C1C2C10C9);  $\theta_5$ (C3C1C2C6). See Figure S1 for atomic numbering and Table S2 for specific numbers of these dihedral angles.

## 9. Cartesian Coordinates

In xyz format (unit: Ångstrom)

### All structures including LIIC points

#### CASSCF method

TPE-4mM

S<sub>0</sub>

C	0.67404206	0.03799359	0.01071806
C	-0.68454633	0.01632018	-0.00267393
C	1.48492019	-1.22849583	0.09264642
C	2.40125175	-1.52728657	-0.91135388
C	1.38589188	-2.07532580	1.18549736
C	3.18738932	-2.66841200	-0.86256243
H	2.50379477	-0.85077337	-1.74193159
C	2.18008660	-3.20954781	1.25838328
H	0.69003339	-1.85505945	1.97423798
C	3.06773036	-3.50669118	0.24201478
H	3.67844533	-4.39079284	0.30856752
C	-1.48060214	-1.25362075	-0.07968547
C	-1.34221750	-2.13854906	-1.12947042
C	-2.44078255	-1.53459523	0.92415148
C	-2.13180224	-3.30544594	-1.17627086
H	-0.62767448	-1.94766229	-1.90847820
C	-3.20145902	-2.66883383	0.89153960
H	-2.56974089	-0.83119446	1.72791913
C	-3.03364933	-3.56573726	-0.18956203
H	-2.01456995	-3.99036585	-1.99742130
H	-3.63304419	-4.45939998	-0.22973227
C	1.48670793	1.28919568	-0.05217568
C	1.29928611	2.24044812	-1.05922492
C	2.51303195	1.50423450	0.88698637
C	2.09969000	3.36407125	-1.10795484
H	0.53149486	2.09905961	-1.79681183
C	3.29880408	2.63441386	0.85781912
H	2.68382441	0.76578713	1.65073058
C	3.08765686	3.57442651	-0.15832126
H	1.95082685	4.08682300	-1.89137857
H	3.69900454	4.45908209	-0.20531531
C	-1.52505391	1.26695324	0.05990913
C	-1.48059544	2.09863640	1.16329610
C	-2.41255986	1.55979054	-0.96969379
C	-2.30146223	3.21686911	1.22349835
H	-0.79859791	1.88971219	1.96735297

C	-3.23009352	2.67982993	-0.93027963
H	-2.46895029	0.89785661	-1.81669057
C	-3.16369541	3.50745534	0.18582893
H	-2.25958347	3.86242340	2.08303864
H	-3.79283829	4.37964740	0.24154599
C	-4.21416669	-2.97765700	1.96897435
H	-5.21151591	-3.07756126	1.55056094
H	-3.97872756	-3.91187296	2.47096973
H	-4.24470851	-2.19528263	2.71804563
C	4.37990112	2.86386772	1.88894931
H	5.35316319	2.97057064	1.41867888
H	4.19353778	3.77151570	2.45604432
H	4.43898359	2.03999080	2.59081467
C	-4.18475859	2.99105661	-2.06042594
H	-5.21681201	2.94238000	-1.72539528
H	-4.01699050	3.98989762	-2.45171840
H	-4.06992836	2.29004813	-2.87892886
H	2.10293745	-3.86124579	2.11061798
C	4.14505679	-3.00101490	-1.98368220
H	5.06985336	-3.41879625	-1.60033077
H	3.71297255	-3.73276187	-2.66123870
H	4.39229095	-2.12028174	-2.56505769

S<sub>1</sub>

C	-0.71190620	-0.08893080	0.04625810
C	0.71333678	-0.08976118	-0.04723036
C	-1.42108516	1.15504806	0.45397055
C	-2.51901142	1.65167763	-0.29767194
C	-1.01169602	1.88558204	1.55878992
C	-3.17208547	2.80377476	0.04406507
H	-2.83114781	1.10608358	-1.17068054
C	-1.68101773	3.06637257	1.92021767
H	-0.18506076	1.53952502	2.15120606
C	-2.73781965	3.51727318	1.18229096
H	-3.24382044	4.42567057	1.46217714
C	1.42370533	1.15196968	-0.45972403
C	1.01524869	1.87845028	-1.56755130
C	2.52198357	1.65052616	0.29012630
C	1.68588833	3.05705349	-1.93366449
H	0.18835122	1.53085270	-2.15870195
C	3.17640803	2.80046910	-0.05624180
H	2.83336748	1.10816325	1.16541479
C	2.74307632	3.50980244	-1.19742687
H	1.36014487	3.60224892	-2.80220554
H	3.25005195	4.41654700	-1.48088767
C	-1.46048551	-1.26092746	-0.23924453
C	-0.88445041	-2.35821612	-0.96049588
C	-2.78782478	-1.46216348	0.25985915
C	-1.59725288	-3.55051570	-1.13638229

H	0.01418787	-2.20587478	-1.51878824
C	-3.46000738	-2.63643924	0.09797022
H	-3.24644816	-0.67242652	0.82196990
C	-2.84787398	-3.70587240	-0.61319920
H	-1.14447567	-4.34519334	-1.70239276
H	-3.38494415	-4.62845173	-0.74684532
C	1.46085025	-1.26136407	0.24262774
C	0.88383191	-2.35546134	0.96793985
C	2.78800228	-1.46565484	-0.25574119
C	1.59554388	-3.54775879	1.14819694
H	-0.01464957	-2.20023891	1.52569179
C	3.45910016	-2.63995008	-0.08955894
H	3.24734634	-0.67841777	-0.82076117
C	2.84600612	-3.70619721	0.62555688
H	1.14205224	-4.33992761	1.71714536
H	3.38221873	-4.62878276	0.76255893
C	4.33396173	3.32842223	0.75911541
H	5.23363834	3.41023678	0.15563312
H	4.11698886	4.31804313	1.15111102
H	4.55447001	2.67935352	1.59857395
C	-4.83949470	-2.83629146	0.67609769
H	-5.55044443	-3.09923136	-0.10217681
H	-4.84274064	-3.64471950	1.40192194
H	-5.19669608	-1.94061035	1.16919472
C	4.83838278	-2.84318760	-0.66699490
H	5.54906121	-3.10419600	0.11217547
H	4.84080115	-3.65409236	-1.39005708
H	5.19649947	-1.94956157	-1.16314868
H	-1.35459191	3.61471079	2.78652103
C	-4.32865240	3.33009929	-0.77374583
H	-5.22595388	3.42454152	-0.16864053
H	-4.10639325	4.31386154	-1.17742253
H	-4.55581746	2.67319411	-1.60528530

### S<sub>1</sub>S<sub>0</sub> -cyc (C4C5)

C	0.020028200	0.031920300	0.003147200
C	1.414242500	0.012310900	0.012012900
C	-0.674945200	0.024044900	-1.270004800
C	-2.051807800	0.264279200	-1.341786100
C	0.020433000	-0.371074000	-2.493279200
C	-2.785259100	-0.165625700	-2.430637800
H	-2.544938300	0.746735800	-0.518221500
C	-0.781051100	-0.673950500	-3.623512200
H	0.848859500	0.268930000	-2.747838400
C	-2.148137000	-0.709716900	-3.564448800
H	-2.742574300	-1.094004800	-4.374203100
C	2.097505300	-0.717956900	-0.999625200
C	1.266911300	-1.634454500	-1.747843700
C	3.453268200	-0.551880000	-1.335064200



C	1.883116300	-2.333368200	-2.833677800
H	0.487395300	-2.148317400	-1.157634400
C	4.031399000	-1.270699600	-2.352121000
H	4.034151200	0.182262200	-0.786940800
C	3.213081700	-2.178529500	-3.074244500
H	1.289778900	-3.029789600	-3.400732600
H	3.683309300	-2.782274900	-3.844241600
C	-0.722843100	0.427455500	1.225724600
C	-1.002368600	-0.544966700	2.196884800
C	-1.156206900	1.735650100	1.441263700
C	-1.678505800	-0.205507100	3.354037000
H	-0.670679700	-1.559987800	2.035680000
C	-1.843496300	2.084241200	2.603633000
H	-0.956321000	2.490573300	0.692055500
C	-2.098350200	1.108128700	3.557242600
H	-1.881787100	-0.955469600	4.105425600
H	-2.622091200	1.374475300	4.464539000
C	2.208755200	0.733298000	1.037953600
C	2.059508600	2.108811700	1.206699000
C	3.113673800	0.031688400	1.827057300
C	2.818218700	2.774061000	2.156363200
H	1.368154500	2.651912900	0.582981400
C	3.863770800	0.688484800	2.795893100
H	3.216072300	-1.034881100	1.685689100
C	3.710764400	2.064999700	2.951124200
H	2.708768300	3.840846300	2.285116900
H	4.290043100	2.581947800	3.702518300
C	5.493018300	-1.173496100	-2.687857500
H	5.932171900	-0.263989700	-2.279597700
H	6.047921400	-2.024536400	-2.283251500
H	5.644568000	-1.160454300	-3.768264500
C	-2.325560500	3.497319700	2.801403500
H	-3.324603000	3.611303800	2.380835700
H	-2.369132600	3.747709000	3.858761800
H	-1.666818200	4.210010900	2.309237900
C	4.811945500	-0.088528800	3.669549500
H	5.338924200	-0.846147800	3.093082000
H	5.549716200	0.567731300	4.125107700
H	4.260060300	-0.588087900	4.464813400
H	-0.264399600	-0.896920400	-4.552021100
C	-4.282972000	-0.047937200	-2.426966300
H	-4.601550200	0.584940400	-3.251984500
H	-4.725120200	-1.033185600	-2.555048500
H	-4.645936100	0.376246300	-1.495954000

S<sub>1</sub>S<sub>0</sub> -cyc (C8C9)

C	0.011631800	0.018643400	-0.008767700
C	1.426493300	0.012326800	-0.008748700
C	-0.591361900	-0.023319800	-1.383409100

C	-1.313471800	-1.128982300	-1.810521800
C	-0.452214300	1.068637800	-2.249066700
C	-1.883273500	-1.177577500	-3.077879500
H	-1.427014800	-1.960225000	-1.129055800
C	-1.014611100	1.030490500	-3.516569500
H	0.099460600	1.943814100	-1.933694600
C	-1.726699700	-0.090535600	-3.930330300
H	-2.156670800	-0.124996300	-4.921354900
C	2.134210300	-1.004065000	-0.810244900
C	1.649479000	-2.314166900	-0.830932200
C	3.307377000	-0.691476400	-1.510934100
C	2.331319000	-3.300872700	-1.536470400
H	0.750522100	-2.544072900	-0.285080500
C	3.977200700	-1.665948600	-2.229373500
H	3.671548800	0.325204800	-1.500251000
C	3.484517800	-2.977274600	-2.226793300
H	1.955147700	-4.313038100	-1.552745500
H	4.012403200	-3.742686300	-2.779343900
C	-0.632584900	0.936322200	0.922163100
C	0.019298900	1.245452900	2.175211800
C	-1.855500100	1.564206800	0.630926400
C	-0.646065900	2.127610300	3.070338400
H	0.576593700	0.451068800	2.644131600
C	-2.433591700	2.450362500	1.511152200
H	-2.380383300	1.269693700	-0.261606000
C	-1.781722500	2.795560400	2.718853300
H	-0.189331200	2.298484900	4.037947900
H	-2.234848900	3.521255200	3.373245900
C	2.173012300	0.948778200	0.761748600
C	1.445033200	2.096203200	1.294322600
C	3.427201800	0.615040800	1.319324800
C	2.117442100	2.890061700	2.295972000
H	0.866305500	2.680768000	0.561747900
C	4.049352100	1.408394600	2.243938800
H	3.888666000	-0.316308100	1.010995200
C	3.369397800	2.573861300	2.695992400
H	1.610505500	3.766968900	2.661153500
H	3.883885900	3.230982100	3.388006500
C	5.220622700	-1.339006400	-3.014253100
H	6.027265500	-2.026184100	-2.764738100
H	5.021777000	-1.417475800	-4.082189200
H	5.559435300	-0.326890600	-2.806098900
C	-3.763106600	3.069884900	1.185838500
H	-4.393364700	2.368671400	0.645200200
H	-4.278598700	3.376184200	2.091899300
H	-3.610495600	3.948456200	0.561196400
C	5.434112600	1.119742900	2.747719500
H	6.185038400	1.644078000	2.150259600
H	5.545139400	1.442558000	3.782858100
H	5.652326100	0.053249000	2.703090700

H	-0.897300900	1.868765500	-4.189724200
C	-2.650036400	-2.401572000	-3.501501700
H	-3.537243100	-2.525275600	-2.881854400
H	-2.964396900	-2.322722900	-4.539349700
H	-2.032253400	-3.291680700	-3.396742100

S<sub>1</sub>S<sub>0</sub> -cyc (C1)

C	0.861481800	1.095552100	0.454808200
C	-0.489118000	0.649671200	0.242420600
C	1.030577500	-0.405111300	1.004456200
C	1.782589400	-1.377903100	0.317428100
C	0.671650700	-0.679801100	2.326607500
C	2.232200800	-2.515285800	0.928908700
H	2.045569100	-1.178683100	-0.699454800
C	1.077924600	-1.856295100	2.947403900
H	0.096198200	0.034887100	2.876448000
C	1.856947700	-2.757020500	2.260036400
H	2.183061600	-3.661568100	2.739295500
C	-1.002809100	-0.393493600	-0.737760400
C	-0.574482700	-0.387543600	-2.068922100
C	-1.865198900	-1.407706400	-0.305253100
C	-1.034296200	-1.376948500	-2.941991400
H	0.098462800	0.362319000	-2.420361700
C	-2.317233300	-2.386964800	-1.171625400
H	-2.132987000	-1.446994300	0.730792200
C	-1.891615500	-2.354848800	-2.504227300
H	-0.697478200	-1.377102000	-3.960929200
H	-2.236165700	-3.114216000	-3.181113000
C	1.712258400	1.480412200	-0.626159700
C	1.194189300	2.316517100	-1.645735100
C	3.106314300	1.277224300	-0.632124900
C	2.018703600	2.889755900	-2.583021100
H	0.142833900	2.543652500	-1.640611200
C	3.920675900	1.871365600	-1.569639400
H	3.536665300	0.678143300	0.147127600
C	3.385060300	2.675098600	-2.572125000
H	1.585171000	3.525753000	-3.333672800
H	4.020095300	3.127980800	-3.304608900
C	-1.541893700	1.302077100	1.067388800
C	-1.091421900	2.192187400	2.045716500
C	-2.920741700	1.186660000	0.831899300
C	-1.993071500	2.890483900	2.820204300
H	-0.027455600	2.289572800	2.121205900
C	-3.824195800	1.905131600	1.586585600
H	-3.281487200	0.572800000	0.035585200
C	-3.346230600	2.739944100	2.595797400
H	-1.640884800	3.557962400	3.580500600
H	-4.048091600	3.290619100	3.194781800
C	-3.252058200	-3.474562700	-0.688666300

H	-4.106525000	-3.556191400	-1.351242100
H	-2.739686500	-4.430084500	-0.662120900
H	-3.612798500	-3.251325600	0.308160800
C	5.424183500	1.695191000	-1.485452400
H	5.837734200	1.483439400	-2.465251300
H	5.879064000	2.609903800	-1.116272300
H	5.689861400	0.888354000	-0.812815500
C	-5.312973400	1.817825600	1.327816400
H	-5.844269400	1.572517700	2.241447200
H	-5.687756000	2.765708300	0.956636000
H	-5.528719800	1.053082800	0.592538300
H	0.790136000	-2.055391800	3.960639500
C	3.106367700	-3.508730100	0.193642000
H	4.119719200	-3.476807300	0.580632400
H	2.724639400	-4.517753900	0.309175600
H	3.137022100	-3.272375100	-0.862643400

S<sub>1</sub>S<sub>0</sub> -cyc (C2)

C	0.518517700	-0.622159700	0.241872900
C	-0.827177000	-1.098444700	0.405651700
C	1.554804800	-1.284241000	1.082926000
C	2.938466500	-1.151479500	0.886642100
C	1.085285100	-2.204432600	2.025167900
C	3.826713800	-1.889216300	1.643705500
H	3.317206100	-0.510041100	0.117845100
C	1.972944500	-2.917684500	2.804047000
H	0.019415600	-2.315203000	2.071552400
C	3.331398200	-2.756104000	2.617643100
H	4.022439000	-3.321892800	3.218800200
C	-1.648526100	-1.465847200	-0.706873200
C	-1.097904000	-2.265109700	-1.738965500
C	-3.046254000	-1.286042900	-0.730308000
C	-1.898355200	-2.827237000	-2.706632500
H	-0.041733900	-2.476689700	-1.723844100
C	-3.833917500	-1.862885700	-1.702378700
H	-3.501379000	-0.717783800	0.060229200
C	-3.267915800	-2.631949700	-2.716880800
H	-1.441851100	-3.437948200	-3.467291200
H	-3.883366700	-3.073584400	-3.475713400
C	1.048983600	0.453769100	-0.692943800
C	0.650805000	0.480824100	-2.032977700
C	1.896011200	1.461887700	-0.211095400
C	1.127310600	1.494462900	-2.869715900
H	-0.013808300	-0.262295600	-2.419477100
C	2.365330000	2.463591200	-1.044541900
H	2.139791000	1.477838100	0.833464900
C	1.973142900	2.463863500	-2.388440800
H	0.809622100	1.523435200	-3.896023100
H	2.330411700	3.243595800	-3.038232700

C	-1.031016300	0.379395400	0.993917300
C	-0.703039500	0.626438200	2.329915000
C	-1.788429100	1.356670300	0.314805700
C	-1.139894000	1.782318000	2.970586100
H	-0.123951000	-0.091157800	2.876028800
C	-2.265297000	2.473642000	0.947715700
H	-2.032083400	1.178604200	-0.712826700
C	-1.918981900	2.690806100	2.291014000
H	-0.871217100	1.962551700	3.994467700
H	-2.264525400	3.581677300	2.786566300
C	-5.339342900	-1.695746300	-1.654164000
H	-5.718862700	-1.410592300	-2.631097500
H	-5.803590600	-2.636781300	-1.368542400
H	-5.627225200	-0.938186900	-0.932620500
C	3.292066100	3.538512400	-0.521592200
H	4.238686400	3.502161300	-1.053626600
H	2.849362000	4.519695700	-0.662366300
H	3.485519000	3.395005000	0.535985000
C	-3.137083800	3.472589600	0.218705200
H	-4.165763400	3.388235800	0.558107700
H	-2.792862800	4.486888100	0.399258000
H	-3.109831400	3.283574100	-0.848676900
H	1.605443000	-3.608247000	3.538270600
C	5.319564200	-1.786547900	1.422253800
H	5.819914900	-1.494131000	2.341239800
H	5.718121600	-2.744100700	1.100356600
H	5.541779000	-1.047835600	0.660505600

TPE-4oM

S<sub>0</sub>

C	-0.00416473	-0.48649118	0.00056568
C	-0.00423775	0.87719448	0.00194162
C	1.29071381	-1.27995655	-0.06854972
C	1.64826906	-2.17991027	0.97300158
C	2.15207843	-1.16078348	-1.18003451
C	2.82815347	-2.91870637	0.87400075
C	3.31996052	-1.92699078	-1.23201934
C	3.66247942	-2.79496401	-0.23044494
H	4.56763095	-3.37289666	-0.29435185
C	1.24542374	1.69780466	0.17572907
C	2.10873422	1.48378094	1.24511246
C	1.52936159	2.74756659	-0.69653422
C	3.23076012	2.27678078	1.42726967
H	1.90564502	0.69337181	1.94275793
C	2.65354388	3.53503935	-0.52338947
H	0.86390240	2.94997093	-1.51607730

C	3.51043974	3.30207149	0.54113986
H	3.88209993	2.09190489	2.26297053
H	4.38131273	3.91756220	0.68083441
C	-1.29847160	-1.28035471	0.06640635
C	-2.15523825	-1.16176250	1.17258617
C	-1.64870737	-2.17733943	-0.96501698
C	-3.31922395	-1.92571538	1.22959972
C	-2.81791298	-2.91553759	-0.87164883
C	-3.65585119	-2.79792159	0.22168174
H	-3.96310055	-1.82504444	2.08639639
H	-4.55894139	-3.37941489	0.28077346
C	-1.25214174	1.69993485	-0.17299834
C	-2.11548371	1.48734998	-1.24284075
C	-1.53317528	2.75184593	0.69759655
C	-3.23474529	2.28370624	-1.42654728
H	-1.91484431	0.69496173	-1.93878513
C	-2.65489725	3.54263845	0.52292298
H	-0.86748869	2.95332679	1.51720807
C	-3.51183084	3.31099869	-0.54176780
H	-3.88619985	2.09982840	-2.26236877
H	-4.38073606	3.92897463	-0.68275020
H	3.96320397	-1.82548095	-2.08975894
H	-3.07691978	-3.58931830	-1.66903961
H	3.09449196	-3.59139994	1.66955575
H	2.85648521	4.33346292	-1.21502018
H	-2.85569619	4.34255912	1.21345314
C	1.92144756	-0.25050688	-2.37269804
H	2.66891387	0.53438168	-2.39428668
H	2.01396289	-0.81747220	-3.29377199
H	0.95468944	0.22427736	-2.37244389
C	0.81849230	-2.36925495	2.22642157
H	-0.11041804	-2.88653013	2.02381451
H	1.37176562	-2.95571622	2.95056916
H	0.57347312	-1.42612324	2.69662800
C	-1.92335496	-0.25095333	2.36273261
H	-2.66220449	0.54271752	2.37482345
H	-2.03362792	-0.81444212	3.28406976
H	-0.95096846	0.21150387	2.37058184
C	-0.81388615	-2.36747838	-2.21336142
H	-0.55041320	-1.42396859	-2.67246104
H	0.10697073	-2.89936871	-2.00817824
H	-1.36953871	-2.94051550	-2.94592931

S<sub>1</sub>

C	-0.02556158	-0.46930518	-0.01526019
C	-0.01382563	1.03564923	0.02895294
C	1.18402558	-1.13820548	-0.54778486
C	1.76814894	-2.21669392	0.17214619
C	1.86005025	-0.71234143	-1.72202981

C	2.94030685	-2.80968211	-0.28247773
C	3.03871039	-1.32124222	-2.12330833
C	3.58966012	-2.37214933	-1.41716365
H	4.50192291	-2.83833139	-1.74481409
C	1.08564154	1.73166360	0.67539202
C	1.87565529	1.06775065	1.63951016
C	1.54198118	3.01029848	0.24462115
C	2.94223619	1.70047486	2.24999526
H	1.62862459	0.06547896	1.91173713
C	2.63132852	3.60764738	0.82078247
H	1.06303973	3.49896886	-0.58042142
C	3.32463112	2.96636808	1.84910813
H	3.49732726	1.18473178	3.01206868
H	4.17737279	3.44189593	2.29905524
C	-1.18089602	-1.17793011	0.50822660
C	-1.95072646	-0.72326549	1.63219585
C	-1.69341413	-2.34234291	-0.17465431
C	-3.12630718	-1.36142274	1.99596694
C	-2.85745476	-2.94545182	0.25377920
C	-3.59743882	-2.47115434	1.32808692
H	-3.66964051	-0.99084154	2.84887446
H	-4.50884333	-2.95590033	1.62851861
C	-1.09005070	1.75842112	-0.59525610
C	-1.96526669	1.08676726	-1.47699590
C	-1.41764195	3.10047675	-0.25700634
C	-3.01544420	1.74942855	-2.08625042
H	-1.79583191	0.05380110	-1.68422970
C	-2.48387675	3.73750032	-0.83094898
H	-0.85903657	3.60858289	0.50218023
C	-3.27587501	3.06815972	-1.76919119
H	-3.64668063	1.22335223	-2.77793720
H	-4.11173933	3.57423358	-2.21786318
H	3.52215798	-0.97707647	-3.02144770
H	-3.22205992	-3.79935678	-0.29186746
H	3.36097962	-3.62219715	0.28468598
H	2.96280679	4.56706677	0.46687157
H	-2.72537690	4.74479763	-0.54552934
C	1.30465248	0.35926105	-2.63095877
H	1.88656010	0.41761862	-3.54328848
H	0.27828865	0.15016965	-2.91023816
H	1.32228781	1.34837343	-2.18521529
C	1.19156321	-2.76972795	1.45909448
H	0.33516893	-3.41254709	1.28802862
H	1.94249472	-3.35566352	1.97779600
H	0.85520306	-1.98792424	2.12809926
C	-1.45776787	0.36573019	2.55205347
H	-2.13584527	0.48924184	3.38851850
H	-0.47963778	0.12706118	2.95928285
H	-1.36825863	1.33795301	2.07821801
C	-1.06155584	-2.90202566	-1.43110075



H	-0.81322790	-2.11658012	-2.13700071
H	-0.14313413	-3.44640651	-1.24517167
H	-1.75186531	-3.58198440	-1.91835883

S<sub>1</sub>S<sub>0</sub>-cyc (C4C5)

C	0.082519200	-0.698712000	0.423360900
C	-0.089306900	0.693531800	0.229766100
C	-1.090730200	-1.441023400	0.884108900
C	-1.467029100	-2.748095300	0.457119200
C	-1.984306500	-0.750285100	1.820083900
C	-2.721504800	-3.228443400	0.763411100
C	-3.195771600	-1.407269800	2.191524800
C	-3.652166800	-2.514654100	1.538777700
H	-4.632627100	-2.919572700	1.719001100
C	-1.346783400	1.350493000	0.374392300
C	-2.527567900	0.506021300	0.522502400
C	-1.408135400	2.704585000	0.781898900
C	-3.715294800	1.149575000	1.033919700
H	-2.720969200	-0.220297300	-0.288880200
C	-2.568712100	3.282344100	1.207375200
H	-0.491487600	3.280918000	0.762440300
C	-3.732702500	2.473771800	1.306413500
H	-4.607295000	0.552533300	1.113114800
H	-4.666372300	2.937078000	1.600973900
C	0.943838200	-1.294205900	-0.661924600
C	0.558065300	-1.227961400	-2.024346500
C	2.163726700	-1.898683900	-0.331651900
C	1.404309600	-1.737208400	-2.996919900
C	2.993821200	-2.405707500	-1.330382000
C	2.624488000	-2.319629500	-2.658520400
H	1.113598800	-1.672035500	-4.037639700
H	3.273843100	-2.703509200	-3.431146600
C	1.075881300	1.505090400	-0.190678100
C	2.309067100	1.330648800	0.435196200
C	0.941712400	2.462842600	-1.194636300
C	3.398897900	2.103194700	0.059447700
H	2.401263300	0.594580900	1.214674600
C	2.037820000	3.220594600	-1.583974900
H	-0.013964100	2.589391600	-1.678764500
C	3.261624000	3.045586900	-0.950354500
H	4.352250900	1.966035400	0.546787300
H	4.111554900	3.641658900	-1.247651200
H	-3.793777700	-0.941737900	2.967778100
H	3.933355600	-2.865660100	-1.057336800
H	-2.995749400	-4.216206900	0.411569500
H	-2.624185900	4.327012200	1.448176000
H	1.938746700	3.943285200	-2.379007700
C	-1.293830400	0.001574500	2.948367400
H	-1.026535500	1.013388600	2.662949400

H	-1.942713700	0.054697300	3.820592800
H	-0.387803200	-0.534584600	3.227175200
C	-0.469539000	-3.708756900	-0.137173200
H	-0.892912000	-4.712021800	-0.162297800
H	-0.184380300	-3.427684500	-1.141223400
H	0.422770400	-3.737411400	0.481497700
C	-0.750471100	-0.613872700	-2.453529600
H	-0.694417600	0.471823200	-2.410620500
H	-0.997734600	-0.901388800	-3.473552200
H	-1.565212000	-0.938366300	-1.812455100
C	2.563430800	-2.048676300	1.111892700
H	3.559180400	-1.638729200	1.281580000
H	1.860133800	-1.538099300	1.759511200
H	2.580504100	-3.102904700	1.390448500

### S<sub>1</sub>S<sub>0</sub>-cyc (C8C9)

C	0.082838700	-0.698579700	0.423109900
C	-0.088727900	0.693708900	0.229780500
C	0.943782800	-1.294599900	-0.662092500
C	2.163675700	-1.899134700	-0.331803600
C	0.557550800	-1.228890100	-2.024457700
C	2.993448000	-2.406755100	-1.330452700
C	1.403492600	-1.738877600	-2.996923400
C	2.623710900	-2.321304200	-2.658556900
H	3.272881000	-2.705581900	-3.431157200
C	1.076280500	1.505820900	-0.190531300
C	2.309501800	1.331518800	0.435364300
C	0.942070900	2.463941200	-1.194082300
C	3.399154700	2.104639100	0.060158000
H	2.401660200	0.595114200	1.214523200
C	2.038000100	3.222269200	-1.582940500
H	-0.013710000	2.590049600	-1.678218500
C	3.261792000	3.047441800	-0.949176600
H	4.352471500	1.967624700	0.547634300
H	4.111513700	3.643852200	-1.246185100
C	-1.090477000	-1.440947600	0.883890000
C	-1.983885900	-0.750282400	1.819930700
C	-1.467283700	-2.747846200	0.456576300
C	-3.195259300	-1.406829800	2.191388500
C	-2.721708100	-3.228068300	0.763305200
C	-3.652043500	-2.514276300	1.538674900
H	-3.793120200	-0.941080100	2.967568600
H	-4.632823200	-2.918191100	1.719286100
C	-1.346445300	1.350224700	0.375008500
C	-2.527144000	0.505630100	0.522603900
C	-1.408244600	2.704335700	0.782557900
C	-3.715205400	1.149021300	1.033752900
H	-2.720418900	-0.220581200	-0.288777900
C	-2.569131400	3.281878000	1.207513500

H	-0.491872200	3.281110000	0.763418200
C	-3.733081000	2.473132200	1.305939700
H	-4.607056900	0.551763400	1.112745800
H	-4.666941300	2.936241700	1.600084800
H	1.112259000	-1.674267700	-4.037508100
H	-2.995800400	-4.215929500	0.411634000
H	3.933034400	-2.866614900	-1.057535400
H	1.939041600	3.945087000	-2.377866200
H	-2.625051500	4.326515900	1.448286200
C	-0.750815500	-0.614656900	-2.453904100
H	-0.694517500	0.470998200	-2.410889000
H	-0.997692400	-0.902068300	-3.474033500
H	-1.565953500	-0.939015200	-1.813291400
C	2.563481300	-2.048516800	1.111775200
H	1.860303300	-1.537455800	1.759040000
H	2.580343200	-3.102632900	1.390928400
H	3.559304200	-1.638634400	1.281127200
C	-1.292773000	0.001727600	2.947716600
H	-1.025302000	1.013344300	2.661789500
H	-1.941113200	0.055420500	3.820293900
H	-0.386796200	-0.534653900	3.226106800
C	-0.470129500	-3.709004300	-0.137471300
H	-0.184650800	-3.428152300	-1.141385900
H	0.421956300	-3.738005300	0.481496600
H	-0.893962700	-4.712119800	-0.162605700

### S<sub>1</sub>S<sub>0</sub>-cyc (C1)

C	0.012775100	-0.098276000	0.047176500
C	1.424710700	-0.019040700	-0.091507600
C	-0.840788500	-1.077628600	0.663587200
C	-2.133115800	-1.399460400	0.166571000
C	-0.482523500	-1.656118700	1.914773100
C	-2.917469400	-2.335266600	0.812327700
C	-1.303458400	-2.592783300	2.516669400
C	-2.512388000	-2.969350600	1.971044500
H	-3.134961900	-3.696725000	2.450914200
C	2.149138600	1.210103200	0.419318300
C	1.452074500	2.045287300	1.289678900
C	3.497034900	1.475106500	0.179985600
C	2.073075800	3.116301200	1.895883900
H	0.421782800	1.818741200	1.459642400
C	4.114588100	2.566116200	0.765610400
H	4.072684200	0.831346800	-0.446749700
C	3.404115900	3.387657400	1.622301900
H	1.522839100	3.741370700	2.569982800
H	3.885222000	4.230471400	2.078910400
C	0.157082900	-0.022661100	-1.570682700
C	0.060557900	1.265311900	-2.196745200
C	0.116325900	-1.179494700	-2.396358400

C	-0.034876900	1.347570100	-3.572277900
C	-0.023146500	-1.040495800	-3.770461100
C	-0.069131900	0.203542700	-4.354401300
H	-0.108734200	2.309790100	-4.039221200
H	-0.149419200	0.289233100	-5.421107400
C	2.421985900	-1.069919100	-0.622535400
C	2.672733000	-2.220646900	0.096919100
C	3.120421500	-0.859040400	-1.831286000
C	3.617758600	-3.156304200	-0.371920800
H	2.133661800	-2.433923000	0.994064400
C	4.024521600	-1.771557300	-2.282121600
H	2.898630300	0.016449000	-2.407340500
C	4.284725800	-2.937842300	-1.540880000
H	3.793888300	-4.049425900	0.195022000
H	4.996048900	-3.651305900	-1.906673500
H	-0.990961400	-3.014731100	3.454905100
H	-0.081697800	-1.921029300	-4.378857000
H	-3.884900000	-2.557283500	0.400868000
H	5.147833800	2.764065600	0.563434000
H	4.531926500	-1.606980800	-3.211597400
C	0.713148400	-1.177081500	2.726001800
H	0.391625800	-0.427317500	3.444620500
H	1.157533800	-1.997112800	3.282444000
H	1.487282500	-0.719125000	2.133192200
C	-2.732805500	-0.689491100	-1.036355400
H	-2.403108200	-1.110850800	-1.978251100
H	-3.813775300	-0.766421200	-1.000157300
H	-2.469006100	0.359911000	-1.034998700
C	-0.036328300	2.555604900	-1.416336300
H	0.947248100	2.930228600	-1.162110100
H	-0.544118500	3.306267100	-2.010138100
H	-0.581086100	2.380829800	-0.506058700
C	0.179295000	-2.597002600	-1.871783100
H	1.098887000	-3.064324800	-2.202044400
H	0.120849000	-2.641991700	-0.803522400
H	-0.655446900	-3.159123700	-2.276757100

### S<sub>1</sub>S<sub>0</sub>-cyc (C2)

C	0.053415500	-0.084164100	-0.022443300
C	1.500732400	-0.052811700	0.036337000
C	-0.606900300	-0.156111500	-1.331988500
C	-2.039178200	-0.334080000	-1.474267500
C	0.166467800	-0.086250800	-2.550328400
C	-2.636029200	-0.229327100	-2.715457100
C	-0.497019100	0.025085300	-3.774427000
C	-1.873636300	0.001720400	-3.855926000
H	-2.364828200	0.109956700	-4.816458300
C	2.223189300	-0.883222100	1.010071900
C	2.178439100	-2.273254100	0.784630000

C	3.216914900	-0.416435700	1.881927300
C	3.004178300	-3.147311300	1.459604900
H	1.483864000	-2.654609100	0.044169800
C	4.065347900	-1.304528700	2.535856000
H	3.359727000	0.644296100	2.021070000
C	3.959841600	-2.674125300	2.353989600
H	2.917334400	-4.209604600	1.266493900
H	4.620963900	-3.358333000	2.864263700
C	-0.915097700	0.136981600	1.142271400
C	-1.064836700	-0.836493800	2.155621900
C	-1.590070000	1.367704300	1.252246300
C	-1.828790400	-0.522369400	3.288516600
C	-2.316899800	1.651474200	2.411447600
C	-2.428527700	0.716132700	3.429599400
H	-1.927631600	-1.263584700	4.072310100
H	-2.993998600	0.951170700	4.320540400
C	1.351813200	1.424621900	0.550159800
C	1.596477400	2.405814900	-0.420310600
C	1.275706900	1.833090000	1.891675200
C	1.790834600	3.733546500	-0.068391400
H	1.671443300	2.125106700	-1.463252500
C	1.467846300	3.146964700	2.257854100
H	1.068716800	1.079649800	2.629447800
C	1.722897800	4.099076000	1.272038600
H	1.995372800	4.486513000	-0.821272900
H	1.867194500	5.132582000	1.553813700
H	0.099075900	0.107637000	-4.669381300
H	-3.706926500	-0.347422800	-2.808054200
H	-2.797408600	2.615078100	2.493949500
H	1.419660400	3.433071800	3.297704500
H	4.830129800	-0.910576300	3.194378400
C	-2.987560700	-0.749054500	-0.376662000
H	-2.514366700	-1.440940200	0.302359500
H	-3.328740400	0.116910400	0.174744700
H	-3.848784700	-1.247281300	-0.818657900
C	1.670118400	-0.139919700	-2.657117400
H	1.975727000	-0.165693700	-1.580048800
H	1.909029000	-1.053815200	-3.204670300
H	2.013751700	0.728262000	-3.233260200
C	-0.508221500	-2.234466000	2.061638400
H	-0.564287300	-2.625887100	1.045755600
H	0.529289800	-2.241579300	2.365758900
H	-1.071431300	-2.913904500	2.702662100
C	-1.523397500	2.437465000	0.197595400
H	-2.536680900	2.744039000	-0.059604200
H	-0.977931400	3.290046000	0.593258800
H	-1.027875800	2.115377100	-0.707120800

## OM2/MRCI method

TPE-4mM

S<sub>0</sub>

C	0.663026700	-0.009855100	-0.022002100
C	-0.694077600	-0.023025800	-0.017180300
C	1.474862300	-1.248428200	0.034644800
C	2.557623200	-1.404830700	-0.823152900
C	1.163434200	-2.234603300	0.980416000
C	3.336039200	-2.572306500	-0.754984100
H	2.809331000	-0.621717000	-1.545187200
C	1.946607100	-3.392897300	1.041777200
H	0.304551000	-2.115041900	1.644142900
C	3.019837700	-3.561558100	0.186434100
H	3.631612600	-4.471871800	0.243093000
C	-1.480900400	-1.267479800	-0.087693200
C	-1.204247500	-2.230444500	-1.067074700
C	-2.553617000	-1.456350100	0.810527900
C	-1.967940800	-3.370623400	-1.123232800
H	-0.375825700	-2.074701300	-1.761273800
C	-3.303342100	-2.606336400	0.752170600
H	-2.780519200	-0.673432700	1.542335400
C	-3.016011700	-3.577149900	-0.213034700
H	-1.756840300	-4.139042600	-1.878844600
H	-3.608639400	-4.497649100	-0.260842400
C	1.452022800	1.237281200	-0.073103100
C	1.153580400	2.222483100	-1.024536500
C	2.535253800	1.411491800	0.814566100
C	1.921539200	3.384000000	-1.075201800
H	0.309816800	2.086993100	-1.704945800
C	3.295058900	2.585794200	0.760550100
H	2.779593400	0.624974900	1.535501700
C	2.989876100	3.573303400	-0.185402900
H	1.690652600	4.158822000	-1.816533100
H	3.586957900	4.489915400	-0.236023900
C	-1.498623700	1.218948500	0.070960000
C	-1.230414700	2.146730300	1.085958800
C	-2.525738200	1.450785700	-0.843639200
C	-1.997833700	3.311312900	1.173945200
H	-0.416212200	1.967295300	1.792781800
C	-3.286848300	2.626983000	-0.751612400
H	-2.739551100	0.719633800	-1.630356700
C	-3.017203600	3.554182800	0.263840600
H	-1.792570200	4.033955300	1.973598700
H	-3.615355700	4.469439000	0.336806400
C	-4.458210100	-2.818307600	1.693261500
H	-5.395080800	-2.593373500	1.164416800
H	-4.474792400	-3.860838000	2.044583000
H	-4.369945300	-2.154299200	2.566974500

C	4.455390600	2.771787200	1.685796900
H	5.372416500	2.421608900	1.186386300
H	4.570463400	3.835365000	1.946248200
H	4.308126000	2.194297600	2.611058900
C	-4.403193000	2.876216900	-1.713511300
H	-5.335284800	2.465674500	-1.293766600
H	-4.532857400	3.956776500	-1.882089600
H	-4.200410600	2.387074000	-2.678290500
H	1.700895600	-4.170428000	1.775505700
C	4.516986200	-2.741065300	-1.653670200
H	5.419148500	-2.364074200	-1.142755300
H	4.664106200	-3.805009600	-1.899540100
H	4.376600300	-2.175025800	-2.587894800

S<sub>1</sub>

C	0.710263000	-0.003706300	-0.006674800
C	-0.715274100	-0.009451900	-0.002406500
C	1.442218900	-1.185272500	0.393712100
C	2.707545200	-1.460272000	-0.188604300
C	0.863464400	-2.122123200	1.272250400
C	3.364619700	-2.657033800	0.107195200
H	3.143878800	-0.763255200	-0.910892200
C	1.547543000	-3.305345300	1.572884000
H	-0.110864300	-1.919514100	1.722849300
C	2.787471400	-3.572465900	0.998924900
H	3.319770000	-4.501914400	1.236103800
C	-1.444020800	-1.186392700	-0.406396400
C	-0.865529200	-2.119893200	-1.296127900
C	-2.710044000	-1.479300700	0.168744500
C	-1.536546500	-3.277758500	-1.605696700
H	0.111722800	-1.905057600	-1.735934600
C	-3.349690300	-2.646811300	-0.131237500
H	-3.145147600	-0.777294100	0.889007800
C	-2.776575500	-3.557650300	-1.036306000
H	-1.091966600	-3.998498600	-2.305991700
H	-3.309947100	-4.481244800	-1.284682100
C	1.436426200	1.182553600	-0.403354800
C	0.854939000	2.124455200	-1.274977400
C	2.700391300	1.464320700	0.180480900
C	1.535729600	3.306744100	-1.575954000
H	-0.120625900	1.921078000	-1.724002300
C	3.356415700	2.659629000	-0.117486100
H	3.140522200	0.762077300	0.895987400
C	2.778442600	3.576713900	-1.006156300
H	1.083974100	4.031231500	-2.265712800
H	3.309582200	4.504028100	-1.245596200
C	-1.444329200	1.173330500	0.414202800
C	-0.863563400	2.100762700	1.298121300
C	-2.706252700	1.464627200	-0.167460800

C	-1.543822600	3.283454200	1.613275500
H	0.109627400	1.890851400	1.748304300
C	-3.365026300	2.659506400	0.145841300
H	-3.146578700	0.776005800	-0.896606400
C	-2.787118700	3.562788500	1.047140200
H	-1.088421700	4.000123000	2.309139200
H	-3.314973000	4.488693400	1.296681100
C	-4.681558500	-2.987047200	0.484980900
H	-5.441478400	-3.042905900	-0.305208900
H	-4.610709700	-3.954908100	0.998443800
H	-4.981677400	-2.221262100	1.216350100
C	4.681142600	2.977552700	0.502703800
H	5.446104900	3.034624000	-0.286357800
H	4.624930000	3.947012800	1.020895800
H	4.974718900	2.204226400	1.229068300
C	-4.688018800	2.979424400	-0.473523700
H	-5.455046400	3.034958900	0.314766700
H	-4.633230000	3.951442800	-0.988336800
H	-4.981515300	2.208949100	-1.203517800
H	1.096967600	-4.028978400	2.262591600
C	4.686830900	-2.974901300	-0.515395200
H	5.458557400	-3.033061200	0.269119800
H	4.631205700	-3.945071400	-1.034670900
H	4.977863600	-2.201404800	-1.243584800

### S<sub>1</sub>S<sub>0</sub>-cyc (C4C5)

C	-0.693857200	-0.136230400	0.334750300
C	0.685333800	-0.057890100	0.013165700
C	-1.384137000	-1.320584100	-0.007645200
C	-2.805578600	-1.355156400	0.024331400
C	-0.657149000	-2.575146100	-0.268814600
C	-3.441373100	-2.574775600	0.155574600
H	-3.370806900	-0.434613100	-0.000135300
C	-1.438114500	-3.761386300	-0.307148500
H	-0.034963500	-2.522475000	-1.165742000
C	-2.759704300	-3.818265100	0.060996800
H	-3.282446200	-4.746836800	0.236409700
C	1.466105500	-1.204405100	0.088623100
C	0.814434400	-2.301630700	0.794283200
C	2.759993700	-1.370200800	-0.493865100
C	1.533528400	-3.550337000	0.840412700
H	0.175634200	-1.984344900	1.706317200
C	3.427410800	-2.553783000	-0.380126300
H	3.180945400	-0.531077300	-1.071746400
C	2.795001000	-3.624074200	0.336858300
H	1.085336000	-4.388999900	1.364178200
H	3.385670300	-4.551262600	0.487522200
C	-1.444275900	1.103298300	0.608975700
C	-1.454980800	1.604242500	1.921097900



C	-2.151348100	1.792263300	-0.392943300
C	-2.148945100	2.774465200	2.221382600
H	-0.898796800	1.072439100	2.700101600
C	-2.856489400	2.961104600	-0.087328600
H	-2.156836400	1.407956600	-1.422971400
C	-2.851907800	3.455585100	1.223773600
H	-2.145133800	3.169465400	3.245775200
H	-3.394282200	4.377765000	1.463980100
C	1.326734800	1.212270200	-0.418491100
C	0.857340000	1.905101100	-1.541982200
C	2.404950400	1.705682000	0.329399100
C	1.489008900	3.083266800	-1.929542600
H	0.017995700	1.506309000	-2.119517900
C	3.014792000	2.904880800	-0.049665100
H	2.747924200	1.160067500	1.213689700
C	2.558025700	3.592540500	-1.184928800
H	1.139181700	3.622872200	-2.817143600
H	3.035826200	4.532497100	-1.483124600
C	4.803301200	-2.759107300	-0.919479500
H	5.034916700	-1.991533000	-1.678606300
H	5.551189400	-2.685288800	-0.105457600
H	4.891074400	-3.756311000	-1.390336600
C	-3.641139000	3.671134000	-1.147246700
H	-4.662381100	3.260657400	-1.173392300
H	-3.693134100	4.749309800	-0.931326400
H	-3.170929800	3.530225700	-2.132858400
C	4.144067200	3.457000200	0.762095100
H	4.812061200	2.645789300	1.087086400
H	4.727390800	4.181576700	0.172996400
H	3.732141400	3.963713200	1.647358200
H	-0.919034200	-4.689190900	-0.625097500
C	-4.919709500	-2.612625500	0.390565300
H	-5.393584000	-3.150264400	-0.439334700
H	-5.115631600	-3.149588300	1.326389900
H	-5.339942800	-1.601601300	0.457102800

### S<sub>1</sub>S<sub>0</sub>-cyc (C8C9)

C	-0.779093900	0.005198700	0.516692500
C	0.644372900	-0.036477300	0.318985700
C	-1.491491900	-1.114684700	-0.159745000
C	-2.159405400	-2.055360000	0.643942900
C	-1.535605900	-1.253750100	-1.557730600
C	-2.847303800	-3.122770500	0.059848000
H	-2.133664000	-1.936231900	1.733303000
C	-2.212516800	-2.323676500	-2.139231700
H	-1.023237500	-0.523374500	-2.195384800
C	-2.869697800	-3.259952400	-1.334778400
H	-3.398539000	-4.103018500	-1.794934500
C	1.361458700	-1.288302700	0.612138300

C	0.964789100	-2.042872100	1.724538200
C	2.427716600	-1.703903700	-0.198688400
C	1.659809800	-3.208389800	2.037268800
H	0.123908600	-1.695873100	2.328702400
C	3.099194500	-2.891538600	0.107356900
H	2.709230900	-1.108517200	-1.072623700
C	2.717049200	-3.636183100	1.231568700
H	1.365303800	-3.804025200	2.907828100
H	3.249448500	-4.564518700	1.475076600
C	-1.371457000	1.288549300	0.323851100
C	-0.630851800	2.515209900	0.633408900
C	-2.710597300	1.437207700	-0.161255300
C	-1.316181000	3.758586400	0.512751100
H	0.022797300	2.463162400	1.504608800
C	-3.272275700	2.682102700	-0.332583900
H	-3.301982500	0.538145400	-0.304481600
C	-2.546986700	3.882099700	-0.079413100
H	-0.780298900	4.665295800	0.849353300
H	-3.001329400	4.845974000	-0.283232100
C	1.347468300	1.070094400	-0.147607500
C	0.546196300	2.182749900	-0.678942600
C	2.695709700	1.325169600	0.266024900
C	1.226870700	3.447304800	-0.891677900
H	-0.169592100	1.891306300	-1.533237100
C	3.299347000	2.526510700	0.036626500
H	3.222151000	0.526962800	0.814546300
C	2.546803700	3.568178300	-0.598196900
H	0.675535600	4.257808200	-1.363440800
H	3.079362200	4.502966100	-0.857563200
C	4.215221700	-3.365316300	-0.769305600
H	3.801364200	-3.703614300	-1.730339500
H	4.926461600	-2.545246200	-0.947604700
H	4.752442900	-4.203845100	-0.298546600
C	-4.695619700	2.804896900	-0.781276100
H	-5.324200800	2.892499800	0.114277900
H	-4.825991000	3.700926600	-1.401900200
H	-5.002033700	1.920236200	-1.352464100
C	4.716998400	2.785385600	0.428813700
H	5.160387400	3.571518100	-0.208775100
H	4.762116500	3.118904900	1.483828800
H	5.319917600	1.865796000	0.324995800
H	-2.231392200	-2.438995300	-3.230254000
C	-3.572754500	-4.121288700	0.909207200
H	-3.327705200	-5.143107700	0.583219000
H	-3.288048500	-4.008682400	1.966983900
H	-4.656904700	-3.958273400	0.813056100

S<sub>1</sub>S<sub>0</sub>-pyr(C1)

C	0.843698400	1.048168800	0.497833400
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C	-0.512720500	0.668988000	0.193706300
C	1.028308500	-0.383557300	1.002675000
C	1.787318800	-1.336995600	0.283008500
C	0.651428600	-0.665309300	2.321845600
C	2.225517300	-2.501432300	0.924170000
H	2.049333900	-1.147101900	-0.760417000
C	1.060078900	-1.850560100	2.938409900
H	0.046496900	0.055705000	2.885633500
C	1.862465300	-2.758107100	2.245458800
H	2.205968800	-3.673569100	2.742466900
C	-0.991915900	-0.388328000	-0.739361200
C	-0.551463400	-0.379022200	-2.068207900
C	-1.850285700	-1.402945600	-0.272326500
C	-1.003404900	-1.371937300	-2.941555400
H	0.129181100	0.397568100	-2.418071700
C	-2.305291300	-2.383922700	-1.161065000
H	-2.125073100	-1.450835700	0.786202800
C	-1.884970800	-2.361788300	-2.497090000
H	-0.651170600	-1.379606900	-3.977641900
H	-2.239419000	-3.131361700	-3.193264600
C	1.701550800	1.431593700	-0.636123600
C	1.160996300	2.264769100	-1.634226900
C	3.088818500	1.239034700	-0.606839300
C	1.988086000	2.867406000	-2.577519000
H	0.089936600	2.497395800	-1.632605600
C	3.912404500	1.860591800	-1.545305100
H	3.526760100	0.619048100	0.180716000
C	3.358587200	2.659238300	-2.551912000
H	1.548870100	3.517572700	-3.347588400
H	4.005189700	3.127011800	-3.302281700
C	-1.537640300	1.293474200	1.039052300
C	-1.060818500	2.168585500	2.027833300
C	-2.914854600	1.162628000	0.807347000
C	-1.966897200	2.877693600	2.811147500
H	0.024792600	2.268297700	2.109474700
C	-3.808589900	1.898496200	1.582436800
H	-3.285265000	0.532216500	-0.007914600
C	-3.330763400	2.742033100	2.594872100
H	-1.601678600	3.555083000	3.587953700
H	-4.045228600	3.311830800	3.202140400
C	-3.246848300	-3.445653500	-0.687073900
H	-4.106637800	-3.515895200	-1.371530900
H	-2.722427500	-4.411974600	-0.661288900
H	-3.615557900	-3.213601000	0.324719600
C	5.399215200	1.700704800	-1.473720100
H	5.810124800	1.490328700	-2.474473000
H	5.842159400	2.636178300	-1.094278100
H	5.670841100	0.878323400	-0.793538200
C	-5.281853400	1.815495300	1.328591000
H	-5.808791000	1.574735500	2.263854200

H	-5.639225300	2.785891100	0.952123900
H	-5.505992600	1.038905600	0.581555900
H	0.758075100	-2.062759600	3.969142500
C	3.094982600	-3.479578500	0.191106000
H	4.115026800	-3.423941300	0.599472800
H	2.707549700	-4.501413100	0.317841800
H	3.126734600	-3.242709600	-0.883286000

S<sub>1</sub>S<sub>0</sub>-pyr (C2)

C	0.545437500	-0.641106200	0.194852900
C	-0.811530600	-1.054738200	0.446480200
C	1.550278900	-1.276848800	1.055285500
C	2.931466300	-1.126832200	0.866248900
C	1.054843100	-2.182269200	2.007798900
C	3.808629100	-1.881975100	1.641693700
H	3.320229200	-0.466054700	0.083645400
C	1.944955700	-2.905278200	2.796558000
H	-0.032194400	-2.291134900	2.059022300
C	3.312689500	-2.758976600	2.616396800
H	4.015206800	-3.343745500	3.222878200
C	-1.639253400	-1.422281600	-0.713896200
C	-1.068560600	-2.216597300	-1.726896600
C	-3.030145400	-1.254218800	-0.702990800
C	-1.869316800	-2.807004400	-2.700422200
H	0.006557400	-2.427838700	-1.716606100
C	-3.826394100	-1.854888300	-1.677697500
H	-3.492104500	-0.667230800	0.096171400
C	-3.243183000	-2.618943500	-2.694734300
H	-1.406807600	-3.429914200	-3.479984200
H	-3.870039500	-3.075652800	-3.468581000
C	1.040107500	0.451033500	-0.691471900
C	0.630047200	0.476324300	-2.030449400
C	1.881600400	1.458707700	-0.179479300
C	1.097991400	1.492620800	-2.867740600
H	-0.042327200	-0.291241000	-2.415277100
C	2.356983000	2.460411700	-1.033709700
H	2.130225500	1.483128800	0.886619400
C	1.969228200	2.470020700	-2.379911400
H	0.761998600	1.533359700	-3.908313600
H	2.337017000	3.259434700	-3.045396600
C	-1.030215300	0.356065400	0.991877200
C	-0.681128800	0.612145500	2.324654900
C	-1.793039900	1.313751800	0.281635500
C	-1.119658000	1.775696600	2.961332800
H	-0.071590500	-0.110275100	2.882504500
C	-2.258455300	2.456065900	0.941688900
H	-2.035979500	1.143278200	-0.769547900
C	-1.921525000	2.688565000	2.274274100
H	-0.835531800	1.969699300	4.001093300

H	-2.283144200	3.589853300	2.784494700
C	-5.315205200	-1.699485200	-1.642832000
H	-5.690805400	-1.414211400	-2.639304400
H	-5.771770300	-2.658533600	-1.348064100
H	-5.610232000	-0.927277600	-0.914929500
C	3.288504400	3.514102400	-0.523199200
H	4.241293300	3.463438100	-1.073669800
H	2.837419000	4.506480200	-0.669848000
H	3.489704200	3.370934000	0.549652300
C	-3.124892400	3.440579500	0.214766100
H	-4.159770700	3.333916500	0.571251400
H	-2.776922200	4.465932200	0.407531200
H	-3.097613700	3.254470900	-0.869086800
H	1.562888000	-3.601882400	3.547468700
C	5.286154000	-1.785555500	1.420664400
H	5.786083200	-1.496253400	2.356835800
H	5.668207800	-2.764112500	1.092824400
H	5.517460600	-1.037226300	0.647236500

#### S<sub>0</sub>-final (C4C5)

C	-0.711838700	0.189210300	-0.099988200
C	0.717193500	0.187825700	0.107229600
C	-1.416128500	1.368412600	-0.094299300
C	-2.839117600	1.373299800	-0.313201500
C	-0.721605300	2.657700500	0.247595000
C	-3.509712300	2.540025300	-0.521633100
H	-3.360498700	0.410192900	-0.354364600
C	-1.469150900	3.843845800	-0.280739200
H	-0.726126100	2.743843600	1.387222900
C	-2.777423200	3.794285300	-0.585186400
H	-3.323500400	4.682297400	-0.928333200
C	1.424393700	1.365075900	0.098331700
C	0.731977700	2.657636600	-0.236413900
C	2.849485800	1.365796500	0.305554200
C	1.483603500	3.838126900	0.299904000
H	0.743675600	2.751619000	-1.375381300
C	3.524621000	2.530790800	0.511948800
H	3.369229600	0.401385100	0.335047300
C	2.794596100	3.785529200	0.592631800
H	0.931410000	4.783682600	0.400104500
H	3.343034000	4.669172400	0.942917900
C	-1.390452700	-1.108544800	-0.314963600
C	-1.439812500	-1.663383000	-1.600629400
C	-1.974738600	-1.781696900	0.767960800
C	-2.081698200	-2.883442600	-1.800846900
H	-0.981680900	-1.132128200	-2.439894900
C	-2.614427700	-3.006997500	0.561054800
H	-1.919585700	-1.347249600	1.771798900
C	-2.664758500	-3.559340800	-0.726430100

H	-2.133594300	-3.316481100	-2.807237400
H	-3.157681800	-4.524756100	-0.888644500
C	1.392814000	-1.111719600	0.320870100
C	1.456615300	-1.658837300	1.609271900
C	1.961145600	-1.793285900	-0.765066300
C	2.098831700	-2.878747300	1.809317500
H	1.014591000	-1.118697100	2.451530800
C	2.600116000	-3.019239600	-0.558433000
H	1.896619000	-1.364013100	-1.770492800
C	2.666193100	-3.563097500	0.731800800
H	2.164685900	-3.304272900	2.818065600
H	3.158296800	-4.529099600	0.893697200
C	5.000395800	2.571247700	0.725390200
H	5.429912400	1.558397000	0.683986100
H	5.467922200	3.190882600	-0.057414700
H	5.222848300	3.014473400	1.710229000
C	-3.258202600	-3.731596000	1.702420600
H	-4.350224500	-3.617715400	1.631841700
H	-3.000963500	-4.800224700	1.663476500
H	-2.916396500	-3.319323300	2.664113400
C	3.188679400	-3.771515900	-1.711582600
H	3.384422800	-3.093087200	-2.555921100
H	4.134107800	-4.249332900	-1.413964700
H	2.475731600	-4.545579000	-2.030928100
H	-0.916120200	4.790153200	-0.367581600
C	-4.982790800	2.583344900	-0.752499300
H	-5.459164200	3.199318500	0.027864600
H	-5.192605300	3.032103100	-1.737591200
H	-5.413757700	1.570718700	-0.721746400

### S<sub>0</sub>-final (C8C9)

C	0.708498800	0.196441000	0.119279700
C	-0.718139200	0.192465700	-0.107033400
C	1.385876500	-1.100982100	0.339128600
C	1.923975000	-1.803212600	-0.750061600
C	1.475841000	-1.630548100	1.633164100
C	2.553069900	-3.033516700	-0.541547900
H	1.836564000	-1.388608200	-1.759924200
C	2.118840900	-2.849443700	1.837142200
H	1.049415200	-1.079239000	2.476182100
C	2.655186200	-3.554159400	0.756071300
H	3.144726500	-4.521052800	0.919976300
C	-1.387036300	-1.108353500	-0.332550600
C	-1.482700200	-1.628769300	-1.630088400
C	-1.913893200	-1.821433000	0.754767600
C	-2.113438200	-2.853216400	-1.838069900
H	-1.074197100	-1.063697300	-2.472902100
C	-2.538139900	-3.053647100	0.540963000
H	-1.820903600	-1.414783900	1.767219300

C	-2.636499100	-3.569965800	-0.758436000
H	-2.199913600	-3.260573000	-2.852746600
H	-3.122622800	-4.537912400	-0.927221900
C	1.409078600	1.378069400	0.115933200
C	0.707688500	2.657383600	-0.252462100
C	2.828514800	1.388216200	0.352383600
C	1.472052100	3.865154600	0.193469100
H	0.678157500	2.704535900	-1.395159600
C	3.501449000	2.560076600	0.520376700
H	3.344845700	0.425087100	0.440845000
C	2.782484100	3.822538800	0.490343600
H	0.938019600	4.826362900	0.197209700
H	3.338586300	4.728410900	0.764748200
C	-1.425094400	1.370274200	-0.102375600
C	-0.731585800	2.652197000	0.271665900
C	-2.842970100	1.373634700	-0.349652100
C	-1.500582800	3.857549300	-0.173568900
H	-0.705503100	2.696920600	1.414264100
C	-3.519356600	2.542284800	-0.527191900
H	-3.354028400	0.407926300	-0.440697900
C	-2.806321700	3.808155000	-0.491301800
H	-0.971488700	4.821564800	-0.170211400
H	-3.363893600	4.711466800	-0.770951500
C	-3.087678900	-3.835052000	1.693908200
H	-3.285435300	-3.172317200	2.550136500
H	-4.026444600	-4.332400700	1.406866200
H	-2.351504500	-4.595824600	1.991972000
C	4.972101500	2.606149600	0.765609800
H	5.462415100	3.177597500	-0.039762400
H	5.174669900	3.103914100	1.728562700
H	5.396986900	1.590626300	0.792644700
C	-4.987665500	2.581256400	-0.787582300
H	-5.407644300	1.563791400	-0.817177500
H	-5.488834600	3.151845600	0.011701600
H	-5.182514100	3.076480300	-1.753433700
H	2.211431200	-3.257971200	2.850843600
C	3.149069400	-3.788032900	-1.689287200
H	4.245561600	-3.711070000	-1.642534500
H	2.856510300	-4.847022600	-1.636557100
H	2.802161800	-3.372190800	-2.647767600

TPE-4oM

S<sub>0</sub>

C	0.007558900	-0.469648400	0.008598000
C	0.015936100	0.893327200	0.006885000
C	1.255799200	-1.267159500	-0.039461200

C	1.561293100	-2.193626200	0.979229400
C	2.130314900	-1.138682400	-1.139485100
C	2.706422200	-2.996548900	0.874968900
C	3.269683200	-1.955666800	-1.224443500
C	3.549416800	-2.885487300	-0.228710700
H	4.437210700	-3.524774200	-0.307533100
C	1.244109000	1.693666200	0.163155200
C	2.243581500	1.302418000	1.066689800
C	1.402377900	2.883729700	-0.563758600
C	3.372871100	2.083198100	1.229986400
H	2.134144900	0.370407600	1.629349400
C	2.540748600	3.649638600	-0.399625300
H	0.620720500	3.198550000	-1.262721300
C	3.533618700	3.258958800	0.498408300
H	4.150184900	1.778992200	1.942068700
H	4.430101600	3.872280300	0.628810100
C	-1.257195600	-1.242683300	0.053404500
C	-2.136191300	-1.096163500	1.147489700
C	-1.570455900	-2.168712400	-0.962535400
C	-3.290520400	-1.892113300	1.226341400
C	-2.727787300	-2.953744200	-0.860944500
C	-3.578666700	-2.821742700	0.234271100
H	-3.968850900	-1.776414500	2.079920900
H	-4.477656500	-3.445958200	0.310097400
C	-1.224287200	1.682900300	-0.165503400
C	-2.134851400	1.340622700	-1.175640500
C	-1.464504500	2.794917600	0.649527700
C	-3.282837200	2.107320300	-1.353632100
H	-1.951392100	0.467930400	-1.808533300
C	-2.622500100	3.545533000	0.471478500
H	-0.743478300	3.067851300	1.425361900
C	-3.529037900	3.203822700	-0.533113100
H	-3.995796200	1.843040000	-2.141918800
H	-4.436412100	3.802950100	-0.675339500
H	3.942676500	-1.858052000	-2.083596300
H	-2.962680100	-3.679908400	-1.648010900
H	2.935394300	-3.719698700	1.666135800
H	2.666879800	4.574823300	-0.976506400
H	-2.820913100	4.408953900	1.115674100
C	1.921950100	-0.128772800	-2.222320400
H	2.512422900	0.767050500	-1.982005200
H	2.262179500	-0.534261200	-3.189593000
H	0.863127600	0.155574900	-2.306831600
C	0.700733100	-2.326903300	2.193324200
H	-0.274978200	-2.741365100	1.911356800
H	1.175509700	-2.994195000	2.932190200
H	0.556036600	-1.336695400	2.656674400
C	-1.912737000	-0.097444200	2.238255400
H	-2.458890900	0.822977300	1.989146900
H	-2.289892300	-0.492962500	3.196437300



H	-0.844793800	0.141869000	2.347955200
C	-0.707961000	-2.321765200	-2.174576300
H	-0.552027900	-1.336785800	-2.644272400
H	0.263153500	-2.744402200	-1.890374800
H	-1.188369700	-2.987390500	-2.911684700

S<sub>1</sub>

C	0.001699700	-0.473352100	0.003663400
C	0.010016200	0.949911200	0.002604500
C	1.183308200	-1.200267700	-0.422041900
C	1.638697500	-2.302173400	0.358228300
C	1.973170900	-0.783310700	-1.521432800
C	2.850783700	-2.924245100	0.039208100
C	3.178816200	-1.436603100	-1.820713400
C	3.620380300	-2.498268400	-1.040561700
H	4.568810200	-2.999097700	-1.271570200
C	1.119998400	1.667619300	0.595813700
C	1.928122500	1.025314300	1.557324600
C	1.481019600	2.963169500	0.167738200
C	3.034987700	1.668561800	2.078308200
H	1.667179500	0.013393100	1.887685800
C	2.602607200	3.575631200	0.675328000
H	0.898530600	3.457766100	-0.619737700
C	3.379504200	2.942144000	1.649657400
H	3.654045600	1.160741500	2.828034000
H	4.258174500	3.448003000	2.062155500
C	-1.182350500	-1.197927400	0.423370800
C	-1.974276900	-0.783198400	1.522780600
C	-1.641299700	-2.296863200	-0.357411700
C	-3.179022500	-1.435592200	1.821806200
C	-2.850052500	-2.922556100	-0.037281900
C	-3.621157200	-2.497488300	1.041819300
H	-3.776508600	-1.098662300	2.678705000
H	-4.569067600	-2.999206600	1.271731400
C	-1.099345500	1.672376700	-0.603990400
C	-1.909798500	1.024002800	-1.561960300
C	-1.470925200	2.961050900	-0.160421000
C	-3.042938700	1.670650500	-2.087667500
H	-1.657353200	0.010765300	-1.891130500
C	-2.613511600	3.583055700	-0.682708900
H	-0.910586000	3.452008000	0.642598400
C	-3.390085100	2.948460700	-1.657138100
H	-3.659234600	1.155894700	-2.834567100
H	-4.273067700	3.451089900	-2.066519000
H	3.775073000	-1.098337500	-2.676771500
H	-3.199359200	-3.757159100	-0.659437500
H	3.203144200	-3.755884900	0.662527000
H	2.898015200	4.568423900	0.311131500
H	-2.903546000	4.575228700	-0.312800400

C	1.515808900	0.303612100	-2.435752300
H	1.651076400	1.275138100	-1.941849100
H	2.099608800	0.291593700	-3.371950100
H	0.449343300	0.174755400	-2.685960400
C	0.917574800	-2.782805300	1.576374900
H	0.030452000	-3.362744700	1.285817500
H	1.583168600	-3.427033000	2.178964300
H	0.593309800	-1.933173900	2.198899900
C	-1.517061700	0.306880900	2.433961300
H	-1.649691900	1.277469800	1.934630000
H	-2.102280200	0.300208400	3.369325000
H	-0.452370700	0.176866100	2.684004500
C	-0.916822500	-2.781546500	-1.573031900
H	-0.590244800	-1.934279600	-2.197066200
H	-0.032034400	-3.360125100	-1.276755700
H	-1.581939800	-3.426301200	-2.175454200

S<sub>1</sub>S<sub>0</sub>-cyc (C4C5)

C	0.102572700	-0.712883700	0.450552300
C	-0.087461500	0.698513800	0.244871100
C	-1.074016900	-1.404003600	0.872309000
C	-1.465822200	-2.731065600	0.451091200
C	-1.998755100	-0.714550100	1.800654300
C	-2.714689800	-3.222496100	0.771866400
C	-3.193238000	-1.398999600	2.195213500
C	-3.666088100	-2.505760300	1.530230900
H	-4.659808900	-2.905762900	1.691090800
C	-1.320638700	1.340044800	0.357636900
C	-2.499821900	0.480240700	0.535688600
C	-1.397065700	2.708218800	0.766184200
C	-3.695032200	1.112375500	1.056556000
H	-2.703003600	-0.254007000	-0.336386800
C	-2.553848600	3.271606900	1.200466000
H	-0.461926500	3.298052600	0.747061700
C	-3.716520000	2.444890500	1.299675600
H	-4.598282200	0.512489300	1.147877400
H	-4.670708800	2.930371700	1.580680200
C	0.917934700	-1.280915200	-0.658844900
C	0.546129000	-1.223288900	-2.024789200
C	2.151917100	-1.889107600	-0.321046500
C	1.395717000	-1.733423500	-3.011229100
C	2.987037100	-2.401131600	-1.318715500
C	2.617354800	-2.315404800	-2.662674900
H	1.109505900	-1.669438100	-4.070326000
H	3.280982600	-2.706213100	-3.442289600
C	1.074535600	1.508371500	-0.178679300
C	2.308932000	1.314713800	0.449926500
C	0.926895200	2.464214100	-1.189635800
C	3.399583100	2.097691700	0.066234000

H	2.400545300	0.560455800	1.232371700
C	2.032830200	3.221023300	-1.581978700
H	-0.039876800	2.588439900	-1.684918600
C	3.259344900	3.043599400	-0.945475900
H	4.367624700	1.959724100	0.556514000
H	4.122110600	3.649620700	-1.249010000
H	-3.796506600	-0.946161900	3.005217000
H	3.941071100	-2.870655000	-1.046982600
H	-2.995423100	-4.237516300	0.427625200
H	-2.625660300	4.324261100	1.447939500
H	1.935211000	3.950918600	-2.390779800
C	-1.299481100	-0.010266000	2.940167200
H	-1.028549300	1.016954000	2.641373400
H	-1.960524600	0.047092600	3.822290700
H	-0.374858800	-0.549421400	3.209999800
C	-0.473022900	-3.692598600	-0.119264800
H	-0.899765100	-4.713344300	-0.155404000
H	-0.196817200	-3.386657300	-1.135381100
H	0.430557600	-3.713154800	0.506328700
C	-0.751220700	-0.611905600	-2.449295100
H	-0.682022800	0.487520800	-2.405865400
H	-0.999676200	-0.906993500	-3.482394000
H	-1.568440200	-0.944092300	-1.786793100
C	2.554072000	-2.039253900	1.112163800
H	3.566076300	-1.626005200	1.268015000
H	1.828184900	-1.516311500	1.746419000
H	2.566262700	-3.109755400	1.379030800

### S<sub>1</sub>S<sub>0</sub>-cyc (C8C9)

C	0.102835700	-0.712687100	0.450367300
C	-0.086667700	0.698774200	0.244943000
C	0.917856000	-1.281329400	-0.658924200
C	2.151905600	-1.889572900	-0.321124900
C	0.545457500	-1.224187000	-2.024871300
C	2.986699300	-2.402206000	-1.318666200
C	1.394847700	-1.735115400	-3.011137100
C	2.616615200	-2.317079700	-2.662636500
H	3.280120200	-2.708238400	-3.442247500
C	1.075001600	1.509288200	-0.178586200
C	2.309413800	1.315717400	0.450028300
C	0.927465300	2.465442000	-1.189012100
C	3.399890800	2.099311200	0.066840800
H	2.400726700	0.561030300	1.232118100
C	2.033230400	3.222848900	-1.580934300
H	-0.039683500	2.588885700	-1.684065100
C	3.259791100	3.045646400	-0.944316900
H	4.367889000	1.961444200	0.557308300
H	4.122151700	3.651920300	-1.247598300
C	-1.073807700	-1.403912600	0.872134500

C	-1.998412400	-0.714538500	1.800387800
C	-1.466282100	-2.730942100	0.450582300
C	-3.192512200	-1.398532200	2.194913400
C	-2.715111900	-3.222075700	0.771733700
C	-3.666161200	-2.505216400	1.529845200
H	-3.795439500	-0.945572700	3.004985200
H	-4.659976800	-2.904667100	1.691145700
C	-1.320303700	1.339531200	0.358392100
C	-2.499508800	0.479685300	0.535813200
C	-1.397015800	2.707822700	0.766911600
C	-3.694949800	1.111870200	1.056481300
H	-2.702512900	-0.254425500	-0.336086500
C	-2.554248600	3.270932200	1.200634900
H	-0.462365300	3.298430200	0.748179300
C	-3.716965700	2.444142900	1.299195300
H	-4.598006700	0.511781500	1.147668900
H	-4.671277900	2.929430300	1.579703400
H	1.107832700	-1.671628200	-4.069992600
H	-2.995342800	-4.237266700	0.427634800
H	3.940751900	-2.871627800	-1.047208900
H	1.935817200	3.952795900	-2.389673500
H	-2.626682600	4.323536600	1.448088400
C	-0.751680800	-0.612745600	-2.449738200
H	-0.682106500	0.486566900	-2.406128900
H	-0.999671200	-0.907798500	-3.482894400
H	-1.569342800	-0.944742000	-1.787818000
C	2.554081900	-2.039095100	1.112133200
H	1.828311700	-1.515656300	1.745813200
H	2.566050500	-3.109576000	1.379606500
H	3.566162200	-1.625847700	1.267442600
C	-1.298372000	-0.009984300	2.939336200
H	-1.027223800	1.017052600	2.640081300
H	-1.958726800	0.048007300	3.821905300
H	-0.373884300	-0.549456400	3.208654000
C	-0.473711800	-3.692862200	-0.119515900
H	-0.197222400	-3.387218600	-1.135348200
H	0.429624600	-3.713718200	0.506386300
H	-0.900941300	-4.713515200	-0.155706300

### S<sub>1</sub>S<sub>0</sub>-pyr(C1)

C	0.00792910	-0.00359750	0.00419210
C	1.44643430	-0.06133480	-0.03004980
C	-0.78335850	-1.09178590	0.59893800
C	-2.08087840	-1.38992030	0.11350360
C	-0.42805550	-1.62836450	1.86236110
C	-2.89963550	-2.30915540	0.77964100
C	-1.26703510	-2.54479700	2.51482490
C	-2.47782310	-2.92811840	1.95396570
H	-3.10968580	-3.67243640	2.44949830

C	2.14409640	1.16765460	0.42301390
C	1.40481700	1.99487870	1.26842380
C	3.50394970	1.45149720	0.17032250
C	2.01868260	3.08950890	1.86300770
H	0.35694660	1.74469280	1.43838830
C	4.10444570	2.54831800	0.76804630
H	4.09364540	0.80901810	-0.49488720
C	3.36602460	3.36892040	1.60616370
H	1.45157750	3.73179490	2.54597500
H	3.83871640	4.24328850	2.07254470
C	0.14715270	-0.00225700	-1.53095660
C	0.05542500	1.27212500	-2.15967360
C	0.07673950	-1.16664950	-2.34134810
C	-0.03518470	1.36316020	-3.56250840
C	-0.04651960	-1.04212700	-3.74189030
C	-0.08378990	0.21437920	-4.34283810
H	-0.10074170	2.35017460	-4.03415940
H	-0.17014020	0.29498670	-5.43591430
C	2.40175230	-1.07895730	-0.57543660
C	2.65387780	-2.26909230	0.12908010
C	3.07279260	-0.85145690	-1.78681720
C	3.57470180	-3.17560470	-0.35458860
H	2.11089280	-2.47923430	1.05178480
C	3.99343700	-1.76216420	-2.25768930
H	2.81828320	0.03252210	-2.38096030
C	4.26591360	-2.93029600	-1.53813200
H	3.76062120	-4.10649540	0.19539620
H	4.99691350	-3.64989760	-1.91241870
H	-0.95900080	-2.96517540	3.48269720
H	-0.11108220	-1.94471250	-4.35780970
H	-3.89722930	-2.53549740	0.37686010
H	5.15417750	2.77361670	0.56631940
H	4.51239960	-1.57905210	-3.20518460
C	0.76014730	-1.17091560	2.64690870
H	0.41274930	-0.43519060	3.39292960
H	1.23055600	-2.01626220	3.18328020
H	1.52107860	-0.67785160	2.02373260
C	-2.65085920	-0.70059150	-1.08516600
H	-2.28729580	-1.17383390	-2.00912670
H	-3.75553200	-0.76152100	-1.06743620
H	-2.35115930	0.35504720	-1.08103700
C	-0.03407030	2.53354420	-1.37173860
H	0.97658550	2.91418340	-1.14110080
H	-0.57493870	3.30400410	-1.95052980
H	-0.57120540	2.33287500	-0.43744800
C	0.14944450	-2.56037520	-1.81105970
H	1.09151050	-3.03091070	-2.14579350
H	0.09575520	-2.58472660	-0.71811220
H	-0.69418590	-3.14566010	-2.21537620

S<sub>1</sub>S<sub>0</sub>-pyr (C2)

C	0.035648300	-0.103713300	-0.014378100
C	1.481578100	-0.037595700	0.030341200
C	-0.617274200	-0.138371100	-1.329316800
C	-2.036390300	-0.327053900	-1.475806900
C	0.145797000	-0.069876100	-2.538827900
C	-2.635533200	-0.227545300	-2.725303300
C	-0.500884500	0.019546900	-3.778794500
C	-1.883528600	0.001709700	-3.877922500
H	-2.380522300	0.115410900	-4.849129800
C	2.197096800	-0.873455300	1.027593000
C	2.149702000	-2.259908100	0.780625100
C	3.211668500	-0.407774200	1.878424900
C	2.988870800	-3.141403700	1.449511700
H	1.444592700	-2.651566800	0.034528100
C	4.063563600	-1.292545700	2.531925600
H	3.362186200	0.667705100	2.012747100
C	3.946852500	-2.663879700	2.341428800
H	2.910790500	-4.221743300	1.259499200
H	4.617844000	-3.358399400	2.856905400
C	-0.910349800	0.098432200	1.140061800
C	-1.063823200	-0.859081200	2.167093500
C	-1.571625700	1.345773600	1.241142500
C	-1.827885400	-0.539145500	3.304846700
C	-2.307535400	1.646326200	2.404601000
C	-2.424855900	0.713243200	3.431034100
H	-1.930011400	-1.280382600	4.103536600
H	-3.000998000	0.957787800	4.331856900
C	1.383056200	1.434101800	0.511704200
C	1.627405000	2.422071600	-0.456896700
C	1.296689800	1.813544100	1.867651400
C	1.792866600	3.737487000	-0.077333000
H	1.700626500	2.137983100	-1.508960700
C	1.466984300	3.131338500	2.234538500
H	1.084777400	1.053405300	2.625379300
C	1.723787000	4.105277400	1.269503900
H	1.988092800	4.507507500	-0.835335700
H	1.871990300	5.149385500	1.562904500
H	0.103492200	0.091269600	-4.685680500
H	-3.720122700	-0.344028300	-2.817938300
H	-2.799386700	2.620588200	2.487781300
H	1.405924200	3.420236000	3.290570000
H	4.841277300	-0.902384200	3.203835500
C	-2.972853400	-0.746861700	-0.381633100
H	-2.484652700	-1.444718500	0.303261200
H	-3.316575100	0.130598100	0.171512000
H	-3.850188300	-1.252818200	-0.821787000
C	1.639463600	-0.128390200	-2.580252100
H	1.979178800	-0.158694300	-1.532545500

H	1.909900700	-1.034532500	-3.150210700
H	2.023088200	0.743362200	-3.141628100
C	-0.508453400	-2.239266800	2.063741700
H	-0.573487100	-2.617058600	1.028441400
H	0.540618200	-2.232392500	2.375513100
H	-1.074673400	-2.924716500	2.717158800
C	-1.507092400	2.416078700	0.199216500
H	-2.535674500	2.729398300	-0.055344500
H	-0.964275800	3.284001200	0.603151000
H	-1.008311900	2.087950000	-0.721879700

### S<sub>0</sub>-final (C4C5)

C	-0.056881500	-0.531583900	0.025639900
C	-0.040898700	0.914553700	-0.140537900
C	-1.245305300	-1.193403400	0.191837100
C	-1.336395500	-2.635840500	0.391524500
C	-2.539370100	-0.405332800	0.281578500
C	-2.531460500	-3.273197300	0.231962300
C	-3.729370100	-1.213663400	-0.163347800
C	-3.720048700	-2.557463000	-0.160437500
H	-4.597070900	-3.143666800	-0.461000000
C	-1.192238700	1.619901000	-0.362667700
C	-2.481893500	0.881354200	-0.568904800
C	-1.168744600	3.055734700	-0.513735300
C	-3.668284500	1.764886500	-0.344708500
H	-2.512832000	0.571504800	-1.670270700
C	-2.318938300	3.769585500	-0.561932700
H	-0.193878000	3.554515400	-0.563191700
C	-3.592410300	3.106536600	-0.388452600
H	-4.640776100	1.277886300	-0.181806800
H	-4.478734400	3.738377700	-0.254623000
C	1.267296600	-1.180092000	-0.095155100
C	1.684087600	-1.652292700	-1.357775700
C	2.137045800	-1.280247000	1.008738800
C	2.944301500	-2.241453700	-1.499757100
C	3.396152400	-1.870093400	0.847875900
C	3.797947700	-2.345315000	-0.400429100
H	3.261489300	-2.627979300	-2.475358500
H	4.789116700	-2.798614700	-0.520087000
C	1.255112400	1.624343000	-0.021464800
C	1.528482200	2.366988000	1.140626800
C	2.198285000	1.577611000	-1.059656900
C	2.733039400	3.055393000	1.257850700
H	0.783572400	2.412291800	1.941238500
C	3.400240000	2.268771800	-0.932770700
H	1.992562300	0.985590700	-1.955190600
C	3.672807400	3.004708800	0.224742400
H	2.942231700	3.647989000	2.155529700
H	4.623645600	3.540099700	0.322841000

H	-4.640472200	-0.670128500	-0.447964800
H	4.075307800	-1.948291800	1.704623900
H	-2.615581200	-4.357976400	0.375051100
H	-2.316242100	4.857998400	-0.686627600
H	4.141128600	2.231171700	-1.739265400
C	-2.739487800	-0.069660100	1.770422900
H	-1.907516700	0.556849900	2.123567000
H	-3.682755700	0.475535400	1.918820200
H	-2.768772500	-0.995569900	2.362383500
C	-0.149710400	-3.465695200	0.765565000
H	-0.469751400	-4.483679500	1.050575100
H	0.543443500	-3.541879900	-0.082545300
H	0.371470100	-3.011955100	1.619407500
C	0.761062000	-1.561059600	-2.532345700
H	0.414207600	-0.523796700	-2.653368600
H	1.271811000	-1.880359200	-3.455330100
H	-0.109146700	-2.208667100	-2.360733000
C	1.736841400	-0.745925200	2.347596700
H	2.084772800	0.293928600	2.425668400
H	0.644364500	-0.770291100	2.461033400
H	2.196104600	-1.342070300	3.152141900

#### S<sub>0</sub>-final (C8C9)

C	-0.061976800	-0.532315400	0.021965200
C	-0.032376600	0.915430500	-0.123187200
C	1.256573600	-1.192089400	-0.097700000
C	2.124788200	-1.303145600	1.006088700
C	1.670403800	-1.663966400	-1.361334700
C	3.379350200	-1.902021000	0.843937400
C	2.927510800	-2.259108000	-1.505246600
C	3.780396100	-2.373336200	-0.406042400
H	4.769217700	-2.830543500	-0.527652400
C	1.271283300	1.611356600	-0.007314000
C	1.560489000	2.341775600	1.158401600
C	2.204402500	1.567431800	-1.054663400
C	2.770896800	3.021125600	1.270441100
H	0.823017500	2.385632800	1.965919000
C	3.412223700	2.249806000	-0.933262600
H	1.986304000	0.983882500	-1.952849300
C	3.700561000	2.973724900	0.227948300
H	2.991712600	3.605768100	2.170448300
H	4.653998100	3.505336400	0.319963600
C	-1.256270600	-1.185851500	0.179391500
C	-2.543129000	-0.387442200	0.271240500
C	-1.360722900	-2.628754600	0.368829300
C	-3.737272200	-1.180828700	-0.189497800
C	-2.560600900	-3.253102400	0.196723900
C	-3.740169300	-2.524641200	-0.200305100
H	-4.640621100	-0.625785200	-0.476541600



H	-4.616464000	-3.101061600	-0.519869200
C	-1.176750400	1.633910300	-0.341690800
C	-2.472821400	0.909498200	-0.559524400
C	-1.140115800	3.069719400	-0.491049300
C	-3.650969800	1.801308300	-0.324075900
H	-2.505235300	0.627908000	-1.669528700
C	-2.283629700	3.793765200	-0.541248800
H	-0.160898100	3.560029900	-0.536326000
C	-3.563506900	3.142329000	-0.368213400
H	-4.626785100	1.322024400	-0.159309100
H	-4.443051400	3.782351200	-0.230085200
H	3.241172200	-2.645385000	-2.482107800
H	-2.654901700	-4.338101600	0.332317000
H	4.055021600	-1.991297500	1.702376900
H	4.146093200	2.212310100	-1.746019400
H	-2.271594800	4.881962600	-0.665310600
C	0.749042800	-1.562211800	-2.535622200
H	0.410159300	-0.522304100	-2.657386700
H	1.258732600	-1.882867300	-3.459309200
H	-0.127267000	-2.203143400	-2.370200900
C	1.725723100	-0.776335700	2.347617700
H	0.632777800	-0.794373200	2.460238600
H	2.178018000	-1.382865200	3.148752200
H	2.078986400	0.260582100	2.438498700
C	-2.750694200	-0.072809100	1.764031000
H	-1.918056700	0.544187300	2.132253600
H	-3.690444100	0.477638700	1.915768000
H	-2.789731100	-1.007689600	2.340780600
C	-0.186157700	-3.469970700	0.752406000
H	0.522941400	-3.544717700	-0.082287800
H	0.323218200	-3.032106800	1.621843400
H	-0.519330300	-4.489209200	1.019527200
C	-0.042730038	-0.520949174	0.017677113
C	-0.017886723	0.953394720	-0.102834233
C	1.287062566	-1.205703760	-0.118239383
C	2.171565605	-1.312035123	0.970145122
C	1.656471155	-1.715420749	-1.380691569
C	3.411643714	-1.930440123	0.782728527
C	2.905212821	-2.321439747	-1.534196215
C	3.782254641	-2.429545256	-0.459276815
H	4.748110501	-2.905138011	-0.590098335
C	1.282215276	1.688716226	0.015832012
C	1.530765591	2.485485255	1.141898494
C	2.250496514	1.648197024	-0.995138777
C	2.715888013	3.209202798	1.261804465
H	0.781761705	2.536289684	1.924964874
C	3.435797147	2.369763292	-0.877364867
H	2.075064170	1.046922571	-1.878878129
C	3.674415906	3.150449571	0.252487258
H	2.887984572	3.819098448	2.141934336

H	4.598035309	3.711156788	0.343291229
C	-1.217496756	-1.198796129	0.183396492
C	-2.537677081	-0.404166104	0.306898546
C	-1.329504984	-2.665813430	0.387674174
C	-3.721578055	-1.206633609	-0.205858854
C	-2.526184700	-3.267323267	0.179319394
C	-3.708765806	-2.542248616	-0.241763109
H	-4.610707988	-0.661527030	-0.500467235
H	-4.577765497	-3.102935137	-0.569673035
C	-1.163198413	1.652860552	-0.331498274
C	-2.466316830	0.902470999	-0.523043115
C	-1.177393857	3.096459262	-0.532944748
C	-3.680799673	1.787684135	-0.343280471
H	-2.476810473	0.568564330	-1.584205471
C	-2.330567329	3.793228660	-0.589084024
H	-0.227023143	3.608136201	-0.613027887
C	-3.611500340	3.123903310	-0.413634515
H	-4.643168868	1.308681949	-0.205672110
H	-4.508542525	3.728220918	-0.330475138
H	3.187039839	-2.713377284	-2.506040515
H	-2.608355222	-4.339842088	0.322856910
H	4.087529233	-2.021168346	1.627043327
H	4.173335355	2.323078122	-1.670895145
H	-2.315614712	4.868009683	-0.731412913
C	0.718254122	-1.632930996	-2.561067456
H	0.366781601	-0.609867910	-2.731419815
H	1.213930408	-1.977564072	-3.472131039
H	-0.173504752	-2.249601099	-2.407879564
C	1.814166387	-0.794345058	2.341813854
H	0.734374729	-0.792456176	2.507548173
H	2.278940352	-1.407336961	3.119626446
H	2.166243977	0.233576312	2.476859734
C	-2.761054064	-0.103097510	1.816544997
H	-1.944417901	0.512148281	2.206084599
H	-3.702148254	0.429064695	1.978832700
H	-2.793339665	-1.041043941	2.376672738
C	-0.184177256	-3.536433160	0.854119825
H	0.588289253	-3.673763430	0.094948437
H	0.307740575	-3.120079824	1.736258420
H	-0.570027865	-4.524210654	1.120811251

### B3LYP method

TPE-4mM

S<sub>0</sub>

C	0.682811000	0.001607000	0.000364000
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C	-0.682817000	0.001577000	-0.000413000
C	1.490115000	-1.250944000	0.128606000
C	2.561279000	-1.496648000	-0.748525000
C	1.244134000	-2.177392000	1.153338000
C	3.355114000	-2.642090000	-0.645918000
H	2.774275000	-0.773277000	-1.531903000
C	2.037190000	-3.317519000	1.277940000
H	0.433142000	-1.998257000	1.852031000
C	3.081429000	-3.552605000	0.384891000
H	3.695315000	-4.444639000	0.491070000
C	-1.490061000	-1.251015000	-0.128644000
C	-1.244034000	-2.177461000	-1.153375000
C	-2.561193000	-1.496787000	0.748501000
C	-2.037012000	-3.317640000	-1.277949000
H	-0.433066000	-1.998266000	-1.852079000
C	-3.354959000	-2.642282000	0.645919000
H	-2.774233000	-0.773437000	1.531886000
C	-3.081225000	-3.552791000	-0.384878000
H	-1.842053000	-4.023813000	-2.081166000
H	-3.695031000	-4.444881000	-0.491057000
C	1.490983000	1.253598000	-0.127499000
C	1.243759000	2.182187000	-1.150363000
C	2.560491000	1.499482000	0.751235000
C	2.032656000	3.325423000	-1.269919000
H	0.430983000	2.005176000	-1.847489000
C	3.354129000	2.645506000	0.649891000
H	2.771368000	0.777302000	1.536338000
C	3.075537000	3.560760000	-0.374930000
H	1.831755000	4.037276000	-2.066617000
H	3.682675000	4.458225000	-0.473424000
C	-1.491051000	1.253524000	0.127483000
C	-1.243909000	2.182073000	1.150397000
C	-2.560562000	1.499390000	-0.751261000
C	-2.032899000	3.325243000	1.270012000
H	-0.431135000	2.005078000	1.847529000
C	-3.354276000	2.645350000	-0.649871000
H	-2.771385000	0.777236000	-1.536402000
C	-3.075782000	3.560556000	0.375027000
H	-1.832078000	4.037052000	2.066769000
H	-3.683000000	4.457960000	0.473585000
C	-4.475474000	-2.901563000	1.627273000
H	-5.392550000	-3.216247000	1.115397000
H	-4.211809000	-3.700423000	2.333017000
H	-4.707487000	-2.007349000	2.214405000
C	4.502654000	2.880672000	1.604695000
H	5.465481000	2.629169000	1.140113000
H	4.559355000	3.930716000	1.913881000
H	4.405544000	2.267850000	2.506577000
C	-4.502713000	2.880597000	-1.604762000
H	-5.465789000	2.631324000	-1.139509000

H	-4.557947000	3.930210000	-1.915706000
H	-4.406715000	2.266138000	-2.505642000
H	1.842257000	-4.023686000	2.081167000
C	4.475646000	-2.901331000	-1.627261000
H	5.392701000	-3.216073000	-1.115387000
H	4.211961000	-3.700123000	-2.333075000
H	4.707705000	-2.007088000	-2.214334000

S<sub>0</sub>-final (C4C5)

C	0.729304000	0.118881000	0.067922000
C	-0.731429000	0.116496000	-0.068020000
C	1.431752000	1.298634000	-0.042452000
C	2.863091000	1.387600000	0.133492000
C	0.655954000	2.572586000	-0.393038000
C	3.541452000	2.566200000	0.125285000
H	3.406796000	0.467980000	0.323450000
C	1.477542000	3.831976000	-0.257733000
H	0.370900000	2.500215000	-1.465677000
C	2.804393000	3.814351000	-0.057411000
H	3.362300000	4.748431000	-0.019764000
C	-1.437872000	1.293721000	0.043481000
C	-0.666399000	2.569719000	0.396224000
C	-2.869435000	1.378135000	-0.133154000
C	-1.492239000	3.826535000	0.262741000
H	-0.381138000	2.496670000	1.468730000
C	-3.551703000	2.554463000	-0.123587000
H	-3.409935000	0.456968000	-0.324659000
C	-2.818904000	3.804759000	0.061613000
H	-0.987246000	4.775434000	0.418609000
H	-3.379892000	4.737042000	0.025219000
C	1.428327000	1.177901000	0.332554000
C	1.199453000	1.880777000	1.523823000
C	2.318921000	1.727164000	-0.603404000
C	1.849285000	3.090718000	1.765481000
H	0.512091000	1.474880000	2.260556000
C	2.979367000	2.939809000	-0.377227000
H	2.492327000	1.193649000	-1.535413000
C	2.731346000	3.618249000	0.823313000
H	1.665206000	3.626456000	2.693439000
H	3.229111000	4.565965000	1.018217000
C	-1.425525000	1.182686000	-0.334055000
C	-1.197208000	1.881018000	-1.528539000
C	-2.315569000	1.735139000	0.599907000
C	-1.849794000	3.087852000	-1.776058000
H	-0.513659000	1.469871000	-2.265911000
C	-2.974032000	2.948733000	0.370620000
H	-2.492598000	1.202229000	1.531614000
C	-2.732453000	3.618494000	-0.835626000
H	-1.673259000	3.615562000	-2.710042000

H	-3.237623000	4.560601000	-1.038062000
C	-5.040459000	2.621885000	-0.331506000
H	-5.470811000	1.628737000	-0.491857000
H	-5.544442000	3.073628000	0.534601000
H	-5.293327000	3.246691000	-1.199619000
C	3.946974000	3.498637000	-1.395772000
H	4.988755000	3.352647000	-1.080300000
H	3.802645000	4.576033000	-1.537216000
H	3.828621000	3.012365000	-2.369501000
C	-3.900268000	3.536149000	1.411260000
H	-4.276537000	2.767060000	2.093907000
H	-4.762788000	4.029121000	0.948657000
H	-3.386365000	4.291122000	2.021399000
H	0.969205000	4.779397000	-0.411640000
C	5.030151000	2.638189000	0.332120000
H	5.532073000	3.091867000	-0.534181000
H	5.281751000	3.263373000	1.200318000
H	5.463715000	1.646296000	0.491609000

#### S<sub>0</sub>-final (C8C9)

C	-0.729431000	0.118352000	-0.067891000
C	0.731281000	0.117209000	0.067927000
C	-1.427292000	-1.179036000	-0.332642000
C	-2.316761000	-1.729522000	0.603441000
C	-1.197894000	-1.881408000	-1.524283000
C	-2.975828000	-2.943086000	0.377146000
H	-2.490288000	-1.196518000	1.535747000
C	-1.846082000	-3.092068000	-1.765904000
H	-0.511119000	-1.474499000	-2.261009000
C	-2.727132000	-3.620996000	-0.823355000
H	-3.223410000	-4.569520000	-1.017990000
C	1.426455000	-1.181389000	0.334148000
C	1.199013000	-1.879316000	1.529103000
C	2.316554000	-1.733561000	-0.599810000
C	1.852573000	-3.085476000	1.777021000
H	0.515434000	-1.468233000	2.266483000
C	2.975950000	-2.946661000	-0.370152000
H	2.492944000	-1.200903000	-1.531797000
C	2.735340000	-3.615924000	0.836490000
H	1.676846000	-3.612832000	2.711356000
H	3.241322000	-4.557524000	1.039208000
C	-1.432874000	1.297484000	0.042553000
C	-0.658078000	2.572075000	0.393162000
C	-2.864302000	1.385234000	-0.133280000
C	-1.480774000	3.830748000	0.257991000
H	-0.372825000	2.499855000	1.465749000
C	-3.543643000	2.563261000	-0.125057000
H	-3.407203000	0.465122000	-0.323163000
C	-2.807608000	3.812010000	0.057661000

H	-0.973273000	4.778613000	0.411959000
H	-3.366279000	4.745637000	0.020055000
C	1.436741000	1.295001000	-0.043641000
C	0.664150000	2.570391000	-0.396240000
C	2.868253000	1.380572000	0.132774000
C	1.488966000	3.827855000	-0.262780000
H	0.378789000	2.497130000	-1.468714000
C	3.549554000	2.557457000	0.123097000
H	3.409523000	0.459836000	0.324198000
C	2.815684000	3.807151000	-0.061887000
H	0.983161000	4.776362000	-0.418397000
H	3.375908000	4.739896000	-0.025497000
C	3.901587000	-3.534092000	-1.411293000
H	4.757006000	-4.039263000	-0.948788000
H	3.383341000	-4.278752000	-2.030406000
H	4.288542000	-2.762986000	-2.085689000
C	-5.032377000	2.634063000	-0.331947000
H	-5.465237000	1.641774000	-0.490896000
H	-5.534628000	3.087893000	0.534079000
H	-5.284412000	3.258563000	-1.200519000
C	5.038306000	2.626067000	0.330622000
H	5.541750000	3.077632000	-0.535901000
H	5.290970000	3.251588000	1.198275000
H	5.469397000	1.633315000	0.491439000
H	-1.661375000	-3.627645000	-2.693831000
C	-3.944054000	-3.501715000	1.395197000
H	-4.985751000	-3.316032000	1.100652000
H	-3.829751000	-4.586283000	1.504430000
H	-3.797046000	-3.046317000	2.379959000

TPE-4oM

S<sub>0</sub>

C	0.000000000	-0.472102000	-0.000016000
C	-0.000015000	0.896969000	-0.000036000
C	1.281589000	-1.266794000	-0.086494000
C	1.611442000	-2.224133000	0.912931000
C	2.154269000	-1.113124000	-1.197481000
C	2.777713000	-2.984565000	0.786467000
C	3.307547000	-1.905339000	-1.285585000
C	3.626693000	-2.835962000	-0.306471000
H	4.526219000	-3.440152000	-0.391436000
C	1.242053000	1.706180000	0.202042000
C	2.159130000	1.402105000	1.222941000
C	1.496978000	2.838645000	-0.594243000
C	3.294677000	2.184802000	1.427222000
H	1.976034000	0.548060000	1.866137000

C	2.636556000	3.616778000	-0.397319000
H	0.794405000	3.104385000	-1.378544000
C	3.542204000	3.292755000	0.615023000
H	3.984649000	1.929804000	2.227367000
H	4.427728000	3.902376000	0.774061000
C	-1.281561000	-1.266842000	0.086492000
C	-2.154256000	-1.113170000	1.197474000
C	-1.611368000	-2.224213000	-0.912903000
C	-3.307510000	-1.905410000	1.285590000
C	-2.777630000	-2.984673000	-0.786431000
C	-3.626624000	-2.836065000	0.306492000
H	-3.959606000	-1.781628000	2.147414000
H	-4.526136000	-3.440275000	0.391467000
C	-1.242101000	1.706165000	-0.202084000
C	-2.159252000	1.402033000	-1.222899000
C	-1.496962000	2.838679000	0.594151000
C	-3.294807000	2.184726000	-1.427147000
H	-1.976211000	0.547948000	-1.866057000
C	-2.636548000	3.616809000	0.397260000
H	-0.794333000	3.104460000	1.378387000
C	-3.542270000	3.292729000	-0.614997000
H	-3.984836000	1.929686000	-2.227229000
H	-4.427800000	3.902347000	-0.774010000
H	3.959632000	-1.781561000	-2.147417000
H	-3.022182000	-3.702283000	-1.565995000
H	3.022292000	-3.702149000	1.566047000
H	2.814751000	4.479753000	-1.033773000
H	-2.814694000	4.479824000	1.033674000
C	1.925103000	-0.136539000	-2.331565000
H	2.521033000	0.772839000	-2.189970000
H	2.232107000	-0.583521000	-3.283823000
H	0.884823000	0.178217000	-2.420348000
C	0.773947000	-2.439219000	2.155161000
H	-0.181275000	-2.925691000	1.933388000
H	1.313152000	-3.071037000	2.867952000
H	0.540194000	-1.497061000	2.661277000
C	-1.925149000	-0.136525000	2.331510000
H	-2.521018000	0.772875000	2.189780000
H	-2.232294000	-0.583424000	3.283769000
H	-0.884865000	0.178217000	2.420381000
C	-0.773844000	-2.439341000	-2.155103000
H	-0.540009000	-1.497156000	-2.661148000
H	0.181312000	-2.925945000	-1.933322000
H	-1.313091000	-3.071070000	-2.867941000

S<sub>0</sub>-final (C4C5)

C	-0.042710000	-0.520952000	0.017658000
C	-0.017897000	0.953401000	-0.102826000
C	-1.217477000	-1.198841000	0.183263000

C	-1.329509000	-2.665889000	0.387355000
C	-2.537656000	-0.404204000	0.306888000
C	-2.526220000	-3.267348000	0.179029000
C	-3.721616000	-1.206605000	-0.205806000
C	-3.708837000	-2.542214000	-0.241843000
H	-4.577885000	-3.102848000	-0.569712000
C	-1.163219000	1.652862000	-0.331478000
C	-2.466346000	0.902479000	-0.522972000
C	-1.177424000	3.096449000	-0.533027000
C	-3.680814000	1.787695000	-0.343071000
H	-2.476912000	0.568645000	-1.584159000
C	-2.330600000	3.793218000	-0.589118000
H	-0.227061000	3.608118000	-0.613233000
C	-3.611517000	3.123910000	-0.413486000
H	-4.643166000	1.308705000	-0.205310000
H	-4.508543000	3.728240000	-0.330236000
C	1.287106000	-1.205674000	-0.118140000
C	1.656681000	-1.715382000	-1.380542000
C	2.171456000	-1.312018000	0.970371000
C	2.905440000	-2.321414000	-1.533879000
C	3.411563000	-1.930413000	0.783115000
C	3.782336000	-2.429522000	-0.458844000
H	3.187403000	-2.713338000	-2.505690000
H	4.748208000	-2.905117000	-0.589536000
C	1.282204000	1.688751000	0.015764000
C	1.530692000	2.485693000	1.141730000
C	2.250524000	1.648117000	-0.995161000
C	2.715793000	3.209450000	1.261588000
H	0.781641000	2.536605000	1.924748000
C	3.435802000	2.369729000	-0.877437000
H	2.075134000	1.046733000	-1.878832000
C	3.674361000	3.150573000	0.252317000
H	2.887843000	3.819469000	2.141641000
H	4.597968000	3.711309000	0.343076000
H	-4.610775000	-0.661464000	-0.500262000
H	4.087339000	-2.021131000	1.627515000
H	-2.608385000	-4.339887000	0.322413000
H	-2.315661000	4.867988000	-0.731534000
H	4.173375000	2.322957000	-1.670930000
C	-2.760908000	-0.103229000	1.816570000
H	-1.944247000	0.511995000	2.206085000
H	-3.701997000	0.428911000	1.978968000
H	-2.793147000	-1.041212000	2.376641000
C	-0.184177000	-3.536647000	0.853544000
H	-0.570038000	-4.524490000	1.119979000
H	0.588278000	-3.673796000	0.094334000
H	0.307758000	-3.120543000	1.735790000
C	0.718590000	-1.632972000	-2.561025000
H	0.366517000	-0.610067000	-2.731030000
H	1.214595000	-1.976972000	-3.472151000



H	-0.172816000	-2.250251000	-2.408194000
C	1.813788000	-0.794377000	2.341986000
H	2.164021000	0.234248000	2.476407000
H	0.734065000	-0.794389000	2.508253000
H	2.280042000	-1.406181000	3.119837000

S<sub>0</sub>-final (C8C9)

C	-0.045905000	-0.521347000	0.023877000
C	-0.005848000	0.947690000	-0.089041000
C	1.282521000	-1.220316000	-0.108161000
C	2.162152000	-1.343421000	0.987409000
C	1.657405000	-1.723653000	-1.376217000
C	3.401778000	-1.968104000	0.799757000
C	2.906554000	-2.335161000	-1.526091000
C	3.778998000	-2.457677000	-0.446128000
H	4.745269000	-2.938403000	-0.575938000
C	1.303034000	1.677075000	0.018606000
C	1.574453000	2.456593000	1.155276000
C	2.255689000	1.658511000	-1.011916000
C	2.762786000	3.181067000	1.266809000
H	0.839798000	2.494319000	1.955266000
C	3.443292000	2.382111000	-0.903739000
H	2.064585000	1.075850000	-1.907231000
C	3.703627000	3.143534000	0.237183000
H	2.949664000	3.776073000	2.157191000
H	4.629783000	3.706118000	0.320457000
C	-1.235377000	-1.198198000	0.175624000
C	-2.550600000	-0.387414000	0.305377000
C	-1.362338000	-2.659577000	0.362253000
C	-3.743158000	-1.169040000	-0.222894000
C	-2.574888000	-3.245590000	0.151238000
C	-3.747914000	-2.508180000	-0.263309000
H	-4.628820000	-0.613261000	-0.514782000
H	-4.626946000	-3.056546000	-0.594033000
C	-1.149590000	1.670502000	-0.312563000
C	-2.465002000	0.934270000	-0.502346000
C	-1.145819000	3.106100000	-0.517043000
C	-3.670733000	1.835839000	-0.322160000
H	-2.481584000	0.617375000	-1.570601000
C	-2.295768000	3.821608000	-0.584067000
H	-0.190195000	3.613171000	-0.588441000
C	-3.583528000	3.173779000	-0.407939000
H	-4.642866000	1.373177000	-0.183094000
H	-4.476585000	3.789682000	-0.333196000
H	3.193688000	-2.722148000	-2.501140000
H	-2.665532000	-4.322046000	0.276873000
H	4.073655000	-2.072387000	1.648866000
H	4.165672000	2.352202000	-1.715343000
H	-2.260341000	4.898219000	-0.727749000

C	0.727855000	-1.634146000	-2.567866000
H	0.379343000	-0.609388000	-2.742195000
H	1.231038000	-1.979050000	-3.476797000
H	-0.169202000	-2.248465000	-2.426608000
C	1.804063000	-0.839252000	2.368019000
H	0.723381000	-0.835148000	2.536059000
H	2.268020000	-1.462814000	3.140239000
H	2.160234000	0.186966000	2.518045000
C	-2.780985000	-0.114398000	1.824687000
H	-1.961365000	0.484936000	2.235900000
H	-3.718706000	0.424034000	1.996123000
H	-2.826100000	-1.063382000	2.366802000
C	-0.231556000	-3.567390000	0.804904000
H	0.539422000	-3.704320000	0.042039000
H	0.271625000	-3.185008000	1.697847000
H	-0.638125000	-4.554643000	1.048205000

## OM2/MRCI: LIIC path

TPE-4mM

S<sub>0</sub>-S<sub>1</sub>S<sub>0</sub>-cyc(C4C5)\_S<sub>0</sub>-final(C4C5)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.357180000	0.000000000	0.000000000
C	-0.799570000	0.000000000	-1.247810000
C	-1.883800000	-0.860940000	-1.373810000
C	-0.475230000	0.896680000	-2.274830000
C	-2.650610000	-0.846140000	-2.550830000
H	-2.145660000	-1.544010000	-0.559690000
C	-1.246900000	0.905130000	-3.442410000
H	0.384810000	1.562700000	-2.178590000
C	-2.321480000	0.046030000	-3.580670000
H	-2.924180000	0.061090000	-4.498640000
C	2.155780000	-0.132230000	-1.231860000
C	1.885010000	-1.155580000	-2.149720000
C	3.233470000	0.752640000	-1.452740000
C	2.659530000	-1.268420000	-3.278340000
H	1.052660000	-1.838990000	-1.969230000
C	3.994110000	0.637180000	-2.591190000
H	3.455360000	1.520270000	-0.703410000
C	3.712780000	-0.372350000	-3.517670000
H	2.453210000	-2.059170000	-4.011900000
H	4.314140000	-0.465840000	-4.428960000
C	-0.801240000	0.010890000	1.240310000
C	-0.515750000	-0.893380000	2.272650000
C	-1.882950000	0.909200000	1.361310000

C	-1.295120000	-0.886200000	3.427630000
H	0.326860000	-1.582080000	2.178080000
C	-2.654300000	0.913610000	2.529300000
H	-2.117080000	1.592540000	0.538950000
C	-2.362080000	0.014900000	3.563750000
H	-1.074400000	-1.590440000	4.239150000
H	-2.968200000	0.009910000	4.475800000
C	2.149940000	0.144810000	1.244230000
C	1.876350000	1.203730000	2.119880000
C	3.171500000	-0.760860000	1.529530000
C	2.632740000	1.344810000	3.286460000
H	1.066440000	1.903700000	1.898930000
C	3.921480000	-0.615170000	2.707450000
H	3.389600000	-1.582220000	0.838860000
C	3.646460000	0.444190000	3.582480000
H	2.423310000	2.178660000	3.968100000
H	4.236290000	0.559180000	4.498820000
C	5.154310000	1.563520000	-2.836390000
H	6.087070000	1.043120000	-2.577270000
H	5.182260000	1.864650000	-3.894260000
H	5.062710000	2.468180000	-2.215690000
C	-3.813090000	1.850250000	2.659520000
H	-4.728440000	1.337530000	2.324520000
H	-3.937550000	2.161500000	3.708290000
H	-3.656940000	2.746450000	2.040060000
C	5.031930000	-1.567530000	3.013260000
H	5.969450000	-1.170720000	2.592380000
H	5.150500000	-1.684760000	4.101850000
H	4.830480000	-2.553910000	2.568690000
H	-0.991050000	1.600170000	-4.251570000
C	-3.833050000	-1.748200000	-2.688200000
H	-4.737000000	-1.217110000	-2.344910000
H	-3.970710000	-2.044100000	-3.740610000
H	-3.701480000	-2.654790000	-2.076910000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.363980000	0.000000000	0.000000000
C	-0.783720000	0.000000000	-1.248780000
C	-1.948340000	-0.760560000	-1.336950000
C	-0.358110000	0.785020000	-2.339210000
C	-2.669500000	-0.785870000	-2.539300000
H	-2.299270000	-1.334920000	-0.475850000
C	-1.107800000	0.761690000	-3.523620000
H	0.500450000	1.450030000	-2.223710000
C	-2.237650000	-0.025980000	-3.632890000
H	-2.805470000	-0.055300000	-4.570120000
C	2.148960000	-0.200640000	-1.220070000
C	1.801770000	-1.232420000	-2.112120000

C	3.275070000	0.614660000	-1.476280000
C	2.559890000	-1.414560000	-3.252010000
H	0.964490000	-1.899190000	-1.861450000
C	4.015750000	0.425180000	-2.616580000
H	3.544410000	1.392270000	-0.752080000
C	3.661740000	-0.593370000	-3.513910000
H	2.299170000	-2.208530000	-3.962320000
H	4.255510000	-0.749640000	-4.423410000
C	-0.792720000	0.055060000	1.244350000
C	-0.556230000	-0.872700000	2.268610000
C	-1.813780000	1.018510000	1.383800000
C	-1.322580000	-0.825660000	3.431330000
H	0.240290000	-1.612770000	2.160210000
C	-2.574020000	1.061750000	2.558150000
H	-2.011520000	1.723890000	0.569820000
C	-2.329500000	0.138830000	3.583640000
H	-1.138490000	-1.547790000	4.236380000
H	-2.926220000	0.165870000	4.501670000
C	2.156620000	0.214780000	1.234760000
C	1.894980000	1.328650000	2.043290000
C	3.166160000	-0.685820000	1.577120000
C	2.652810000	1.532390000	3.198870000
H	1.095800000	2.025100000	1.776330000
C	3.916030000	-0.478100000	2.744920000
H	3.371750000	-1.551580000	0.938990000
C	3.654570000	0.637260000	3.552320000
H	2.454300000	2.409120000	3.827750000
H	4.244090000	0.800460000	4.461510000
C	5.227330000	1.269080000	-2.899300000
H	6.105120000	0.808740000	-2.423060000
H	5.395210000	1.341160000	-3.985140000
H	5.091990000	2.285210000	-2.496130000
C	-3.671400000	2.067600000	2.705730000
H	-4.618250000	1.617970000	2.367830000
H	-3.772760000	2.372040000	3.758950000
H	-3.461080000	2.960500000	2.097530000
C	5.009330000	-1.428350000	3.113640000
H	5.933310000	-1.134730000	2.590960000
H	5.190790000	-1.405100000	4.199590000
H	4.742490000	-2.454460000	2.818760000
H	-0.782690000	1.377010000	-4.373360000
C	-3.919730000	-1.596720000	-2.646290000
H	-4.788880000	-0.950820000	-2.439450000
H	-4.017690000	-2.013980000	-3.660730000
H	-3.910300000	-2.423150000	-1.919150000

Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.370770000	0.000000000	0.000000000

C	-0.767920000	0.000000000	-1.249550000
C	-2.003590000	-0.649800000	-1.307670000
C	-0.252710000	0.659130000	-2.393730000
C	-2.686880000	-0.723880000	-2.526990000
H	-2.430530000	-1.102740000	-0.411170000
C	-0.986670000	0.600980000	-3.589510000
H	0.600500000	1.330450000	-2.274190000
C	-2.167130000	-0.110160000	-3.671870000
H	-2.707710000	-0.189210000	-4.619890000
C	2.142220000	-0.268110000	-1.204360000
C	1.720450000	-1.302400000	-2.071050000
C	3.313420000	0.473450000	-1.490960000
C	2.461480000	-1.553270000	-3.218320000
H	0.881480000	-1.951070000	-1.754880000
C	4.033150000	0.211070000	-2.628810000
H	3.628900000	1.257590000	-0.791700000
C	3.608370000	-0.810970000	-3.497320000
H	2.148360000	-2.346310000	-3.906000000
H	4.193320000	-1.030020000	-4.401420000
C	-0.784170000	0.099530000	1.246740000
C	-0.600910000	-0.848320000	2.263930000
C	-1.740400000	1.124360000	1.401970000
C	-1.354500000	-0.761810000	3.432690000
H	0.146170000	-1.636960000	2.143760000
C	-2.489940000	1.206280000	2.581010000
H	-1.897970000	1.849230000	0.595650000
C	-2.297450000	0.262420000	3.598520000
H	-1.210310000	-1.499370000	4.232030000
H	-2.884870000	0.321220000	4.521230000
C	2.163300000	0.284140000	1.221350000
C	1.913690000	1.448560000	1.959370000
C	3.160610000	-0.607620000	1.621150000
C	2.672900000	1.714130000	3.100650000
H	1.125420000	2.138300000	1.646090000
C	3.910280000	-0.338540000	2.775660000
H	3.353620000	-1.514200000	1.038360000
C	3.662500000	0.828330000	3.511890000
H	2.485360000	2.630230000	3.674110000
H	4.251620000	1.039330000	4.411450000
C	5.291640000	0.968080000	-2.943340000
H	6.098770000	0.620050000	-2.281610000
H	5.583510000	0.801970000	-3.992860000
H	5.141330000	2.048610000	-2.786690000
C	-3.521530000	2.277710000	2.743110000
H	-4.495110000	1.893330000	2.400800000
H	-3.603050000	2.574530000	3.800190000
H	-3.255240000	3.163260000	2.146100000
C	4.986080000	-1.282190000	3.208060000
H	5.888210000	-1.106560000	2.601380000
H	5.233950000	-1.124910000	4.269450000

H	4.658110000	-2.323340000	3.068850000
H	-0.600490000	1.128400000	-4.473920000
C	-3.997700000	-1.437010000	-2.607390000
H	-4.813840000	-0.699660000	-2.544290000
H	-4.076020000	-1.976730000	-3.563460000
H	-4.102030000	-2.155680000	-1.780730000

Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.377570000	0.000000000	0.000000000
C	-0.752180000	0.000000000	-1.250150000
C	-2.048390000	-0.530070000	-1.286270000
C	-0.160790000	0.521050000	-2.437790000
C	-2.703090000	-0.659310000	-2.513700000
H	-2.536570000	-0.851530000	-0.366430000
C	-0.885870000	0.426640000	-3.639430000
H	0.685420000	1.203380000	-2.330610000
C	-2.111970000	-0.202970000	-3.697010000
H	-2.633830000	-0.335040000	-4.647270000
C	2.135550000	-0.334420000	-1.184810000
C	1.641510000	-1.365420000	-2.027290000
C	3.348340000	0.329730000	-1.496390000
C	2.364950000	-1.684160000	-3.178130000
H	0.803530000	-1.995330000	-1.650650000
C	4.046290000	-0.004120000	-2.627670000
H	3.708480000	1.117070000	-0.821500000
C	3.553000000	-1.024240000	-3.468310000
H	2.001730000	-2.472290000	-3.844260000
H	4.127890000	-1.305760000	-4.363400000
C	-0.775590000	0.144220000	1.247490000
C	-0.649510000	-0.819980000	2.258400000
C	-1.663220000	1.226350000	1.415980000
C	-1.390660000	-0.694420000	3.431550000
H	0.045090000	-1.654120000	2.128400000
C	-2.402530000	1.346760000	2.598070000
H	-1.777070000	1.967850000	0.616730000
C	-2.266110000	0.385560000	3.608410000
H	-1.289450000	-1.444700000	4.225790000
H	-2.844410000	0.475810000	4.534520000
C	2.169990000	0.352670000	1.204050000
C	1.932470000	1.563030000	1.868460000
C	3.154860000	-0.526400000	1.661420000
C	2.693010000	1.889430000	2.992180000
H	1.155280000	2.242810000	1.508770000
C	3.904210000	-0.196780000	2.799470000
H	3.335200000	-1.470070000	1.136490000
C	3.670230000	1.016870000	3.461330000
H	2.516510000	2.841250000	3.507820000
H	4.258870000	1.275140000	4.348780000

C	5.347010000	0.662210000	-2.967780000
H	6.075820000	0.471540000	-2.165170000
H	5.741720000	0.265320000	-3.917960000
H	5.207520000	1.751090000	-3.071930000
C	-3.364350000	2.479790000	2.772030000
H	-4.359620000	2.162430000	2.423610000
H	-3.429370000	2.768410000	3.832490000
H	-3.040670000	3.353800000	2.186380000
C	4.962200000	-1.129260000	3.296010000
H	5.834170000	-1.083080000	2.625290000
H	5.279220000	-0.847860000	4.312370000
H	4.578180000	-2.160290000	3.314490000
H	-0.447710000	0.859260000	-4.552370000
C	-4.066900000	-1.268630000	-2.571260000
H	-4.815740000	-0.465960000	-2.655390000
H	-4.146260000	-1.926250000	-3.449580000
H	-4.272060000	-1.855340000	-1.663880000

#### Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.384370000	0.000000000	0.000000000
C	-0.736500000	0.000000000	-1.250550000
C	-2.081710000	-0.402900000	-1.272940000
C	-0.083930000	0.373050000	-2.471030000
C	-2.718260000	-0.591200000	-2.499340000
H	-2.614950000	-0.585670000	-0.342020000
C	-0.807290000	0.242580000	-3.673100000
H	0.755280000	1.068010000	-2.392990000
C	-2.073690000	-0.300630000	-3.708110000
H	-2.585970000	-0.486840000	-4.652160000
C	2.128950000	-0.399350000	-1.161510000
C	1.565410000	-1.421490000	-1.981590000
C	3.379670000	0.184300000	-1.492260000
C	2.270980000	-1.806990000	-3.132320000
H	0.730490000	-2.032740000	-1.549770000
C	4.055140000	-0.219300000	-2.612990000
H	3.782790000	0.971610000	-0.840800000
C	3.495980000	-1.232330000	-3.427360000
H	1.860240000	-2.586470000	-3.778430000
H	4.059560000	-1.575700000	-4.309850000
C	-0.766970000	0.189090000	1.246570000
C	-0.701710000	-0.787460000	2.251800000
C	-1.582680000	1.324080000	1.426070000
C	-1.430850000	-0.623300000	3.427690000
H	-0.062300000	-1.663750000	2.113710000
C	-2.312270000	1.482800000	2.609560000
H	-1.649500000	2.079100000	0.633440000
C	-2.235650000	0.508150000	3.613310000
H	-1.375450000	-1.383360000	4.217290000

H	-2.805070000	0.629540000	4.541540000
C	2.176670000	0.420160000	1.182910000
C	1.951330000	1.671650000	1.770920000
C	3.148910000	-0.442340000	1.697690000
C	2.713130000	2.057710000	2.873910000
H	1.185390000	2.338210000	1.364950000
C	3.897830000	-0.053170000	2.816190000
H	3.316510000	-1.419210000	1.232920000
C	3.677780000	1.202360000	3.400780000
H	2.547730000	3.041460000	3.329560000
H	4.265860000	1.507230000	4.273690000
C	5.393260000	0.353220000	-2.972070000
H	6.043810000	0.353800000	-2.083420000
H	5.866600000	-0.250590000	-3.765420000
H	5.285550000	1.389530000	-3.335040000
C	-3.200730000	2.673100000	2.792930000
H	-4.212450000	2.424130000	2.436530000
H	-3.252720000	2.953210000	3.856370000
H	-2.818690000	3.531300000	2.219080000
C	4.937690000	-0.969810000	3.376990000
H	5.771320000	-1.060930000	2.663770000
H	5.325770000	-0.577330000	4.329860000
H	4.503520000	-1.965730000	3.551210000
H	-0.327020000	0.574890000	-4.608320000
C	-4.126980000	-1.091020000	-2.537840000
H	-4.798690000	-0.250810000	-2.768830000
H	-4.227670000	-1.856470000	-3.320700000
H	-4.416060000	-1.525850000	-1.570400000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.391160000	0.000000000	0.000000000
C	-0.720870000	0.000000000	-1.250780000
C	-2.102640000	-0.269920000	-1.267740000
C	-0.023470000	0.217580000	-2.493280000
C	-2.732270000	-0.518530000	-2.484010000
H	-2.663730000	-0.309800000	-0.337920000
C	-0.752340000	0.052940000	-3.690580000
H	0.809680000	0.923510000	-2.460750000
C	-2.053300000	-0.399180000	-3.705360000
H	-2.565400000	-0.638440000	-4.635100000
C	2.122430000	-0.462670000	-1.134540000
C	1.492600000	-1.470710000	-1.934680000
C	3.407280000	0.037960000	-1.478340000
C	2.180230000	-1.921620000	-3.081770000
H	0.662160000	-2.064120000	-1.453140000
C	4.059700000	-0.433410000	-2.584740000
H	3.851520000	0.822210000	-0.849010000
C	3.437690000	-1.434440000	-3.375020000



H	1.724800000	-2.688990000	-3.709810000
H	3.988710000	-1.838760000	-4.241390000
C	-0.758320000	0.234060000	1.243970000
C	-0.757140000	-0.750560000	2.243860000
C	-1.499210000	1.417230000	1.432470000
C	-1.474790000	-0.548270000	3.420870000
H	-0.175320000	-1.665440000	2.099240000
C	-2.219660000	1.614070000	2.615720000
H	-1.515990000	2.182400000	0.646230000
C	-2.206220000	0.630130000	3.613240000
H	-1.467790000	-1.314970000	4.206100000
H	-2.767090000	0.782310000	4.542320000
C	2.183350000	0.486380000	1.157980000
C	1.970260000	1.774050000	1.667120000
C	3.142760000	-0.355630000	1.729770000
C	2.733260000	2.218440000	2.746280000
H	1.215730000	2.424100000	1.215280000
C	3.891150000	0.091970000	2.825680000
H	3.297540000	-1.361660000	1.327160000
C	3.685130000	1.384270000	3.330420000
H	2.579010000	3.230180000	3.140040000
H	4.272580000	1.734980000	4.186380000
C	5.430250000	0.042940000	-2.955860000
H	6.009380000	0.254380000	-2.042590000
H	5.957230000	-0.728900000	-3.544470000
H	5.369130000	0.965490000	-3.558990000
C	-3.031610000	2.857010000	2.806340000
H	-4.054340000	2.677350000	2.439940000
H	-3.074080000	3.128530000	3.872400000
H	-2.590670000	3.695060000	2.244980000
C	4.912550000	-0.804120000	3.450490000
H	5.699900000	-1.036570000	2.717300000
H	5.372760000	-0.316320000	4.323870000
H	4.434870000	-1.740790000	3.774630000
H	-0.240500000	0.280870000	-4.641840000
C	-4.177350000	-0.903590000	-2.507220000
H	-4.766790000	-0.054030000	-2.880940000
H	-4.318260000	-1.761650000	-3.179150000
H	-4.530070000	-1.171650000	-1.501610000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.397960000	0.000000000	0.000000000
C	-0.705310000	0.000000000	-1.250820000
C	-2.110450000	-0.132860000	-1.270620000
C	0.019540000	0.057230000	-2.504580000
C	-2.744760000	-0.440280000	-2.467910000
H	-2.681510000	-0.028710000	-0.353760000
C	-0.721910000	-0.138050000	-3.692280000

H	0.847750000	0.769280000	-2.532740000
C	-2.051220000	-0.494590000	-3.689280000
H	-2.572480000	-0.783660000	-4.597140000
C	2.115990000	-0.524170000	-1.104020000
C	1.423520000	-1.513270000	-1.887260000
C	3.431030000	-0.108440000	-1.454460000
C	2.093370000	-2.028040000	-3.027330000
H	0.598350000	-2.090280000	-1.361550000
C	4.060010000	-0.645360000	-2.542990000
H	3.914360000	0.669940000	-0.845630000
C	3.378480000	-1.629870000	-3.311900000
H	1.596360000	-2.780190000	-3.639620000
H	3.915740000	-2.093910000	-4.158720000
C	-0.749640000	0.279070000	1.239690000
C	-0.815460000	-0.709130000	2.234300000
C	-1.413300000	1.505490000	1.435470000
C	-1.522200000	-0.469160000	3.410820000
H	-0.293260000	-1.658840000	2.084490000
C	-2.125220000	1.740270000	2.616840000
H	-1.377340000	2.277250000	0.655580000
C	-2.177990000	0.751420000	3.608210000
H	-1.565910000	-1.239190000	4.191740000
H	-2.730670000	0.934050000	4.536890000
C	2.190030000	0.551120000	1.129350000
C	1.989250000	1.869870000	1.557480000
C	3.136410000	-0.266480000	1.757460000
C	2.753390000	2.371100000	2.609790000
H	1.246310000	2.500110000	1.060370000
C	3.884160000	0.238270000	2.827780000
H	3.278310000	-1.297530000	1.418730000
C	3.692290000	1.562100000	3.250470000
H	2.610350000	3.406810000	2.940010000
H	4.279030000	1.957750000	4.087110000
C	5.457910000	-0.266770000	-2.918950000
H	5.977790000	0.158880000	-2.044920000
H	6.014960000	-1.155410000	-3.267960000
H	5.451240000	0.485310000	-3.727800000
C	-2.857940000	3.030960000	2.812820000
H	-3.886080000	2.921080000	2.434320000
H	-2.894460000	3.294100000	3.881170000
H	-2.358000000	3.844540000	2.264940000
C	4.886800000	-0.632540000	3.516000000
H	5.620260000	-1.006430000	2.785690000
H	5.419270000	-0.067430000	4.296780000
H	4.372900000	-1.487260000	3.980590000
H	-0.189500000	-0.017040000	-4.653460000
C	-4.217070000	-0.705810000	-2.479650000
H	-4.723950000	0.125700000	-2.988460000
H	-4.414770000	-1.636750000	-3.027930000
H	-4.610610000	-0.797780000	-1.458330000

## Coord\_8

C	0.00000000	0.00000000	0.00000000
C	1.40476000	0.00000000	0.00000000
C	-0.68981000	0.00000000	-1.25068000
C	-2.10456000	0.00650000	-1.28138000
C	0.04434000	-0.10529000	-2.50517000
C	-2.75512000	-0.35553000	-2.45140000
H	-2.66747000	0.25270000	-0.38878000
C	-0.71635000	-0.32609000	-3.67896000
H	0.86816000	0.60523000	-2.60733000
C	-2.06727000	-0.58287000	-3.66076000
H	-2.60664000	-0.91650000	-4.53988000
C	2.10963000	-0.58365000	-1.07007000
C	1.35860000	-1.54947000	-1.84001000
C	3.45082000	-0.25404000	-1.42054000
C	2.01107000	-2.12636000	-2.96982000
H	0.53889000	-2.11205000	-1.27568000
C	4.05612000	-0.85408000	-2.48787000
H	3.97103000	0.51591000	-0.83028000
C	3.31877000	-1.81798000	-3.23865000
H	1.47580000	-2.86059000	-3.56901000
H	3.84107000	-2.34025000	-4.06261000
C	-0.74093000	0.32405000	1.23371000
C	-0.87626000	-0.66305000	2.22280000
C	-1.32541000	1.58861000	1.43537000
C	-1.57276000	-0.38585000	3.39723000
H	-0.41535000	-1.64366000	2.06889000
C	-2.02947000	1.86116000	2.61323000
H	-1.23434000	2.36320000	0.66204000
C	-2.15107000	0.87199000	3.59822000
H	-1.66920000	-1.15575000	4.17369000
H	-2.69600000	1.08472000	4.52527000
C	2.19671000	0.61419000	1.09710000
C	2.00832000	1.95878000	1.44242000
C	3.12987000	-0.17510000	1.78056000
C	2.77353000	2.51522000	2.46495000
H	1.27711000	2.56595000	0.90091000
C	3.87687000	0.38538000	2.82239000
H	3.25882000	-1.22692000	1.50716000
C	3.69926000	1.73537000	3.16116000
H	2.64175000	3.57076000	2.73027000
H	4.28520000	2.17493000	3.97614000
C	5.47622000	-0.57406000	-2.86135000
H	5.95250000	0.05221000	-2.08833000
H	6.04312000	-1.51966000	-2.95143000
H	5.52486000	-0.04013000	-3.82766000
C	-2.68072000	3.19452000	2.81300000
H	-3.70855000	3.15440000	2.42025000

H	-2.714850000	3.449730000	3.883330000
H	-2.122140000	3.979320000	2.279870000
C	4.860440000	-0.455410000	3.573060000
H	5.532840000	-0.966990000	2.868170000
H	5.464390000	0.167250000	4.251270000
H	4.318220000	-1.207530000	4.165250000
H	-0.174720000	-0.312990000	-4.644130000
C	-4.244920000	-0.497290000	-2.455530000
H	-4.673620000	0.290730000	-3.088640000
H	-4.512780000	-1.477650000	-2.870500000
H	-4.654850000	-0.409700000	-1.440830000

### Coord\_9

C	0.000000000	0.000000000	0.000000000
C	1.411560000	0.000000000	0.000000000
C	-0.674370000	0.000000000	-1.250350000
C	-2.084600000	0.146360000	-1.299740000
C	0.050480000	-0.267230000	-2.495480000
C	-2.762470000	-0.263460000	-2.434910000
H	-2.621380000	0.529580000	-0.441920000
C	-0.735440000	-0.506960000	-3.651650000
H	0.869230000	0.431940000	-2.682520000
C	-2.100690000	-0.660170000	-3.620970000
H	-2.666420000	-1.031220000	-4.465330000
C	2.103340000	-0.640910000	-1.032830000
C	1.298250000	-1.579650000	-1.793520000
C	3.466570000	-0.397960000	-1.376600000
C	1.933960000	-2.216830000	-2.910030000
H	0.483620000	-2.130250000	-1.196120000
C	4.048090000	-1.058520000	-2.419640000
H	4.021290000	0.361310000	-0.802690000
C	3.258940000	-1.998220000	-3.155970000
H	1.363990000	-2.930840000	-3.499020000
H	3.765130000	-2.576950000	-3.953910000
C	-0.732190000	0.368940000	1.226040000
C	-0.939130000	-0.612250000	2.209040000
C	-1.236060000	1.666400000	1.432510000
C	-1.626120000	-0.298270000	3.379800000
H	-0.540810000	-1.619720000	2.051860000
C	-1.932940000	1.976560000	2.605220000
H	-1.087860000	2.439930000	0.666220000
C	-2.125590000	0.991800000	3.583290000
H	-1.777010000	-1.064470000	4.151390000
H	-2.663250000	1.234270000	4.507450000
C	2.203390000	0.675370000	1.061320000
C	2.027440000	2.040470000	1.322380000
C	3.123130000	-0.081720000	1.798900000
C	2.793670000	2.650350000	2.312310000
H	1.308140000	2.621350000	0.737580000

C	3.869280000	0.532910000	2.809390000
H	3.239070000	-1.150010000	1.591970000
C	3.706030000	1.903580000	3.062740000
H	2.673200000	3.721530000	2.511630000
H	4.291110000	2.385920000	3.853790000
C	5.485180000	-0.877060000	-2.783240000
H	5.934970000	-0.080040000	-2.166560000
H	6.046680000	-1.815650000	-2.612050000
H	5.583520000	-0.596130000	-3.848100000
C	-2.500930000	3.347330000	2.807540000
H	-3.522660000	3.376480000	2.398370000
H	-2.536230000	3.595350000	3.879500000
H	-1.884550000	4.099150000	2.290730000
C	4.833480000	-0.273160000	3.621180000
H	5.438200000	-0.914900000	2.963320000
H	5.507190000	0.386140000	4.190230000
H	4.271330000	-0.904550000	4.325170000
H	-0.196090000	-0.601200000	-4.615200000
C	-4.259360000	-0.277850000	-2.435390000
H	-4.618620000	0.444280000	-3.179310000
H	-4.606910000	-1.281430000	-2.710690000
H	-4.660620000	-0.013230000	-1.448860000

### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.418350000	0.000000000	0.000000000
C	-0.659010000	0.000000000	-1.249850000
C	-2.050360000	0.284880000	-1.325290000
C	0.037830000	-0.425800000	-2.476130000
C	-2.765720000	-0.163440000	-2.419000000
H	-2.543590000	0.797160000	-0.511790000
C	-0.778400000	-0.676580000	-3.611650000
H	0.849110000	0.250830000	-2.756060000
C	-2.150120000	-0.722910000	-3.571340000
H	-2.749480000	-1.122600000	-4.375870000
C	2.097130000	-0.695770000	-0.992450000
C	1.242860000	-1.604280000	-1.748340000
C	3.478210000	-0.539320000	-1.322720000
C	1.862670000	-2.299760000	-2.848630000
H	0.432430000	-2.145670000	-1.123320000
C	4.036040000	-1.257640000	-2.338640000
H	4.064910000	0.207330000	-0.762740000
C	3.199400000	-2.170120000	-3.064570000
H	1.261770000	-2.991750000	-3.430560000
H	3.688390000	-2.803280000	-3.833510000
C	-0.723410000	0.413670000	1.216680000
C	-1.003650000	-0.556690000	2.192670000
C	-1.145740000	1.738730000	1.427240000
C	-1.681900000	-0.206360000	3.358180000

H	-0.668820000	-1.586900000	2.032780000
C	-1.836150000	2.086340000	2.593130000
H	-0.938760000	2.507180000	0.668730000
C	-2.101640000	1.110830000	3.563400000
H	-1.888640000	-0.965220000	4.124230000
H	-2.632560000	1.382690000	4.483450000
C	2.210070000	0.734470000	1.022140000
C	2.046640000	2.114690000	1.197820000
C	3.116200000	0.013410000	1.812300000
C	2.813810000	2.776080000	2.152430000
H	1.339390000	2.666090000	0.571060000
C	3.861390000	0.680490000	2.788710000
H	3.219080000	-1.066980000	1.672710000
C	3.712610000	2.066270000	2.955500000
H	2.704690000	3.858640000	2.284930000
H	4.296740000	2.590140000	3.720390000
C	5.484880000	-1.173950000	-2.685000000
H	5.924620000	-0.250300000	-2.269550000
H	6.031640000	-2.042280000	-2.267280000
H	5.621910000	-1.165150000	-3.782710000
C	-2.319600000	3.489160000	2.797140000
H	-3.329390000	3.586570000	2.369420000
H	-2.359560000	3.730970000	3.870330000
H	-1.646690000	4.203950000	2.298500000
C	4.805930000	-0.086230000	3.659930000
H	5.336980000	-0.847070000	3.069180000
H	5.546730000	0.588210000	4.116720000
H	4.232640000	-0.581770000	4.457380000
H	-0.252810000	-0.876030000	-4.568390000
C	-4.258610000	-0.047640000	-2.419810000
H	-4.560930000	0.590180000	-3.258930000
H	-4.690960000	-1.046610000	-2.552500000
H	-4.626490000	0.385650000	-1.481660000

### Coord\_11

C	0.000000000	0.000000000	0.000000000
C	1.424050000	0.000000000	0.000000000
C	-0.667930000	0.000000000	-1.235150000
C	-2.075830000	0.220030000	-1.291760000
C	0.055700000	-0.310630000	-2.488370000
C	-2.777190000	-0.180010000	-2.407470000
H	-2.586560000	0.651180000	-0.438420000
C	-0.777150000	-0.617200000	-3.619820000
H	0.752200000	0.500900000	-2.762430000
C	-2.141190000	-0.675630000	-3.558660000
H	-2.748180000	-1.061230000	-4.369590000
C	2.107070000	-0.595260000	-1.048430000
C	1.274750000	-1.408910000	-1.943720000
C	3.509040000	-0.443880000	-1.292930000

C	1.941610000	-1.894460000	-3.141520000
H	0.585440000	-2.142940000	-1.378970000
C	4.089520000	-1.009340000	-2.389170000
H	4.093680000	0.176030000	-0.595770000
C	3.282400000	-1.748220000	-3.288410000
H	1.353620000	-2.449460000	-3.870600000
H	3.795130000	-2.213680000	-4.151950000
C	-0.718510000	0.325550000	1.247440000
C	-0.988260000	-0.705460000	2.161140000
C	-1.140530000	1.634150000	1.539760000
C	-1.662840000	-0.429900000	3.348600000
H	-0.654180000	-1.723140000	1.934940000
C	-1.824360000	1.906420000	2.729000000
H	-0.935430000	2.446710000	0.829620000
C	-2.082850000	0.871230000	3.637560000
H	-1.867070000	-1.236100000	4.065000000
H	-2.608990000	1.083960000	4.575630000
C	2.195740000	0.635310000	1.098830000
C	2.111990000	2.016100000	1.320550000
C	3.001330000	-0.171930000	1.914350000
C	2.855510000	2.589710000	2.348250000
H	1.483470000	2.636070000	0.674350000
C	3.726250000	0.408290000	2.959130000
H	3.044260000	-1.251200000	1.738090000
C	3.654900000	1.793110000	3.173980000
H	2.808280000	3.671740000	2.517760000
H	4.221420000	2.248670000	3.993990000
C	5.553520000	-0.918310000	-2.661780000
H	6.014400000	-0.139450000	-2.030510000
H	6.043150000	-1.886150000	-2.442080000
H	5.732490000	-0.663980000	-3.722600000
C	-2.305240000	3.293250000	3.026490000
H	-3.340240000	3.399480000	2.667010000
H	-2.279240000	3.484110000	4.110100000
H	-1.670580000	4.037390000	2.520840000
C	4.563820000	-0.448560000	3.855800000
H	5.023210000	-1.267310000	3.282340000
H	5.362190000	0.147010000	4.324700000
H	3.923040000	-0.873330000	4.642540000
H	-0.261410000	-0.827940000	-4.576860000
C	-4.271050000	-0.099310000	-2.423090000
H	-4.581660000	0.571960000	-3.234360000
H	-4.681790000	-1.100580000	-2.607940000
H	-4.659040000	0.280600000	-1.469000000

Coord\_12

C	0.000000000	0.000000000	0.000000000
C	1.432590000	0.000000000	0.000000000
C	-0.680880000	0.000000000	-1.213020000

C	-2.107360000	0.121140000	-1.244000000
C	0.063610000	-0.129570000	-2.497490000
C	-2.797820000	-0.201560000	-2.383150000
H	-2.632380000	0.423480000	-0.338990000
C	-0.777150000	-0.526180000	-3.628260000
H	0.551250000	0.848380000	-2.745870000
C	-2.129780000	-0.604780000	-3.552880000
H	-2.738410000	-0.971360000	-4.379080000
C	2.121870000	-0.436700000	-1.113400000
C	1.327520000	-1.073530000	-2.192680000
C	3.547090000	-0.326540000	-1.239090000
C	2.062980000	-1.219120000	-3.461030000
H	0.849760000	-2.048750000	-1.815720000
C	4.170870000	-0.648960000	-2.407070000
H	4.114590000	0.064760000	-0.383400000
C	3.405640000	-1.075120000	-3.514080000
H	1.497800000	-1.518370000	-4.347860000
H	3.954030000	-1.263940000	-4.452090000
C	-0.711120000	0.189210000	1.281490000
C	-0.965090000	-0.925170000	2.094570000
C	-1.132980000	1.463610000	1.694020000
C	-1.634400000	-0.764410000	3.305780000
H	-0.631890000	-1.916030000	1.770870000
C	-1.807050000	1.619950000	2.908970000
H	-0.930760000	2.336670000	1.061220000
C	-2.055110000	0.502580000	3.717940000
H	-1.834850000	-1.635560000	3.942190000
H	-2.574250000	0.624360000	4.675750000
C	2.173980000	0.471610000	1.194890000
C	2.223940000	1.838430000	1.498750000
C	2.816110000	-0.463990000	2.018590000
C	2.932880000	2.266980000	2.618070000
H	1.723280000	2.560390000	0.846900000
C	3.512800000	-0.027800000	3.149160000
H	2.758120000	-1.530370000	1.777990000
C	3.571190000	1.341220000	3.448230000
H	2.989350000	3.336540000	2.852890000
H	4.112690000	1.683870000	4.337360000
C	5.651780000	-0.576410000	-2.572050000
H	6.116400000	-0.097460000	-1.694610000
H	6.067350000	-1.594100000	-2.682860000
H	5.905360000	0.010330000	-3.472510000
C	-2.284250000	2.971090000	3.344150000
H	-3.349500000	3.076080000	3.088380000
H	-2.160520000	3.086590000	4.431330000
H	-1.713200000	3.763660000	2.836510000
C	4.177430000	-1.018880000	4.052920000
H	4.494100000	-1.905670000	3.483630000
H	5.061380000	-0.570810000	4.531780000
H	3.462600000	-1.326020000	4.830380000



H	-0.263850000	-0.755010000	-4.578530000
C	-4.291330000	-0.167830000	-2.414730000
H	-4.619350000	0.552620000	-3.178200000
H	-4.672810000	-1.165670000	-2.676760000
H	-4.700590000	0.129290000	-1.438840000

Coord\_13

C	0.000000000	0.000000000	0.000000000
C	1.443980000	0.000000000	0.000000000
C	-0.697310000	0.000000000	-1.183350000
C	-2.136990000	-0.012700000	-1.185730000
C	0.037850000	0.121400000	-2.489610000
C	-2.831680000	-0.227430000	-2.337110000
H	-2.657960000	0.108130000	-0.229120000
C	-0.778920000	-0.399380000	-3.632680000
H	0.196830000	1.237510000	-2.677310000
C	-2.117290000	-0.507880000	-3.571800000
H	-2.707810000	-0.848070000	-4.432080000
C	2.141450000	-0.216050000	-1.163180000
C	1.406930000	-0.563510000	-2.428860000
C	3.581530000	-0.215880000	-1.165280000
C	2.226610000	-0.248840000	-3.643460000
H	1.254970000	-1.696230000	-2.420530000
C	4.278210000	-0.214050000	-2.335860000
H	4.101030000	-0.174340000	-0.201180000
C	3.566090000	-0.143060000	-3.601510000
H	1.693600000	-0.156370000	-4.600740000
H	4.158270000	0.044080000	-4.506280000
C	-0.701200000	0.002180000	1.303540000
C	-0.934010000	-1.207890000	1.970430000
C	-1.123380000	1.213770000	1.870160000
C	-1.596820000	-1.203430000	3.195710000
H	-0.601570000	-2.148500000	1.521840000
C	-1.784700000	1.211830000	3.101430000
H	-0.925160000	2.156100000	1.348430000
C	-2.019010000	-0.000150000	3.765840000
H	-1.792180000	-2.148870000	3.716310000
H	-2.529180000	-0.002490000	4.735910000
C	2.144510000	0.231120000	1.283260000
C	2.393070000	1.541190000	1.713770000
C	2.551780000	-0.859000000	2.065920000
C	3.058510000	1.756510000	2.918540000
H	2.075970000	2.385830000	1.095260000
C	3.214960000	-0.636180000	3.276080000
H	2.343220000	-1.879430000	1.727480000
C	3.466030000	0.675070000	3.703200000
H	3.268860000	2.779690000	3.252970000
H	3.977200000	0.851360000	4.656700000
C	5.769300000	-0.218580000	-2.377490000

H	6.189370000	-0.229630000	-1.359900000
H	6.118950000	-1.112850000	-2.919100000
H	6.130500000	0.680300000	-2.904170000
C	-2.257320000	2.494160000	3.713360000
H	-3.348310000	2.570370000	3.593390000
H	-2.007080000	2.515450000	4.784150000
H	-1.781640000	3.355970000	3.220750000
C	3.632670000	-1.789070000	4.135400000
H	3.704570000	-2.710420000	3.537550000
H	4.611480000	-1.587850000	4.596020000
H	2.882020000	-1.932070000	4.926300000
H	-0.244980000	-0.649380000	-4.560730000
C	-4.322680000	-0.248000000	-2.377330000
H	-4.682590000	0.533710000	-3.066330000
H	-4.672260000	-1.229350000	-2.738660000
H	-4.743800000	-0.064600000	-1.376780000

S<sub>0</sub>\_S<sub>1</sub>S<sub>0</sub>-cyc(C8C9)\_S<sub>0</sub>-final(C8C9)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.357180000	0.000000000	0.000000000
C	-0.799570000	0.000000000	-1.247810000
C	-1.883800000	-0.860940000	-1.373810000
C	-0.475230000	0.896680000	-2.274830000
C	-2.650610000	-0.846140000	-2.550830000
H	-2.145660000	-1.544010000	-0.559690000
C	-1.246900000	0.905130000	-3.442410000
H	0.384810000	1.562700000	-2.178590000
C	-2.321480000	0.046030000	-3.580670000
H	-2.924180000	0.061090000	-4.498640000
C	2.155780000	-0.132230000	-1.231860000
C	1.885010000	-1.155580000	-2.149720000
C	3.233470000	0.752640000	-1.452740000
C	2.659530000	-1.268420000	-3.278340000
H	1.052660000	-1.838990000	-1.969230000
C	3.994110000	0.637180000	-2.591190000
H	3.455360000	1.520270000	-0.703410000
C	3.712780000	-0.372350000	-3.517670000
H	2.453210000	-2.059170000	-4.011900000
H	4.314140000	-0.465840000	-4.428960000
C	-0.801240000	0.010890000	1.240310000
C	-0.515750000	-0.893380000	2.272650000
C	-1.882950000	0.909200000	1.361310000
C	-1.295120000	-0.886200000	3.427630000
H	0.326860000	-1.582080000	2.178080000
C	-2.654300000	0.913610000	2.529300000

H	-2.117080000	1.592540000	0.538950000
C	-2.362080000	0.014900000	3.563750000
H	-1.074400000	-1.590440000	4.239150000
H	-2.968200000	0.009910000	4.475800000
C	2.149940000	0.144810000	1.244230000
C	1.876350000	1.203730000	2.119880000
C	3.171500000	-0.760860000	1.529530000
C	2.632740000	1.344810000	3.286460000
H	1.066440000	1.903700000	1.898930000
C	3.921480000	-0.615170000	2.707450000
H	3.389600000	-1.582220000	0.838860000
C	3.646460000	0.444190000	3.582480000
H	2.423310000	2.178660000	3.968100000
H	4.236290000	0.559180000	4.498820000
C	5.154310000	1.563520000	-2.836390000
H	6.087070000	1.043120000	-2.577270000
H	5.182260000	1.864650000	-3.894260000
H	5.062710000	2.468180000	-2.215690000
C	-3.813090000	1.850250000	2.659520000
H	-4.728440000	1.337530000	2.324520000
H	-3.937550000	2.161500000	3.708290000
H	-3.656940000	2.746450000	2.040060000
C	5.031930000	-1.567530000	3.013260000
H	5.969450000	-1.170720000	2.592380000
H	5.150500000	-1.684760000	4.101850000
H	4.830480000	-2.553910000	2.568690000
H	-0.991050000	1.600170000	-4.251570000
C	-3.833050000	-1.748200000	-2.688200000
H	-4.737000000	-1.217110000	-2.344910000
H	-3.970710000	-2.044100000	-3.740610000
H	-3.701480000	-2.654790000	-2.076910000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.366130000	0.000000000	0.000000000
C	-0.776300000	0.000000000	-1.263430000
C	-1.830630000	-0.894700000	-1.422930000
C	-0.466640000	0.922530000	-2.272560000
C	-2.578010000	-0.886220000	-2.611510000
H	-2.081250000	-1.599080000	-0.623310000
C	-1.217220000	0.924220000	-3.452990000
H	0.368030000	1.616900000	-2.150840000
C	-2.261630000	0.031430000	-3.622840000
H	-2.848070000	0.040330000	-4.551130000
C	2.154630000	-0.241310000	-1.221540000
C	1.854980000	-1.327800000	-2.053960000
C	3.244810000	0.603220000	-1.519090000
C	2.620120000	-1.546960000	-3.175910000
H	1.010810000	-1.977060000	-1.812540000

C	3.994940000	0.382140000	-2.652130000
H	3.484640000	1.426370000	-0.837470000
C	3.687610000	-0.693820000	-3.492000000
H	2.392480000	-2.389370000	-3.842070000
H	4.280630000	-0.871600000	-4.396410000
C	-0.778680000	0.121310000	1.242180000
C	-0.451500000	-0.663230000	2.365760000
C	-1.884270000	1.000590000	1.294470000
C	-1.223030000	-0.555140000	3.525190000
H	0.365560000	-1.384800000	2.298590000
C	-2.633920000	1.107560000	2.468590000
H	-2.155330000	1.580540000	0.407860000
C	-2.299800000	0.335210000	3.592140000
H	-0.976130000	-1.172250000	4.399020000
H	-2.887280000	0.419230000	4.511140000
C	2.151620000	0.252030000	1.219520000
C	1.808920000	1.339420000	2.047020000
C	3.204100000	-0.601880000	1.566310000
C	2.544970000	1.566640000	3.220230000
H	1.014340000	2.031050000	1.731780000
C	3.930330000	-0.373450000	2.740670000
H	3.456190000	-1.450410000	0.920220000
C	3.594010000	0.730960000	3.564000000
H	2.290430000	2.421760000	3.857020000
H	4.172510000	0.919890000	4.476740000
C	5.164880000	1.268150000	-2.980270000
H	6.084480000	0.805240000	-2.595190000
H	5.248890000	1.399690000	-4.069540000
H	5.037650000	2.257690000	-2.515090000
C	-3.818070000	2.020030000	2.521770000
H	-4.721650000	1.446800000	2.262880000
H	-3.933960000	2.438120000	3.533320000
H	-3.700950000	2.847680000	1.806490000
C	5.071030000	-1.265890000	3.108900000
H	5.980310000	-0.921730000	2.590240000
H	5.248030000	-1.237510000	4.195930000
H	4.861600000	-2.304800000	2.809490000
H	-0.971450000	1.639060000	-4.247960000
C	-3.727080000	-1.825350000	-2.784610000
H	-4.658200000	-1.320500000	-2.477140000
H	-3.817160000	-2.131220000	-3.839120000
H	-3.589520000	-2.724080000	0.000000000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.375080000	0.000000000	0.000000000
C	-0.752720000	0.000000000	-1.278610000
C	-1.775110000	-0.927400000	-1.471190000
C	-0.458990000	0.946990000	-2.270340000

C	-2.502480000	-0.925490000	-2.671230000
H	-2.013470000	-1.651960000	-0.685720000
C	-1.187860000	0.941830000	-3.463460000
H	0.348620000	1.668750000	-2.123500000
C	-2.200120000	0.016360000	-3.664470000
H	-2.769730000	0.019010000	-4.602980000
C	2.153420000	-0.349570000	-1.201450000
C	1.825050000	-1.491550000	-1.943980000
C	3.255830000	0.447800000	-1.570600000
C	2.580490000	-1.816630000	-3.049290000
H	0.969390000	-2.101050000	-1.645940000
C	3.995200000	0.121310000	-2.688410000
H	3.513560000	1.320300000	-0.960890000
C	3.661940000	-1.013260000	-3.436780000
H	2.331610000	-2.704620000	-3.644320000
H	4.246450000	-1.274770000	-4.326500000
C	-0.756070000	0.232070000	1.233790000
C	-0.387180000	-0.422940000	2.433790000
C	-1.884770000	1.086850000	1.222970000
C	-1.150660000	-0.213800000	3.588940000
H	0.401020000	-1.178030000	2.404370000
C	-2.612480000	1.297570000	2.393780000
H	-2.192210000	1.556840000	0.285790000
C	-2.236840000	0.660930000	3.590230000
H	-0.877470000	-0.738280000	4.515120000
H	-2.805930000	0.835190000	4.506780000
C	2.153330000	0.356040000	1.185620000
C	1.744480000	1.465190000	1.966030000
C	3.236000000	-0.441170000	1.587370000
C	2.462000000	1.776690000	3.138610000
H	0.969720000	2.144940000	1.564510000
C	3.939890000	-0.131400000	2.751340000
H	3.520800000	-1.313120000	0.986260000
C	3.544560000	1.008930000	3.521090000
H	2.164940000	2.648100000	3.731610000
H	4.112650000	1.269990000	4.423980000
C	5.174640000	0.959500000	-3.094510000
H	6.077230000	0.577490000	-2.596640000
H	5.314400000	0.918820000	-4.185380000
H	5.015750000	2.007650000	-2.798550000
C	-3.821170000	2.179050000	2.376770000
H	-4.711240000	1.555860000	2.201900000
H	-3.929110000	2.699340000	3.340260000
H	-3.743370000	2.927280000	1.574590000
C	5.109830000	-0.959120000	3.174490000
H	5.988310000	-0.684300000	2.568120000
H	5.342190000	-0.784890000	4.237660000
H	4.897380000	-2.030540000	3.027950000
H	-0.953120000	1.675440000	-4.244580000
C	-3.615970000	-1.900470000	-2.879580000

H	-4.572200000	-1.422540000	-2.609490000
H	-3.657380000	-2.214780000	-3.934460000
H	-3.473870000	-2.791160000	-2.247680000

Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.384030000	0.000000000	0.000000000
C	-0.728850000	0.000000000	-1.293340000
C	-1.717280000	-0.958990000	-1.518480000
C	-0.452230000	0.970020000	-2.268250000
C	-2.424040000	-0.963890000	-2.729850000
H	-1.942380000	-1.702580000	-0.746750000
C	-1.158770000	0.957940000	-3.473870000
H	0.326660000	1.718200000	-2.096730000
C	-2.136900000	0.000850000	-3.705490000
H	-2.689120000	-0.002780000	-4.654100000
C	2.152170000	-0.456130000	-1.171670000
C	1.795240000	-1.645630000	-1.820580000
C	3.266500000	0.287820000	-1.606700000
C	2.540670000	-2.075290000	-2.899310000
H	0.928440000	-2.210250000	-1.470780000
C	3.994860000	-0.142940000	-2.699460000
H	3.542100000	1.203180000	-1.072540000
C	3.635770000	-1.327940000	-3.352180000
H	2.270650000	-3.002490000	-3.420060000
H	4.211620000	-1.671880000	-4.219460000
C	-0.733420000	0.342170000	1.215100000
C	-0.322870000	-0.175360000	2.475640000
C	-1.884380000	1.167980000	1.147190000
C	-1.078040000	0.134240000	3.617870000
H	0.433550000	-0.962290000	2.494800000
C	-2.589940000	1.482740000	2.305070000
H	-2.227590000	1.523260000	0.173780000
C	-2.173230000	0.989080000	3.557260000
H	-0.778500000	-0.293260000	4.585960000
H	-2.724220000	1.253720000	4.461800000
C	2.155060000	0.456050000	1.142920000
C	1.683500000	1.580840000	1.878330000
C	3.267160000	-0.280240000	1.592610000
C	2.384650000	1.974240000	3.043440000
H	0.932030000	2.246770000	1.398850000
C	3.950230000	0.108900000	2.739700000
H	3.583280000	-1.172010000	1.036430000
C	3.498900000	1.276260000	3.455320000
H	2.047880000	2.857460000	3.594340000
H	4.057710000	1.607230000	4.342420000
C	5.183580000	0.640490000	-3.177880000
H	6.065640000	0.360060000	-2.584540000
H	5.378390000	0.430200000	-4.240580000

H	4.997070000	1.718680000	-3.060150000
C	-3.822270000	2.327600000	2.225340000
H	-4.697090000	1.665930000	2.140920000
H	-3.922900000	2.944350000	3.130520000
H	-3.784010000	2.986760000	1.346420000
C	5.148320000	-0.650160000	3.209800000
H	5.994000000	-0.459670000	2.528480000
H	5.432550000	-0.333320000	4.226870000
H	4.937740000	-1.732640000	3.220790000
H	-0.935960000	1.709300000	-4.241550000
C	-3.499770000	-1.973420000	-2.972880000
H	-4.478940000	-1.523040000	-2.741640000
H	-3.491540000	-2.294600000	-4.026270000
H	-3.354600000	-2.855970000	-2.330360000

### Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.392980000	0.000000000	0.000000000
C	-0.704690000	0.000000000	-1.307640000
C	-1.657170000	-0.989420000	-1.564700000
C	-0.446310000	0.991600000	-2.266360000
C	-2.342720000	-1.001320000	-2.787250000
H	-1.868080000	-1.750850000	-0.806220000
C	-1.129890000	0.972560000	-3.484250000
H	0.302230000	1.765160000	-2.070700000
C	-2.071950000	-0.015030000	-3.745870000
H	-2.606220000	-0.024970000	-4.704430000
C	2.150860000	-0.560100000	-1.132330000
C	1.765550000	-1.788920000	-1.684660000
C	3.276830000	0.124800000	-1.626980000
C	2.500670000	-2.320870000	-2.726990000
H	0.887990000	-2.304070000	-1.288440000
C	3.993930000	-0.408180000	-2.684960000
H	3.570250000	1.076230000	-1.171390000
C	3.609110000	-1.635130000	-3.238660000
H	2.209630000	-3.280700000	-3.170910000
H	4.176130000	-2.059470000	-4.075850000
C	-0.710750000	0.450630000	1.186170000
C	-0.258660000	0.076540000	2.490540000
C	-1.883060000	1.243990000	1.067470000
C	-1.005240000	0.485280000	3.611350000
H	0.463520000	-0.738090000	2.569110000
C	-2.566250000	1.662140000	2.202710000
H	-2.261310000	1.481700000	0.072590000
C	-2.109040000	1.316540000	3.492780000
H	-0.679290000	0.157910000	4.610550000
H	-2.642230000	1.670660000	4.375760000
C	2.156810000	0.551320000	1.091850000
C	1.626420000	1.686340000	1.785240000

C	3.297550000	-0.120650000	1.582080000
C	2.313710000	2.158840000	2.936480000
H	0.900780000	2.338020000	1.236190000
C	3.961400000	0.345460000	2.706150000
H	3.643470000	-1.028850000	1.070420000
C	3.457780000	1.531390000	3.368330000
H	1.940290000	3.049970000	3.447530000
H	4.008620000	1.929630000	4.234000000
C	5.191690000	0.314160000	-3.229420000
H	6.050040000	0.152580000	-2.561520000
H	5.440460000	-0.057950000	-4.235120000
H	4.981640000	1.392390000	-3.293870000
C	-3.821260000	2.466040000	2.068130000
H	-4.679110000	1.778070000	2.079040000
H	-3.915180000	3.172480000	2.905490000
H	-3.822660000	3.027820000	1.123730000
C	5.186520000	-0.341910000	3.214910000
H	5.997940000	-0.248660000	2.473780000
H	5.518730000	0.110800000	4.164230000
H	4.982530000	-1.413100000	3.384760000
H	-0.919880000	1.740620000	-4.238960000
C	-3.378540000	-2.044060000	-3.064240000
H	-4.378360000	-1.621770000	-2.873230000
H	-3.319860000	-2.370490000	-4.114220000
H	-3.231770000	-2.918440000	-2.411020000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.401930000	0.000000000	0.000000000
C	-0.680240000	0.000000000	-1.321480000
C	-1.594830000	-1.018630000	-1.609740000
C	-0.441170000	1.011720000	-2.264740000
C	-2.258540000	-1.037720000	-2.843290000
H	-1.790660000	-1.796720000	-0.863950000
C	-1.101160000	0.985700000	-3.494660000
H	0.275420000	1.809560000	-2.045560000
C	-2.005250000	-0.031230000	-3.785520000
H	-2.520990000	-0.047490000	-4.753870000
C	2.149520000	-0.660630000	-1.083680000
C	1.736020000	-1.920380000	-1.537230000
C	3.286790000	-0.039730000	-1.631170000
C	2.460520000	-2.551400000	-2.533530000
H	0.848060000	-2.382050000	-1.100340000
C	3.992390000	-0.671960000	-2.644820000
H	3.597990000	0.940780000	-1.256530000
C	3.581970000	-1.932160000	-3.096900000
H	2.148580000	-3.537130000	-2.898690000
H	4.140000000	-2.434170000	-3.896560000
C	-0.688050000	0.556460000	1.147170000



C	-0.194630000	0.329700000	2.478070000
C	-1.880750000	1.314920000	0.984090000
C	-0.932300000	0.835590000	3.569150000
H	0.491270000	-0.506010000	2.626360000
C	-2.541380000	1.834870000	2.087000000
H	-2.293240000	1.434090000	-0.017330000
C	-2.044300000	1.640150000	3.396660000
H	-0.579910000	0.610290000	4.588480000
H	-2.560020000	2.081760000	4.248640000
C	2.158590000	0.641160000	1.032910000
C	1.573650000	1.781860000	1.688030000
C	3.327120000	0.036070000	1.555990000
C	2.249950000	2.330330000	2.819390000
H	0.875530000	2.420130000	1.077580000
C	3.973440000	0.576310000	2.651240000
H	3.701240000	-0.885420000	1.088060000
C	3.421910000	1.773000000	3.261780000
H	1.843110000	3.226090000	3.293250000
H	3.966250000	2.235550000	4.100710000
C	5.198950000	-0.016360000	-3.248460000
H	6.030770000	-0.045880000	-2.529840000
H	5.500250000	-0.537600000	-4.170210000
H	4.969450000	1.031340000	-3.493780000
C	-3.818000000	2.594710000	1.905670000
H	-4.657180000	1.893130000	2.015160000
H	-3.905850000	3.383150000	2.666520000
H	-3.859140000	3.052310000	0.907950000
C	5.224440000	-0.037280000	3.190150000
H	6.000710000	-0.051620000	2.406390000
H	5.600400000	0.541180000	4.051230000
H	5.031530000	-1.074440000	3.516730000
H	-0.904770000	1.769380000	-4.236910000
C	-3.252360000	-2.112260000	-3.153420000
H	-4.270410000	-1.718530000	-3.003930000
H	-3.142600000	-2.442290000	-4.197970000
H	-3.105460000	-2.978500000	-2.489500000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.410880000	0.000000000	0.000000000
C	-0.655530000	0.000000000	-1.334860000
C	-1.530330000	-1.046570000	-1.653470000
C	-0.436770000	1.030350000	-2.263460000
C	-2.171540000	-1.073000000	-2.897850000
H	-1.710240000	-1.840110000	-0.919790000
C	-1.072510000	0.997350000	-3.505120000
H	0.246320000	1.851350000	-2.021480000
C	-1.936780000	-0.047690000	-3.824400000
H	-2.433420000	-0.070250000	-4.802330000

C	2.148120000	-0.756860000	-1.026010000
C	1.706670000	-2.039060000	-1.379370000
C	3.296390000	-0.204190000	-1.619130000
C	2.420230000	-2.765040000	-2.320300000
H	0.808690000	-2.443890000	-0.907950000
C	3.990240000	-0.931810000	-2.579180000
H	3.625310000	0.798260000	-1.327180000
C	3.554340000	-2.216420000	-2.927850000
H	2.087530000	-3.769830000	-2.605410000
H	4.103240000	-2.792670000	-3.682790000
C	-0.665340000	0.658700000	1.098370000
C	-0.130870000	0.581050000	2.438160000
C	-1.877400000	1.380800000	0.897280000
C	-0.859260000	1.181440000	3.491430000
H	0.517140000	-0.266780000	2.665450000
C	-2.515280000	2.000020000	1.958270000
H	-2.323240000	1.382370000	-0.095820000
C	-1.979050000	1.956720000	3.269090000
H	-0.480420000	1.058900000	4.519820000
H	-2.477680000	2.482800000	4.080900000
C	2.160390000	0.724930000	0.966660000
C	1.525600000	1.867730000	1.587830000
C	3.355840000	0.188390000	1.514710000
C	2.194080000	2.488750000	2.693690000
H	0.855970000	2.494460000	0.923740000
C	3.986390000	0.799570000	2.575710000
H	3.756450000	-0.743540000	1.089440000
C	3.391950000	2.000000000	3.137320000
H	1.757240000	3.386570000	3.133340000
H	3.931410000	2.523560000	3.944520000
C	5.205350000	-0.347880000	-3.234650000
H	6.008200000	-0.236680000	-2.491340000
H	5.557460000	-1.001030000	-4.048180000
H	4.960450000	0.639150000	-3.654180000
C	-3.812380000	2.713960000	1.738350000
H	-4.631230000	2.011780000	1.947990000
H	-3.894790000	3.575900000	2.414890000
H	-3.893250000	3.062160000	0.700160000
C	5.262060000	0.260890000	3.136120000
H	6.002860000	0.131430000	2.328500000
H	5.677270000	0.951800000	3.890180000
H	5.084440000	-0.719700000	3.613770000
H	-0.890520000	1.795590000	-4.235500000
C	-3.121330000	-2.177880000	-3.240170000
H	-4.155100000	-1.813090000	-3.133380000
H	-2.960010000	-2.509820000	-4.277210000
H	-2.975760000	-3.036100000	-2.565650000

Coord\_8

C	0.00000000	0.00000000	0.00000000
C	1.41983000	0.00000000	0.00000000
C	-0.63055000	0.00000000	-1.34779000
C	-1.46370000	-1.07320000	-1.69581000
C	-0.43302000	1.04747000	-2.26258000
C	-2.08178000	-1.10708000	-2.95079000
H	-1.62693000	-1.88096000	-0.97356000
C	-1.04389000	1.00752000	-3.51568000
H	0.21507000	1.89045000	-1.99859000
C	-1.86652000	-0.06435000	-3.86244000
H	-2.34348000	-0.09317000	-4.84973000
C	2.14669000	-0.84799000	-0.95971000
C	1.67751000	-2.14414000	-1.21224000
C	3.30562000	-0.36701000	-1.59091000
C	2.37982000	-2.96007000	-2.08887000
H	0.76990000	-2.48940000	-0.71271000
C	3.98747000	-1.18528000	-2.48842000
H	3.65218000	0.65015000	-1.38273000
C	3.52625000	-2.48538000	-2.73271000
H	2.02651000	-3.97706000	-2.29324000
H	4.06585000	-3.13179000	-3.43606000
C	-0.64261000	0.75642000	1.04011000
C	-0.06746000	0.82749000	2.37110000
C	-1.87296000	1.44165000	0.80723000
C	-0.78617000	1.51914000	3.37877000
H	0.54148000	-0.02130000	2.68519000
C	-2.48791000	2.15666000	1.81691000
H	-2.35118000	1.32845000	-0.16301000
C	-1.91335000	2.26308000	3.11063000
H	-0.38090000	1.49881000	4.40523000
H	-2.39526000	2.86958000	3.87342000
C	2.16221000	0.80204000	0.89371000
C	1.48264000	1.94441000	1.48564000
C	3.38367000	0.33483000	1.45874000
C	2.14673000	2.63431000	2.56073000
H	0.84194000	2.56227000	0.77513000
C	4.00027000	1.01343000	2.48046000
H	3.80897000	-0.60501000	1.07480000
C	3.36846000	2.21150000	2.99656000
H	1.68353000	3.53234000	2.96930000
H	3.90481000	2.79252000	3.76736000
C	5.21088000	-0.67719000	-3.18795000
H	5.98268000	-0.42146000	-2.44727000
H	5.61177000	-1.44104000	-3.87246000
H	4.95454000	0.22039000	-3.76980000
C	-3.80430000	2.82413000	1.56641000
H	-4.60115000	2.13438000	1.87608000
H	-3.88187000	3.75034000	2.15185000
H	-3.92480000	3.05932000	0.50112000
C	5.29938000	0.54983000	3.05371000

H	6.004930000	0.300840000	2.242100000
H	5.749100000	1.336950000	3.684170000
H	5.140930000	-0.352420000	3.673210000
H	-0.877020000	1.819220000	-4.234790000
C	-2.985560000	-2.240800000	-3.324260000
H	-4.032430000	-1.905250000	-3.261240000
H	-2.772380000	-2.572930000	-4.351630000
H	-2.842740000	-3.091170000	-2.639310000

### Coord\_9

C	0.000000000	0.000000000	0.000000000
C	1.428780000	0.000000000	0.000000000
C	-0.605320000	0.000000000	-1.360240000
C	-1.395030000	-1.098470000	-1.736650000
C	-0.429870000	1.063080000	-2.262160000
C	-1.989310000	-1.139900000	-3.001970000
H	-1.540850000	-1.919210000	-1.025110000
C	-1.015230000	1.016230000	-3.526360000
H	0.181770000	1.926820000	-1.977040000
C	-1.794460000	-0.081160000	-3.899560000
H	-2.251170000	-0.116180000	-4.895960000
C	2.145200000	-0.933230000	-0.885240000
C	1.648560000	-2.234890000	-1.037080000
C	3.314460000	-0.526600000	-1.546670000
C	2.339330000	-3.134940000	-1.840910000
H	0.731720000	-2.518570000	-0.516100000
C	3.984080000	-1.429960000	-2.373150000
H	3.678600000	0.498000000	-1.422700000
C	3.497700000	-2.736640000	-2.512890000
H	1.965570000	-4.157260000	-1.964490000
H	4.027840000	-3.448470000	-3.158160000
C	-0.619890000	0.848700000	0.972840000
C	-0.004490000	1.066000000	2.277530000
C	-1.867380000	1.497490000	0.714080000
C	-0.713070000	1.845040000	3.232130000
H	0.564610000	0.229250000	2.684250000
C	-2.459250000	2.303880000	1.663370000
H	-2.376940000	1.274130000	-0.219290000
C	-1.847230000	2.556090000	2.922120000
H	-0.281410000	1.925200000	4.245870000
H	-2.312840000	3.238020000	3.627570000
C	2.164060000	0.871970000	0.814720000
C	1.445150000	2.012460000	1.382310000
C	3.410580000	0.473980000	1.388730000
C	2.108520000	2.767390000	2.421640000
H	0.833440000	2.624690000	0.631940000
C	4.015100000	1.216190000	2.366520000
H	3.858680000	-0.471630000	1.044640000
C	3.351980000	2.406760000	2.841060000

H	1.622710000	3.664480000	2.802320000
H	3.887090000	3.041430000	3.571050000
C	5.215530000	-1.001060000	-3.108630000
H	5.954580000	-0.602070000	-2.398310000
H	5.662940000	-1.851100000	-3.647430000
H	4.951610000	-0.219450000	-3.835980000
C	-3.793650000	2.925470000	1.389990000
H	-4.566880000	2.261060000	1.797900000
H	-3.866990000	3.906140000	1.878590000
H	-3.953610000	3.045760000	0.311260000
C	5.336380000	0.826870000	2.944050000
H	6.007440000	0.457220000	2.148900000
H	5.815690000	1.691440000	3.436980000
H	5.200590000	0.023390000	3.692790000
H	-0.864150000	1.840290000	-4.234880000
C	-2.845170000	-2.300890000	-3.405440000
H	-3.902440000	-1.994800000	-3.387130000
H	-2.580010000	-2.631490000	-4.420930000
H	-2.706500000	-3.143660000	-2.710350000

#### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.437740000	0.000000000	0.000000000
C	-0.579850000	0.000000000	-1.372220000
C	-1.324380000	-1.122330000	-1.775880000
C	-0.427250000	1.077150000	-2.262240000
C	-1.894190000	-1.171380000	-3.051280000
H	-1.452150000	-1.954810000	-1.074300000
C	-0.986470000	1.023480000	-3.537190000
H	0.146550000	1.960400000	-1.956970000
C	-1.720610000	-0.098060000	-3.935700000
H	-2.156480000	-0.139190000	-4.940930000
C	2.143680000	-1.011840000	-0.803140000
C	1.619850000	-2.310710000	-0.855180000
C	3.322900000	-0.681420000	-1.486750000
C	2.298750000	-3.288220000	-1.578260000
H	0.694170000	-2.531490000	-0.319560000
C	3.980060000	-1.663490000	-2.234210000
H	3.704540000	0.343400000	-1.446770000
C	3.468690000	-2.967940000	-2.270050000
H	1.904720000	-4.309130000	-1.621610000
H	3.989220000	-3.739860000	-2.851200000
C	-0.597170000	0.934700000	0.897100000
C	0.057960000	1.293640000	2.158450000
C	-1.860620000	1.548290000	0.617950000
C	-0.640020000	2.155670000	3.052840000
H	0.586830000	0.483460000	2.661290000
C	-2.429250000	2.440770000	1.498150000
H	-2.400380000	1.221110000	-0.265320000

C	-1.780750000	2.832690000	2.704780000
H	-0.182020000	2.333400000	4.043420000
H	-2.230480000	3.584190000	3.345110000
C	2.165940000	0.934240000	0.730380000
C	1.413430000	2.072510000	1.278500000
C	3.436520000	0.604460000	1.305500000
C	2.079950000	2.888400000	2.277380000
H	0.830670000	2.682700000	0.494170000
C	4.030890000	1.406240000	2.235070000
H	3.905450000	-0.345120000	0.999620000
C	3.342930000	2.585200000	2.672270000
H	1.575470000	3.784110000	2.633230000
H	3.878770000	3.269480000	3.357360000
C	5.219290000	-1.316300000	-2.997280000
H	5.924230000	-0.780420000	-2.344530000
H	5.710760000	-2.225490000	-3.378320000
H	4.951510000	-0.674050000	-3.848800000
C	-3.780330000	3.018160000	1.209150000
H	-4.528360000	2.391640000	1.711860000
H	-3.850040000	4.043020000	1.596240000
H	-3.979510000	3.023370000	0.130690000
C	5.373040000	1.089430000	2.808510000
H	6.010910000	0.601370000	2.050320000
H	5.876910000	2.010590000	3.153050000
H	5.262960000	0.403270000	3.670700000
H	-0.851780000	1.858790000	-4.235830000
C	-2.700290000	-2.358020000	-3.483480000
H	-3.765190000	-2.081510000	-3.510700000
H	-2.383230000	-2.685370000	-4.484850000
H	-2.567140000	-3.193520000	-2.778610000

### Coord\_11

C	0.000000000	0.000000000	0.000000000
C	1.439980000	0.000000000	0.000000000
C	-0.620650000	0.000000000	-1.350710000
C	-1.235570000	-1.176750000	-1.810500000
C	-0.613710000	1.141750000	-2.167900000
C	-1.828360000	-1.212110000	-3.075720000
H	-1.241640000	-2.063630000	-1.166880000
C	-1.204200000	1.103960000	-3.429200000
H	-0.137300000	2.062590000	-1.813470000
C	-1.811500000	-0.069240000	-3.886960000
H	-2.267920000	-0.097740000	-4.883350000
C	2.143810000	-0.793060000	-1.024990000
C	1.852330000	-2.158450000	-1.146310000
C	3.094670000	-0.186570000	-1.858970000
C	2.531970000	-2.920210000	-2.093650000
H	1.103900000	-2.605980000	-0.487970000
C	3.755430000	-0.954570000	-2.822380000

H	3.297460000	0.884630000	-1.761860000
C	3.475240000	-2.323390000	-2.933350000
H	2.317950000	-3.990330000	-2.191740000
H	3.996460000	-2.926660000	-3.687000000
C	-0.631380000	0.640920000	1.084300000
C	0.080030000	0.819870000	2.368430000
C	-1.989170000	1.094960000	0.996820000
C	-0.637590000	1.546680000	3.396230000
H	0.515780000	-0.124540000	2.751170000
C	-2.581110000	1.762780000	2.038340000
H	-2.551460000	0.854570000	0.095480000
C	-1.858340000	2.066560000	3.239350000
H	-0.119960000	1.703210000	4.358340000
H	-2.335740000	2.672130000	4.008590000
C	2.156830000	0.732390000	0.932580000
C	1.404570000	1.685380000	1.782260000
C	3.515690000	0.398170000	1.251270000
C	2.122850000	2.181630000	2.961230000
H	0.940970000	2.538040000	1.166760000
C	4.149460000	0.949210000	2.325090000
H	4.020200000	-0.352430000	0.624490000
C	3.425090000	1.874010000	3.163500000
H	1.598630000	2.868130000	3.629020000
H	3.975740000	2.320330000	4.009510000
C	4.750200000	-0.314550000	-3.739140000
H	5.364750000	0.410390000	-3.184700000
H	5.412670000	-1.073620000	-4.183570000
H	4.213390000	0.207070000	-4.544830000
C	-4.010140000	2.195780000	1.954900000
H	-4.619920000	1.495530000	2.543290000
H	-4.125530000	3.207480000	2.369470000
H	-4.359720000	2.190420000	0.913850000
C	5.570540000	0.631750000	2.654570000
H	6.104150000	0.268280000	1.759810000
H	6.085940000	1.531960000	3.033070000
H	5.610040000	-0.152550000	3.433180000
H	-1.195500000	1.995000000	-4.069240000
C	-2.499950000	-2.456570000	-3.569720000
H	-3.590470000	-2.310160000	-3.553110000
H	-2.177810000	-2.676200000	-4.598420000
H	-2.245500000	-3.314320000	-2.927900000

### Coord\_12

C	0.000000000	0.000000000	0.000000000
C	1.442230000	0.000000000	0.000000000
C	-0.660670000	0.000000000	-1.327990000
C	-1.145870000	-1.207970000	-1.854320000
C	-0.802300000	1.187830000	-2.060280000
C	-1.765480000	-1.225940000	-3.106890000

H	-1.027290000	-2.132640000	-1.278970000
C	-1.427650000	1.167040000	-3.305020000
H	-0.422150000	2.128650000	-1.649380000
C	-1.908560000	-0.034950000	-3.832110000
H	-2.388480000	-0.048680000	-4.817580000
C	2.143930000	-0.526740000	-1.188630000
C	2.134660000	-1.905430000	-1.439420000
C	2.810950000	0.349780000	-2.057360000
C	2.807110000	-2.405460000	-2.551980000
H	1.610240000	-2.574490000	-0.752020000
C	3.470440000	-0.157980000	-3.180490000
H	2.796660000	1.426330000	-1.858930000
C	3.468940000	-1.538170000	-3.424810000
H	2.812390000	-3.483580000	-2.750500000
H	3.986120000	-1.937160000	-4.305720000
C	-0.663880000	0.316410000	1.181070000
C	0.078530000	0.330610000	2.474970000
C	-2.080440000	0.555860000	1.192290000
C	-0.682810000	0.907220000	3.596580000
H	0.408320000	-0.713660000	2.737590000
C	-2.714650000	0.974260000	2.328260000
H	-2.636380000	0.394950000	0.265340000
C	-1.970820000	1.218680000	3.541210000
H	-0.143190000	1.065140000	4.543930000
H	-2.497160000	1.657150000	4.393520000
C	2.147760000	0.488010000	1.080530000
C	1.397310000	1.178180000	2.171620000
C	3.563690000	0.269510000	1.194820000
C	2.168790000	1.320150000	3.429280000
H	1.060250000	2.212420000	1.809360000
C	4.230810000	0.558860000	2.347130000
H	4.085860000	-0.181690000	0.340330000
C	3.496270000	1.085300000	3.479210000
H	1.637510000	1.694770000	4.311340000
H	4.065670000	1.257230000	4.405400000
C	4.165240000	0.767790000	-4.129680000
H	4.552810000	1.646390000	-3.592210000
H	5.005510000	0.255160000	-4.622580000
H	3.448450000	1.100560000	-4.894510000
C	-4.189790000	1.206340000	2.358240000
H	-4.660460000	0.436380000	2.988810000
H	-4.406540000	2.198200000	2.784420000
H	-4.615390000	1.150050000	1.345830000
C	5.702140000	0.351970000	2.486440000
H	6.160500000	0.139800000	1.506710000
H	6.170350000	1.256880000	2.909920000
H	5.898610000	-0.498670000	3.162680000
H	-1.547880000	2.096070000	-3.875820000
C	-2.302730000	-2.503890000	-3.673460000
H	-3.401600000	-2.490030000	-3.619120000



H	-1.991810000	-2.611060000	-4.723160000
H	-1.927970000	-3.367810000	-3.103050000

Coord\_13

C	0.000000000	0.000000000	0.000000000
C	1.444480000	0.000000000	0.000000000
C	-0.699880000	0.000000000	-1.304090000
C	-1.058750000	-1.215690000	-1.906010000
C	-0.990020000	1.214230000	-1.940120000
C	-1.709360000	-1.213590000	-3.142780000
H	-0.815340000	-2.160470000	-1.408510000
C	-1.653680000	1.210670000	-3.164990000
H	-0.702460000	2.157370000	-1.466580000
C	-2.012090000	0.003030000	-3.770090000
H	-2.518600000	0.005480000	-4.742120000
C	2.144030000	-0.228070000	-1.284150000
C	2.443230000	-1.534230000	-1.694050000
C	2.495980000	0.863550000	-2.092110000
C	3.102230000	-1.744500000	-2.903120000
H	2.170270000	-2.379340000	-1.055470000
C	3.149410000	0.645870000	-3.308420000
H	2.244400000	1.879910000	-1.771500000
C	3.451550000	-0.661350000	-3.714110000
H	3.347730000	-2.764130000	-3.224180000
H	3.960770000	-0.833850000	-4.669440000
C	-0.694650000	-0.012240000	1.185060000
C	0.052270000	-0.156200000	2.483400000
C	-2.133630000	-0.000610000	1.190280000
C	-0.775840000	0.265920000	3.657230000
H	0.260340000	-1.272020000	2.626630000
C	-2.827790000	0.159240000	2.350840000
H	-2.654790000	-0.076270000	0.228660000
C	-2.116480000	0.349560000	3.603610000
H	-0.251640000	0.434910000	4.608960000
H	-2.711190000	0.609750000	4.488910000
C	2.138730000	0.215360000	1.165620000
C	1.391660000	0.584130000	2.418650000
C	3.577830000	0.193990000	1.174800000
C	2.217600000	0.368830000	3.649070000
H	1.186760000	1.708210000	2.366940000
C	4.270460000	0.224510000	2.347010000
H	4.099490000	0.102090000	0.214860000
C	3.557120000	0.256100000	3.612830000
H	1.691860000	0.371470000	4.614930000
H	4.149130000	0.144980000	4.530560000
C	3.513670000	1.799800000	-4.190250000
H	3.573010000	2.729680000	-3.604370000
H	4.487180000	1.621770000	-4.671510000
H	2.741990000	1.913250000	-4.965620000

C	-4.318820000	0.175420000	2.391540000
H	-4.679000000	-0.645110000	3.033860000
H	-4.670600000	1.133760000	2.808590000
H	-4.739890000	0.049760000	1.381860000
C	5.761320000	0.201140000	2.392240000
H	6.183540000	0.151070000	1.376510000
H	6.129500000	1.114580000	2.887890000
H	6.103720000	-0.676670000	2.965210000
H	-1.902820000	2.158930000	-3.656700000
C	-2.116100000	-2.500400000	-3.791230000
H	-3.206580000	-2.619260000	-3.706850000
H	-1.832500000	-2.492910000	-4.853940000
H	-1.624450000	-3.353940000	-3.299600000

S<sub>0</sub>\_S<sub>1</sub>S<sub>0</sub>-pyr(C1)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.357180000	0.000000000	0.000000000
C	-0.799570000	0.000000000	-1.247810000
C	-1.883800000	-0.860940000	-1.373810000
C	-0.475230000	0.896680000	-2.274830000
C	-2.650610000	-0.846140000	-2.550830000
H	-2.145660000	-1.544010000	-0.559690000
C	-1.246900000	0.905130000	-3.442410000
H	0.384810000	1.562700000	-2.178590000
C	-2.321480000	0.046030000	-3.580670000
H	-2.924180000	0.061090000	-4.498640000
C	2.155780000	-0.132230000	-1.231860000
C	1.885010000	-1.155580000	-2.149720000
C	3.233470000	0.752640000	-1.452740000
C	2.659530000	-1.268420000	-3.278340000
H	1.052660000	-1.838990000	-1.969230000
C	3.994110000	0.637180000	-2.591190000
H	3.455360000	1.520270000	-0.703410000
C	3.712780000	-0.372350000	-3.517670000
H	2.453210000	-2.059170000	-4.011900000
H	4.314140000	-0.465840000	-4.428960000
C	-0.801240000	0.010890000	1.240310000
C	-0.515750000	-0.893380000	2.272650000
C	-1.882950000	0.909200000	1.361310000
C	-1.295120000	-0.886200000	3.427630000
H	0.326860000	-1.582080000	2.178080000
C	-2.654300000	0.913610000	2.529300000
H	-2.117080000	1.592540000	0.538950000
C	-2.362080000	0.014900000	3.563750000
H	-1.074400000	-1.590440000	4.239150000

H	-2.968200000	0.009910000	4.475800000
C	2.149940000	0.144810000	1.244230000
C	1.876350000	1.203730000	2.119880000
C	3.171500000	-0.760860000	1.529530000
C	2.632740000	1.344810000	3.286460000
H	1.066440000	1.903700000	1.898930000
C	3.921480000	-0.615170000	2.707450000
H	3.389600000	-1.582220000	0.838860000
C	3.646460000	0.444190000	3.582480000
H	2.423310000	2.178660000	3.968100000
H	4.236290000	0.559180000	4.498820000
C	5.154310000	1.563520000	-2.836390000
H	6.087070000	1.043120000	-2.577270000
H	5.182260000	1.864650000	-3.894260000
H	5.062710000	2.468180000	-2.215690000
C	-3.813090000	1.850250000	2.659520000
H	-4.728440000	1.337530000	2.324520000
H	-3.937550000	2.161500000	3.708290000
H	-3.656940000	2.746450000	2.040060000
C	5.031930000	-1.567530000	3.013260000
H	5.969450000	-1.170720000	2.592380000
H	5.150500000	-1.684760000	4.101850000
H	4.830480000	-2.553910000	2.568690000
H	-0.991050000	1.600170000	-4.251570000
C	-3.833050000	-1.748200000	-2.688200000
H	-4.737000000	-1.217110000	-2.344910000
H	-3.970710000	-2.044100000	-3.740610000
H	-3.701480000	-2.654790000	-2.076910000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.366480000	0.000000000	0.000000000
C	-0.712430000	0.000000000	-1.305530000
C	-1.747210000	-0.903840000	-1.535090000
C	-0.372960000	0.956260000	-2.272000000
C	-2.451270000	-0.860990000	-2.749360000
H	-2.017870000	-1.639200000	-0.771260000
C	-1.077690000	0.989600000	-3.480420000
H	0.447620000	1.655620000	-2.095090000
C	-2.106020000	0.094240000	-3.718560000
H	-2.658710000	0.130500000	-4.666720000
C	2.179550000	-0.260580000	-1.203650000
C	1.923900000	-1.382480000	-2.002820000
C	3.246160000	0.608680000	-1.518220000
C	2.709180000	-1.613900000	-3.108940000
H	1.098220000	-2.051170000	-1.751580000
C	4.019240000	0.371810000	-2.632690000
H	3.448780000	1.465380000	-0.866440000
C	3.755930000	-0.740260000	-3.439680000

H	2.513660000	-2.483160000	-3.750180000
H	4.366410000	-0.930340000	-4.329730000
C	-0.786910000	-0.143340000	1.240720000
C	-0.359270000	-1.023810000	2.245110000
C	-1.970850000	0.603990000	1.408730000
C	-1.102650000	-1.146360000	3.417000000
H	0.567360000	-1.588940000	2.118130000
C	-2.707310000	0.484450000	2.592360000
H	-2.309040000	1.272150000	0.610570000
C	-2.278930000	-0.391780000	3.597990000
H	-0.768900000	-1.832860000	4.205130000
H	-2.858380000	-0.494860000	4.521530000
C	2.140700000	0.296900000	1.226880000
C	1.768160000	1.389030000	2.022040000
C	3.226380000	-0.502640000	1.587050000
C	2.493430000	1.675120000	3.181070000
H	0.904380000	1.996270000	1.739340000
C	3.942580000	-0.213970000	2.758180000
H	3.516020000	-1.354680000	0.963060000
C	3.571850000	0.883270000	3.550150000
H	2.206910000	2.534380000	3.799510000
H	4.136700000	1.110410000	4.461470000
C	5.169090000	1.279010000	-2.973680000
H	6.111110000	0.780870000	-2.703560000
H	5.167050000	1.502620000	-4.050910000
H	5.091020000	2.225970000	-2.417440000
C	-3.968720000	1.267520000	2.774490000
H	-4.830370000	0.628050000	2.525920000
H	-4.059490000	1.604130000	3.819040000
H	-3.974840000	2.149530000	2.116110000
C	5.115560000	-1.054310000	3.148660000
H	6.036970000	-0.581900000	2.773120000
H	5.178100000	-1.138790000	4.244830000
H	5.030640000	-2.063480000	2.717910000
H	-0.808700000	1.732470000	-4.241050000
C	-3.583480000	-1.804840000	-2.994600000
H	-4.530040000	-1.318270000	-2.705560000
H	-3.632150000	-2.077270000	-4.060940000
H	-3.459600000	-2.721840000	-2.397530000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.375780000	0.000000000	0.000000000
C	-0.621110000	0.000000000	-1.357140000
C	-1.595460000	-0.944200000	-1.684730000
C	-0.277040000	1.010930000	-2.264400000
C	-2.237700000	-0.876560000	-2.931050000
H	-1.866140000	-1.727470000	-0.970470000
C	-0.915510000	1.066400000	-3.508010000

H	0.495650000	1.741730000	-2.011700000
C	-1.887650000	0.136560000	-3.839900000
H	-2.391210000	0.191510000	-4.814000000
C	2.203260000	-0.384410000	-1.162020000
C	1.962680000	-1.591000000	-1.831790000
C	3.258710000	0.458840000	-1.569710000
C	2.758710000	-1.937540000	-2.902920000
H	1.143710000	-2.237410000	-1.510750000
C	4.044280000	0.104340000	-2.647160000
H	3.442000000	1.391910000	-1.026220000
C	3.799000000	-1.095990000	-3.323110000
H	2.573940000	-2.874510000	-3.443350000
H	4.418590000	-1.379190000	-4.181660000
C	-0.772490000	-0.297450000	1.221740000
C	-0.226090000	-1.134600000	2.206360000
C	-2.041470000	0.284570000	1.411810000
C	-0.938580000	-1.381640000	3.377600000
H	0.769370000	-1.564450000	2.067360000
C	-2.749080000	0.044980000	2.594170000
H	-2.466890000	0.923790000	0.632000000
C	-2.206550000	-0.790900000	3.578520000
H	-0.510040000	-2.034530000	4.148650000
H	-2.763740000	-0.989280000	4.500250000
C	2.131340000	0.446790000	1.190620000
C	1.665340000	1.558110000	1.906510000
C	3.276210000	-0.235630000	1.607430000
C	2.359190000	1.986090000	3.040040000
H	0.753290000	2.063120000	1.577920000
C	3.958810000	0.193040000	2.754060000
H	3.633860000	-1.107750000	1.049990000
C	3.496980000	1.313630000	3.463560000
H	1.999930000	2.859880000	3.596280000
H	4.036860000	1.650570000	4.356020000
C	5.183710000	0.982060000	-3.082880000
H	6.133920000	0.504250000	-2.803880000
H	5.151410000	1.126420000	-4.173030000
H	5.120400000	1.967040000	-2.594820000
C	-4.096780000	0.660250000	2.801880000
H	-4.875070000	-0.098180000	2.621930000
H	-4.187220000	1.030530000	3.835160000
H	-4.249030000	1.501990000	2.109130000
C	5.189320000	-0.523600000	3.209810000
H	6.077480000	0.028430000	2.864480000
H	5.209630000	-0.582940000	4.309140000
H	5.220050000	-1.543500000	2.797390000
H	-0.641860000	1.853220000	-4.220930000
C	-3.308760000	-1.860130000	-3.278130000
H	-4.292800000	-1.419160000	-3.048440000
H	-3.268500000	-2.108390000	-4.350500000
H	-3.189450000	-2.785520000	-2.693330000

## Coord\_4

C	0.00000000	0.00000000	0.00000000
C	1.38508000	0.00000000	0.00000000
C	-0.52605000	0.00000000	-1.40235000
C	-1.42959000	-0.98192000	-1.82121000
C	-0.18740000	1.06038000	-2.25330000
C	-2.01120000	-0.89305000	-3.09500000
H	-1.69186000	-1.80842000	-1.15446000
C	-0.76059000	1.13488000	-3.52705000
H	0.52957000	1.82068000	-1.93062000
C	-1.66731000	0.17233000	-3.94555000
H	-2.12279000	0.24316000	-4.94186000
C	2.22690000	-0.50230000	-1.10764000
C	2.00135000	-1.77857000	-1.63891000
C	3.27113000	0.30443000	-1.60666000
C	2.80811000	-2.23545000	-2.66303000
H	1.18913000	-2.39512000	-1.24984000
C	4.06924000	-0.16248000	-2.63457000
H	3.43506000	1.29989000	-1.18051000
C	3.84197000	-1.43547000	-3.16966000
H	2.63406000	-3.22839000	-3.09542000
H	4.47066000	-1.80725000	-3.98693000
C	-0.75798000	-0.44898000	1.18341000
C	-0.12026000	-1.22871000	2.16123000
C	-2.09268000	-0.04061000	1.36710000
C	-0.80886000	-1.59406000	3.31550000
H	0.92695000	-1.51674000	2.03351000
C	-2.77887000	-0.39547000	2.53234000
H	-2.58581000	0.55961000	0.59635000
C	-2.14782000	-1.17796000	3.50746000
H	-0.30699000	-2.20170000	4.07965000
H	-2.68818000	-1.46807000	4.41484000
C	2.12187000	0.59209000	1.13574000
C	1.56893000	1.70977000	1.77654000
C	3.32045000	0.03463000	1.58884000
C	2.23148000	2.27429000	2.86745000
H	0.61466000	2.10592000	1.41974000
C	3.97000000	0.59818000	2.69410000
H	3.74194000	-0.84765000	1.09572000
C	3.42277000	1.72861000	3.32472000
H	1.80463000	3.15267000	3.36479000
H	3.93804000	2.17135000	4.18513000
C	5.19821000	0.67541000	-3.16280000
H	6.15545000	0.21573000	-2.87654000
H	5.13546000	0.73944000	-4.25922000
H	5.15086000	1.69371000	-2.74642000
C	-4.19456000	0.04371000	2.73583000
H	-4.86806000	-0.81875000	2.60904000

H	-4.318190000	0.450120000	3.752110000
H	-4.467370000	0.822330000	2.007080000
C	5.252610000	0.013630000	3.193650000
H	6.092080000	0.645030000	2.863330000
H	5.245830000	-0.027000000	4.293900000
H	5.395000000	-1.004370000	2.800410000
H	-0.490330000	1.961540000	-4.194380000
C	-3.010860000	-1.914200000	-3.536750000
H	-4.026630000	-1.519820000	-3.370960000
H	-2.882420000	-2.137660000	-4.607440000
H	-2.893390000	-2.845900000	-2.961820000

### Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.394380000	0.000000000	0.000000000
C	-0.427700000	0.000000000	-1.440890000
C	-1.250820000	-1.016880000	-1.943110000
C	-0.103750000	1.104340000	-2.239910000
C	-1.773120000	-0.910610000	-3.240420000
H	-1.496780000	-1.881670000	-1.320550000
C	-0.612790000	1.194460000	-3.539350000
H	0.550320000	1.892140000	-1.853890000
C	-1.445650000	0.200950000	-4.036390000
H	-1.854220000	0.284600000	-5.051690000
C	2.250460000	-0.612940000	-1.041290000
C	2.039890000	-1.942890000	-1.426720000
C	3.283450000	0.146850000	-1.628620000
C	2.857380000	-2.504050000	-2.392430000
H	1.234450000	-2.522140000	-0.972250000
C	4.094120000	-0.425940000	-2.595160000
H	3.427970000	1.189630000	-1.327060000
C	3.884850000	-1.754870000	-2.981460000
H	2.694000000	-3.540450000	-2.710930000
H	4.522630000	-2.209630000	-3.748280000
C	-0.743380000	-0.595480000	1.126090000
C	-0.045000000	-1.310410000	2.112950000
C	-2.122770000	-0.362280000	1.273030000
C	-0.718210000	-1.787500000	3.234850000
H	1.035390000	-1.455940000	2.021300000
C	-2.796000000	-0.827090000	2.406050000
H	-2.661960000	0.193490000	0.499900000
C	-2.104970000	-1.549220000	3.386750000
H	-0.167000000	-2.343530000	4.004680000
H	-2.634670000	-1.926990000	4.267820000
C	2.112300000	0.730460000	1.062850000
C	1.479910000	1.843470000	1.635330000
C	3.358560000	0.302250000	1.530380000
C	2.111730000	2.537240000	2.667570000
H	0.489830000	2.127400000	1.269210000

C	3.976030000	0.993650000	2.578450000
H	3.839140000	-0.581400000	1.097440000
C	3.350140000	2.122060000	3.136460000
H	1.623190000	3.411680000	3.111270000
H	3.841530000	2.665070000	3.952460000
C	5.212600000	0.361910000	-3.212490000
H	6.175660000	-0.082030000	-2.920100000
H	5.119280000	0.345220000	-4.308430000
H	5.182390000	1.408430000	-2.871030000
C	-4.259710000	-0.565490000	2.573530000
H	-4.816410000	-1.512350000	2.488470000
H	-4.447680000	-0.126110000	3.566110000
H	-4.619700000	0.133130000	1.802640000
C	5.304930000	0.545870000	3.098820000
H	6.082350000	1.252430000	2.769440000
H	5.287060000	0.519210000	4.199290000
H	5.551890000	-0.458280000	2.722040000
H	-0.353440000	2.056610000	-4.164360000
C	-2.691890000	-1.967140000	-3.768590000
H	-3.733110000	-1.620270000	-3.670600000
H	-2.476690000	-2.165250000	-4.830120000
H	-2.574010000	-2.903040000	-3.200750000

#### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.403680000	0.000000000	0.000000000
C	-0.326530000	0.000000000	-1.472520000
C	-1.060500000	-1.048990000	-2.049150000
C	-0.025590000	1.142540000	-2.225330000
C	-1.524790000	-0.929390000	-3.366580000
H	-1.282980000	-1.946910000	-1.466310000
C	-0.471670000	1.244600000	-3.546540000
H	0.559150000	1.955830000	-1.783360000
C	-1.223110000	0.221880000	-4.113210000
H	-1.585910000	0.315060000	-5.144770000
C	2.273960000	-0.715120000	-0.963920000
C	2.078310000	-2.081950000	-1.198020000
C	3.295660000	-0.012470000	-1.635270000
C	2.906520000	-2.740190000	-2.094670000
H	1.279680000	-2.616670000	-0.681640000
C	4.118940000	-0.683320000	-2.529450000
H	3.420780000	1.061720000	-1.463580000
C	3.927650000	-2.050610000	-2.761010000
H	2.753750000	-3.806910000	-2.294890000
H	4.574510000	-2.581810000	-3.468950000
C	-0.728690000	-0.734530000	1.050450000
C	-0.002570000	-1.384700000	2.062750000
C	-2.130490000	-0.670780000	1.130070000
C	-0.669880000	-1.966790000	3.137400000



H	1.091360000	-1.393210000	2.032000000
C	-2.799840000	-1.239860000	2.216160000
H	-2.692570000	-0.159850000	0.342560000
C	-2.079410000	-1.901350000	3.217960000
H	-0.095120000	-2.470710000	3.926030000
H	-2.605090000	-2.362320000	4.061060000
C	2.102620000	0.859630000	0.972840000
C	1.399210000	1.959350000	1.485830000
C	3.390080000	0.561080000	1.432080000
C	2.001280000	2.773290000	2.444640000
H	0.380020000	2.131140000	1.129880000
C	3.976810000	1.371600000	2.408400000
H	3.924450000	-0.316680000	1.053620000
C	3.280020000	2.488360000	2.902270000
H	1.457670000	3.637130000	2.841550000
H	3.748600000	3.124820000	3.662450000
C	5.226890000	0.044530000	-3.231320000
H	6.194520000	-0.386150000	-2.933340000
H	5.102980000	-0.052590000	-4.319970000
H	5.214990000	1.113750000	-2.967660000
C	-4.290300000	-1.150100000	2.315500000
H	-4.728110000	-2.159900000	2.265360000
H	-4.568930000	-0.685240000	3.274770000
H	-4.698310000	-0.540630000	1.494430000
C	5.345830000	1.061280000	2.925780000
H	6.050340000	1.835540000	2.585270000
H	5.333210000	1.045840000	4.026450000
H	5.687410000	0.081240000	2.559550000
H	-0.230010000	2.137710000	-4.133610000
C	-2.354070000	-2.019030000	-3.971960000
H	-3.414010000	-1.720500000	-3.944970000
H	-2.054180000	-2.191330000	-5.017120000
H	-2.234040000	-2.956990000	-3.408120000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.412980000	0.000000000	0.000000000
C	-0.223020000	0.000000000	-1.497020000
C	-0.860120000	-1.078170000	-2.138190000
C	0.047710000	1.174760000	-2.210500000
C	-1.267580000	-0.949490000	-3.472840000
H	-1.052840000	-2.003820000	-1.589570000
C	-0.336500000	1.284840000	-3.550100000
H	0.557530000	2.011490000	-1.720690000
C	-0.999920000	0.234650000	-4.176730000
H	-1.317950000	0.333890000	-5.222240000
C	2.297380000	-0.807750000	-0.876560000
C	2.116600000	-2.194110000	-0.955810000
C	3.307770000	-0.172060000	-1.626450000

C	2.955500000	-2.941090000	-1.773630000
H	1.324780000	-2.677390000	-0.381820000
C	4.143700000	-0.932010000	-2.438240000
H	3.413510000	0.917060000	-1.587860000
C	3.970350000	-2.319420000	-2.511230000
H	2.813290000	-4.024570000	-1.852680000
H	4.626280000	-2.919660000	-3.152660000
C	-0.713920000	-0.863840000	0.957490000
C	0.005800000	-1.456600000	2.009780000
C	-2.115100000	-0.956630000	0.940810000
C	-0.665530000	-2.136810000	3.022270000
H	1.093040000	-1.339660000	2.063140000
C	-2.789810000	-1.623860000	1.965270000
H	-2.676040000	-0.485840000	0.128000000
C	-2.071720000	-2.231080000	3.002200000
H	-0.093950000	-2.593910000	3.841530000
H	-2.600150000	-2.770360000	3.795710000
C	2.092840000	0.977460000	0.866920000
C	1.327670000	2.058060000	1.330630000
C	3.414600000	0.804910000	1.295000000
C	1.901400000	2.981590000	2.202690000
H	0.286280000	2.121350000	1.004270000
C	3.972300000	1.724380000	2.186400000
H	3.996910000	-0.061520000	0.964160000
C	3.213290000	2.822570000	2.626180000
H	1.309970000	3.830350000	2.560740000
H	3.660460000	3.544520000	3.320220000
C	5.241100000	-0.273700000	-3.218890000
H	6.211980000	-0.693630000	-2.915330000
H	5.086660000	-0.450260000	-4.293510000
H	5.248670000	0.812280000	-3.035550000
C	-4.284840000	-1.692950000	1.965790000
H	-4.611420000	-2.745130000	1.947830000
H	-4.673470000	-1.212230000	2.878000000
H	-4.698410000	-1.173450000	1.087530000
C	5.374950000	1.548070000	2.676890000
H	5.998440000	2.380130000	2.315860000
H	5.383750000	1.543050000	3.777610000
H	5.798550000	0.599750000	2.312800000
H	-0.118420000	2.204190000	-4.104550000
C	-1.999770000	-2.069920000	-4.145310000
H	-3.071300000	-1.820460000	-4.191760000
H	-1.617840000	-2.215990000	-5.167250000
H	-1.876390000	-3.007770000	-3.582150000

Coord\_8

C	0.000000000	0.000000000	0.000000000
C	1.422280000	0.000000000	0.000000000
C	-0.117680000	0.000000000	-1.514230000

C	-0.651310000	-1.104330000	-2.209210000
C	0.116940000	1.200820000	-2.196250000
C	-1.002880000	-0.971010000	-3.558610000
H	-0.808970000	-2.052170000	-1.688450000
C	-0.206300000	1.314790000	-3.551250000
H	0.547140000	2.058880000	-1.667260000
C	-0.776130000	0.238860000	-4.227530000
H	-1.050180000	0.340520000	-5.285030000
C	2.320720000	-0.889840000	-0.780390000
C	2.154740000	-2.278050000	-0.703250000
C	3.319800000	-0.330410000	-1.602100000
C	3.004330000	-3.104480000	-1.433450000
H	1.369770000	-2.703390000	-0.076760000
C	4.168420000	-1.169470000	-2.322590000
H	3.406190000	0.756810000	-1.697720000
C	4.012970000	-2.558400000	-2.235330000
H	2.872630000	-4.190870000	-1.390030000
H	4.677940000	-3.219510000	-2.803550000
C	-0.699070000	-0.981220000	0.848470000
C	-0.019980000	-1.530390000	1.951150000
C	-2.076370000	-1.210990000	0.709930000
C	-0.705090000	-2.301440000	2.886100000
H	1.040170000	-1.305120000	2.108690000
C	-2.765360000	-1.969560000	1.657690000
H	-2.611980000	-0.771110000	-0.136490000
C	-2.081550000	-2.534820000	2.740210000
H	-0.163540000	-2.722160000	3.744680000
H	-2.619270000	-3.146920000	3.472330000
C	2.082970000	1.081960000	0.746530000
C	1.266050000	2.140660000	1.171870000
C	3.431750000	1.027660000	1.121230000
C	1.813250000	3.161980000	1.945380000
H	0.209520000	2.102600000	0.893740000
C	3.962450000	2.044690000	1.916030000
H	4.055700000	0.175960000	0.830460000
C	3.150770000	3.120360000	2.312640000
H	1.181820000	3.993510000	2.273000000
H	3.578270000	3.918910000	2.931330000
C	5.255250000	-0.589700000	-3.175150000
H	6.228030000	-1.001280000	-2.865430000
H	5.070430000	-0.844020000	-4.229130000
H	5.283390000	0.506750000	-3.074180000
C	-4.242260000	-2.177660000	1.531890000
H	-4.474200000	-3.254810000	1.545920000
H	-4.751600000	-1.690230000	2.379000000
H	-4.618310000	-1.741390000	0.593450000
C	5.392010000	1.994750000	2.356370000
H	5.929340000	2.873310000	1.968490000
H	5.437700000	2.001000000	3.456080000
H	5.882720000	1.082490000	1.984450000

H	-0.016680000	2.255520000	-4.079210000
C	-1.631430000	-2.119820000	-4.287300000
H	-2.707150000	-1.920070000	-4.408840000
H	-1.170680000	-2.239350000	-5.279550000
H	-1.504130000	-3.055370000	-3.721330000

Coord\_9

C	0.000000000	0.000000000	0.000000000
C	1.431580000	0.000000000	0.000000000
C	-0.011020000	0.000000000	-1.524010000
C	-0.435770000	-1.127390000	-2.261400000
C	0.183020000	1.220540000	-2.183200000
C	-0.732110000	-0.993990000	-3.623390000
H	-0.554250000	-2.091740000	-1.761440000
C	-0.079910000	1.334130000	-3.550940000
H	0.529850000	2.097820000	-1.624180000
C	-0.551650000	0.234220000	-4.266020000
H	-0.782250000	0.334530000	-5.333810000
C	2.343990000	-0.960590000	-0.676670000
C	2.192730000	-2.332850000	-0.443640000
C	3.331760000	-0.486010000	-1.562350000
C	3.053010000	-3.228560000	-1.078510000
H	1.414610000	-2.694270000	0.229470000
C	4.193090000	-1.393290000	-2.183810000
H	3.398850000	0.582450000	-1.791150000
C	4.055490000	-2.764990000	-1.936820000
H	2.931740000	-4.303930000	-0.912910000
H	4.729500000	-3.478170000	-2.426130000
C	-0.684130000	-1.084670000	0.724950000
C	-0.078910000	-1.608970000	1.882280000
C	-2.014590000	-1.426160000	0.443930000
C	-0.786730000	-2.462650000	2.723550000
H	0.934140000	-1.297140000	2.159580000
C	-2.726020000	-2.268120000	1.299400000
H	-2.501240000	-1.004430000	-0.440330000
C	-2.107620000	-2.808320000	2.432600000
H	-0.301290000	-2.861410000	3.625420000
H	-2.660640000	-3.486810000	3.091170000
C	2.073010000	1.171350000	0.613400000
C	1.215000000	2.208470000	1.011160000
C	3.441220000	1.223530000	0.913910000
C	1.737860000	3.314750000	1.675910000
H	0.150460000	2.079570000	0.798480000
C	3.947300000	2.325740000	1.601920000
H	4.100080000	0.387840000	0.655460000
C	3.093230000	3.378080000	1.966390000
H	1.074760000	4.129340000	1.981400000
H	3.503080000	4.243560000	2.501680000
C	5.269370000	-0.900380000	-3.100330000

H	6.242640000	-1.305820000	-2.783330000
H	5.054380000	-1.230090000	-4.127290000
H	5.319150000	0.199880000	-3.083270000
C	-4.162020000	-2.589430000	1.024620000
H	-4.323350000	-3.678590000	1.070800000
H	-4.792980000	-2.101280000	1.785230000
H	-4.459580000	-2.223990000	0.029390000
C	5.396800000	2.390490000	1.970280000
H	5.845920000	3.303870000	1.552290000
H	5.493630000	2.409910000	3.066430000
H	5.937820000	1.515020000	1.580140000
H	0.077480000	2.291250000	-4.059170000
C	-1.251640000	-2.168730000	-4.396750000
H	-2.323910000	-2.019240000	-4.594190000
H	-0.715760000	-2.261440000	-5.353280000
H	-1.120410000	-3.099760000	-3.824420000

### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.440880000	0.000000000	0.000000000
C	0.096430000	0.000000000	-1.526270000
C	-0.215290000	-1.147310000	-2.294090000
C	0.246920000	1.233800000	-2.171810000
C	-0.456700000	-1.018470000	-3.666740000
H	-0.291680000	-2.122350000	-1.807350000
C	0.044000000	1.342610000	-3.549840000
H	0.507650000	2.128140000	-1.592290000
C	-0.326280000	0.220490000	-4.292410000
H	-0.513630000	0.315610000	-5.368940000
C	2.367170000	-1.019310000	-0.566710000
C	2.230570000	-2.357960000	-0.180350000
C	3.343650000	-0.637370000	-1.507450000
C	3.101510000	-3.312020000	-0.713360000
H	1.459300000	-2.650070000	0.532810000
C	4.217730000	-1.601200000	-2.023440000
H	3.391510000	0.395710000	-1.866240000
C	4.097930000	-2.937070000	-1.619480000
H	2.990620000	-4.362530000	-0.427450000
H	4.780950000	-3.692980000	-2.025200000
C	-0.669120000	-1.172380000	0.588720000
C	-0.168840000	-1.693300000	1.797420000
C	-1.930580000	-1.596060000	0.150910000
C	-0.906940000	-2.619810000	2.528060000
H	0.777870000	-1.320020000	2.204460000
C	-2.671370000	-2.511740000	0.897960000
H	-2.345920000	-1.177580000	-0.770390000
C	-2.147770000	-3.046480000	2.080200000
H	-0.502030000	-3.013300000	3.471370000
H	-2.721200000	-3.783590000	2.652760000

C	2.062960000	1.244060000	0.469460000
C	1.175090000	2.262930000	0.849540000
C	3.442780000	1.387230000	0.677120000
C	1.676110000	3.440550000	1.396880000
H	0.109650000	2.056690000	0.717450000
C	3.926870000	2.561460000	1.249710000
H	4.129450000	0.566730000	0.443600000
C	3.041380000	3.592670000	1.592370000
H	0.990080000	4.240790000	1.687850000
H	3.435850000	4.514780000	2.037350000
C	5.283450000	-1.202660000	-2.994970000
H	6.255790000	-1.603870000	-2.669030000
H	5.038620000	-1.604770000	-3.988870000
H	5.355920000	-0.105540000	-3.062780000
C	-4.044060000	-2.915750000	0.457740000
H	-4.164290000	-4.008610000	0.534110000
H	-4.787300000	-2.427460000	1.109220000
H	-4.226910000	-2.605960000	-0.583090000
C	5.389200000	2.725430000	1.526400000
H	5.751200000	3.662470000	1.077810000
H	5.549710000	2.760250000	2.614580000
H	5.962240000	1.883860000	1.108330000
H	0.166580000	2.311050000	-4.045550000
C	-0.863060000	-2.216590000	-4.472670000
H	-1.924140000	-2.117820000	-4.745970000
H	-0.256180000	-2.282290000	-5.387920000
H	-0.728510000	-3.140890000	-3.890430000

S<sub>0</sub>\_S<sub>1</sub>S<sub>0</sub>-pyr (C2)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.357180000	0.000000000	0.000000000
C	-0.799570000	0.000000000	-1.247810000
C	-1.883800000	-0.860940000	-1.373810000
C	-0.475230000	0.896680000	-2.274830000
C	-2.650610000	-0.846140000	-2.550830000
H	-2.145660000	-1.544010000	-0.559690000
C	-1.246900000	0.905130000	-3.442410000
H	0.384810000	1.562700000	-2.178590000
C	-2.321480000	0.046030000	-3.580670000
H	-2.924180000	0.061090000	-4.498640000
C	2.155780000	-0.132230000	-1.231860000
C	1.885010000	-1.155580000	-2.149720000
C	3.233470000	0.752640000	-1.452740000
C	2.659530000	-1.268420000	-3.278340000
H	1.052660000	-1.838990000	-1.969230000

C	3.994110000	0.637180000	-2.591190000
H	3.455360000	1.520270000	-0.703410000
C	3.712780000	-0.372350000	-3.517670000
H	2.453210000	-2.059170000	-4.011900000
H	4.314140000	-0.465840000	-4.428960000
C	-0.801240000	0.010890000	1.240310000
C	-0.515750000	-0.893380000	2.272650000
C	-1.882950000	0.909200000	1.361310000
C	-1.295120000	-0.886200000	3.427630000
H	0.326860000	-1.582080000	2.178080000
C	-2.654300000	0.913610000	2.529300000
H	-2.117080000	1.592540000	0.538950000
C	-2.362080000	0.014900000	3.563750000
H	-1.074400000	-1.590440000	4.239150000
H	-2.968200000	0.009910000	4.475800000
C	2.149940000	0.144810000	1.244230000
C	1.876350000	1.203730000	2.119880000
C	3.171500000	-0.760860000	1.529530000
C	2.632740000	1.344810000	3.286460000
H	1.066440000	1.903700000	1.898930000
C	3.921480000	-0.615170000	2.707450000
H	3.389600000	-1.582220000	0.838860000
C	3.646460000	0.444190000	3.582480000
H	2.423310000	2.178660000	3.968100000
H	4.236290000	0.559180000	4.498820000
C	5.154310000	1.563520000	-2.836390000
H	6.087070000	1.043120000	-2.577270000
H	5.182260000	1.864650000	-3.894260000
H	5.062710000	2.468180000	-2.215690000
C	-3.813090000	1.850250000	2.659520000
H	-4.728440000	1.337530000	2.324520000
H	-3.937550000	2.161500000	3.708290000
H	-3.656940000	2.746450000	2.040060000
C	5.031930000	-1.567530000	3.013260000
H	5.969450000	-1.170720000	2.592380000
H	5.150500000	-1.684760000	4.101850000
H	4.830480000	-2.553910000	2.568690000
H	-0.991050000	1.600170000	-4.251570000
C	-3.833050000	-1.748200000	-2.688200000
H	-4.737000000	-1.217110000	-2.344910000
H	-3.970710000	-2.044100000	-3.740610000
H	-3.701480000	-2.654790000	-2.076910000

S<sub>0</sub>-S<sub>1</sub>S<sub>0</sub>(C2)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.357180000	0.000000000	0.000000000
C	-0.799570000	0.000000000	-1.247810000

C	-1.883800000	-0.860940000	-1.373810000
C	-0.475230000	0.896680000	-2.274830000
C	-2.650610000	-0.846140000	-2.550830000
H	-2.145660000	-1.544010000	-0.559690000
C	-1.246900000	0.905130000	-3.442410000
H	0.384810000	1.562700000	-2.178590000
C	-2.321480000	0.046030000	-3.580670000
H	-2.924180000	0.061090000	-4.498640000
C	2.155780000	-0.132230000	-1.231860000
C	1.885010000	-1.155580000	-2.149720000
C	3.233470000	0.752640000	-1.452740000
C	2.659530000	-1.268420000	-3.278340000
H	1.052660000	-1.838990000	-1.969230000
C	3.994110000	0.637180000	-2.591190000
H	3.455360000	1.520270000	-0.703410000
C	3.712780000	-0.372350000	-3.517670000
H	2.453210000	-2.059170000	-4.011900000
H	4.314140000	-0.465840000	-4.428960000
C	-0.801240000	0.010890000	1.240310000
C	-0.515750000	-0.893380000	2.272650000
C	-1.882950000	0.909200000	1.361310000
C	-1.295120000	-0.886200000	3.427630000
H	0.326860000	-1.582080000	2.178080000
C	-2.654300000	0.913610000	2.529300000
H	-2.117080000	1.592540000	0.538950000
C	-2.362080000	0.014900000	3.563750000
H	-1.074400000	-1.590440000	4.239150000
H	-2.968200000	0.009910000	4.475800000
C	2.149940000	0.144810000	1.244230000
C	1.876350000	1.203730000	2.119880000
C	3.171500000	-0.760860000	1.529530000
C	2.632740000	1.344810000	3.286460000
H	1.066440000	1.903700000	1.898930000
C	3.921480000	-0.615170000	2.707450000
H	3.389600000	-1.582220000	0.838860000
C	3.646460000	0.444190000	3.582480000
H	2.423310000	2.178660000	3.968100000
H	4.236290000	0.559180000	4.498820000
C	5.154310000	1.563520000	-2.836390000
H	6.087070000	1.043120000	-2.577270000
H	5.182260000	1.864650000	-3.894260000
H	5.062710000	2.468180000	-2.215690000
C	-3.813090000	1.850250000	2.659520000
H	-4.728440000	1.337530000	2.324520000
H	-3.937550000	2.161500000	3.708290000
H	-3.656940000	2.746450000	2.040060000
C	5.031930000	-1.567530000	3.013260000
H	5.969450000	-1.170720000	2.592380000
H	5.150500000	-1.684760000	4.101850000
H	4.830480000	-2.553910000	2.568690000



H	-0.991050000	1.600170000	-4.251570000
C	-3.833050000	-1.748200000	-2.688200000
H	-4.737000000	-1.217110000	-2.344910000
H	-3.970710000	-2.044100000	-3.740610000
H	-3.701480000	-2.654790000	-2.076910000

Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.366470000	0.000000000	0.000000000
C	-0.779430000	0.000000000	-1.258620000
C	-1.915770000	-0.794220000	-1.378120000
C	-0.365580000	0.821790000	-2.316130000
C	-2.645480000	-0.785160000	-2.577030000
H	-2.241730000	-1.424110000	-0.544340000
C	-1.103370000	0.829210000	-3.504410000
H	0.538430000	1.426790000	-2.217850000
C	-2.230270000	0.037950000	-3.635950000
H	-2.805210000	0.049130000	-4.571440000
C	2.152450000	-0.430140000	-1.170160000
C	1.738760000	-1.528970000	-1.936090000
C	3.333640000	0.264050000	-1.505890000
C	2.481130000	-1.908530000	-3.030090000
H	0.820190000	-2.058490000	-1.673050000
C	4.064770000	-0.113370000	-2.609180000
H	3.658890000	1.099180000	-0.876300000
C	3.647710000	-1.200720000	-3.384150000
H	2.161360000	-2.761900000	-3.643190000
H	4.226280000	-1.503150000	-4.264250000
C	-0.816350000	0.029400000	1.232030000
C	-0.546670000	-0.867230000	2.275050000
C	-1.888250000	0.941060000	1.336540000
C	-1.337320000	-0.843400000	3.422670000
H	0.289780000	-1.564770000	2.193890000
C	-2.672290000	0.959980000	2.495900000
H	-2.102470000	1.627270000	0.511080000
C	-2.398510000	0.066200000	3.539600000
H	-1.127620000	-1.539640000	4.243560000
H	-3.014020000	0.074230000	4.445440000
C	2.071770000	0.308540000	1.272810000
C	1.781410000	1.500360000	1.949760000
C	3.045530000	-0.563870000	1.765100000
C	2.472850000	1.814050000	3.122910000
H	1.009200000	2.174380000	1.568660000
C	3.734740000	-0.242420000	2.944630000
H	3.273150000	-1.492660000	1.232110000
C	3.442090000	0.952920000	3.620750000
H	2.248730000	2.750440000	3.648520000
H	3.983060000	1.204620000	4.540030000
C	5.330250000	0.612220000	-2.975100000

H	6.193820000	-0.005640000	-2.689970000
H	5.356410000	0.802170000	-4.058750000
H	5.388280000	1.576700000	-2.447270000
C	-3.823450000	1.908290000	2.608820000
H	-4.749060000	1.387390000	2.317380000
H	-3.922030000	2.266190000	3.645250000
H	-3.676700000	2.775300000	1.946920000
C	4.796890000	-1.156200000	3.466260000
H	5.771760000	-0.836280000	3.065820000
H	4.831530000	-1.117620000	4.566160000
H	4.604790000	-2.193300000	3.152300000
H	-0.779310000	1.466570000	-4.335750000
C	-3.876470000	-1.620550000	-2.713820000
H	-4.762040000	-1.005320000	-2.482510000
H	-3.965840000	-2.003580000	-3.742920000
H	-3.845630000	-2.473090000	-2.017420000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.375750000	0.000000000	0.000000000
C	-0.759150000	0.000000000	-1.269110000
C	-1.943510000	-0.723560000	-1.386440000
C	-0.260630000	0.739450000	-2.351050000
C	-2.636450000	-0.723360000	-2.605520000
H	-2.330530000	-1.295640000	-0.537090000
C	-0.964380000	0.742720000	-3.558820000
H	0.682470000	1.280710000	-2.246590000
C	-2.139170000	0.023070000	-3.687920000
H	-2.686570000	0.027720000	-4.639670000
C	2.149040000	-0.705760000	-1.036970000
C	1.615920000	-1.843100000	-1.661190000
C	3.416310000	-0.219120000	-1.416000000
C	2.330680000	-2.469860000	-2.658180000
H	0.626410000	-2.206880000	-1.373510000
C	4.123220000	-0.840840000	-2.423120000
H	3.828250000	0.655080000	-0.900900000
C	3.592530000	-1.970440000	-3.055110000
H	1.915740000	-3.355600000	-3.158270000
H	4.152410000	-2.467060000	-3.855490000
C	-0.831380000	0.047650000	1.223290000
C	-0.577480000	-0.841180000	2.276720000
C	-1.893420000	0.972140000	1.311270000
C	-1.379340000	-0.800970000	3.416620000
H	0.252790000	-1.547180000	2.209020000
C	-2.690120000	1.005270000	2.461640000
H	-2.087700000	1.661000000	0.483030000
C	-2.434770000	0.116590000	3.514300000
H	-1.180630000	-1.489070000	4.246660000
H	-3.059640000	0.137410000	4.413630000

C	1.989480000	0.479020000	1.273480000
C	1.691050000	1.767450000	1.736070000
C	2.906250000	-0.323410000	1.961780000
C	2.317770000	2.252710000	2.886870000
H	0.963550000	2.387460000	1.203850000
C	3.535120000	0.171510000	3.114020000
H	3.136430000	-1.330160000	1.599420000
C	3.234140000	1.465700000	3.573980000
H	2.085760000	3.263260000	3.244350000
H	3.726680000	1.852640000	4.473460000
C	5.476790000	-0.333010000	-2.834550000
H	6.248390000	-1.032600000	-2.481210000
H	5.530040000	-0.252380000	-3.931010000
H	5.665610000	0.660300000	-2.398680000
C	-3.833660000	1.964740000	2.557190000
H	-4.768820000	1.438110000	2.309800000
H	-3.906060000	2.368190000	3.578820000
H	-3.697240000	2.801010000	1.854700000
C	4.539810000	-0.666080000	3.839240000
H	5.547110000	-0.411050000	3.474650000
H	4.490640000	-0.473240000	4.922060000
H	4.354950000	-1.735880000	3.659550000
H	-0.575820000	1.316930000	-4.407800000
C	-3.911990000	-1.489180000	-2.745470000
H	-4.765930000	-0.801460000	-2.630140000
H	-3.964020000	-1.961630000	-3.739190000
H	-3.980850000	-2.272390000	-1.974450000

#### Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.385040000	0.000000000	0.000000000
C	-0.738730000	0.000000000	-1.279270000
C	-1.966630000	-0.649390000	-1.398690000
C	-0.161220000	0.650300000	-2.379470000
C	-2.623500000	-0.661010000	-2.636060000
H	-2.411190000	-1.159400000	-0.537900000
C	-0.831140000	0.646370000	-3.605350000
H	0.815830000	1.125660000	-2.264900000
C	-2.049060000	0.001650000	-3.736150000
H	-2.569460000	-0.002780000	-4.702770000
C	2.145560000	-0.942090000	-0.839510000
C	1.520620000	-2.093780000	-1.342150000
C	3.479400000	-0.654860000	-1.188050000
C	2.214230000	-2.935180000	-2.187330000
H	0.477340000	-2.300570000	-1.089230000
C	4.168690000	-1.490300000	-2.044650000
H	3.958720000	0.238590000	-0.774700000
C	3.550080000	-2.638120000	-2.551620000
H	1.725640000	-3.833070000	-2.590150000

H	4.096300000	-3.303900000	-3.229160000
C	-0.846330000	0.065640000	1.214090000
C	-0.608160000	-0.815240000	2.277660000
C	-1.898480000	1.002430000	1.285540000
C	-1.421180000	-0.758930000	3.409500000
H	0.215900000	-1.529340000	2.223460000
C	-2.707820000	1.049480000	2.426550000
H	-2.072770000	1.693720000	0.454820000
C	-2.470870000	0.166050000	3.487880000
H	-1.233420000	-1.438770000	4.248450000
H	-3.105060000	0.199430000	4.380420000
C	1.903520000	0.651000000	1.245190000
C	1.605230000	1.998820000	1.485190000
C	2.754670000	-0.048140000	2.111960000
C	2.167740000	2.649760000	2.586250000
H	0.928930000	2.539630000	0.815750000
C	3.323830000	0.613240000	3.209760000
H	2.980750000	-1.102590000	1.927050000
C	3.023500000	1.967750000	3.444290000
H	1.934250000	3.705380000	2.769280000
H	3.468220000	2.484680000	4.302590000
C	5.591070000	-1.191220000	-2.424390000
H	6.254780000	-1.943000000	-1.971850000
H	5.699160000	-1.220690000	-3.519620000
H	5.884770000	-0.191720000	-2.067770000
C	-3.843730000	2.019610000	2.504670000
H	-4.787690000	1.489660000	2.301670000
H	-3.889730000	2.467370000	3.509080000
H	-3.718550000	2.823680000	1.763510000
C	4.262520000	-0.114210000	4.119830000
H	5.296910000	0.090670000	3.803220000
H	4.130220000	0.226010000	5.158330000
H	4.083130000	-1.198950000	4.075290000
H	-0.382380000	1.152430000	-4.467360000
C	-3.939360000	-1.354710000	-2.782810000
H	-4.749600000	-0.607580000	-2.785670000
H	-3.965920000	-1.916690000	-3.729660000
H	-4.104710000	-2.054260000	-1.948680000

### Coord\_5

C	0.000000000	-1.016210000	0.000000000
C	1.394320000	0.540990000	0.000000000
C	-0.718180000	0.962860000	-1.289100000
C	-1.984780000	-0.025950000	-1.414790000
C	-0.068120000	-0.041820000	-2.401380000
C	-2.606610000	-1.124320000	-2.668460000
H	-2.482910000	-2.281170000	-0.546680000
C	-0.704820000	-1.003570000	-3.643790000
H	0.937510000	-3.294060000	-2.272950000

C	-1.960790000	-2.360010000	-3.780310000
H	-2.455080000	-2.011270000	-4.760260000
C	2.142010000	-0.100420000	-0.589000000
C	1.456100000	-3.166950000	-0.992740000
C	3.521210000	-4.195780000	-0.839920000
C	2.136600000	-3.968170000	-1.640820000
H	0.377800000	0.083350000	-0.828040000
C	4.200540000	-0.789430000	-1.500380000
H	4.046530000	1.031930000	-0.513060000
C	3.522580000	-0.717310000	-1.903060000
H	1.598410000	-1.511260000	-1.964620000
H	4.060810000	1.092580000	-2.421700000
C	-0.861200000	1.725450000	1.204460000
C	-0.638700000	0.214560000	2.277870000
C	-1.903410000	-1.388770000	1.259350000
C	-1.462830000	0.260240000	3.401320000
H	0.179110000	0.819120000	2.237210000
C	-2.725370000	2.189740000	2.390670000
H	-2.057730000	0.251970000	0.426490000
C	-2.506800000	2.996140000	3.460370000
H	-1.285970000	2.629820000	4.248950000
H	-3.150280000	1.068680000	4.345810000
C	1.814330000	-0.820360000	1.187880000
C	1.523790000	2.445360000	1.204230000
C	2.591920000	4.068220000	2.209990000
C	2.022730000	3.083740000	2.230420000
H	0.904570000	-1.886180000	0.415550000
C	3.102120000	-2.653480000	3.228630000
H	2.807660000	-2.026630000	2.203450000
C	2.810860000	-0.890870000	3.236230000
H	1.793710000	2.072880000	2.238260000
H	3.208470000	1.542010000	4.033930000
C	5.670720000	2.563610000	-1.778320000
H	6.218170000	2.843430000	-1.210140000
H	5.858490000	0.480530000	-2.854240000
H	6.037640000	0.651990000	-1.482870000
C	-3.853670000	0.956320000	2.451300000
H	-4.805640000	-0.602080000	2.292920000
H	-3.873090000	0.974420000	3.436180000
H	-3.740640000	-1.217710000	1.673430000
C	3.966960000	-0.425430000	4.299300000
H	5.022700000	-1.867120000	4.039070000
H	3.752760000	-1.820560000	5.268390000
H	3.791620000	-1.016210000	4.388230000
H	-0.200730000	0.540990000	-4.514230000
C	-3.958330000	0.962860000	-2.825470000
H	-4.714280000	-0.025950000	-2.946960000
H	-3.971940000	-0.041820000	-3.714730000
H	-4.214860000	-1.124320000	-1.940530000

## Coord\_6

C	0.00000000	0.00000000	0.00000000
C	1.40361000	0.00000000	0.00000000
C	-0.69750000	0.00000000	-1.29861000
C	-1.99762000	-0.49224000	-1.43459000
C	0.01794000	0.45438000	-2.41683000
C	-2.58582000	-0.53560000	-2.70249000
H	-2.54493000	-0.86693000	-0.56322000
C	-0.58655000	0.42750000	-3.67406000
H	1.04662000	0.79362000	-2.27103000
C	-1.87522000	-0.05925000	-3.82012000
H	-2.34461000	-0.08874000	-4.81177000
C	2.13839000	-1.24075000	-0.30000000
C	1.42463000	-2.40714000	-0.62263000
C	3.54054000	-1.23221000	-0.40123000
C	2.10118000	-3.54008000	-1.03912000
H	0.33117000	-2.40440000	-0.58661000
C	4.21821000	-2.36187000	-0.83030000
H	4.08901000	-0.31937000	-0.14822000
C	3.51151000	-3.52758000	-1.14539000
H	1.53920000	-4.44827000	-1.29870000
H	4.04782000	-4.42347000	-1.47754000
C	-0.87599000	0.10077000	1.19439000
C	-0.66910000	-0.76378000	2.27737000
C	-1.90824000	1.06062000	1.23275000
C	-1.50427000	-0.67615000	3.39209000
H	0.14245000	-1.49298000	2.25027000
C	-2.74278000	1.13457000	2.35401000
H	-2.04260000	1.75619000	0.39806000
C	-2.54257000	0.26208000	3.43178000
H	-1.33828000	-1.33912000	4.24817000
H	-3.19528000	0.31983000	4.30985000
C	1.72238000	0.97805000	1.10252000
C	1.44640000	2.33690000	0.90070000
C	2.41920000	0.56606000	2.25239000
C	1.88249000	3.28494000	1.82978000
H	0.88954000	2.65905000	0.01393000
C	2.87126000	1.52356000	3.17013000
H	2.61896000	-0.49596000	2.41971000
C	2.59672000	2.88620000	2.95648000
H	1.66328000	4.34642000	1.66675000
H	2.94796000	3.63476000	3.67658000
C	5.71386000	-2.35377000	-0.95206000
H	6.14449000	-3.09961000	-0.26621000
H	6.00160000	-2.60222000	-1.98577000
H	6.11825000	-1.36058000	-0.70161000
C	-3.86350000	2.12454000	2.39712000
H	-4.82265000	1.59510000	2.28344000
H	-3.85620000	2.65680000	3.36021000

H	-3.763530000	2.860380000	1.584580000
C	3.655130000	1.098220000	4.372810000
H	4.726200000	1.254090000	4.173340000
H	3.360790000	1.693380000	5.250400000
H	3.482830000	0.033710000	4.591270000
H	-0.032510000	0.784370000	-4.548370000
C	-3.968740000	-1.078750000	-2.873070000
H	-4.661480000	-0.256420000	-3.111880000
H	-3.982210000	-1.811280000	-3.695010000
H	-4.309090000	-1.573390000	-1.950180000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.412900000	0.000000000	0.000000000
C	-0.676700000	0.000000000	-1.307780000
C	-2.004860000	-0.410180000	-1.457920000
C	0.096290000	0.349180000	-2.425930000
C	-2.561160000	-0.472970000	-2.737920000
H	-2.596550000	-0.712470000	-0.587290000
C	-0.477380000	0.306940000	-3.696160000
H	1.142370000	0.619280000	-2.259520000
C	-1.793150000	-0.097680000	-3.855390000
H	-2.239160000	-0.142730000	-4.857030000
C	2.134690000	-1.283590000	0.010380000
C	1.427450000	-2.472840000	-0.238000000
C	3.536700000	-1.317880000	0.089140000
C	2.109710000	-3.668090000	-0.400210000
H	0.339300000	-2.446700000	-0.352590000
C	4.221230000	-2.512400000	-0.085000000
H	4.084620000	-0.388730000	0.274110000
C	3.517530000	-3.698780000	-0.319660000
H	1.550730000	-4.592860000	-0.602100000
H	4.058060000	-4.643270000	-0.447280000
C	-0.890690000	0.117880000	1.183880000
C	-0.699360000	-0.738320000	2.276160000
C	-1.912980000	1.088510000	1.205740000
C	-1.545510000	-0.635470000	3.381830000
H	0.105920000	-1.474510000	2.262620000
C	-2.760070000	1.175420000	2.316600000
H	-2.027400000	1.785950000	0.369580000
C	-2.578160000	0.308600000	3.402140000
H	-1.390340000	-1.289850000	4.246130000
H	-3.240070000	0.378150000	4.272570000
C	1.628160000	1.122740000	0.991090000
C	1.372630000	2.438410000	0.582210000
C	2.237850000	0.882910000	2.237980000
C	1.746560000	3.511340000	1.395230000
H	0.882710000	2.630170000	-0.379310000
C	2.632520000	1.963930000	3.036400000

H	2.416650000	-0.143220000	2.569940000
C	2.381460000	3.279630000	2.613520000
H	1.541800000	4.537630000	1.070100000
H	2.686990000	4.125000000	3.241640000
C	5.719130000	-2.548540000	-0.018940000
H	6.039990000	-3.240880000	0.775190000
H	6.121170000	-2.893960000	-0.984670000
H	6.123060000	-1.546490000	0.194440000
C	-3.873220000	2.174580000	2.342160000
H	-4.838690000	1.648890000	2.273150000
H	-3.839140000	2.746830000	3.281300000
H	-3.787200000	2.874640000	1.497020000
C	3.329160000	1.718620000	4.339470000
H	4.409230000	1.876990000	4.201010000
H	2.956890000	2.413350000	5.107210000
H	3.159310000	0.686840000	4.681590000
H	0.120740000	0.583910000	-4.569870000
C	-3.970430000	-0.938390000	-2.925190000
H	-4.592930000	-0.101650000	-3.278340000
H	-3.996590000	-1.747570000	-3.671240000
H	-4.385400000	-1.315070000	-1.977560000

#### Coord\_8

C	0.000000000	0.000000000	0.000000000
C	1.422180000	0.000000000	0.000000000
C	-0.655780000	0.000000000	-1.316620000
C	-2.006240000	-0.326430000	-1.484580000
C	0.166310000	0.240270000	-2.428860000
C	-2.532670000	-0.410650000	-2.774540000
H	-2.637140000	-0.553780000	-0.618560000
C	-0.378280000	0.180420000	-3.710190000
H	1.224080000	0.441190000	-2.238910000
C	-1.715360000	-0.140590000	-3.885990000
H	-2.139810000	-0.202860000	-4.895880000
C	2.130930000	-1.249400000	0.323570000
C	1.464640000	-2.476840000	0.156660000
C	3.509490000	-1.250470000	0.586650000
C	2.162220000	-3.672280000	0.258670000
H	0.402460000	-2.490110000	-0.108610000
C	4.209220000	-2.448040000	0.678030000
H	4.033030000	-0.296320000	0.700170000
C	3.540420000	-3.668080000	0.529260000
H	1.633100000	-4.625870000	0.118890000
H	4.091110000	-4.611530000	0.613620000
C	-0.905300000	0.134680000	1.172960000
C	-0.729450000	-0.713050000	2.274240000
C	-1.917620000	1.115590000	1.178340000
C	-1.586530000	-0.595310000	3.370540000
H	0.069540000	-1.455890000	2.274280000



C	-2.777230000	1.215120000	2.278480000
H	-2.012160000	1.814740000	0.341070000
C	-2.613570000	0.354080000	3.371470000
H	-1.442130000	-1.241000000	4.242830000
H	-3.284650000	0.435170000	4.233990000
C	1.532170000	1.248580000	0.856480000
C	1.301960000	2.493700000	0.256290000
C	2.049270000	1.191370000	2.167890000
C	1.614300000	3.672590000	0.937820000
H	0.882810000	2.547550000	-0.755560000
C	2.387200000	2.376650000	2.832120000
H	2.202910000	0.223360000	2.651400000
C	2.165300000	3.616860000	2.217180000
H	1.427860000	4.642210000	0.462950000
H	2.425670000	4.544120000	2.741790000
C	5.685750000	-2.448550000	0.936410000
H	5.910850000	-3.063080000	1.822660000
H	6.209330000	-2.869200000	0.062910000
H	6.051110000	-1.424000000	1.108840000
C	-3.882850000	2.222990000	2.286480000
H	-4.853760000	1.703340000	2.261980000
H	-3.821970000	2.833620000	3.199590000
H	-3.811660000	2.886320000	1.410840000
C	2.991220000	2.322020000	4.202260000
H	4.073800000	2.500340000	4.121090000
H	2.543690000	3.093680000	4.846130000
H	2.823680000	1.336050000	4.660660000
H	0.257600000	0.374780000	-4.578980000
C	-3.963300000	-0.797160000	-2.981420000
H	-4.510580000	0.038170000	-3.444360000
H	-4.014630000	-1.674470000	-3.644280000
H	-4.441980000	-1.048110000	-2.022330000

### Coord\_9

C	0.000000000	0.000000000	0.000000000
C	1.431470000	0.000000000	0.000000000
C	-0.634750000	0.000000000	-1.325130000
C	-2.001530000	-0.241450000	-1.514360000
C	0.227470000	0.128530000	-2.425870000
C	-2.500420000	-0.348800000	-2.812120000
H	-2.666150000	-0.391830000	-0.656660000
C	-0.290130000	0.049150000	-3.716360000
H	1.291210000	0.260750000	-2.209750000
C	-1.642550000	-0.187250000	-3.911870000
H	-2.047540000	-0.268100000	-4.928270000
C	2.127100000	-1.139430000	0.620610000
C	1.535160000	-2.414590000	0.556160000
C	3.459260000	-1.033960000	1.045480000
C	2.256980000	-3.545790000	0.918390000

H	0.519250000	-2.526630000	0.162380000
C	4.181890000	-2.170380000	1.398830000
H	3.935120000	-0.049230000	1.074790000
C	3.579060000	-3.432400000	1.353920000
H	1.783760000	-4.536450000	0.856030000
H	4.145300000	-4.323650000	1.646260000
C	-0.919820000	0.151160000	1.161630000
C	-0.759390000	-0.688010000	2.271620000
C	-1.922190000	1.141850000	1.150590000
C	-1.627320000	-0.555690000	3.358250000
H	0.033320000	-1.437140000	2.285220000
C	-2.794270000	1.253670000	2.239670000
H	-1.996900000	1.842560000	0.312570000
C	-2.648810000	0.398510000	3.339810000
H	-1.493640000	-1.192600000	4.238290000
H	-3.329000000	0.490870000	4.194150000
C	1.434920000	1.351560000	0.702410000
C	1.233780000	2.503380000	-0.069920000
C	1.854950000	1.480840000	2.045490000
C	1.484930000	3.767830000	0.468370000
H	0.888450000	2.416710000	-1.107590000
C	2.136620000	2.749800000	2.564260000
H	1.980060000	0.589320000	2.664580000
C	1.948380000	3.891070000	1.778310000
H	1.319820000	4.662880000	-0.141190000
H	2.163950000	4.884330000	2.190730000
C	5.613500000	-2.058080000	1.825790000
H	5.762750000	-2.578070000	2.785960000
H	6.258040000	-2.521530000	1.061340000
H	5.904040000	-1.002050000	1.941780000
C	-3.892400000	2.269760000	2.230110000
H	-4.867820000	1.758370000	2.249840000
H	-3.804750000	2.917070000	3.115190000
H	-3.836900000	2.895550000	1.326110000
C	2.643580000	2.889930000	3.967860000
H	3.722010000	3.104160000	3.936500000
H	2.123870000	3.713980000	4.478540000
H	2.478640000	1.961210000	4.534000000
H	0.376810000	0.158810000	-4.576110000
C	-3.947290000	-0.655560000	-3.041310000
H	-4.416470000	0.162670000	-3.608060000
H	-4.035620000	-1.590610000	-3.615100000
H	-4.477300000	-0.775170000	-2.083920000

Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.440750000	0.000000000	0.000000000
C	-0.613610000	0.000000000	-1.333300000
C	-1.990560000	-0.155750000	-1.547010000

C	0.279310000	0.014890000	-2.417280000
C	-2.464490000	-0.287570000	-2.850460000
H	-2.683110000	-0.227590000	-0.701160000
C	-0.213710000	-0.085630000	-3.714970000
H	1.343340000	0.079350000	-2.172680000
C	-1.575370000	-0.236840000	-3.933070000
H	-1.963230000	-0.337310000	-4.954230000
C	2.123200000	-0.959530000	0.883320000
C	1.636820000	-2.279190000	0.952050000
C	3.386860000	-0.686130000	1.423100000
C	2.390490000	-3.281920000	1.555420000
H	0.686670000	-2.538200000	0.471700000
C	4.139020000	-1.697700000	2.019630000
H	3.793010000	0.326830000	1.348490000
C	3.631460000	-2.998950000	2.105710000
H	1.997560000	-4.308460000	1.593750000
H	4.217830000	-3.787680000	2.589900000
C	-0.934250000	0.167300000	1.149890000
C	-0.789150000	-0.663210000	2.268300000
C	-1.926680000	1.167290000	1.122500000
C	-1.667880000	-0.516630000	3.344970000
H	-0.002720000	-1.418280000	2.295460000
C	-2.811190000	1.291040000	2.200200000
H	-1.981670000	1.869430000	0.284080000
C	-2.683860000	0.441860000	3.307170000
H	-1.544860000	-1.144690000	4.232520000
H	-3.373120000	0.545220000	4.153070000
C	1.336940000	1.428440000	0.533320000
C	1.167410000	2.469100000	-0.389740000
C	1.656420000	1.741760000	1.876180000
C	1.357580000	3.797870000	-0.002830000
H	0.898140000	2.243970000	-1.429660000
C	1.882090000	3.073140000	2.241800000
H	1.750580000	0.940970000	2.613020000
C	1.730730000	4.097470000	1.308410000
H	1.215870000	4.604260000	-0.730240000
H	1.901680000	5.140330000	1.602750000
C	5.502730000	-1.407730000	2.565670000
H	5.600550000	-1.821590000	3.582800000
H	6.259560000	-1.874160000	1.913930000
H	5.686030000	-0.322260000	2.602110000
C	-3.901890000	2.314890000	2.173090000
H	-4.880860000	1.813930000	2.236650000
H	-3.787550000	2.997100000	3.028250000
H	-3.862910000	2.902440000	1.242900000
C	2.288540000	3.405760000	3.646280000
H	3.356120000	3.669670000	3.653980000
H	1.700100000	4.256720000	4.019350000
H	2.126980000	2.544100000	4.310790000
H	0.477280000	-0.062060000	-4.561780000

C	-3.922370000	-0.514060000	-3.104430000
H	-4.312780000	0.271850000	-3.767730000
H	-4.058530000	-1.494770000	-3.584730000
H	-4.490140000	-0.498990000	-2.161520000

TPE-4oM

S<sub>0</sub>-S<sub>1</sub>S<sub>0</sub>-cyc(C4C5)-S<sub>0</sub>-final(C4C5)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.363000000	0.000000000	0.000000000
C	-0.789760000	0.000000000	-1.254080000
C	-1.715610000	-1.028920000	-1.525220000
C	-0.654530000	1.064840000	-2.170140000
C	-2.511350000	-0.968720000	-2.678500000
C	-1.464390000	1.105990000	-3.316990000
C	-2.393720000	0.101020000	-3.563320000
H	-3.027440000	0.145700000	-4.457450000
C	2.170680000	-0.205010000	-1.216140000
C	1.784440000	-1.146560000	-2.181910000
C	3.362600000	0.513950000	-1.395350000
C	2.571940000	-1.354700000	-3.299100000
H	0.851070000	-1.703560000	-2.056320000
C	4.135290000	0.304630000	-2.521670000
H	3.673490000	1.242630000	-0.639700000
C	3.749590000	-0.631160000	-3.481050000
H	2.271630000	-2.096340000	-4.049830000
H	4.368240000	-0.797160000	-4.367940000
C	-0.780850000	0.005490000	1.260730000
C	-0.641110000	-1.053520000	2.182740000
C	-1.707510000	1.033850000	1.528270000
C	-1.444240000	-1.086340000	3.334320000
C	-2.499770000	0.978410000	2.683810000
C	-2.374370000	-0.082820000	3.577680000
H	-1.333780000	-1.912850000	4.046220000
H	-3.004200000	-0.122780000	4.475070000
C	2.145150000	0.219970000	1.237400000
C	1.798560000	1.265310000	2.105620000
C	3.254650000	-0.586170000	1.516190000
C	2.558410000	1.487290000	3.250490000
H	0.927800000	1.891420000	1.892140000
C	3.998360000	-0.363710000	2.670960000
H	3.531030000	-1.389890000	0.827760000
C	3.652340000	0.675920000	3.535380000
H	2.290700000	2.303100000	3.930450000

H	4.246060000	0.852930000	4.440180000
H	-1.361560000	1.938060000	-4.022460000
H	-3.226370000	1.774800000	2.883240000
H	-3.234070000	-1.767510000	-2.880830000
H	5.061950000	0.875190000	-2.664540000
H	4.859730000	-1.000530000	2.899760000
C	0.355440000	2.153970000	-1.998040000
H	1.254570000	1.889830000	-2.573100000
H	-0.046730000	3.107600000	-2.378340000
H	0.633380000	2.279550000	-0.941590000
C	-1.855700000	-2.208280000	-0.618670000
H	-2.275800000	-1.887940000	0.342680000
H	-2.520990000	-2.964480000	-1.068310000
H	-0.866990000	-2.666620000	-0.449840000
C	0.357590000	-2.153200000	2.008300000
H	1.274950000	-1.883850000	2.549980000
H	-0.041440000	-3.095500000	2.420190000
H	0.603330000	-2.304840000	0.946970000
C	-1.853730000	2.211370000	0.618100000
H	-0.867230000	2.673610000	0.450020000
H	-2.270750000	1.889830000	-0.343750000
H	-2.521370000	2.967390000	1.065180000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.371440000	0.000000000	0.000000000
C	-0.766820000	0.000000000	-1.261250000
C	-1.727470000	-1.000490000	-1.538430000
C	-0.572050000	1.043580000	-2.202630000
C	-2.474190000	-0.944950000	-2.721300000
C	-1.355250000	1.080740000	-3.371670000
C	-2.286570000	0.084600000	-3.635790000
H	-2.880910000	0.112040000	-4.555450000
C	2.175660000	-0.190470000	-1.210090000
C	1.741470000	-1.074190000	-2.220000000
C	3.379610000	0.517760000	-1.374040000
C	2.509460000	-1.238980000	-3.366750000
H	0.830990000	-1.672030000	-2.057610000
C	4.134090000	0.353780000	-2.516840000
H	3.709450000	1.206210000	-0.587550000
C	3.701190000	-0.541820000	-3.525010000
H	2.179250000	-1.934480000	-4.147040000
H	4.307520000	-0.684060000	-4.426180000
C	-0.751910000	-0.102280000	1.274940000
C	-0.595270000	-1.229630000	2.110090000
C	-1.666630000	0.905720000	1.645240000
C	-1.363880000	-1.345420000	3.278920000
C	-2.425860000	0.767410000	2.815380000
C	-2.279180000	-0.357470000	3.625290000

H	-1.238700000	-2.223460000	3.923980000
H	-2.881130000	-0.460920000	4.536460000
C	2.144750000	0.198170000	1.246340000
C	1.787380000	1.224600000	2.131900000
C	3.253560000	-0.611460000	1.517450000
C	2.538420000	1.426560000	3.286850000
H	0.917040000	1.851850000	1.921720000
C	3.987360000	-0.410000000	2.683020000
H	3.534890000	-1.402700000	0.816750000
C	3.632230000	0.612220000	3.563990000
H	2.263400000	2.227990000	3.980600000
H	4.218350000	0.772980000	4.476830000
H	-1.217390000	1.902280000	-4.085370000
H	-3.142190000	1.549180000	3.094560000
H	-3.221080000	-1.722130000	-2.927100000
H	5.071360000	0.907750000	-2.643100000
H	4.847080000	-1.050430000	2.907080000
C	0.401230000	2.153730000	-1.954770000
H	1.362400000	1.889680000	-2.419880000
H	0.031600000	3.090490000	-2.404150000
H	0.559990000	2.311460000	-0.877710000
C	-1.973570000	-2.127470000	-0.588660000
H	-2.602230000	-1.782280000	0.242830000
H	-2.481860000	-2.959880000	-1.102220000
H	-1.013460000	-2.494040000	-0.189810000
C	0.387650000	-2.318690000	1.818600000
H	1.336670000	-2.083000000	2.320790000
H	0.009330000	-3.282810000	2.198150000
H	0.570860000	-2.410270000	0.737560000
C	-1.838180000	2.142940000	0.822790000
H	-0.884500000	2.694440000	0.779020000
H	-2.149060000	1.873290000	-0.193640000
H	-2.601840000	2.801350000	1.270590000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.379870000	0.000000000	0.000000000
C	-0.743840000	0.000000000	-1.268010000
C	-1.738190000	-0.970560000	-1.553060000
C	-0.489290000	1.019710000	-2.232660000
C	-2.435480000	-0.922620000	-2.763150000
C	-1.245630000	1.051860000	-3.423030000
C	-2.178240000	0.064110000	-3.704390000
H	-2.732910000	0.072910000	-4.647110000
C	2.180630000	-0.176090000	-1.203870000
C	1.700900000	-0.997010000	-2.255750000
C	3.396430000	0.520960000	-1.352870000
C	2.451320000	-1.113730000	-3.428690000
H	0.819330000	-1.642100000	-2.068310000

C	4.133580000	0.403660000	-2.509450000
H	3.744640000	1.167320000	-0.537430000
C	3.656280000	-0.443540000	-3.563010000
H	2.093380000	-1.760140000	-4.237060000
H	4.251480000	-0.559490000	-4.477010000
C	-0.722540000	-0.212290000	1.279170000
C	-0.548740000	-1.400800000	2.022120000
C	-1.624980000	0.765340000	1.750190000
C	-1.282130000	-1.602640000	3.201020000
C	-2.350400000	0.541380000	2.927960000
C	-2.182130000	-0.640480000	3.648670000
H	-1.141950000	-2.526770000	3.775200000
H	-2.755570000	-0.809970000	4.568140000
C	2.144320000	0.176100000	1.254830000
C	1.776180000	1.183330000	2.157240000
C	3.252380000	-0.637010000	1.518230000
C	2.518380000	1.364950000	3.321840000
H	0.906340000	1.811790000	1.950330000
C	3.976220000	-0.456890000	2.694130000
H	3.538650000	-1.415570000	0.805510000
C	3.612010000	0.547640000	3.591220000
H	2.236040000	2.151750000	4.029020000
H	4.190470000	0.691910000	4.511730000
H	-1.072900000	1.861940000	-4.144100000
H	-3.056190000	1.300750000	3.285360000
H	-3.205840000	-1.677200000	-2.973580000
H	5.081070000	0.940230000	-2.620230000
H	4.834240000	-1.100960000	2.913370000
C	0.437550000	2.154830000	-1.918220000
H	1.448130000	1.895970000	-2.268380000
H	0.105420000	3.071510000	-2.433750000
H	0.476660000	2.346040000	-0.835140000
C	-2.089460000	-2.037600000	-0.567620000
H	-2.893000000	-1.684970000	0.094320000
H	-2.427680000	-2.946370000	-1.090280000
H	-1.205080000	-2.288900000	0.039930000
C	0.417630000	-2.467390000	1.615100000
H	1.394690000	-2.258040000	2.074230000
H	0.063250000	-3.453500000	1.959550000
H	0.537780000	-2.496750000	0.521430000
C	-1.822810000	2.055570000	1.020140000
H	-0.916280000	2.676920000	1.110440000
H	-2.024150000	1.854500000	-0.038880000
H	-2.672570000	2.612930000	1.449670000

Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.388300000	0.000000000	0.000000000
C	-0.720850000	0.000000000	-1.274360000

C	-1.747660000	-0.939200000	-1.569100000
C	-0.406420000	0.993240000	-2.260190000
C	-2.395400000	-0.901720000	-2.803950000
C	-1.135790000	1.019370000	-3.470990000
C	-2.069070000	0.039620000	-3.768990000
H	-2.583960000	0.028440000	-4.732250000
C	2.185580000	-0.161870000	-1.197490000
C	1.662950000	-0.915230000	-2.288840000
C	3.413060000	0.523540000	-1.331870000
C	2.398030000	-0.979470000	-3.484140000
H	0.815530000	-1.612600000	-2.089460000
C	4.133800000	0.454090000	-2.499460000
H	3.779040000	1.126080000	-0.489460000
C	3.615420000	-0.336930000	-3.594270000
H	2.014650000	-1.573980000	-4.318880000
H	4.200830000	-0.424240000	-4.519430000
C	-0.692760000	-0.323550000	1.273160000
C	-0.501520000	-1.565590000	1.919150000
C	-1.582580000	0.613930000	1.841870000
C	-1.199070000	-1.855840000	3.100540000
C	-2.273440000	0.302230000	3.019950000
C	-2.083310000	-0.929420000	3.646750000
H	-1.043610000	-2.820260000	3.600230000
H	-2.627650000	-1.166930000	4.568700000
C	2.143850000	0.153780000	1.262880000
C	1.764980000	1.141500000	2.181610000
C	3.251130000	-0.662790000	1.518510000
C	2.498260000	1.302480000	3.355450000
H	0.895730000	1.771300000	1.977960000
C	3.964930000	-0.504330000	2.704260000
H	3.542320000	-1.428510000	0.794030000
C	3.591670000	0.482230000	3.617050000
H	2.208620000	2.074420000	4.075690000
H	4.162450000	0.609760000	4.544880000
H	-0.928410000	1.817100000	-4.198560000
H	-2.968440000	1.031600000	3.453300000
H	-3.188440000	-1.632740000	-3.020140000
H	5.091110000	0.972550000	-2.595940000
H	4.821180000	-1.152110000	2.918600000
C	0.465390000	2.157000000	-1.889630000
H	1.512540000	1.909050000	-2.121770000
H	0.175150000	3.050390000	-2.467790000
H	0.386010000	2.382150000	-0.814830000
C	-2.202390000	-1.939070000	-0.555740000
H	-3.140780000	-1.602030000	-0.090520000
H	-2.369530000	-2.917350000	-1.032080000
H	-1.434340000	-2.053260000	0.225650000
C	0.447550000	-2.598150000	1.399310000
H	1.448890000	-2.407340000	1.812900000
H	0.120200000	-3.605940000	1.705510000



H	0.504380000	-2.564200000	0.300280000
C	-1.807630000	1.950030000	1.208450000
H	-0.962020000	2.619530000	1.439090000
H	-1.897660000	1.832450000	0.121900000
H	-2.732260000	2.406770000	1.600470000

Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.396740000	0.000000000	0.000000000
C	-0.697830000	0.000000000	-1.280300000
C	-1.755780000	-0.906470000	-1.586510000
C	-0.323620000	0.964200000	-2.285160000
C	-2.354110000	-0.882240000	-2.843590000
C	-1.025990000	0.983330000	-3.515480000
C	-1.959380000	0.011180000	-3.829460000
H	-2.434580000	-0.021260000	-4.810760000
C	2.190520000	-0.147800000	-1.190960000
C	1.627840000	-0.829050000	-2.318950000
C	3.429490000	0.525530000	-1.311050000
C	2.350080000	-0.836810000	-3.532330000
H	0.819060000	-1.582090000	-2.121790000
C	4.134770000	0.504920000	-2.486820000
H	3.812590000	1.082590000	-0.443730000
C	3.579100000	-0.222720000	-3.618060000
H	1.943650000	-1.376760000	-4.391570000
H	4.156210000	-0.279230000	-4.552470000
C	-0.662580000	-0.435060000	1.256720000
C	-0.453650000	-1.722590000	1.801650000
C	-1.539460000	0.452860000	1.919210000
C	-1.114760000	-2.102820000	2.977640000
C	-2.195060000	0.052040000	3.089940000
C	-1.982830000	-1.221760000	3.618750000
H	-0.943770000	-3.101420000	3.399710000
H	-2.497510000	-1.528660000	4.537070000
C	2.143350000	0.131210000	1.270460000
C	1.753760000	1.099150000	2.205020000
C	3.249800000	-0.688810000	1.518290000
C	2.478090000	1.239200000	3.387650000
H	0.885190000	1.730370000	2.004610000
C	3.953510000	-0.552330000	2.713410000
H	3.545880000	-1.441500000	0.782300000
C	3.571210000	0.416010000	3.641450000
H	2.181150000	1.996050000	4.120590000
H	4.134270000	0.526560000	4.576230000
H	-0.784230000	1.767820000	-4.248680000
H	-2.879010000	0.744090000	3.596260000
H	-3.169000000	-1.588740000	-3.066670000
H	5.101490000	1.004640000	-2.570210000
H	4.807930000	-1.203840000	2.922750000

C	0.485830000	2.159790000	-1.870040000
H	1.556740000	1.929000000	-1.983080000
H	0.241260000	3.026760000	-2.506840000
H	0.290690000	2.418480000	-0.817310000
C	-2.311390000	-1.832330000	-0.553150000
H	-3.341490000	-1.538040000	-0.297530000
H	-2.317560000	-2.865500000	-0.931060000
H	-1.691380000	-1.791610000	0.356000000
C	0.477420000	-2.709920000	1.172810000
H	1.499160000	-2.529570000	1.539610000
H	0.180050000	-3.738550000	1.437360000
H	0.470950000	-2.612660000	0.075750000
C	-1.792620000	1.827240000	1.386080000
H	-1.020910000	2.521530000	1.759410000
H	-1.771290000	1.805600000	0.289890000
H	-2.779790000	2.187760000	1.721870000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.405170000	0.000000000	0.000000000
C	-0.674820000	0.000000000	-1.285840000
C	-1.762430000	-0.872440000	-1.605270000
C	-0.241080000	0.932620000	-2.307550000
C	-2.311780000	-0.864130000	-2.881980000
C	-0.916510000	0.943810000	-3.556430000
C	-1.849520000	-0.021120000	-3.885730000
H	-2.285290000	-0.076010000	-4.882520000
C	2.195430000	-0.133900000	-1.184270000
C	1.595790000	-0.738740000	-2.345780000
C	3.445720000	0.526910000	-1.290430000
C	2.307940000	-0.686460000	-3.572550000
H	0.829440000	-1.548870000	-2.165700000
C	4.136540000	0.555970000	-2.471510000
H	3.845260000	1.036960000	-0.400350000
C	3.547800000	-0.101720000	-3.633660000
H	1.880970000	-1.169360000	-4.454210000
H	4.118220000	-0.125490000	-4.575250000
C	-0.632020000	-0.545780000	1.229810000
C	-0.405150000	-1.870440000	1.670220000
C	-1.495650000	0.283560000	1.981230000
C	-1.029270000	-2.341390000	2.832710000
C	-2.115310000	-0.206950000	3.136780000
C	-1.880790000	-1.514880000	3.564120000
H	-0.842510000	-3.367790000	3.174530000
H	-2.365300000	-1.891890000	4.472540000
C	2.142820000	0.108420000	1.277570000
C	1.742530000	1.056300000	2.227430000
C	3.248380000	-0.715040000	1.517550000
C	2.457850000	1.175130000	3.418430000

H	0.874740000	1.689050000	2.030270000
C	3.941940000	-0.600840000	2.721550000
H	3.549350000	-1.454550000	0.770330000
C	3.550640000	0.349010000	3.664410000
H	2.153620000	1.916680000	4.163690000
H	4.105940000	0.442370000	4.605750000
H	-0.640680000	1.714190000	-4.294400000
H	-2.788000000	0.440770000	3.712360000
H	-3.147620000	-1.545210000	-3.113040000
H	5.112200000	1.036400000	-2.543050000
H	4.794490000	-1.256130000	2.925810000
C	0.500030000	2.162660000	-1.860320000
H	1.582160000	1.955660000	-1.855140000
H	0.304270000	3.000170000	-2.551340000
H	0.193260000	2.453560000	-0.842700000
C	-2.415520000	-1.717880000	-0.559890000
H	-3.494310000	-1.495590000	-0.511790000
H	-2.280190000	-2.783460000	-0.794260000
H	-1.964830000	-1.510730000	0.422820000
C	0.507240000	-2.801830000	0.937300000
H	1.545430000	-2.623740000	1.257240000
H	0.242650000	-3.849840000	1.156580000
H	0.437790000	-2.642330000	-0.150630000
C	-1.777750000	1.688260000	1.551470000
H	-1.091950000	2.383030000	2.065630000
H	-1.646780000	1.771950000	0.465920000
H	-2.814200000	1.960920000	1.813580000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.413610000	0.000000000	0.000000000
C	-0.651800000	0.000000000	-1.290960000
C	-1.767530000	-0.837180000	-1.625330000
C	-0.158970000	0.898530000	-2.327310000
C	-2.268590000	-0.847360000	-2.919060000
C	-0.807610000	0.900880000	-3.593800000
C	-1.739830000	-0.057190000	-3.937710000
H	-2.136600000	-0.135650000	-4.947480000
C	2.200330000	-0.120170000	-1.177430000
C	1.566980000	-0.644590000	-2.369040000
C	3.461750000	0.527720000	-1.270010000
C	2.272020000	-0.529190000	-3.604120000
H	0.846260000	-1.511080000	-2.221190000
C	4.139120000	0.607060000	-2.453510000
H	3.877020000	0.989310000	-0.359420000
C	3.521940000	0.025160000	-3.640460000
H	1.827110000	-0.952760000	-4.505940000
H	4.087410000	0.035820000	-4.586930000
C	-0.601090000	-0.654680000	1.192460000

C	-0.356050000	-2.007790000	1.525620000
C	-1.451180000	0.107580000	2.027150000
C	-0.942670000	-2.569400000	2.666350000
C	-2.034260000	-0.472420000	3.159510000
C	-1.777280000	-1.806090000	3.482630000
H	-0.739920000	-3.616960000	2.925830000
H	-2.231160000	-2.253290000	4.374720000
C	2.142250000	0.085400000	1.284210000
C	1.731290000	1.012970000	2.248860000
C	3.246890000	-0.741490000	1.516280000
C	2.437560000	1.110320000	3.447760000
H	0.864370000	1.647360000	2.054930000
C	3.930230000	-0.649850000	2.728660000
H	3.552720000	-1.467640000	0.758090000
C	3.529970000	0.281280000	3.685890000
H	2.126050000	1.836360000	4.204960000
H	4.077460000	0.357230000	4.633430000
H	-0.498070000	1.656300000	-4.335700000
H	-2.695460000	0.124380000	3.800030000
H	-3.124400000	-1.502120000	-3.159180000
H	5.123260000	1.067770000	-2.514460000
H	4.780840000	-1.308950000	2.927740000
C	0.509200000	2.164930000	-1.861110000
H	1.590510000	1.988550000	-1.740540000
H	0.364710000	2.970080000	-2.601650000
H	0.096190000	2.485770000	-0.890650000
C	-2.513840000	-1.596270000	-0.575920000
H	-3.601440000	-1.474900000	-0.718660000
H	-2.263510000	-2.664600000	-0.631780000
H	-2.242750000	-1.219250000	0.421690000
C	0.537030000	-2.873140000	0.694540000
H	1.587620000	-2.689180000	0.968780000
H	0.307860000	-3.938410000	0.864860000
H	0.405200000	-2.653490000	-0.377400000
C	-1.763010000	1.534290000	1.703180000
H	-1.173880000	2.205120000	2.351850000
H	-1.525840000	1.729060000	0.650370000
H	-2.834730000	1.731200000	1.876190000

### Coord\_8

C	0.000000000	0.000000000	0.000000000
C	1.422040000	0.000000000	0.000000000
C	-0.628780000	0.000000000	-1.295690000
C	-1.770970000	-0.800770000	-1.646650000
C	-0.077480000	0.861980000	-2.344430000
C	-2.224700000	-0.831860000	-2.954740000
C	-0.699560000	0.854630000	-3.627560000
C	-1.630650000	-0.096900000	-3.985360000
H	-1.989040000	-0.199980000	-5.005590000

C	2.205210000	-0.106600000	-1.170440000
C	1.541600000	-0.546900000	-2.388440000
C	3.477580000	0.527940000	-1.249830000
C	2.242720000	-0.365880000	-3.626410000
H	0.869230000	-1.466730000	-2.287860000
C	4.142530000	0.658020000	-2.432830000
H	3.907820000	0.939770000	-0.321030000
C	3.501890000	0.156930000	-3.637870000
H	1.782570000	-0.728020000	-4.545960000
H	4.064250000	0.203450000	-4.586770000
C	-0.569820000	-0.760720000	1.144820000
C	-0.306370000	-2.133390000	1.368720000
C	-1.406080000	-0.073450000	2.056320000
C	-0.855040000	-2.784720000	2.479410000
C	-1.951980000	-0.741940000	3.157470000
C	-1.672410000	-2.092680000	3.374330000
H	-0.636080000	-3.846630000	2.655020000
H	-2.095220000	-2.609470000	4.243630000
C	2.141650000	0.062180000	1.290380000
C	1.720040000	0.969190000	2.269270000
C	3.245310000	-0.768120000	1.514490000
C	2.417210000	1.044790000	3.475620000
H	0.854080000	1.605320000	2.078600000
C	3.918390000	-0.699340000	2.734720000
H	3.556000000	-1.480770000	0.745600000
C	3.509180000	0.212850000	3.705890000
H	2.098440000	1.755120000	4.244390000
H	4.048840000	0.271180000	4.659220000
H	-0.356720000	1.594270000	-4.372550000
H	-2.601500000	-0.202190000	3.857980000
H	-3.099460000	-1.459460000	-3.204980000
H	5.134670000	1.098640000	-2.484460000
H	4.767000000	-1.362280000	2.928530000
C	0.514550000	2.165810000	-1.872850000
H	1.583700000	2.026970000	-1.641520000
H	0.423120000	2.935900000	-2.657980000
H	0.001780000	2.513440000	-0.960400000
C	-2.605470000	-1.468120000	-0.601160000
H	-3.667640000	-1.473630000	-0.904750000
H	-2.270830000	-2.503740000	-0.456080000
H	-2.513540000	-0.927100000	0.352180000
C	0.566800000	-2.923270000	0.446340000
H	1.625690000	-2.725560000	0.677260000
H	0.375500000	-4.002990000	0.564050000
H	0.373470000	-2.646530000	-0.603200000
C	-1.748380000	1.366650000	1.839880000
H	-1.265290000	1.989830000	2.612270000
H	-1.410190000	1.674180000	0.843050000
H	-2.840870000	1.503370000	1.911150000

## Coord\_9

C	0.00000000	0.00000000	0.00000000
C	1.43047000	0.00000000	0.00000000
C	-0.60578000	0.00000000	-1.30001000
C	-1.77267000	-0.76328000	-1.66917000
C	0.00320000	0.82302000	-2.35891000
C	-2.18028000	-0.81756000	-2.98899000
C	-0.59264000	0.80515000	-3.65769000
C	-1.52233000	-0.14015000	-4.02866000
H	-1.84311000	-0.26878000	-5.05686000
C	2.21007000	-0.09320000	-1.16331000
C	1.51984000	-0.44602000	-2.40372000
C	3.49321000	0.52760000	-1.22989000
C	2.22037000	-0.19746000	-3.63887000
H	0.89820000	-1.41380000	-2.36486000
C	4.14680000	0.70867000	-2.40945000
H	3.93762000	0.88847000	-0.28526000
C	3.48796000	0.29254000	-3.62541000
H	1.74777000	-0.49630000	-4.57353000
H	4.04916000	0.37604000	-4.57412000
C	-0.53820000	-0.86289000	1.08714000
C	-0.25614000	-2.24606000	1.20052000
C	-1.36037000	-0.25788000	2.06827000
C	-0.76645000	-2.98531000	2.27295000
C	-1.86854000	-1.01300000	3.13022000
C	-1.56628000	-2.37195000	3.23954000
H	-0.53109000	-4.05462000	2.36373000
H	-1.95762000	-2.95704000	4.07963000
C	2.14102000	0.03876000	1.29605000
C	1.70879000	0.92499000	2.28867000
C	3.24366000	-0.79495000	1.51216000
C	2.39680000	0.97859000	3.50201000
H	0.84387000	1.56296000	2.10127000
C	3.90641000	-0.74927000	2.73973000
H	3.55918000	-1.49393000	0.73283000
C	3.48829000	0.14375000	3.72438000
H	2.07078000	1.67302000	4.28196000
H	4.02008000	0.18427000	4.68311000
H	-0.21694000	1.52821000	-4.40495000
H	-2.50619000	-0.53596000	3.88522000
H	-3.07290000	-1.41719000	-3.25037000
H	5.14644000	1.12894000	-2.45305000
H	4.75297000	-1.41610000	2.92817000
C	0.51726000	2.16443000	-1.89573000
H	1.56380000	2.06994000	-1.56003000
H	0.48004000	2.89697000	-2.72043000
H	-0.08791000	2.53485000	-1.05078000
C	-2.68955000	-1.33408000	-0.63541000
H	-3.69958000	-1.48693000	-1.05890000

H	-2.302590000	-2.297750000	-0.281080000
H	-2.766830000	-0.644800000	0.217850000
C	0.596560000	-2.951790000	0.194570000
H	1.659610000	-2.732880000	0.385710000
H	0.445400000	-4.042450000	0.256160000
H	0.342880000	-2.621900000	-0.826760000
C	-1.733830000	1.186770000	1.960360000
H	-1.364560000	1.740240000	2.841310000
H	-1.301470000	1.604330000	1.043120000
H	-2.832340000	1.281770000	1.920730000

### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.438910000	0.000000000	0.000000000
C	-0.582800000	0.000000000	-1.303930000
C	-1.772540000	-0.724780000	-1.692850000
C	0.082900000	0.781700000	-2.370740000
C	-2.135490000	-0.804400000	-3.021760000
C	-0.487110000	0.752550000	-3.684200000
C	-1.415210000	-0.186790000	-4.067580000
H	-1.699320000	-0.341820000	-5.101310000
C	2.214920000	-0.079960000	-1.156030000
C	1.501830000	-0.342310000	-2.414650000
C	3.508620000	0.526690000	-1.210200000
C	2.205280000	-0.024950000	-3.640970000
H	0.933120000	-1.350360000	-2.450900000
C	4.151940000	0.758840000	-2.383410000
H	3.966410000	0.835540000	-0.252190000
C	3.480400000	0.430860000	-3.602660000
H	1.723100000	-0.258870000	-4.588000000
H	4.042450000	0.552160000	-4.548450000
C	-0.506270000	-0.960190000	1.019780000
C	-0.205400000	-2.344690000	1.022160000
C	-1.314090000	-0.443980000	2.062700000
C	-0.676980000	-3.169240000	2.048240000
C	-1.784010000	-1.283080000	3.077610000
C	-1.458990000	-2.641230000	3.078900000
H	-0.425030000	-4.238900000	2.053850000
H	-1.818530000	-3.292660000	3.883450000
C	2.140360000	0.015150000	1.301240000
C	1.697530000	0.880380000	2.307050000
C	3.241930000	-0.821940000	1.509280000
C	2.376340000	0.911750000	3.526890000
H	0.833750000	1.520300000	2.122930000
C	3.894290000	-0.799630000	2.743660000
H	3.562260000	-1.507130000	0.719790000
C	3.467300000	0.074030000	3.741330000
H	2.043080000	1.590110000	4.317640000
H	3.991180000	0.096540000	4.705080000

H	-0.079040000	1.458240000	-4.432920000
H	-2.409620000	-0.873820000	3.881100000
H	-3.044820000	-1.375260000	-3.295280000
H	5.158570000	1.158600000	-2.420240000
H	4.738740000	-1.470360000	2.926620000
C	0.518480000	2.159840000	-1.929730000
H	1.532990000	2.116270000	-1.497600000
H	0.535950000	2.852560000	-2.788950000
H	-0.171050000	2.548280000	-1.160260000
C	-2.765280000	-1.194850000	-0.678450000
H	-3.704980000	-1.507690000	-1.172840000
H	-2.356420000	-2.046100000	-0.121140000
H	-2.994200000	-0.382670000	0.025970000
C	0.626320000	-2.958470000	-0.058870000
H	1.689380000	-2.711510000	0.097100000
H	0.517360000	-4.055840000	-0.056610000
H	0.313710000	-2.580120000	-1.046920000
C	-1.719350000	0.996200000	2.063560000
H	-1.469930000	1.460410000	3.033880000
H	-1.201200000	1.516460000	1.248990000
H	-2.809140000	1.070220000	1.907930000

#### Coord\_11

C	0.000000000	0.000000000	0.000000000
C	1.442650000	0.000000000	0.000000000
C	-0.608080000	0.000000000	-1.278110000
C	-1.900260000	-0.580230000	-1.584340000
C	0.113230000	0.642240000	-2.411280000
C	-2.303290000	-0.722830000	-2.892560000
C	-0.468400000	0.484930000	-3.728500000
C	-1.543020000	-0.328310000	-3.964130000
H	-1.886830000	-0.566850000	-4.966540000
C	2.204700000	-0.112760000	-1.155560000
C	1.489030000	-0.402060000	-2.414660000
C	3.552980000	0.371170000	-1.194920000
C	2.222340000	-0.103360000	-3.640620000
H	1.001070000	-1.448830000	-2.427520000
C	4.220120000	0.545300000	-2.363970000
H	4.030920000	0.630140000	-0.234420000
C	3.519880000	0.275820000	-3.599820000
H	1.723930000	-0.281030000	-4.594400000
H	4.087210000	0.399310000	-4.539510000
C	-0.531090000	-0.787560000	1.144250000
C	-0.358130000	-2.187770000	1.259190000
C	-1.208010000	-0.099340000	2.178680000
C	-0.837670000	-2.867370000	2.383180000
C	-1.685540000	-0.794660000	3.294190000
C	-1.493880000	-2.173330000	3.402520000
H	-0.692960000	-3.952490000	2.472350000



H	-1.859440000	-2.711630000	4.284460000
C	2.145060000	0.078050000	1.299510000
C	1.898730000	1.165220000	2.147010000
C	3.055690000	-0.920110000	1.666370000
C	2.578140000	1.253240000	3.362730000
H	1.185060000	1.933140000	1.843100000
C	3.712440000	-0.831010000	2.894380000
H	3.223840000	-1.773840000	1.004450000
C	3.479060000	0.257370000	3.734080000
H	2.398990000	2.104090000	4.027120000
H	4.003830000	0.326550000	4.694720000
H	0.029980000	0.997410000	-4.571090000
H	-2.209800000	-0.254690000	4.092540000
H	-3.287880000	-1.176380000	-3.109970000
H	5.259080000	0.861300000	-2.393600000
H	4.408430000	-1.618270000	3.199680000
C	0.496950000	2.077110000	-2.100910000
H	1.429370000	2.099030000	-1.512610000
H	0.658650000	2.643540000	-3.033290000
H	-0.299600000	2.563680000	-1.513560000
C	-2.904330000	-0.865850000	-0.513800000
H	-3.892430000	-1.085850000	-0.960350000
H	-2.584000000	-1.730240000	0.080600000
H	-3.005760000	0.006330000	0.147150000
C	0.334840000	-2.967280000	0.186860000
H	1.413290000	-2.740820000	0.194700000
H	0.200600000	-4.050180000	0.345350000
H	-0.077230000	-2.704120000	-0.800870000
C	-1.453910000	1.372800000	2.075380000
H	-0.964890000	1.892400000	2.916630000
H	-1.056500000	1.743840000	1.122480000
H	-2.538000000	1.571150000	2.119010000

## Coord\_12

C	0.000000000	0.000000000	0.000000000
C	1.450130000	0.000000000	0.000000000
C	-0.655950000	0.000000000	-1.225120000
C	-2.080780000	-0.246510000	-1.385170000
C	0.117280000	0.331210000	-2.473600000
C	-2.598580000	-0.503230000	-2.626340000
C	-0.544130000	-0.097110000	-3.727850000
C	-1.819560000	-0.551640000	-3.752820000
H	-2.289660000	-0.915170000	-4.669350000
C	2.184350000	-0.178360000	-1.151340000
C	1.463660000	-0.522210000	-2.409700000
C	3.606450000	0.042910000	-1.163730000
C	2.257210000	-0.261340000	-3.631910000
H	1.146880000	-1.626310000	-2.380260000
C	4.303320000	0.089960000	-2.325670000

H	4.110890000	0.200510000	-0.199710000
C	3.585090000	-0.034800000	-3.584700000
H	1.742360000	-0.320670000	-4.597500000
H	4.169470000	0.095650000	-4.507540000
C	-0.579960000	-0.400420000	1.304520000
C	-0.684020000	-1.764500000	1.657840000
C	-0.989510000	0.584720000	2.228670000
C	-1.197720000	-2.126960000	2.906860000
C	-1.501070000	0.204490000	3.474250000
C	-1.599500000	-1.145170000	3.814560000
H	-1.285700000	-3.186650000	3.177200000
H	-1.991990000	-1.435890000	4.796000000
C	2.154440000	0.203290000	1.286930000
C	2.384350000	1.509940000	1.744910000
C	2.602920000	-0.895060000	2.033950000
C	3.065560000	1.711410000	2.943950000
H	2.037680000	2.359020000	1.149930000
C	3.274680000	-0.681930000	3.236280000
H	2.404380000	-1.910570000	1.681390000
C	3.507260000	0.618110000	3.690670000
H	3.259270000	2.728950000	3.299540000
H	4.034960000	0.780050000	4.637660000
H	0.038620000	-0.035710000	-4.660240000
H	-1.818750000	0.970850000	4.191330000
H	-3.675500000	-0.696210000	-2.748960000
H	5.385950000	0.228550000	-2.343030000
H	3.616490000	-1.535960000	3.830510000
C	0.387180000	1.836860000	-2.500480000
H	1.126540000	2.097100000	-1.727290000
H	0.781960000	2.140150000	-3.482480000
H	-0.544000000	2.389690000	-2.302610000
C	-3.033720000	-0.155480000	-0.236270000
H	-4.077060000	-0.172150000	-0.600840000
H	-2.886100000	-1.002720000	0.445560000
H	-2.870660000	0.782030000	0.312900000
C	-0.270790000	-2.830100000	0.692070000
H	0.799650000	-2.725960000	0.456070000
H	-0.446790000	-3.831350000	1.118340000
H	-0.850940000	-2.732400000	-0.237260000
C	-0.887140000	2.037900000	1.888000000
H	-0.021420000	2.469470000	2.413640000
H	-0.758590000	2.162730000	0.804760000
H	-1.800040000	2.566540000	2.207380000

### Coord\_13

C	0.000000000	0.000000000	0.000000000
C	1.455740000	0.000000000	0.000000000
C	-0.689470000	0.000000000	-1.184320000
C	-2.146190000	0.027940000	-1.261750000

C	0.068950000	0.080120000	-2.496600000
C	-2.774250000	-0.292530000	-2.429100000
C	-0.696330000	-0.542010000	-3.634480000
C	-2.031490000	-0.690280000	-3.599190000
H	-2.589150000	-1.120610000	-4.440010000
C	2.169150000	-0.227410000	-1.145320000
C	1.444860000	-0.612720000	-2.401570000
C	3.613020000	-0.213040000	-1.138750000
C	2.283950000	-0.380460000	-3.618290000
H	1.262440000	-1.741210000	-2.345000000
C	4.315030000	-0.267090000	-2.295950000
H	4.124850000	-0.131960000	-0.172810000
C	3.622570000	-0.266450000	-3.565580000
H	1.770890000	-0.347640000	-4.590470000
H	4.225240000	-0.129480000	-4.471520000
C	-0.615900000	-0.092830000	1.341880000
C	-0.936280000	-1.365570000	1.859940000
C	-0.831860000	1.055260000	2.129490000
C	-1.491510000	-1.477530000	3.138460000
C	-1.385630000	0.924440000	3.408310000
C	-1.710800000	-0.335600000	3.910420000
H	-1.760630000	-2.463760000	3.534330000
H	-2.136570000	-0.430420000	4.916370000
C	2.161490000	0.296180000	1.269580000
C	2.769580000	1.552070000	1.441810000
C	2.243930000	-0.666340000	2.287600000
C	3.453280000	1.837090000	2.620760000
H	2.715330000	2.293910000	0.638910000
C	2.929240000	-0.371640000	3.463190000
H	1.755780000	-1.636010000	2.160190000
C	3.531180000	0.878900000	3.635090000
H	3.941790000	2.809210000	2.751460000
H	4.062280000	1.108490000	4.565460000
H	-0.133890000	-0.831450000	-4.532500000
H	-1.554360000	1.815820000	4.023420000
H	-3.869130000	-0.279720000	-2.502380000
H	5.410530000	-0.267420000	-2.305280000
H	2.992090000	-1.118870000	4.262220000
C	0.230250000	1.577930000	-2.812670000
H	0.821450000	2.061510000	-2.021440000
H	0.744550000	1.715240000	-3.774780000
H	-0.757450000	2.057550000	-2.867540000
C	-3.000240000	0.394450000	-0.089980000
H	-4.047550000	0.537580000	-0.410280000
H	-2.971490000	-0.401980000	0.665290000
H	-2.641240000	1.331050000	0.357750000
C	-0.721700000	-2.588720000	1.024610000
H	0.318730000	-2.617630000	0.667470000
H	-0.927920000	-3.500590000	1.608280000
H	-1.394180000	-2.557690000	0.156900000

C	-0.458290000	2.411800000	1.621130000
H	0.569610000	2.632970000	1.941990000
H	-0.507440000	2.438820000	0.523940000
H	-1.137300000	3.176230000	2.031240000

S<sub>0</sub>-S<sub>1</sub>S<sub>0</sub>-cyc(C8C9)-S<sub>0</sub>-final(C8C9)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.363000000	0.000000000	0.000000000
C	-0.789760000	0.000000000	-1.254080000
C	-1.715610000	-1.028920000	-1.525220000
C	-0.654530000	1.064840000	-2.170140000
C	-2.511350000	-0.968720000	-2.678500000
C	-1.464390000	1.105990000	-3.316990000
C	-2.393720000	0.101020000	-3.563320000
H	-3.027440000	0.145700000	-4.457450000
C	2.170680000	-0.205010000	-1.216140000
C	1.784440000	-1.146560000	-2.181910000
C	3.362600000	0.513950000	-1.395350000
C	2.571940000	-1.354700000	-3.299100000
H	0.851070000	-1.703560000	-2.056320000
C	4.135290000	0.304630000	-2.521670000
H	3.673490000	1.242630000	-0.639700000
C	3.749590000	-0.631160000	-3.481050000
H	2.271630000	-2.096340000	-4.049830000
H	4.368240000	-0.797160000	-4.367940000
C	-0.780850000	0.005490000	1.260730000
C	-0.641110000	-1.053520000	2.182740000
C	-1.707510000	1.033850000	1.528270000
C	-1.444240000	-1.086340000	3.334320000
C	-2.499770000	0.978410000	2.683810000
C	-2.374370000	-0.082820000	3.577680000
H	-1.333780000	-1.912850000	4.046220000
H	-3.004200000	-0.122780000	4.475070000
C	2.145150000	0.219970000	1.237400000
C	1.798560000	1.265310000	2.105620000
C	3.254650000	-0.586170000	1.516190000
C	2.558410000	1.487290000	3.250490000
H	0.927800000	1.891420000	1.892140000
C	3.998360000	-0.363710000	2.670960000
H	3.531030000	-1.389890000	0.827760000
C	3.652340000	0.675920000	3.535380000
H	2.290700000	2.303100000	3.930450000
H	4.246060000	0.852930000	4.440180000
H	-1.361560000	1.938060000	-4.022460000
H	-3.226370000	1.774800000	2.883240000

H	-3.234070000	-1.767510000	-2.880830000
H	5.061950000	0.875190000	-2.664540000
H	4.859730000	-1.000530000	2.899760000
C	0.355440000	2.153970000	-1.998040000
H	1.254570000	1.889830000	-2.573100000
H	-0.046730000	3.107600000	-2.378340000
H	0.633380000	2.279550000	-0.941590000
C	-1.855700000	-2.208280000	-0.618670000
H	-2.275800000	-1.887940000	0.342680000
H	-2.520990000	-2.964480000	-1.068310000
H	-0.866990000	-2.666620000	-0.449840000
C	0.357590000	-2.153200000	2.008300000
H	1.274950000	-1.883850000	2.549980000
H	-0.041440000	-3.095500000	2.420190000
H	0.603330000	-2.304840000	0.946970000
C	-1.853730000	2.211370000	0.618100000
H	-0.867230000	2.673610000	0.450020000
H	-2.270750000	1.889830000	-0.343750000
H	-2.521370000	2.967390000	1.065180000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.371430000	0.000000000	0.000000000
C	-0.760030000	0.000000000	-1.273270000
C	-1.673960000	-1.035980000	-1.561030000
C	-0.607550000	1.058660000	-2.194750000
C	-2.436350000	-0.991910000	-2.736770000
C	-1.382340000	1.083540000	-3.365210000
C	-2.296860000	0.068760000	-3.630230000
H	-2.902380000	0.099730000	-4.544140000
C	2.167730000	-0.287400000	-1.207500000
C	1.774290000	-1.298370000	-2.096440000
C	3.350860000	0.425650000	-1.452520000
C	2.550300000	-1.582370000	-3.206830000
H	0.847330000	-1.850220000	-1.915970000
C	4.110930000	0.140830000	-2.572830000
H	3.663550000	1.210710000	-0.756660000
C	3.719580000	-0.865540000	-3.455270000
H	2.245710000	-2.377750000	-3.897930000
H	4.328150000	-1.091230000	-4.336330000
C	-0.758890000	0.111090000	1.262130000
C	-0.560000000	-0.844240000	2.292040000
C	-1.720280000	1.130450000	1.451760000
C	-1.337210000	-0.775610000	3.463350000
C	-2.463840000	1.178560000	2.636610000
C	-2.269280000	0.237690000	3.640690000
H	-1.192490000	-1.528970000	4.248300000
H	-2.860140000	0.291840000	4.561630000
C	2.153040000	0.305790000	1.207820000

C	1.748160000	1.363410000	2.047670000
C	3.285630000	-0.459130000	1.524390000
C	2.487670000	1.640700000	3.201510000
H	0.897580000	1.996610000	1.752680000
C	4.011090000	-0.184140000	2.674980000
H	3.588660000	-1.276930000	0.862120000
C	3.608660000	0.885150000	3.513380000
H	2.182020000	2.464400000	3.854110000
H	4.191030000	1.114820000	4.415100000
H	-1.264120000	1.909450000	-4.076020000
H	-3.214160000	1.967730000	2.774550000
H	-3.149170000	-1.796410000	-2.951970000
H	5.029710000	0.707120000	-2.770070000
H	4.892540000	-0.781110000	2.927330000
C	0.385590000	2.158950000	-1.997230000
H	1.320070000	1.885440000	-2.508650000
H	0.002810000	3.098610000	-2.428890000
H	0.597950000	2.318010000	-0.929720000
C	-1.839990000	-2.201620000	-0.640850000
H	-2.153520000	-1.848160000	0.349070000
H	-2.601740000	-2.895920000	-1.033800000
H	-0.883850000	-2.743950000	-0.550550000
C	0.402580000	-1.980920000	2.138120000
H	1.376730000	-1.678360000	2.548190000
H	0.038420000	-2.863670000	2.690480000
H	0.532230000	-2.250990000	1.079350000
C	-1.971990000	2.171780000	0.408420000
H	-1.026320000	2.675490000	0.152260000
H	-2.387650000	1.704410000	-0.492620000
H	-2.682650000	2.930010000	0.780110000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.379860000	0.000000000	0.000000000
C	-0.729820000	0.000000000	-1.291750000
C	-1.631500000	-1.043000000	-1.595730000
C	-0.559820000	1.052420000	-2.218290000
C	-2.359750000	-1.015060000	-2.792830000
C	-1.298810000	1.061080000	-3.411070000
C	-2.198050000	0.036530000	-3.694090000
H	-2.774710000	0.053820000	-4.626710000
C	2.164700000	-0.369510000	-1.193150000
C	1.764300000	-1.443740000	-2.000270000
C	3.338730000	0.331930000	-1.503780000
C	2.528690000	-1.803620000	-3.098570000
H	0.844090000	-1.985480000	-1.765240000
C	4.086020000	-0.028540000	-2.612850000
H	3.652990000	1.168510000	-0.871820000
C	3.689300000	-1.099240000	-3.413210000

H	2.220000000	-2.647990000	-3.726220000
H	4.287680000	-1.384600000	-4.284290000
C	-0.736930000	0.216900000	1.254290000
C	-0.478680000	-0.622060000	2.378720000
C	-1.731910000	1.220490000	1.371290000
C	-1.229760000	-0.448050000	3.559750000
C	-2.426400000	1.379130000	2.573220000
C	-2.163070000	0.571370000	3.670350000
H	-1.050980000	-1.121160000	4.409530000
H	-2.714690000	0.724130000	4.602650000
C	2.160860000	0.388510000	1.172380000
C	1.701290000	1.453980000	1.986450000
C	3.315920000	-0.333290000	1.522280000
C	2.423190000	1.783680000	3.145350000
H	0.875890000	2.094240000	1.617680000
C	4.024810000	-0.007080000	2.665330000
H	3.644180000	-1.163360000	0.885580000
C	3.569520000	1.084250000	3.477080000
H	2.082690000	2.612170000	3.772830000
H	4.142060000	1.364270000	4.372210000
H	-1.164890000	1.880800000	-4.126800000
H	-3.199730000	2.155760000	2.653410000
H	-3.062400000	-1.825250000	-3.020550000
H	4.996590000	0.528620000	-2.864340000
H	4.925450000	-0.562960000	2.937410000
C	0.415650000	2.163850000	-1.996260000
H	1.381500000	1.882710000	-2.441700000
H	0.055930000	3.088490000	-2.477380000
H	0.561620000	2.355920000	-0.922650000
C	-1.824430000	-2.194720000	-0.662980000
H	-2.027930000	-1.819360000	0.347350000
H	-2.672680000	-2.817020000	-0.994690000
H	-0.915310000	-2.819300000	-0.647990000
C	0.438360000	-1.802080000	2.260240000
H	1.457400000	-1.491790000	2.534280000
H	0.113250000	-2.606090000	2.942150000
H	0.451880000	-2.189990000	1.230180000
C	-2.088210000	2.105840000	0.220030000
H	-1.189700000	2.635730000	-0.132180000
H	-2.497080000	1.504010000	-0.601170000
H	-2.840380000	2.854560000	0.524490000

#### Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.388290000	0.000000000	0.000000000
C	-0.699170000	0.000000000	-1.309510000
C	-1.588270000	-1.050000000	-1.629290000
C	-0.511340000	1.046120000	-2.240730000
C	-2.281620000	-1.038190000	-2.846640000

C	-1.213880000	1.038600000	-3.454540000
C	-2.097390000	0.004340000	-3.754840000
H	-2.644580000	0.007970000	-4.705090000
C	2.161600000	-0.450940000	-1.173100000
C	1.754470000	-1.581900000	-1.893910000
C	3.326210000	0.233220000	-1.548670000
C	2.507140000	-2.017290000	-2.974780000
H	0.841340000	-2.108600000	-1.605070000
C	4.060550000	-0.202710000	-2.641200000
H	3.641830000	1.116140000	-0.984310000
C	3.658750000	-1.331110000	-3.354840000
H	2.194500000	-2.905660000	-3.535540000
H	4.246850000	-1.675800000	-4.211760000
C	-0.714950000	0.322070000	1.237190000
C	-0.397300000	-0.389560000	2.441190000
C	-1.742300000	1.304160000	1.287440000
C	-1.122170000	-0.107360000	3.621320000
C	-2.387620000	1.578630000	2.493030000
C	-2.056070000	0.914400000	3.664560000
H	-0.909560000	-0.694070000	4.527000000
H	-2.568360000	1.168570000	4.595350000
C	2.168610000	0.467750000	1.131360000
C	1.658320000	1.537250000	1.922760000
C	3.345520000	-0.209490000	1.510050000
C	2.365730000	1.916350000	3.083210000
H	0.862200000	2.185700000	1.488280000
C	4.039550000	0.166470000	2.642420000
H	3.697490000	-1.050180000	0.898160000
C	3.535700000	1.272600000	3.427720000
H	1.993680000	2.747010000	3.688110000
H	4.100150000	1.600510000	4.313060000
H	-1.063950000	1.852100000	-4.174730000
H	-3.183190000	2.338120000	2.519700000
H	-2.973850000	-1.854020000	-3.086510000
H	4.962600000	0.340490000	-2.946390000
H	4.958440000	-0.347460000	2.930300000
C	0.445630000	2.168660000	-1.995120000
H	1.438700000	1.881630000	-2.372530000
H	0.112490000	3.077310000	-2.523550000
H	0.524760000	2.393180000	-0.920400000
C	-1.809000000	-2.187590000	-0.685100000
H	-1.900690000	-1.802360000	0.337720000
H	-2.732520000	-2.728810000	-0.951810000
H	-0.960810000	-2.890810000	-0.741660000
C	0.465860000	-1.615630000	2.375480000
H	1.517740000	-1.323890000	2.514790000
H	0.183450000	-2.323580000	3.173210000
H	0.364720000	-2.115410000	1.399470000
C	-2.201430000	2.018180000	0.056400000
H	-1.356320000	2.557530000	-0.396980000



H	-2.598200000	1.295830000	-0.668270000
H	-2.992850000	2.747920000	0.303610000

Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.396720000	0.000000000	0.000000000
C	-0.668080000	0.000000000	-1.326550000
C	-1.544280000	-1.056950000	-1.661700000
C	-0.462170000	1.039750000	-2.262040000
C	-2.202030000	-1.061280000	-2.898160000
C	-1.127600000	1.016120000	-3.495590000
C	-1.994990000	-0.027810000	-3.812450000
H	-2.512130000	-0.037800000	-4.779210000
C	2.158410000	-0.531280000	-1.147360000
C	1.744820000	-1.712140000	-1.777890000
C	3.313300000	0.129960000	-1.586730000
C	2.485630000	-2.222280000	-2.835990000
H	0.839080000	-2.218940000	-1.436440000
C	4.034530000	-0.380810000	-2.657410000
H	3.630050000	1.053800000	-1.093270000
C	3.627940000	-1.559980000	-3.280220000
H	2.169220000	-3.149400000	-3.326840000
H	4.205650000	-1.963360000	-4.118800000
C	-0.692980000	0.425770000	1.210900000
C	-0.316050000	-0.149580000	2.478190000
C	-1.751350000	1.381720000	1.200730000
C	-1.014670000	0.242470000	3.646330000
C	-2.347660000	1.775450000	2.395590000
C	-1.948620000	1.262630000	3.621700000
H	-0.768510000	-0.252740000	4.598380000
H	-2.421650000	1.619240000	4.537730000
C	2.176290000	0.543120000	1.085100000
C	1.619590000	1.613520000	1.857350000
C	3.374410000	-0.088520000	1.487970000
C	2.316000000	2.038940000	3.016150000
H	0.856030000	2.272240000	1.365320000
C	4.055350000	0.335540000	2.606690000
H	3.748520000	-0.938400000	0.899970000
C	3.507910000	1.449700000	3.366500000
H	1.915890000	2.869700000	3.601230000
H	4.066190000	1.822980000	4.239090000
H	-0.961400000	1.823360000	-4.219760000
H	-3.164650000	2.513920000	2.373340000
H	-2.883610000	-1.882720000	-3.149790000
H	4.927740000	0.143640000	-3.015330000
H	4.991500000	-0.135940000	2.906440000
C	0.475540000	2.173380000	-1.993840000
H	1.491550000	1.882180000	-2.301490000
H	0.172370000	3.065150000	-2.567170000

H	0.487710000	2.429670000	-0.922980000
C	-1.793700000	-2.180240000	-0.707230000
H	-1.773530000	-1.797690000	0.320440000
H	-2.780100000	-2.632570000	-0.905930000
H	-1.019540000	-2.956650000	-0.831150000
C	0.486120000	-1.420110000	2.484080000
H	1.558870000	-1.172750000	2.495730000
H	0.249500000	-2.016970000	3.381440000
H	0.273210000	-2.020710000	1.585470000
C	-2.310700000	1.913900000	-0.079850000
H	-1.525050000	2.445130000	-0.636380000
H	-2.690300000	1.087010000	-0.693980000
H	-3.138340000	2.617760000	0.121400000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.405150000	0.000000000	0.000000000
C	-0.636580000	0.000000000	-1.342850000
C	-1.499570000	-1.063870000	-1.692940000
C	-0.412310000	1.033320000	-2.282210000
C	-2.121050000	-1.084330000	-2.947330000
C	-1.040070000	0.993630000	-3.534170000
C	-1.890940000	-0.059910000	-3.866850000
H	-2.377500000	-0.083470000	-4.849010000
C	2.155160000	-0.610130000	-1.116010000
C	1.735350000	-1.833770000	-1.652830000
C	3.300010000	0.022650000	-1.617550000
C	2.464170000	-2.417530000	-2.682840000
H	0.837320000	-2.315920000	-1.260360000
C	4.007960000	-0.561980000	-2.661060000
H	3.617680000	0.981780000	-1.197830000
C	3.596860000	-1.784670000	-3.189510000
H	2.144160000	-3.377960000	-3.101130000
H	4.164100000	-2.245810000	-4.005580000
C	-0.671010000	0.527160000	1.175570000
C	-0.235090000	0.094940000	2.488800000
C	-1.758960000	1.453460000	1.111580000
C	-0.907530000	0.597240000	3.633540000
C	-2.306700000	1.967870000	2.280660000
C	-1.841030000	1.611680000	3.540680000
H	-0.628160000	0.197530000	4.621940000
H	-2.275070000	2.069960000	4.428530000
C	2.183910000	0.614300000	1.033920000
C	1.585440000	1.683200000	1.790870000
C	3.402570000	0.028830000	1.456350000
C	2.274660000	2.151800000	2.945080000
H	0.857030000	2.354980000	1.249360000
C	4.072220000	0.499240000	2.558680000
H	3.797180000	-0.829000000	0.891230000

C	3.486790000	1.615250000	3.294530000
H	1.850140000	2.981150000	3.513240000
H	4.041020000	2.031310000	4.151640000
H	-0.857320000	1.794600000	-4.261850000
H	-3.144240000	2.682210000	2.214360000
H	-2.791750000	-1.911340000	-3.210340000
H	4.892010000	-0.060990000	-3.070350000
H	5.024630000	0.070330000	2.866340000
C	0.505410000	2.177990000	-1.992410000
H	1.539950000	1.884360000	-2.228880000
H	0.235400000	3.052080000	-2.608010000
H	0.450840000	2.465330000	-0.930380000
C	-1.778520000	-2.172680000	-0.729410000
H	-1.648210000	-1.805660000	0.295800000
H	-2.814460000	-2.529770000	-0.857760000
H	-1.090480000	-3.015050000	-0.916140000
C	0.500260000	-1.213800000	2.585560000
H	1.582210000	-1.034950000	2.482270000
H	0.311920000	-1.687220000	3.564380000
H	0.179730000	-1.899640000	1.784710000
C	-2.415090000	1.798420000	-0.187030000
H	-1.694720000	2.303640000	-0.845460000
H	-2.772700000	0.884520000	-0.679530000
H	-3.275210000	2.472240000	-0.019720000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.413580000	0.000000000	0.000000000
C	-0.604680000	0.000000000	-1.358400000
C	-1.454180000	-1.070760000	-1.723000000
C	-0.361800000	1.026830000	-2.301220000
C	-2.038740000	-1.107330000	-2.994120000
C	-0.951360000	0.971150000	-3.570240000
C	-1.785360000	-0.091940000	-3.918010000
H	-2.240850000	-0.129030000	-4.914440000
C	2.151830000	-0.687090000	-1.079130000
C	1.726040000	-1.946170000	-1.519370000
C	3.286330000	-0.088170000	-1.640750000
C	2.442780000	-2.602010000	-2.516020000
H	0.836050000	-2.399070000	-1.077890000
C	3.980860000	-0.745280000	-2.651820000
H	3.604700000	0.900410000	-1.297190000
C	3.565540000	-2.004030000	-3.082930000
H	2.119330000	-3.590120000	-2.859550000
H	4.122210000	-2.521680000	-3.872380000
C	-0.649050000	0.625440000	1.131400000
C	-0.154610000	0.340940000	2.472460000
C	-1.765040000	1.519690000	1.020290000
C	-0.801010000	0.952570000	3.582210000

C	-2.264920000	2.154070000	2.148200000
C	-1.733650000	1.957010000	3.420980000
H	-0.488800000	0.651250000	4.596620000
H	-2.129120000	2.514350000	4.267320000
C	2.191450000	0.680970000	0.978190000
C	1.556160000	1.746720000	1.723850000
C	3.429990000	0.141800000	1.415580000
C	2.242280000	2.255380000	2.870790000
H	0.865000000	2.434830000	1.140710000
C	4.090180000	0.656690000	2.498970000
H	3.843380000	-0.722930000	0.872230000
C	3.472890000	1.769010000	3.212860000
H	1.797160000	3.082360000	3.424950000
H	4.025320000	2.225240000	4.051960000
H	-0.751820000	1.765810000	-4.300960000
H	-3.122070000	2.841970000	2.042860000
H	-2.698350000	-1.939870000	-3.268110000
H	4.855440000	-0.272340000	-3.110680000
H	5.057800000	0.270090000	2.810640000
C	0.535230000	2.182500000	-1.990830000
H	1.583800000	1.888120000	-2.155050000
H	0.301410000	3.038170000	-2.645870000
H	0.414500000	2.500050000	-0.942550000
C	-1.763420000	-2.164920000	-0.751660000
H	-1.526500000	-1.826310000	0.264140000
H	-2.834860000	-2.422070000	-0.807970000
H	-1.172400000	-3.064350000	-0.996430000
C	0.509430000	-0.994960000	2.678730000
H	1.589390000	-0.905870000	2.478320000
H	0.371260000	-1.335480000	3.719300000
H	0.086560000	-1.746680000	1.992050000
C	-2.513680000	1.677300000	-0.264420000
H	-1.864120000	2.138950000	-1.020170000
H	-2.844820000	0.694960000	-0.627230000
H	-3.401860000	2.319740000	-0.118890000

### Coord\_8

C	0.000000000	0.810090000	0.000000000
C	1.422000000	-2.216900000	0.000000000
C	-0.572410000	-3.784790000	-1.373200000
C	-1.408130000	-2.789520000	-1.751850000
C	-0.310670000	0.719800000	-2.319050000
C	-1.955180000	0.585260000	-3.038470000
C	-0.861550000	1.580720000	-3.603790000
C	-1.678350000	1.304030000	-3.965880000
H	-2.102330000	2.332220000	-4.975430000
C	2.148430000	2.293990000	-1.036850000
C	1.716920000	1.102800000	-1.378200000
C	3.272280000	2.945970000	-1.656010000

C	2.421440000	0.742850000	-2.336310000
H	0.835280000	1.804560000	-0.890120000
C	3.953210000	0.249680000	-2.629410000
H	3.591120000	2.350180000	-1.390530000
C	3.533960000	2.512540000	-2.960800000
H	2.094720000	0.807100000	-2.603310000
H	4.079980000	-0.621140000	-3.719590000
C	-0.627110000	1.910870000	1.078710000
C	-0.074780000	3.174360000	2.428970000
C	-1.769490000	2.404620000	0.927110000
C	-0.695380000	1.737010000	3.492130000
C	-2.222490000	2.992120000	1.998400000
C	-1.626810000	-1.968310000	3.262620000
H	-0.350740000	-0.489310000	4.521970000
H	-1.984310000	0.462190000	4.054490000
C	2.198930000	2.186890000	0.918290000
C	1.532040000	1.893440000	1.656730000
C	3.456660000	3.023500000	1.366110000
C	2.219360000	2.533740000	2.793870000
H	0.879900000	-2.156980000	1.039480000
C	4.109230000	-1.859390000	2.428180000
H	3.887070000	-2.311300000	0.843370000
C	3.466680000	-3.103020000	3.122400000
H	1.757590000	-0.761990000	3.336910000
H	4.019690000	-0.779980000	3.941110000
H	-0.644980000	-0.963250000	-4.337050000
H	-3.098260000	-1.557380000	1.859070000
H	-2.603500000	1.556120000	-3.323070000
H	4.818020000	1.957520000	-3.135680000
H	5.091000000	0.524340000	2.740030000
C	0.565030000	2.168580000	-1.989120000
H	1.623040000	0.810090000	-2.080320000
H	0.370210000	-2.216900000	-2.680530000
H	0.379050000	-3.784790000	-0.959420000
C	-1.748390000	-2.789520000	-0.774000000
H	-1.410110000	0.719800000	0.225760000
H	-2.840770000	0.585260000	-0.757150000
H	-1.263820000	1.580720000	-1.071850000
C	0.514780000	1.304030000	2.761560000
H	1.582260000	2.332220000	2.486360000
H	0.428080000	2.293990000	3.843220000
H	-0.004170000	1.102800000	2.200830000
C	-2.605600000	2.945970000	-0.312250000
H	-2.031950000	0.742850000	-1.157550000
H	-2.906160000	1.804560000	-0.540370000
H	-3.516780000	0.249680000	-0.176820000

Coord\_9

C	0.000000000	0.000000000	0.000000000
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C	1.430430000	0.000000000	0.000000000
C	-0.539770000	0.000000000	-1.387220000
C	-1.361460000	-1.084410000	-1.779480000
C	-0.258950000	1.013650000	-2.335680000
C	-1.870440000	-1.153180000	-3.080360000
C	-0.770710000	0.926240000	-3.634780000
C	-1.570010000	-0.155790000	-4.010440000
H	-1.962080000	-0.219760000	-5.031940000
C	2.144960000	-0.833760000	-0.989290000
C	1.707970000	-2.140980000	-1.230050000
C	3.257850000	-0.318060000	-1.663020000
C	2.400170000	-2.934870000	-2.144540000
H	0.835000000	-2.522310000	-0.698150000
C	3.925040000	-1.114470000	-2.593630000
H	3.576950000	0.711320000	-1.477110000
C	3.502140000	-2.422150000	-2.823540000
H	2.070350000	-3.960950000	-2.333690000
H	4.037420000	-3.047900000	-3.547700000
C	-0.605190000	0.809490000	1.017850000
C	0.004210000	0.824760000	2.358520000
C	-1.772230000	1.636830000	0.832160000
C	-0.590900000	1.647120000	3.363660000
C	-2.179570000	2.500440000	1.831660000
C	-1.520850000	2.617980000	3.066240000
H	-0.214290000	1.546530000	4.398270000
H	-1.841130000	3.358470000	3.791290000
C	2.206350000	0.799690000	0.854620000
C	1.513310000	1.857220000	1.589850000
C	3.482570000	0.351800000	1.308440000
C	2.206310000	2.436720000	2.714760000
H	0.901880000	2.588620000	0.945580000
C	4.129370000	0.949720000	2.347000000
H	3.928170000	-0.524510000	0.805140000
C	3.468490000	2.040750000	3.023980000
H	1.731970000	3.258180000	3.249410000
H	4.024570000	2.569350000	3.820080000
H	-0.536900000	1.708210000	-4.370070000
H	-3.072920000	3.131560000	1.663360000
H	-2.507290000	-1.996650000	-3.375150000
H	4.779760000	-0.710730000	-3.144750000
H	5.124190000	0.645510000	2.655320000
C	0.594820000	2.191150000	-1.987270000
H	1.657650000	1.900290000	-2.005040000
H	0.441590000	3.008160000	-2.711820000
H	0.344810000	2.566340000	-0.980900000
C	-1.733410000	-2.148840000	-0.796470000
H	-1.300720000	-1.904380000	0.180980000
H	-2.831920000	-2.199370000	-0.705820000
H	-1.363140000	-3.129740000	-1.142290000
C	0.517440000	-0.513710000	2.831320000

H	1.562770000	-0.651240000	2.507140000
H	0.482940000	-0.572470000	3.932930000
H	-0.090550000	-1.328790000	2.403190000
C	-2.690010000	1.440250000	-0.331730000
H	-2.196910000	1.766240000	-1.255770000
H	-2.956300000	0.378040000	-0.423180000
H	-3.618560000	2.026720000	-0.195760000

### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.438860000	0.000000000	0.000000000
C	-0.506780000	0.000000000	-1.400470000
C	-1.314200000	-1.091190000	-1.805870000
C	-0.206670000	1.006980000	-2.351100000
C	-1.784590000	-1.176010000	-3.119750000
C	-0.678930000	0.903810000	-3.663180000
C	-1.460470000	-0.187580000	-4.051650000
H	-1.820260000	-0.264900000	-5.083940000
C	2.141410000	-0.902720000	-0.936650000
C	1.699200000	-2.222380000	-1.075690000
C	3.243040000	-0.435920000	-1.661540000
C	2.378960000	-3.081490000	-1.941640000
H	0.835210000	-2.561850000	-0.503130000
C	3.896340000	-1.298360000	-2.544360000
H	3.562190000	0.604630000	-1.556190000
C	3.470090000	-2.618680000	-2.671620000
H	2.046210000	-4.117660000	-2.052050000
H	3.994540000	-3.295430000	-3.357320000
C	-0.583310000	0.893780000	0.949260000
C	0.082190000	1.056320000	2.261690000
C	-1.773190000	1.688290000	0.735510000
C	-0.487840000	1.977410000	3.197660000
C	-2.136340000	2.656900000	1.648650000
C	-1.416110000	2.924400000	2.833070000
H	-0.079750000	1.976820000	4.226430000
H	-1.700090000	3.745610000	3.479760000
C	2.213690000	0.851270000	0.787580000
C	1.500200000	1.905210000	1.523420000
C	3.507700000	0.447530000	1.243120000
C	2.203460000	2.515500000	2.633750000
H	0.931290000	2.663410000	0.858740000
C	4.150580000	1.083840000	2.256140000
H	3.966640000	-0.433870000	0.758090000
C	3.478600000	2.158620000	2.918330000
H	1.720710000	3.334800000	3.162550000
H	4.040280000	2.719360000	3.689680000
H	-0.427680000	1.679410000	-4.399990000
H	-3.046170000	3.259170000	1.456210000
H	-2.409810000	-2.024890000	-3.424330000

H	4.740680000	-0.935380000	-3.137410000
H	5.157350000	0.819020000	2.557380000
C	0.624620000	2.195290000	-1.985290000
H	1.687610000	1.908610000	-1.929530000
H	0.515350000	2.992200000	-2.739580000
H	0.312140000	2.597750000	-1.006870000
C	-1.718460000	-2.140540000	-0.819080000
H	-1.199880000	-1.960500000	0.130100000
H	-2.808320000	-2.088310000	-0.654460000
H	-1.468560000	-3.143400000	-1.207700000
C	0.518520000	-0.249520000	2.884620000
H	1.533010000	-0.513560000	2.539690000
H	0.536370000	-0.165660000	3.985080000
H	-0.170890000	-1.059690000	2.590350000
C	-2.766120000	1.334760000	-0.324960000
H	-2.357680000	1.572210000	-1.314190000
H	-2.994910000	0.260570000	-0.280580000
H	-3.705900000	1.901490000	-0.179350000

#### Coord\_11

C	0.000000000	0.000000000	0.000000000
C	1.424050000	0.000000000	0.000000000
C	-0.667930000	0.000000000	-1.235150000
C	-2.075830000	0.220030000	-1.291760000
C	0.055700000	-0.310630000	-2.488370000
C	-2.777190000	-0.180010000	-2.407470000
H	-2.586560000	0.651180000	-0.438420000
C	-0.777150000	-0.617200000	-3.619820000
H	0.752200000	0.500900000	-2.762430000
C	-2.141190000	-0.675630000	-3.558660000
H	-2.748180000	-1.061230000	-4.369590000
C	2.107070000	-0.595260000	-1.048430000
C	1.274750000	-1.408910000	-1.943720000
C	3.509040000	-0.443880000	-1.292930000
C	1.941610000	-1.894460000	-3.141520000
H	0.585440000	-2.142940000	-1.378970000
C	4.089520000	-1.009340000	-2.389170000
H	4.093680000	0.176030000	-0.595770000
C	3.282400000	-1.748220000	-3.288410000
H	1.353620000	-2.449460000	-3.870600000
H	3.795130000	-2.213680000	-4.151950000
C	-0.718510000	0.325550000	1.247440000
C	-0.988260000	-0.705460000	2.161140000
C	-1.140530000	1.634150000	1.539760000
C	-1.662840000	-0.429900000	3.348600000
H	-0.654180000	-1.723140000	1.934940000
C	-1.824360000	1.906420000	2.729000000
H	-0.935430000	2.446710000	0.829620000
C	-2.082850000	0.871230000	3.637560000



H	-1.867070000	-1.236100000	4.065000000
H	-2.608990000	1.083960000	4.575630000
C	2.195740000	0.635310000	1.098830000
C	2.111990000	2.016100000	1.320550000
C	3.001330000	-0.171930000	1.914350000
C	2.855510000	2.589710000	2.348250000
H	1.483470000	2.636070000	0.674350000
C	3.726250000	0.408290000	2.959130000
H	3.044260000	-1.251200000	1.738090000
C	3.654900000	1.793110000	3.173980000
H	2.808280000	3.671740000	2.517760000
H	4.221420000	2.248670000	3.993990000
C	5.553520000	-0.918310000	-2.661780000
H	6.014400000	-0.139450000	-2.030510000
H	6.043150000	-1.886150000	-2.442080000
H	5.732490000	-0.663980000	-3.722600000
C	-2.305240000	3.293250000	3.026490000
H	-3.340240000	3.399480000	2.667010000
H	-2.279240000	3.484110000	4.110100000
H	-1.670580000	4.037390000	2.520840000
C	4.563820000	-0.448560000	3.855800000
H	5.023210000	-1.267310000	3.282340000
H	5.362190000	0.147010000	4.324700000
H	3.923040000	-0.873330000	4.642540000
H	-0.261410000	-0.827940000	-4.576860000
C	-4.271050000	-0.099310000	-2.423090000
H	-4.581660000	0.571960000	-3.234360000
H	-4.681790000	-1.100580000	-2.607940000
H	-4.659040000	0.280600000	-1.469000000

### Coord\_12

C	0.000000000	0.000000000	0.000000000
C	1.432590000	0.000000000	0.000000000
C	-0.680880000	0.000000000	-1.213020000
C	-2.107360000	0.121140000	-1.244000000
C	0.063610000	-0.129570000	-2.497490000
C	-2.797820000	-0.201560000	-2.383150000
H	-2.632380000	0.423480000	-0.338990000
C	-0.777150000	-0.526180000	-3.628260000
H	0.551250000	0.848380000	-2.745870000
C	-2.129780000	-0.604780000	-3.552880000
H	-2.738410000	-0.971360000	-4.379080000
C	2.121870000	-0.436700000	-1.113400000
C	1.327520000	-1.073530000	-2.192680000
C	3.547090000	-0.326540000	-1.239090000
C	2.062980000	-1.219120000	-3.461030000
H	0.849760000	-2.048750000	-1.815720000
C	4.170870000	-0.648960000	-2.407070000
H	4.114590000	0.064760000	-0.383400000

C	3.405640000	-1.075120000	-3.514080000
H	1.497800000	-1.518370000	-4.347860000
H	3.954030000	-1.263940000	-4.452090000
C	-0.711120000	0.189210000	1.281490000
C	-0.965090000	-0.925170000	2.094570000
C	-1.132980000	1.463610000	1.694020000
C	-1.634400000	-0.764410000	3.305780000
H	-0.631890000	-1.916030000	1.770870000
C	-1.807050000	1.619950000	2.908970000
H	-0.930760000	2.336670000	1.061220000
C	-2.055110000	0.502580000	3.717940000
H	-1.834850000	-1.635560000	3.942190000
H	-2.574250000	0.624360000	4.675750000
C	2.173980000	0.471610000	1.194890000
C	2.223940000	1.838430000	1.498750000
C	2.816110000	-0.463990000	2.018590000
C	2.932880000	2.266980000	2.618070000
H	1.723280000	2.560390000	0.846900000
C	3.512800000	-0.027800000	3.149160000
H	2.758120000	-1.530370000	1.777990000
C	3.571190000	1.341220000	3.448230000
H	2.989350000	3.336540000	2.852890000
H	4.112690000	1.683870000	4.337360000
C	5.651780000	-0.576410000	-2.572050000
H	6.116400000	-0.097460000	-1.694610000
H	6.067350000	-1.594100000	-2.682860000
H	5.905360000	0.010330000	-3.472510000
C	-2.284250000	2.971090000	3.344150000
H	-3.349500000	3.076080000	3.088380000
H	-2.160520000	3.086590000	4.431330000
H	-1.713200000	3.763660000	2.836510000
C	4.177430000	-1.018880000	4.052920000
H	4.494100000	-1.905670000	3.483630000
H	5.061380000	-0.570810000	4.531780000
H	3.462600000	-1.326020000	4.830380000
H	-0.263850000	-0.755010000	-4.578530000
C	-4.291330000	-0.167830000	-2.414730000
H	-4.619350000	0.552620000	-3.178200000
H	-4.672810000	-1.165670000	-2.676760000
H	-4.700590000	0.129290000	-1.438840000

### Coord\_13

C	0.000000000	0.000000000	0.000000000
C	1.455310000	0.000000000	0.000000000
C	-0.617590000	0.000000000	-1.344160000
C	-0.820500000	-1.196880000	-2.058850000
C	-0.952570000	1.234140000	-1.940310000
C	-1.374580000	-1.152050000	-3.343320000
C	-1.504690000	1.260280000	-3.224720000

C	-1.710610000	0.070340000	-3.924950000
H	-2.133080000	0.095840000	-4.936120000
C	2.162570000	-0.360340000	-1.251880000
C	2.778810000	-1.619450000	-1.356410000
C	2.242320000	0.548070000	-2.318660000
C	3.468080000	-1.961600000	-2.517020000
H	2.726900000	-2.318330000	-0.515720000
C	2.933610000	0.196760000	-3.475340000
H	1.746950000	1.519560000	-2.243500000
C	3.543810000	-1.057170000	-3.579840000
H	3.964410000	-2.935370000	-2.594580000
H	4.082880000	-1.330050000	-4.493660000
C	-0.690130000	0.071800000	1.181860000
C	0.068790000	0.081550000	2.495570000
C	-2.146560000	0.037970000	1.262120000
C	-0.698810000	0.776170000	3.589190000
C	-2.774910000	0.432600000	2.406050000
C	-2.034620000	0.916270000	3.545230000
H	-0.136390000	1.130080000	4.463800000
H	-2.594000000	1.407170000	4.350460000
C	2.168570000	0.303790000	1.128060000
C	1.443290000	0.766340000	2.357710000
C	3.612560000	0.308110000	1.120120000
C	2.283020000	0.610600000	3.586280000
H	1.273210000	1.892110000	2.230610000
C	4.314600000	0.445330000	2.270210000
H	4.124760000	0.171000000	0.160860000
C	3.623250000	0.513310000	3.539000000
H	1.769940000	0.628390000	4.558660000
H	4.228280000	0.436630000	4.450240000
H	-1.785150000	2.217260000	-3.680110000
H	-3.869710000	0.416090000	2.481090000
H	-1.535270000	-2.082670000	-3.899680000
H	2.992300000	0.900680000	-4.312950000
H	5.409760000	0.461480000	2.278310000
C	-0.752960000	2.508720000	-1.182820000
H	0.286800000	2.575500000	-0.828530000
H	-0.969450000	3.380020000	-1.822950000
H	-1.424880000	2.527700000	-0.314350000
C	-0.438350000	-2.515120000	-1.464960000
H	-0.489760000	-2.474110000	-0.368050000
H	-1.112440000	-3.308860000	-1.825310000
H	0.591300000	-2.752870000	-1.767520000
C	0.228680000	-1.391760000	2.913050000
H	0.822680000	-1.928520000	2.158990000
H	0.742020000	-1.464970000	3.882720000
H	-0.759670000	-1.865190000	2.997910000
C	-2.997780000	-0.420920000	0.122280000
H	-2.974460000	0.311620000	-0.695020000
H	-2.638540000	-1.390130000	-0.250120000

H	-4.045140000	-0.540560000	0.453820000
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S<sub>0</sub>\_S<sub>1</sub>S<sub>0</sub>-pyr(C1)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.363000000	0.000000000	0.000000000
C	-0.789760000	0.000000000	-1.254080000
C	-1.715610000	-1.028920000	-1.525220000
C	-0.654530000	1.064840000	-2.170140000
C	-2.511350000	-0.968720000	-2.678500000
C	-1.464390000	1.105990000	-3.316990000
C	-2.393720000	0.101020000	-3.563320000
H	-3.027440000	0.145700000	-4.457450000
C	2.170680000	-0.205010000	-1.216140000
C	1.784440000	-1.146560000	-2.181910000
C	3.362600000	0.513950000	-1.395350000
C	2.571940000	-1.354700000	-3.299100000
H	0.851070000	-1.703560000	-2.056320000
C	4.135290000	0.304630000	-2.521670000
H	3.673490000	1.242630000	-0.639700000
C	3.749590000	-0.631160000	-3.481050000
H	2.271630000	-2.096340000	-4.049830000
H	4.368240000	-0.797160000	-4.367940000
C	-0.780850000	0.005490000	1.260730000
C	-0.641110000	-1.053520000	2.182740000
C	-1.707510000	1.033850000	1.528270000
C	-1.444240000	-1.086340000	3.334320000
C	-2.499770000	0.978410000	2.683810000
C	-2.374370000	-0.082820000	3.577680000
H	-1.333780000	-1.912850000	4.046220000
H	-3.004200000	-0.122780000	4.475070000
C	2.145150000	0.219970000	1.237400000
C	1.798560000	1.265310000	2.105620000
C	3.254650000	-0.586170000	1.516190000
C	2.558410000	1.487290000	3.250490000
H	0.927800000	1.891420000	1.892140000
C	3.998360000	-0.363710000	2.670960000
H	3.531030000	-1.389890000	0.827760000
C	3.652340000	0.675920000	3.535380000
H	2.290700000	2.303100000	3.930450000
H	4.246060000	0.852930000	4.440180000
H	-1.361560000	1.938060000	-4.022460000
H	-3.226370000	1.774800000	2.883240000
H	-3.234070000	-1.767510000	-2.880830000
H	5.061950000	0.875190000	-2.664540000
H	4.859730000	-1.000530000	2.899760000

C	0.355440000	2.153970000	-1.998040000
H	1.254570000	1.889830000	-2.573100000
H	-0.046730000	3.107600000	-2.378340000
H	0.633380000	2.279550000	-0.941590000
C	-1.855700000	-2.208280000	-0.618670000
H	-2.275800000	-1.887940000	0.342680000
H	-2.520990000	-2.964480000	-1.068310000
H	-0.866990000	-2.666620000	-0.449840000
C	0.357590000	-2.153200000	2.008300000
H	1.274950000	-1.883850000	2.549980000
H	-0.041440000	-3.095500000	2.420190000
H	0.603330000	-2.304840000	0.946970000
C	-1.853730000	2.211370000	0.618100000
H	-0.867230000	2.673610000	0.450020000
H	-2.270750000	1.889830000	-0.343750000
H	-2.521370000	2.967390000	1.065180000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.371560000	0.000000000	0.000000000
C	-0.786560000	0.000000000	-1.254650000
C	-1.853490000	-0.905100000	-1.438810000
C	-0.474930000	0.917430000	-2.281620000
C	-2.621380000	-0.855590000	-2.610950000
C	-1.256140000	0.954520000	-3.448150000
C	-2.330900000	0.086950000	-3.608590000
H	-2.942430000	0.130670000	-4.517840000
C	2.161060000	-0.491040000	-1.145500000
C	1.673420000	-1.540700000	-1.936880000
C	3.414370000	0.070530000	-1.439090000
C	2.423470000	-2.010840000	-2.999830000
H	0.693010000	-1.972930000	-1.717090000
C	4.150220000	-0.399580000	-2.510640000
H	3.803710000	0.883770000	-0.817640000
C	3.663930000	-1.446370000	-3.296250000
H	2.042810000	-2.834520000	-3.616350000
H	4.252930000	-1.821180000	-4.139100000
C	-0.688120000	0.164720000	1.310680000
C	-0.545390000	-0.830650000	2.302660000
C	-1.545250000	1.259630000	1.550630000
C	-1.268780000	-0.729730000	3.502710000
C	-2.263300000	1.335900000	2.753750000
C	-2.126960000	0.340760000	3.723960000
H	-1.155410000	-1.506430000	4.268130000
H	-2.695810000	0.405080000	4.660140000
C	2.179960000	0.481740000	1.145310000
C	1.901200000	1.729390000	1.722700000
C	3.246760000	-0.288270000	1.623640000
C	2.686100000	2.190600000	2.773820000

H	1.062230000	2.327980000	1.357990000
C	4.016840000	0.177790000	2.682720000
H	3.464600000	-1.258400000	1.167550000
C	3.740420000	1.420450000	3.255200000
H	2.469890000	3.164360000	3.226630000
H	4.354750000	1.787630000	4.085360000
H	-1.014860000	1.674980000	-4.238190000
H	-2.935800000	2.183050000	2.931650000
H	-3.453610000	-1.556950000	-2.743690000
H	5.125480000	0.045660000	-2.743120000
H	4.844910000	-0.427660000	3.067000000
C	0.700300000	1.839450000	-2.213260000
H	1.542640000	1.369020000	-2.741600000
H	0.461300000	2.798470000	-2.702980000
H	1.000650000	2.034540000	-1.173560000
C	-2.175110000	-1.948290000	-0.418440000
H	-2.577910000	-1.472720000	0.484680000
H	-2.921600000	-2.657810000	-0.814420000
H	-1.261590000	-2.507550000	-0.158600000
C	0.367010000	-2.004320000	2.143720000
H	1.343030000	-1.757520000	2.585670000
H	-0.051930000	-2.882440000	2.663990000
H	0.509150000	-2.252700000	1.082110000
C	-1.697660000	2.372570000	0.563870000
H	-0.718180000	2.847620000	0.388640000
H	-2.086700000	1.984560000	-0.384840000
H	-2.392120000	3.137890000	0.950190000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.380130000	0.000000000	0.000000000
C	-0.783350000	0.000000000	-1.255220000
C	-1.971760000	-0.754380000	-1.365430000
C	-0.324490000	0.730460000	-2.373900000
C	-2.716730000	-0.723910000	-2.552550000
C	-1.081390000	0.753120000	-3.556550000
C	-2.277940000	0.050940000	-3.645900000
H	-2.869990000	0.086110000	-4.568050000
C	2.151230000	-0.754870000	-1.007660000
C	1.573370000	-1.873650000	-1.622240000
C	3.456360000	-0.368290000	-1.357210000
C	2.286990000	-2.585900000	-2.570290000
H	0.554250000	-2.166180000	-1.355160000
C	4.156740000	-1.079900000	-2.313790000
H	3.915590000	0.499740000	-0.872170000
C	3.580260000	-2.197820000	-2.922190000
H	1.835090000	-3.461940000	-3.051380000
H	4.140180000	-2.765330000	-3.672650000
C	-0.590730000	0.334280000	1.333120000

C	-0.455940000	-0.588790000	2.395660000
C	-1.367260000	1.498230000	1.524450000
C	-1.098110000	-0.343280000	3.621340000
C	-2.009730000	1.717260000	2.753710000
C	-1.872820000	0.796820000	3.798370000
H	-0.990350000	-1.063750000	4.440590000
H	-2.379660000	0.974070000	4.755670000
C	2.214500000	0.713690000	0.998890000
C	2.004900000	2.080020000	1.239730000
C	3.236800000	0.035300000	1.673940000
C	2.814430000	2.749860000	2.148490000
H	1.199060000	2.610030000	0.725610000
C	4.033030000	0.713140000	2.587340000
H	3.394480000	-1.031380000	1.488830000
C	3.827660000	2.073990000	2.821770000
H	2.650690000	3.816400000	2.338550000
H	4.462380000	2.606810000	3.538340000
H	-0.723580000	1.331290000	-4.416790000
H	-2.619610000	2.617010000	2.893810000
H	-3.643080000	-1.306510000	-2.625960000
H	5.172730000	-0.773540000	-2.589570000
H	4.826400000	0.181730000	3.124160000
C	0.985990000	1.450470000	-2.389900000
H	1.737830000	0.792230000	-2.850880000
H	0.907630000	2.375350000	-2.986540000
H	1.321300000	1.707950000	-1.374670000
C	-2.450460000	-1.623640000	-0.248030000
H	-2.811300000	-1.000860000	0.580640000
H	-3.272840000	-2.274500000	-0.592100000
H	-1.623870000	-2.258770000	0.108130000
C	0.355040000	-1.838540000	2.278350000
H	1.378430000	-1.635860000	2.627310000
H	-0.085370000	-2.635360000	2.901940000
H	0.394550000	-2.181110000	1.234760000
C	-1.514620000	2.538610000	0.461150000
H	-0.539510000	3.020590000	0.278800000
H	-1.874080000	2.084090000	-0.469260000
H	-2.231980000	3.313490000	0.780930000

#### Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.388690000	0.000000000	0.000000000
C	-0.780150000	0.000000000	-1.255780000
C	-2.066690000	-0.581170000	-1.307230000
C	-0.209620000	0.511990000	-2.443230000
C	-2.795290000	-0.576100000	-2.504480000
C	-0.948870000	0.512110000	-3.637060000
C	-2.239730000	-0.002150000	-3.672290000
H	-2.816660000	0.018370000	-4.604160000

C	2.141200000	-0.980750000	-0.809250000
C	1.485830000	-2.135410000	-1.254240000
C	3.487830000	-0.767800000	-1.154040000
C	2.164950000	-3.056450000	-2.033810000
H	0.436720000	-2.288600000	-0.988610000
C	4.154790000	-1.688280000	-1.942160000
H	4.007230000	0.129530000	-0.800280000
C	3.500340000	-2.842900000	-2.380080000
H	1.652220000	-3.959850000	-2.385550000
H	4.032450000	-3.576290000	-2.995470000
C	-0.489210000	0.508870000	1.326320000
C	-0.372420000	-0.331100000	2.459500000
C	-1.175090000	1.738800000	1.446780000
C	-0.932350000	0.065710000	3.686410000
C	-1.740920000	2.107830000	2.679010000
C	-1.613280000	1.272210000	3.795920000
H	-0.838080000	-0.590500000	4.559460000
H	-2.057410000	1.567910000	4.755410000
C	2.248780000	0.904810000	0.806790000
C	2.109300000	2.296460000	0.689580000
C	3.225120000	0.373650000	1.659340000
C	2.943000000	3.134830000	1.416330000
H	1.337710000	2.716550000	0.039830000
C	4.047190000	1.221570000	2.386540000
H	3.321410000	-0.711380000	1.762710000
C	3.913970000	2.605940000	2.261630000
H	2.832470000	4.221420000	1.326860000
H	4.568800000	3.272200000	2.832930000
H	-0.501420000	0.923310000	-4.550240000
H	-2.280520000	3.057720000	2.764090000
H	-3.797380000	-1.022080000	-2.530560000
H	5.203060000	-1.519360000	-2.213250000
H	4.804740000	0.806800000	3.060480000
C	1.200820000	1.002570000	-2.521180000
H	1.832100000	0.182480000	-2.896730000
H	1.273820000	1.855420000	-3.218100000
H	1.582240000	1.312210000	-1.537200000
C	-2.672340000	-1.245010000	-0.112920000
H	-2.967850000	-0.488800000	0.626210000
H	-3.564250000	-1.825470000	-0.407440000
H	-1.939840000	-1.929670000	0.341880000
C	0.323690000	-1.651900000	2.410970000
H	1.382170000	-1.513370000	2.679200000
H	-0.138870000	-2.350120000	3.129830000
H	0.262890000	-2.082390000	1.401970000
C	-1.306910000	2.696810000	0.307160000
H	-0.333870000	3.181130000	0.118300000
H	-1.634540000	2.174430000	-0.598800000
H	-2.044040000	3.480090000	0.553080000



## Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.397250000	0.000000000	0.000000000
C	-0.776940000	0.000000000	-1.256330000
C	-2.135270000	-0.390560000	-1.265860000
C	-0.135240000	0.271450000	-2.486910000
C	-2.855200000	-0.414890000	-2.467750000
C	-0.865190000	0.243790000	-3.685960000
C	-2.219890000	-0.066150000	-3.685650000
H	-2.787350000	-0.064480000	-4.623290000
C	2.130960000	-1.154850000	-0.560580000
C	1.412190000	-2.320260000	-0.849390000
C	3.508150000	-1.095170000	-0.843620000
C	2.059610000	-3.405720000	-1.416620000
H	0.342040000	-2.349710000	-0.630970000
C	4.144400000	-2.180740000	-1.419160000
H	4.076970000	-0.187970000	-0.611210000
C	3.425830000	-3.345690000	-1.700100000
H	1.497600000	-4.317980000	-1.649650000
H	3.932090000	-4.209340000	-2.145630000
C	-0.384070000	0.682920000	1.289600000
C	-0.294280000	-0.060930000	2.492090000
C	-0.970460000	1.969920000	1.317080000
C	-0.771330000	0.489660000	3.694960000
C	-1.458860000	2.492160000	2.528020000
C	-1.349510000	1.753220000	3.713980000
H	-0.697550000	-0.092580000	4.620790000
H	-1.730490000	2.169600000	4.655990000
C	2.282770000	1.046440000	0.579810000
C	2.214050000	2.367320000	0.109160000
C	3.212060000	0.713280000	1.574220000
C	3.071460000	3.327110000	0.624920000
H	1.477600000	2.639430000	-0.650430000
C	4.059610000	1.682360000	2.086030000
H	3.246140000	-0.309910000	1.960890000
C	3.999250000	2.993000000	1.607200000
H	3.014600000	4.358860000	0.259400000
H	4.673890000	3.754850000	2.010200000
H	-0.358820000	0.470410000	-4.632680000
H	-1.921430000	3.485200000	2.541040000
H	-3.912170000	-0.710390000	-2.459870000
H	5.215990000	-2.132810000	-1.640650000
H	4.780460000	1.423060000	2.869180000
C	1.335890000	0.513690000	-2.602210000
H	1.821400000	-0.435870000	-2.877520000
H	1.544650000	1.259820000	-3.388950000
H	1.772630000	0.862520000	-1.654950000
C	-2.833110000	-0.824870000	-0.017360000
H	-3.042210000	0.045630000	0.618810000

H	-3.786980000	-1.323510000	-0.265400000
H	-2.197180000	-1.532630000	0.535350000
C	0.275400000	-1.440360000	2.538610000
H	1.355950000	-1.382990000	2.743480000
H	-0.209050000	-2.023050000	3.341420000
H	0.117930000	-1.949460000	1.578290000
C	-1.077200000	2.833690000	0.102350000
H	-0.104570000	3.317220000	-0.092270000
H	-1.370240000	2.241210000	-0.771470000
H	-1.831550000	3.622120000	0.265990000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.405820000	0.000000000	0.000000000
C	-0.773740000	0.000000000	-1.256870000
C	-2.175230000	-0.188140000	-1.242520000
C	-0.104480000	0.019200000	-2.503320000
C	-2.894860000	-0.243280000	-2.443200000
C	-0.834530000	-0.038170000	-3.701110000
C	-2.220560000	-0.133990000	-3.684850000
H	-2.784950000	-0.153110000	-4.623890000
C	2.120530000	-1.266100000	-0.275070000
C	1.353630000	-2.426080000	-0.423360000
C	3.516810000	-1.322250000	-0.448940000
C	1.972940000	-3.623300000	-0.746050000
H	0.271510000	-2.360970000	-0.290290000
C	4.125680000	-2.520570000	-0.779210000
H	4.123450000	-0.417810000	-0.326160000
C	3.358280000	-3.678660000	-0.919440000
H	1.374170000	-4.532990000	-0.872410000
H	3.841270000	-4.630350000	-1.169700000
C	-0.275870000	0.850820000	1.223360000
C	-0.220740000	0.218150000	2.491480000
C	-0.755220000	2.180140000	1.137360000
C	-0.614570000	0.920670000	3.644900000
C	-1.165600000	2.854650000	2.302340000
C	-1.082500000	2.225900000	3.552290000
H	-0.567290000	0.423700000	4.620730000
H	-1.400090000	2.761840000	4.456930000
C	2.316470000	1.132700000	0.330310000
C	2.318800000	2.291270000	-0.463240000
C	3.197970000	1.038530000	1.416010000
C	3.199400000	3.321060000	-0.175680000
H	1.618130000	2.384150000	-1.295840000
C	4.070560000	2.075650000	1.695690000
H	3.169410000	0.152860000	2.058410000
C	4.083430000	3.220240000	0.894790000
H	3.196450000	4.226580000	-0.793600000
H	4.777540000	4.036390000	1.116020000

H	-0.302470000	-0.005940000	-4.660680000
H	-1.545400000	3.879350000	2.227530000
H	-3.984000000	-0.378920000	-2.415700000
H	5.211230000	-2.563750000	-0.913860000
H	4.754120000	2.003120000	2.548770000
C	1.385470000	0.003450000	-2.630130000
H	1.705870000	-1.038030000	-2.794210000
H	1.708740000	0.612790000	-3.492880000
H	1.884300000	0.376340000	-1.723500000
C	-2.927120000	-0.377080000	0.035690000
H	-3.031900000	0.583860000	0.557740000
H	-3.934080000	-0.782980000	-0.169690000
H	-2.385750000	-1.082570000	0.682760000
C	0.213030000	-1.200380000	2.656500000
H	1.302150000	-1.236820000	2.819750000
H	-0.292090000	-1.651670000	3.528510000
H	-0.036320000	-1.776540000	1.755850000
C	-0.828500000	2.935830000	-0.149430000
H	0.144600000	3.416900000	-0.349400000
H	-1.083930000	2.270660000	-0.981470000
H	-1.597870000	3.723410000	-0.076900000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.414380000	0.000000000	0.000000000
C	-0.770540000	0.000000000	-1.257400000
C	-2.185120000	0.020130000	-1.237820000
C	-0.118640000	-0.233870000	-2.492060000
C	-2.912980000	-0.064510000	-2.431450000
C	-0.858390000	-0.319410000	-3.682030000
C	-2.242190000	-0.198170000	-3.669770000
H	-2.810190000	-0.237660000	-4.605750000
C	2.109910000	-1.306890000	0.031420000
C	1.311090000	-2.453440000	0.009650000
C	3.513460000	-1.427990000	-0.000400000
C	1.906590000	-3.704370000	-0.049160000
H	0.226080000	-2.333550000	0.030760000
C	4.098800000	-2.681070000	-0.065460000
H	4.145600000	-0.532780000	0.023330000
C	3.299030000	-3.823620000	-0.080030000
H	1.284350000	-4.606350000	-0.079190000
H	3.761930000	-4.816970000	-0.119930000
C	-0.165210000	1.007080000	1.129090000
C	-0.150880000	0.502220000	2.455890000
C	-0.531340000	2.358550000	0.912150000
C	-0.461360000	1.350540000	3.534930000
C	-0.863280000	3.180230000	2.006740000
C	-0.813110000	2.676470000	3.312900000
H	-0.445410000	0.951330000	4.555570000

H	-1.06720000	3.32753000	4.16061000
C	2.34987000	1.16069000	0.07150000
C	2.42321000	2.07696000	-0.99066000
C	3.18319000	1.33242000	1.18592000
C	3.32645000	3.12388000	-0.93631000
H	1.75872000	1.96939000	-1.85035000
C	4.08035000	2.38329000	1.22949000
H	3.09195000	0.64916000	2.03626000
C	4.16641000	3.28159000	0.16253000
H	3.37738000	3.84067000	-1.76449000
H	4.87962000	4.10967000	0.19838000
H	-0.33500000	-0.48315000	-4.63336000
H	-1.15563000	4.22089000	1.83072000
H	-4.01040000	-0.03566000	-2.39919000
H	5.18867000	-2.77501000	-0.08767000
H	4.72627000	2.51799000	2.10413000
C	1.34725000	-0.50763000	-2.60427000
H	1.48985000	-1.59981000	-2.65036000
H	1.75902000	-0.05932000	-3.52646000
H	1.91212000	-0.12737000	-1.74036000
C	-2.95096000	0.08358000	0.04469000
H	-2.93746000	1.10726000	0.44413000
H	-4.00071000	-0.21934000	-0.12266000
H	-2.49799000	-0.59638000	0.77998000
C	0.13973000	-0.92952000	2.75818000
H	1.22375000	-1.06697000	2.90484000
H	-0.38390000	-1.23539000	3.68119000
H	-0.19564000	-1.55991000	1.92480000
C	-0.56410000	2.99064000	-0.44093000
H	0.40949000	3.46894000	-0.64670000
H	-0.77890000	2.25068000	-1.21926000
H	-1.34649000	3.76826000	-0.46791000

### Coord\_8

C	0.00000000	0.00000000	0.00000000
C	1.42294000	0.00000000	0.00000000
C	-0.76734000	0.00000000	-1.25793000
C	-2.16442000	0.22811000	-1.25185000
C	-0.17705000	-0.47686000	-2.45389000
C	-2.90860000	0.11795000	-2.43290000
C	-0.93552000	-0.58556000	-3.62995000
C	-2.28353000	-0.25129000	-3.64138000
H	-2.86149000	-0.30833000	-4.57008000
C	2.09910000	-1.27362000	0.34155000
C	1.28527000	-2.40463000	0.43707000
C	3.49789000	-1.40051000	0.46641000
C	1.86186000	-3.64874000	0.64810000
H	0.20634000	-2.27625000	0.33390000
C	4.06397000	-2.64758000	0.67304000

H	4.142710000	-0.516430000	0.398120000
C	3.249230000	-3.772330000	0.773680000
H	1.230000000	-4.542300000	0.708170000
H	3.695680000	-4.759080000	0.948490000
C	-0.052680000	1.146620000	1.009290000
C	-0.083630000	0.786920000	2.383780000
C	-0.300890000	2.495320000	0.648340000
C	-0.310770000	1.770760000	3.364690000
C	-0.554040000	3.454970000	1.649020000
C	-0.542020000	3.091630000	3.000140000
H	-0.329710000	1.482380000	4.421900000
H	-0.732570000	3.850090000	3.772170000
C	2.382950000	1.130620000	-0.183270000
C	2.526920000	1.742210000	-1.440020000
C	3.168060000	1.577580000	0.889520000
C	3.452240000	2.754790000	-1.611980000
H	1.898780000	1.425610000	-2.274750000
C	4.089240000	2.589760000	0.705400000
H	3.014520000	1.145550000	1.883670000
C	4.248110000	3.179860000	-0.551760000
H	3.556780000	3.233980000	-2.592880000
H	4.980020000	3.978770000	-0.695270000
H	-0.454850000	-0.938570000	-4.552440000
H	-0.755440000	4.492260000	1.361820000
H	-3.989930000	0.310970000	-2.410850000
H	5.148410000	-2.745570000	0.774410000
H	4.697450000	2.938740000	1.547260000
C	1.222450000	-0.998970000	-2.526090000
H	1.181760000	-2.098620000	-2.451920000
H	1.693070000	-0.729100000	-3.489180000
H	1.854210000	-0.628800000	-1.705090000
C	-2.903490000	0.541900000	0.009570000
H	-2.762370000	1.597760000	0.280910000
H	-3.984260000	0.351200000	-0.125260000
H	-2.529190000	-0.092330000	0.824740000
C	0.058920000	-0.627000000	2.835820000
H	1.124240000	-0.866370000	2.992770000
H	-0.480160000	-0.776120000	3.788360000
H	-0.355780000	-1.298460000	2.073810000
C	-0.287550000	2.987300000	-0.761760000
H	0.685760000	3.463510000	-0.975160000
H	-0.458970000	2.171820000	-1.472120000
H	-1.080990000	3.742440000	-0.895210000

#### Coord\_9

C	0.000000000	0.000000000	0.000000000
C	1.431510000	0.000000000	0.000000000
C	-0.764140000	0.000000000	-1.258450000
C	-2.113480000	0.429670000	-1.284130000

C	-0.277150000	-0.699280000	-2.390760000
C	-2.881140000	0.300470000	-2.447740000
C	-1.062000000	-0.822990000	-3.547710000
C	-2.341660000	-0.286500000	-3.601620000
H	-2.935100000	-0.356100000	-4.519380000
C	2.088100000	-1.166920000	0.637460000
C	1.276590000	-2.282860000	0.847740000
C	3.470010000	-1.238290000	0.913470000
C	1.839630000	-3.459940000	1.321190000
H	0.212510000	-2.193970000	0.623670000
C	4.021460000	-2.418720000	1.384740000
H	4.114370000	-0.365190000	0.755190000
C	3.209740000	-3.526440000	1.596850000
H	1.212330000	-4.345990000	1.470670000
H	3.643810000	-4.458780000	1.980040000
C	0.061110000	1.264880000	0.867430000
C	-0.017820000	1.067330000	2.273980000
C	-0.066000000	2.582210000	0.354910000
C	-0.161730000	2.172470000	3.134810000
C	-0.240110000	3.666700000	1.239710000
C	-0.269810000	3.458870000	2.620500000
H	-0.217740000	2.007800000	4.216860000
H	-0.396840000	4.313940000	3.299420000
C	2.415700000	1.045710000	-0.421210000
C	2.629610000	1.312670000	-1.784390000
C	3.152930000	1.757520000	0.536960000
C	3.576410000	2.243400000	-2.164720000
H	2.037730000	0.792780000	-2.539620000
C	4.097520000	2.683170000	0.144850000
H	2.937820000	1.605420000	1.599730000
C	4.328460000	2.926320000	-1.212630000
H	3.734040000	2.453510000	-3.229700000
H	5.078630000	3.658320000	-1.520590000
H	-0.656330000	-1.350580000	-4.422110000
H	-0.348200000	4.678470000	0.835690000
H	-3.922280000	0.652390000	-2.450480000
H	5.090690000	-2.472570000	1.604940000
H	4.668200000	3.238370000	0.897570000
C	1.015810000	-1.450740000	-2.399190000
H	0.793710000	-2.514320000	-2.207030000
H	1.513200000	-1.369230000	-3.383400000
H	1.712060000	-1.108120000	-1.619330000
C	-2.785990000	0.982730000	-0.068320000
H	-2.512910000	2.038510000	0.072680000
H	-3.884490000	0.912150000	-0.176960000
H	-2.477720000	0.410650000	0.816670000
C	-0.025850000	-0.294210000	2.880670000
H	1.007530000	-0.629640000	3.075070000
H	-0.576460000	-0.278750000	3.838400000
H	-0.512500000	-0.994180000	2.190880000

C	-0.002560000	2.917420000	-1.098840000
H	0.969010000	3.392710000	-1.323440000
H	-0.128350000	2.028130000	-1.724800000
H	-0.805080000	3.634330000	-1.343130000

Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.440070000	0.000000000	0.000000000
C	-0.760940000	0.000000000	-1.258960000
C	-2.033550000	0.618840000	-1.333660000
C	-0.414550000	-0.891540000	-2.305660000
C	-2.830400000	0.479280000	-2.475880000
C	-1.231390000	-1.019430000	-3.439620000
C	-2.412160000	-0.298070000	-3.553320000
H	-3.025270000	-0.373330000	-4.457330000
C	2.076930000	-0.991740000	0.901820000
C	1.285180000	-2.091790000	1.231350000
C	3.429930000	-0.950600000	1.303460000
C	1.840360000	-3.144590000	1.946880000
H	0.244440000	-2.087120000	0.905240000
C	3.971580000	-2.006660000	2.019160000
H	4.060560000	-0.089190000	1.051850000
C	3.181140000	-3.097250000	2.346170000
H	1.231880000	-4.022580000	2.190740000
H	3.607170000	-3.929890000	2.921210000
C	0.175520000	1.358040000	0.707800000
C	0.047750000	1.338020000	2.125900000
C	0.171140000	2.613020000	0.042580000
C	-0.013060000	2.546580000	2.847100000
C	0.076320000	3.805530000	0.791680000
C	0.003010000	3.766850000	2.182520000
H	-0.106900000	2.517270000	3.938560000
H	-0.060490000	4.704750000	2.752680000
C	2.448120000	0.911920000	-0.630780000
C	2.730930000	0.819750000	-2.004780000
C	3.138110000	1.857910000	0.142840000
C	3.698610000	1.627410000	-2.565950000
H	2.175020000	0.117290000	-2.627590000
C	4.105460000	2.656120000	-0.427920000
H	2.862560000	1.991990000	1.194180000
C	4.407370000	2.539730000	-1.788750000
H	3.908570000	1.556720000	-3.640450000
H	5.175330000	3.172280000	-2.238650000
H	-0.929850000	-1.699570000	-4.248860000
H	0.062660000	4.767830000	0.270170000
H	-3.808260000	0.980020000	-2.517210000
H	5.015940000	-1.971810000	2.337750000
H	4.639050000	3.393910000	0.181630000
C	0.735360000	-1.844660000	-2.229110000

H	0.341110000	-2.830050000	-1.925660000
H	1.226400000	-1.953580000	-3.214300000
H	1.490520000	-1.546250000	-1.486690000
C	-2.602050000	1.391520000	-0.186210000
H	-2.197940000	2.414450000	-0.174510000
H	-3.703500000	1.447230000	-0.275820000
H	-2.345100000	0.893640000	0.757350000
C	-0.110960000	0.064980000	2.883660000
H	0.877860000	-0.353820000	3.141270000
H	-0.668370000	0.248600000	3.819990000
H	-0.661680000	-0.652330000	2.264100000
C	0.287030000	2.775790000	-1.436960000
H	1.254900000	3.251050000	-1.678430000
H	0.208390000	1.817840000	-1.960540000
H	-0.522600000	3.435840000	-1.792740000

S<sub>0</sub>-S<sub>1</sub>S<sub>0</sub>-pyr(C2)

Coord\_1

C	0.000000000	0.000000000	0.000000000
C	1.363000000	0.000000000	0.000000000
C	-0.789760000	0.000000000	-1.254080000
C	-1.715610000	-1.028920000	-1.525220000
C	-0.654530000	1.064840000	-2.170140000
C	-2.511350000	-0.968720000	-2.678500000
C	-1.464390000	1.105990000	-3.316990000
C	-2.393720000	0.101020000	-3.563320000
H	-3.027440000	0.145700000	-4.457450000
C	2.170680000	-0.205010000	-1.216140000
C	1.784440000	-1.146560000	-2.181910000
C	3.362600000	0.513950000	-1.395350000
C	2.571940000	-1.354700000	-3.299100000
H	0.851070000	-1.703560000	-2.056320000
C	4.135290000	0.304630000	-2.521670000
H	3.673490000	1.242630000	-0.639700000
C	3.749590000	-0.631160000	-3.481050000
H	2.271630000	-2.096340000	-4.049830000
H	4.368240000	-0.797160000	-4.367940000
C	-0.780850000	0.005490000	1.260730000
C	-0.641110000	-1.053520000	2.182740000
C	-1.707510000	1.033850000	1.528270000
C	-1.444240000	-1.086340000	3.334320000
C	-2.499770000	0.978410000	2.683810000
C	-2.374370000	-0.082820000	3.577680000
H	-1.333780000	-1.912850000	4.046220000
H	-3.004200000	-0.122780000	4.475070000
C	2.145150000	0.219970000	1.237400000



C	1.798560000	1.265310000	2.105620000
C	3.254650000	-0.586170000	1.516190000
C	2.558410000	1.487290000	3.250490000
H	0.927800000	1.891420000	1.892140000
C	3.998360000	-0.363710000	2.670960000
H	3.531030000	-1.389890000	0.827760000
C	3.652340000	0.675920000	3.535380000
H	2.290700000	2.303100000	3.930450000
H	4.246060000	0.852930000	4.440180000
H	-1.361560000	1.938060000	-4.022460000
H	-3.226370000	1.774800000	2.883240000
H	-3.234070000	-1.767510000	-2.880830000
H	5.061950000	0.875190000	-2.664540000
H	4.859730000	-1.000530000	2.899760000
C	0.355440000	2.153970000	-1.998040000
H	1.254570000	1.889830000	-2.573100000
H	-0.046730000	3.107600000	-2.378340000
H	0.633380000	2.279550000	-0.941590000
C	-1.855700000	-2.208280000	-0.618670000
H	-2.275800000	-1.887940000	0.342680000
H	-2.520990000	-2.964480000	-1.068310000
H	-0.866990000	-2.666620000	-0.449840000
C	0.357590000	-2.153200000	2.008300000
H	1.274950000	-1.883850000	2.549980000
H	-0.041440000	-3.095500000	2.420190000
H	0.603330000	-2.304840000	0.946970000
C	-1.853730000	2.211370000	0.618100000
H	-0.867230000	2.673610000	0.450020000
H	-2.270750000	1.889830000	-0.343750000
H	-2.521370000	2.967390000	1.065180000

## Coord\_2

C	0.000000000	0.000000000	0.000000000
C	1.372460000	0.000000000	0.000000000
C	-0.779240000	0.000000000	-1.258880000
C	-1.791790000	-0.959510000	-1.487880000
C	-0.539560000	0.989610000	-2.239200000
C	-2.574680000	-0.888890000	-2.647570000
C	-1.339860000	1.039820000	-3.391950000
C	-2.360930000	0.116720000	-3.587470000
H	-2.988570000	0.171130000	-4.485360000
C	2.169300000	-0.502190000	-1.135670000
C	1.641210000	-1.489210000	-1.982560000
C	3.453150000	0.007060000	-1.384960000
C	2.386750000	-1.963760000	-3.046720000
H	0.630530000	-1.871720000	-1.807860000
C	4.189090000	-0.457220000	-2.459740000
H	3.866690000	0.778680000	-0.727620000
C	3.662410000	-1.461060000	-3.298110000

H	1.973250000	-2.742180000	-3.700560000
H	4.247230000	-1.836140000	-4.143280000
C	-0.794190000	0.032850000	1.255000000
C	-0.688610000	-1.017260000	2.191860000
C	-1.687290000	1.095410000	1.505690000
C	-1.485850000	-1.002510000	3.348300000
C	-2.472980000	1.088310000	2.667940000
C	-2.375870000	0.039510000	3.581840000
H	-1.400520000	-1.821070000	4.072400000
H	-2.998930000	0.038230000	4.484790000
C	2.077660000	0.381520000	1.253770000
C	1.747790000	1.586720000	1.891070000
C	3.108190000	-0.420770000	1.760090000
C	2.442870000	1.973600000	3.031500000
H	0.940390000	2.211270000	1.499250000
C	3.789580000	-0.030130000	2.906910000
H	3.370170000	-1.353960000	1.253260000
C	3.458630000	1.170290000	3.542480000
H	2.187890000	2.914840000	3.530780000
H	4.000930000	1.477730000	4.444380000
H	-1.154850000	1.814310000	-4.144060000
H	-3.170660000	1.912580000	2.855940000
H	-3.364300000	-1.630220000	-2.814700000
H	5.189900000	-0.050520000	-2.654830000
H	4.588820000	-0.660580000	3.311730000
C	0.571280000	1.984600000	-2.130050000
H	1.423390000	1.617650000	-2.721060000
H	0.248110000	2.957470000	-2.536990000
H	0.881810000	2.110640000	-1.082510000
C	-2.038800000	-2.086690000	-0.537700000
H	-2.466620000	-1.698240000	0.394150000
H	-2.740200000	-2.814830000	-0.979030000
H	-1.091260000	-2.603420000	-0.316620000
C	0.258880000	-2.161340000	2.021510000
H	1.200930000	-1.917880000	2.531130000
H	-0.167500000	-3.075400000	2.468220000
H	0.468480000	-2.351010000	0.958070000
C	-1.806580000	2.261170000	0.576700000
H	-0.830070000	2.764530000	0.488860000
H	-2.128520000	1.923710000	-0.415870000
H	-2.540790000	2.988340000	0.963690000

### Coord\_3

C	0.000000000	0.000000000	0.000000000
C	1.381920000	0.000000000	0.000000000
C	-0.768680000	0.000000000	-1.263590000
C	-1.862240000	-0.880110000	-1.455710000
C	-0.431520000	0.901540000	-2.301780000
C	-2.630890000	-0.799220000	-2.622460000

C	-1.221210000	0.961240000	-3.460930000
C	-2.326220000	0.132050000	-3.612360000
H	-2.946430000	0.197010000	-4.514700000
C	2.167830000	-0.772070000	-0.983190000
C	1.535730000	-1.775370000	-1.735530000
C	3.518690000	-0.475480000	-1.222000000
C	2.246000000	-2.488250000	-2.685630000
H	0.471810000	-1.982850000	-1.579130000
C	4.226630000	-1.171130000	-2.186430000
H	4.009620000	0.316710000	-0.647730000
C	3.590990000	-2.208380000	-2.921570000
H	1.748070000	-3.279110000	-3.261510000
H	4.147890000	-2.770360000	-3.677350000
C	-0.807500000	0.059950000	1.248540000
C	-0.736060000	-0.980450000	2.199590000
C	-1.666180000	1.155040000	1.482400000
C	-1.526240000	-0.919230000	3.359750000
C	-2.443790000	1.195110000	2.650330000
C	-2.374960000	0.159360000	3.582990000
H	-1.465930000	-1.729300000	4.095480000
H	-2.990210000	0.195780000	4.490540000
C	2.006480000	0.547980000	1.244210000
C	1.710180000	1.863080000	1.632790000
C	2.942500000	-0.202670000	1.969420000
C	2.342490000	2.411730000	2.741210000
H	0.978380000	2.448350000	1.069670000
C	3.563670000	0.351760000	3.080650000
H	3.176490000	-1.225100000	1.659110000
C	3.265190000	1.663290000	3.468260000
H	2.113510000	3.439220000	3.045720000
H	3.757520000	2.099050000	4.345350000
H	-0.959310000	1.668410000	-4.254780000
H	-3.111760000	2.045840000	2.826840000
H	-3.482450000	-1.475200000	-2.758800000
H	5.281860000	-0.930260000	-2.370780000
H	4.289140000	-0.235910000	3.654020000
C	0.771290000	1.788270000	-2.247980000
H	1.566970000	1.323350000	-2.849580000
H	0.531210000	2.774190000	-2.681060000
H	1.110840000	1.907470000	-1.208420000
C	-2.213250000	-1.944810000	-0.465980000
H	-2.643560000	-1.487970000	0.432550000
H	-2.948520000	-2.643340000	-0.900350000
H	-1.312180000	-2.513680000	-0.190710000
C	0.158500000	-2.166450000	2.034060000
H	1.123140000	-1.951580000	2.512220000
H	-0.293300000	-3.051000000	2.514050000
H	0.330460000	-2.390950000	0.970180000
C	-1.758970000	2.308810000	0.535660000
H	-0.801740000	2.854550000	0.525130000

H	-1.983420000	1.957780000	-0.478930000
H	-2.554120000	3.003310000	0.857250000

Coord\_4

C	0.000000000	0.000000000	0.000000000
C	1.391380000	0.000000000	0.000000000
C	-0.758100000	0.000000000	-1.268220000
C	-1.926010000	-0.791530000	-1.429090000
C	-0.331740000	0.801760000	-2.357330000
C	-2.679030000	-0.700730000	-2.603530000
C	-1.109660000	0.871230000	-3.523430000
C	-2.289550000	0.146740000	-3.637950000
H	-2.900820000	0.222840000	-4.545510000
C	2.166280000	-0.997360000	-0.767290000
C	1.473170000	-2.007610000	-1.455090000
C	3.557330000	-0.887730000	-0.918330000
C	2.158360000	-2.919350000	-2.240260000
H	0.381450000	-2.064100000	-1.380850000
C	4.247990000	-1.779690000	-1.721790000
H	4.097260000	-0.084290000	-0.407290000
C	3.542510000	-2.833630000	-2.379920000
H	1.608790000	-3.713850000	-2.762190000
H	4.080180000	-3.551610000	-3.006620000
C	-0.820770000	0.086780000	1.241360000
C	-0.783460000	-0.943160000	2.205890000
C	-1.644260000	1.212700000	1.458510000
C	-1.565440000	-0.836620000	3.368730000
C	-2.412340000	1.298670000	2.631190000
C	-2.371790000	0.276550000	3.581310000
H	-1.530050000	-1.637710000	4.115500000
H	-2.978220000	0.349610000	4.492550000
C	1.931920000	0.714780000	1.207920000
C	1.684840000	2.089530000	1.342560000
C	2.759070000	0.059420000	2.132770000
C	2.256560000	2.791970000	2.393840000
H	1.039850000	2.601270000	0.623570000
C	3.322210000	0.768600000	3.183500000
H	2.952400000	-1.011650000	2.023610000
C	3.072620000	2.140660000	3.316860000
H	2.065920000	3.866250000	2.499410000
H	3.516550000	2.698750000	4.149040000
H	-0.777170000	1.502200000	-4.353700000
H	-3.049880000	2.174430000	2.796210000
H	-3.586810000	-1.304190000	-2.713750000
H	5.336110000	-1.684080000	-1.834940000
H	3.963200000	0.256750000	3.910030000
C	0.952600000	1.567540000	-2.350700000
H	1.683060000	1.010940000	-2.958070000
H	0.799260000	2.559660000	-2.809090000

H	1.316550000	1.673350000	-1.317700000
C	-2.377160000	-1.783820000	-0.404310000
H	-2.804470000	-1.258850000	0.457110000
H	-3.144080000	-2.451380000	-0.832970000
H	-1.527370000	-2.398000000	-0.073380000
C	0.056590000	-2.168490000	2.045780000
H	1.041660000	-1.984700000	2.493150000
H	-0.418650000	-3.022480000	2.557480000
H	0.189680000	-2.424480000	0.982970000
C	-1.710960000	2.354350000	0.495090000
H	-0.782040000	2.943340000	0.558130000
H	-1.836380000	1.992540000	-0.532830000
H	-2.560830000	3.012280000	0.746670000

### Coord\_5

C	0.000000000	0.000000000	0.000000000
C	1.400840000	0.000000000	0.000000000
C	-0.747500000	0.000000000	-1.272760000
C	-1.982210000	-0.694660000	-1.408310000
C	-0.241450000	0.691570000	-2.405410000
C	-2.718230000	-0.594530000	-2.591000000
C	-1.006360000	0.770930000	-3.579030000
C	-2.250920000	0.160530000	-3.664180000
H	-2.851610000	0.248100000	-4.577750000
C	2.164640000	-1.163360000	-0.500670000
C	1.456830000	-2.190460000	-1.148780000
C	3.567940000	-1.189000000	-0.500190000
C	2.129790000	-3.253290000	-1.729010000
H	0.363320000	-2.141730000	-1.208030000
C	4.253350000	-2.232940000	-1.101390000
H	4.126410000	-0.370630000	-0.034950000
C	3.522350000	-3.305680000	-1.706670000
H	1.564020000	-4.057930000	-2.217610000
H	4.051520000	-4.142360000	-2.172980000
C	-0.834020000	0.113310000	1.233470000
C	-0.830750000	-0.905440000	2.210750000
C	-1.621580000	1.268370000	1.434120000
C	-1.603490000	-0.754830000	3.375290000
C	-2.378780000	1.398870000	2.610680000
C	-2.366500000	0.390920000	3.576970000
H	-1.592910000	-1.546480000	4.132500000
H	-2.963170000	0.499480000	4.491090000
C	1.854290000	0.877250000	1.144930000
C	1.670440000	2.264120000	1.032180000
C	2.559740000	0.354390000	2.241040000
C	2.183660000	3.108470000	2.004390000
H	1.122170000	2.673350000	0.179860000
C	3.066870000	1.205600000	3.209720000
H	2.701010000	-0.726830000	2.327990000

C	2.881040000	2.589910000	3.094730000
H	2.042460000	4.192220000	1.916100000
H	3.278150000	3.261170000	3.864350000
H	-0.610510000	1.317770000	-4.440080000
H	-2.985260000	2.298200000	2.764320000
H	-3.675810000	-1.119100000	-2.679990000
H	5.351640000	-2.241520000	-1.093580000
H	3.613830000	0.797600000	4.067250000
C	1.112570000	1.325320000	-2.437280000
H	1.769870000	0.684620000	-3.046280000
H	1.049080000	2.316170000	-2.919830000
H	1.495340000	1.412130000	-1.409060000
C	-2.528720000	-1.605040000	-0.353370000
H	-2.947290000	-1.012880000	0.467200000
H	-3.325070000	-2.240520000	-0.777460000
H	-1.734450000	-2.257260000	0.034190000
C	-0.046650000	-2.167450000	2.056490000
H	0.956550000	-2.017010000	2.473810000
H	-0.543410000	-2.990070000	2.598330000
H	0.046520000	-2.451480000	0.996090000
C	-1.662640000	2.397850000	0.455090000
H	-0.770690000	3.030530000	0.587220000
H	-1.688320000	2.028450000	-0.577590000
H	-2.560430000	3.015290000	0.632820000

### Coord\_6

C	0.000000000	0.000000000	0.000000000
C	1.410300000	0.000000000	0.000000000
C	-0.736870000	0.000000000	-1.277210000
C	-2.030030000	-0.590510000	-1.393590000
C	-0.161760000	0.572400000	-2.445700000
C	-2.747690000	-0.481820000	-2.585040000
C	-0.912370000	0.661550000	-3.627400000
C	-2.210380000	0.173170000	-3.690980000
H	-2.798750000	0.272270000	-4.611370000
C	2.162920000	-1.258890000	-0.199370000
C	1.487970000	-2.326230000	-0.818330000
C	3.550160000	-1.348530000	-0.005810000
C	2.163160000	-3.486120000	-1.164470000
H	0.418440000	-2.233750000	-1.042660000
C	4.242890000	-2.492520000	-0.373720000
H	4.095780000	-0.501890000	0.422490000
C	3.533610000	-3.600510000	-0.938540000
H	1.617740000	-4.318560000	-1.629710000
H	4.066200000	-4.513730000	-1.221470000
C	-0.847220000	0.139520000	1.224870000
C	-0.877930000	-0.867350000	2.214150000
C	-1.598250000	1.322040000	1.409320000
C	-1.640440000	-0.673990000	3.379520000

C	-2.343260000	1.495600000	2.589020000
C	-2.359210000	0.502300000	3.570170000
H	-1.654520000	-1.455760000	4.146540000
H	-2.945260000	0.645180000	4.486410000
C	1.773900000	1.030770000	1.056100000
C	1.665250000	2.387610000	0.712740000
C	2.346580000	0.669360000	2.287940000
C	2.121800000	3.359070000	1.587600000
H	1.222140000	2.672000000	-0.244850000
C	2.799430000	1.647220000	3.156740000
H	2.426060000	-0.387810000	2.557550000
C	2.690200000	3.000620000	2.810100000
H	2.039500000	4.419160000	1.318600000
H	3.041870000	3.773470000	3.502310000
H	-0.461210000	1.117420000	-4.513360000
H	-2.918120000	2.417030000	2.731430000
H	-3.748040000	-0.921990000	-2.657850000
H	5.328130000	-2.548770000	-0.212800000
H	3.244130000	1.364750000	4.117840000
C	1.248840000	1.064810000	-2.507080000
H	1.826020000	0.348730000	-3.114260000
H	1.277650000	2.046330000	-3.012230000
H	1.644040000	1.128110000	-1.481590000
C	-2.666190000	-1.410020000	-0.313740000
H	-3.070140000	-0.752260000	0.462360000
H	-3.489810000	-2.012500000	-0.734280000
H	-1.931050000	-2.092580000	0.130940000
C	-0.151040000	-2.163320000	2.066020000
H	0.867930000	-2.048260000	2.454060000
H	-0.667410000	-2.953990000	2.636410000
H	-0.098610000	-2.471870000	1.009220000
C	-1.614070000	2.439350000	0.415760000
H	-0.767330000	3.115720000	0.611830000
H	-1.540160000	2.065970000	-0.613270000
H	-2.552500000	3.012470000	0.516560000

### Coord\_7

C	0.000000000	0.000000000	0.000000000
C	1.419760000	0.000000000	0.000000000
C	-0.726220000	0.000000000	-1.281570000
C	-2.068730000	-0.480130000	-1.385060000
C	-0.093670000	0.445790000	-2.478000000
C	-2.766750000	-0.363860000	-2.585720000
C	-0.828630000	0.544450000	-3.668310000
C	-2.167970000	0.184390000	-3.718260000
H	-2.742240000	0.294790000	-4.646250000
C	2.161110000	-1.277090000	0.118190000
C	1.565670000	-2.411950000	-0.462590000
C	3.504450000	-1.349080000	0.518490000

C	2.258000000	-3.609780000	-0.556530000
H	0.544940000	-2.344500000	-0.859390000
C	4.216800000	-2.534920000	0.403610000
H	4.006100000	-0.457030000	0.906290000
C	3.576750000	-3.700090000	-0.115230000
H	1.768950000	-4.491550000	-0.993340000
H	4.124910000	-4.643540000	-0.200290000
C	-0.860400000	0.165390000	1.215580000
C	-0.924970000	-0.828950000	2.216060000
C	-1.574330000	1.373700000	1.384230000
C	-1.676320000	-0.594200000	3.381470000
C	-2.305960000	1.588760000	2.566380000
C	-2.350080000	0.610560000	3.561080000
H	-1.714920000	-1.365720000	4.157670000
H	-2.924710000	0.786510000	4.478780000
C	1.691100000	1.170910000	0.943140000
C	1.667180000	2.462990000	0.394050000
C	2.121930000	0.990400000	2.270290000
C	2.068430000	3.544800000	1.157120000
H	1.336010000	2.607760000	-0.637090000
C	2.521730000	2.077790000	3.025170000
H	2.131840000	-0.014520000	2.702370000
C	2.499450000	3.364500000	2.472330000
H	2.052580000	4.553910000	0.726960000
H	2.806750000	4.225700000	3.075280000
H	-0.330960000	0.903650000	-4.573150000
H	-2.848680000	2.530840000	2.697810000
H	-3.802260000	-0.715050000	-2.647460000
H	5.265960000	-2.574260000	0.727560000
H	2.857430000	1.935260000	4.058870000
C	1.359360000	0.789470000	-2.559710000
H	1.850560000	0.007640000	-3.162330000
H	1.482130000	1.753120000	-3.085450000
H	1.759900000	0.825980000	-1.534720000
C	-2.787940000	-1.200470000	-0.285860000
H	-3.171310000	-0.479390000	0.442290000
H	-3.636730000	-1.769170000	-0.703740000
H	-2.114880000	-1.905350000	0.215900000
C	-0.256420000	-2.156100000	2.074210000
H	0.775900000	-2.078230000	2.433770000
H	-0.790500000	-2.914460000	2.671580000
H	-0.245310000	-2.485590000	1.022020000
C	-1.565330000	2.478920000	0.377210000
H	-0.771560000	3.198460000	0.631420000
H	-1.392780000	2.105490000	-0.640060000
H	-2.536680000	3.003990000	0.398790000

Coord\_8

C	0.000000000	0.000000000	0.000000000
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C	1.429210000	0.000000000	0.000000000
C	-0.715540000	0.000000000	-1.285850000
C	-2.097680000	-0.364670000	-1.382800000
C	-0.038000000	0.313390000	-2.502200000
C	-2.774840000	-0.241990000	-2.593030000
C	-0.755940000	0.421070000	-3.701660000
C	-2.123810000	0.193940000	-3.745920000
H	-2.682130000	0.315090000	-4.682270000
C	2.159220000	-1.215840000	0.432320000
C	1.686830000	-2.438270000	-0.081660000
C	3.432050000	-1.188900000	1.023270000
C	2.410350000	-3.610600000	0.082660000
H	0.738060000	-2.462540000	-0.633260000
C	4.175240000	-2.353540000	1.168340000
H	3.860070000	-0.237560000	1.354000000
C	3.649500000	-3.592200000	0.719790000
H	2.011520000	-4.558540000	-0.305220000
H	4.224520000	-4.516010000	0.837700000
C	-0.873530000	0.190900000	1.205610000
C	-0.971830000	-0.790320000	2.216480000
C	-1.549910000	1.423340000	1.358930000
C	-1.711190000	-0.515600000	3.381220000
C	-2.267040000	1.678250000	2.542960000
C	-2.339240000	0.715580000	3.549890000
H	-1.774150000	-1.276510000	4.165940000
H	-2.901730000	0.923300000	4.468460000
C	1.606240000	1.293600000	0.808510000
C	1.673840000	2.494940000	0.084240000
C	1.888300000	1.303300000	2.188130000
C	2.020560000	3.669280000	0.724840000
H	1.459690000	2.493360000	-0.987060000
C	2.235670000	2.482170000	2.818780000
H	1.823030000	0.371670000	2.757830000
C	2.307860000	3.675380000	2.091390000
H	2.076570000	4.606990000	0.157550000
H	2.571410000	4.610730000	2.596190000
H	-0.221190000	0.679110000	-4.619280000
H	-2.777200000	2.639530000	2.663720000
H	-3.837440000	-0.500570000	-2.648850000
H	5.166190000	-2.311940000	1.641580000
H	2.457260000	2.486320000	3.892430000
C	1.442390000	0.502950000	-2.595020000
H	1.843030000	-0.334290000	-3.191130000
H	1.659930000	1.439800000	-3.138930000
H	1.840710000	0.510760000	-1.568280000
C	-2.892470000	-0.978250000	-0.270050000
H	-3.249280000	-0.196860000	0.406870000
H	-3.764440000	-1.512530000	-0.686010000
H	-2.283690000	-1.697220000	0.288260000
C	-0.362600000	-2.145820000	2.080880000

H	0.68060000	-2.10670000	2.41280000
H	-0.91257000	-2.87172000	2.70368000
H	-0.39316000	-2.49264000	1.03418000
C	-1.51648000	2.51661000	0.33953000
H	-0.78289000	3.27831000	0.64556000
H	-1.24709000	2.14740000	-0.65819000
H	-2.51268000	2.99011000	0.28040000

### Coord\_9

C	0.00000000	0.00000000	0.00000000
C	1.43867000	0.00000000	0.00000000
C	-0.70484000	0.00000000	-1.29003000
C	-2.11632000	-0.24531000	-1.38679000
C	0.00458000	0.17691000	-2.51835000
C	-2.77152000	-0.11755000	-2.60686000
C	-0.69500000	0.29291000	-3.72742000
C	-2.07802000	0.20157000	-3.77384000
H	-2.61858000	0.33264000	-4.71924000
C	2.15725000	-1.07800000	0.72330000
C	1.84627000	-2.39071000	0.31876000
C	3.33492000	-0.88182000	1.46133000
C	2.61290000	-3.47104000	0.73340000
H	0.99037000	-2.56232000	-0.34764000
C	4.11832000	-1.95942000	1.85851000
H	3.66234000	0.13274000	1.70825000
C	3.74681000	-3.27190000	1.51832000
H	2.33442000	-4.48935000	0.42646000
H	4.35812000	-4.12352000	1.83326000
C	-0.88662000	0.21603000	1.19498000
C	-1.01849000	-0.75150000	2.21539000
C	-1.52506000	1.47095000	1.33352000
C	-1.74509000	-0.43829000	3.37885000
C	-2.22667000	1.76403000	2.51894000
C	-2.32686000	0.81724000	3.53678000
H	-1.83224000	-1.18826000	4.17143000
H	-2.87653000	1.05539000	4.45570000
C	1.51969000	1.39524000	0.65539000
C	1.68267000	2.48926000	-0.21048000
C	1.64834000	1.59429000	2.04476000
C	1.97490000	3.73796000	0.30047000
H	1.58875000	2.34254000	-1.28885000
C	1.94321000	2.84638000	2.54424000
H	1.50465000	0.74935000	2.72462000
C	2.11427000	3.92903000	1.67745000
H	2.10589000	4.59124000	-0.37753000
H	2.33416000	4.92395000	2.07804000
H	-0.13310000	0.44660000	-4.65173000
H	-2.70391000	2.74305000	2.62941000
H	-3.85276000	-0.28093000	-2.66188000

H	5.030510000	-1.782000000	2.445470000
H	2.047250000	2.996260000	3.625370000
C	1.496600000	0.209080000	-2.613140000
H	1.803400000	-0.672760000	-3.201520000
H	1.808730000	1.109900000	-3.172290000
H	1.884820000	0.187690000	-1.582470000
C	-2.978430000	-0.745390000	-0.266490000
H	-3.302760000	0.092600000	0.356140000
H	-3.871660000	-1.244690000	-0.681170000
H	-2.435350000	-1.470050000	0.347330000
C	-0.469380000	-2.132510000	2.085890000
H	0.582180000	-2.133460000	2.391000000
H	-1.033460000	-2.826020000	2.732580000
H	-0.541780000	-2.493030000	1.045420000
C	-1.467600000	2.552500000	0.302800000
H	-0.800780000	3.354800000	0.653860000
H	-1.103940000	2.191990000	-0.667960000
H	-2.480280000	2.971140000	0.162270000

#### Coord\_10

C	0.000000000	0.000000000	0.000000000
C	1.448130000	0.000000000	0.000000000
C	-0.694120000	0.000000000	-1.294130000
C	-2.124220000	-0.123280000	-1.396970000
C	0.033570000	0.038140000	-2.526570000
C	-2.756490000	0.008050000	-2.627050000
C	-0.646340000	0.161520000	-3.745670000
C	-2.030760000	0.207070000	-3.801900000
H	-2.551800000	0.346900000	-4.756960000
C	2.155200000	-0.871280000	0.972660000
C	2.036950000	-2.253210000	0.724110000
C	3.215760000	-0.455470000	1.792680000
C	2.855250000	-3.174490000	1.364620000
H	1.291990000	-2.609560000	-0.000660000
C	4.046150000	-1.380550000	2.417410000
H	3.419300000	0.611530000	1.924730000
C	3.861120000	-2.744420000	2.227480000
H	2.722090000	-4.249440000	1.174640000
H	4.515310000	-3.470690000	2.720300000
C	-0.899680000	0.240760000	1.183680000
C	-1.064920000	-0.712570000	2.212790000
C	-1.499880000	1.516550000	1.308090000
C	-1.778080000	-0.362370000	3.374420000
C	-2.185020000	1.846010000	2.494500000
C	-2.313070000	0.915450000	3.521940000
H	-1.889230000	-1.101130000	4.174190000
H	-2.849350000	1.182650000	4.440760000
C	1.431820000	1.472860000	0.487560000
C	1.690990000	2.452250000	-0.485890000

C	1.404780000	1.850820000	1.846400000
C	1.927980000	3.757350000	-0.108630000
H	1.718650000	2.169020000	-1.540370000
C	1.646310000	3.158110000	2.210840000
H	1.181880000	1.098320000	2.608590000
C	1.917400000	4.122910000	1.240540000
H	2.134660000	4.520480000	-0.870550000
H	2.093120000	5.162890000	1.533410000
H	-0.067610000	0.208990000	-4.670690000
H	-2.629070000	2.841360000	2.595130000
H	-3.847610000	-0.058550000	-2.686260000
H	4.861240000	-1.028720000	3.065770000
H	1.631150000	3.445580000	3.268920000
C	1.521010000	-0.088220000	-2.614430000
H	1.732070000	-1.003630000	-3.194580000
H	1.926520000	0.767220000	-3.185440000
H	1.891180000	-0.137850000	-1.577840000
C	-3.044630000	-0.504030000	-0.275240000
H	-3.330690000	0.386120000	0.290310000
H	-3.957320000	-0.967850000	-0.689120000
H	-2.567890000	-1.225940000	0.392580000
C	-0.576600000	-2.116230000	2.089100000
H	0.480820000	-2.158320000	2.368190000
H	-1.153080000	-2.777590000	2.758190000
H	-0.690760000	-2.486830000	1.055450000
C	-1.418750000	2.586650000	0.267120000
H	-0.824660000	3.427440000	0.656010000
H	-0.964150000	2.239560000	-0.669750000
H	-2.439320000	2.947460000	0.045300000