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Origins of the Stereocontrol in the [2+2] Cycloaddition between Achiral Ketenes and Chiral α-Alkoxy Aldehydes. A Pericyclic Alternative to the Aldol Reaction

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Supporting Information

	Total Energy	ZPVE
1a		
HF/6-31G*	-1069.49205	0.01711
MP2/6-31G*//HF/6-31G*	-1070.17406	
B3LYP/6-31G*	-1071.76037	0.01538
HF(L1A1)/6-31G*	-1069.49205	0.01706
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-1070.17407	
B3LYP(L1A1)/6-31G*	-1071.76038	0.01534
1b		
HF/6-31G*	-151.72467	0.03421
MP2/6-31G*//HF/6-31G*	-152.14448	
B3LYP/6-31G*	-152.59847	0.03174
1c		
HF/6-31G*	-229.79467	0.09618
MP2/6-31G*//HF/6-31G*	-230.47777	
B3LYP/6-31G*	-231.22925	0.08996
2a conformation **A**		
HF/6-31G*	-305.82747	0.12668
MP2/6-31G*//HF/6-31G*	-306.69078	
B3LYP/6-31G*	-307.65823	0.11770
HF(L1A1)/6-31G*	-305.82836	0.12660
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-306.69141	
B3LYP(L1A1)/6-31G*	-307.65883	0.11763
Structure **H**		
HF/6-31G*	-313.16311	0.13023
MP2/6-31G*//HF/6-31G*	-314.02881	
B3LYP/6-31G*	-315.04699	0.12146

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2a conformation **B**		
HF/6-31G*	-305.82714	0.12660
MP2/6-31G*//HF/6-31G*	-306.69029	
B3LYP/6-31G*	-307.65783	0.11760
HF(L1A1)/6-31G*	-305.82923	0.12658
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-306.69205	
B3LYP(L1A1)/6-31G*	-307.65951	0.11757
***syn*-TSa**		
HF/6-31G*	-1375.25842	0.14587
MP2/6-31G*//HF/6-31G*	-1376.83001	
B3LYP/6-31G*	-1379.38925	0.13499
HF(L1A1)/6-31G*	-1375.26442	0.14599
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-1376.83227	
B3LYP(L1A1)/6-31G*	-1379.39223	0.13510
***syn*-TS'a**		
HF/6-31G*	-1382.61485	0.14849
MP2/6-31G*//HF/6-31G*	-1384.19056	
B3LYP/6-31G*	-1386.78195	0.13763
***anti*-TSa**		
HF/6-31G*	-1375.25723	0.14599
MP2/6-31G*//HF/6-31G*	-1376.82922	
B3LYP/6-31G*	-1379.38790	0.13486
HF(L1A1)/6-31G*	-1375.26431	0.14614
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-1376.83224	
B3LYP(L1A1)/6-31G*	-1379.39134	0.13503
***anti*-TS'a**		
HF/6-31G*	-1382.60427	0.14831
MP2/6-31G*//HF/6-31G*	-1384.18080	
B3LYP/6-31G*	-1386.77337	0.13758
***syn*-TSc**		
HF/6-31G*	-457.48185	0.16452
MP2/6-31G*//HF/6-31G*	-458.79560	
B3LYP/6-31G*	-460.21781	0.15351
***syn*-TS'c**		
HF/6-31G*	-464.85667	0.16772
MP2/6-31G*//HF/6-31G*	-466.16444	
B3LYP/6-31G*	-467.63178	0.15728

***syn*-TS'c·2H$_2$O**		
HF/6-31G*	-616.94946	0.21920
B3LYP/6-31G*	-620.52252	
B3LYP(SCIPCM)/6-31G*	-620.58789	
***anti*-TSc**		
HF/6-31G*	-457.47825	0.16482
MP2/6-31G*//HF/6-31G*	-458.79058	
B3LYP/6-31G*	-460.21458	0.15389
***anti*-TS'c**		
HF/6-31G*	-464.85403	0.16753
MP2/6-31G*//HF/6-31G*	-466.16236	
B3LYP/6-31G*	-467.63099	0.15668
***anti*-TS'c 2H$_2$O**		
HF/6-31G*	-616.94730	0.21876
B3LYP/6-31G*	-620.52107	
B3LYP(SCIPCM)/6-31G*	-620.58581	
***syn*-TSe**		
HF/6-31G*	-535.54561	0.22506
MP2/6-31G*//HF/6-31G*	-537.12678	
B3LYP/6-31G*	-538.84462	0.20979
***syn*-TS'e**		
HF/6-31G*	-542.92839	0.22863
MP2/6-31G*//HF/6-31G*	-544.50913	
B3LYP/6-31G*	-546.26573	0.21415
***anti*-TSe**		
HF/6-31G*	-535.54306	0.22554
MP2/6-31G*//HF/6-31G*	-535.34233	
B3LYP/6-31G*	-538.84185	0.20974
***anti*-TS'e**		
HF/6-31G*	-542.92307	0.22860
MP2/6-31G*//HF/6-31G*	-544.50436	
B3LYP/6-31G*	-546.26350	0.21364
***syn*-3a**		
HF/6-31G*	-1375.36731	0.15072
MP2/6-31G*//HF/6-31G*	-1376.93310	
B3LYP/6-31G*	-1379.47064	0.13924
HF(L1A1)/6-31G*	-1375.37057	0.15066
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-1376.93578	

B3LYP(L1A1)/6-31G*	-1379.47282	0.13923
***anti*-3a**		
HF/6-31G*	-1375.37420	0.15063
MP2/6-31G*//HF/6-31G*	-1376.93945	
B3LYP/6-31G*	-1379.47642	0.13911
HF(L1A1)/6-31G*	-1375.37708	0.15057
MP2(L1A1)/6-31G*//HF(L1A1)/6-31G*	-1376.74179	
B3LYP(L1A1)/6-31G*	-1379.47840	0.13910
***syn*-3c**		
HF/6-31G*	-457.59404	0.17068
MP2/6-31G*//HF/6-31G*	-458.89147	
B3LYP/6-31G*	-460.30277	0.15851
***anti*-3c**		
HF/6-31G*	-457.59622	0.17052
MP2/6-31G*//HF/6-31G*	-458.89302	
B3LYP/6-31G*	-460.30460	0.15837
***syn*-3e**		
HF/6-31G*	-535.66136	0.23084
MP2/6-31G*//HF/6-31G*	-537.22694	
B3LYP/6-31G*	-538.93014	0.21493
***anti*-3e**		
HF/6-31G*	-535.66781	0.23056
MP2/6-31G*//HF/6-31G*	-537.23814	
B3LYP/6-31G*	-538.93550	0.21472

(*R*)-4-[(*S*)-1-Benzyloxyethyl]-3,3-dichloro-2-oxetanone (***syn*-3b**). Was obtained from dichloroacetyl chloride (2 eqs.) following the general procedure. The crude product was purified by flash chromatography (Ethyl acetate-hexanes 1:20) as a pale yelow oil. Yield: 70%. $[\alpha]_D^{25}$= +28.0 (c=0.15, CH_2Cl_2). IR(film) 1859 cm^{-1} ^{1}H-NMR ($CDCl_3$) δ 7.38-7.25 (m, 5H); 4.70 (d, 1H, J= 8.2 Hz); 4.66 (d, 1H, J= 11.0 Hz); 4.63 (d, 1H, J= 11.0 Hz); 3.85 (dq, 1H, J= 6.3 Hz, J'= 8.2 Hz); 1.38 (d, 3H, J= 6.3 Hz). ^{13}C-NMR($CDCl_3$) δ 160.8, 137.4, 128.5, 127.9, 127.7, 89.8, 79.3, 73.3, 72.2, 16.1.

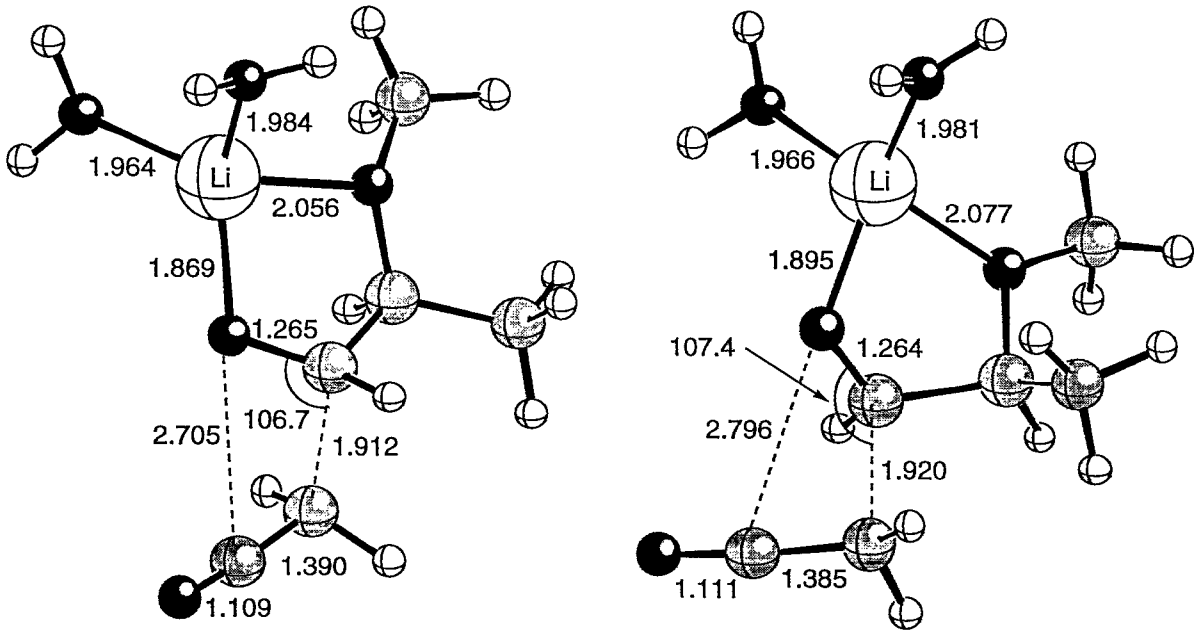
(4*S*,5*S*)-3,3-Dichloro-4-hydroxy-5-methyl-2-oxolanone (**4**). Was obtained from ***syn*-3b** as a colorless oil after 24 h following the general procedure. Yield: 68%. $[\alpha]_D^{25}$= -14.8 (c= 0.60, CH_2Cl_2). IR(film) 1779 cm^{-1}. ^{1}H-NMR($CDCl_3$) δ 4.97 (dq, 1H, J= 3.2 Hz, J'= 6.6 Hz). 4.36 (d, 1H, J= 3.2 Hz), 1.52 (d, 3H, J= 6.6 Hz). ^{13}C-NMR($CDCl_3$) δ 167.1, 81.4, 77.9, 77.4, 13.7.

(4*S*,5*S*)-3,3-Dichloro-4-[4-chlorobenzoyloxy]-5-methyl-2-oxolanone (**5**). Triethylamine (0.3 mL, 2 mmol) was added over a solution of compound **4** (0.4 g, 2 mmol) in CH_2Cl_2 (10 mL) at 0-5°C. p-Nitrobenzoyl chloride (0.44 g, 2.4 mmol) was added in one portion and the ice-water but was removed. The reaction mixture was stirred for 12 h at room temperature and then washed with 0.1 N HCl (2x10 mL) and saturated solution of $NaHCO_3$ (2x10 mL). The organic layer was dried ($MgSO_4$) and the solvent was evaporated under reduced pressure. The title product was crystallized from ethyl acetate-hexanes as pale yelow needles. Yield: 72%. m.p. 101-102°C (from Ethyl acetate-hexanes). IR(film) 1736, 1800 cm^{-1}. ^{1}H-NMR($CDCl_3$) δ 8.34 (d, 2H, J= 9.0 Hz), 8.24 (d, 2H, J= 9.0 Hz), 5.94 (d, 1H, J= 3.4 Hz), 5.22 (dq, 1H, J= 3.4 Hz, J'= 6.5 Hz), 1.51 (d, 3H, J= 6.5 Hz). ^{13}C-NMR($CDCl_3$) δ 165.7, 162.6, 151.2, 133.0, 131.3, 123.9, 78.2, 77.8, 76.2, 14.2. Anal. Calcd. for $C_{12}H_9NO_6Cl_2$: C, 43.13; H, 2.72; N, 4.19. Found: C; 44.01, H, 2.74; N, 4.19 %.

Table 1. Main Geometric Features[a-c] of Saddle Points **TSa,c,e** and **TS'a,c,e**.

Method	r(O1-C2)	r(C3-C4)	ω	ξ	ϕ	α_N	α'_N
				***syn*-TSa**			
HF/6-31G*	1.500	2.452	53.1	68.5	178.5	67.7	103.1
B3LYP/6-31G*	1.556	2.585	60.2	65.7	175.0	65.6	105.0
HF(L1A1)/6-31G*	1.463	2.423	49.8	70.7	170.7	68.0	103.4
B3LYP(L1A1)/6-31G*	1.526	2.546	57.0	65.4	175.7	66.2	105.2
				***syn*-TS'a**			
HF/6-31G*	2.697	1.910	47.4	27.8	95.9	106.1	69.3
B3LYP/6-31G*	2.573	1.774	48.5	20.4	97.2	105.3	69.4
				***anti*-TSa**			
HF/6-31G*	1.499	2.441	51.9	9.6	121.6	68.0	103.5
B3LYP/6-31G*	1.553	2.582	59.4	10.3	121.6	65.6	105.3
HF(L1A1)/6-31G*	1.456	2.417	48.6	1.0	113.2	68.2	103.6
B3LYP(L1A1)/6-31G*	1.519	2.541	56.2	4.8	116.2	66.3	105.4
				***anti*-TS'a**			
HF/6-31G*	2.754	1.979	37.2	69.9	184.3	106.9	70.3
B3LYP/6-31G*	2.736	1.765	45.3	70.4	184.2	108.3	65.4
				***syn*-TSc**			
HF/6-31G*	1.978	2.002	37.9	61.6	179.9	89.7	86.9
B3LYP/6-31G*	1.798	2.258	49.8	61.1	179.6	79.3	95.6
				***syn*-TS'c**			
HF/6-31G*	2.827	1.980	51.3	32.8	147.4	106.9	67.9
B3LYP/6-31G*	2.598	1.686	48.9	43.1	156.9	106.4	66.9
				***anti*-TSc**			
HF/6-31G*	2.106	1.907	34.9	46.9	158.7	94.4	82.3
B3LYP/6-31G*	1.801	2.249	48.8	52.9	163.2	79.7	95.5
				***anti*-TS'c**			
HF/6-31G*	2.916	2.035	57.6	78.0	167.7	107.3	66.8
B3LYP/6-31G*	2.975	1.914	63.4	78.0	168.2	108.8	62.0
				***syn*-TSe**			
HF/6-31G*	2.216	1.922	38.0	67.3	174.6	98.0	81.5
B3LYP/6-31G*	1.788	2.419	45.8	62.5	181.1	76.9	100.8
				***syn*-TS'e**			
HF/6-31G*	2.714	2.014	48.9	21.8	96.7	108.3	74.4
B3LYP/6-31G*	2.560	1.729	49.4	18.6	98.6	108.0	70.8
				***anti*-TSe**			
HF/6-31G*	2.362	1.820	36.1	23.5	135.7	103.2	76.3
B3LYP/6-31G*	1.692	2.495	60.3	6.6	118.4	72.4	103.1
				***anti*-TS'e**			
HF/6-31G*	2.827	2.074	45.4	68.7	182.9	109.0	72.8
B3LYP/6-31G*	2.872	1.939	51.5	69.4	183.0	110.8	68.0

[a]See Figure 4 for atom numbering and for the geometries of the corresponding saddle points. [b]Definition of dihedral angles: ω=O1-C4-C3-C2, ξ=C3-C4-C6-H7, ϕ=C3-C4-C6-O8, α_N=C3-C4-O1, $\alpha_{N'}$=O1-C2-C3.[c]Distances and angles are given in Å and deg, respectively.



syn-TS'c·2H_2O *anti*-TS'c·2H_2O

Figure 1. Computer plot of transition structures ***syn*-TS'c·2H_2O** and ***anti*-TS'c·2H_2O** computed at the HF/6-31G* level. Bond distances and angles are given in A and deg., respectively.

Table 2. Relative energies (kcal/mol)[a,b] of transition structures ***syn*-TS'c·2H_2O** and ***anti*-TS'c·2H_2O** computed at different theoretical levels.

Method	***syn*-TS'c·2H_2O**	***anti*-TS'c·2H_2O**
HF/6-31G*	0.00	+1.11
B3LYP/6-31G*	0.00	+0.66
B3LYP(SCIPCM)/6-31G*[c]	0.00	+1.06

[a]Single-point energies calculated on fully optimized HF/6-31G* geometries. [b]ZPVE corrections, computed at the HF/6-31G* level and scaled by 0.89, have been included. [c]Computed with ε=4.20 (diethyl ether).

1a (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.037383	0.000000
2	6	-0.000006	1.346042	0.000000
3	8	-0.000001	2.487073	0.000000
4	17	-1.488288	-0.829336	0.000000
5	17	1.488291	-0.829319	0.000000

1a (HF/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000010	.036753	.000000
2	6	.000010	1.345653	.000000
3	8	-.000005	2.486486	.000000
4	17	-1.488806	-.828992	.000000
5	17	1.488801	-.829026	.000000

1a (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.030352	.000000
2	6	.000000	1.351632	.000000
3	8	.000000	2.521600	.000000
4	17	1.506949	-.837199	.000000
5	17	-1.506950	-.837196	.000000

1a (B3lyp/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.030352	.000000
2	6	.000000	1.351632	.000000
3	8	.000000	2.521600	.000000
4	17	1.506949	-.837199	.000000
5	17	-1.506950	-.837196	.000000

1b (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.000000	.000000	-1.199586
2	6	.000000	.000000	.106289
3	8	.000000	.000000	1.251082
4	1	.000000	.933626	-1.724436
5	1	.000000	-.933626	-1.724436

1b (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	.000000	.000000	1.272387

2	6	.000000	.000000	.101178
3	6	.000000	.000000	-1.213679
4	1	.000000	.939370	-1.752043
5	1	.000000	-.939370	-1.752043

1c (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	.000000	.000000	2.125722
2	6	.000000	.000000	.974162
3	6	.000000	.000000	-.329928
4	6	.000000	-1.306514	-1.091433
5	6	.000000	1.306514	-1.091433
6	1	.000000	-2.164783	-.429588
7	1	.000000	2.164783	-.429588
8	1	-.877155	-1.377471	-1.728703
9	1	-.877155	1.377471	-1.728703
10	1	.877155	-1.377471	-1.728703
11	1	.877155	1.377471	-1.728703

1c (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	.000000	.000000	2.156065
2	6	.000000	.000000	.978770
3	6	.000000	.000000	-.338060
4	6	.000000	-1.307754	-1.102043
5	6	.000000	1.307754	-1.102043
6	1	.000000	-2.176960	-.437466
7	1	.000000	2.176960	-.437466
8	1	-.885590	-1.380158	-1.748335
9	1	-.885590	1.380158	-1.748335
10	1	.885590	-1.380158	-1.748335
11	1	.885590	1.380158	-1.748335

2a (HF/6-31G* epsi=1) conformation A

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.957745	-.705206	-.356728
2	8	1.886903	-1.194697	.197135
3	6	.075315	.363060	.266450
4	1	.694973	-.974288	-1.385793
5	1	.023532	.173707	1.335658
6	8	-1.196532	.340474	-.310040
7	6	.682656	1.737689	.011290
8	1	.752059	1.929791	-1.054146
9	1	1.673362	1.801102	.445701
10	1	.051244	2.499421	.451872
11	6	-2.034172	-.684884	.138658
12	1	-2.218941	-.601411	1.206555
13	1	-1.617390	-1.669312	-.063499
14	1	-2.971069	-.589188	-.391124

2a (HF/6-31G* epsi=9.08) conformation A

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	.957166	-.728705	-.336467
2	8	1.942073	-1.135088	.190180
3	6	.066145	.346679	.262329
4	1	.645412	-1.086892	-1.323640
5	1	-.000570	.169526	1.333103
6	8	-1.194360	.318729	-.332540
7	6	.679495	1.718959	.004868
8	1	.755771	1.905259	-1.061097
9	1	1.667341	1.781085	.445948
10	1	.046259	2.483866	.436708
11	6	-2.065008	-.663835	.151347
12	1	-2.268066	-.520035	1.209078
13	1	-1.666184	-1.666086	.007903
14	1	-2.988457	-.574433	-.401585

2a (B3lyp/6-31G* epsi=1) conformation A

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.955371	-.691699	-.364648
2	8	1.876137	-1.244182	.192447
3	6	.077244	.382153	.276940
4	1	.695870	-.903234	-1.428243
5	1	.034532	.188728	1.360415
6	8	-1.219087	.372944	-.296887
7	6	.691424	1.758912	.014183
8	1	.764255	1.947635	-1.062322
9	1	1.691264	1.820569	.454090
10	1	.055379	2.532130	.455094
11	6	-2.017937	-.717569	.130963
12	1	-2.174799	-.697440	1.220342
13	1	-1.576441	-1.689965	-.136816
14	1	-2.983077	-.619309	-.371670

2a (B3lyp/6-31G* epsi=9.08) conformation A

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.953300	-0.710962	-0.350409
2	8	1.923940	-1.194799	0.187724
3	6	0.068759	0.368096	0.273006
4	1	0.651003	-0.993398	-1.385793
5	1	0.014650	0.184709	1.358001
6	8	-1.218658	0.357849	-0.314873
7	6	0.690667	1.742449	0.009552
8	1	0.762217	1.930329	-1.067135
9	1	1.691323	1.797313	0.448510
10	1	0.058776	2.518590	0.450722
11	6	-2.044119	-0.701343	0.142199
12	1	-2.215284	-0.636358	1.227349
13	1	-1.616564	-1.690879	-0.083273
14	1	-3.000015	-0.604144	-0.377278

Structure H (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.004851	.534757	.396846

2	6	1.483878	.246992	.333031
3	8	1.918239	-.776956	-.119118
4	3	.574810	-1.969455	-.684534
5	8	-.648444	-.628818	-.074056
6	1	2.156971	1.013586	.704447
7	1	-.251883	.691853	1.442189
8	1	-.109620	1.631517	-1.467612
9	6	-.322522	1.788415	-.416304
10	1	-1.364291	2.056996	-.307709
11	1	.266186	2.627367	-.063080
12	6	-2.058531	-.688088	.139873
13	1	-2.377831	-1.682140	-.132528
14	1	-2.281433	-.511049	1.183651
15	1	-2.566943	.033962	-.481044

Structure H (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.007854	.537857	.395308
2	6	1.490744	.259981	.333207
3	8	1.945457	-.781872	-.123146
4	3	.578785	-1.969187	-.663945
5	8	-.648607	-.651068	-.079472
6	1	2.166297	1.047046	.702311
7	1	-.255916	.695969	1.454052
8	1	-.107308	1.653517	-1.476377
9	6	-.333196	1.797710	-.415230
10	1	-1.390513	2.050746	-.307510
11	1	.245613	2.650460	-.045894
12	6	-2.078002	-.690563	.139487
13	1	-2.410297	-1.688996	-.148869
14	1	-2.299599	-.521414	1.198123
15	1	-2.583832	.053848	-.479686

syn-TSa (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.146949	-.942843	.771027
2	8	-.254303	-.579196	1.124464
3	6	-.862607	-.493852	.021035
4	6	1.510173	.038476	-.198475
5	8	1.553500	-1.979149	1.130654
6	17	3.046162	-.251967	-.972906
7	17	1.289284	1.742125	.211252
8	6	-1.954865	.513137	-.184457
9	1	-.688938	-1.226107	-.746717
10	1	-1.433334	1.373412	-.597315
11	8	-2.802302	.071972	-1.195443
12	6	-2.632730	.940884	1.116731
13	1	-1.913246	1.423847	1.763788
14	1	-3.062948	.105168	1.654666
15	1	-3.418192	1.647909	.880851
16	6	-3.738844	-.922372	-.870715
17	1	-4.523605	-.539231	-.229608
18	1	-4.173383	-1.250739	-1.802567
19	1	-3.272541	-1.776532	-.383268

syn-TSa (HF/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.162278	-.959158	-.743080
2	8	.213110	-.664874	-1.120252
3	6	.860509	-.510146	-.034862
4	6	-1.474340	.058384	.223135
5	8	-1.647582	-1.969519	-1.086312
6	17	-3.003848	-.199171	1.048734
7	17	-1.309443	1.737840	-.309978
8	6	1.970849	.491135	.062907
9	1	.703706	-1.194160	.778166
10	1	1.453748	1.423619	.279084
11	8	2.733107	.214792	1.187227
12	6	2.733969	.665452	-1.253608
13	1	2.066255	1.034661	-2.020339
14	1	3.176887	-.258352	-1.603296
15	1	3.520917	1.392376	-1.100317
16	6	3.738771	-.766865	1.083555
17	1	4.555840	-.436050	.456219
18	1	4.106745	-.930683	2.084091
19	1	3.347889	-1.704782	.693962

syn-TSa (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.167405	-1.004903	.692310
2	8	-.270017	-.617158	1.136501
3	6	-.911324	-.506983	.025413
4	6	1.603350	.060338	-.136470
5	8	1.553917	-2.112415	.928721
6	17	3.167691	-.170849	-.876546
7	17	1.232806	1.753279	.192744
8	6	-1.997155	.510179	-.140682
9	1	-.706159	-1.196775	-.793447
10	1	-1.464229	1.403557	-.515415
11	8	-2.853815	.138596	-1.204311
12	6	-2.687738	.899698	1.173586
13	1	-1.956443	1.330168	1.862190
14	1	-3.151623	.041011	1.667136
15	1	-3.457151	1.647430	.962443
16	6	-3.758504	-.922348	-.920717
17	1	-4.531729	-.624404	-.201258
18	1	-4.235769	-1.175099	-1.869694
19	1	-3.242230	-1.815263	-.535263

syn-TSa (B3lyp/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.171420	-1.007772	.695220
2	8	-.240393	-.672110	1.142842
3	6	-.897120	-.516953	.036642
4	6	1.567642	.072104	-.147353
5	8	1.617753	-2.097102	.924248
6	17	3.118275	-.143605	-.940271
7	17	1.236509	1.757253	.259509
8	6	-1.993923	.493731	-.071269
9	1	-.703096	-1.182237	-.803546
10	1	-1.462574	1.430835	-.323253
11	8	-2.789581	.220707	-1.204552

12	6	-2.745955	.732774	1.247982
13	1	-2.050408	1.084015	2.014358
14	1	-3.228932	-.176119	1.616921
15	1	-3.508805	1.498868	1.086376
16	6	-3.737030	-.834444	-1.058759
17	1	-4.551816	-.565243	-.376353
18	1	-4.151504	-1.006290	-2.053653
19	1	-3.266636	-1.764461	-.702991

syn-TS'a (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.484905	-.308700	.592615
2	6	.267964	-1.076369	.053439
3	8	.321352	-1.506049	-1.140014
4	3	1.699422	-.835417	-2.084026
5	8	2.187818	.182240	-.539691
6	1	-.153893	-1.731237	.812050
7	1	1.185724	.529142	1.209976
8	6	2.350486	-1.266908	1.408044
9	1	2.617896	-2.140236	.823397
10	1	3.260775	-.780629	1.734494
11	1	1.817858	-1.594707	2.293241
12	6	3.049337	1.286599	-.309325
13	1	3.480359	1.558945	-1.260828
14	1	2.484778	2.122965	.082009
15	1	3.841424	1.022501	.376980
16	6	-1.180049	.168707	.104196
17	6	-2.164707	-.626550	-.574835
18	8	-2.836920	-1.336771	-1.082554
19	17	-1.731073	.511161	1.733004
20	17	-.848857	1.591396	-.872179

syn-TS'a (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.460520	-.662341	-.205882
2	6	-.180402	-.742190	.678585
3	8	-.230200	-.162439	1.851587
4	3	-1.663245	.892908	2.043638
5	8	-2.221136	.465451	.284033
6	1	.215030	-1.774120	.650605
7	1	-1.210366	-.475634	-1.258161
8	6	-2.252480	-1.964691	-.080473
9	1	-2.453445	-2.201205	.969803
10	1	-3.206061	-1.896979	-.611934
11	1	-1.688090	-2.793453	-.519868
12	6	-3.170982	1.005506	-.650215
13	1	-3.657771	1.848094	-.155713
14	1	-2.656757	1.357559	-1.551216
15	1	-3.925649	.260662	-.918532
16	6	1.142204	.064100	-.184887
17	6	2.135474	-.011110	.851433
18	8	2.869360	-.243522	1.683231
19	17	1.763452	-.812102	-1.605532
20	17	.762953	1.775913	-.496708

anti-TSa (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.025110	1.254423	.210012
2	8	.401066	1.020246	.611892
3	6	.903823	.358795	-.334461
4	6	-1.498992	-.058576	-.082204
5	8	-1.362463	2.354166	.004721
6	17	-3.103498	-.096850	-.770138
7	17	-1.280272	-1.315700	1.143225
8	6	2.037825	-.602790	-.090300
9	1	.681181	.629676	-1.351182
10	1	2.095699	-.803210	.973244
11	8	3.180551	.054265	-.554811
12	6	1.856378	-1.884656	-.887276
13	1	1.798084	-1.663555	-1.946713
14	1	.961764	-2.412133	-.583309
15	1	2.718161	-2.518107	-.719641
16	6	3.815070	.919097	.357620
17	1	4.136447	.376415	1.240576
18	1	3.166985	1.735354	.659377
19	1	4.678566	1.321733	-.149593

anti-TSa (HF/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.022426	1.245011	.236122
2	8	.376488	1.030897	.606087
3	6	.892914	.350330	-.332801
4	6	-1.482054	-.072226	-.105815
5	8	-1.414997	2.339702	.092682
6	17	-3.089783	-.089495	-.815396
7	17	-1.319517	-1.322427	1.139181
8	6	2.049325	-.577967	-.074029
9	1	.678517	.611363	-1.352245
10	1	2.135642	-.739216	.993796
11	8	3.144046	.117315	-.589935
12	6	1.894195	-1.891614	-.824058
13	1	1.807999	-1.708563	-1.888742
14	1	1.026294	-2.441137	-.482771
15	1	2.782103	-2.486986	-.655007
16	6	3.897139	.882959	.327357
17	1	4.313501	.248953	1.101602
18	1	3.296186	1.662863	.783982
19	1	4.699021	1.333115	-.236287

anti-TSa (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.023443	1.242064	.189116
2	8	.432664	.959675	.669899
3	6	.950581	.317229	-.316339
4	6	-1.594172	-.037218	-.029290
5	8	-1.320181	2.367939	-.085162
6	17	-3.222184	-.010364	-.662418
7	17	-1.282457	-1.431909	1.011155
8	6	2.101201	-.622641	-.091940
9	1	.713420	.615960	-1.337912
10	1	2.160332	-.862768	.978559
11	8	3.266446	.081323	-.522696

12	6	1.975064	-1.884745	-.935879
13	1	1.912540	-1.628464	-1.998349
14	1	1.084380	-2.453418	-.652878
15	1	2.861883	-2.506287	-.782353
16	6	3.768315	1.027946	.419015
17	1	4.028874	.538352	1.367815
18	1	3.052117	1.834973	.621355
19	1	4.668652	1.452985	-.029207

anti-TSa (B3lyp/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.010536	1.241929	.197504
2	8	.424568	.979416	.643494
3	6	.933421	.298070	-.331388
4	6	-1.570987	-.045689	-.038075
5	8	-1.349637	2.364596	-.053043
6	17	-3.202646	-.019269	-.684222
7	17	-1.287605	-1.425212	1.031564
8	6	2.093110	-.623249	-.090488
9	1	.698910	.579769	-1.357231
10	1	2.163046	-.846149	.982367
11	8	3.227933	.118175	-.538750
12	6	1.999202	-1.897943	-.918340
13	1	1.931622	-1.657088	-1.984069
14	1	1.124501	-2.487574	-.627747
15	1	2.902309	-2.493029	-.757038
16	6	3.772406	1.024112	.422443
17	1	4.079227	.490844	1.331933
18	1	3.062863	1.817213	.692649
19	1	4.649185	1.471312	-.049227

anti-TS'a (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.527885	.430245	-.103610
2	6	-.474729	-.635783	-.450879
3	8	-.556158	-1.710202	.207620
4	3	-2.321591	-2.147610	.304749
5	8	-2.724691	-.332293	-.304939
6	1	-.251265	-.689778	-1.511744
7	6	-3.860390	.387826	-.765252
8	1	-4.672624	-.317923	-.847664
9	1	-4.130854	1.165921	-.064601
10	1	-3.656999	.819209	-1.736386
11	6	1.330786	.104070	-.122896
12	6	1.517513	-.224921	1.246389
13	8	1.519564	-.528726	2.308343
14	17	2.384628	-.919265	-1.085807
15	17	1.547544	1.820108	-.408103
16	6	-1.497478	.964861	1.319762
17	1	-2.405493	1.515595	1.530271
18	1	-1.423027	.156891	2.038591
19	1	-.675133	1.653662	1.468896
20	1	-1.503376	1.236902	-.824416

anti-TS'a (B3lyp/6-31G* epsi=1)

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	-1.492675	.416479	-.119782
2	6	-.357262	-.616150	-.400147
3	8	-.441594	-1.711090	.307472
4	3	-2.170312	-2.188460	.344720
5	8	-2.665260	-.433073	-.294467
6	1	-.227880	-.735501	-1.496441
7	6	-3.849504	.246527	-.745967
8	1	-4.636646	-.506089	-.817580
9	1	-4.153461	1.021745	-.035380
10	1	-3.678873	.691117	-1.732041
11	6	1.243805	.083494	-.151027
12	6	1.455592	.014287	1.261214
13	8	1.461014	-.084851	2.390399
14	17	2.409737	-1.059419	-.870462
15	17	1.445200	1.762635	-.707414
16	6	-1.511398	1.045049	1.268627
17	1	-2.455978	1.568974	1.441041
18	1	-1.402078	.283928	2.048068
19	1	-.720809	1.795863	1.377729
20	1	-1.511907	1.184672	-.900388

syn-TSc (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.464030	-.032872	.010253
2	8	.606519	-.688045	.754638
3	6	.205582	-.198765	-.349146
4	6	1.672203	1.009225	-.513901
5	8	3.258575	-.809334	.144923
6	1	2.183988	1.517719	-1.323424
7	1	1.341225	1.668615	.267254
8	6	-1.086215	.623672	-.429530
9	1	.316023	-.787150	-1.260152
10	1	-1.005917	1.304691	-1.268040
11	8	-2.122254	-.251040	-.802196
12	6	-1.391862	1.409191	.839445
13	1	-.697885	2.234489	.960181
14	1	-1.320452	.786115	1.720303
15	1	-2.390172	1.827644	.773825
16	6	-2.571818	-1.185364	.144915
17	1	-3.129548	-.706190	.943346
18	1	-3.235189	-1.857684	-.381792
19	1	-1.756313	-1.751424	.577361

syn-TSc (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.464030	-.032872	.010253
2	8	.606519	-.688045	.754638
3	6	.205582	-.198765	-.349146
4	6	1.672203	1.009225	-.513901
5	8	3.258574	-.809334	.144923
6	1	2.183988	1.517719	-1.323424
7	1	1.341225	1.668615	.267254
8	6	-1.086215	.623672	-.429530
9	1	.316023	-.787150	-1.260152
10	1	-1.005917	1.304691	-1.268040
11	8	-2.122254	-.251040	-.802196

12	6	-1.391862	1.409191	.839445
13	1	-.697885	2.234489	.960181
14	1	-1.320452	.786115	1.720303
15	1	-2.390172	1.827644	.773825
16	6	-2.571818	-1.185364	.144915
17	1	-3.129548	-.706190	.943346
18	1	-3.235189	-1.857684	-.381792
19	1	-1.756313	-1.751424	.577361

syn-TS'c (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.965735	.462986	.125929
2	6	.357526	-.105890	-.441308
3	8	.563866	-1.342962	-.324619
4	3	-.963959	-2.275313	-.222798
5	8	-1.901269	-.602466	-.032759
6	1	.671384	.378782	-1.360630
7	1	-.872263	.649275	1.189486
8	1	-1.612681	1.511184	-1.643918
9	6	-1.390127	1.727381	-.604893
10	1	-2.259414	2.185654	-.152196
11	1	-.589834	2.458902	-.574189
12	6	-3.206749	-.367988	.474511
13	1	-3.731352	-1.311682	.452110
14	1	-3.155452	-.008951	1.495534
15	1	-3.736737	.343328	-.141305
16	6	1.682047	.809860	.710866
17	6	2.848872	.208863	.276225
18	8	3.720662	-.323073	-.161024
19	1	1.722718	1.883401	.596917
20	1	1.434429	.472771	1.705828

syn-TS'c (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.975598	.462843	.190473
2	6	.422829	-.033507	-.307468
3	8	.677995	-1.318792	-.102880
4	3	-.823456	-2.246546	-.215204
5	8	-1.865434	-.633602	-.143692
6	1	.580290	.327147	-1.343720
7	1	-.967950	.545598	1.288865
8	6	-1.404796	1.777175	-.448861
9	1	-1.507988	1.664145	-1.532580
10	1	-2.351383	2.144130	-.044602
11	1	-.658360	2.555932	-.256628
12	6	-3.224658	-.470285	.298298
13	1	-3.727571	-1.423319	.123965
14	1	-3.254562	-.228578	1.367150
15	1	-3.734072	.308270	-.274245
16	6	1.573645	.825559	.575812
17	6	2.771946	.190308	.191799
18	8	3.696820	-.319775	-.218105
19	1	1.657215	1.906308	.403569
20	1	1.379492	.604798	1.630933

syn-TS'c-2H2O (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.042060	1.383107	-.191145
2	6	-.873716	.221693	.391476
3	8	-.492178	-.952579	.115893
4	8	2.527617	-1.591271	1.599752
5	8	2.122690	-2.013325	-1.480843
6	1	1.564647	-2.453126	-2.111048
7	1	2.992617	-2.383436	-1.570317
8	1	2.434086	-2.431106	2.034275
9	1	2.783510	-.966817	2.268315
10	3	1.371993	-1.074241	.071716
11	8	1.293743	.979830	.055127
12	1	-1.212932	.425553	1.407040
13	1	-.184304	1.421676	-1.267189
14	1	-.122769	2.710870	1.503721
15	6	-.361993	2.727502	.446034
16	1	.194242	3.532503	-.016628
17	1	-1.413993	2.966213	.337252
18	6	2.301200	1.751296	-.564827
19	1	3.233542	1.224067	-.426411
20	1	2.104115	1.855258	-1.626354
21	1	2.381384	2.730159	-.111936
22	6	-2.559754	.468906	-.476142
23	6	-3.176702	-.725740	-.124795
24	8	-3.590932	-1.691021	.231839
25	1	-3.156118	1.314296	-.163807
26	1	-2.323382	.462951	-1.529807

anti-TSc (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.391006	-.096028	.108941
2	8	.681894	-1.091495	.155546
3	6	.175413	-.041307	-.340149
4	6	1.650804	1.041164	.471835
5	8	3.225284	-.687723	-.365554
6	1	2.216909	1.955615	.343013
7	1	1.190545	.942634	1.436658
8	6	-1.138462	.512086	.196906
9	1	.311358	.167451	-1.398497
10	1	-1.143081	.390028	1.277481
11	8	-2.160709	-.253654	-.380732
12	6	-1.397602	1.958485	-.188473
13	1	-1.348627	2.076588	-1.265803
14	1	-.679413	2.629672	.266940
15	1	-2.392204	2.241466	.133530
16	6	-2.437847	-1.491568	.220770
17	1	-2.709263	-1.359422	1.265458
18	1	-1.596199	-2.167800	.158174
19	1	-3.281646	-1.910250	-.310012

anti-TSc (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.319974	-.169840	.072640
2	8	.721397	-.946105	.346997
3	6	.129145	.000789	-.282916
4	6	1.935629	1.094103	.516020

5	8	3.102894	-.806115	-.533831
6	1	2.684684	1.879142	.407195
7	1	1.312375	1.153304	1.396473
8	6	-1.204339	.540377	.203297
9	1	.337453	.169911	-1.346968
10	1	-1.242650	.445773	1.299299
11	8	-2.206528	-.281109	-.398696
12	6	-1.469176	1.971703	-.241095
13	1	-1.399971	2.051110	-1.331277
14	1	-.746609	2.660209	.205675
15	1	-2.478981	2.266325	.058470
16	6	-2.386529	-1.553701	.214737
17	1	-2.651161	-1.445160	1.276956
18	1	-1.491645	-2.182947	.137619
19	1	-3.213824	-2.031619	-.315310

anti-TS'c (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.984461	.480635	-.289299
2	6	.290302	-.383096	-.274272
3	8	.438461	-1.146789	.709842
4	3	-1.188041	-1.803511	1.181939
5	8	-1.983258	-.519497	-.048087
6	1	.579135	-.740271	-1.257219
7	6	-3.255965	-.293902	-.637139
8	1	-3.889438	-1.120242	-.353101
9	1	-3.688865	.629389	-.277313
10	1	-3.165362	-.263455	-1.715042
11	6	1.774540	1.006538	-.189927
12	6	2.871422	.177714	-.202251
13	8	3.681719	-.585018	-.233735
14	1	1.772577	1.692380	-1.024067
15	1	1.645761	1.456825	.780410
16	1	-.758331	1.199778	1.736600
17	1	-2.103709	1.909237	.859917
18	6	-1.080045	1.568472	.768899
19	1	-.480107	2.429893	.505028
20	1	-1.137674	.889260	-1.281253

anti-TS'c (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-.967690	.478667	-.295356
2	6	.335654	-.375595	-.223916
3	8	.431203	-1.155185	.791323
4	3	-1.208818	-1.808644	1.156461
5	8	-1.980393	-.550427	-.075939
6	1	.608591	-.783858	-1.213102
7	6	-3.262615	-.282715	-.669652
8	1	-3.906650	-1.128642	-.423034
9	1	-3.699747	.635937	-.266175
10	1	-3.166263	-.203111	-1.757566
11	6	1.720583	.941815	-.124550
12	6	2.877764	.205903	-.215817
13	8	3.746703	-.528988	-.315840
14	1	1.629342	1.669322	-.934809
15	1	1.594325	1.369497	.871009
16	1	-.819668	1.216101	1.742104
17	1	-2.147306	1.924462	.803962

18	6	-1.111219	1.578306	.749842
19	1	-.501263	2.451850	.499247
20	1	-1.099872	.872884	-1.310694

anti-TS'c-H2O (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.056805	-1.439108	-.233076
2	6	-.826593	-.196334	-.440225
3	8	-.503081	.844229	.199670
4	8	1.909950	2.425900	-1.113727
5	8	2.404206	1.295586	1.840810
6	1	2.022335	1.775329	2.566574
7	1	3.177394	.857184	2.174657
8	1	1.209181	2.925981	-1.515323
9	1	2.684241	2.975283	-1.120714
10	3	1.383170	1.027758	.164226
11	8	1.332368	-.913260	-.572518
12	1	-1.104294	-.088098	-1.488788
13	6	2.240958	-1.804883	-1.180492
14	1	3.148317	-1.252160	-1.371835
15	1	2.462879	-2.642861	-.530800
16	1	1.842483	-2.171069	-2.119293
17	6	-2.549062	-.751945	.200191
18	6	-3.260611	.420557	.007839
19	8	-3.738829	1.399451	-.208672
20	1	-3.000249	-1.579164	-.329641
21	1	-2.398375	-.921196	1.254332
22	1	.179148	-1.216625	1.908664
23	1	.930486	-2.677996	1.289275
24	6	.085247	-2.009985	1.176736
25	1	-.805977	-2.587630	1.392511
26	1	-.214459	-2.205313	-.952647

syn-TSe (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.113948	-.767683	-.159289
2	8	.018206	-.995217	-1.148387
3	6	.163979	-.435805	-.011127
4	6	-1.427473	.408549	.244039
5	8	-2.660977	-1.722312	-.316388
6	6	-1.837357	.804303	1.666641
7	6	-1.572757	1.519087	-.801393
8	6	1.304331	.594203	.203822
9	1	.155870	-1.072955	.886724
10	1	.958371	1.408944	.830243
11	8	2.308036	-.008563	.987518
12	6	1.849777	1.160225	-1.101967
13	1	1.129517	1.819142	-1.570603
14	1	2.071048	.372209	-1.807432
15	1	2.749319	1.732634	-.899242
16	6	3.038387	-1.051970	.400987
17	1	3.757361	-.678148	-.321538
18	1	3.578213	-1.540843	1.201212
19	1	2.396336	-1.773337	-.090862
20	1	-1.158466	1.579679	2.000404
21	1	-2.846976	1.200498	1.723234
22	1	-1.749532	-.026225	2.358116
23	1	-.979513	2.366456	-.481914

24	1	-1.213461	1.177003	-1.761209
25	1	-2.599849	1.858227	-.899352

syn-TSe (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.710987	-.779330	-.495992
2	8	-.205918	-.497777	-1.216249
3	6	.414113	-.396463	-.097471
4	6	-1.930738	.372811	.267022
5	8	-2.116841	-1.898024	-.594007
6	6	-3.099618	.279293	1.222593
7	6	-1.557932	1.776185	-.142753
8	6	1.545579	.587285	.101727
9	1	.288198	-1.158362	.677076
10	1	1.094376	1.503193	.512147
11	8	2.400823	.137574	1.143585
12	6	2.252991	.956666	-1.209397
13	1	1.545762	1.432038	-1.894080
14	1	2.662920	.079055	-1.717341
15	1	3.065751	1.657778	-.997687
16	6	3.244932	-.958594	.818979
17	1	4.034220	-.677436	.109293
18	1	3.709870	-1.271912	1.756579
19	1	2.684708	-1.809266	.402189
20	1	-2.896985	.886047	2.115080
21	1	-4.029128	.670594	.780246
22	1	-3.285715	-.751204	1.536752
23	1	-1.169860	2.352776	.710284
24	1	-.827908	1.808801	-.952020
25	1	-2.450762	2.316599	-.493397

syn-TS'e (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.252657	-.013337	.599873
2	6	-.052196	-.796938	.391791
3	8	-.087958	-1.602961	-.580968
4	3	1.298427	-1.480800	-1.706594
5	8	1.915899	.005980	-.658525
6	1	-.485501	-1.115341	1.334609
7	1	1.071282	1.007474	.907871
8	6	2.087718	-.725413	1.663405
9	1	2.262608	-1.760505	1.391032
10	1	3.044565	-.238167	1.800836
11	1	1.572921	-.706136	2.617091
12	6	2.969595	.944512	-.801870
13	1	3.276486	.923883	-1.836772
14	1	2.621824	1.939583	-.554103
15	1	3.810854	.685029	-.174937
16	6	-1.444484	.626203	.086319
17	6	-2.435541	-.295424	-.201097
18	8	-3.143969	-1.133611	-.393713
19	6	-1.724956	1.406298	1.376689
20	6	-1.049701	1.465149	-1.133730
21	1	-1.819716	2.182275	-1.395118
22	1	-.151809	2.021328	-.898848
23	1	-.850086	.845809	-1.999273
24	1	-2.502479	2.149395	1.240385
25	1	-2.012496	.755312	2.194291

26	1	-.824058	1.930897	1.670081

syn-TS'e (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.242646	.109265	.598092
2	6	-.155387	-.585943	.459108
3	8	-.201089	-1.588663	-.407974
4	3	1.268269	-1.786149	-1.361880
5	8	1.951933	-.159235	-.637588
6	1	-.501259	-.833001	1.481153
7	1	1.158157	1.199642	.698294
8	6	1.989535	-.459990	1.804233
9	1	2.031035	-1.553758	1.756366
10	1	3.010536	-.072587	1.866280
11	1	1.475880	-.180212	2.729839
12	6	3.088096	.682180	-.884773
13	1	3.473217	.413364	-1.870371
14	1	2.787295	1.736395	-.890053
15	1	3.871175	.528066	-.136412
16	6	-1.337583	.584746	-.012908
17	6	-2.412594	-.323682	-.160713
18	8	-3.245056	-1.097037	-.163866
19	6	-1.675557	1.617128	1.089529
20	6	-.965408	1.221524	-1.371124
21	1	-2.482575	2.289938	.786269
22	1	-1.947226	1.134876	2.032798
23	1	-.780688	2.223371	1.258511
24	1	-1.777007	1.844815	-1.756508
25	1	-.092697	1.860833	-1.215794
26	1	-.719436	.454827	-2.107968

anti-TSe (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.972951	-.909259	-.169354
2	8	-.127575	-1.510833	.200657
3	6	-.242167	-.378435	-.362588
4	6	1.448190	.360890	.177186
5	8	2.502533	-1.764099	-.654450
6	6	2.248558	1.450351	-.549584
7	6	1.325146	.568864	1.689037
8	6	-1.375238	.554635	.078749
9	1	-.125654	-.315443	-1.450929
10	1	-1.428622	.551264	1.163732
11	8	-2.558805	.020671	-.455080
12	6	-1.279293	1.977001	-.448698
13	1	-1.128141	1.978466	-1.523514
14	1	-.472541	2.531222	.015656
15	1	-2.207795	2.495368	-.243081
16	6	-3.157464	-1.030863	.254864
17	1	-3.390276	-.724175	1.272873
18	1	-2.524021	-1.904947	.285220
19	1	-4.081842	-1.261414	-.258149
20	1	.814821	1.506766	1.871420
21	1	.761077	-.234641	2.139331
22	1	2.298034	.631926	2.169015
23	1	1.758209	2.401225	-.388539
24	1	3.266886	1.542244	-.180022
25	1	2.286541	1.277125	-1.619703

anti-TSe (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.615937	-1.044221	-.060749
2	8	-.064873	-1.213869	.526920
3	6	-.430058	-.327577	-.321623
4	6	1.845894	.310951	.190855
5	8	1.989422	-1.958969	-.716193
6	6	3.094093	.852994	-.478744
7	6	1.457302	1.021384	1.467955
8	6	-1.537169	.660833	-.007889
9	1	-.242493	-.486511	-1.391939
10	1	-1.565700	.843400	1.075797
11	8	-2.752660	.037676	-.432773
12	6	-1.403075	1.961588	-.785848
13	1	-1.350029	1.758188	-1.860731
14	1	-.501799	2.505357	-.487632
15	1	-2.277708	2.591499	-.599954
16	6	-3.249111	-.960658	.452449
17	1	-3.444121	-.541174	1.450681
18	1	-2.557635	-1.806007	.555178
19	1	-4.188896	-1.311482	.019495
20	1	1.225396	2.076714	1.273717
21	1	.610846	.555831	1.972775
22	1	2.302511	1.016740	2.173243
23	1	2.959766	1.921981	-.688355
24	1	3.982456	.765946	.165426
25	1	3.309406	.339064	-1.419762

anti-TS'e (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.180124	.168530	.453291
2	6	.145967	-.772751	-.188612
3	8	.171230	-.839264	-1.441814
4	3	1.908569	-.808288	-1.975227
5	8	2.386512	-.330780	-.143222
6	1	-.020462	-1.681504	.379801
7	6	3.566549	-.233758	.640569
8	1	4.375121	-.637478	.050598
9	1	3.782634	.797014	.886380
10	1	3.458292	-.814241	1.547436
11	6	-1.758899	-.224507	.421457
12	6	-1.936243	.784529	-.484567
13	8	-1.956962	1.572486	-1.279447
14	6	-2.529987	-1.496609	.036005
15	6	-1.830125	.158686	1.900116
16	6	1.041953	1.650712	.143232
17	1	1.941342	2.176563	.437886
18	1	.883710	1.816722	-.915288
19	1	.223274	2.099419	.691293
20	1	1.228845	-.002368	1.521508
21	1	-3.592996	-1.385181	.215082
22	1	-2.369048	-1.766055	-.999424
23	1	-2.175105	-2.310014	.658130
24	1	-2.857136	.187783	2.246073
25	1	-1.313544	-.599991	2.477528
26	1	-1.372917	1.115663	2.115599

anti-TS'e (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.156675	0.192084	0.439593
2	6	0.074174	-0.771697	-0.127953
3	8	0.121511	-0.958237	-1.400602
4	3	1.847922	-1.000543	-1.899507
5	8	2.366926	-0.374726	-0.155359
6	1	-0.034895	-1.667635	0.513316
7	6	3.574683	-0.167335	0.595191
8	1	4.381715	-0.636517	0.030448
9	1	3.788638	0.899065	0.713478
10	1	3.495537	-0.641956	1.578460
11	6	-1.702253	-0.219304	0.420305
12	6	-1.916653	0.827141	-0.446786
13	8	-1.956428	1.637526	-1.257013
14	6	-2.545450	-1.453018	0.019513
15	6	-1.731130	0.120559	1.916852
16	6	1.041626	1.662569	0.055586
17	1	1.963210	2.196916	0.302320
18	1	0.855574	1.778454	-1.016132
19	1	0.238501	2.160703	0.607907
20	1	1.233405	0.074146	1.526869
21	1	-3.610700	-1.281107	0.194806
22	1	-2.379614	-1.723016	-1.025169
23	1	-2.224216	-2.287897	0.649847
24	1	-2.760532	0.185694	2.281340
25	1	-1.236995	-0.693554	2.456737
26	1	-1.219496	1.055832	2.154281

syn3a (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.039378	-.056676	-.027662
2	6	-.394723	.060871	-.600954
3	17	2.259150	-.624938	-1.162805
4	17	1.238326	-.822579	1.550136
5	6	.926583	1.469082	.073199
6	8	-.329214	1.485960	-.374612
7	1	-.421106	-.127361	-1.662828
8	8	1.620704	2.344778	.406482
9	6	-1.594856	-.591673	.069891
10	1	-1.567726	-.387950	1.135073
11	6	-1.612050	-2.093667	-.181563
12	8	-2.749855	-.050115	-.501017
13	1	-2.481437	-2.524753	.298966
14	1	-1.685635	-2.291665	-1.245274
15	1	-.725984	-2.581943	.206190
16	6	-3.392983	.973038	.212416
17	1	-4.279948	1.231141	-.348219
18	1	-3.689575	.629152	1.199980
19	1	-2.766843	1.850333	.312701

syn3a (HF/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.043484	-.061837	-.022658

2	6	-.385911	.063980	-.604851
3	17	2.268181	-.638797	-1.150863
4	17	1.229451	-.824599	1.556627
5	6	.941996	1.464298	.070473
6	8	-.308930	1.492085	-.378884
7	1	-.406666	-.122717	-1.666899
8	8	1.647597	2.336487	.396983
9	6	-1.599135	-.573459	.055701
10	1	-1.577862	-.370286	1.120908
11	6	-1.639214	-2.074824	-.196548
12	8	-2.728966	.002174	-.531020
13	1	-2.522094	-2.490965	.271898
14	1	-1.702827	-2.272583	-1.260800
15	1	-.767655	-2.579270	.203913
16	6	-3.436283	.936611	.239645
17	1	-4.283658	1.250360	-.352410
18	1	-3.798462	.487297	1.160066
19	1	-2.827752	1.801322	.478128

syn3a (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.034475	-0.053425	-0.032620
2	6	-0.410388	0.058160	-0.599601
3	17	2.265523	-0.612657	-1.198930
4	17	1.240752	-0.856472	1.554326
5	6	0.932153	1.486524	0.095699
6	8	-0.353103	1.517269	-0.366475
7	1	-0.444940	-0.123338	-1.676036
8	8	1.633013	2.379657	0.448158
9	6	-1.602376	-0.612669	0.082045
10	1	-1.566959	-0.403998	1.160677
11	6	-1.590005	-2.119963	-0.169399
12	8	-2.802404	-0.103853	-0.480279
13	1	-2.457334	-2.571508	0.319756
14	1	-1.662867	-2.324155	-1.242976
15	1	-0.682659	-2.589889	0.220931
16	6	-3.365455	1.024911	0.179587
17	1	-4.329866	1.207364	-0.300963
18	1	-3.533828	0.816700	1.246844
19	1	-2.738692	1.918231	0.084538

syn3a (B3lyp/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.035356	-0.055947	-0.029106
2	6	-0.406987	0.055436	-0.601435
3	17	2.271482	-0.618734	-1.191127
4	17	1.236838	-0.853934	1.559543
5	6	0.936167	1.484115	0.090988
6	8	-0.345452	1.518056	-0.372765
7	1	-0.438133	-0.127330	-1.677570
8	8	1.641827	2.377354	0.438650
9	6	-1.605341	-0.608258	0.075674
10	1	-1.573363	-0.400920	1.154514
11	6	-1.603148	-2.115311	-0.177521
12	8	-2.793726	-0.083345	-0.495062
13	1	-2.474816	-2.561004	0.308910
14	1	-1.675710	-2.318199	-1.251243
15	1	-0.700733	-2.593386	0.214858

16	6	-3.379310	1.014887	0.195302
17	1	-4.327946	1.218200	-0.307274
18	1	-3.581834	0.759991	1.246068
19	1	-2.750536	1.911943	0.158673

anti3a (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.542189	1.113930	-.400991
2	8	.489092	1.822179	.019345
3	6	-.221991	.679513	.533517
4	6	.943115	-.221089	.059300
5	8	2.523548	1.466777	-.922069
6	17	.645324	-1.346725	-1.260891
7	17	1.855574	-.991684	1.354674
8	1	-.282708	.728138	1.609212
9	6	-1.608126	.537888	-.066025
10	6	-2.463678	1.758494	.257601
11	8	-2.108006	-.633884	.507293
12	1	-1.523420	.429008	-1.143206
13	1	-2.014772	2.659119	-.143711
14	1	-2.573393	1.868093	1.331199
15	1	-3.452202	1.655560	-.174476
16	6	-3.138113	-1.276289	-.188049
17	1	-2.830958	-1.524624	-1.199815
18	1	-4.037089	-.669400	-.229738
19	1	-3.358165	-2.188210	.347563

anti3a (HF/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.555236	1.114850	-.376299
2	8	.498604	1.822154	.020592
3	6	-.226237	.676820	.522193
4	6	.942592	-.222301	.055001
5	8	2.556860	1.468190	-.863664
6	17	.664553	-1.327352	-1.284939
7	17	1.835729	-1.013407	1.354457
8	1	-.293295	.722303	1.597403
9	6	-1.610249	.535745	-.083259
10	6	-2.472338	1.747965	.255202
11	8	-2.088099	-.648492	.476820
12	1	-1.524159	.441181	-1.162295
13	1	-2.020069	2.657363	-.122741
14	1	-2.596345	1.835408	1.329203
15	1	-3.454642	1.654787	-.191376
16	6	-3.181881	-1.250103	-.162855
17	1	-2.964962	-1.436256	-1.210790
18	1	-4.076653	-.642746	-.086614
19	1	-3.356311	-2.191826	.335523

anti3a (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.565142	1.120170	-.399339
2	8	.499639	1.851578	.056228
3	6	-.221410	.668690	.555191

4	6	.947280	-.225621	.056027
5	8	2.559673	1.489438	-.934950
6	17	.622290	-1.351103	-1.290384
7	17	1.878589	-1.027063	1.354062
8	1	-.281889	.698241	1.645187
9	6	-1.611743	.540841	-.052068
10	6	-2.459810	1.779628	.246380
11	8	-2.134586	-.638460	.541694
12	1	-1.516161	.410408	-1.140286
13	1	-1.997275	2.675659	-.178752
14	1	-2.568554	1.916398	1.327740
15	1	-3.458743	1.674421	-.188245
16	6	-3.175765	-1.258473	-.193666
17	1	-2.843740	-1.529616	-1.206530
18	1	-4.067615	-.620543	-.270816
19	1	-3.440935	-2.168007	.350265

anti3a (B3lyp/6-31G* epsi=9.08)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.574883	1.121532	-0.379739
2	8	0.505044	1.851040	0.056028
3	6	-0.225595	0.665403	0.545262
4	6	0.947351	-0.226335	0.052068
5	8	2.585344	1.492185	-0.888517
6	17	0.640255	-1.335756	-1.309382
7	17	1.863888	-1.043262	1.354569
8	1	-0.290991	0.692715	1.634813
9	6	-1.614609	0.537904	-0.065593
10	6	-2.466765	1.771074	0.245632
11	8	-2.119657	-0.651582	0.517867
12	1	-1.519330	0.419419	-1.155835
13	1	-2.004541	2.673841	-0.165743
14	1	-2.582245	1.892939	1.328000
15	1	-3.462809	1.671386	-0.195630
16	6	-3.212250	-1.237972	-0.174597
17	1	-2.949079	-1.459951	-1.219088
18	1	-4.104462	-0.598115	-0.159236
19	1	-3.440918	-2.171705	0.343314

syn3c (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.407040	1.195337	.021017
2	6	.198130	.411304	.553903
3	1	1.889328	1.876142	.708748
4	1	1.284290	1.672210	-.943076
5	6	2.040305	-.180042	-.056871
6	8	.948049	-.816402	.393433
7	1	-.019674	.562113	1.601632
8	8	3.072367	-.639159	-.372132
9	6	-1.087860	.430004	-.254759
10	1	-.849656	.173105	-1.286461
11	6	-1.736990	1.807408	-.202340
12	8	-2.013928	-.477894	.264617
13	1	-2.654320	1.795975	-.777430
14	1	-1.987277	2.066035	.821068
15	1	-1.086785	2.576432	-.606064
16	6	-1.948964	-1.799051	-.201685
17	1	-2.802166	-2.316298	.214563

18	1	-2.015126	-1.831299	-1.286649
19	1	-1.040482	-2.296532	.110742

syn3c (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.391228	1.210495	0.050937
2	6	0.179609	0.405227	0.558209
3	1	1.862181	1.892773	0.762564
4	1	1.264188	1.715005	-0.911481
5	6	2.057890	-0.160110	-0.057086
6	8	0.950723	-0.847047	0.383706
7	1	-0.051886	0.531323	1.619681
8	8	3.116655	-0.608860	-0.380361
9	6	-1.104680	0.435121	-0.265390
10	1	-0.850365	0.185269	-1.310147
11	6	-1.751594	1.819281	-0.203088
12	8	-2.065659	-0.481968	0.232005
13	1	-2.672612	1.817349	-0.792158
14	1	-2.012338	2.071007	0.830743
15	1	-1.086448	2.595346	-0.595685
16	6	-1.906607	-1.832487	-0.184783
17	1	-2.797778	-2.364445	0.158625
18	1	-1.849729	-1.904967	-1.281797
19	1	-1.014038	-2.300829	0.244063

anti3c (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.185204	-.172561	-.133364
2	8	1.423228	.908059	.117797
3	6	.336839	.114815	.640134
4	6	1.151148	-1.156367	.380612
5	8	3.264360	-.206074	-.590890
6	1	.757244	-1.830521	-.367585
7	1	1.465136	-1.715380	1.251181
8	1	.171098	.347099	1.682387
9	6	-.935483	.309509	-.162442
10	6	-1.461648	1.735309	-.046124
11	8	-1.822761	-.645450	.349853
12	1	-.716897	.088030	-1.207248
13	1	-.701301	2.441095	-.358977
14	1	-1.736696	1.949859	.981512
15	1	-2.334623	1.887398	-.670472
16	6	-2.951758	-.925924	-.423059
17	1	-2.675537	-1.204776	-1.437477
18	1	-3.635688	-.084444	-.466070
19	1	-3.457165	-1.759335	.044136

anti3c (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.207044	-.180109	-.135048
2	8	1.434260	.934133	.125119
3	6	.334012	.103238	.646882
4	6	1.156654	-1.165459	.375592
5	8	3.308361	-.209032	-.596091

6	1	.753646	-1.840593	-.383511
7	1	1.468704	-1.742156	1.249528
8	1	.166704	.330899	1.703463
9	6	-.943777	.304972	-.157810
10	6	-1.464603	1.738582	-.047043
11	8	-1.845836	-.663795	.364867
12	1	-.723093	.074865	-1.215084
13	1	-.695512	2.443262	-.378333
14	1	-1.726913	1.966956	.992128
15	1	-2.352664	1.891459	-.668269
16	6	-2.986007	-.908300	-.437072
17	1	-2.703987	-1.188993	-1.464139
18	1	-3.660159	-.041579	-.484482
19	1	-3.520943	-1.742116	.024537

syn3e (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.505317	1.072008	1.353115
2	6	-1.333710	.416694	-.018237
3	6	-2.273464	1.040024	-1.049998
4	6	.094920	.098966	-.547416
5	6	1.357467	.523661	.186518
6	8	2.461339	-.127328	-.378410
7	6	2.876396	-1.321937	.226099
8	6	-1.427647	-1.099737	.044875
9	8	-2.238784	-1.892177	.353268
10	8	-.181310	-1.312915	-.393207
11	6	1.604050	2.019957	.039079
12	1	.219297	.315712	-1.599901
13	1	-.834527	.661787	2.098690
14	1	-1.344563	2.142611	1.299135
15	1	-2.519162	.903265	1.697864
16	1	-2.197914	.544458	-2.011890
17	1	-3.301707	.966288	-.714618
18	1	-2.035637	2.089820	-1.190733
19	1	1.275075	.261844	1.237880
20	1	.793370	2.610674	.449482
21	1	1.724851	2.275608	-1.008210
22	1	2.518646	2.287164	.553913
23	1	3.768631	-1.639899	-.295228
24	1	3.123183	-1.161648	1.273372
25	1	2.124330	-2.096135	.152825

syn3e (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.503264	1.106939	1.333156
2	6	-1.329588	.427749	-.030147
3	6	-2.259960	1.043828	-1.080902
4	6	.109522	.098202	-.544354
5	6	1.368802	.532769	.201857
6	8	2.513092	-.104943	-.353778
7	6	2.842830	-1.373086	.198132
8	6	-1.446748	-1.099663	.057528
9	8	-2.280550	-1.896550	.377662
10	8	-.171686	-1.346019	-.382710
11	6	1.602519	2.036695	.055889
12	1	.246024	.303557	-1.611150
13	1	-.819376	.711825	2.090591

14	1	-1.351231	2.189182	1.260330
15	1	-2.524615	.934365	1.688808
16	1	-2.161968	.544651	-2.051009
17	1	-3.303481	.956441	-.760257
18	1	-2.033002	2.107528	-1.218798
19	1	1.277606	.264702	1.265859
20	1	.778666	2.622352	.474633
21	1	1.718052	2.299309	-1.001424
22	1	2.525668	2.312339	.573143
23	1	3.795376	-1.663788	-.253010
24	1	2.973615	-1.309110	1.289762
25	1	2.087143	-2.133856	-.023823

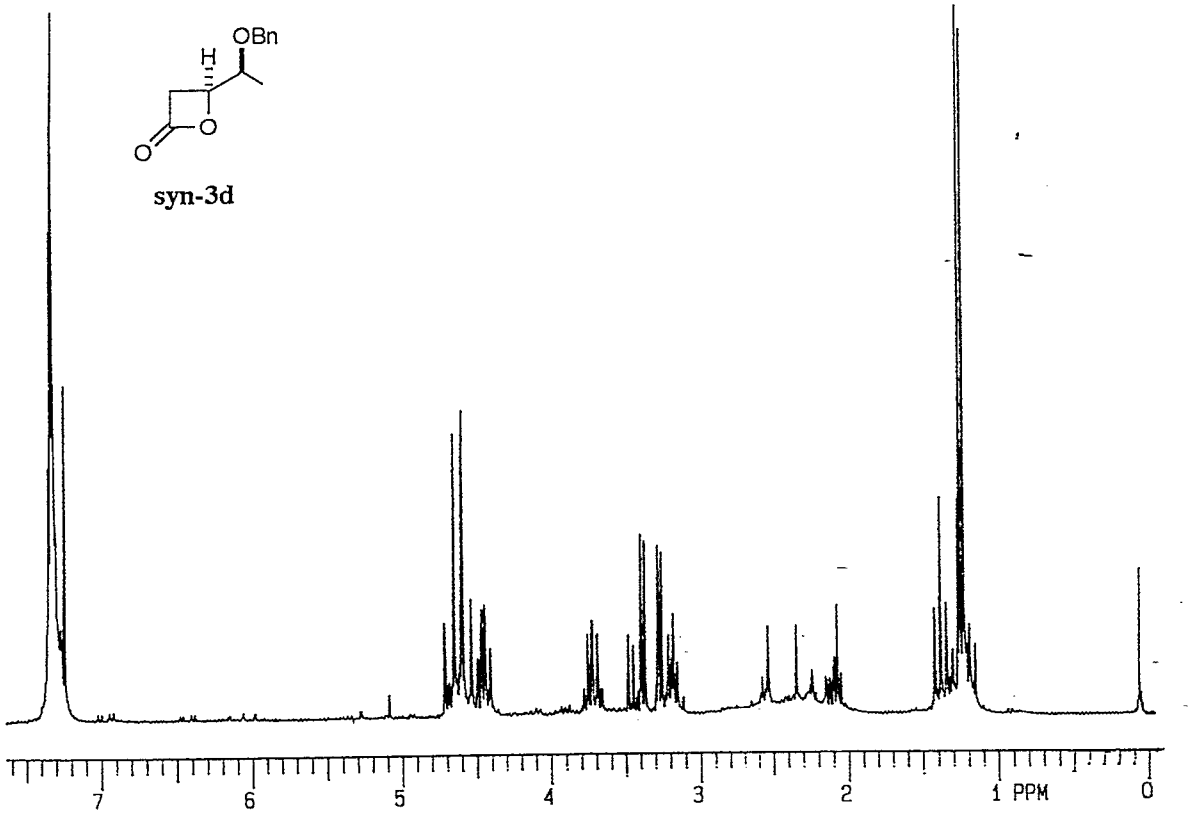
anti3e (HF/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.891348	.614800	-.290153
2	8	.936716	1.482155	.085977
3	6	.058429	.434964	.547388
4	6	1.114353	-.622652	.135575
5	8	2.935768	.851126	-.773020
6	6	.794394	-1.579396	-1.011201
7	6	1.755200	-1.360941	1.310606
8	1	-.075367	.512366	1.618035
9	6	-1.296725	.498281	-.132694
10	6	-2.022609	1.795150	.210923
11	8	-1.973674	-.641107	.325153
12	1	-1.162812	.441359	-1.210436
13	1	-1.415865	2.648431	-.067634
14	1	-2.223154	1.841733	1.276433
15	1	-2.966766	1.871382	-.316400
16	6	-3.123086	-1.006989	-.378432
17	1	-2.916261	-1.119407	-1.440299
18	1	-3.924726	-.286364	-.253061
19	1	-3.448842	-1.958664	.017528
20	1	.071993	-2.320713	-.692329
21	1	.398842	-1.067859	-1.880597
22	1	1.701553	-2.087859	-1.317508
23	1	1.068324	-2.105356	1.699500
24	1	2.661904	-1.862502	.992046
25	1	2.012875	-.683246	2.117768

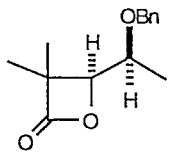
anti3e (B3lyp/6-31G* epsi=1)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.910259	.609983	-.296691
2	8	.946019	1.508291	.105962
3	6	.059068	.424473	.562565
4	6	1.119546	-.632969	.135605
5	8	2.969762	.854264	-.795707
6	6	.779297	-1.589068	-1.010711
7	6	1.772424	-1.376940	1.306396
8	1	-.074612	.493884	1.647210
9	6	-1.299182	.496827	-.124059
10	6	-2.022221	1.803404	.211534
11	8	-1.992883	-.659508	.337249
12	1	-1.156473	.433556	-1.215002
13	1	-1.404414	2.658455	-.079642
14	1	-2.218625	1.862246	1.288043
15	1	-2.976930	1.880223	-.318352

16	6	-3.160500	-.981560	-.394622
17	1	-2.945592	-1.092991	-1.469043
18	1	-3.953148	-.230175	-.272764
19	1	-3.522114	-1.936414	-.004408
20	1	.048420	-2.332462	-.678662
21	1	.369235	-1.068545	-1.881709
22	1	1.687042	-2.108471	-1.335350
23	1	1.094974	-2.149013	1.688667
24	1	2.698842	-1.861202	.980067
25	1	2.018068	-.698358	2.130819



- Figure 2 -



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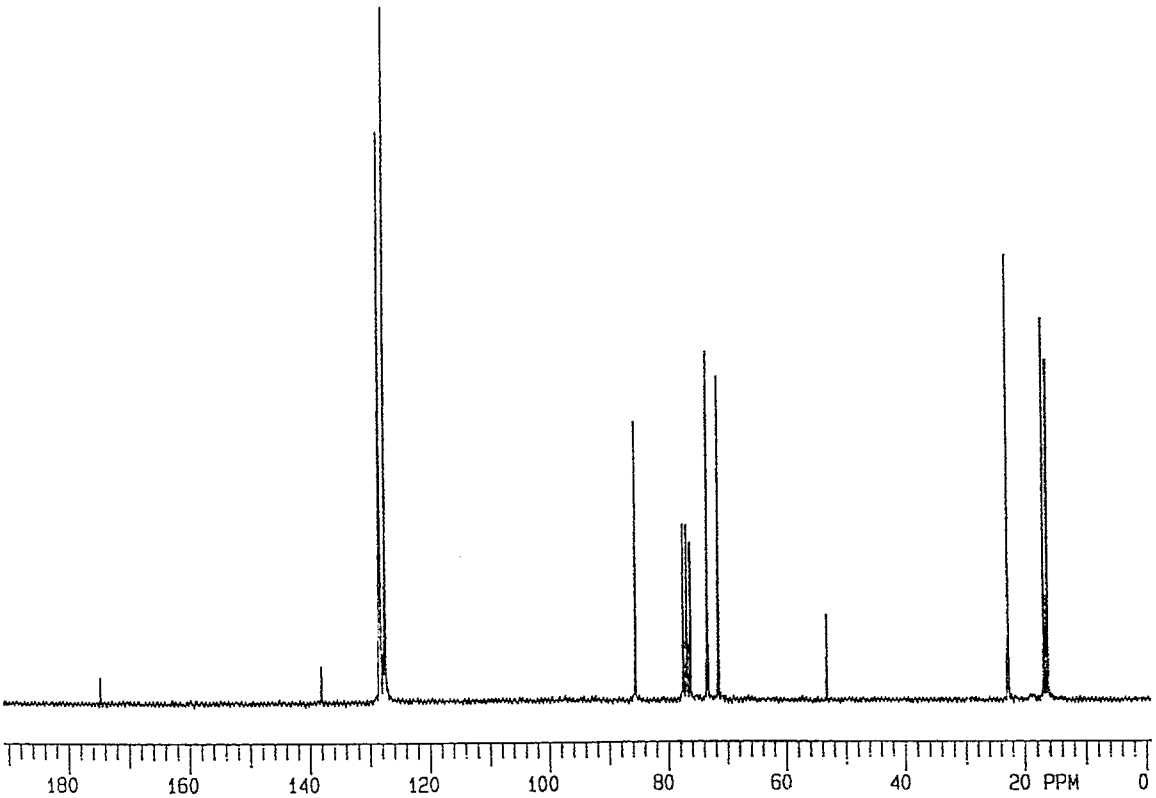

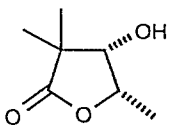

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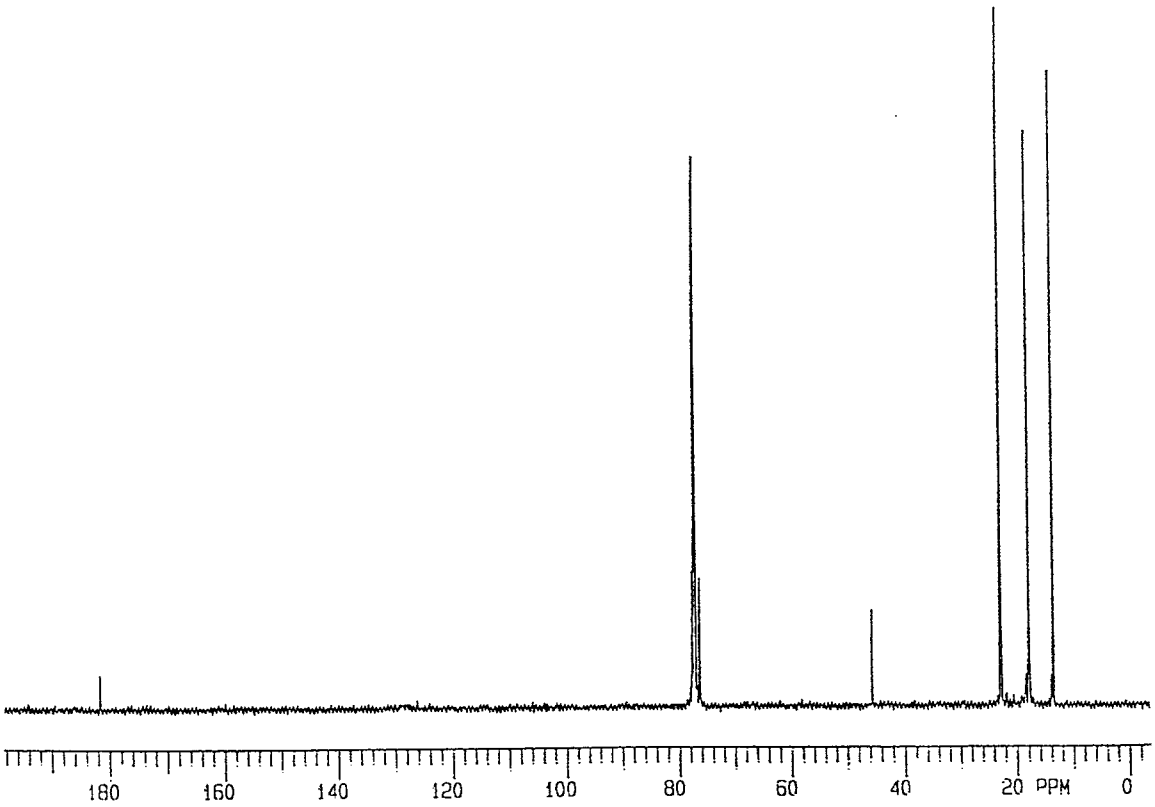

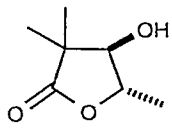
OH
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anti-8

4.0
3.5
3.0
2.5
2.0
1.5
1.0
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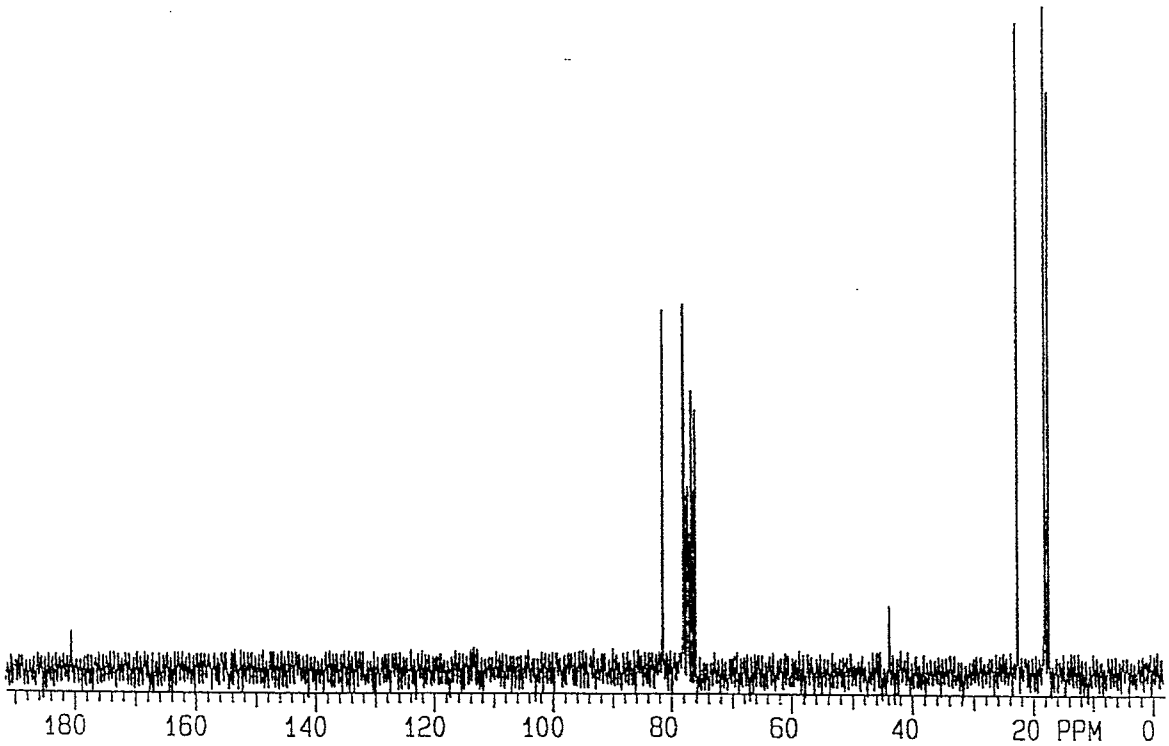
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100
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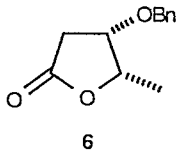
60
40
20 PPM 0



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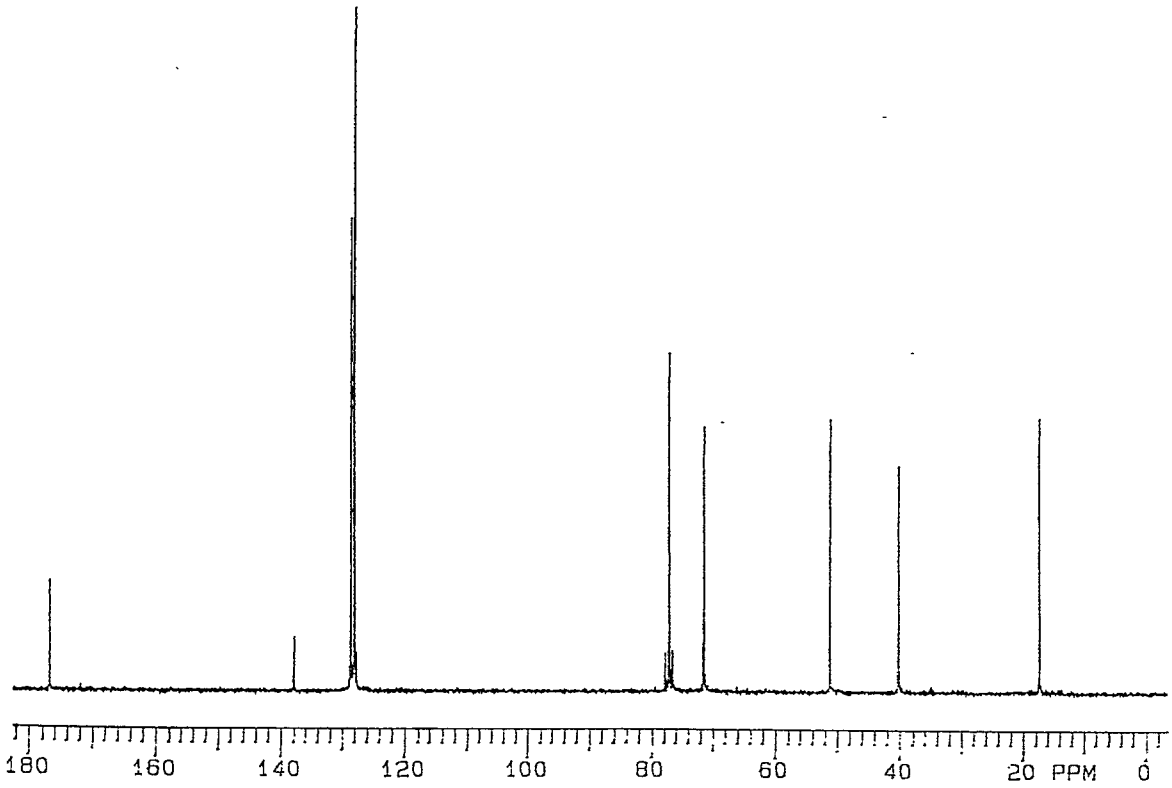

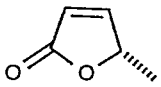

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