

Supplementary Information for

**The phosphorescent properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization**

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Table S1 Main geometry parameters for **1c–4c** in the optimized S<sub>0</sub> and T<sub>1</sub> states

	<b>1c</b>		<b>2c</b>		<b>3c</b>		<b>4c</b>	
	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>
Bond [Å]								
Pt-N <sub>1</sub>	2.010	2.014	2.009	2.013	2.018	2.019	2.015	2.017
Pt-O <sub>2</sub>	2.103	2.107	2.097	2.102	2.102	2.104	2.104	2.094
Pt-O <sub>3</sub>	2.021	2.018	2.019	2.016	2.014	2.016	2.015	2.014
Pt-C <sub>4</sub>	1.997	1.984	1.993	1.982	1.964	1.959	1.964	1.959
C <sub>4</sub> -C <sub>5</sub>	1.379	1.401	1.393	1.405	1.390	1.392	1.394	1.397
C <sub>5</sub> -C <sub>6</sub>	1.429	1.422	1.422	1.416	1.431	1.427	1.430	1.420
C <sub>4</sub> -C <sub>7</sub>	1.449	1.416	1.445	1.412	1.413	1.407	1.409	1.404
C <sub>7</sub> -C <sub>8</sub>	1.472	1.419	1.471	1.422	1.466	1.411	1.463	1.413
Rc	1.530	1.563	1.530	1.563	1.533	1.562	1.533	1.562
Angle [deg.]								
N <sub>1</sub> -Pt-O <sub>2</sub>	91.0	91.8	90.8	91.5	93.6	94.0	93.8	93.1
O <sub>2</sub> -Pt-O <sub>3</sub>	89.9	90.5	90.2	91.7	91.8	91.7	91.8	92.0
O <sub>3</sub> -Pt-C <sub>4</sub>	97.6	96.2	97.6	96.3	93.6	93.3	93.4	92.9
N <sub>1</sub> -Pt-C <sub>4</sub>	81.3	81.5	81.2	81.4	81.1	81.0	80.9	82.2
Dihedral [deg.]								
O <sub>3</sub> -Pt-C <sub>4</sub> -C <sub>7</sub>	10.9	7.0	12.1	8.1	0.5	0.1	0.2	0.1
O <sub>2</sub> -Pt-N <sub>1</sub> -C <sub>6</sub>	168.0	173.0	174.1	172.5	180.0	179.9	179.7	179.4
Pt-O <sub>2</sub> -O <sub>3</sub> -C <sub>9</sub>	180.0	180.0	178.5	179.4	179.8	179.9	179.8	179.9

Table S2 The calculated composition(percentage) of the selected frontier MOs for open and closed

forms of 1-4

		acac	Pt	thpy/tthpy	DTE
<b>1c</b>	L	1	2	26	71
	H	1	0	27	72
	H-1	6	23	46	25
<b>1o</b>	L+3	1	2	21	76
	L	2	7	85	6
	H	5	22	56	17
	H-1	3	10	21	66
<b>2c</b>	H-5	4	88	5	3
	L	1	2	31	66
	H	0	0	33	67
	H-1	6	23	45	26
<b>2o</b>	L+3	1	1	31	67
	L	1	6	85	8
	H	1	6	41	52
	H-1	4	10	26	60
	H-5	4	88	6	2
<b>3c</b>	L	0	1	29	70
	H	0	0	25	75
	H-1	2	13	52	33
<b>3o</b>	L+3	1	2	43	54
	L	1	7	86	6
	H	1	8	69	22
	H-1	10	22	38	30
	H-6	2	91	1	6
<b>4c</b>	L	1	2	31	66
	H	0	0	33	67
	H-1	6	23	45	26
<b>4o</b>	L+3	0	2	29	69
	L	1	6	84	9
	H	1	8	39	52
	H-1	7	23	35	35
	H-6	1	92	0	7

Table S3. The main transitions, oscillator strengths and vertical excitation energy(eV) of **1o**

State	Transition(CI)	Energy	<i>f</i>
T <sub>1</sub>	H→L (0.68)	1.76	-
S <sub>2</sub>	H-1→L (0.63)	3.68	0.1760
S <sub>3</sub>	H-2→L (0.20)	4.01	0.0525
S <sub>4</sub>	H-2→L (0.54)	4.13	0.1123
	H-3→L (-0.20)		
S <sub>5</sub>	H-5→L (0.63)	4.20	0.0254
S <sub>6</sub>	H-6→L (-0.24)	4.32	0.0297
	H-3→L (0.31)		
S <sub>7</sub>	H-6→L (-0.20)	4.38	0.0161
	H-3→L (0.28)		
	H-5→L (0.25)		
S <sub>9</sub>	H-3→L(-0.37)	4.52	0.1245
	H-4→L (0.45)		
S <sub>10</sub>	H-4→L (-0.20)	4.62	0.0626

Table S4. The main transitions, oscillator strengths and vertical excitation energy(eV) of **2o**

State	Transition(Cl)	Energy	<i>f</i>
T <sub>1</sub>	H→L (0.67)	1.75	-
S <sub>2</sub>	H-1→L (0.63)	3.51	0.1727
S <sub>3</sub>	H-2→L (0.49)	3.93	0.0510
	H-8→L (0.18)		
S <sub>4</sub>	H-2→L (-0.35)	4.02	0.1178
	H-5→L (0.18)		
S <sub>5</sub>	H-6→L (0.23)	4.05	0.0190
	H-5→L (0.59)		
S <sub>6</sub>	H-6→L (0.31)	4.19	0.0545
	H-3→L (0.47)		
	H-8→L (0.18)		
	H-2→L (-0.19)		
S <sub>7</sub>	H-4→L (0.37)	4.38	0.0549
S <sub>8</sub>	H-4→L (0.34)	4.39	0.0702

Table S5. The main transitions, oscillator strengths and vertical excitation energy(eV) of **3o**

State	Transition(CI)	Energy	<i>f</i>
T <sub>1</sub>	H→L (0.68)	1.71	-
S <sub>2</sub>	H-1→L (0.49)	3.77	0.6943
	H-2→L (0.20)		
S <sub>3</sub>	H-2→L (0.50)	3.94	0.2318
S <sub>4</sub>	H-2→L (0.35)	4.08	0.0.01
	H-1→L (-0.33)		
S <sub>5</sub>	H-6→L (0.45)	4.25	0.0968
	H-3→L (-0.38)		
S <sub>6</sub>	H-6→L (0.49)	4.27	0.0821
	H-3→L (0.31)		
S <sub>10</sub>	H-5→L (0.20)	4.60	0.0205
	H-3→L (0.30)		

Table S6. The main transitions, oscillator strengths and vertical excitation energy(eV) of **4o**

State	Transition(Cl)	Energy	<i>f</i>
T <sub>1</sub>	H→L (0.68)	1.71	-
S <sub>2</sub>	H-1→L (0.53)	3.66	0.3394
	H-2→L (0.28)		
S <sub>3</sub>	H-2→L (0.52)	3.85	0.1665
S <sub>4</sub>	H-3→L (-0.22)	3.98	0.0089
	H-2→L (0.23)		
	H-1→L (-0.28)		
S <sub>5</sub>	H-6→L (0.65)	4.12	0.0206
S <sub>6</sub>	H-6→L (0.54)	4.15	0.2073
	H-3→L (0.49)		
	H-1→L (0.23)		
S <sub>9</sub>	H-3→L (-0.20)	4.47	0.0179
S <sub>10</sub>	H-3→L (-0.21)	4.52	0.0756



Table S7 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **1o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	18.00		
S <sub>3</sub>	-10.28		10.30
S <sub>4</sub>	51.71		29.03
S <sub>5</sub>	-55.57		-254.83
S <sub>6</sub>	14.00		-24.73
S <sub>7</sub>	-8.86		-94.68
S <sub>8</sub>			
S <sub>9</sub>	6.63		
S <sub>10</sub>	-10.86		
$k_r^\alpha$	108.22		691.44
$k_r$		266.55	

Table S8 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **2o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	30.59		
S <sub>3</sub>	-65.26		16.80
S <sub>4</sub>	17.94		-79.27
S <sub>5</sub>	-46.33		-267.68
S <sub>6</sub>	41.81		-84.93
S <sub>7</sub>	11.30		
S <sub>8</sub>	10.14		
S <sub>9</sub>			
S <sub>10</sub>			
$k_r^\alpha$	47.04		3329
$k_r$		1125.35	

Table S9 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **3o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	-27.50		
S <sub>3</sub>	-22.19		
S <sub>4</sub>	-3.26		
S <sub>5</sub>	44.52		-168.07
S <sub>6</sub>	-16.68		-181.97
S <sub>7</sub>			
S <sub>8</sub>			
S <sub>9</sub>			
S <sub>10</sub>	-19.24		
$k_r^\alpha$	363.63		2953.04
$k_r$		1105.35	

Table S10 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **4o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	-36.39		
S <sub>3</sub>	-23.88		
S <sub>4</sub>	-39.28		
S <sub>5</sub>	-15.10		-253.84
S <sub>6</sub>	12.57		-212.06
S <sub>7</sub>			
S <sub>8</sub>			
S <sub>9</sub>	-14.00		
S <sub>10</sub>	-15.35		
$k_r^\alpha$	557.66		5416.01
$k_r$		1991.22	

Table S11 Main optimized geometry parameters for <sup>3</sup>MC in **1o-4o**..

Item	1o	2o	3o	4o
Bond (Å)				
Pt-N <sub>1</sub>	2.264	2.254	2.253	2.247
Pt-O <sub>2</sub>	2.130	2.134	2.122	2.121
Pt-O <sub>3</sub>	2.207	2.205	1.211	2.208
Pt-C <sub>4</sub>	1.998	1.996	1.997	1.997
C <sub>4</sub> -C <sub>5</sub>	1.383	1.386	1.387	1.391
C <sub>5</sub> -C <sub>6</sub>	1.443	1.438	1.442	1.436
C <sub>4</sub> -C <sub>7</sub>	1.430	1.428	1.415	1.414
C <sub>7</sub> -C <sub>8</sub>	1.387	1.389	1.386	1.386
Rc	3.469	3.471	3.471	3.471
Angle [deg.]				
N <sub>1</sub> -Pt-O <sub>2</sub>	101.5	98.6	101.1	99.9
O <sub>2</sub> -Pt-O <sub>3</sub>	87.5	87.8	87.7	87.6
O <sub>3</sub> -Pt-C <sub>4</sub>	98.9	98.0	98.8	98.2
N <sub>1</sub> -Pt-C <sub>4</sub>	78.4	78.6	78.4	78.5
Dihedral [deg.]				
O <sub>3</sub> -Pt-C <sub>4</sub> -C <sub>7</sub>	92.6	90.5	95.3	95.49
O <sub>2</sub> -Pt-N <sub>1</sub> -C <sub>6</sub>	174.4	174.5	174.3	175.0
Pt-O <sub>2</sub> -O <sub>3</sub> -C <sub>9</sub>	171.0	170.8	170.5	168.5

Table S12. Main geometry parameters for **5**, **6** in the optimized S<sub>0</sub> and T<sub>1</sub> states. Rc represents the distance between two reactive C atoms on DTE.

	<b>5o</b>		<b>5c</b>		<b>6o</b>		<b>6c</b>	
	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>
Bond [Å]								
Pt-N <sub>1</sub>	2.018	2.008	2.019	2.017	2.018	2.009	2.019	2.016
Pt-O <sub>2</sub>	2.096	2.099	2.096	2.097	2.096	2.099	2.096	2.097
Pt-O <sub>3</sub>	2.013	2.020	2.010	2.014	2.012	2.019	2.010	2.015
Pt-C <sub>4</sub>	1.957	1.944	1.960	1.959	1.957	1.947	1.960	1.959
C <sub>4</sub> -C <sub>5</sub>	1.391	1.464	1.395	1.397	1.391	1.459	1.395	1.402
C <sub>5</sub> -C <sub>6</sub>	1.425	1.398	1.426	1.419	1.426	1.399	1.425	1.416
C <sub>4</sub> -C <sub>7</sub>	1.413	1.376	1.410	1.404	1.413	1.372	1.410	1.377
C <sub>7</sub> -C <sub>8</sub>	1.389	1.423	1.472	1.414	1.391	1.433	1.478	1.429
Rc	3.475	3.428	1.538	1.576	3.494	3.439	1.544	1.585
Angle [deg.]								
N <sub>1</sub> -Pt-O <sub>2</sub>	93.5	92.9	93.4	93.4	93.0	93.5	93.4	93.5
O <sub>2</sub> -Pt-O <sub>3</sub>	91.9	91.9	91.8	91.8	91.9	91.7	91.8	91.8
O <sub>3</sub> -Pt-C <sub>4</sub>	93.8	93.0	93.8	93.7	93.0	92.5	93.8	93.6
N <sub>1</sub> -Pt-C <sub>4</sub>	80.8	82.2	81.0	81.0	82.1	82.2	81.0	81.0
Dihedral [deg.]								
O <sub>3</sub> -Pt-C <sub>4</sub> -C <sub>7</sub>	0.5	0.4	1.2	0.3	0.6	0.7	0.8	0.3
O <sub>2</sub> -Pt-N <sub>1</sub> -C <sub>6</sub>	179.3	179.8	180.0	179.2	179.5	179.8	180.0	179.3
Pt-O <sub>2</sub> -O <sub>3</sub> -C <sub>9</sub>	179.8	179.7	179.5	179.8	179.7	179.6	179.3	179.8

Table S13. Electron transition configurations, excitation energies, oscillator strengths ( $f$ ), andassignment for absorption and emission bands of isomers in **5**, **6**.

	State	Major contrib. <sup>a</sup>	Energy(nm/eV)	$f$	Assignment
<b>5o</b>	T <sub>1</sub>	H→L (90.1%) H-1→L (5.7%)	724/1.71	-	<sup>3</sup> LLCT/ <sup>3</sup> MLCT
	S <sub>1</sub>	H→L (91.5%) H-1→L (3.3%)	448/2.76	0.4483	LLCT/MLCT
	S <sub>2</sub>	H-1→L (85.4%) H→L (5.0%)	377/3.28	0.0986	LLCT/MLCT
	S <sub>9</sub>	H→L+3 (60.7%) H-1→L+1 (29.1%)	272/4.55	0.0320	ILCT/LLCT
<b>5c</b>	T <sub>1</sub>	H→L (74.5%) H→L+1 (20.7%)	2721/0.45	-	<sup>3</sup> ILCT/ <sup>3</sup> LLCT
	S <sub>1</sub>	H→L (99.2%)	639/1.94	0.1409	ILCT/LLCT
	S <sub>3</sub>	H-1→L (89.6%)	432/2.87	0.2334	LLCT/MLCT
<b>6o</b>	T <sub>1</sub>	H→L (90.6%) H→L (4.2%)	752/1.65	-	<sup>3</sup> LLCT/ <sup>3</sup> MLCT
	S <sub>1</sub>	H→L (92.6%) H-1→L (2.5%)	455/2.73	0.5370	LLCT/MLCT
	S <sub>2</sub>	H-1→L (85.5%) H→L (4.1%)	384/3.23	0.1233	LLCT/MLCT
	S <sub>8</sub>	H→L+3 (80.3%) H-1→L+2 (9.0%)	316/3.93	0.0737	ILCT/LLCT
<b>6c</b>	T <sub>1</sub>	H→L (77.02%) H→L+1 (15.08%)	5001/0.25	-	<sup>3</sup> ILCT/ <sup>3</sup> LLCT
	S <sub>1</sub>	H→L (99.0%)	616/2.01	0.2123	ILCT/LLCT
	S <sub>2</sub>	H→L+1 (72.4%) H-1→L (19.9%)	437/2.84	0.1738	LLCT/MLCT
	S <sub>3</sub>	H-1→L (72.4%) H→L+1 (19.0%)	426/2.91	0.1337	LLCT/MLCT

Table S14 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **5o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	-32.60		
S <sub>3</sub>	-29.07		
S <sub>4</sub>	-3.96		
S <sub>5</sub>	33.95		-239.72
S <sub>6</sub>	37.77		-165.26
S <sub>7</sub>	-8.99		
S <sub>8</sub>			
S <sub>9</sub>			
S <sub>10</sub>	18.46		
$k_r^\alpha$	105.84		4662.09
$k_r$		1589.31	



Table S15 SOC matrix elements  $\langle T_m^\alpha | H_{\text{SOC}} | S_n \rangle$  ( $\text{cm}^{-1}$ ) and the radiative decay rate rate ( $k_r / \text{s}^{-1}$ ) of **6o**

calculated at the T1 optimized geometry

	$\langle T_1^x   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^y   H_{\text{SOC}}   S_n \rangle$	$\langle T_1^z   H_{\text{SOC}}   S_n \rangle$
S <sub>1</sub>			
S <sub>2</sub>	-23.70		
S <sub>3</sub>	-20.68		
S <sub>4</sub>	-3.70		
S <sub>5</sub>	-6.08		-202.35
S <sub>6</sub>	-16.68		-208.82
S <sub>7</sub>	-18.33		
S <sub>8</sub>			
S <sub>9</sub>			
S <sub>10</sub>			17.71
$k_r^\alpha$	310.61		5133.38
$k_r$		1814.66	

Table S16. The relative energies of  $^3\text{ESo}$ ,  $^3\text{MC}$ ,  $^3\text{ESc}$  state and the energy barriers in nonradiative decay

process of **5** and **6**. Ground state of open-ring form is treated as zero point.

	$^3\text{ESo}$	$^3\text{MC}$	$^3\text{ESc}$	$\Delta E_1$	$\Delta E_2$	$\Delta E_3$	$\Delta E_4$
<b>5</b>	1.89	2.41	1.62	0.77	0.04	0.54	0.05
<b>6</b>	1.86	2.42	2.04	0.78	0.04	0.72	0.07

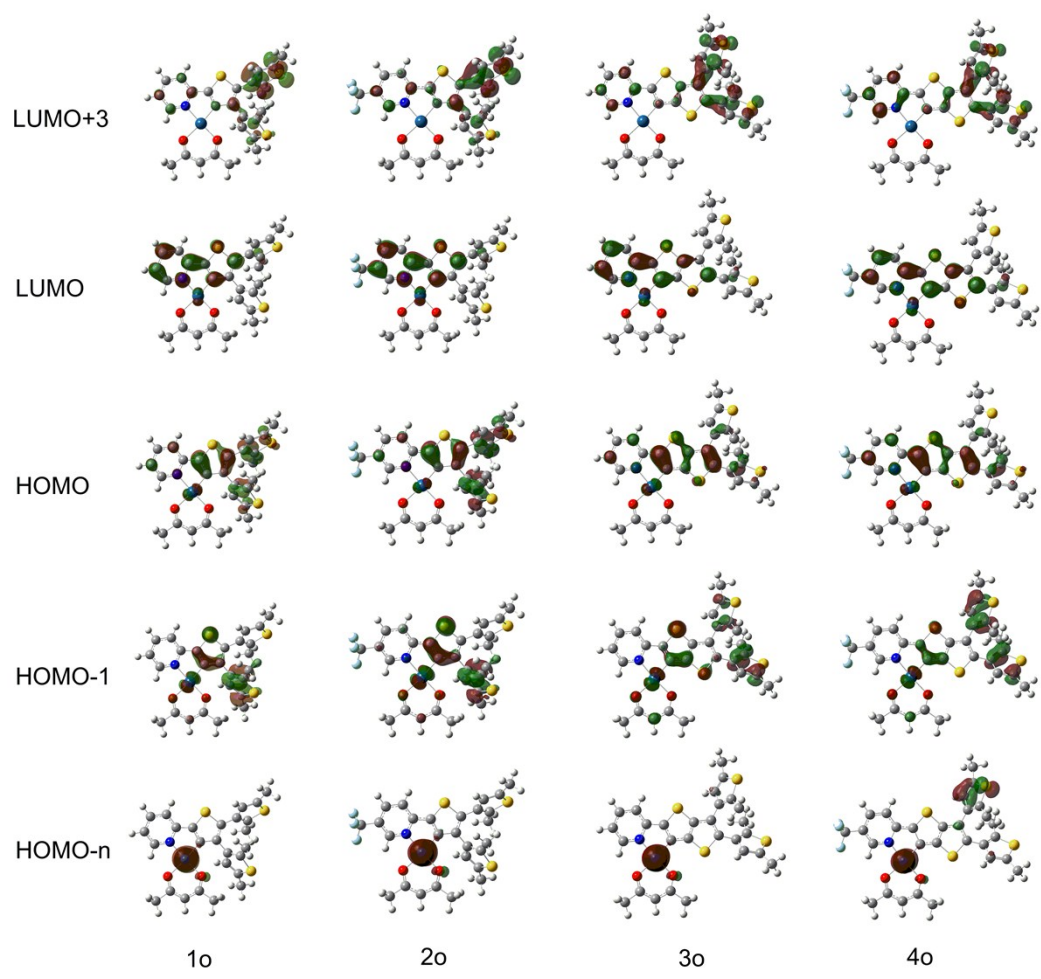


Fig. S1 The selected molecular orbitals in **1o**, **2o**(n=5) and **3o**, **4o**(n=6)

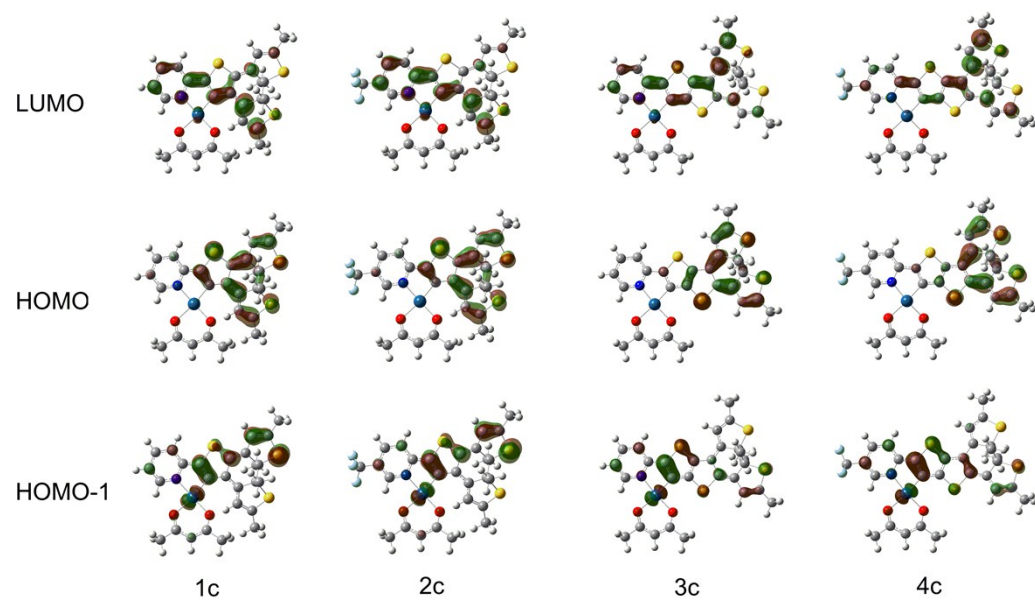


Fig. S2 The selected molecular orbitals in **1c-4c**.

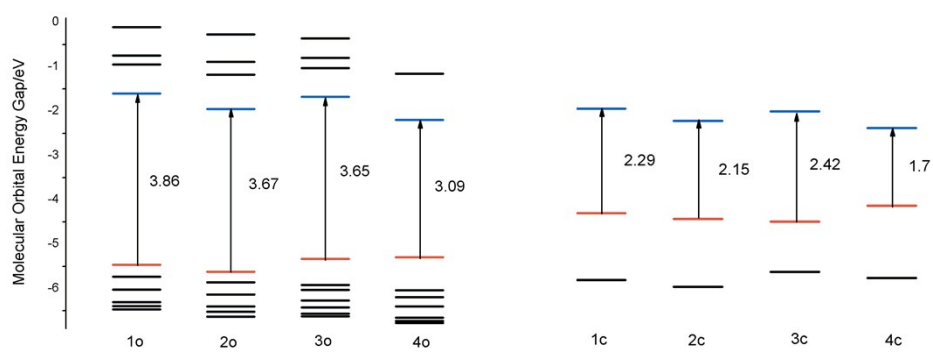


Fig. S3 Calculated energy levels of molecular orbitals and energy gaps(eV) between HOMO(orange)

and LUMO(blue) in **1-4**.

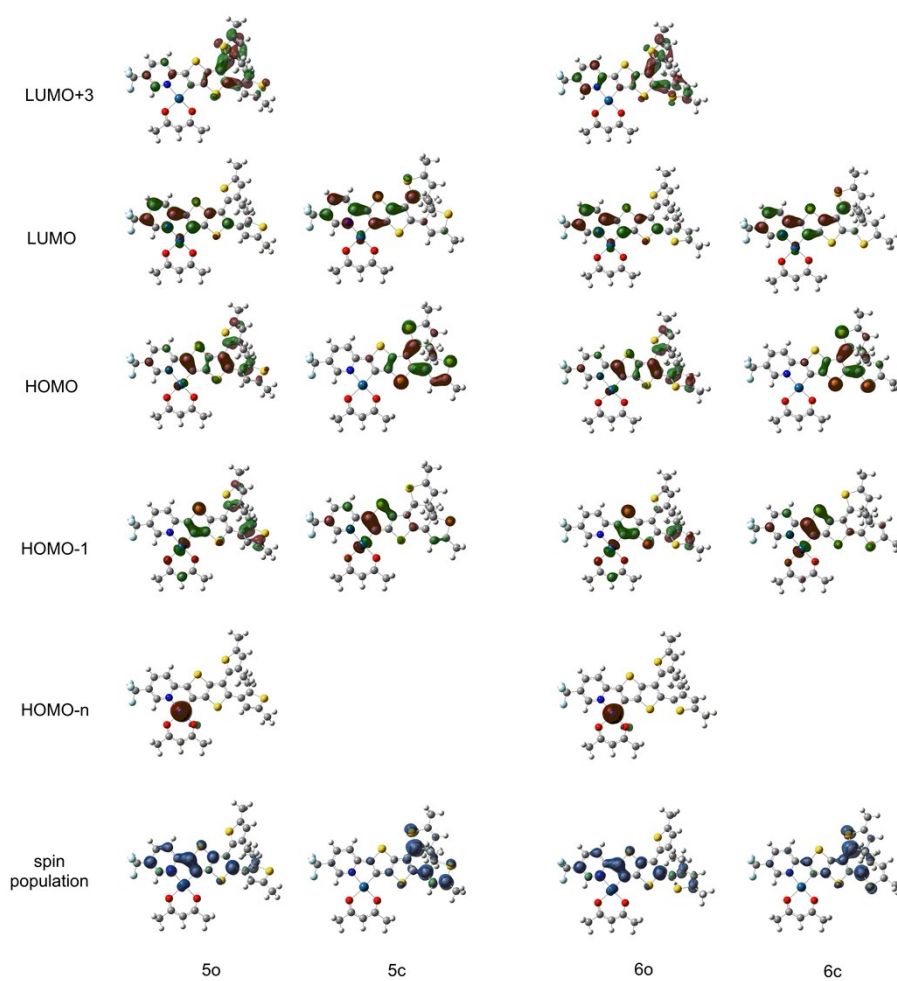
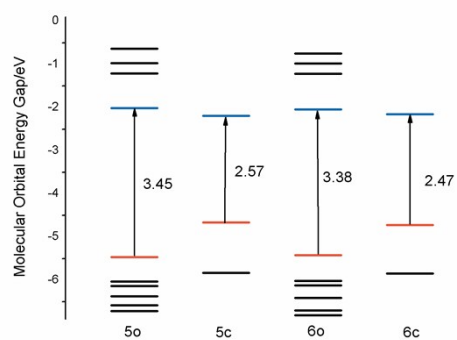


Fig. S4 The selected molecular orbitals and spin population distribution in each isomer of **5**( $n=5$ ), **6**( $n=4$ ).



**Fig. S5** Calculated energy levels of molecular orbitals and energy gaps(eV) between HOMO(orange) and LUMO(blue) in **5, 6**.

## Cartesian coordinates of the optimized geometries

### 1-<sup>1</sup>GSo

C	-3.70212300	-2.60547800	0.29500400
H	-4.49990800	-1.87055900	0.27144300
C	-3.93607800	-3.96640500	0.40400300
H	-4.95374700	-4.33252100	0.47970800
C	-2.84309900	-4.83481700	0.40946500
H	-2.99349900	-5.90744700	0.48995200
C	-1.56077800	-4.31992000	0.31164900
H	-0.69216300	-4.97067500	0.31408500
C	-1.37971400	-2.93732200	0.21018000
C	-0.14739000	-2.21268700	0.12862700
C	-0.20070100	-0.82769900	0.07674700
C	1.11452500	-0.25821600	0.07187700
C	2.11198400	-1.22528400	0.08851700
C	2.90191700	1.31948600	-1.99989000
H	3.96575000	1.13329900	-1.80643500
H	2.82616900	2.01136100	-2.84594500
H	2.45025600	0.36734600	-2.29293900
C	2.20685500	1.85016300	-0.79108500
C	1.40247600	1.18682800	0.10072400
C	0.91585700	2.04301000	1.14305800
H	0.25023300	1.69141000	1.92484300
C	1.36080500	3.32757200	1.06418600
C	1.07444600	4.46927700	1.98365500
H	0.62214800	5.32008600	1.45922300
H	1.98272300	4.83662300	2.47660900
H	0.37663200	4.14535400	2.76192700
C	3.80964300	0.53178300	2.08440800
H	3.68669000	1.58600900	1.80858200
H	4.50224300	0.47764600	2.93108800
H	2.83240100	0.16651100	2.41244800
C	4.29046100	-0.28485400	0.93332500
C	3.56776000	-1.07099800	0.06504100
C	4.39998600	-1.73637100	-0.89719600
H	4.00348500	-2.39208800	-1.66653500
C	5.72647900	-1.44646400	-0.78051900
C	6.86317600	-1.93777600	-1.61423400
H	7.60040700	-2.48676900	-1.01652800
H	7.38972800	-1.11501500	-2.11206000
H	6.48616600	-2.61337600	-2.38791000
C	-6.04005900	1.64539600	-0.37054000
H	-6.44821100	0.98320600	-1.14206100
H	-6.38318000	2.66554100	-0.55609600
H	-6.43611600	1.30321200	0.59202600
C	-4.53908400	1.52832500	-0.35935000
C	-3.75905900	2.67255600	-0.57909400
H	-4.28768300	3.60160200	-0.75885100
C	-2.36023500	2.72848700	-0.61003200
C	-1.67417900	4.03161400	-0.91105300
H	-0.94924600	4.24154600	-0.11857000
H	-2.37338800	4.86465200	-1.00918200
H	-1.10084000	3.92754300	-1.83894000
N	-2.46318600	-2.10470700	0.20117500
O	-4.09933600	0.35292700	-0.14892700
O	-1.54274700	1.76792600	-0.41259000
S	1.46364200	-2.83778900	0.13159800
S	2.37901300	3.51716400	-0.33335300
S	5.97642100	-0.34621400	0.53956000
Pt	-2.05393000	-0.14384900	-0.04404700

### 1-<sup>1</sup>GSc

C	3.85589500	2.41998200	0.46909200
H	4.61880100	1.65554500	0.56812500
C	4.13889600	3.77560800	0.52241400
H	5.15792200	4.10524100	0.69034600
C	3.09357000	4.68517900	0.35035500
H	3.28489700	5.75387700	0.38032900
C	1.80691200	4.21686300	0.14131000
H	0.97482000	4.90035600	0.00726000
C	1.57381500	2.83727400	0.10931700
C	0.32008700	2.16714200	-0.03507600
C	0.29030200	0.79216100	0.06007000
C	-1.07607600	0.30884700	0.03443700
C	-2.03503700	1.40977600	-0.15007000
C	-3.05078900	-1.28590100	-1.78459300
H	-2.74191800	-0.32345300	-2.20429500
H	-4.04564000	-1.53264500	-2.16369700
H	-2.34470400	-2.05413500	-2.11179000
C	-3.03794300	-1.21619300	-0.24733500
C	-1.58651900	-0.96395900	0.18604400
C	-0.97188500	-2.14072000	0.69349900
H	0.07169400	-2.17447700	0.97232400
C	-1.80290700	-3.20237000	0.86306700
C	-1.43759700	-4.54205000	1.40191300
H	-1.58156100	-5.32448200	0.64580800
H	-2.06172100	-4.80934500	2.26360400
H	-0.39046700	-4.55350500	1.71857800
C	-3.96058600	-0.10668800	1.87203700
H	-2.94195900	-0.02920100	2.26804700
H	-4.42643600	-1.01307700	2.26465500
H	-4.53266900	0.76181900	2.20979100
C	-3.92289200	-0.11099200	0.33258500
C	-3.38000100	1.24600700	-0.10445300
C	-4.43799900	2.19222300	-0.30422200
H	-4.26944800	3.26121100	-0.40133500
C	-5.67089600	1.64204900	-0.41152700
C	-6.96229900	2.34915700	-0.63331800
H	-7.65087900	2.18659600	0.20518000
H	-7.46449300	1.98371300	-1.53786900
H	-6.79588300	3.42481100	-0.74230200
C	6.11398100	-1.79391000	-0.21185300
H	6.56392700	-1.09048600	-0.92095800
H	6.46187100	-2.80398900	-0.43850400
H	6.46036100	-1.51134000	0.78844800
C	4.61565700	-1.66750800	-0.27071800
C	3.84017300	-2.79224100	-0.58994000
H	4.36912400	-3.71432100	-0.80092300
C	2.44663700	-2.82675700	-0.68549300
C	1.76226200	-4.09737100	-1.10992100
H	0.96660700	-4.34099700	-0.39862000
H	2.45278400	-4.93929200	-1.19146000
H	1.28014900	-3.93487100	-2.08056400
N	2.61276000	1.96565800	0.27025500
O	4.16953300	-0.50298900	-0.02391500
O	1.63076500	-1.86798100	-0.45930200
S	-1.22673300	2.97090400	-0.28383700
S	-3.46541000	-2.89511900	0.39974700
S	-5.67224600	-0.12039300	-0.27829700
Pt	2.13557400	0.02903400	0.02046500



1-<sup>3</sup>Eso

C	-3.46062710	2.54891059	-0.55208482
H	-4.29615210	1.85786759	-0.62636582
C	-3.63680410	3.92595259	-0.57665182
H	-4.63040210	4.34991959	-0.67165882
C	-2.50220310	4.73189759	-0.47369582
H	-2.59550610	5.81436459	-0.48992882
C	-1.25079510	4.14912359	-0.35450282
H	-0.35576110	4.75873359	-0.27740082
C	-1.14235110	2.75121559	-0.33868582
C	0.07700590	1.98920559	-0.24206982
C	0.06134390	0.60669859	-0.25642682
C	1.37937090	0.06248959	-0.12635882
C	2.35910090	1.04292559	-0.04678182
C	3.05430590	-1.47430941	2.09784618
H	4.12473590	-1.31596541	1.91653018
H	2.95329390	-2.13739041	2.96412818
H	2.61868890	-0.50509041	2.35784618
C	2.36161590	-2.03528541	0.90041118
C	1.62884890	-1.38871541	-0.06705382
C	1.08151590	-2.29833741	-1.03300682
H	0.47591090	-1.96967641	-1.87237782
C	1.40334390	-3.60579741	-0.81891682
C	1.01972190	-4.80034341	-1.62858982
H	0.44976690	-5.52939641	-1.04018582
H	1.89524890	-5.31990441	-2.03698182
H	0.39307990	-4.48656541	-2.46891982
C	4.16850390	-0.70957641	-1.95092282
H	4.07236790	-1.75857141	-1.64528382
H	4.88671590	-0.65992941	-2.77624682
H	3.19161190	-0.38901641	-2.32436482
C	4.58816990	0.16116459	-0.81507682
C	3.81647090	0.93387059	0.02456318
C	4.60703190	1.67523859	0.96606018
H	4.17196090	2.33423359	1.71162818
C	5.94831490	1.46024659	0.85947418
C	7.05393190	2.05012659	1.67056318
H	7.74263690	2.63868059	1.05275018
H	7.64546790	1.28054459	2.18043618
H	6.63748290	2.71381459	2.43452918
C	-5.75913910	-2.06146341	-0.48222782
H	-6.11411010	-1.48375141	-1.34140382
H	-6.56234610	-2.16072241	0.25158218
H	-5.49481010	-3.05905141	-0.85205282
C	-4.52477810	-1.40913141	0.09002518
C	-4.45085910	-1.22050641	1.47827518
H	-5.31477410	-1.52907741	2.05558018
C	-3.36093010	-0.71794641	2.20729918
C	-3.47540510	-0.64532241	3.71276518
H	-2.72742310	-1.30768141	4.16218418
H	-4.46685310	-0.92968641	4.07280518
H	-3.24523810	0.37229859	4.04413118
N	-2.25888910	1.99171359	-0.43440182
O	-3.64544210	-1.10006641	-0.77208282
O	-2.24638910	-0.31122141	1.75993918
S	1.67427390	2.64108759	-0.09528182
S	2.38784790	-3.74461641	0.60266618
S	6.26550890	0.33486659	-0.42177982
Pt	-1.75600810	-0.20989441	-0.38084182

1-<sup>3</sup>ESc

C	3.97560800	2.31522400	0.29219500
H	4.70833800	1.51535900	0.28222800
C	4.32618100	3.65225100	0.37792400
H	5.37137100	3.93047300	0.45100500
C	3.31014200	4.61328700	0.36308100
C	3.55293200	5.67010600	0.42550500
H	1.99049500	4.21106500	0.26922000
H	1.18210800	4.93525900	0.25756500
C	1.68769800	2.84385600	0.19212700
C	0.40518600	2.23255100	0.11898000
C	0.32749200	0.83367000	0.11258100
C	-1.02166400	0.40489200	0.13564800
C	-1.93918500	1.48626700	0.08789500
C	-3.00043900	-0.98004100	-1.87900700
H	-2.72429600	0.04110300	-2.16187300
H	-3.99424100	-1.19494200	-2.28297700
H	-2.27871200	-1.67130400	-2.32223900
C	-2.97889300	-1.12465500	-0.35502300
C	-1.58096600	-0.93370100	0.20593800
C	-1.09802400	-2.02671300	0.90670400
H	-0.13181700	-2.01974600	1.39818300
C	-1.93802000	-3.12904800	0.95997100
C	-1.68997400	-4.42877300	1.63941700
H	-1.67789500	-5.26597900	0.92763400
H	-2.46601600	-4.65350100	2.38320900
H	-0.72390600	-4.40681900	2.15394700
C	-3.92165500	-0.23891000	1.87610200
H	-2.90566900	-0.20453900	2.28191400
H	-4.37917300	-1.19545700	2.14424500
H	-4.50498000	0.57120500	2.32255100
C	-3.88073600	-0.06127200	0.35251800
C	-3.33424400	1.31689500	0.02845300
C	-4.32776600	2.24002000	-0.33515900
H	-4.12549600	3.29250900	-0.51556200
C	-5.57802800	1.70294900	-0.52751100
C	-6.80869800	2.42191300	-0.95602100
H	-7.59676000	2.35407300	-0.19524800
H	-7.21733000	1.99624100	-1.88135500
H	-6.59122800	3.47959300	-1.13116100
C	5.96330900	-2.07703800	-0.40889700
H	6.40692100	-1.43821100	-1.18043700
H	6.22987400	-3.11732100	-0.60763800
H	6.39566100	-1.77265900	0.55074000
C	4.47508900	-1.85261400	-0.37476800
C	3.61071700	-2.93764800	-0.58586100
H	4.06789900	-3.90139900	-0.77789500
C	2.21279700	-2.89181000	-0.58838400
C	1.42914000	-4.14341800	-0.87623200
H	0.71094000	-4.31641200	-0.06821400
H	2.06726300	-5.02157700	-0.99474000
H	0.84421900	-3.99658400	-1.79093600
N	2.69918300	1.91985600	0.20221600
O	4.12376100	-0.65097500	-0.15359200
O	1.47066000	-1.87403700	-0.37364300
S	-1.13648700	3.02906700	0.07015400
S	-3.43562100	-2.85902800	0.08523400
S	-5.63227700	-0.02602600	-0.25049500
Pt	2.12445000	0.00195100	-0.01968800

**1-<sup>3</sup>MC**

C	-3.65657600	2.36304200	-0.60387800
H	-4.46230100	1.63502500	-0.64215800
C	-3.89539900	3.73108100	-0.61894800
H	-4.91060800	4.10874700	-0.67165000
C	-2.79572800	4.58834100	-0.56277100
H	-2.93912900	5.66509300	-0.57485300
C	-1.51457000	4.06303800	-0.48978900
H	-0.64645200	4.71353500	-0.44386100
C	-1.34366800	2.67267500	-0.47199000
C	-0.08977600	1.96264700	-0.38584600
C	-0.05441300	0.58081700	-0.35081200
C	1.28128900	0.09084000	-0.20453100
C	2.22723100	1.10504200	-0.16385400
C	3.05065800	-1.27231900	2.04344700
H	4.10495700	-1.07201700	1.81380600
H	3.01033600	-1.89463600	2.94375500
H	2.57852400	-0.31130500	2.26835400
C	2.34690900	-1.92017400	0.89803800
C	1.57402000	-1.34496600	-0.08223900
C	1.03911700	-2.31397600	-0.99615300
H	0.41125500	-2.04274700	-1.83954400
C	1.40924600	-3.59887500	-0.72942900
C	1.04909500	-4.84285600	-1.47204600
H	0.51101600	-5.55611100	-0.83639000
H	1.93417300	-5.35617600	-1.86658900
H	0.40074900	-4.59052000	-2.31667600
C	4.06702800	-0.73644900	-1.93635800
H	3.96530800	-1.76539800	-1.56995400
H	4.79545300	-0.73539700	-2.75410800
H	3.09430000	-0.43819400	-2.33803100
C	4.46956200	0.19850500	-0.84652000
C	3.68356100	1.02433300	-0.07345900
C	4.45320500	1.80765800	0.85118700
H	4.00360100	2.50849900	1.54823200
C	5.79393000	1.56959100	0.80124000
C	6.87849000	2.18290800	1.62348400
H	7.61231700	2.71043500	1.00273900
H	7.42155000	1.43159700	2.20881600
H	6.44575000	2.90561500	2.32169300
C	-5.88961200	-2.06978300	-0.43206600
H	-6.21786000	-1.54181100	-1.33358300
H	-6.70481400	-2.09070200	0.29472700
H	-5.65350900	-3.09760800	-0.73023600
C	-4.64078800	-1.41552700	0.10437700
C	-4.60996400	-1.02966700	1.45315600
H	-5.51273700	-1.20503500	2.02700200
C	-3.51690200	-0.50096900	2.16028000
C	-3.67968700	-0.22775200	3.63692000
H	-2.96146100	-0.83822400	4.19481800
H	-4.68831600	-0.44171900	3.99794200
H	-3.43605000	0.82076200	3.83765400
N	-2.42648100	1.86223500	-0.53497400
O	-3.70836500	-1.28497600	-0.74908900
O	-2.36325500	-0.22154900	1.71255700
S	1.48626100	2.67609500	-0.26948600
S	2.42763800	-3.64018800	0.67677700
S	6.13705400	0.37158000	-0.40806000
Pt	-1.83628900	-0.32087400	-0.42822000

**1-<sup>3</sup>MECP<sub>1</sub>**

C	-3.46062710	2.54891059	-0.55208482
H	-4.29615210	1.85786759	-0.62636582
C	-3.63680410	3.92595259	-0.57665182
H	-4.63040210	4.34991959	-0.67165882
C	-2.50220310	4.73189759	-0.47369582
H	-2.59550610	5.81436459	-0.48992882
C	-1.25079510	4.14912359	-0.35450282
H	-0.35576110	4.75873359	-0.27740082
C	-1.14235110	2.75121559	-0.33868582
C	0.07700590	1.98920559	-0.24206982
C	0.06134390	0.60669859	-0.25642682
C	1.37937090	0.06248959	-0.12635882
C	2.35910090	1.04292559	-0.04678182
C	3.05430590	-1.47430941	2.09784618
H	4.12473590	-1.31596541	1.91653018
H	2.95329390	-2.13739041	-2.96412818
H	2.61868890	-0.50509041	2.35784618
C	2.36161590	-2.03528541	0.90041118
C	1.62884890	-1.38871541	-0.06705382
C	1.08151590	-2.29833741	-1.03300682
H	0.47591090	-1.96967641	-1.87237782
C	1.40334390	-3.60579741	-0.81891682
C	1.01972190	-4.80034341	-1.62858982
H	0.44976690	-5.52939641	-1.04018582
H	1.89524890	-5.31990441	-2.03698182
H	0.39307990	-4.48656541	-2.46891982
C	4.16850390	-0.70957641	-1.95092282
H	4.07236790	-1.75857141	-1.64528382
H	4.88671590	-0.65992941	-2.77624682
H	3.19161190	-0.38901641	-2.32436482
C	4.58816990	0.16116459	-0.81507682
C	3.81647090	0.93387059	0.02456318
C	4.60703190	1.67523859	0.96606018
H	4.17196090	2.33423359	1.71162818
C	5.94831490	1.46024659	0.85947418
C	7.05393190	2.05012659	1.67056318
H	7.74263690	2.63868059	1.05275018
H	7.64546790	1.28054459	2.18043618
H	6.63748290	2.71381459	2.43452918
C	-5.75913910	-2.06146341	-0.48222782
H	-6.11411010	-1.48375141	-1.34140382
H	-6.56234610	-2.16072241	0.25158218
H	-5.49481010	-3.05905141	-0.85205282
C	-4.52477810	-1.40913141	0.09002518
C	-4.45085910	-1.22050641	1.47827518
H	-5.31477410	-1.52907741	2.05558018
C	-3.36093010	-0.71794641	2.20729918
C	-3.47540510	-0.64532241	3.71276518
H	-2.72742310	-1.30768141	4.16218418
H	-4.46685310	-0.92968641	4.07280518
H	-3.24523810	0.37229859	4.04413118
N	-2.25888910	1.99171359	-0.43440182
O	-3.64544210	-1.10006641	-0.77208282
O	-2.24638910	-0.31122141	1.75993918
S	1.67427390	2.64108759	-0.09528182
S	2.38784790	-3.74461641	0.60266618
S	6.26550890	0.33486659	-0.42177982
Pt	-1.75600810	-0.20989441	-0.38084182

1-TS<sub>1</sub>

C	3.45553700	-3.11908300	0.09320100
H	4.34558700	-2.49790300	0.14817200
C	3.51888800	-4.50544900	0.03233100
H	4.47820000	-5.01124400	0.04366400
C	2.31796400	-5.21269900	-0.03142300
H	2.32292100	-6.29793800	-0.07949300
C	1.11208600	-4.52597400	-0.04526100
H	0.16829700	-5.05793100	-0.11785700
C	1.11942800	-3.12736500	0.01605100
C	-0.03915600	-2.26242900	-0.03585700
C	0.09131900	-0.89162400	-0.15240500
C	-1.18058000	-0.23707000	-0.16137600
C	-2.24481900	-1.12264200	-0.08648500
C	-2.84157600	1.53989500	1.85524900
H	-3.90279700	1.45948900	1.58798400
H	-2.75470800	2.22847700	2.70237200
H	-2.51197700	0.54926400	2.18265800
C	-2.01202400	1.98629300	0.69832400
C	-1.29397700	1.22920300	-0.19477200
C	-0.59461600	2.03306200	-1.15556900
H	0.02475600	1.60719000	-1.93942700
C	-0.78176300	3.37453100	-1.00590500
C	-0.20561000	4.48982300	-1.81393100
H	0.43198200	5.14479100	-1.20749900
H	-0.98358800	5.11577200	-2.26694500
H	0.40914600	4.07826100	-2.62026300
C	-3.72733600	0.73883100	-2.14637700
H	-3.50700400	1.77679000	-1.86763400
H	-4.40360500	0.75134900	-3.00765800
H	-2.78267400	0.28025100	-2.45276100
C	-4.30974200	-0.02627900	-1.00635800
C	-3.68188000	-0.85955600	-0.10662800
C	-4.59799200	-1.44761400	0.82914100
H	-4.28293000	-2.12455400	1.61762800
C	-5.89233000	-1.05592000	0.66207800
C	-7.09275800	-1.44884800	1.45779500
H	-7.85386300	-1.93411400	0.83544200
H	-7.56398000	-0.58436400	1.94015600
H	-6.79909700	-2.15343800	2.24160200
C	6.00524900	1.62814400	-0.38893400
H	6.57873600	0.77366400	-0.01298600
H	6.44688800	2.55077800	-0.00575300
H	6.08750200	1.61518000	-1.48126500
C	4.55827000	1.46128900	0.00320700
C	3.94996300	2.46524900	0.77421700
H	4.55643500	3.33242600	1.00959500
C	2.63495300	2.47151200	1.26249500
C	2.13350900	3.68720700	2.00257500
H	1.21238800	4.03333300	1.52046300
H	2.86401600	4.49928300	2.02789600
H	1.87058100	3.40419100	3.02769900
N	2.29747900	-2.46393300	0.09704000
O	4.01390200	0.39958100	-0.43306900
O	1.76689500	1.54832700	1.15732000
S	-1.69647300	-2.77211700	0.02752900
S	-1.83219400	3.67682400	0.34498400
S	-6.00856800	0.04816700	-0.67324100
Pt	1.96679200	-0.18840600	-0.17461200

1-TS<sub>2</sub>

C	3.87773700	2.41632800	0.27859100
H	4.63442500	1.63883100	0.27426900
C	4.18893700	3.76434700	0.35529200
H	5.22550700	4.07362100	0.42612900
C	3.14420100	4.69580400	0.33431900
H	3.35641000	5.75967400	0.38870700
C	1.83763200	4.25478800	0.24463400
H	1.00785900	4.95429200	0.22873900
C	1.57364500	2.87692900	0.17709000
C	0.31140500	2.23311600	0.11127100
C	0.27623800	0.82986300	0.10555700
C	-1.04855200	0.35370300	0.10078100
C	-2.02623200	1.41141500	0.11081500
C	-3.09186600	-0.90379800	-1.99292800
H	-4.17693100	-1.00129500	-2.10667000
H	-2.61007200	-1.44961800	-2.81310000
H	-2.82816500	0.15107800	-2.08977200
C	-2.62225100	-1.44126000	-0.67607900
C	-1.49609700	-1.02498400	0.06438700
C	-1.01546400	-2.04308300	0.93824100
H	-0.18645500	-1.87950800	1.61745300
C	-1.72236300	-3.20831400	0.89075500
C	-1.54378500	-4.43232800	1.72291100
H	-1.37510300	-5.32479200	1.10729900
H	-2.42340200	-4.63059600	2.34805500
H	-0.68041400	-4.30777300	2.38374600
C	-3.76138000	-0.52040900	2.00809400
H	-3.97965400	-1.59401400	2.06060400
H	-4.37074800	-0.01543600	2.77041700
H	-2.71034100	-0.37110500	2.26313500
C	-4.05345900	0.03513900	0.64887500
C	-3.41262200	1.26107100	0.15643700
C	-4.37047200	2.17318000	-0.38464100
H	-4.10213300	3.14589300	-0.78707900
C	-5.63055700	1.66851500	-0.49522900
C	-6.81871200	2.30883400	-1.12147100
H	-7.64451500	2.40520000	-0.40557400
H	-7.19075400	1.71407300	-1.96520200
H	-6.56477800	3.30734800	-1.48883300
C	5.98775100	-1.94035300	-0.34719300
H	6.42318800	-1.30824100	-1.12890200
H	6.28085700	-2.97806400	-0.52072600
H	6.40421500	-1.60475600	0.60904900
C	4.49418400	-1.75071600	-0.33080200
C	3.65822600	-2.85913800	-0.53319700
H	4.14045600	-3.81455400	-0.70484000
C	2.25907900	-2.84709700	-0.55507000
C	1.51019700	-4.12196200	-0.83241800
H	0.79427300	-4.30151500	-0.02399800
H	2.17172200	-4.98423200	-0.93895100
H	0.92350600	-4.00040500	-1.74963500
N	2.61487700	1.98192100	0.19227800
O	4.11296100	-0.55409900	-0.13246600
O	1.49050600	-1.84478000	-0.36634400
S	-1.25694600	2.99373100	0.05811400
S	-3.00225400	-3.10198400	-0.29368900
S	-5.74804800	0.03235000	0.14960400
Pt	2.09529000	0.04885100	-0.02062000

**1-<sup>3</sup>MECP<sub>2</sub>**

C	3.95632400	2.33222700	0.33146200
H	4.69674200	1.53968900	0.33660500
C	4.29042200	3.67371700	0.42016100
H	5.33090800	3.96363200	0.51301200
C	3.26546100	4.62256000	0.38231100
H	3.49488000	5.68228500	0.44569600
C	1.95173200	4.20442000	0.26442400
H	1.13631700	4.92009000	0.23503800
C	1.66736700	2.83428100	0.18661300
C	0.39106200	2.20680700	0.09667700
C	0.32090200	0.81102700	0.09970600
C	-1.03629400	0.37894400	0.11543900
C	-1.95230700	1.46369400	0.05501200
C	-3.05948900	-1.02794100	-1.86382100
H	-2.77775500	-0.01688000	-2.17606800
H	-4.06207400	-1.24194200	-2.24652400
H	-2.35391900	-1.73750300	-2.30440000
C	-3.01647500	-1.14109500	-0.33731300
C	-1.60442000	-0.95455700	0.19648200
C	-1.10939100	-2.06020300	0.87861100
H	-0.12785800	-2.06564600	1.33888300
C	-1.95842100	-3.15056400	0.96019000
C	-1.71272100	-4.44947000	1.64327500
H	-1.74965000	-5.29430000	0.94177700
H	-2.46348800	-4.64779500	2.41989200
H	-0.72699600	-4.44635300	2.11925900
C	-3.93793000	-0.21837200	1.88598000
H	-2.91941300	-0.19450100	2.28688200
H	-4.40818900	-1.16462700	2.16851600
H	-4.50684100	0.60488200	2.32722000
C	-3.90580000	-0.06083500	0.36028900
C	-3.35145200	1.30533700	0.00721000
C	-4.33920200	2.23272400	-0.36443800
H	-4.12870200	3.28031600	-0.56384800
C	-5.59679000	1.70526900	-0.53706000
C	-6.82540600	2.42599200	-0.96891400
H	-7.60941600	2.37799900	-0.20236800
H	-7.24437400	1.98922600	-1.88445400
H	-6.60124100	3.47892500	-1.16326900
C	6.02659600	-1.98783000	-0.38115000
H	6.47218600	-1.32134000	-1.12776900
H	6.31328800	-3.01770100	-0.60412200
H	6.44044600	-1.70461000	0.59314400
C	4.53354400	-1.79316000	-0.36441600
C	3.69629100	-2.89171600	-0.60672000
H	4.17776800	-3.84045700	-0.81357100
C	2.29755000	-2.88031200	-0.62286100
C	1.55842900	-4.14774900	-0.95870100
H	0.78848500	-4.33653400	-0.20409400
H	2.22315700	-5.01112700	-1.03021600
H	1.04012900	-4.01798600	-1.91571400
N	2.68646700	1.92380800	0.21838700
O	4.15114700	-0.60398500	-0.12766100
O	1.52633300	-1.88807600	-0.39002400
S	-1.14933400	3.00699200	0.02945200
S	-3.48328400	-2.86316100	0.13785600
S	-5.66049000	-0.01997600	-0.23021100
Pt	2.13759900	0.00142600	-0.01462800

## 2-1GSo

C	-3.71957300	-1.07536800	0.15201900
H	-4.25005000	-0.12941900	0.14308200
C	-4.36878000	-2.29553000	0.22729400
C	-3.60874200	-3.47063900	0.21928500
H	-4.09879500	-4.43765800	0.27952000
C	-2.23339900	-3.38522500	0.14319200
H	-1.61789600	-4.27859400	0.13928900
C	-1.62009500	-2.12656800	0.07659300
C	-0.22622300	-1.82880500	0.02656800
C	0.15963900	-0.49319800	0.01459200
C	1.58458800	-0.36569100	0.05443700
C	2.22729100	-1.59865400	0.05793800
C	3.84444800	0.63523200	-1.91533400
H	4.79088800	0.12169100	-1.70451500
H	4.01610400	1.34071900	-2.73563800
H	3.13032000	-0.11995600	-2.25629900
C	3.30718800	1.32089800	-0.70404800
C	2.30631900	0.91587600	0.14246500
C	2.07138600	1.85144400	1.20356700
H	1.30322300	1.70187000	1.95563700
C	2.89275300	2.93748300	1.18211500
C	2.93791600	4.08884600	2.13235400
H	2.76346100	5.04788400	1.62905200
H	3.90533000	4.16059300	2.64383100
H	2.16237000	3.96452300	2.89434600
C	4.34611600	-0.50736100	2.12876700
H	4.56734600	0.53788900	1.88156900
H	4.96826600	-0.79634900	2.98241800
H	3.29710200	-0.55355300	2.43411600
C	4.57115000	-1.40704400	0.96101900
C	3.65795800	-1.90763200	0.06068300
C	4.26002200	-2.77865600	-0.90868400
H	3.69524000	-3.25833900	-1.70236600
C	5.60767900	-2.92196300	-0.76547900
C	6.55086200	-3.72541400	-1.59816000
H	7.06501300	-4.49251100	-1.00720700
H	7.31970500	-3.09804900	-2.06422400
H	5.99776100	-4.22936100	-2.39639900
C	-4.59512900	3.69003600	-0.42854800
H	-5.17552400	3.21557100	-1.22750700
H	-4.59873100	4.77200400	-0.57687500
H	-5.09577700	3.45482300	0.51713100
C	-3.20708100	3.10932800	-0.41216800
C	-2.10350100	3.95515700	-0.59236500
H	-2.31095800	5.00774100	-0.74628300
C	-0.75773300	3.56962400	-0.62184100
C	0.30461500	4.59679300	-0.89550100
H	1.09105400	4.50421000	-0.14036500
H	-0.08792200	5.61577200	-0.90863500
H	0.77075300	4.37910900	-1.86327200
N	-2.38783100	-0.99313500	0.08032200
O	-3.16044500	1.84911200	-0.23602900
O	-0.28420600	2.39556700	-0.44974400
S	1.10825700	-2.92815700	0.03873300
S	3.96850900	2.83946000	-0.18136100
S	6.16025300	-1.98715900	0.58945600
C	-5.86193900	-2.36061800	0.27195200
Pt	-1.37821900	0.74109200	-0.11961200
F	-6.28258400	-3.25140000	1.18612200
F	-6.40756800	-1.17345200	0.57364600
F	-6.37584000	-2.74866600	-0.90890900

## 2-1GSc

C	-3.76358800	-1.03998100	0.24944400
H	-4.29243800	-0.10115100	0.36869000
C	-4.40905600	-2.26529700	0.24775100
C	-3.65480200	-3.42997500	0.05725600
H	-4.14270600	-4.39998900	0.05218700
C	-2.28971100	-3.33139900	-0.11447200
H	-1.67932300	-4.21638500	-0.25889200
C	-1.67808600	-2.06807000	-0.09179400
C	-0.29041600	-1.77181000	-0.18998200
C	0.11372500	-0.45786100	-0.03620600
C	1.55611800	-0.37036900	-0.00392300
C	2.18613000	-1.68373700	-0.21121100
C	3.95347300	0.69376800	-1.69590400
H	3.41620700	-0.13548000	-2.16615000
H	4.99203100	0.67785300	-2.03536500
H	3.49124100	1.63424600	-2.00820700
C	3.86450300	0.57519400	-0.16389800
C	2.38551100	0.71134200	0.22009800
C	2.09301100	1.98467200	0.77451700
H	1.08932900	2.28608500	1.03846400
C	3.17444300	2.77433400	1.01387400
C	3.16344300	4.13751800	1.61378500
H	3.54371800	4.88304700	0.90388800
H	3.80258500	4.18601700	2.50394700
H	2.14693100	4.41970400	1.90289200
C	4.36861700	-0.81764600	1.92853800
H	3.35351400	-0.62431800	2.29281200
H	5.05044500	-0.09041000	2.37458700
H	4.66570700	-1.82164000	2.24357400
C	4.39453600	-0.74924900	0.39009300
C	3.52243700	-1.89213200	-0.12233900
C	4.29366700	-3.08136400	-0.33623800
H	3.84761900	-4.06054500	-0.48713800
C	5.63232300	-2.88160300	-0.38430500
C	6.69312900	-3.90336000	-0.60204500
H	7.36479300	-3.96563700	0.26313200
H	7.31199300	-3.65371000	-1.47298400
H	6.24721000	-4.88844400	-0.76696300
C	-4.75209700	3.64121200	-0.29514400
H	-5.35719400	3.12375300	-1.04763100
H	-4.80255000	4.71762600	-0.47183700
H	-5.19142500	3.41599300	0.68281900
C	-3.34594700	3.10962700	-0.33944600
C	-2.28159400	3.98528500	-0.60087500
H	-2.52911100	5.02529500	-0.77851700
C	-0.93170900	3.63461600	-0.68455500
C	0.08549000	4.67792700	-1.05727700
H	0.94071700	4.61606200	-0.37708500
H	-0.32685300	5.68899500	-1.04383100
H	0.46318800	4.46275300	-2.06365800
N	-2.44199600	-0.94618400	0.08758700
O	-3.24406100	1.85801400	-0.13619300
O	-0.41770100	2.47854200	-0.49186500
S	0.98785000	-2.95840600	-0.43575000
S	4.70487900	2.05158900	0.56725200
S	6.10345900	-1.19196200	-0.16955800
Pt	-1.44195500	0.78753900	-0.08250100
C	-5.89372300	-2.34170600	0.39897900
F	-6.41202800	-1.19190800	0.85606300
F	-6.49880300	-2.61475200	-0.77138700
F	-6.24728000	-3.31957300	1.25068300

2-<sup>3</sup>ESo

C	-3.69670600	-1.10624800	0.15492600
H	-4.24436800	-0.16891500	0.16041300
C	-4.32705400	-2.33884200	0.24049200
C	-3.55445500	-3.52527900	0.21361100
H	-4.04311200	-4.49161600	0.28474200
C	-2.19368900	-3.43069400	0.09890300
H	-1.56725300	-4.31624200	0.07781200
C	-1.58426500	-2.15087000	0.01935900
C	-0.22555400	-1.85654100	-0.08309200
C	0.18440600	-0.44020600	-0.05488700
C	1.55849400	-0.32111000	0.03658100
C	2.24832200	-1.56870100	0.00603000
C	3.84740400	0.67707300	-1.89346000
H	4.80643900	0.19434800	-1.66961900
H	4.00443300	1.38079800	-2.71618200
H	3.15375600	-0.09715600	-2.23199300
C	3.28583000	1.36863100	-0.68904400
C	2.27985900	0.96567800	0.14576600
C	2.02319000	1.90809000	1.20083500
H	1.24862600	1.75631000	1.94627300
C	2.83706000	2.99529800	1.17801000
C	2.86739200	4.15935500	2.12073200
H	2.69883600	5.10935100	1.60218300
H	3.82807200	4.23371900	2.64063700
H	2.08217100	4.03914700	2.87144200
C	4.39010200	-0.30643900	2.00832100
H	4.62472700	0.71406700	1.68387000
H	5.02635400	-0.54785700	2.86503800
H	3.34789700	-0.31740800	2.33605700
C	4.58583800	-1.30327600	0.90995600
C	3.64672200	-1.89365700	0.07714000
C	4.23336500	-2.92274800	-0.75412600
H	3.66330400	-3.49340800	-1.48095000
C	5.57103600	-3.07031400	-0.59086300
C	6.50203000	-3.99912000	-1.30572300
H	6.97966600	-4.69850200	-0.61228700
H	7.29376600	-3.45246400	-1.82706100
H	5.94373600	-4.57899900	-2.04463900
C	-4.62253100	3.72444700	-0.34340400
H	-5.22194700	3.25988400	-1.13195200
H	-4.61864000	4.80630400	-0.48120500
H	-5.09705200	3.48279700	0.61253200
C	-3.23384100	3.13090700	-0.36751200
C	-2.13459200	3.98831300	-0.54251700
H	-2.35135300	5.04250800	-0.65642100
C	-0.78482000	3.61608900	-0.61779300
C	0.25615700	4.67837600	-0.87236800
H	1.04564300	4.57868700	-0.12149600
H	-0.15975200	5.68655700	-0.85145500
H	0.71743300	4.49650800	-1.84838000
N	-2.37439200	-1.00362400	0.05153400
O	-3.18969500	1.87116100	-0.22732400
O	-0.29228200	2.44844700	-0.50509500
S	1.10593200	-2.94889400	-0.20807600
S	3.92805500	2.90005500	-0.17488800
S	6.15657700	-1.96904100	0.62509500
C	-5.81055000	-2.43332000	0.36783300
Pt	-1.36435000	0.74062700	-0.16514700
F	-6.16968300	-3.03201600	1.51686000
F	-6.39927700	-1.23095500	0.33971900
F	-6.34320200	-3.17059800	-0.62142400

2-<sup>3</sup>ESc

C	-3.81980500	-0.95758400	0.16884100
H	-4.31775700	0.00564900	0.17872100
C	-4.51319600	-2.15440300	0.21920700
C	-3.79358900	-3.35876300	0.18328800
H	-4.31905900	-4.30804800	0.22367100
C	-2.41930700	-3.32215200	0.10588100
H	-1.83724900	-4.23750500	0.08127200
C	-1.75616200	-2.08226800	0.06565100
C	-0.36242000	-1.83695200	0.01783900
C	0.08646800	-0.50579100	0.05000100
C	1.49674500	-0.45355800	0.10907100
C	2.09543100	-1.74156600	0.04390200
C	3.82438200	0.41259700	-1.82454500
H	3.29216300	-0.48712000	-2.15108300
H	4.85005200	0.36452500	-2.20222500
H	3.32702900	1.28576200	-2.25501200
C	3.80122300	0.51267300	-0.29656900
C	2.38801600	0.68476200	0.23107900
C	2.19079000	1.85068000	0.95369400
H	1.24314000	2.08997900	1.42298200
C	3.29151500	2.68677900	1.06044400
C	3.37820200	3.98814700	1.77549900
H	3.61194900	4.81504000	1.09066900
H	4.16304700	3.97777500	2.54342100
H	2.42613700	4.21272900	2.26685300
C	4.41565400	-0.65383200	1.91962900
H	3.41652000	-0.42933300	2.30623200
H	5.10200800	0.14033300	2.22639800
H	4.75260100	-1.60108100	2.34982100
C	4.36857900	-0.77131300	0.38988300
C	3.48405000	-1.94567800	0.01379900
C	4.20684500	-3.09161700	-0.35785300
H	3.73887800	-4.04835900	-0.57349400
C	5.55829400	-2.89861000	-0.51228400
C	6.56428800	-3.90735200	-0.94284500
H	7.32528100	-4.06671600	-0.16857900
H	7.09007400	-3.58187000	-1.84923700
H	6.07968100	-4.86550800	-1.15110900
C	-4.56506700	3.79683100	-0.46494400
H	-5.14485800	3.32065600	-1.26327800
H	-4.54474000	4.87599300	-0.63106600
H	-5.08197600	3.58721300	0.47796700
C	-3.18959000	3.18852600	-0.42178200
C	-2.06619300	4.01005600	-0.60223700
H	-2.25035200	5.06402200	-0.77487800
C	-0.73027600	3.59656700	-0.60034300
C	0.36012300	4.60144700	-0.85349800
H	1.08247400	4.56691200	-0.03127700
H	-0.02192200	5.61832400	-0.96400000
H	0.90359600	4.31874500	-1.76180500
N	-2.48704500	-0.91938000	0.09546100
O	-3.16970900	1.93223700	-0.22383200
O	-0.28498900	2.41376000	-0.40715200
S	0.91318800	-3.01501900	-0.03130400
S	4.68977000	2.04919000	0.21232600
S	6.06182500	-1.25575300	-0.18213800
Pt	-1.41863400	0.77748100	-0.08516600
C	-6.00538100	-2.16820500	0.26477400
F	-6.51176900	-0.96320900	0.56733800
F	-6.53675500	-2.53898100	-0.91533100
F	-6.45821400	-3.04505500	1.17865500

**2-<sup>3</sup>MC**

C	3.56032100	-1.08071700	-0.39812900
H	4.15234100	-0.17179700	-0.44545300
C	4.14394700	-2.33960500	-0.33992900
C	3.30592600	-3.45767500	-0.28978900
H	3.73373200	-4.45502200	-0.25667900
C	1.93476600	-3.28463800	-0.29129700
H	1.26844400	-4.14056400	-0.25603000
C	1.40408500	-1.98530700	-0.33719300
C	0.01241100	-1.62413000	-0.31879500
C	-0.38048700	-0.29468200	-0.34041200
C	-1.79818500	-0.16477500	-0.22618300
C	-2.44967200	-1.38924200	-0.15789500
C	-3.86381100	0.74397700	1.99279100
H	-4.83277100	0.27570700	1.77892200
H	-3.98062400	1.37761300	2.87836800
H	-3.16003800	-0.05778700	2.23551600
C	-3.35471300	1.52345100	0.82653200
C	-2.45591700	1.14762600	-0.14336800
C	-2.18974300	2.20059500	-1.08117300
H	-1.51063100	2.08358400	-1.92050200
C	-2.88405800	3.34980700	-0.84331800
C	-2.86050800	4.62621500	-1.61715200
H	-2.53123300	5.47093500	-1.00055800
H	-3.84794500	4.87879500	-2.02158700
H	-2.16553800	4.53216900	-2.45705500
C	-4.67968000	-0.12813400	-1.99206800
H	-4.83568300	0.90183100	-1.64822100
H	-5.38436500	-0.32743700	-2.80615600
H	-3.66327600	-0.18513000	-2.39239500
C	-4.84046200	-1.10873300	-0.87975800
C	-3.87806100	-1.68417700	-0.07918400
C	-4.43066800	-2.61601500	0.86279500
H	-3.82441000	-3.15767000	1.58260400
C	-5.78670700	-2.73304600	0.79856600
C	-6.68769100	-3.58292400	1.63181100
H	-7.25061300	-4.29972200	1.02244800
H	-7.41522900	-2.98137800	2.18920000
H	-6.09353000	-4.14907100	2.35536000
C	4.71813700	3.57619600	-0.34232300
H	5.19820100	3.08214300	-1.19364300
H	5.46874400	3.79874300	0.41928800
H	4.29791000	4.51800900	-0.71305500
C	3.59769500	2.70869400	0.17325800
C	3.56917200	2.38795800	1.53951900
H	4.38440500	2.77241400	2.14150700
C	2.57094600	1.67926400	2.22847800
C	2.70340500	1.52166400	3.72453100
H	1.85474500	2.01378400	4.21194700
H	3.63293400	1.94403600	4.11273700
H	2.65089000	0.45850400	3.98106800
N	2.24414100	-0.92269200	-0.39835900
O	2.76074400	2.34980400	-0.71356500
O	1.52466200	1.14246700	1.74952000
S	-1.32809100	-2.71801900	-0.19531100
S	-3.88156700	3.15648700	0.56499800
S	-6.41108000	-1.69639700	-0.44702800
Pt	1.11354600	1.02693600	-0.41341400
C	5.62997100	-2.48935900	-0.27632200
F	6.25986800	-1.42653300	-0.80040100
F	6.04097300	-3.58169200	-0.94107500
F	6.06294000	-2.61953600	0.99070400

**2-<sup>3</sup>MECP<sub>1</sub>**

C	3.44111001	-1.18455156	-0.38099486
H	4.04984201	-0.29156256	-0.48554886
C	4.00478601	-2.45240056	-0.31653186
C	3.14730901	-3.55014056	-0.19323086
H	3.55738901	-4.55478356	-0.15295886
C	1.78203401	-3.34846956	-0.13675686
H	1.10022301	-4.18801756	-0.04397186
C	1.27271501	-2.04089856	-0.20155286
C	-0.11085699	-1.65847556	-0.16116186
C	-0.48503399	-0.32683756	-0.23284186
C	-1.90315999	-0.17326656	-0.14531086
C	-2.57041599	-1.38660056	-0.03462086
C	-3.93559899	0.91845744	2.02796214
H	-4.91528599	0.45315844	1.86181214
H	-4.03102699	1.61524144	2.86759914
H	-3.24007899	0.12604544	2.32074614
C	-3.42928699	1.60712144	0.80469514
C	-2.54625999	1.15151244	-0.14545086
C	-2.26369099	2.14010044	-1.14617586
H	-1.58903099	1.95832244	-1.97737286
C	-2.92810299	3.31839944	-0.97302986
C	-2.87885899	4.54833844	-1.81829786
H	-2.52319099	5.41817344	-1.25341886
H	-3.86304099	4.80429444	-2.22839286
H	-2.19429999	4.39267744	-2.65778186
C	-4.75783399	-0.28860656	-2.03038786
H	-4.94905799	0.75985844	-1.77125286
H	-5.42658599	-0.56269156	-2.85321286
H	-3.72701999	-0.35088756	-2.39111086
C	-4.94165899	-1.19171756	-0.85713386
C	-4.00190499	-1.68431556	0.02188814
C	-4.57288399	-2.57645856	0.99086814
H	-3.98474699	-3.05566456	1.76805814
C	-5.91919399	-2.74609456	0.86744914
C	-6.83458499	-3.58435856	1.69759414
H	-7.30201599	-4.38341456	1.10938614
H	-7.63972699	-2.99088456	2.14627014
H	-6.27097499	-4.05362356	2.50936314
C	4.41978101	3.78490644	-0.32980286
H	4.90178801	3.34384644	-1.20792286
H	5.17674401	4.04489044	0.41386514
H	3.92410001	4.70488744	-0.66228486
C	3.37814901	2.83463544	0.20611414
C	3.33719001	2.59349744	1.58834414
H	4.09720001	3.08259644	2.18715014
C	2.38740901	1.83307244	2.28920514
C	2.49560701	1.75951444	3.79448214
H	1.61247301	2.22921744	4.24127014
H	3.39326701	2.25206944	4.17541114
H	2.49419801	0.71032944	4.10627614
N	2.12962001	-0.99689856	-0.32375586
O	2.60918701	2.34357044	-0.67739886
O	1.40503301	1.18301844	1.81654314
S	-1.46451499	-2.72887056	-0.00638386
S	-3.91798699	3.23258344	0.44900514
S	-6.51174399	-1.80722256	-0.46548086
Pt	1.02626301	0.97052044	-0.33654986
C	5.48994401	-2.63148256	-0.31784486
F	6.11321201	-1.60158156	-0.90921986
F	5.84532601	-3.75480756	-0.96174486
F	5.98047301	-2.72602256	0.93054614

**2-TS<sub>1</sub>**

C	3.82691400	-1.26674400	0.08171400
H	4.41859100	-0.35907000	0.15947900
C	4.41425100	-2.51977800	-0.05875700
C	3.57974700	-3.63481000	-0.15913900
H	4.00753400	-4.62558700	-0.27885100
C	2.20650600	-3.46365200	-0.13036000
H	1.54118500	-4.31429400	-0.23983400
C	1.67896700	-2.17247500	0.01228000
C	0.27507600	-1.82670100	-0.00437500
C	-0.16030800	-0.51227200	-0.08895100
C	-1.58948400	-0.43195000	-0.11889500
C	-2.20300800	-1.67389300	-0.07492000
C	-3.87447100	0.51251600	1.85594900
H	-4.81122500	0.01303900	1.57849600
H	-4.08116100	1.17867000	2.70025800
H	-3.17901000	-0.26206800	2.19261600
C	-3.28177100	1.25409400	0.70486100
C	-2.29296800	0.85905600	-0.16276000
C	-1.97641300	1.86887100	-1.13042700
H	-1.21277500	1.73487600	-1.89066000
C	-2.71730800	3.00625200	-1.01446900
C	-2.65095400	4.24724700	-1.84198100
H	-2.37804000	5.12466100	-1.24279200
H	-3.60731500	4.46842100	-2.33060500
H	-1.89280400	4.12682500	-2.62180400
C	-4.30916800	-0.56290500	-2.13720000
H	-4.53573500	0.47107600	-1.84945900
H	-4.92818600	-0.82096900	-3.00283900
H	-3.25892400	-0.59053000	-2.44145400
C	-4.53164900	-1.50935100	-1.00615100
C	-3.62237500	-2.02006100	-0.10593600
C	-4.22136800	-2.93778300	0.82127100
H	-3.66090700	-3.43174700	1.60932500
C	-5.56213400	-3.10769000	0.64714800
C	-6.50109800	-3.96234200	1.43218000
H	-6.98554600	-4.71902100	0.80388800
H	-7.29329900	-3.37016400	1.90501800
H	-5.95137500	-4.48216600	2.22251200
C	4.34012700	4.07806200	-0.36004200
H	5.15293300	3.55452000	0.15513600
H	4.37917700	5.13922500	-0.10416000
H	4.51197800	3.95969700	-1.43550600
C	3.02754300	3.43364700	0.00712500
C	2.02613400	4.22281000	0.59727000
H	2.24645700	5.27509200	0.73627300
C	0.77101500	3.77658700	1.03104000
C	-0.20694800	4.76798300	1.60885400
H	-1.17028700	4.64572700	1.10254100
H	0.13361200	5.80196900	1.51483200
H	-0.37117100	4.53779300	2.66751400
N	2.51147900	-1.11161100	0.12988400
O	2.94787600	2.19753500	-0.27133100
O	0.33376900	2.58163500	1.00147600
S	-1.03441200	-2.96225000	0.01977800
S	-3.82548800	2.85627000	0.31595500
S	-6.11280000	-2.13931100	-0.68493500
Pt	1.25620100	0.89472300	-0.05410400
C	5.90143400	-2.67751900	-0.04531800
F	6.52582700	-1.53780700	-0.37790100
F	6.29875400	-3.63097500	-0.90433300
F	6.35259200	-3.03732800	1.16968000

**2-TS<sub>2</sub>**

C	-3.78851100	-0.98207600	0.15253200
H	-4.29585400	-0.02367700	0.15555800
C	-4.47250000	-2.18525800	0.19867000
C	-3.74139600	-3.38488900	0.17322900
H	-4.25955500	-4.33839300	0.20958200
C	-2.36774400	-3.33646100	0.11104800
H	-1.77679800	-4.24632900	0.09554200
C	-1.71315500	-2.08985200	0.07440900
C	-0.32358400	-1.83755200	0.04048700
C	0.11380500	-0.50107300	0.06538700
C	1.51900700	-0.42995800	0.09193100
C	2.14869000	-1.72348000	0.09164100
C	3.88396400	0.21654400	-1.94185300
H	4.95195600	0.00046800	-2.05288300
H	3.58834600	0.90705700	-2.74064000
H	3.32613800	-0.71211200	-2.07622100
C	3.57938900	0.82365100	-0.60589900
C	2.34737600	0.75847000	0.09178700
C	2.16028600	1.86429500	0.96619300
H	1.29763300	1.94867300	1.61716100
C	3.18314200	2.76825300	0.96163700
C	3.34359900	3.98485000	1.80719400
H	3.46939100	4.88988200	1.19975600
H	4.21944500	3.91023600	2.46379100
H	2.45855400	4.11848200	2.43669400
C	4.31486200	-0.40777600	2.05931000
H	4.83299100	0.55457400	2.14899300
H	4.73455500	-1.08822300	2.81238100
H	3.25984000	-0.25369400	2.29449700
C	4.46739600	-0.98790100	0.68634300
C	3.52410100	-1.97077200	0.14945500
C	4.19618400	-3.08924500	-0.42793500
H	3.67390600	-3.92916500	-0.87695500
C	5.50642000	-2.95359500	-0.50521900
C	6.52195400	-3.87579700	-1.15354200
H	7.27199100	-4.23301600	-0.43711600
H	7.06342000	-3.37448400	-1.96541000
H	6.00321700	-4.74422500	-1.56932600
C	-4.56454400	3.77522100	-0.43699600
H	-5.13485400	3.30570100	-1.24605100
H	-4.55044300	4.85662400	-0.58882700
H	-5.08738400	3.54960900	0.49891300
C	-3.18515900	3.17556400	-0.39110900
C	-2.06632200	4.00662200	-0.55375800
H	-2.25653600	5.06146900	-0.71423800
C	-0.72708700	3.60235600	-0.54840800
C	0.35689600	4.62065100	-0.77399000
H	1.04853600	4.60260500	0.07473600
H	-0.03566400	5.63090800	-0.90646500
H	0.93768400	4.33726900	-1.65846600
N	-2.45639200	-0.93126100	0.09358200
O	-3.15845000	1.91727000	-0.20779500
O	-0.27484100	2.42043700	-0.37042700
S	0.96181100	-3.01571100	-0.00478200
S	4.41798000	2.29796900	-0.18284400
S	6.10671000	-1.44966200	0.21621700
Pt	-1.39965800	0.77251300	-0.07363100
C	-5.96369400	-2.21267100	0.22979300
F	-6.48172900	-2.60582000	-0.94980900
F	-6.48576000	-1.00860700	0.51019200
F	-6.41870300	-3.08105300	1.15155500



**2-<sup>3</sup>MECP<sub>2</sub>**

C	-3.81980500	-0.95758400	0.16884100
H	-4.31775700	0.00564900	0.17872100
C	-4.51319600	-2.15440300	0.21920700
C	-3.79358900	-3.35876300	0.18328800
H	-4.31905900	-4.30804800	0.22367100
C	-2.41930700	-3.32215200	0.10588100
H	-1.83724900	-4.23750500	0.08127200
C	-1.75616200	-2.08226800	0.06565100
C	-0.36242000	-1.83695200	0.01783900
C	0.08646800	-0.50579100	0.05000100
C	1.49674500	-0.45355800	0.10907100
C	2.09543100	-1.74156600	0.04390200
C	3.82438200	0.41259700	-1.82454500
H	3.29216300	-0.48712000	-2.15108300
H	4.85005200	0.36452500	-2.20222500
H	3.32702900	1.28576200	-2.25501200
C	3.80122300	0.51267300	-0.29656900
C	2.38801600	0.68476200	0.23107900
C	2.19079000	1.85068000	0.95369400
H	1.24314000	2.08997900	1.42298200
C	3.29151500	2.68677900	1.06044400
C	3.37820200	3.98814700	1.77549900
H	3.61194900	4.81504000	1.09066900
H	4.16304700	3.97777500	2.54342100
H	2.42613700	4.21272900	2.26685300
C	4.41565400	-0.65383200	1.91962900
H	3.41652000	-0.42933300	2.30623200
H	5.10200800	0.14033300	2.22639800
H	4.75260100	-1.60108100	2.34982100
C	4.36857900	-0.77131300	0.38988300
C	3.48405000	-1.94567800	0.01379900
C	4.20684500	-3.09161700	-0.35785300
H	3.73887800	-4.04835900	-0.57349400
C	5.55829400	-2.89861000	-0.51228400
C	6.56428800	-3.90735200	-0.94284500
H	7.32528100	-4.06671600	-0.16857900
H	7.09007400	-3.58187000	-1.84923700
H	6.07968100	-4.86550800	-1.15110900
C	-4.56506700	3.79683100	-0.46494400
H	-5.14485800	3.32065600	-1.26327800
H	-4.54474000	4.87599300	-0.63106600
H	-5.08197600	3.58721300	0.47796700
C	-3.18959000	3.18852600	-0.42178200
C	-2.06619300	4.01005600	-0.60223700
H	-2.25035200	5.06402200	-0.77487800
C	-0.73027600	3.59656700	-0.60034300
C	0.36012300	4.60144700	-0.85349800
H	1.08247400	4.56691200	-0.03127700
H	-0.02192200	5.61832400	-0.96400000
H	0.90359600	4.31874500	-1.76180500
N	-2.48704500	-0.91938000	0.09546100
O	-3.16970900	1.93223700	-0.22383200
O	-0.28498900	2.41376000	-0.40715200
S	0.91318800	-3.01501900	-0.03130400
S	4.68977000	2.04919000	0.21232600
S	6.06182500	-1.25575300	-0.18213800
Pt	-1.41863400	0.77748100	-0.08516600
C	-6.00538100	-2.16820500	0.26477400
F	-6.51176900	-0.96320900	0.56733800
F	-6.53675500	-2.53898100	-0.91533100
F	-6.45821400	-3.04505500	1.17865500

**3-1GSo**

Pt	3.02790300	-0.17840700	0.01117400
S	-0.41218600	2.66623000	-0.11225900
S	-0.82412900	-1.48058800	0.09061900
S	-5.79416400	2.59734100	-0.80436700
S	-5.73871500	-2.92341200	0.75866200
C	2.34722100	-4.40284400	0.26623300
O	5.03297500	-0.81430600	0.03095100
O	2.35742600	-2.07611000	0.12857200
N	3.51019600	1.77816400	-0.10281200
C	4.76675600	2.23836700	-0.14066200
H	5.53821000	1.47605500	-0.10776200
C	5.05168600	3.59177300	-0.21626000
H	6.08311700	3.92433100	-0.24515300
C	3.98861800	4.49589000	-0.25327900
H	4.17734000	5.56386600	-0.31252300
C	2.68698600	4.02441300	-0.21396300
H	1.84331700	4.70663900	-0.24143700
C	2.45252400	2.64698900	-0.13774800
C	1.19297900	1.96805700	-0.08966300
C	1.22099900	0.58316300	-0.01517100
C	-0.10565300	0.09061600	0.02991600
C	-1.09233700	1.07251500	-0.00718600
C	-2.43229800	0.58552600	-0.00963500
C	-2.43656700	-0.79909100	0.05522600
C	-5.43633600	4.52142000	1.22670800
H	-5.54012300	5.37703500	0.54899800
H	-4.73867300	4.80446700	2.02059300
H	-6.41618600	4.34585500	1.68634700
C	-4.92645200	3.30953100	0.51913700
C	-3.78940200	2.59746500	0.76288100
H	-3.09475300	2.85356800	1.55754400
C	-3.60649700	1.46709600	-0.10285300
C	-4.61869400	1.34232900	-1.02571200
C	-4.78500100	0.33681400	-2.11593200
H	-5.21474400	0.78929900	-3.01590900
H	-5.43508300	-0.49227200	-1.81020600
H	-3.81240100	-0.09033200	-2.37751600
C	-4.87576300	-0.59896000	2.05780300
H	-5.34294900	-1.04874200	2.94023500
H	-5.52832800	0.20819500	1.70303400
H	-3.93001900	-0.14246600	2.36458700
C	-4.62597900	-1.61728900	0.99645200
C	-3.56785400	-1.72467400	0.12055900
C	-3.66687900	-2.88637800	-0.71804800
H	-2.92696400	-3.13386600	-1.47347900
C	-4.78377400	-3.63704400	-0.50314800
C	-5.21363900	-4.88713900	-1.19718100
H	-6.17760400	-4.76351500	-1.70464200
H	-5.31455700	-5.72732500	-0.50004500
H	-4.47014700	-5.16327700	-1.95079900
C	6.86389200	-2.27530400	0.10442900
C	5.37707700	-2.03620000	0.10363000
C	4.50884400	-3.13781100	0.17902400
H	4.97025300	-4.11682100	0.23608900
C	3.11062600	-3.10924200	0.18638200
H	7.31749800	-1.73746100	0.94421400
H	7.29777100	-1.86467800	-0.81412200
H	7.12052200	-3.33421300	0.17750700
H	3.00494200	-5.27054600	0.34727200
H	1.67524000	-4.37554500	1.13067300
H	1.71992600	-4.50943100	-0.62573200

**3-1GSc**

Pt	3.10923600	-0.18886200	-0.00682500
S	-0.28939800	2.69025600	0.07253900
S	-0.70653500	-1.50142700	-0.05304800
S	-6.18754300	1.66401900	-0.03397100
S	-6.12997700	-1.97189300	-0.00053300
C	2.39321900	-4.41177900	-0.13367200
O	5.10745000	-0.84092500	-0.02198500
O	2.42411500	-2.08232800	-0.06807100
N	3.61544000	1.76394300	0.05233100
C	4.87793000	2.20894200	0.06703500
H	5.63941000	1.43631500	0.04577500
C	5.18028000	3.56020200	0.10631100
H	6.21603400	3.88012500	0.11688000
C	4.12945700	4.47892600	0.13100500
H	4.33231000	5.54545000	0.16175200
C	2.82173200	4.02324800	0.11573500
H	1.98724600	4.71700500	0.13396000
C	2.57010700	2.64748500	0.07584400
C	1.30307100	1.98163400	0.05288100
C	1.30740300	0.59208400	0.01613500
C	-0.02338200	0.11720400	0.00853500
C	-0.99122400	1.11000500	0.03467800
C	-2.34622700	0.63929800	-0.02056800
C	-2.34397100	-0.82673200	0.01641200
C	-5.68961000	4.42251900	-0.02877700
H	-6.32035400	4.60974500	-0.90663600
H	-4.89572000	5.17427600	-0.00593300
H	-6.32225800	4.56029200	0.85683600
C	-5.10926000	3.05190800	-0.06831900
C	-3.79309900	2.71875900	-0.11761300
H	-3.01384500	3.47507100	-0.10799700
C	-3.53187400	1.31550000	-0.13849500
C	-4.79625900	0.50662900	-0.43032900
C	-4.83890700	0.23753800	-1.94639100
H	-5.76511100	-0.26533400	-2.23469000
H	-3.99107200	-0.38825500	-2.24270900
H	-4.77393800	1.19077400	-2.47834500
C	-4.86007500	-0.49956900	1.93492400
H	-5.80858500	-0.03350500	2.21250200
H	-4.03999700	0.15756100	2.24313500
C	-4.76502200	-1.44953800	2.46820900
H	-4.78516500	-0.76771600	0.42167300
C	-3.49210400	-1.53792000	0.14568900
C	-3.70650700	-2.95507900	0.14702600
H	-2.89496800	-3.67719800	0.16621300
C	-5.00611300	-3.32980600	0.07807700
C	-5.54783900	-4.71668600	0.04929600
H	-6.15642500	-4.88678300	-0.84755200
H	-6.19205000	-4.90809500	0.91637000
H	-4.73271700	-5.44586900	0.05574600
C	6.92764600	-2.31666600	-0.05798100
C	5.44266500	-2.06716800	-0.05655700
C	4.56601500	-3.16368300	-0.09187300
H	5.01915800	-4.14780900	-0.11871900
C	3.16805400	-3.12321500	-0.09565800
H	7.37101500	-1.87291800	0.84034900
H	7.37894300	-1.81624200	-0.92186000
H	7.17622700	-3.37948800	-0.09082700
C	3.04352400	-5.28775500	-0.17658800
H	1.75702300	-4.47824800	0.75577800
H	1.72966100	-4.41037300	-1.00511200

**3-<sup>3</sup>ESo**

Pt	-3.02383600	-0.17799000	-0.01886000
S	0.40786600	2.69717600	0.09791100
S	0.79465100	-1.51346700	-0.13056400
S	5.78706000	2.52473200	0.81606500
S	5.81035100	-2.82765200	-0.66660200
C	-2.36059900	-4.40792600	-0.27441900
O	-5.03518100	-0.80791100	-0.01640200
O	-2.36212200	-2.08477800	-0.14296100
N	-3.50624100	1.76862200	0.10183300
C	-4.75424000	2.24029000	0.15213300
H	-5.53451700	1.48633700	0.12175500
C	-5.03504900	3.59638100	0.23820800
C	-3.96609500	4.51670300	0.27517100
H	-4.16230100	5.58229500	0.34349800
C	-2.67462100	4.05072300	0.22379300
H	-1.82892800	4.73132500	0.24968200
C	-2.42921500	2.65880400	0.13442000
C	-1.19747200	2.00571200	0.07044100
C	-1.21875900	0.53974800	-0.01578600
C	0.07090700	0.07274900	-0.06419900
C	1.09000400	1.06346100	-0.02472200
C	2.39409300	0.59189000	-0.01769500
C	2.41428400	-0.82673400	-0.09832100
C	5.45335900	4.50409500	-1.16586400
H	5.57535600	5.34158600	-0.46896300
H	4.75794400	4.81703800	-1.95042600
H	6.42807700	4.31898800	-1.63235800
C	4.92371700	3.28678500	-0.48333600
C	3.77022900	2.60545800	-0.73627900
H	3.07615000	2.89017500	-1.52149600
C	3.57415700	1.45780400	0.10167100
C	4.58969400	1.28723200	1.01379700
C	4.74685600	0.24516200	2.07087400
H	5.14300200	0.67235500	2.99812900
H	5.42210100	-0.55742900	1.74958400
H	3.77744300	-0.21099200	2.28929300
C	4.99521200	-0.46545400	-1.91766200
H	5.51176400	-0.87385000	-2.79302300
H	5.62683500	0.32233900	-1.48861700
H	4.06898900	0.00714200	-2.25628600
C	4.68530600	-1.53691700	-0.92706100
C	3.54968100	-1.72277200	-0.15721300
C	3.60449100	-2.94307500	0.60391400
H	2.80920200	-3.25518400	1.27423900
C	4.75918800	-3.64629500	0.45079100
C	5.16595300	-4.92170200	1.11065900
H	6.06988500	-4.79590800	1.71820200
H	5.36872700	-5.71213800	0.37848100
H	4.36290800	-5.26824500	1.76788300
C	-6.86973100	-2.25981000	-0.06441300
C	-5.38202700	-2.02925200	-0.08212600
C	-4.51953100	-3.13551700	-0.16495600
H	-4.98616600	-4.11245600	-0.21399300
C	-3.12088200	-3.11319300	-0.18908600
H	-7.32802100	-1.71727400	-0.89852300
H	-7.28709800	-1.84395800	0.85936600
H	-7.13678300	-3.31650000	-0.13356100
H	-3.01739300	-5.27729000	-0.34555900
H	-1.69840400	-4.37987800	-1.14631500
H	-1.72284200	-4.50890900	0.61070800
H	-6.06694800	3.92606100	0.27609500

**3-<sup>3</sup>ESc**

Pt	-3.12016800	-0.18503200	-0.01008500
S	0.29144200	2.69677500	0.09070300
S	0.69912600	-1.47293100	-0.09509200
S	6.21340500	1.64444000	0.14894100
S	6.14323200	-1.96152600	0.02570700
C	-2.36892700	-4.39742000	-0.23072500
O	-5.11498400	-0.85423900	-0.01825100
O	-2.42298900	-2.07348800	-0.11408700
N	-3.62611000	1.76657800	0.09216800
C	-4.88744400	2.21408700	0.12992100
H	-5.65141800	1.44389500	0.10245700
C	-5.18722900	3.56450100	0.19928000
H	-6.22219800	3.88561100	0.22839600
C	-4.13321800	4.48163000	0.22999700
H	-4.33450200	5.54757500	0.28432000
C	-2.82709900	4.02581900	0.19051100
H	-1.99061100	4.71708200	0.21264100
C	-2.57576200	2.64953000	0.12052100
C	-1.31212600	1.98746600	0.07225300
C	-1.32429800	0.59675000	0.00443800
C	-0.00366700	0.11390800	-0.03933700
C	0.98602000	1.10786400	-0.00670200
C	2.30813500	0.61892600	-0.01565000
C	2.30820100	-0.79066500	-0.07692400
C	5.77890500	4.30603300	-0.65155900
H	6.34042200	4.73437700	0.18942700
H	4.99312000	5.01460700	-0.93059800
H	6.47784700	4.22223800	-1.49444900
C	5.18325500	2.98910000	-0.30209300
C	3.83835700	2.64036600	-0.29863600
H	3.07361000	3.35217300	-0.59888100
C	3.56274400	1.32853100	0.05152000
C	4.77862800	0.52318200	0.46853100
C	4.73771600	0.21151100	1.96981900
H	5.64923700	-0.30405900	2.28634300
H	3.87817500	-0.42756800	2.19732800
H	4.64195400	1.14184500	2.53594700
C	4.88336400	-0.47301400	-1.89940300
H	5.83654200	0.00750700	-2.13858300
H	4.06756200	0.19349400	-2.19796100
H	4.80159200	-1.40320500	-2.46838200
C	4.78700000	-0.77601100	-0.39877300
C	3.50576400	-1.53978300	-0.10946000
C	3.70625400	-2.90258100	0.13794100
H	2.89164800	-3.60545000	0.29211200
C	5.02340800	-3.29128700	0.24377200
C	5.53988900	-4.65493400	0.53928100
H	6.15758100	-4.66035500	1.44656700
H	6.16624300	-5.03326900	-0.27879400
H	4.70969100	-5.35214300	0.68540600
C	-6.92355400	-2.33939400	-0.07064700
C	-5.44035100	-2.08183600	-0.07759600
C	-4.55600800	-3.17186700	-0.14534600
H	-5.00219800	-4.15849600	-0.19074300
C	-3.15882100	-3.11990100	-0.15894000
H	-7.38419300	-1.81489500	-0.91495600
H	-7.35721100	-1.92159400	0.84466300
H	-7.16999300	-3.40161200	-0.13073800
H	-3.00597200	-5.28202800	-0.29282800
H	-1.70841100	-4.36379100	-1.10382000
H	-1.72900700	-4.47490000	0.65519900

**3-<sup>3</sup>MC**

Pt	-2.85008700	-0.61619300	-0.56206000
S	0.41362800	2.43777800	0.09729600
S	1.06514700	-1.64046700	-0.43615600
S	5.79261500	2.48732500	1.17315400
S	6.13754300	-2.70196800	-0.79318100
C	-4.72433700	-1.18038800	3.45135500
O	-4.70264100	-1.53020500	-1.04888200
O	-3.38445100	-0.87332700	1.56807200
N	-3.48008600	1.53210600	-0.31195200
C	-4.72349100	2.00419100	-0.29896600
H	-5.50919400	1.27079000	-0.45770900
C	-4.99800300	3.34900200	-0.08912800
C	-3.92049900	4.21375500	0.10943500
H	-4.09209500	5.27362900	0.27460400
C	-2.62599700	3.71809300	0.09883600
H	-1.77629200	4.37547900	0.25568300
C	-2.41717700	2.34815400	-0.11176400
C	-1.14667600	1.66656700	-0.13365200
C	-1.08831600	0.29418800	-0.32625000
C	0.26618000	-0.11440900	-0.28941200
C	1.19354000	0.90119400	-0.07962900
C	2.55133700	0.47368600	-0.01049300
C	2.63382200	-0.89590900	-0.20769000
C	5.44666000	4.62105500	-0.63918200
H	5.49676800	5.39532100	0.13546500
H	4.76970000	4.97241500	-1.42366600
H	6.44820300	4.52610000	-1.07507300
C	4.95134900	3.32193300	-0.09551700
C	3.84859900	2.61143500	-0.46677900
H	3.17658800	2.93556900	-1.25597200
C	3.67264500	1.38381100	0.25499200
C	4.65118600	1.18190000	1.20012100
C	4.81137300	0.05496800	2.16472300
H	5.17595800	0.40656300	3.13563600
H	5.51131600	-0.70271600	1.79085800
H	3.84765400	-0.43996700	2.31580900
C	5.20111600	-0.32296400	-1.93956700
H	5.76611300	-0.63751100	-2.82326700
H	5.76277100	0.47676000	-1.44109300
H	4.25083500	0.10604400	-2.27052800
C	4.94214200	-1.46906400	-1.02113400
C	3.82194200	-1.74410800	-0.26777900
C	3.94033600	-2.97238200	0.46576700
H	3.15797600	-3.34835600	1.11819900
C	5.13312800	-3.60869500	0.29538400
C	5.60224400	-4.88503300	0.91128700
H	6.49995100	-4.73758300	1.52317600
H	5.84072300	-5.64012100	0.15301300
H	4.81749900	-5.29144200	1.55627100
C	-6.87969900	-2.36938500	-0.88194200
C	-5.64145500	-1.80178100	-0.23523500
C	-5.62525600	-1.63489900	1.15771600
H	-6.53303800	-1.90197500	1.68641400
C	-4.54251100	-1.22065600	1.95250200
H	-6.63298100	-3.33458500	-1.33850000
H	-7.20431900	-1.70612600	-1.69059000
H	-7.70079300	-2.51156200	-0.17579000
H	-5.73442900	-1.45689100	3.76203200
H	-4.00523900	-1.86221000	3.91787100
H	-4.49474000	-0.17279400	3.81357300
H	-6.02277500	3.70352400	-0.08140700

**3-<sup>3</sup>MECP<sub>1</sub>**

Pt	-2.85008700	-0.61619300	-0.56206000
S	0.41362800	2.43777800	0.09729600
S	1.06514700	-1.64046700	-0.43615600
S	5.79261500	2.48732500	1.17315400
S	6.13754300	-2.70196800	-0.79318100
C	-4.72433700	-1.18038800	3.45135500
O	-4.70264100	-1.53020500	-1.04888200
O	-3.38445100	-0.87332700	1.56807200
N	-3.48008600	1.53210600	-0.31195200
C	-4.72349100	2.00419100	-0.29896600
H	-5.50919400	1.27079000	-0.45770900
C	-4.99800300	3.34900200	-0.08912800
C	-3.92049900	4.21375500	0.10943500
H	-4.09209500	5.27362900	0.27460400
C	-2.62599700	3.71809300	0.09883600
H	-1.77629200	4.37547900	0.25568300
C	-2.41717700	2.34815400	-0.11176400
C	-1.14667600	1.66656700	-0.13365200
C	-1.08831600	0.29418800	-0.32625000
C	0.26618000	-0.11440900	-0.28941200
C	1.19354000	0.90119400	-0.07962900
C	2.55133700	0.47368600	-0.01049300
C	2.63382200	-0.89590900	-0.20769000
C	5.44666000	4.62105500	-0.63918200
H	5.49676800	5.39532100	0.13546500
H	4.76970000	4.97241500	-1.42366600
H	6.44820300	4.52610000	-1.07507300
C	4.95134900	3.32193300	-0.09551700
C	3.84859900	2.61143500	-0.46677900
H	3.17658800	2.93556900	-1.25597200
C	3.67264500	1.38381100	0.25499200
C	4.65118600	1.18190000	1.20012100
C	4.81137300	0.05496800	2.16472300
H	5.17595800	0.40656300	3.13563600
H	5.51131600	-0.70271600	1.79085800
H	3.84765400	-0.43996700	2.31580900
C	5.20111600	-0.32296400	-1.93956700
H	5.76611300	-0.63751100	-2.82326700
H	5.76277100	0.47676000	-1.44109300
H	4.25083500	0.10604400	-2.27052800
C	4.94214200	-1.46906400	-1.02113400
C	3.82194200	-1.74410800	-0.26777900
C	3.94033600	-2.97238200	0.46576700
H	3.15797600	-3.34835600	1.11819900
C	5.13312800	-3.60869500	0.29538400
C	5.60224400	-4.88503300	0.91128700
H	6.49995100	-4.73758300	1.52317600
H	5.84072300	-5.64012100	0.15301300
H	4.81749900	-5.29144200	1.55627100
C	-6.87969900	-2.36938500	-0.88194200
C	-5.64145500	-1.80178100	-0.23523500
C	-5.62525600	-1.63489900	1.15771600
H	-6.53303800	-1.90197500	1.68641400
C	-4.54251100	-1.22065600	1.95250200
H	-6.63298100	-3.33458500	-1.33850000
H	-7.20431900	-1.70612600	-1.69059000
H	-7.70079300	-2.51156200	-0.17579000
H	-5.73442900	-1.45689100	3.76203200
H	-4.00523900	-1.86221000	3.91787100
H	-4.49474000	-0.17279400	3.81357300
H	-6.02277500	3.70352400	-0.08140700

**3-TS<sub>1</sub>**

Pt	-3.01718800	-0.20295400	-0.22912300
S	0.45983200	2.66362800	0.24300000
S	0.78251900	-1.44732700	-0.33174200
S	5.87709900	2.33841400	0.98177800
S	5.74730900	-2.87602900	-0.92584800
C	-2.86718900	-4.43279800	1.28244200
O	-4.98210900	-0.93003600	-0.58745000
O	-2.59378000	-2.21329900	0.59805700
N	-3.50902700	2.07925100	0.28712100
C	-4.69477000	2.67773900	0.32696500
H	-5.55598900	2.01522500	0.35564800
C	-4.82826200	4.06203300	0.34593100
C	-3.66541600	4.82974000	0.30871200
H	-3.72289200	5.91448000	0.32033900
C	-2.42766900	4.20373200	0.24346200
H	-1.51294900	4.78603700	0.18504300
C	-2.36917600	2.80511100	0.22872500
C	-1.16348900	2.00887800	0.12007500
C	-1.21434000	0.63849000	-0.09713900
C	0.10870900	0.13382000	-0.15044000
C	1.11758800	1.07737800	0.00126500
C	2.44194500	0.55324200	-0.00637300
C	2.41117100	-0.81949900	-0.20029200
C	5.58426600	4.47944500	-0.83182400
H	5.72310800	5.25579500	-0.07016400
H	4.89552900	4.86840700	-1.58782200
H	6.55519800	4.31322900	-1.31325000
C	5.02958500	3.22188100	-0.24918100
C	3.86158800	2.58826500	-0.55405700
H	3.17282400	2.95316900	-1.31036500
C	3.63883100	1.38115900	0.18900400
C	4.65011300	1.11663600	1.08253700
C	4.78169700	-0.01206500	2.04938900
H	5.21474300	0.32109100	2.99848900
H	5.41180200	-0.81689300	1.65058500
H	3.79586000	-0.44099100	2.25097700
C	4.92845600	-0.44795900	-2.05948200
H	5.42071100	-0.81186300	-2.96749200
H	5.57500400	0.31059200	-1.60085200
H	3.99747200	0.04967400	-2.34614700
C	4.63180600	-1.56371300	-1.11541600
C	3.53096400	-1.75172200	-0.30909800
C	3.59730200	-2.97730900	0.43540300
H	2.82212300	-3.28938700	1.12886800
C	4.73361900	-3.69786100	0.22031500
C	5.14171600	-4.99563700	0.83497500
H	6.07626800	-4.90321900	1.40076200
H	5.28965100	-5.77647300	0.07971400
H	4.36305100	-5.33631800	1.52395100
C	-6.91027400	-2.25255100	-0.67506200
C	-5.46243500	-2.06947000	-0.29636300
C	-4.78251000	-3.13849500	0.31055900
H	-5.35355800	-4.04417200	0.48019900
C	-3.43422600	-3.16484500	0.69343500
H	-7.01598600	-2.12846400	-1.75852100
H	-7.50895900	-1.46732900	-0.20100800
H	-7.30521100	-3.22936500	-0.38722100
H	-3.59658900	-5.24516500	1.32287800
H	-2.00505200	-4.74943100	0.68587100
H	-2.49989900	-4.22489500	2.29333800
H	-5.81106900	4.51791500	0.39728000

**3-TS<sub>2</sub>**

Pt	-3.08708600	-0.17999500	-0.01291900
S	0.33041000	2.69252700	0.09451800
S	0.72017800	-1.49287500	-0.09979300
S	6.04114100	1.94050800	0.62484700
S	6.06342200	-2.19514700	-0.34465800
C	-2.35289300	-4.39511600	-0.23189000
O	-5.08533800	-0.84176100	-0.01540600
O	-2.39861800	-2.07114600	-0.11867700
N	-3.58666400	1.77258700	0.09202900
C	-4.84616400	2.22452000	0.13067000
H	-5.61282900	1.45702300	0.10192300
C	-5.14177200	3.57586500	0.20264700
C	-4.08464500	4.49032900	0.23566000
H	-4.28289800	5.56716000	0.29228700
C	-2.78043900	4.03074000	0.19536600
H	-1.94172500	4.71931100	0.21888000
C	-2.53283500	2.65306200	0.12216700
C	-1.27267300	1.98853700	0.07222200
C	-1.28707000	0.59378900	-0.00314300
C	0.02804300	0.10867400	-0.05642400
C	1.02120100	1.10038800	-0.02335900
C	2.34171100	0.61887000	0.00897600
C	2.35092300	-0.81340900	-0.11041600
C	5.72994100	4.26018200	-0.94924900
H	6.18673900	4.91352100	-0.19608300
H	4.97564900	4.83984400	-1.48937800
H	6.51784500	3.98043200	-1.65961700
C	5.09983700	3.06010100	-0.33063300
C	3.81056100	2.62662100	-0.44759200
H	3.07270800	3.15006800	-1.04879700
C	3.55067600	1.37505800	0.18386000
C	4.69452500	0.84546100	0.83857500
C	4.71058100	-0.02011600	2.06284400
H	4.67381700	0.60427800	2.96396600
H	5.61646000	-0.63437300	2.10953500
H	3.84462600	-0.68419200	2.07656500
C	4.92428100	-0.24851300	-1.95767400
H	5.00399900	-0.91984400	-2.82343300
H	5.82140300	0.38178600	-1.93577500
H	4.05568300	0.39525500	-2.11044700
C	4.77872300	-1.03711700	-0.69259900
C	3.50195700	-1.59565900	-0.24386400
C	3.63703800	-2.95221500	0.18394700
H	2.80254000	-3.54179000	0.55300500
C	4.91988400	-3.40595500	0.22833200
C	5.40996400	-4.71654300	0.73497200
H	6.09553800	-4.58475700	1.58153200
H	5.95609900	-5.26781800	-0.04062700
H	4.56942100	-5.33265000	1.06616500
C	-6.89976900	-2.31995200	-0.06419000
C	-5.41547000	-2.06810700	-0.07442400
C	-4.53569100	-3.16150600	-0.14446500
H	-4.98571100	-4.14645700	-0.18887600
C	-3.13813400	-3.11467200	-0.16101100
H	-7.36030700	-1.79359000	-0.90740400
H	-7.32981300	-1.90064800	0.85214400
H	-7.15049400	-3.38121700	-0.12389100
H	-2.99290800	-5.27684400	-0.30413000
H	-1.68331800	-4.35939000	-1.09783700
H	-1.72193300	-4.47939800	0.65989000
H	-6.17579000	3.89998600	0.23211700

**3-<sup>3</sup>MECP<sub>2</sub>**

Pt	2.43005900	0.94300500	-0.05469600
S	-0.46525600	-2.45836000	0.06640100
S	-1.56390800	1.57992800	-0.11085400
S	-6.48601200	-2.40365600	0.14143700
S	-7.01191800	1.15870700	0.08774900
C	1.02240800	4.98031000	-0.22567400
O	4.27834000	1.91682000	-0.07022400
O	1.46130300	2.69598700	-0.13479200
N	3.24445400	-0.89658600	0.02618400
C	4.55766100	-1.13006400	0.05084600
H	5.19552200	-0.24334100	0.01945900
C	4.18251100	-3.50075000	0.12693200
H	4.56462300	-4.52379900	0.15474300
C	2.82417400	-3.26155800	0.10060600
H	2.10755300	-4.08407700	0.10905400
C	2.34750600	-1.93753200	0.05430700
C	0.99816300	-1.49454400	0.02557800
C	0.78367500	-0.11336700	-0.03342500
C	-0.59915100	0.14237200	-0.05670800
C	-1.41203000	-1.00778100	-0.01214300
C	-2.79543800	-0.74365400	-0.01418300
C	-3.02710300	0.64082700	-0.07251500
C	-5.64204000	-4.93687900	-0.73959000
H	-6.10454200	-5.47316700	0.10727400
H	-4.75339700	-5.50264600	-1.05404500
H	-6.37215000	-4.95677700	-1.56712600
C	-5.26296900	-3.54924600	-0.36879600
C	-3.98864900	-2.97836100	-0.36305300
H	-3.11171100	-3.53993400	-0.69684100
C	-3.92833100	-1.65779600	0.04421500
C	-5.25309600	-1.07203800	0.48398200
C	-5.27946600	-0.77420700	1.98441100
H	-6.27202600	-0.41001000	2.28815600
H	-4.53318700	-0.00430700	2.23343900
H	-5.04591600	-1.68677000	2.55001200
C	-5.56265100	-0.08069300	-1.86781800
H	-6.42897700	-0.72464600	-2.07858900
H	-4.64916500	-0.59989500	-2.19512700
H	-5.66225000	0.85256900	-2.43937500
C	-5.48232100	0.22608000	-0.37089000
C	-4.34740300	1.18516200	-0.07413400
C	-4.76453600	2.48059300	0.23498400
H	-4.06780000	3.30153400	0.42163500
C	-6.13574500	2.64562600	0.35452000
C	-6.87246300	3.89271100	0.68860300
H	-7.48118600	3.77277500	1.60097300
H	-7.56450700	4.17857300	-0.12175500
H	-6.17079700	4.72333500	0.84860600
C	5.85108500	3.65034300	-0.11917100
C	4.42496800	3.17405400	-0.11643700
C	3.38246400	4.11991200	-0.16376500
H	3.67131500	5.16984200	-0.19997300
C	2.00698700	3.84681600	-0.17052800
H	6.37695900	3.20926500	-0.98004000
H	6.35696400	3.28141100	0.78649700
H	5.93518900	4.74299400	-0.16274900
H	1.50842600	5.96299000	-0.25125600
H	0.38681900	4.86253700	-1.11689600
H	0.35664100	4.92308800	0.64932600
C	5.07502600	-2.41699500	0.10571700
H	6.13379010	-2.56957214	0.13099132

## 4-1GSo

Pt	-2.32752600	-0.97929900	-0.04950900
S	0.52127400	2.46038700	0.08349700
S	1.68403700	-1.54837900	-0.09056100
S	5.86750500	3.33460600	0.74505700
S	6.83131200	-1.95582700	-0.65439400
C	-0.87981800	-5.00024500	-0.27710100
O	-4.17699300	-1.96529800	-0.09190200
O	-1.32271000	-2.71958600	-0.15062000
N	-3.16737700	0.85334900	0.04776500
C	-4.48594000	1.06755100	0.07229300
H	-5.10726700	0.17918600	0.03607900
C	-5.01435200	2.34489800	0.13564100
C	-4.14046000	3.43854800	0.17610600
H	-4.53392900	4.44961400	0.22259900
C	-2.77904800	3.21872200	0.15173100
H	-2.07911800	4.04715300	0.18123700
C	-2.28798900	1.90613600	0.08637600
C	-0.92904800	1.47834800	0.05332600
C	-0.69979600	0.10697800	-0.01108100
C	0.69227200	-0.13332200	-0.04213100
C	1.47959800	1.01622700	-0.00410800
C	2.88385100	0.78204600	0.01004300
C	3.14106100	-0.57941400	-0.04927000
C	5.13557600	5.17310100	-1.26533800
H	5.11135200	6.03340000	-0.58614100
H	4.37982200	5.33386500	-2.03997400
H	6.11905500	5.16357800	-1.74977000
C	4.85530800	3.89302400	-0.55022100
C	3.84545600	3.00293900	-0.76682000
H	3.09698200	3.13808700	-1.54209000
C	3.87932000	1.85801900	0.09739000
C	4.92269400	1.90173800	0.99207600
C	5.28751400	0.92849800	2.06263400
H	5.64467600	1.43821300	2.96364800
H	6.06993200	0.23474200	1.73059100
H	4.41298100	0.32819500	2.32992000
C	5.52111700	0.12979000	-1.99019600
H	6.08116900	-0.20709900	-2.86874500
H	5.99099800	1.04793500	-1.61638400
H	4.50644400	0.38963500	-2.30543900
C	5.46684600	-0.92744200	-0.93967200
C	4.43159400	-1.26255200	-0.09458400
C	4.75349300	-2.37153900	0.75805300
H	4.06244200	-2.77017400	1.49470400
C	6.01497800	-2.85692100	0.58538500
C	6.68752400	-3.97653500	1.30820800
H	7.58074300	-3.63678700	1.84546900
H	6.99800200	-4.77521200	0.62440800
H	5.99779800	-4.40781600	2.03980700
C	-5.71649200	-3.72690300	-0.17395800
C	-4.29636800	-3.23053500	-0.15633500
C	-3.24265500	-4.15810200	-0.21076600
H	-3.51840700	-5.20485500	-0.26323600
C	-1.87351900	-3.87460200	-0.20723800
H	-6.23898300	-3.29280500	-1.03350100
H	-6.23161100	-3.37647600	0.72715200
H	-5.78411600	-4.81557900	-0.22566800
H	-1.35812200	-5.98080300	-0.31874000
H	-0.24798600	-4.86791700	-1.16206700
H	-0.22170200	-4.95485500	0.59735000
C	-6.49207500	2.56368800	0.18356200
F	-6.88316200	3.45148300	-0.74730800
F	-7.17715900	1.42954100	-0.02020600
F	-6.87798600	3.06034500	1.37248400

## 4-1GSc

Pt	2.42207700	0.93883200	-0.03743300
S	-0.46458400	-2.46692100	0.04816700
S	-1.55867400	1.58152200	-0.07623100
S	-6.48260700	-2.41246400	0.12489300
S	-7.01429000	1.15680800	0.05330900
C	0.98397700	4.96988800	-0.21301700
O	4.27882800	1.92757500	-0.05485200
O	1.42229800	2.68625900	-0.11654900
N	3.24430800	-0.90373400	0.03919800
C	4.56260400	-1.13615700	0.06422600
H	5.18831500	-0.24986400	0.04133100
C	5.08182200	-2.41943300	0.11559100
C	4.19509600	-3.49814300	0.14140800
H	4.57019500	-4.51660800	0.18179400
C	2.83063200	-3.26381400	0.11502700
H	2.11997300	-4.08391900	0.13393600
C	2.35611900	-1.94813300	0.06318600
C	0.99793500	-1.50246400	0.03097200
C	0.78035800	-0.12966800	-0.01859900
C	-0.60476100	0.12860100	-0.04747600
C	-1.41257300	-1.01451300	-0.02380400
C	-2.80276300	-0.75069500	-0.01664500
C	-3.03463400	0.64038800	-0.05839200
C	-5.60314800	-4.96590300	-0.66605000
H	-6.09244900	-5.48001000	0.17174800
H	-4.70959500	-5.53556600	-0.93892500
H	-6.30031100	-4.99715900	-1.51373600
C	-5.23543400	-3.56852500	-0.31348200
C	-3.96905600	-3.00280700	-0.30032400
H	-3.09415200	-3.57771900	-0.59272600
C	-3.91930000	-1.65893400	0.04756800
C	-5.25567100	-1.07115100	0.46519600
C	-5.26930500	-0.77834700	1.97013700
H	-6.25498400	-0.42729300	2.28951200
H	-4.52940600	-0.00788500	2.21121000
H	-5.02068600	-1.68769300	2.52387500
C	-5.52055800	-0.07507100	-1.88858200
H	-6.38105900	-0.70289200	-2.13741300
H	-4.60608000	-0.59510700	-2.19266000
H	-5.59166800	0.86278700	-2.44632400
C	-5.47949100	0.22040600	-0.38458100
C	-4.34376700	1.18303700	-0.07794800
C	-4.76600100	2.48724400	0.19955800
H	-4.07840200	3.31103800	0.37277600
C	-6.13077100	2.65121700	0.30675300
C	-6.86767800	3.90262000	0.63023300
H	-7.47754000	3.78476600	1.53516300
H	-7.54819100	4.18966700	-0.18170600
H	-6.16549100	4.72519100	0.79495700
C	5.81732700	3.69094400	-0.11059400
C	4.39690000	3.19252800	-0.10710300
C	3.34432300	4.12201800	-0.15837700
H	3.62109900	5.16902900	-0.19991100
C	1.97479400	3.84019600	-0.15947800
H	6.35098700	3.25215000	-0.96075300
H	6.32157500	3.34759400	0.79951300
H	5.88476300	4.77942900	-0.16776700
H	1.46538200	5.94779000	-0.27740100
H	0.32620500	4.83118500	-1.07773000
H	0.35215600	4.93680200	0.68145500
C	6.60760600	-2.62640300	0.14291500
F	6.88169500	-3.94726000	0.19498400
F	7.15356600	-2.09715700	-0.97257800
F	7.12509500	-2.01622600	1.23029300

4-<sup>3</sup>ESo

Pt	-2.32081400	-0.98200500	-0.05992200
S	0.51353900	2.47851800	0.04590200
S	1.68801300	-1.58032600	-0.11793600
S	5.82163700	3.33920200	0.79170900
S	6.86739300	-1.92568100	-0.58974700
C	-0.91854100	-5.02672000	-0.27338800
O	-4.18362200	-1.95144000	-0.06900500
O	-1.33010500	-2.73978200	-0.16126800
N	-3.15502400	0.84183300	0.03456000
C	-4.46673700	1.06890500	0.07124200
H	-5.09783000	0.18695900	0.04310100
C	-4.99147100	2.35056300	0.14070700
C	-4.11304600	3.46211300	0.17723600
H	-4.51147400	4.46996700	0.23267900
C	-2.76184400	3.24033500	0.13954300
H	-2.05929800	4.06765000	0.16579900
C	-2.26157200	1.91811900	0.06503300
C	-0.92848300	1.50039900	0.01679200
C	-0.67856600	0.05840000	-0.05050000
C	0.68001800	-0.15895600	-0.08148100
C	1.49196100	1.00314900	-0.04860600
C	2.86307500	0.78637100	-0.02329600
C	3.14750900	-0.60331900	-0.08146500
C	5.13184600	5.18792100	-1.22402400
H	5.09007900	6.04350400	-0.53989200
H	4.39367800	5.35192900	-2.01463900
H	6.12622500	5.18303900	-1.68552300
C	4.83819200	3.90303500	-0.52332600
C	3.83648500	3.01140200	-0.76900200
H	3.10742700	3.14636400	-1.56256900
C	3.85709100	1.86055400	0.08702200
C	4.88019900	1.90029500	1.00613300
C	5.22416700	0.92608400	2.08375600
H	5.52357100	1.43816700	3.00424400
H	6.04380200	0.26208700	1.78243300
H	4.35864400	0.29665900	2.30805500
C	5.62215000	0.20789200	-1.89705900
H	6.21518500	-0.11048300	-2.76103300
H	6.08550700	1.11113400	-1.48145700
H	4.62485300	0.48490400	-2.24960000
C	5.51783800	-0.88237400	-0.88439300
C	4.43362300	-1.26805200	-0.11459000
C	4.71554800	-2.43650600	0.67606600
H	3.99005400	-2.88023200	1.35120200
C	5.98608300	-2.90557600	0.54434300
C	6.62796100	-4.06099600	1.23729300
H	7.48848500	-3.74696000	1.83957100
H	6.98155800	-4.81649500	0.52593100
H	5.90424000	-4.53777700	1.90489000
C	-5.73734800	-3.70063900	-0.11229500
C	-4.31291500	-3.21582600	-0.12032600
C	-3.26894800	-4.15431200	-0.18133900
H	-3.55681400	-5.19840500	-0.22051600
C	-1.89615600	-3.88673300	-0.19956500
H	-6.27110900	-3.26315000	-0.96309500
H	-6.23340800	-3.34408000	0.79712300
H	-5.81523300	-4.78880300	-0.16054900
H	-1.40981400	-6.00144800	-0.29709000
H	-0.29938500	-4.91170700	-1.16969800
H	-0.24604000	-4.98061400	0.59001200
C	-6.46400900	2.57247400	0.19089000
F	-6.87195600	3.38932800	-0.79935400
F	-7.15725100	1.42901800	0.08388100
F	-6.83617200	3.16339400	1.34298100

4-<sup>3</sup>ESc

Pt	2.42835900	0.94695300	-0.04763900
S	-0.47161500	-2.45180400	0.03136400
S	-1.57074800	1.59442600	-0.06565600
S	-6.48643900	-2.41110400	0.10627800
S	-7.02260800	1.16087700	0.07991800
C	1.07786500	5.00690500	-0.22795500
O	4.29900900	1.88894800	-0.07081200
O	1.46027700	2.71032400	-0.12863500
N	3.23643600	-0.89951800	0.02695500
C	4.54989500	-1.13615400	0.05318500
H	5.18406700	-0.25627400	0.02885800
C	5.05946000	-2.42360600	0.10036400
C	4.16682100	-3.50231000	0.12094100
H	4.54276400	-4.52033700	0.14998800
C	2.80915300	-3.25941700	0.09375400
H	2.09748600	-4.07829400	0.10536100
C	2.33916000	-1.93788900	0.04692000
C	0.99002100	-1.48633500	0.01549600
C	0.77434200	-0.10951300	-0.02683800
C	-0.61060500	0.14474600	-0.04907200
C	-1.41866500	-0.99975500	-0.02944900
C	-2.80915300	-0.74130100	-0.01721400
C	-3.04383100	0.65009900	-0.04861300
C	-5.60220700	-4.95988000	-0.69648800
H	-6.08130100	-5.48345900	0.14134800
H	-4.70838400	-5.52302900	-0.98143300
H	-6.30649900	-4.98902000	-1.53817300
C	-5.23754200	-3.56331500	-0.33668300
C	-3.97283700	-2.99514400	-0.31679800
H	-3.09690700	-3.56780000	-0.61130700
C	-3.92528600	-1.65255500	0.04069900
C	-5.26350600	-1.07089300	0.46294200
C	-5.28508500	-0.79753200	1.97167000
H	-6.27404800	-0.45539200	2.29052000
H	-4.54991700	-0.02808600	2.23018300
H	-5.03714500	-1.71342900	2.51495200
C	-5.54080900	-0.04904500	-1.88004100
H	-6.40444800	-0.67223500	-2.12912200
H	-4.63020900	-0.56728200	-2.19856300
H	-5.61566800	0.89436000	-2.42799200
C	-5.48960100	0.22955500	-0.37282600
C	-4.35423000	1.19069700	-0.06034900
C	-4.77735500	2.49333100	0.22608600
H	-4.09102600	3.31746200	0.40248200
C	-6.14216600	2.65434800	0.33922200
C	-6.88061400	3.90273300	0.67173400
H	-7.48782500	3.77924800	1.57758300
H	-7.56405700	4.19283400	-0.13651200
H	-6.18021800	4.72614200	0.83903600
C	5.87716800	3.62095000	-0.12478200
C	4.44727800	3.15168700	-0.11888300
C	3.41462800	4.10252700	-0.16522900
H	3.71472800	5.14319900	-0.20371900
C	2.03920400	3.85195800	-0.16909500
H	6.39897100	3.18432200	-0.98348500
H	6.38175900	3.25841500	0.77761200
H	5.96249300	4.70859900	-0.16957800
H	1.58686500	5.97238500	-0.25184300
H	0.44832500	4.90949700	-1.11922100
H	0.41318800	4.97057200	0.64199300
C	6.53499000	-2.65203300	0.17904800
F	6.90175600	-3.72406500	-0.54290300
F	7.22949200	-1.59661000	-0.27092200
F	6.93755900	-2.88130300	1.44191300



4-<sup>3</sup>MC

Pt	-2.12227800	-1.29899000	-0.57777200
S	0.64858200	2.21279400	0.06256500
S	1.91349100	-1.72092000	-0.46324000
S	5.92135200	3.09865900	1.18060200
S	7.09734400	-1.98524100	-0.74325800
C	-3.88367400	-1.98580800	3.46140900
O	-3.84742900	-2.44914300	-1.02509100
O	-2.59277500	-1.59502900	1.55956600
N	-3.06197800	0.72580700	-0.32004500
C	-4.36018500	0.99819400	-0.28299900
H	-5.03236800	0.15989300	-0.43528300
C	-4.82817200	2.28340400	-0.05160900
C	-3.89258700	3.30694200	0.13923900
H	-4.22865000	4.32383800	0.32025000
C	-2.54379300	3.01542300	0.10252600
H	-1.80437800	3.79492700	0.25547100
C	-2.12971700	1.69111400	-0.12500800
C	-0.77686600	1.21237300	-0.16360600
C	-0.51162000	-0.13956500	-0.35842300
C	0.88791700	-0.33533300	-0.32437600
C	1.64909600	0.81205500	-0.11536500
C	3.05486600	0.59901900	-0.03953000
C	3.34697400	-0.74297000	-0.22953700
C	5.28285600	5.14141100	-0.65729700
H	5.19258600	5.91817900	0.11116000
H	4.57684500	5.37716900	-1.45920200
H	6.29641800	5.20348000	-1.07062300
C	4.98643100	3.78365100	-0.11200800
C	4.01612500	2.90697400	-0.49808600
H	3.31901200	3.11715900	-1.30395000
C	4.01914000	1.67230700	0.23265300
C	4.99723600	1.63176600	1.19854800
C	5.30962600	0.55021200	2.17755700
H	5.59101500	0.96088100	3.15290400
H	6.12920300	-0.08959400	1.82754600
H	4.43259700	-0.08940900	2.31250900
C	5.82791600	0.21636200	-1.92135700
H	6.44938300	-0.01252200	-2.79337900
H	6.25379900	1.09387700	-1.41931600
H	4.83004900	0.49543400	-2.27182700
C	5.73068500	-0.95262200	-0.99996600
C	4.65187300	-1.39793700	-0.26755200
C	4.94444200	-2.59147300	0.47440700
H	4.21740600	-3.08250900	1.11422700
C	6.22503600	-3.03438000	0.33102500
C	6.87592900	-4.21924700	0.96399300
H	7.73202200	-3.93083900	1.58514000
H	7.23750700	-4.93383000	0.21529700
H	6.15447000	-4.73665400	1.60327600
C	-5.92547300	-3.50424000	-0.82413200
C	-4.75261900	-2.79238800	-0.20013400
C	-4.75035300	-2.58227100	1.18717300
H	-5.62528700	-2.92262000	1.72868600
C	-3.70898600	-2.04567900	1.96294600
H	-5.58011100	-4.45165100	-1.25322500
H	-6.31832700	-2.90218600	-1.65011300
H	-6.72596900	-3.70959100	-0.11010400
H	-4.84736400	-2.38126600	3.78994000
H	-3.07850200	-2.55348100	3.93959900
H	-3.78578200	-0.94629400	3.79200800
C	-6.29131800	2.58392600	-0.00958400
F	-6.64765700	3.43409600	-0.98852000
F	-7.03597800	1.47675000	-0.14450900
F	-6.63740800	3.16910900	1.15053600

4-<sup>3</sup>MECP<sub>1</sub>

Pt	-2.13276100	-1.24866400	-0.53792200
S	0.64810200	2.24441000	0.12121400
S	1.89519100	-1.68839600	-0.43919000
S	5.83371700	3.18329700	1.27144500
S	7.02009500	-2.05296400	-0.91940400
C	-3.62256000	-2.49978500	3.46439400
O	-3.82096200	-2.41272000	-1.03897800
O	-2.48199100	-1.77958800	1.56529400
N	-3.06412300	0.77406700	-0.28111500
C	-4.36045500	1.05999800	-0.28257600
H	-5.03526800	0.22924400	-0.46357400
C	-4.82497400	2.34910800	-0.06584200
C	-3.88533600	3.36141400	0.16451900
H	-4.21923700	4.37940200	0.34308100
C	-2.53966400	3.05839500	0.16639500
H	-1.79628000	3.82833000	0.34696600
C	-2.12908200	1.73276800	-0.06433000
C	-0.78115300	1.25090000	-0.09611400
C	-0.52436700	-0.09998700	-0.30209900
C	0.87391000	-0.30304600	-0.28334300
C	1.64103800	0.84118200	-0.07809900
C	3.04771800	0.62631000	-0.02101600
C	3.33285100	-0.71665900	-0.21682800
C	5.20101900	5.21663500	-0.57775200
H	5.06273100	5.98508500	0.19216900
H	4.51345900	5.43967300	-1.39939400
H	6.22409000	5.31452500	-0.95971000
C	4.92805500	3.84604800	-0.05131900
C	3.99984500	2.94204900	-0.47582500
H	3.32640000	3.13440200	-1.30631800
C	4.00728700	1.70652200	0.25323700
C	4.95300800	1.69066600	1.25188400
C	5.24581900	0.62282100	2.25245100
H	5.48607200	1.04765100	3.23284900
H	6.08535200	-0.01165400	1.94255300
H	4.37148300	-0.02502600	2.36462300
C	5.74757600	0.17817200	-2.03077100
H	6.33791400	-0.07252000	-2.91829300
H	6.19329400	1.06536600	-1.56460300
H	4.73946400	0.45232000	-2.35589400
C	5.67708700	-0.97474000	-1.08685800
C	4.62909100	-1.38838700	-0.29360300
C	4.92734700	-2.59526900	0.42410500
H	4.22351500	-3.06793500	1.10304800
C	6.18100600	-3.08007100	0.19878100
C	6.83483600	-4.28894700	0.78103900
H	7.72468000	-4.02922100	1.36664600
H	7.14743400	-4.99723500	0.00456300
H	6.13456800	-4.80519900	1.44442800
C	-5.78616000	-3.67087900	-0.87318200
C	-4.64272400	-2.93395800	-0.22150000
C	-4.57340200	-2.89678200	1.17931600
H	-5.38558500	-3.37148400	1.71743700
C	-3.53377900	-2.36805600	1.96204800
H	-5.39729700	-4.57179100	-1.36187700
H	-6.22537000	-3.04626400	-1.65738300
H	-6.56064500	-3.96366100	-0.16072300
H	-4.54479600	-2.98491100	3.79172600
H	-2.76380600	-3.07541300	3.82568500
H	-3.55494900	-1.50445600	3.91566500
C	-6.28465500	2.66870400	-0.08022300
F	-6.57973100	3.56589800	-1.03634100
F	-7.03420400	1.57922000	-0.30008200
F	-6.68030400	3.20757500	1.08588200

4-TS <sub>1</sub>			
Pt	-2.28129300	-1.12349900	-0.30535100
S	0.49931000	2.42079700	0.17627100
S	1.71279700	-1.53068000	-0.33479600
S	5.84341300	3.28555200	0.98945600
S	6.87835800	-1.85548700	-0.81847100
C	-1.34648000	-5.21186600	1.27627400
O	-4.09451300	-2.19790600	-0.61586500
O	-1.49752400	-2.99039400	0.56534400
N	-3.24487700	0.97113400	0.17344300
C	-4.53373300	1.28585400	0.18568000
H	-5.22962300	0.45240700	0.20349700
C	-4.96690600	2.60602200	0.17967600
C	-4.00434900	3.61919700	0.14895500
H	-4.31137500	4.66084500	0.13516400
C	-2.66291300	3.28552500	0.11413800
H	-1.90220800	4.05785400	0.06033100
C	-2.29029200	1.93230500	0.12140300
C	-0.94192600	1.42604100	0.04222700
C	-0.69003400	0.07372800	-0.15910900
C	0.70891700	-0.13179600	-0.18513900
C	1.48624400	1.01189300	-0.03247500
C	2.89228400	0.78777300	-0.01483200
C	3.16268400	-0.56148400	-0.18762800
C	5.14261200	5.27756500	-0.88108400
H	5.10150300	6.08014800	-0.13530100
H	4.40107900	5.49826500	-1.65471500
H	6.13519400	5.31038900	-1.34556400
C	4.85489700	3.94279800	-0.27750700
C	3.85535100	3.06858100	-0.58689700
H	3.12211500	3.26296600	-1.36417100
C	3.87873100	1.85732800	0.18177100
C	4.90249500	1.83333300	1.09942500
C	5.25073000	0.77831800	2.09534400
H	5.58631200	1.21511400	3.04181900
H	6.04380400	0.11702300	1.72477300
H	4.37437900	0.15469500	2.29497600
C	5.57619600	0.31909100	-2.01340200
H	6.16046500	0.05902700	-2.90224100
H	6.02662200	1.20891000	-1.55641500
H	4.56633100	0.59372700	-2.33179700
C	5.50957300	-0.81974900	-1.05236900
C	4.45952500	-1.23032100	-0.26084100
C	4.77393800	-2.40111500	0.50786000
H	4.07063500	-2.86346100	1.19396700
C	6.04396100	-2.86025400	0.32614700
C	6.71184500	-4.02854700	0.97222600
H	7.59315100	-3.72617900	1.54997100
H	7.03974500	-4.77024600	0.23445500
H	6.01264600	-4.51914800	1.65589300
C	-5.76045700	-3.84091800	-0.61190200
C	-4.36071800	-3.39241800	-0.27842100
C	-3.48679800	-4.30512900	0.33799600
H	-3.88101500	-5.29429500	0.54076900
C	-2.15002700	-4.07922700	0.68815800
H	-5.90077000	-3.80145400	-1.69791700
H	-6.47772000	-3.14177600	-0.16903700
H	-5.97753200	-4.85186000	-0.26041700
H	-1.91035200	-6.14581800	1.33263700
H	-0.44882500	-5.36645700	0.66826100
H	-1.01072100	-4.93003000	2.28019500
C	-6.42104900	2.94651800	0.24880000
F	-6.74321400	3.89320400	-0.64919900
F	-7.19716700	1.87823500	0.01462000
F	-6.75966300	3.43118000	1.45703500

4-TS <sub>2</sub>			
Pt	-2.38882800	-0.95436800	-0.05632200
S	0.49147400	2.46214900	0.02380000
S	1.59047200	-1.59994600	-0.10416600
S	6.22489600	2.71157000	0.63105700
S	6.98171900	-1.35124800	-0.26088800
C	-0.99223700	-4.99695200	-0.24550600
O	-4.25068000	-1.92027200	-0.05050300
O	-1.40601800	-2.70945900	-0.14819200
N	-3.20933200	0.88616900	0.02879900
C	-4.52417100	1.11615100	0.06582100
H	-5.15578300	0.23456200	0.04585700
C	-5.03968500	2.39923100	0.12336000
C	-4.15252200	3.48672800	0.14525400
H	-4.53606000	4.50176600	0.18808000
C	-2.79592500	3.25362300	0.10745500
H	-2.08779800	4.07566000	0.12187500
C	-2.31562500	1.93322500	0.04742300
C	-0.96830400	1.49370200	0.00310100
C	-0.74416900	0.11131300	-0.05364300
C	0.63255300	-0.14103800	-0.09215500
C	1.44186400	1.00879500	-0.06706800
C	2.82183800	0.76112900	-0.01652600
C	3.07981500	-0.64982500	-0.10902100
C	5.55605700	4.91060600	-1.00270600
H	5.86866300	5.64965600	-0.25518400
H	4.72843300	5.33722200	-1.57682600
H	6.40167200	4.75817500	-1.68465600
C	5.12775300	3.63214800	-0.36899300
C	3.93455900	2.98110300	-0.49952300
H	3.13153400	3.35667500	-1.12704900
C	3.88021800	1.71783500	0.15773600
C	5.08270500	1.40627200	0.84526500
C	5.22195900	0.57722600	2.08685000
H	5.07940000	1.20618900	2.97392600
H	6.21223800	0.11358600	2.15238800
H	4.46956200	-0.21280300	2.10947800
C	5.54284600	0.33057200	-1.92970500
H	5.77481400	-0.32775700	-2.77755900
H	6.30079500	1.12267600	-1.90089200
H	4.57126700	0.79117200	-2.11862300
C	5.51717300	-0.45043900	-0.65140600
C	4.35379300	-1.21838000	-0.20755800
C	4.72148400	-2.51809000	0.25667400
H	4.00052500	-3.23934800	0.63073500
C	6.06459600	-2.73222100	0.32867800
C	6.77198100	-3.92104400	0.87698800
H	7.40234700	-3.64833600	1.73257200
H	7.42685500	-4.37925500	0.12560200
H	6.04971800	-4.67316100	1.20699200
C	-5.81111500	-3.66492400	-0.07520600
C	-4.38526300	-3.18444300	-0.09337800
C	-3.34345600	-4.12535900	-0.15292800
H	-3.63239800	-5.16944600	-0.18457600
C	-1.97123700	-3.85798100	-0.17709900
H	-6.35028900	-3.22528100	-0.92141100
H	-6.29930800	-3.30839600	0.83852400
H	-5.89226400	-4.75286600	-0.12371400
H	-1.48264900	-5.97221200	-0.26622000
H	-0.37188300	-4.88445900	-1.14129600
H	-0.32131000	-4.94700200	0.61896200
C	-6.51253100	2.63417200	0.18386000
F	-6.90865500	3.50371700	-0.76348600
F	-7.21338200	1.50309200	0.01679400
F	-6.88099200	3.16532200	1.36458100

**4-<sup>3</sup>MECP<sub>2</sub>**

Pt	2.43005900	0.94300500	-0.05469600
S	-0.46525600	-2.45836000	0.06640100
S	-1.56390800	1.57992800	-0.11085400
S	-6.48601200	-2.40365600	0.14143700
S	-7.01191800	1.15870700	0.08774900
C	1.02240800	4.98031000	-0.22567400
O	4.27834000	1.91682000	-0.07022400
O	1.46130300	2.69598700	-0.13479200
N	3.24445400	-0.89658600	0.02618400
C	4.55766100	-1.13006400	0.05084600
H	5.19552200	-0.24334100	0.01945900
C	5.07502600	-2.41699500	0.10571700
C	4.18251100	-3.50075000	0.12693200
H	4.56462300	-4.52379900	0.15474300
C	2.82417400	-3.26155800	0.10060600
H	2.10755300	-4.08407700	0.10905400
C	2.34750600	-1.93753200	0.05430700
C	0.99816300	-1.49454400	0.02557800
C	0.78367500	-0.11336700	-0.03342500
C	-0.59915100	0.14237200	-0.05670800
C	-1.41203000	-1.00778100	-0.01214300
C	-2.79543800	-0.74365400	-0.01418300
C	-3.02710300	0.64082700	-0.07251500
C	-5.64204000	-4.93687900	-0.73959000
H	-6.10454200	-5.47316700	0.10727400
H	-4.75339700	-5.50264600	-1.05404500
H	-6.37215000	-4.95677700	-1.56712600
C	-5.26296900	-3.54924600	-0.36879600
C	-3.98864900	-2.97836100	-0.36305300
H	-3.11171100	-3.53993400	-0.69684100
C	-3.92833100	-1.65779600	0.04421500
C	-5.25309600	-1.07203800	0.48398200
C	-5.27946600	-0.77420700	1.98441100
H	-6.27202600	-0.41001000	2.28815600
H	-4.53318700	-0.00430700	2.23343900
H	-5.04591600	-1.68677000	2.55001200
C	-5.56265100	-0.08069300	-1.86781800
H	-6.42897700	-0.72464600	-2.07858900
H	-4.64916500	-0.59989500	-2.19512700
H	-5.66225000	0.85256900	-2.43937500
C	-5.48232100	0.22608000	-0.37089000
C	-4.34740300	1.18516200	-0.07413400
C	-4.76453600	2.48059300	0.23498400
H	-4.06780000	3.30153400	0.42163500
C	-6.13574500	2.64562600	0.35452000
C	-6.87246300	3.89271100	0.68860300
H	-7.48118600	3.77277500	1.60097300
H	-7.56450700	4.17857300	-0.12175500
H	-6.17079700	4.72333500	0.84860600
C	5.85108500	3.65034300	-0.11917100
C	4.42496800	3.17405400	-0.11643700
C	3.38246400	4.11991200	-0.16376500
H	3.67131500	5.16984200	-0.19997300
C	2.00698700	3.84681600	-0.17052800
H	6.37695900	3.20926500	-0.98004000
H	6.35696400	3.28141100	0.78649700
H	5.93518900	4.74299400	-0.16274900
H	1.50842600	5.96299000	-0.25125600
H	0.38681900	4.86253700	-1.11689600
H	0.35664100	4.92308800	0.64932600
C	6.55418900	-2.64312000	0.18562700
F	6.92360900	-3.70271900	-0.54280900
F	7.24340700	-1.58655000	-0.25051900
F	6.95227900	-2.88356900	1.44144000

**5-1GSo**

Pt	-2.29287400	-0.98550300	-0.06172300
S	0.51297100	2.49411200	0.10587500
S	1.71437000	-1.55569000	-0.09850600
C	-0.85831700	-5.01680200	-0.31456100
O	-4.14780100	-1.96825300	-0.10310000
O	-1.28790700	-2.73459500	-0.17546300
N	-3.14205100	0.83061300	0.04813400
C	-4.45576100	1.04680200	0.07795100
H	-5.07956700	0.16030500	0.03417400
C	-4.99114300	2.32331800	0.15928000
C	-4.12175000	3.44104100	0.21522000
H	-4.52844600	4.44509600	0.27911800
C	-2.76856000	3.23048600	0.18466700
H	-2.07289000	4.06301700	0.22477100
C	-2.25729900	1.91318600	0.09836700
C	-0.92068700	1.50621600	0.05505100
C	-0.65948300	0.06778400	-0.02897700
C	0.70089000	-0.13860400	-0.05627800
C	1.50478000	1.02808600	-0.00281100
C	2.87821300	0.81471000	0.02992900
C	5.83176600	5.23004800	-0.61652000
C	5.26710300	3.92751300	-0.15456100
C	3.88550200	1.86209800	0.17283200
C	4.93631700	1.93865300	1.05929600
C	5.24122000	0.94300800	2.13520400
H	5.54349000	1.45543700	3.05507300
H	6.06107800	0.27671900	1.83935700
H	4.37506800	0.31502500	2.35854500
C	-5.68815700	-3.72773700	-0.18638400
C	-4.26729100	-3.23277800	-0.17223800
C	-3.21587400	-4.16281600	-0.23431700
H	-3.49555600	-5.20835700	-0.29024300
C	-1.84498500	-3.88503200	-0.23503600
H	-6.21410600	-3.28697700	-1.04038700
H	-6.19836200	-3.38220700	0.71942700
H	-5.75762700	-4.81597500	-0.24477700
H	-1.34217700	-5.99467900	-0.35531200
H	-0.23216700	-4.88565100	-1.20374800
H	-0.19388400	-4.97701800	0.55536600
C	-6.46567200	2.53290900	0.20203400
F	-6.87324000	3.36041900	-0.77942900
F	-7.14899300	1.38560400	0.07399400
F	-6.85086500	3.10441300	1.35970100
C	5.71371600	3.11851700	0.85324700
S	3.85795200	3.24367000	-0.88965400
H	6.58210200	3.36585200	1.45729500
S	6.88962200	-1.91050900	-0.52181000
C	5.67023000	0.23475800	-1.83191100
H	6.27926300	-0.07913700	-2.68628500
H	6.12566800	1.13602100	-1.40264400
H	4.67972600	0.51232500	-2.20229800
C	5.54870100	-0.85885200	-0.82528500
C	4.72389900	-2.41403200	0.72207800
H	3.98998300	-2.85582000	1.38929700
C	5.99295300	-2.88954600	0.60074800
C	6.62201300	-4.05085000	1.29558100
C	4.45523500	-1.24121900	-0.06718200
C	3.16907100	-0.57591800	-0.04371100
H	5.88991300	-4.52508700	1.95581600
H	6.97677700	-4.80649600	0.58493200
H	7.47943500	-3.74391300	1.90589700
H	5.11638400	6.05066100	-0.48784600
H	6.11144300	5.20040400	-1.67597700
H	6.72813600	5.46927700	-0.03675500

**5-1GSc**

Pt	2.39017600	0.95962100	-0.03553200
S	-0.48970400	-2.45644200	0.12377600
S	-1.59194700	1.58899800	-0.02683100
C	0.98469100	4.99900700	-0.24013400
O	4.24962600	1.92589200	-0.10550300
O	1.40251000	2.71285200	-0.12159300
N	3.21341100	-0.88012300	0.04904900
C	4.52928100	-1.10863500	0.05853000
H	5.15937400	-0.22672000	0.01742600
C	5.04659900	-2.39081500	0.11321400
C	4.16083200	-3.47757200	0.16058300
H	4.54537800	-4.49237700	0.20052800
C	2.80306600	-3.24535900	0.15142800
H	2.09591300	-4.06756900	0.18570100
C	2.32136700	-1.92608900	0.09486300
C	0.97160400	-1.48682700	0.07823200
C	0.74928700	-0.10871900	0.02095700
C	-0.63195700	0.14281100	0.00616500
C	-1.43999100	-1.00488400	0.04905900
C	-2.82637300	-0.74587600	0.05849400
C	-6.44539300	-4.60012600	-0.65517400
C	-5.74653800	-3.33422400	-0.29115300
C	-3.94522400	-1.63273400	0.15576500
C	-5.31435000	-1.09093800	0.50071200
C	-5.39784300	-0.78339000	2.00774500
H	-6.40005700	-0.43274400	2.27490500
H	-4.67241200	-0.01136200	2.28349700
H	-5.17664600	-1.68960800	2.57910400
C	5.80697400	3.67033500	-0.21071900
C	4.38184500	3.18933900	-0.17105500
C	3.33781100	4.12905700	-0.20896200
H	3.62480400	5.17264000	-0.26479600
C	1.96586100	3.86112800	-0.18544900
H	6.31022500	3.23367200	-1.08039900
H	6.33324200	3.31099900	0.68035100
H	5.88564700	4.75841600	-0.25994000
H	1.47391300	5.97402900	-0.28526400
H	0.34088900	4.87672700	-1.11798900
H	0.33733200	4.95909200	0.64261600
C	6.52089900	-2.62454000	0.14245600
F	6.89662800	-3.49852100	-0.80880800
F	7.21660200	-1.49363600	-0.04604200
F	6.91555800	-3.14883900	1.31757500
C	-6.27633400	-2.18343700	0.14216700
S	-3.97673400	-3.27435900	-0.40703400
H	-7.34597600	-2.05544100	0.28970400
S	-7.04028100	1.15926200	0.02613400
C	-5.50472800	-0.10462200	-1.85563500
H	-6.35075900	-0.75210800	-2.10569100
H	-4.57848100	-0.61926500	-2.13244300
H	-5.57925500	0.81716000	-2.43907800
C	-5.49253100	0.21926600	-0.35619000
C	-4.79970300	2.48255400	0.25301700
H	-4.11775800	3.30337800	0.45894700
C	-6.16791000	2.64449400	0.32996400
C	-6.91009400	3.89037700	0.66208800
C	-4.37092800	1.18376700	-0.03020000
C	-3.06059100	0.64784300	0.00189900
H	-6.21100200	4.70796600	0.86063400
H	-7.57083200	4.19594400	-0.15937300
H	-7.54146900	3.75459700	1.54961300
H	-6.11805800	-5.43093100	-0.01908500
H	-6.24080600	-4.88274500	-1.69452100
H	-7.52608900	-4.48076900	-0.53677900

**5-<sup>3</sup>ESo**

Pt	-2.29287400	-0.98550300	-0.06172300
S	0.51297100	2.49411200	0.10587500
S	1.71437000	-1.55569000	-0.09850600
C	-0.85831700	-5.01680200	-0.31456100
O	-4.14780100	-1.96825300	-0.10310000
O	-1.28790700	-2.73459500	-0.17546300
N	-3.14205100	0.83061300	0.04813400
C	-4.45576100	1.04680200	0.07795100
H	-5.07956700	0.16030500	0.03417400
C	-4.99114300	2.32331800	0.15928000
C	-4.12175000	3.44104100	0.21522000
H	-4.52844600	4.44509600	0.27911800
C	-2.76856000	3.23048600	0.18466700
H	-2.07289000	4.06301700	0.22477100
C	-2.25729900	1.91318600	0.09836700
C	-0.92068700	1.50621600	0.05505100
C	-0.65948300	0.06778400	-0.02897700
C	0.70089000	-0.13860400	-0.05627800
C	1.50478000	1.02808600	-0.00281100
C	2.87821300	0.81471000	0.02992900
C	5.83176600	5.23004800	-0.61652000
C	5.26710300	3.92751300	-0.15456100
C	3.88550200	1.86209800	0.17283200
C	4.93631700	1.93865300	1.05929600
C	5.24122000	0.94300800	2.13520400
H	5.54349000	1.45543700	3.05507300
H	6.06107800	0.27671900	1.83935700
H	4.37506800	0.31502500	2.35854500
C	-5.68815700	-3.72773700	-0.18638400
C	-4.26729100	-3.23277800	-0.17223800
C	-3.21587400	-4.16281600	-0.23431700
H	-3.49555600	-5.20835700	-0.29024300
C	-1.84498500	-3.88503200	-0.23503600
H	-6.21410600	-3.28697700	-1.04038700
H	-6.19836200	-3.38220700	0.71942700
H	-5.75762700	-4.81597500	-0.24477700
H	-1.34217700	-5.99467900	-0.35531200
H	-0.23216700	-4.88565100	-1.20374800
H	-0.19388400	-4.97701800	0.55536600
C	-6.46567200	2.53290900	0.20203400
F	-6.87324000	3.36041900	-0.77942900
F	-7.14899300	1.38560400	0.07399400
F	-6.85086500	3.10441300	1.35970100
C	5.71371600	3.11851700	0.85324700
S	3.85795200	3.24367000	-0.88965400
H	6.58210200	3.36585200	1.45729500
S	6.88962200	-1.91050900	-0.52181000
C	5.67023000	0.23475800	-1.83191100
H	6.27926300	-0.07913700	-2.68628500
H	6.12566800	1.13602100	-1.40264400
H	4.67972600	0.51232500	-2.20229800
C	5.54870100	-0.85885200	-0.82528500
C	4.72389900	-2.41403200	0.72207800
H	3.98998300	-2.85582000	1.38929700
C	5.99295300	-2.88954600	0.60074800
C	6.62201300	-4.05085000	1.29558100
C	4.45523500	-1.24121900	-0.06718200
C	3.16907100	-0.57591800	-0.04371100
H	5.88991300	-4.52508700	1.95581600
H	6.97677700	-4.80649600	0.58493200
H	7.47943500	-3.74391300	1.90589700
H	5.11638400	6.05066100	-0.48784600
H	6.11144300	5.20040400	-1.67597700

H 6.72813600 5.46927700 -0.03675500

**5-<sup>3</sup>ESc**

Pt	2.39017600	0.95962100	-0.03553200
S	-0.48970400	-2.45644200	0.12377600
S	-1.59194700	1.58899800	-0.02683100
C	0.98469100	4.99900700	-0.24013400
O	4.24962600	1.92589200	-0.10550300
O	1.40251000	2.71285200	-0.12159300
N	3.21341100	-0.88012300	0.04904900
C	4.52928100	-1.10863500	0.05853000
H	5.15937400	-0.22672000	0.01742600
C	5.04659900	-2.39081500	0.11321400
C	4.16083200	-3.47757200	0.16058300
H	4.54537800	-4.49237700	0.20052800
C	2.80306600	-3.24535900	0.15142800
H	2.09591300	-4.06756900	0.18570100
C	2.32136700	-1.92608900	0.09486300
C	0.97160400	-1.48682700	0.07823200
C	0.74928700	-0.10871900	0.02095700
C	-0.63195700	0.14281100	0.00616500
C	-1.43999100	-1.00488400	0.04905900
C	-2.82637300	-0.74587600	0.05849400
C	-6.44539300	-4.60012600	-0.65517400
C	-5.74653800	-3.33422400	-0.29115300
C	-3.94522400	-1.63273400	0.15576500
C	-5.31435000	-1.09093800	0.50071200
C	-5.39784300	-0.78339000	2.00774500
H	-6.40005700	-0.43274400	2.27490500
H	-4.67241200	-0.01136200	2.28349700
H	-5.17664600	-1.68960800	2.57910400
C	5.80697400	3.67033500	-0.21071900
C	4.38184500	3.18933900	-0.17105500
C	3.33781100	4.12905700	-0.20896200
H	3.62480400	5.17264000	-0.26479600
C	1.96586100	3.86112800	-0.18544900
H	6.31022500	3.23367200	-1.08039900
H	6.33324200	3.31099900	0.68035100
H	5.88564700	4.75841600	-0.25994000
H	1.47391300	5.97402900	-0.28526400
H	0.34088900	4.87672700	-1.11798900
H	0.33733200	4.95909200	0.64261600
C	6.52089900	-2.62454000	0.14245600
F	6.89662800	-3.49852100	-0.80880800
F	7.21660200	-1.49363600	-0.04604200
F	6.91555800	-3.14883900	1.31757500
C	-6.27633400	-2.18343700	0.14216700
S	-3.97673400	-3.27435900	-0.40703400
H	-7.34597600	-2.05544100	0.28970400
S	-7.04028100	1.15926200	0.02613400
C	-5.50472800	-0.10462200	-1.85563500
H	-6.35075900	-0.75210800	-2.10569100
H	-4.57848100	-0.61928500	-2.13244300
H	-5.57925500	0.81716000	-2.43907800
C	-5.49253100	0.21926600	-0.35619000
C	-4.79970300	2.48255400	0.25301700
H	-4.11775800	3.30337800	0.45894700
C	-6.16791000	2.64449400	0.32996400
C	-6.91009400	3.89037700	0.66208800
C	-4.37092800	1.18376700	-0.03020000
C	-3.06059100	0.64784300	0.00189900
H	-6.21100200	4.70796600	0.86063400
H	-7.57083200	4.19594400	-0.15937300
H	-7.54146900	3.75459700	1.54961300
H	-6.11805800	-5.43093100	-0.01908500
H	-6.24080600	-4.88274500	-1.69452100

H	-7.52608900	-4.48076900	-0.53677900
<b>5-<sup>3</sup>MC</b>			
Pt	-2.29287400	-0.98550300	-0.06172300
S	0.51297100	2.49411200	0.10587500
S	1.71437000	-1.55569000	-0.09850600
C	-3.03299257	-1.10047241	4.15873420
O	-4.14780100	-1.96825300	-0.10310000
O	-2.32320655	-0.87018960	1.95520562
N	-3.14205100	0.83061300	0.04813400
C	-4.45576100	1.04680200	0.07795100
H	-5.07956700	0.16030500	0.03417400
C	-4.99114300	2.32331800	0.15928000
C	-4.12175000	3.44104100	0.21522000
H	-4.52844600	4.44509600	0.27911800
C	-2.76856000	3.23048600	0.18466700
H	-2.07289000	4.06301700	0.22477100
C	-2.25729900	1.91318600	0.09836700
C	-0.92068700	1.50621600	0.05505100
C	-0.65948300	0.06778400	-0.02897700
C	0.70089000	-0.13860400	-0.05627800
C	1.50478000	1.02808600	-0.00281100
C	2.87821300	0.81471000	0.02992900
C	5.83176600	5.23004800	-0.61652000
C	5.26710300	3.92751300	-0.15456100
C	3.88550200	1.86209800	0.17283200
C	4.93631700	1.93865300	1.05929600
C	5.24122000	0.94300800	2.13520400
H	5.54349000	1.45543700	3.05507300
H	6.06107800	0.27671900	1.83935700
H	4.37506800	0.31502500	2.35854500
C	-6.11953252	-2.95026942	0.68641588
C	-4.81469665	-2.24654400	0.94374560
C	-4.43951264	-1.95852200	2.26684140
H	-5.12811811	-2.26732807	3.04463767
C	-3.27013120	-1.31824332	2.69003328
H	-5.92458419	-3.88342001	0.14656592
H	-6.74260964	-2.32619032	0.03642060
H	-6.66874662	-3.17406179	1.60335569
H	-3.85010046	-1.47710411	4.77720639
H	-2.10075190	-1.59674426	4.44952540
H	-2.89958294	-0.02969014	4.34702692
C	-6.46567200	2.53290900	0.20203400
F	-6.87324000	3.36041900	-0.77942900
F	-7.14899300	1.38560400	0.07399400
F	-6.85086500	3.10441300	1.35970100
C	5.71371600	3.11851700	0.85324700
S	3.85795200	3.24367000	-0.88965400
H	6.58210200	3.36585200	1.45729500
S	6.88962200	-1.91050900	-0.52181000
C	5.67023000	0.23475800	-1.83191100
H	6.27926300	-0.07913700	-2.68628500
H	6.12566800	1.13602100	-1.40264400
H	4.67972600	0.51232500	-2.20229800
C	5.54870100	-0.85885200	-0.82528500
C	4.72389900	-2.41403200	0.72207800
H	3.98998300	-2.85582000	1.38929700
C	5.99295300	-2.88954600	0.60074800
C	6.62201300	-4.05085000	1.29558100
C	4.45523500	-1.24121900	-0.06718200
C	3.16907100	-0.57591800	-0.04371100
H	5.88991300	-4.52508700	1.95581600
H	6.97677700	-4.80649600	0.58493200
H	7.47943500	-3.74391300	1.90589700
H	5.11638400	6.05066100	-0.48784600
H	6.11144300	5.20040400	-1.67597700

H	6.72813600	5.46927700	-0.03675500
<b>5-<sup>3</sup>MECP<sub>1</sub></b>			
Pt	-2.09209000	-1.29710600	-0.58426400
S	0.65425700	2.22361300	0.10743300
S	1.94180300	-1.69696500	-0.46048600
C	-3.85996100	-2.01263700	3.44678600
O	-3.81024800	-2.45390100	-1.04193300
O	-2.56593900	-1.60641500	1.56032300
N	-3.04426800	0.72051900	-0.31408300
C	-4.34416500	0.98548100	-0.28253100
H	-5.01076700	0.14518000	-0.44762000
C	-4.82047500	2.26575300	-0.04099000
C	-3.89176700	3.29231900	0.16598700
H	-4.23449700	4.30551200	0.35501700
C	-2.54113800	3.00846100	0.13468300
H	-1.80688000	3.79047600	0.29921900
C	-2.11874200	1.68881300	-0.10356000
C	-0.76274400	1.21771200	-0.13915300
C	-0.48888700	-0.12956900	-0.35068000
C	0.91171900	-0.31603100	-0.31335800
C	1.66543400	0.83215500	-0.08333000
C	3.07315400	0.62025500	0.00124000
C	5.94473500	5.14000500	0.05846000
C	5.39187100	3.77885200	0.32529300
C	4.04621200	1.66141300	0.32278200
C	5.04408600	1.65214700	1.27053100
C	5.31157100	0.53634100	2.23142800
H	5.58978800	0.93326700	3.21380800
H	6.13266700	-0.10255900	1.88303900
H	4.43289300	-0.10307000	2.35111600
C	-5.88348700	-3.52019600	-0.85123800
C	-4.71555000	-2.80590500	-0.22082700
C	-4.71753700	-2.60281100	1.16752800
H	-5.59206000	-2.95024800	1.70518800
C	-3.68092600	-2.06464000	1.94854200
H	-5.53232900	-4.46312900	-1.28544800
H	-6.27799500	-2.91524600	-1.67432400
H	-6.68420500	-3.73399900	-0.13995300
H	-4.82197900	-2.41568900	3.77097500
H	-3.05240700	-2.57718600	3.92464200
H	-3.76970200	-0.97397300	3.78219300
C	-6.28551100	2.55818600	-0.00662800
F	-6.64086100	3.40910600	-0.98519600
F	-7.02325300	1.44732200	-0.14906100
F	-6.64140500	3.13808300	1.15318300
C	5.80312100	2.86235600	1.25168800
S	4.04433700	3.16086300	-0.56863600
H	6.62985400	3.05103300	1.93087400
S	7.12001500	-1.98257000	-0.68377000
C	5.89172900	0.25187500	-1.84044500
H	6.53269000	0.03688100	-2.70178000
H	6.31102300	1.11586700	-1.30961600
H	4.90459700	0.54397900	-2.20962900
C	5.76732800	-0.93286800	-0.94356200
C	4.94370500	-2.58873000	0.49064200
H	4.20285900	-3.08325500	1.11162500
C	6.22205200	-3.04121800	0.35946400
C	6.85203900	-4.24259200	0.98228200
C	4.67318300	-1.37994800	-0.23539700
C	3.37071100	-0.72031800	-0.20703500
H	6.11560000	-4.76431300	1.60061400
H	7.21958800	-4.94740400	0.22725600
H	7.70023600	-3.97274700	1.62231600
H	5.19700400	5.92323400	0.22997800
H	6.29734300	5.24256100	-0.97447300

H	6.79160400	5.33034200	0.72447500
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5-TS <sub>1</sub>			
Pt	-2.29287400	-0.98550300	-0.06172300
S	0.51297100	2.49411200	0.10587500
S	1.71437000	-1.55569000	-0.09850600
C	-3.03299257	-1.10047241	4.15873420
O	-4.14780100	-1.96825300	-0.10310000
O	-2.32320655	-0.87018960	1.95520562
N	-3.14205100	0.83061300	0.04813400
C	-4.45576100	1.04680200	0.07795100
H	-5.07956700	0.16030500	0.03417400
C	-4.99114300	2.32331800	0.15928000
C	-4.12175000	3.44104100	0.21522000
H	-4.52844600	4.44509600	0.27911800
C	-2.76856000	3.23048600	0.18466700
H	-2.07289000	4.06301700	0.22477100
C	-2.25729900	1.91318600	0.09836700
C	-0.92068700	1.50621600	0.05505100
C	-0.65948300	0.06778400	-0.02897700
C	0.70089000	-0.13860400	-0.05627800
C	1.50478000	1.02808600	-0.00281100
C	2.87821300	0.81471000	0.02992900
C	5.83176600	5.23004800	-0.61652000
C	5.26710300	3.92751300	-0.15456100
C	3.88550200	1.86209800	0.17283200
C	4.93631700	1.93865300	1.05929600
C	5.24122000	0.94300800	2.13520400
H	5.54349000	1.45543700	3.05507300
H	6.06107800	0.27671900	1.83935700
H	4.37506800	0.31502500	2.35854500
C	-6.11953252	-2.95026942	0.68641588
C	-4.81469665	-2.24654400	0.94374560
C	-4.43951264	-1.95852200	2.26684140
H	-5.12811811	-2.26732807	3.04463767
C	-3.27013120	-1.31824332	2.69003328
H	-5.92458419	-3.88342001	0.14656592
H	-6.74260964	-2.32619032	0.03642060
H	-6.66874662	-3.17406179	1.60335569
H	-3.85010046	-1.47710411	4.77720639
H	-2.10075190	-1.59674426	4.44952540
H	-2.89958294	-0.02969014	4.34702692
C	-6.46567200	2.53290900	0.20203400
F	-6.87324000	3.36041900	-0.77942900
F	-7.14899300	1.38560400	0.07399400
F	-6.85086500	3.10441300	1.35970100
C	5.71371600	3.11851700	0.85324700
S	3.85795200	3.24367000	-0.88965400
H	6.58210200	3.36585200	1.45729500
S	6.88962200	-1.91050900	-0.52181000
C	5.67023000	0.23475800	-1.83191100
H	6.27926300	-0.07913700	-2.68628500
H	6.12566800	1.13602100	-1.40264400
H	4.67972600	0.51232500	-2.20229800
C	5.54870100	-0.85885200	-0.82528500
C	4.72389900	-2.41403200	0.72207800
H	3.98998300	-2.85582000	1.38929700
C	5.99295300	-2.88954600	0.60074800
C	6.62201300	-4.05085000	1.29558100
C	4.45523500	-1.24121900	-0.06718200
C	3.16907100	-0.57591800	-0.04371100
H	5.88991300	-4.52508700	1.95581600
H	6.97677700	-4.80649600	0.58493200
H	7.47943500	-3.74391300	1.90589700
H	5.11638400	6.05066100	-0.48784600
H	6.11444300	5.20040400	-1.67597700

H	6.72813600	5.46927700	-0.03675500
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5-TS <sub>2</sub>			
Pt	2.36644000	0.96116800	-0.03772700
S	-0.49710300	-2.46527000	0.09082400
S	-1.61497400	1.58905400	-0.04579100
C	0.94805500	4.99624500	-0.21362900
O	4.22336900	1.93479700	-0.07970400
O	1.37440500	2.71104300	-0.11648100
N	3.19650100	-0.87595100	0.03847800
C	4.51325800	-1.09905100	0.05071500
H	5.13981600	-0.21427500	0.01729700
C	5.03562100	-2.37959600	0.09928400
C	4.15467800	-3.47041600	0.13802400
H	4.54336100	-4.48378600	0.17308600
C	2.79585800	-3.24356500	0.12610900
H	2.09200200	-4.06887700	0.15323800
C	2.30934800	-1.92615900	0.07502800
C	0.95757700	-1.49176100	0.05475500
C	0.72808700	-0.11324000	-0.00212100
C	-0.65341500	0.13282400	-0.02850800
C	-1.45250800	-1.01827200	0.01099000
C	-2.84042500	-0.77144300	0.06919800
C	-6.38892400	-4.69280100	-0.49048300
C	-5.66415300	-3.44925300	-0.10288200
C	-3.91211500	-1.68525200	0.26668300
C	-5.17505100	-1.34047600	0.84473000
C	-5.29486500	-0.51422900	2.09817700
H	-5.21501400	-1.17471300	2.97044800
H	-6.26540500	-0.00890000	2.14476900
H	-4.50589300	0.23569600	2.17226700
C	5.77544200	3.68572000	-0.15099900
C	4.35165700	3.19940900	-0.13112000
C	3.30472500	4.13560300	-0.16976700
H	3.58817500	5.18080500	-0.21197400
C	1.93354400	3.86205600	-0.16239000
H	6.29008100	3.25761000	-1.01824500
H	6.29292000	3.32142600	0.74323300
H	5.85071700	4.77443000	-0.19083600
H	1.43346600	5.97363300	-0.24764200
H	0.30962400	4.87813700	-1.09589400
H	0.29563700	4.94595900	0.66486100
C	6.51106100	-2.60707000	0.13246100
F	6.89210900	-3.48151500	-0.81605800
F	7.20224600	-1.47366600	-0.05685900
F	6.90490500	-3.12696300	1.30969700
C	-6.13401500	-2.38145300	0.59613900
S	-3.97471800	-3.25057200	-0.51462100
H	-7.15032200	-2.33946100	0.97766300
S	-7.00428500	1.30434500	-0.30333300
C	-5.49460800	-0.37090600	-1.91221300
H	-5.75062200	0.28725500	-2.75199500
H	-6.20765800	-1.20363800	-1.89953800
H	-4.49758500	-0.77620400	-2.09708100
C	-5.51951200	0.39309700	-0.61872500
C	-4.77148900	2.48958700	0.27342800
H	-4.06700900	3.22097900	0.65936400
C	-6.11922300	2.69738600	0.29780000
C	-6.84998600	3.88944700	0.80779100
C	-4.38035700	1.19299400	-0.16892100
C	-3.09771000	0.63630700	-0.04605600
H	-5.91679400	-5.58283300	-0.05777600
H	-6.40507900	-4.82798700	-1.57860500
H	-7.42312300	-4.64731900	-0.13728800
H	-7.50261800	3.62588800	1.64951400
H	-7.48591700	4.33279800	0.03161500

H	-6.14219700	4.65121700	1.14705900
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H	-7.52608900	-4.48076900	-0.53677900
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<b>5-<sup>3</sup>MECP<sub>2</sub></b>			
Pt	2.39017600	0.95962100	-0.03553200
S	-0.48970400	-2.45644200	0.12377600
S	-1.59194700	1.58899800	-0.02683100
C	0.98469100	4.99900700	-0.24013400
O	4.24962600	1.92589200	-0.10550300
O	1.40251000	2.71285200	-0.12159300
N	3.21341100	-0.88012300	0.04904900
C	4.52928100	-1.10863500	0.05853000
H	5.15937400	-0.22672000	0.01742600
C	5.04659900	-2.39081500	0.11321400
C	4.16083200	-3.47757200	0.16058300
H	4.54537800	-4.49237700	0.20052800
C	2.80306600	-3.24535900	0.15142800
H	2.09591300	-4.06756900	0.18570100
C	2.32136700	-1.92608900	0.09486300
C	0.97160400	-1.48682700	0.07823200
C	0.74928700	-0.10871900	0.02095700
C	-0.63195700	0.14281100	0.00616500
C	-1.43999100	-1.00488400	0.04905900
C	-2.82637300	-0.74587600	0.05849400
C	-6.44539300	-4.60012600	-0.65517400
C	-5.74653800	-3.33422400	-0.29115300
C	-3.94522400	-1.63273400	0.15576500
C	-5.31435000	-1.09093800	0.50071200
C	-5.39784300	-0.78339000	2.00774500
H	-6.40005700	-0.43274400	2.27490500
H	-4.67241200	-0.01136200	2.28349700
H	-5.17664600	-1.68960800	2.57910400
C	5.80697400	3.67033500	-0.21071900
C	4.38184500	3.18933900	-0.17105500
C	3.33781100	4.12905700	-0.20896200
H	3.62480400	5.17264000	-0.26479600
C	1.96586100	3.86112800	-0.18544900
H	6.31022500	3.23367200	-1.08039900
H	6.33324200	3.31099900	0.68035100
H	5.88564700	4.75841600	-0.25994000
H	1.47391300	5.97402900	-0.28526400
H	0.34088900	4.87672700	-1.11798900
H	0.33733200	4.95909200	0.64261600
C	6.52089900	-2.62454000	0.14245600
F	6.89662800	-3.49852100	-0.80880800
F	7.21660200	-1.49363600	-0.04604200
F	6.91555800	-3.14883900	1.31757500
C	-6.27633400	-2.18343700	0.14216700
S	-3.97673400	-3.27435900	-0.40703400
H	-7.34597600	-2.05544100	0.28970400
S	-7.04028100	1.15926200	0.02613400
C	-5.50472800	-0.10462200	-1.85563500
H	-6.35075900	-0.75210800	-2.10569100
H	-4.57848100	-0.61926500	-2.13244300
H	-5.57925500	0.81716000	-2.43907800
C	-5.49253100	0.21926600	-0.35619000
C	-4.79970300	2.48255400	0.25301700
H	-4.11775800	3.30337800	0.45894700
C	-6.16791000	2.64449400	0.32996400
C	-6.91009400	3.89037700	0.66208800
C	-4.37092800	1.18376700	-0.03020000
C	-3.06059100	0.64784300	0.00189900
H	-6.21100200	4.70796600	0.86063400
H	-7.57083200	4.19594400	-0.15937300
H	-7.54146900	3.75459700	1.54961300
H	-6.11805800	-5.43093100	-0.01908500
H	-6.24080600	-4.88274500	-1.69452100



**6-1GSo**

Pt	-3.00562000	-1.03834700	-0.09784000
S	-0.19445300	2.42733000	0.18935400
S	0.98713400	-1.61523400	-0.25553900
C	-1.57179300	-5.05408800	-0.50828500
O	-4.85737200	-2.01514400	-0.15394700
O	-2.00061700	-2.77833500	-0.28629500
N	-3.85237600	0.77455300	0.09537900
C	-5.16482400	0.98839300	0.15041900
H	-5.79001900	0.10469700	0.07738300
C	-5.69711800	2.26174600	0.29827800
C	-4.82748300	3.37141300	0.39148300
H	-5.23160500	4.37128800	0.51198600
C	-3.47322500	3.16285800	0.33487200
H	-2.77649100	3.99213900	0.40620300
C	-2.96722200	1.84989000	0.18375700
C	-1.63122300	1.44523700	0.10957500
C	-1.37283700	0.00889000	-0.04470600
C	-0.01706300	-0.19833000	-0.10859200
C	0.79061800	0.96613600	-0.00955100
C	2.15868700	0.74817700	-0.01393200
C	2.44751900	-0.64103800	-0.17643400
C	5.10787700	5.16391900	-0.30750000
C	4.54216900	3.82964000	0.03062900
C	3.16974300	1.78110800	0.20137000
C	4.19998400	1.79518900	1.11901800
C	4.47199300	0.73298100	2.13797000
H	4.77036800	1.18423800	3.08984200
H	5.28381700	0.07077000	1.81333600
H	3.59049200	0.11137600	2.31341200
C	4.97568700	0.27857200	-1.88078500
H	5.61126200	0.02940900	-2.73682800
H	5.41591500	1.15145000	-1.38338500
H	3.99373400	0.57466200	-2.25842800
C	4.87242500	-0.89208100	-0.95532400
C	3.73029200	-1.27763800	-0.26005100
C	5.61712400	-2.86117300	0.05260500
C	6.50184600	-3.99868700	0.41956000
C	-6.39975100	-3.77002200	-0.28010000
C	-4.97876500	-3.27777600	-0.26495400
C	-3.92876900	-4.20471300	-0.37043300
H	-4.20949000	-5.24767500	-0.45802600
C	-2.55798800	-3.92773000	-0.37820700
H	-6.93410700	-3.30076600	-1.11345800
H	-6.89958700	-3.45401400	0.64209500
H	-6.47116800	-4.85554600	-0.37366100
H	-2.05530900	-6.03091200	-0.56949500
H	-0.96182000	-4.89594200	-1.40435300
H	-0.89186000	-5.03869000	0.35027700
C	-7.17487500	2.46961900	0.32418700
F	-7.61135400	3.06167900	-0.80307200
F	-7.84600900	1.31600500	0.45550300
F	-7.53500800	3.27281300	1.34101900
C	4.98304200	2.97933300	1.00399000
C	5.94035600	-1.80405800	-0.75253600
S	3.15726800	3.21208500	-0.78338500
S	3.99201000	-2.77139100	0.61391400
H	5.83820500	3.19773000	1.63414300
H	6.91441400	-1.69757900	-1.21720400
H	6.03882875	5.31838728	0.19684948
H	5.28197207	5.26795655	-1.35810321
H	4.45235525	5.96161016	-0.02664408

**6-1GSc**

H	6.10682222	-4.93694508	0.09012414
H	6.63347749	-4.08004022	1.47831153
H	7.47052624	-3.88081622	-0.01937630
Pt	2.39017600	0.95962100	-0.03553200
S	-0.48970400	-2.45644200	0.12377600
S	-1.59194700	1.58899800	-0.02683100
C	0.98469100	4.99900700	-0.24013400
O	4.24962600	1.92589200	-0.10550300
O	1.40251000	2.71285200	-0.12159300
N	3.21341100	-0.88012300	0.04904900
C	4.52928100	-1.10863500	0.05853000
H	5.15937400	-0.22672000	0.01742600
C	5.04659900	-2.39081500	0.11321400
C	4.16083200	-3.47757200	0.16058300
H	4.54537800	-4.49237700	0.20052800
C	2.80306600	-3.24535900	0.15142800
H	2.09591300	-4.06756900	0.18570100
C	2.32136700	-1.92608900	0.09486300
C	0.97160400	-1.48682700	0.07823200
C	0.74928700	-0.10871900	0.02095700
C	-0.63195700	0.14281100	0.00616500
C	-1.43999100	-1.00488400	0.04905900
C	-2.82637300	-0.74587600	0.05849400
C	-6.44539300	-4.60012600	-0.65517400
C	-5.74653800	-3.33422400	-0.29115300
C	-3.94522400	-1.63273400	0.15576500
C	-5.31435000	-1.09093800	0.50071200
C	-5.39784300	-0.78339000	2.00774500
H	-6.40005700	-0.43274400	2.27490500
H	-4.67241200	-0.01136200	2.28349700
H	-5.17664600	-1.68960800	2.57910400
C	5.80697400	3.67033500	-0.21071900
C	4.38184500	3.18933900	-0.17105500
C	3.33781100	4.12905700	-0.20896200
H	3.62480400	5.17264000	-0.26479600
C	1.96586100	3.86112800	-0.18544900
H	6.31022500	3.23367200	-1.08039900
H	6.33324200	3.31099900	0.68035100
H	5.88564700	4.75841600	-0.25994000
H	1.47391300	5.97402900	-0.28526400
H	0.34088900	4.87672700	-1.11798900
H	0.33733200	4.95909200	0.64261600
C	6.52089900	-2.62454000	0.14245600
F	6.89662800	-3.49852100	-0.80880800
F	7.21660200	-1.49363600	-0.04604200
F	6.91555800	-3.14883900	1.31757500
C	-6.27633400	-2.18343700	0.14216700
S	-3.97673400	-3.27435900	-0.40703400
H	-7.34597600	-2.05544100	0.28970400
S	-7.04028100	1.15926200	0.02613400
C	-5.50472800	-0.10462200	-1.85563500
H	-6.35075900	-0.75210800	-2.10569100
H	-4.57848100	-0.61926500	-2.13244300
H	-5.57925500	0.81716000	-2.43907800
C	-5.49253100	0.21926600	-0.35619000
C	-4.79970300	2.48255400	0.25301700
H	-4.11775800	3.30337800	0.45894700
C	-6.16791000	2.64449400	0.32996400
C	-6.91009400	3.89037700	0.66208800
C	-4.37092800	1.18376700	-0.03020000
C	-3.06059100	0.64784300	0.00189900
H	-6.21100200	4.70796600	0.86063400
H	-7.57083200	4.19594400	-0.15937300
H	-7.54146900	3.75459700	1.54961300

H	-6.11805800	-5.43093100	-0.01908500
H	-6.24080600	-4.88274500	-1.69452100
H	-7.52608900	-4.48076900	-0.53677900

**6-3ESo**

Pt	-2.26064900	-0.97778600	-0.06739000
S	0.54064600	2.51211100	0.05051900
S	1.73859800	-1.54190100	-0.15937800
C	-0.81166700	-5.00358200	-0.30422600
O	-4.11152200	-1.96863300	-0.06325700
O	-1.25089700	-2.72208800	-0.18493400
N	-3.11201600	0.83832200	0.04266200
C	-4.42561100	1.05088700	0.09142200
H	-5.04725700	0.16215200	0.06402500
C	-4.96323800	2.32660700	0.17709100
C	-4.09589900	3.44419000	0.21327400
H	-4.50304400	4.44756800	0.28528000
C	-2.74188300	3.23673200	0.16313000
H	-2.04780300	4.07095300	0.19196700
C	-2.22986900	1.92062100	0.07464800
C	-0.89145300	1.51645300	0.01510200
C	-0.62850300	0.08410900	-0.06719900
C	0.72783100	-0.12124100	-0.10907400
C	1.53389000	1.05093900	-0.06468700
C	2.90145800	0.84226500	-0.03454000
C	3.19948100	-0.55691000	-0.11959500
C	5.84693200	5.28134500	-0.53410900
C	5.27847800	3.96736000	-0.11092000
C	3.90392400	1.88767900	0.14056900
C	4.93059900	1.95380100	1.05636900
C	5.21422700	0.94055400	2.12180700
H	5.50183000	1.43766100	3.05458700
H	6.03771000	0.27732700	1.82879300
H	4.34346100	0.31104400	2.32157800
C	5.77424300	0.31238500	-1.79265100
H	6.43255600	0.03384400	-2.62267000
H	6.20204500	1.19997100	-1.31004500
H	4.80459500	0.60184600	-2.20526900
C	5.64178400	-0.82938900	-0.83534100
C	4.47888300	-1.19192000	-0.16076300
C	6.38106900	-2.78914900	0.23862100
C	7.25221000	-3.91698500	0.67881000
C	-5.64499500	-3.73579000	-0.09764000
C	-4.22635200	-3.23431900	-0.11663300
C	-3.17198400	-4.16026900	-0.18915900
H	-3.44764500	-5.20767700	-0.22780500
C	-1.80273600	-3.87620300	-0.21971800
H	-6.19049500	-3.30427000	-0.94405200
H	-6.13805900	-3.38548100	0.81581400
H	-5.71055100	-4.82477600	-0.14597000
H	-1.29122400	-5.98414600	-0.32828300
H	-0.19981200	-4.87758700	-1.20402600
H	-0.13386200	-4.95229100	0.55473300
C	-6.43921000	2.53167900	0.20161700
F	-6.88049600	3.11273400	-0.93113500
F	-7.11120300	1.37945800	0.34605300
F	-6.80357500	3.34634000	1.20973900
C	5.70426300	3.14232300	0.89321400
C	6.70276800	-1.73932700	-0.58136100
S	3.89345800	3.28895600	-0.89505400
S	4.73125500	-2.67371400	0.74592600
H	6.55423600	3.38415600	1.52502300
H	7.68726100	-1.63311800	-1.02838000
H	6.72437200	5.51683200	0.07541300
H	6.15734400	5.27156000	-1.58535400
H	5.12212600	6.09472900	-0.41257200

H	6.84604700	-4.88691800	0.36845400
H	7.36491800	-3.94263500	1.76922500
H	8.24767400	-3.80903900	0.23827400

**6-3ESc**

Pt	2.35770600	0.94981900	-0.03702600
S	-0.50364000	-2.48848400	0.11428100
S	-1.61797000	1.56185700	-0.05628700
C	0.92544900	4.98030000	-0.25319900
O	4.21162100	1.92952400	-0.09236000
O	1.35846200	2.69694200	-0.13252900
N	3.19092500	-0.88379800	0.05797800
C	4.50703400	-1.10543700	0.08138400
H	5.13283800	-0.22015000	0.04422300
C	5.03217500	-2.38405800	0.15386500
C	4.15158900	-3.47691700	0.20086100
H	4.54245800	-4.48813400	0.26277400
C	2.79362500	-3.25356000	0.17472200
H	2.09124500	-4.07975800	0.21314700
C	2.30233200	-1.93662200	0.10164700
C	0.95365300	-1.50749900	0.07118200
C	0.72134000	-0.12634900	0.00706200
C	-0.65399100	0.11712000	-0.01800200
C	-1.46510100	-1.03958400	0.02459000
C	-2.84031200	-0.79341700	0.02268100
C	-3.08865100	0.61258500	-0.03971000
C	-6.47332200	-4.64331400	-0.65425900
C	-5.76762700	-3.37978700	-0.29478500
C	-3.96263700	-1.68183700	0.13322600
C	-5.32021400	-1.14345400	0.51321300
C	-5.38446300	-0.82167100	2.01840900
H	-6.38161900	-0.45794000	2.29076100
H	-4.65301000	-0.04928900	2.27751000
H	-5.16500900	-1.71981100	2.60305100
C	-5.64364200	-0.14963900	-1.82595800
H	-6.52564400	-0.76650200	-2.02825400
H	-4.75287200	-0.69705700	-2.15028000
H	-5.71889900	0.77325800	-2.40902700
C	-5.55639500	0.18219300	-0.32227800
C	-4.38468600	1.10876400	-0.07855100
C	-6.58374200	2.27021200	0.31893800
C	-7.59589100	3.31782700	0.63506600
C	5.75659600	3.68532600	-0.18744700
C	4.33459500	3.19375600	-0.15793300
C	3.28434200	4.12619800	-0.20437600
H	3.56457600	5.17174600	-0.25828400
C	1.91386700	3.84908600	-0.19155800
H	6.26860500	3.25378200	-1.05459300
H	6.27971100	3.32826600	0.70637800
H	5.82775800	4.77405000	-0.23452200
H	1.40844700	5.95844900	-0.29851300
H	0.28585300	4.85166900	-1.13316800
H	0.27426200	4.93829200	0.62664200
C	6.50733700	-2.60721300	0.14782600
F	6.92706600	-3.13902500	-1.01607400
F	7.19214100	-1.46865400	0.33428300
F	6.87611200	-3.46919100	1.11307500
C	-6.28684300	-2.23891700	0.17774500
C	-6.77089400	0.96876000	0.07129100
S	-4.00488500	-3.30633400	-0.47062200
S	-4.87337700	2.74723000	0.21587000
H	-7.35145400	-2.12628200	0.36716800
H	-7.75986800	0.51802400	0.06240300
H	-6.30776700	-4.90625000	-1.70565800
H	-6.11720700	-5.48341300	-0.04655000
H	-7.54938400	-4.53308100	-0.49227700

H	-8.59680300	2.87764800	0.65855100
H	-7.58859400	4.11632500	-0.11627700
H	-7.39892600	3.78154400	1.60879400

**6-<sup>3</sup>MC**

Pt	-1.90705662	-1.43656047	-0.59316504
S	0.83929038	2.08415853	0.09853196
S	2.12683638	-1.83641947	-0.46938704
C	-3.85996100	-2.01263700	3.44678600
O	-3.81024800	-2.45390100	-1.04193300
O	-2.56593900	-1.60641500	1.55032300
N	-2.85923462	0.58106453	-0.32298404
C	-4.15913162	0.84602653	-0.29143204
H	-4.82573362	0.00572553	-0.45652104
C	-4.63544162	2.12629853	-0.04989104
C	-3.70673362	3.15286453	0.15708596
H	-4.04946362	4.16605753	0.34611596
C	-2.35610462	2.86900653	0.12578196
H	-1.62184662	3.65102153	0.29031796
C	-1.93370862	1.54935853	-0.11246104
C	-0.57771062	1.07825753	-0.14805404
C	-0.30385362	-0.26902347	-0.35958104
C	1.09675238	-0.45548547	-0.32225904
C	1.85046738	0.69270053	-0.09223104
C	3.25818738	0.48080053	-0.00766104
C	6.12976838	5.00055053	0.04955896
C	5.57690438	3.63939753	0.31639196
C	4.23124538	1.52195853	0.31388096
C	5.22911938	1.51269253	1.26162996
C	5.49660438	0.39688653	2.22252696
H	5.77482138	0.79381253	3.20490696
H	6.31770038	-0.24201347	1.87413796
H	4.61792638	-0.24252447	2.34221496
C	-5.88348700	-3.52019600	-0.85123800
C	-4.71555000	-2.80590500	-0.22082700
C	-4.71753700	-2.60281100	1.16752800
H	-5.59206000	-2.95024800	1.70518800
C	-3.68092600	-2.06464000	1.94854200
H	-5.53232900	-4.46312900	-1.28544800
H	-6.27799500	-2.91524600	-1.67432400
H	-6.68420500	-3.73399900	-0.13995300
H	-4.82197900	-2.41568900	3.77097500
H	-3.05240700	-2.57718600	3.92464200
H	-3.76970200	-0.97397300	3.78219300
C	-6.10047762	2.41873153	-0.01552904
F	-6.45582762	3.26965153	-0.99409704
F	-6.83821962	1.30786753	-0.15796204
F	-6.45637162	2.99862853	1.14428196
C	5.98815438	2.72290153	1.24278696
S	4.22937038	3.02140853	-0.57753704
H	6.81488738	2.91157853	1.92197296
S	4.60837621	-3.16810267	0.70637229
C	6.91093515	-4.60457858	1.39491226
H	6.26931348	-5.48728158	1.30486532
H	7.06609433	-4.40228468	2.46218536
H	7.88716269	-4.84244323	0.96311212
C	6.32064524	-3.42723393	0.69569263
C	6.02419433	-1.48741277	-0.57960564
C	3.55574438	-0.85977247	-0.21593604
H	5.38203738	5.78377953	0.22107696
H	6.48237638	5.10310653	-0.98337404
H	6.97663738	5.19088753	0.71557396
C	6.46909474	-0.27385877	-1.41683338
H	7.34524398	0.15851501	-0.98058181
H	6.68686751	-0.59010792	-2.41556332
H	5.68429169	0.45319991	-1.43606493

C	4.72082675	-1.73786239	-0.27198241
C	6.94928870	-2.43419317	-0.02347976
H	8.01489750	-2.36151363	-0.08747643

**6-<sup>3</sup>MECP<sub>1</sub>**

Pt	-1.90705662	-1.43656047	-0.59316504
S	0.83929038	2.08415853	0.09853196
S	2.12683638	-1.83641947	-0.46938704
C	-3.33247659	-2.98403297	3.41188313
O	-3.81024800	-2.45390100	-1.04193300
O	-2.29432884	-2.10118951	1.52008033
N	-2.85923462	0.58106453	-0.32298404
C	-4.15913162	0.84602653	-0.29143204
H	-4.82573362	0.00572553	-0.45652104
C	-4.63544162	2.12629853	-0.04989104
C	-3.70673362	3.15286453	0.15708596
H	-4.04946362	4.16605753	0.34611596
C	-2.35610462	2.86900653	0.12578196
H	-1.62184662	3.65102153	0.29031796
C	-1.93370862	1.54935853	-0.11246104
C	-0.57771062	1.07825753	-0.14805404
C	-0.30385362	-0.26902347	-0.35958104
C	1.09675238	-0.45548547	-0.32225904
C	1.85046738	0.69270053	-0.09223104
C	3.25818738	0.48080053	-0.00766104
C	6.12976838	5.00055053	0.04955896
C	5.57690438	3.63939753	0.31639196
C	4.23124538	1.52195853	0.31388096
C	5.22911938	1.51269253	1.26162996
C	5.49660438	0.39688653	2.22252696
H	5.77482138	0.79381253	3.20490696
H	6.31770038	-0.24201347	1.87413796
H	4.61792638	-0.24252447	2.34221496
C	-5.80273882	-3.66615561	-0.86279991
C	-4.59522358	-3.02982343	-0.22350750
C	-4.43671933	-3.12799870	1.16718252
H	-5.22569045	-3.63706709	1.70843585
C	-3.33447068	-2.70384773	1.92831137
H	-5.47094616	-4.47048836	-1.52908466
H	-6.31695775	-2.92598795	-1.48473428
H	-6.50257884	-4.07726426	-0.13204619
H	-4.23197383	-3.50737381	3.74361666
H	-2.45194549	-3.58489148	3.66256105
H	-3.24207077	-2.03718930	3.95482080
C	-6.10047762	2.41873153	-0.01552904
F	-6.45582762	3.26965153	-0.99409704
F	-6.83821962	1.30786753	-0.15796204
F	-6.45637162	2.99862853	1.14428196
C	5.98815438	2.72290153	1.24278696
S	4.22937038	3.02140853	-0.57753704
H	6.81488738	2.91157853	1.92197296
S	4.60837621	-3.16810267	0.70637229
C	6.91093515	-4.60457858	1.39491226
H	6.26931348	-5.48728158	1.30486532
H	7.06609433	-4.40228468	2.46218536
H	7.88716269	-4.84244323	0.96311212
C	6.32064524	-3.42723393	0.69569263
C	6.02419433	-1.48741277	-0.57960564
C	3.55574438	-0.85977247	-0.21593604
H	5.38203738	5.78377953	0.22107696
H	6.48237638	5.10310653	-0.98337404
H	6.97663738	5.19088753	0.71557396
C	6.46909474	-0.27385877	-1.41683338
H	7.34524398	0.15851501	-0.98058181
H	6.68686751	-0.59010792	-2.41556332
H	5.68429169	0.45319991	-1.43606493

C	4.72082675	-1.73786239	-0.27198241
C	6.94928870	-2.43419317	-0.02347976
H	8.01489750	-2.36151363	-0.08747643

C	4.72082675	-1.73786239	-0.27198241
C	6.94928870	-2.43419317	-0.02347976
H	8.01489750	-2.36151363	-0.08747643

**6-TS<sub>1</sub>**

Pt	-1.90705662	-1.43656047	-0.59316504
S	0.83929038	2.08415853	0.09853196
S	2.12683638	-1.83641947	-0.46938704
C	-3.76646744	-2.19380094	3.46097881
O	-3.81024800	-2.45390100	-1.04193300
O	-2.51766884	-1.69890608	1.55528674
N	-2.85923462	0.58106453	-0.32298404
C	-4.15913162	0.84602653	-0.29143204
H	-4.82573362	0.00572553	-0.45652104
C	-4.63544162	2.12629853	-0.04989104
C	-3.70673362	3.15286453	0.15708596
H	-4.04946362	4.16605753	0.34611596
C	-2.35610462	2.86900653	0.12578196
H	-1.62184662	3.65102153	0.29031796
C	-1.93370862	1.54935853	-0.11246104
C	-0.57771062	1.07825753	-0.14805404
C	-0.30385362	-0.26902347	-0.35958104
C	1.09675238	-0.45548547	-0.32225904
C	1.85046738	0.69270053	-0.09223104
C	3.25818738	0.48080053	-0.00766104
C	6.12976838	5.00055053	0.04955896
C	5.57690438	3.63939753	0.31369196
C	4.23124538	1.52195853	0.31388096
C	5.22911938	1.51269253	1.26162996
C	5.49660438	0.39688653	2.22252696
H	5.77482138	0.79381253	3.20490696
H	6.31770038	-0.24201347	1.87413796
H	4.61792638	-0.24252447	2.34221496
C	-5.86910956	-3.54752690	-0.85025350
C	-4.69427829	-2.84757235	-0.21658040
C	-4.66795515	-2.70043622	1.17856790
H	-5.52741174	-3.07785408	1.72029787
C	-3.61954708	-2.18380382	1.95837860
H	-5.51893386	-4.46872559	-1.32956852
H	-6.28686442	-2.91395206	-1.63964277
H	-6.65222201	-3.79766617	-0.13125933
H	-4.71752664	-2.61908068	3.78908183
H	-2.94364415	-2.76904197	3.89831733
H	-3.67836145	-1.16860205	3.83604148
C	-6.10047762	2.41873153	-0.01552904
F	-6.45582762	3.26965153	-0.99409704
F	-6.83821962	1.30786753	-0.15796204
F	-6.45637162	2.99862853	1.14428196
C	5.98815438	2.72290153	1.24278696
C	4.22937038	3.02140853	-0.57753704
H	6.81488738	2.91157853	1.92197296
S	4.60837621	-3.16810267	0.70637229
C	6.91093515	-4.60457858	1.39491226
H	6.26931348	-5.48728158	1.30486532
H	7.06609433	-4.40228468	2.46218536
H	7.88716269	-4.84244323	0.96311212
C	6.32064524	-3.42723393	0.69569263
C	6.02419433	-1.48741277	-0.57960564
C	3.55574438	-0.85977247	-0.21593604
H	5.38203738	5.78377953	0.22107696
H	6.48237638	5.10310653	-0.98337404
H	6.97663738	5.19088753	0.71557396
C	6.46909474	-0.27385877	-1.41683338
H	7.34524398	0.15851501	-0.98058181
H	6.68686751	-0.59010792	-2.41556332
H	5.68429169	0.45319991	-1.43606493

**6-TS<sub>2</sub>**

Pt	2.34595300	0.95134700	-0.04831600
S	-0.51191500	-2.48074800	0.05886600
S	-1.63193700	1.57172700	-0.10040900
C	0.91362000	4.97920700	-0.26370100
O	4.19937400	1.93184100	-0.06524700
O	1.34839100	2.69637600	-0.14946200
N	3.17960700	-0.88334900	0.04869500
C	4.49634900	-1.10240600	0.08668700
H	5.12094400	-0.21588800	0.06051300
C	5.02125000	-2.38096800	0.16110400
C	4.14298900	-3.47337500	0.19476100
H	4.53368000	-4.48450100	0.25863900
C	2.78367300	-3.25060200	0.15323600
H	2.08149100	-4.07729800	0.18113500
C	2.29486000	-1.93556500	0.07843500
C	0.94199300	-1.50473700	0.03415300
C	0.71104300	-0.12764800	-0.03072400
C	-0.67088200	0.11632500	-0.07159100
C	-1.46872400	-1.03561600	-0.03565100
C	-2.85751700	-0.79097100	0.00824700
C	-3.11026200	0.61801600	-0.10663600
C	-6.44912600	-4.68350500	-0.49665800
C	-5.71727500	-3.43563700	-0.13736700
C	-3.93756000	-1.69417900	0.21059200
C	-5.21956600	-1.28950200	0.74127000
C	-5.30195900	-0.53327300	2.04706400
H	-6.25082100	0.00751000	2.12743700
H	-4.48443100	0.18220400	2.15360500
H	-5.23820700	-1.24366800	2.87988400
C	-5.52476800	-0.40071100	-1.93555100
H	-6.26239400	-1.21068900	-1.94796100
H	-4.53968600	-0.82516500	-2.13799000
H	-5.76476200	0.29406000	-2.74976600
C	-5.55576200	0.33478100	-0.61646100
C	-4.40055700	1.13674400	-0.21763600
C	-6.59403100	2.28993300	0.24057600
C	-7.62962000	3.28307400	0.64121100
C	5.74501400	3.68890300	-0.12101300
C	4.32303100	3.19692900	-0.12107300
C	3.27320700	4.12856100	-0.18051400
H	3.55310600	5.17467900	-0.22358000
C	1.90297200	3.84980000	-0.19228200
H	6.27639900	3.25442000	-0.97486500
H	6.24818700	3.33554500	0.78571700
H	5.81667400	4.77747600	-0.17010500
H	1.39542900	5.95846000	-0.29502700
H	0.28896500	4.85424200	-1.15481400
H	0.24768900	4.93020500	0.60461900
C	6.49823800	-2.60209000	0.17150300
F	6.93146900	-3.11778400	-0.99368100
F	7.17718400	-1.46461300	0.38107400
F	6.85400400	-3.47486600	1.13080100
C	-6.18728700	-2.33844800	0.50599600
C	-6.76620300	1.05400500	-0.28664400
S	-4.01046900	-3.28200200	-0.51911700
S	-4.88613800	2.70301800	0.40421400
H	-7.21192300	-2.27062000	0.86132200
H	-7.75242600	0.65493100	-0.50890900
H	-6.44694400	-4.85393400	-1.58002700
H	-5.99369500	-5.56337800	-0.02693100
H	-7.48894700	-4.61645300	-0.16376000

H	-8.62825000	2.88396600	0.44063100
H	-7.51724400	4.22317500	0.08764900
H	-7.56597400	3.52449400	1.70944300

H	-8.59680300	2.87764800	0.65855100
H	-7.58859400	4.11632500	-0.11627700
H	-7.39892600	3.78154400	1.60879400

**6-<sup>3</sup>MECP<sub>2</sub>**

Pt	2.35770600	0.94981900	-0.03702600
S	-0.50364000	-2.48848400	0.11428100
S	-1.61797000	1.56185700	-0.05628700
C	0.92544900	4.98030000	-0.25319900
O	4.21162100	1.92952400	-0.09236000
O	1.35846200	2.69694200	-0.13252900
N	3.19092500	-0.88379800	0.05797800
C	4.50703400	-1.10543700	0.08138400
H	5.13283800	-0.22015000	0.04422300
C	5.03217500	-2.38405800	0.15386500
C	4.15158900	-3.47691700	0.20086100
H	4.54245800	-4.48813400	0.26277400
C	2.79362500	-3.25356000	0.17472200
H	2.09124500	-4.07975800	0.21314700
C	2.30233200	-1.93662200	0.10164700
C	0.95365300	-1.50749900	0.07118200
C	0.72134000	-0.12634900	0.00706200
C	-0.65399100	0.11712000	-0.01800200
C	-1.46510100	-1.03958400	0.02459000
C	-2.84031200	-0.79341700	0.02268100
C	-3.08865100	0.61258500	-0.03971000
C	-6.47332200	-4.64331400	-0.65425900
C	-5.76762700	-3.37978700	-0.29478500
C	-3.96263700	-1.68183700	0.13322600
C	-5.31907131	-1.14986776	0.51725528
C	-5.38332031	-0.82808476	2.02245128
H	-6.38047631	-0.46435376	2.29480328
H	-4.65186731	-0.05570276	2.28155228
H	-5.16386631	-1.72622476	2.60709328
C	-5.64478469	-0.14322524	-1.83000028
H	-6.52678669	-0.76008824	-2.03229628
H	-4.75401469	-0.69064324	-2.15432228
H	-5.72004169	0.77967176	-2.41306928
C	-5.55753769	0.18860676	-0.32632028
C	-4.38468600	1.10876400	-0.07855100
C	-6.58374200	2.27021200	0.31893800
C	-7.59589100	3.31782700	0.63506600
C	5.75659600	3.68532600	-0.18744700
C	4.33459500	3.19375600	-0.15793300
C	3.28434200	4.12619800	-0.20437600
H	3.56457600	5.17174600	-0.25828400
C	1.91386700	3.84908600	-0.19155800
H	6.26860500	3.25378200	-1.05459300
H	6.27971100	3.32826600	0.70637800
H	5.82775800	4.77405000	-0.23452200
H	1.40844700	5.95844900	-0.29851300
H	0.28585300	4.85166900	-1.13316800
H	0.27426200	4.93829200	0.62664200
C	6.50733700	-2.60721300	0.14782600
F	6.92706600	-3.13902500	-1.01607400
F	7.19214100	-1.46865400	0.33428300
F	6.87611200	-3.46919100	1.11307500
C	-6.28684300	-2.23891700	0.17774500
C	-6.77089400	0.96876000	0.07129100
S	-4.00488500	-3.30633400	-0.47062200
S	-4.87337700	2.74723000	0.21587000
H	-7.35145400	-2.12626200	0.36716800
H	-7.75986800	0.51802400	0.06240300
H	-6.30776700	-4.90625000	-1.70565800
H	-6.11720700	-5.48341300	-0.04655000
H	-7.54938400	-4.53308100	-0.49227700