Cyclic Vinyl *p*-Tolyl Sulfilimines as Chiral Dienophiles: Theoretical Study on the Stereoselectivity, Lewis Acid Catalysis and Solvent Effects in Their Diels-Alder Reactions

José L. García Ruano,[a*] Fernando R. Clemente,[b] Lorena González Gutiérrez,[a] Ruth Gordillo,[b]

Ana M. Martín Castro,[a] and Jesús H. Rodríguez Ramos[a*]

[a]*Departamento de Química Orgánica, Universidad Autónoma de Madrid, Cantoblanco, 28049-Madrid, Spain*

[b]*Departamento de Química Orgánica, Universidad de Extremadura, 06071 Badajoz, Spain*

SUPPORTING INFORMATION

- **Table A.** Interfrontier MO Gaps for the Reactions of **1** and **2** with **3-7** (in eV).
- **Table B.** B3LYP/6-31G(d) Thermodynamic Energies (in kcal/mol) and Entropies (in eu) for structures **5-7** from **4** and **8**.
- **Table C.** B3LYP/6-31G(d) Thermodynamic Activation and Reaction Energies (in kcal/mol) as well as the corresponding Entropies (in eu) for the Reactions of **4** with Cyclopentadiene and Furan.
- **Table D.** B3LYP/6-31G(d) Thermodynamic Activation Energies (in kcal/mol) and Entropies (in eu) for the Reactions of **4** with Cyclopentadiene and Furan in the presence of BF_3.
- **Table E.** Computed Bond Distances for Dienes **1** and **2**.
- **Table F.** Computed Bond Distances for Dienophiles **3-7** and **21-23**.
- **Table G.** Computed Bond Distances for Transition Structures **TS9-TS10** and **TS17-TS20**.
- **Table H.** Computed Bond Distances of BF_3-Coordinated Transition Structures **TS11-TS16** and **TS24-TS35**.
- **Cartesian Coordinates of all the Optimized Structures with their Computed Heats of Formation (semiempirical) or Electronic Energies (DFT).**

* Corresponding author. FAX 3491 397 3966. E-mail: joseluis.garcia.ruano@uam.es

Table A. Interfrontier MO Gaps for the Reactions of **1** and **2** with **3-7** (in eV).

		3	**4**	**5**	**6**	**7**
1	Normal elec. demand	4.4	4.2	3.0	3.1	3.2
	Inverse elec. demand	5.9	6.0	7.4	7.5	7.3
2	Normal elec. demand	4.7	4.5	3.4	3.4	3.5
	Inverse elec. demand	6.7	6.7	8.2	8.3	8.1

Table B. B3LYP/6-31G(d) Thermodynamic Energies (in kcal/mol) and Entropies (in eu) for structures **5-7** from **4** and **8**.

	5	**6**	**7**
ΔE	-15.3	-19.9	-20.7
ΔE_0	-13.9	-18.4	-19.1
ΔE_{298}	-13.4	-17.9	-18.6
ΔH_{298}	-14.0	-18.5	-19.2
ΔG_{298}	-3.5	-7.5	-8.1
ΔS_{298}	-35.2	-37.1	-37.3

Table C. B3LYP/6-31G(d) Thermodynamic Activation and Reaction Energies (in kcal/mol) as well as the corresponding Entropies (in eu) for the Reactions of **4** with Cyclopentadiene and Furan.

	endo-TS9	**exo-TS9**	**endo-TS10**	**exo-TS10**	**endo-9**	**exo-9**	**endo-10**	**exo-10**
ΔE	17.0	17.5	22.4	22.7	-21.9	-23.1	-4.2	-6.1
ΔE_0	18.6	19.3	23.7	24.0	-17.0	-18.1	-0.4	-2.4
ΔE_{298}	18.6	19.2	23.7	24.0	-17.6	-18.7	-0.9	-2.8
ΔH_{298}	18.0	18.6	23.1	23.4	-18.2	-19.3	-1.5	-3.4
ΔG_{298}	31.8	32.5	36.9	37.2	-3.1	-4.2	13.2	11.3
ΔS_{298}	-46.4	-46.8	-46.2	-46.1	-50.3	-50.7	-49.2	-49.2

Table D. B3LYP/6-31G(d) Thermodynamic Activation Energies (in kcal/mol) and Entropies (in eu) for the Reactions of **4** with Cyclopentadiene and Furan in the presence of BF_3.

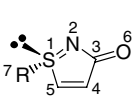
	endo-TS11	**exo-TS11**	**endo-TS12**	**exo-TS12**	**endo-TS13**	**exo-TS13**	**endo-TS14**	**exo-TS14**	**endo-TS15**	**exo-TS15**	**endo-TS16**	**exo-TS16**
ΔE	11.0	14.2	10.0	12.0	12.8	13.7	16.5	19.2	14.6	15.6	18.3	20.2
ΔE_0	12.9	16.0	11.9	14.0	14.5	15.5	18.0	20.6	16.1	17.2	19.7	21.5
ΔE_{298}	12.7	15.9	11.7	13.9	14.4	15.4	17.8	20.6	16.0	17.1	19.6	21.5
ΔH_{298}	12.1	15.3	11.1	13.3	13.8	14.8	17.3	20.0	15.4	15.9	19.0	20.9
ΔG_{298}	27.0	29.2	26.0	28.1	28.2	29.2	32.2	33.8	30.2	31.0	33.0	34.8
ΔS_{298}	-49.8	-46.5	-49.8	-49.6	-48.3	-48.2	-50.0	-46.5	-49.4	-50.9	-47.0	-46.7

Table E. Computed Bond Distances for Dienes **1** and **2**.

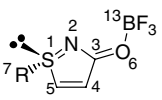
1. X = CH_2
2. X = O

Method	**Structure**	1-2	2-3	1-5
B3LYP/6-31G(d)	**1**	1.35	1.47	1.51
AM1	**1**	1.36	1.47	1.51
SM5.4/AM1	**1**	1.36	1.47	1.51
B3LYP/6-31G(d)	**2**	1.36	1.44	1.36
B3LYP/6-31+G(d)	**2**	1.36	1.44	1.37
AM1	**2**	1.38	1.45	1.40
SM5.4/AM1	**2**	1.38	1.45	1.40

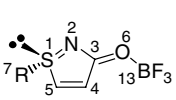
Table F. Computed Bond Distances for Dienophiles **3-7** and **21-23**.[a]



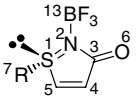
3. R = *p*-MeC_6H_4
4. R = Me



21. R = *p*-MeC_6H_4
5. R = Me



22. R = *p*-MeC_6H_4
6. R = Me

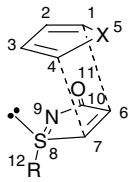
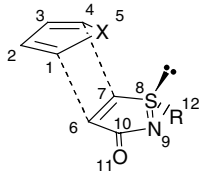
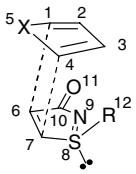
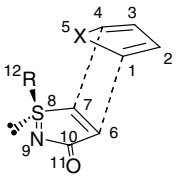


23. R = *p*-MeC_6H_4
7. R = Me

Method	**Structure**	1-2	2-3	3-4	4-5	5-1	3-6	1-7	A-13
B3LYP/6-31G(d)	**3**	1.64	1.39	1.53	1.33	1.82	1.82	1.82	
AM1	**3**	1.66	1.38	1.54	1.33	1.76	1.24	1.73	
SM5.4/AM1	**3**	1.55	1.40	1.53	1.34	1.79	1.24	1.71	
B3LYP/6-31G(d)	**4**	1.63	1.39	1.53	1.33	1.81	1.22	1.84	
B3LYP/6-31+G(d)	**4**	1.64	1.38	1.53	1.33	1.81	1.22	1.84	
B3LYP/6-31G(d)	**5**	1.66	1.34	1.50	1.33	1.80	1.26	1.83	1.67
B3LYP/6-31+G(d)	**5**	1.66	1.34	1.50	1.34	1.80	1.26	1.83	1.62
AM1	**21**	1.68	1.36	1.53	1.34	1.76	1.28	1.72	1.80
B3LYP/6-31G(d)	**6**	1.66	1.34	1.51	1.33	1.80	1.26	1.83	1.62
B3LYP/6-31+G(d)	**6**	1.67	1.34	1.50	1.34	1.80	1.27	1.83	1.59
AM1	**22**	1.68	1.36	1.53	1.34	1.76	1.28	1.72	1.78
B3LYP/6-31G(d)	**7**	1.67	1.40	1.51	1.33	1.80	1.21	1.84	1.66
B3LYP/6-31+G(d)	**7**	1.67	1.40	1.51	1.33	1.80	1.21	1.84	1.65
AM1	**23**	1.67	1.40	1.53	1.33	1.76	1.23	1.73	1.76

[a]Structures 5-6 and 21-22, A = 6; Structures 7 and 23, A = 2.

Table G. Computed Bond Distances for Transition Structures **TS9-TS10** and **TS17-TS20**.

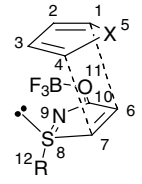





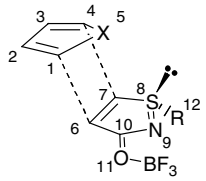
R = Me { **endo-TS9.** X = CH_2 / **endo-TS10.** X = O } **exo-TS9.** X = CH_2 / **exo-TS10.** X = O

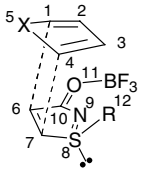
R = *p*-MeC_6H_4 { **endo-TS17.** X = CH_2 / **endo-TS19.** X = O } **exo-TS17.** X = CH_2 / **exo-TS19.** X = O / **endo-TS18.** X = CH_2 / **endo-TS20.** X = O / **exo-TS18.** X = CH_2 / **exo-TS20.** X = O

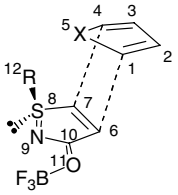
Method	**Structure**	1-2	2-3	3-4	4-5	5-1	1-6	4-7	6-7	7-8	8-9	9-10	10-6	10-11	8-12
B3LYP/6-31G(d)	**endo-TS9**	1.40	1.40	1.40	1.51	1.51	2.25	2.22	1.39	1.82	1.64	1.39	1.52	1.22	1.85
AM1	**endo-TS17**	1.42	1.41	1.41	1.51	1.52	2.05	2.21	1.40	1.76	1.66	1.38	1.53	1.25	1.73
SM5.4/AM1	**endo-TS17**	1.42	1.41	1.42	1.51	1.52	2.10	2.18	1.40	1.77	1.56	1.39	1.52	1.25	1.71
B3LYP/6-31G(d)	**exo-TS9**	1.40	1.40	1.40	1.51	1.51	2.23	2.26	1.39	1.82	1.64	1.39	1.53	1.22	1.85
AM1	**exo-TS17**	1.41	1.41	1.42	1.52	1.51	2.07	2.20	1.40	1.76	1.66	1.38	1.53	1.25	1.73
SM5.4/AM1	**exo-TS17**	1.41	1.41	1.42	1.52	1.51	2.08	2.22	1.40	1.76	1.56	1.39	1.53	1.25	1.71
AM1	**endo-TS18**	1.42	1.41	1.41	1.51	1.52	2.02	2.25	1.40	1.75	1.66	1.38	1.54	1.25	1.73
SM5.4/AM1	**endo-TS18**	1.42	1.41	1.41	1.51	1.52	2.00	2.31	1.40	1.74	1.57	1.39	1.53	1.25	1.71
B3LYP/6-31G(d)	**exo-TS18**	1.42	1.41	1.41	1.51	1.52	2.04	2.24	1.40	1.76	1.66	1.38	1.54	1.25	1.73
B3LYP/6-31+G(d)	**exo-TS18**	1.42	1.41	1.41	1.51	1.52	2.03	2.30	1.40	1.74	1.57	1.39	1.53	1.25	1.71
AM1	**endo-TS10**	1.42	1.38	1.42	1.37	1.38	2.11	2.13	1.40	1.83	1.64	1.39	1.53	1.22	1.85
SM5.4/AM1	**endo-TS10**	1.42	1.38	1.43	1.37	1.38	2.11	2.13	1.40	1.83	1.65	1.39	1.52	1.23	1.84
AM1	**endo-TS19**	1.45	1.40	1.43	1.39	1.42	1.99	2.22	1.40	1.75	1.66	1.38	1.54	1.25	1.73
SM5.4/AM1	**endo-TS19**	1.44	1.40	1.44	1.39	1.41	2.02	2.20	1.41	1.76	1.56	1.39	1.53	1.25	1.71
B3LYP/6-31G(d)	**exo-TS10**	1.42	1.38	1.42	1.37	1.37	2.12	2.15	1.40	1.83	1.64	1.39	1.53	1.22	1.85
B3LYP/6-31+G(d)	**exo-TS10**	1.42	1.38	1.42	1.37	1.37	2.13	2.14	1.40	1.83	1.64	1.38	1.53	1.23	1.84
AM1	**exo-TS19**	1.45	1.39	1.44	1.39	1.41	2.02	2.19	1.40	1.76	1.66	1.38	1.54	1.25	1.73
SM5.4/AM1	**exo-TS19**	1.44	1.39	1.43	1.40	1.41	2.04	2.21	1.41	1.76	1.56	1.39	1.53	1.25	1.71
AM1	**endo-TS20**	1.44	1.40	1.43	1.39	1.42	1.95	2.29	1.40	1.74	1.66	1.38	1.54	1.25	1.73
SM5.4/AM1	**endo-TS20**	1.44	1.40	1.42	1.38	1.42	1.92	2.43	1.41	1.72	1.57	1.39	1.54	1.25	1.71
AM1	**exo-TS20**	1.45	1.40	1.43	1.39	1.41	2.00	2.23	1.40	1.76	1.66	1.37	1.54	1.25	1.73
SM5.4/AM1	**exo-TS20**	1.45	1.40	1.43	1.39	1.42	1.99	2.30	1.41	1.74	1.57	1.39	1.53	1.25	1.71

Table H. Computed Bond Distances of BF_3-Coordinated Transition Structures **TS11-TS16** and **TS24-TS35**.[a]



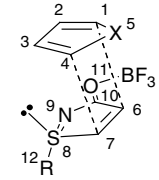


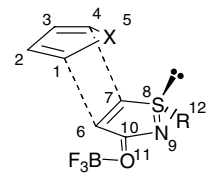


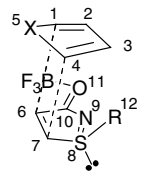


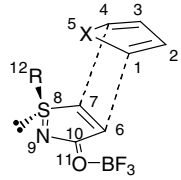
R = Me { **endo-TS11.** X = CH_2 / **endo-TS14.** X = O } **exo-TS11.** X = CH_2 / **exo-TS14.** X = O

R = *p*-MeC_6H_4 { **endo-TS24.** X = CH_2 / **endo-TS30.** X = O } { **exo-TS24.** X = CH_2 / **exo-TS30.** X = O } **endo-TS25.** X = CH_2 / **endo-TS31.** X = O **exo-TS25.** X = CH_2 / **exo-TS31.** X = O



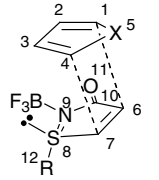


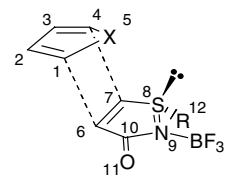


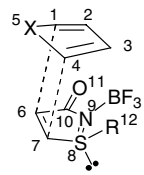


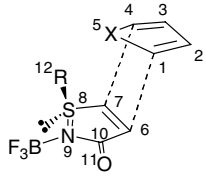
R = Me { **endo-TS12.** X = CH_2 / **endo-TS15.** X = O } **exo-TS12.** X = CH_2 / **exo-TS15.** X = O

R = *p*-MeC_6H_4 { **endo-TS26.** X = CH_2 / **endo-TS32.** X = O } { **exo-TS26.** X = CH_2 / **exo-TS32.** X = O } **endo-TS27.** X = CH_2 / **endo-TS33.** X = O **exo-TS27.** X = CH_2 / **exo-TS33.** X = O









R = Me { **endo-TS13.** X = CH_2 / **endo-TS16.** X = O } **exo-TS13.** X = CH_2 / **exo-TS16.** X = O

R = *p*-MeC_6H_4 { **endo-TS28.** X = CH_2 / **endo-TS34.** X = O } { **exo-TS28.** X = CH_2 / **exo-TS34.** X = O } **endo-TS28.** X = CH_2 / **endo-TS34.** X = O **exo-TS28.** X = CH_2 / **exo-TS34.** X = O

Table H. Computed Bond Distances of BF_3-Coordinated Transition Structures **TS11-TS16** and **TS24-TS35** (Continuing).[a]

Method	**Structure**	1-2	2-3	3-4	4-5	5-1	1-6	4-7	6-7	7-8	8-9	9-10	10-6	10-11	8-12	A-B
B3LYP/6-31G(d)	**endo-TS11**	1.40	1.40	1.41	1.51	1.51	2.29	2.18	1.39	1.81	1.67	1.34	1.47	1.27	1.84	1.61
AM1	**endo-TS24**	1.42	1.41	1.41	1.51	1.52	2.07	2.21	1.40	1.76	1.68	1.35	1.52	1.29	1.73	1.75
B3LYP/6-31G(d)	**exo-TS11**	1.40	1.40	1.41	1.51	1.50	2.28	2.23	1.40	1.81	1.66	1.35	1.49	1.26	1.83	1.64
AM1	**exo-TS24**	1.42	1.41	1.41	1.51	1.52	2.09	2.20	1.40	1.76	1.68	1.36	1.52	1.28	1.73	1.76
AM1	**endo-TS25**	1.42	1.41	1.41	1.51	1.52	2.03	2.26	1.40	1.75	1.68	1.35	1.52	1.29	1.72	1.75
AM1	**exo-TS25**	1.42	1.41	1.41	1.51	1.52	2.06	2.23	1.40	1.76	1.68	1.35	1.52	1.28	1.73	1.75
B3LYP/6-31G(d)	**endo-TS12**	1.39	1.41	1.41	1.52	1.51	2.35	2.16	1.39	1.81	1.66	1.35	1.48	1.27	1.84	1.58
AM1	**endo-TS26**	1.42	1.41	1.41	1.51	1.52	2.09	2.17	1.40	1.76	1.68	1.36	1.52	1.29	1.73	1.74
B3LYP/6-31G(d)	**exo-TS12**	1.40	1.40	1.41	1.51	1.50	2.37	2.17	1.40	1.82	1.66	1.35	1.49	1.27	1.84	1.58
AM1	**exo-TS26**	1.42	1.41	1.41	1.51	1.52	2.11	2.18	1.40	1.76	1.68	1.36	1.52	1.29	1.73	1.75
AM1	**endo-TS27**	1.42	1.41	1.41	1.51	1.52	2.06	2.22	1.41	1.75	1.68	1.36	1.52	1.29	1.72	1.75
AM1	**exo-TS27**	1.42	1.41	1.41	1.51	1.52	2.09	2.21	1.40	1.76	1.68	1.36	1.52	1.28	1.73	1.76
B3LYP/6-31G(d)	**endo-TS13**	1.40	1.40	1.41	1.51	1.51	2.24	2.21	1.39	1.80	1.67	1.41	1.50	1.21	1.82	1.64
AM1	**endo-TS28**	1.42	1.41	1.41	1.51	1.52	2.04	2.24	1.40	1.75	1.66	1.40	1.52	1.24	1.73	1.73
B3LYP/6-31G(d)	**exo-TS13**	1.40	1.40	1.40	1.51	1.51	2.25	2.25	1.39	1.80	1.67	1.41	1.50	1.21	1.83	1.64
AM1	**exo-TS28**	1.42	1.41	1.41	1.51	1.52	2.06	2.23	1.40	1.75	1.67	1.41	1.52	1.24	1.73	1.73
AM1	**endo-TS29**	1.42	1.41	1.41	1.51	1.52	2.01	2.29	1.40	1.74	1.67	1.40	1.52	1.24	1.73	1.74
AM1	**exo-TS29**	1.42	1.41	1.41	1.51	1.52	2.04	2.26	1.40	1.75	1.66	1.40	1.52	1.24	1.73	1.74
B3LYP/6-31G(d)	**endo-TS14**	1.42	1.38	1.43	1.37	1.37	2.12	2.11	1.41	1.82	1.67	1.34	1.49	1.27	1.83	1.61
B3LYP/6-31+G(d)	**endo-TS14**	1.42	1.38	1.43	1.38	1.37	2.15	2.08	1.41	1.82	1.67	1.34	1.49	1.27	1.83	1.59
AM1	**endo-TS30**	1.45	1.40	1.44	1.39	1.42	2.00	2.23	1.41	1.75	1.68	1.35	1.53	1.29	1.73	1.75
B3LYP/6-31G(d)	**exo-TS14**	1.42	1.38	1.43	1.37	1.37	2.17	2.10	1.41	1.83	1.66	1.34	1.50	1.26	1.83	1.63
B3LYP/6-31+G(d)	**exo-TS14**	1.42	1.38	1.43	1.38	1.37	2.18	2.08	1.41	1.83	1.66	1.34	1.49	1.27	1.83	1.60
AM1	**exo-TS30**	1.45	1.39	1.44	1.39	1.41	2.04	2.19	1.41	1.76	1.68	1.35	1.52	1.28	1.73	1.76
AM1	**endo-TS31**	1.45	1.40	1.43	1.39	1.42	1.96	2.31	1.41	1.74	1.68	1.35	1.53	1.29	1.72	1.75
AM1	**exo-TS31**	1.45	1.39	1.44	1.39	1.41	2.02	2.21	1.41	1.76	1.68	1.35	1.52	1.29	1.72	1.76
B3LYP/6-31G(d)	**endo-TS15**	1.42	1.38	1.43	1.38	1.37	2.19	2.05	1.41	1.82	1.66	1.35	1.49	1.27	1.83	1.57
B3LYP/6-31+G(d)	**endo-TS15**	1.42	1.38	1.43	1.38	1.36	2.24	2.02	1.42	1.82	1.67	1.35	1.48	1.28	1.83	1.56
AM1	**endo-TS32**	1.45	1.39	1.44	1.39	1.41	2.03	2.18	1.41	1.75	1.68	1.36	1.52	1.29	1.73	1.74
B3LYP/6-31G(d)	**exo-TS15**	1.42	1.38	1.43	1.38	1.36	2.23	2.05	1.41	1.83	1.66	1.35	1.49	1.27	1.83	1.58
B3LYP/6-31+G(d)	**exo-TS15**	1.42	1.38	1.43	1.38	1.36	2.25	2.04	1.41	1.83	1.66	1.34	1.48	1.28	1.83	1.56
AM1	**exo-TS32**	1.45	1.39	1.44	1.40	1.41	2.06	2.16	1.41	1.76	1.67	1.36	1.52	1.29	1.73	1.74
AM1	**endo-TS33**	1.45	1.39	1.43	1.39	1.42	1.99	2.25	1.41	1.74	1.68	1.36	1.52	1.29	1.72	1.75
AM1	**exo-TS33**	1.45	1.39	1.44	1.39	1.41	2.05	2.18	1.41	1.76	1.68	1.36	1.52	1.29	1.72	1.74
B3LYP/6-31G(d)	**endo-TS16**	1.43	1.37	1.43	1.37	1.38	2.09	2.13	1.41	1.81	1.67	1.41	1.50	1.21	1.83	1.64
B3LYP/6-31+G(d)	**endo-TS16**	1.42	1.38	1.43	1.37	1.38	2.10	2.12	1.41	1.81	1.67	1.40	1.50	1.22	1.83	1.63
AM1	**endo-TS34**	1.45	1.40	1.43	1.38	1.42	1.96	2.29	1.40	1.74	1.67	1.40	1.52	1.24	1.73	1.73
B3LYP/6-31G(d)	**exo-TS16**	1.42	1.38	1.42	1.37	1.37	2.12	2.14	1.41	1.82	1.66	1.40	1.51	1.21	1.83	1.65
B3LYP/6-31+G(d)	**exo-TS16**	1.43	1.38	1.43	1.37	1.37	2.13	2.13	1.41	1.82	1.67	1.40	1.51	1.22	1.83	1.64
AM1	**exo-TS34**	1.45	1.39	1.44	1.39	1.41	2.02	2.22	1.40	1.75	1.66	1.40	1.52	1.24	1.73	1.74
AM1	**endo-TS35**	1.45	1.40	1.43	1.38	1.42	1.94	2.34	1.40	1.73	1.67	1.40	1.53	1.24	1.73	1.74
AM1	**exo-TS35**	1.45	1.40	1.43	1.39	1.41	1.99	2.26	1.40	1.75	1.66	1.40	1.53	1.24	1.73	1.74

[a]Structures 5-6 and 21-22, A-B = 6-B; Structures 7 and 23, A-B = 2-B.

CARTESIAN COORDINATES OF ALL THE OPTIMIZED STRUCTURES

Structure 1. AM1 Geometry.
AM1 HF = 0.0589259
B3LYP/6-31G(d) Energy = -194.0997221

C	0.999702	-0.735903	-0.000026
C	0.999684	0.735927	0.000125
C	-0.285152	1.180010	-0.000142
C	-1.225807	-0.000015	0.000063
C	-0.285123	-1.180017	-0.000015
H	1.913378	-1.328571	0.000021
H	1.913344	1.328619	-0.000023
H	-0.646627	2.205842	-0.000023
H	-1.876656	0.000026	0.909080
H	-1.876688	-0.000068	-0.909003
H	-0.646574	-2.205857	-0.000078

Structure 1. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -194.101058

C	1.181208	-0.281617	-0.000038
C	0.735049	0.991219	0.000059
C	-0.735008	0.991248	-0.000057
C	-1.181220	-0.281569	0.000032
C	-0.000025	-1.217479	0.000003
H	1.347089	1.887545	0.000093
H	-1.347011	1.887600	-0.000086
H	-2.214012	-0.610954	0.000059
H	-0.000020	-1.881967	0.878006
H	-0.000056	-1.881984	-0.877987
H	2.213986	-0.611046	-0.000069

Structure 1. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 33.209685

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.360349
C	1.391074	0.000000	1.840474
C	2.230139	-0.000055	0.769754
C	1.421840	0.000064	-0.504085
H	-0.858943	-0.000050	2.032436
H	1.652583	-0.000016	2.899289
H	3.319699	-0.000087	0.763739
H	1.634984	0.909301	-1.121433
H	1.635015	-0.909058	-1.121592
H	-0.853925	0.000014	-0.676746

Structure 2. AM1 Geometry.
AM1 HF = 0.0045813
B3LYP/6-31G(d) Energy = -230.0178912

C	1.118294	-0.348657	-0.000067
C	0.723877	0.973558	0.000147
C	-0.723877	0.973558	-0.000170
C	-1.118294	-0.348657	0.000113
O	0.000000	-1.183348	-0.000020
H	1.356655	1.855846	0.000032
H	-1.356656	1.855846	-0.000025
H	-2.069222	-0.871861	0.000032
H	2.069222	-0.871861	-0.000014

Structure 2. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -230.0205816

O	0.000006	-1.161137	-0.000071
C	-1.094835	-0.347440	0.000032
C	-0.718012	0.959979	0.000017
C	0.718002	0.959986	-0.000047
C	1.094839	-0.347429	0.000075
H	-1.373738	1.819561	0.000025
H	1.373720	1.819574	-0.000089
H	2.049890	-0.850296	0.000122
H	-2.049882	-0.850314	0.000049

Structure 2. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -230.0314377

O	-.000001	-1.160988	-.000026
C	1.097401	-.348230	-.000008
C	.718567	.960759	.000022
C	-.718566	.960760	.000022
C	-1.097402	-.348229	-.000009
H	1.375238	1.820218	.000042
H	-1.375236	1.820219	.000046
H	-2.052384	-.851442	-.000024
H	2.052383	-.851445	-.000024

Structure 2. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = -1.459157

O	.000000	.000000	.000000
C	.000000	.000000	1.400238
C	1.295968	.000000	1.870416
C	2.162235	.000168	.708541
C	1.342034	.000159	-.399621
H	1.627712	.000042	2.907313
H	3.250757	.000194	.729432
H	1.494035	.000265	-1.478034
H	-.989965	-.000086	1.854212

Structure 3. AM1 Geometry.
AM1 Energy = 0.1298347
B3LYP/6-31G(d) Energy = -914.5577236

C	-1.334589	1.320183	-0.158059
C	-0.449134	0.269083	-0.415031
C	-0.891094	-1.052601	-0.372419
C	-2.225664	-1.320815	-0.066294
C	-3.120379	-0.278409	0.198232
C	-2.663201	1.046409	0.148426
S	1.167676	0.679074	-0.868921
C	1.785816	1.413636	0.608656
C	2.740129	0.620243	1.093247
C	2.933858	-0.649529	0.245090
O	3.797563	-1.485554	0.556251
C	-4.531489	-0.568951	0.539577
N	2.079972	-0.706892	-0.834005
H	-0.204083	-1.891608	-0.579874
H	-2.575017	-2.364447	-0.034180
H	-3.360457	1.873382	0.351018
H	-0.988425	2.364888	-0.195669
H	-5.202551	0.265012	0.217327
H	-4.876461	-1.512148	0.048357
H	-4.634420	-0.693524	1.647734
H	1.380197	2.365106	0.934742
H	3.372586	0.765334	1.972764

Structure 3. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -914.5675308

C	-2.925132	.707241	-.003831
N	-2.109462	.302389	-1.052721
O	-3.711216	1.638969	-.044779
C	-2.753541	-.162794	1.237897
C	-1.833965	-1.110372	1.108746
H	-3.339197	.043348	2.126586
H	-1.465312	-1.869109	1.786551
S	-1.223820	-.998343	-.601253
C	.484982	-.440287	-.296624
C	.773920	.918640	-.191275
C	2.093434	1.308854	.023792
C	3.126740	.364250	.127440
C	2.803844	-.993481	.004654
C	1.489111	-1.403925	-.219202
H	-.023627	1.648076	-.295216
H	2.327070	2.367523	.108319
C	4.555951	.807417	.331612
H	3.590739	-1.740329	.074720
H	1.256987	-2.460438	-.331218
H	5.177284	-.005896	.719167
H	5.003381	1.141816	-.613489
H	4.617701	1.646766	1.032659

Structure 3. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 18.068251

C	.000000	.000000	.000000
C	.000000	.000000	1.403389
C	1.222108	.000000	2.078243
C	2.424597	.012718	1.376064
C	2.424251	.017847	-.024916
C	1.198740	.009574	-.704853
S	-1.534375	.120216	2.141842
N	-1.476588	-.078630	3.680620
C	-2.044138	-1.288974	4.081791
C	-2.502444	-2.105240	2.874653
C	-2.253396	-1.466098	1.729190
O	-2.191814	-1.633544	5.264264
C	3.701666	.041360	-.773368
H	-2.981120	-3.076050	3.060027
H	-2.460235	-1.782294	.702210
H	1.253245	-.010324	3.177230
H	3.377511	.013971	1.928474
H	1.185546	.006835	-1.808599
H	-.958667	-.011476	-.551991
H	3.603382	-.498920	-1.748200
H	3.994934	1.101452	-.986566
H	4.522572	-.435195	-.182503

Structure 4. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -683.5142033

N	0.340327	-1.046294	-0.383915
S	-1.003820	-0.141465	-0.598706
C	-0.305933	1.454007	-0.091921
C	0.971890	1.221978	0.186219
C	1.382030	-0.244600	0.059987
C	-2.099228	-0.455401	0.850932
O	2.512608	-0.626902	0.311270
H	-0.894935	2.362298	-0.096949
H	1.699432	1.959787	0.504869
H	-2.465241	-1.479441	0.751719
H	-1.516829	-0.343479	1.767382
H	-2.937019	0.247638	0.818213

Structure 4. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -683.5312212

N	.339674	-1.043867	-.368338
S	-1.008894	-.133532	-.591685
C	-.302079	1.458178	-.089506
C	.979120	1.224929	.182055
C	1.381279	-.241520	.060531
C	-2.105854	-.461173	.851685
O	2.516012	-.626953	.310264
H	-.887108	2.369704	-.098902
H	1.711841	1.962896	.489504
H	-2.467939	-1.485848	.742029
H	-1.526928	-.354398	1.771368
H	-2.945840	.239711	.820093

Structure 5. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1008.0917756

C	0.072015	0.667778	0.015809
N	0.578816	-0.489250	0.474780
S	2.223316	-0.337420	0.589101
C	2.342353	1.327156	-0.088025
C	1.088546	1.732767	-0.288776
C	2.863617	-1.353359	-0.794857
O	-1.143525	0.918727	-0.180263
H	3.288856	1.839943	-0.198446
H	0.779812	2.704982	-0.654889
H	2.627132	-2.390080	-0.546757
H	2.362096	-1.054731	-1.716707
H	3.946323	-1.213949	-0.853775
B	-2.354871	-0.217320	-0.030469
F	-3.447201	0.497392	-0.417024
F	-1.984190	-1.209713	-0.898085
F	-2.335898	-0.573452	1.287446

Structure 5. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1008.1365564

C	.077672	.653789	.017241
N	.589012	-.499835	.460768
S	2.237884	-.337084	.583388
C	2.337705	1.330616	-.088863
C	1.078779	1.729765	-.282699
C	2.878144	-1.360420	-.794481
O	-1.147198	.897787	-.175956
H	3.279440	1.854011	-.195612
H	.760859	2.703487	-.638231
H	2.648075	-2.396276	-.535283
H	2.372787	-1.072178	-1.717837
H	3.960163	-1.215382	-.856244
B	-2.341451	-.190766	-.029733
F	-3.447927	.522777	-.418996
F	-2.007651	-1.216153	-.895908
F	-2.353618	-.565446	1.296503

Structure 6. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1008.0991927

C	-0.071751	-0.368488	-0.281506
N	-1.178107	-1.088831	-0.531740
S	-2.488343	-0.069756	-0.518143
C	-1.598511	1.418770	-0.053396
C	-0.305793	1.096544	-0.016155
C	-3.359985	-0.494727	1.035513
O	1.068852	-0.907271	-0.271033
H	-2.099416	2.370156	0.069274
H	0.516610	1.768385	0.185891
H	-3.752015	-1.505321	0.904280
H	-2.649166	-0.458292	1.862583
H	-4.180624	0.214178	1.173691
B	2.389173	-0.055397	0.111029
F	3.398878	-0.956015	0.047074
F	2.445953	0.955637	-0.830868
F	2.126770	0.441640	1.375253

Structure 6. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1008.1422872

C	-.079740	-.349631	-.254225
N	-1.175278	-1.079248	-.504734
S	-2.498080	-.068501	-.513293
C	-1.619995	1.425373	-.043545
C	-.323581	1.112112	.003874
C	-3.389208	-.505540	1.025847
O	1.066638	-.887839	-.236346
H	-2.127152	2.374989	.071971
H	.489849	1.794275	.214549
H	-3.774980	-1.517240	.882432
H	-2.691754	-.469526	1.864622
H	-4.215418	.199209	1.153708
B	2.388971	-.075102	.089835
F	3.395124	-.994880	.037587
F	2.473974	.921712	-.880753
F	2.188200	.478748	1.355831

Structure 7. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1008.1003594

C	-0.626790	1.490570	0.141530
N	0.055487	0.300035	-0.114762
S	-0.953098	-0.957640	-0.529854
C	-2.444429	0.024948	-0.338123
C	-2.109811	1.274732	-0.027501
C	-1.046708	-2.037752	0.951344
O	-0.108902	2.543442	0.442081
H	-3.410566	-0.425328	-0.528636
H	-2.798416	2.099888	0.112783
H	-0.075615	-2.531200	0.999834
H	-1.223481	-1.419846	1.833033
H	-1.851924	-2.760507	0.791932
B	1.669745	-0.080920	-0.062009
F	1.593520	-1.470218	-0.334058
F	2.314749	0.608876	-1.041653
F	2.103963	0.172571	1.207038

Structure 7. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1008.1003594

C	-.624227	1.478654	.145599
N	.054025	.279775	-.087646
S	-.962489	-.974333	-.518238
C	-2.446476	.023167	-.339722
C	-2.105615	1.272806	-.031483
C	-1.071091	-2.052797	.963459
O	-.101393	2.532765	.439303
H	-3.414311	-.422125	-.535846
H	-2.789286	2.104052	.098623
H	-.109357	-2.564928	1.025678
H	-1.249843	-1.433595	1.844206
H	-1.883157	-2.766723	.795482
B	1.663401	-.064324	-.069803
F	1.639408	-1.456234	-.360624
F	2.283784	.660381	-1.053326
F	2.127110	.179090	1.201657

Structure 8. AM1 Geometry.
AM1 Energy = -0.2940995
B3LYP/6-31(d) Energy = -324.5496592

B	0.000000	0.000000	0.000038
F	0.000000	-1.171901	-0.676605
F	0.000000	0.000000	1.353189
F	0.000000	1.171901	-0.676605

Structure 8. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -324.5532219

B	0.000000	0.000000	0.000000
F	0.000000	1.317760	0.000000
F	1.141213	-0.658880	0.000000
F	-1.141213	-0.658880	0.000000

Structure 8. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -324.5795545

B	.000000	.000000	.000000
F	.000000	1.321350	.000000
F	1.144323	-.660675	.000000
F	-1.144323	-.660675	.000000

Structure *endo*-TS9. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -877.5882132

C	1.599972	-1.528819	0.052920
C	-0.261207	-0.748548	-0.861483
C	0.027808	0.592401	-1.065893
C	2.156035	0.683847	-0.332942
C	1.939411	0.504563	1.034982
C	1.615460	-0.840714	1.274874
C	2.386696	-0.685717	-0.926585
S	-1.462156	-0.765730	0.509856
N	-1.376370	0.822860	0.895901
C	-0.672478	1.518147	-0.084687
O	-0.563385	2.734364	-0.125423
C	-3.012116	-1.000691	-0.468021
H	1.506420	-2.606980	-0.036506
H	1.300232	-1.246404	2.230017
H	1.889007	1.300476	1.768784
H	2.506491	1.606151	-0.782076
H	2.124009	-0.802488	-1.980390
H	3.454209	-0.939652	-0.818025
H	-0.331625	-1.526095	-1.612811
H	0.336656	1.000547	-2.020405
H	-3.846263	-0.842274	0.219697
H	-3.043447	-0.268808	-1.277630
H	-3.037003	-2.024536	-0.855263

Structure *exo*-TS9. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -877.5874576

C	1.981525	0.919940	0.142860
C	0.047900	0.582778	-0.918947
C	-0.172534	-0.766950	-0.677646
C	1.616106	-1.320109	0.591395
C	2.582444	-1.211264	-0.417895
C	2.798518	0.147480	-0.693595
C	1.551063	0.025114	1.275637
S	-1.560240	-0.816455	0.502084
N	-1.665579	0.792677	0.797008
C	-0.861385	1.493496	-0.100139
O	-0.826707	2.711594	-0.186823
C	-2.918567	-1.237360	-0.674485
H	1.341290	-2.250306	1.079316
H	2.994383	-2.039499	-0.985520
H	3.401856	0.532627	-1.509357
H	1.994832	2.001934	0.209128
H	2.338609	0.048134	2.047194
H	0.611232	0.293590	1.760098
H	-0.085113	-1.585531	-1.379361
H	0.428240	0.969310	-1.854064
H	-3.857177	-1.127241	-0.126266
H	-2.885701	-0.545732	-1.518717
H	-2.796320	-2.274242	-1.003375

Structure *endo*-TS10. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -913.4990856

C	1.634429	-1.479051	-0.040138
C	-0.222639	-0.767382	-0.814548
C	0.086476	0.582741	-1.025969
C	2.100411	0.594094	-0.387183
C	1.934892	0.464084	1.017085
C	1.644033	-0.862273	1.242836
O	2.296818	-0.660324	-0.917307
S	-1.462952	-0.748738	0.526727
N	-1.388713	0.847073	0.887644
C	-0.648571	1.522919	-0.076417
O	-0.519607	2.737302	-0.123609
C	-2.984618	-1.003784	-0.485121
H	1.689295	-2.535497	-0.271090
H	1.336889	-1.326430	2.170382
H	1.887396	1.285063	1.718935
H	2.563894	1.405895	-0.931083
H	-0.343561	-1.514451	-1.591131
H	0.340157	0.966384	-2.007660
H	-3.836557	-0.827184	0.175707
H	-2.991997	-0.291098	-1.312316
H	-3.001469	-2.036298	-0.848824

Structure *endo*-TS10. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -913.5243306

C	1.631748	-1.481876	-.034246
C	-.219420	-.765079	-.807616
C	.092153	.587865	-1.018732
C	2.111207	.591036	-.394660
C	1.950855	.468051	1.011646
C	1.651470	-.856469	1.245697
O	2.295530	-.669457	-.919244
S	-1.468401	-.753050	.524080
N	-1.399084	.851627	.880372
C	-.649880	1.522008	-.073433
O	-.525646	2.741903	-.121541
C	-2.990962	-1.004707	-.484688
H	1.678416	-2.539855	-.260128
H	1.344785	-1.312673	2.177930
H	1.912427	1.292956	1.710374
H	2.574348	1.397538	-.946770
H	-.338585	-1.510660	-1.586738
H	.343071	.973635	-2.000804
H	-3.840541	-.833314	.181097
H	-3.002732	-.288214	-1.308948
H	-3.005272	-2.036545	-.851417

Structure *exo*-TS10. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -913.4985666

C	-1.855936	0.836523	-0.274593
C	-0.110658	0.596538	0.903580
C	0.129361	-0.766431	0.689056
C	-1.537673	-1.274227	-0.563795
C	-2.575837	-1.170818	0.402439
C	-2.774431	0.178892	0.589786
O	-1.428827	-0.070448	-1.208653
S	1.523410	-0.795138	-0.499974
N	1.647002	0.812595	-0.769085
C	0.821031	1.508532	0.100614
O	0.766835	2.727005	0.182967
C	2.874008	-1.251517	0.670629
H	-1.258461	-2.135961	-1.157234
H	-2.996328	-1.991853	0.967919
H	-3.388148	0.665155	1.336703
H	-1.827319	1.872793	-0.583658
H	0.110237	-1.548188	1.438780
H	-0.473345	0.985413	1.846678
H	3.815080	-1.127491	0.129768
H	2.842429	-0.585516	1.535479
H	2.749029	-2.297725	0.967953

Structure *exo*-TS10. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -913.5233488

C	-1.862788	.841686	-.291403
C	-.113537	.609809	.892018
C	.121597	-.759147	.687231
C	-1.544476	-1.277231	-.549056
C	-2.581816	-1.157566	.419238
C	-2.779396	.196230	.586503
O	-1.438255	-.081732	-1.211750
S	1.518811	-.808249	-.497443
N	1.655129	.805546	-.767184
C	.832748	1.505845	.095134
O	.802401	2.729452	.186297
C	2.873346	-1.257283	.669876
H	-1.268889	-2.147962	-1.131281
H	-3.003283	-1.970359	.996817
H	-3.392442	.694815	1.326514
H	-1.839530	1.872324	-.620140
H	.101294	-1.532925	1.445971
H	-.476650	1.006295	1.832164
H	3.810659	-1.147087	.118856
H	2.852280	-.578707	1.525572
H	2.742451	-2.299059	.981265

Structure *endo*-9. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -877.6500932

C	1.871555	0.434155	1.061165
C	1.857012	0.621173	-0.448628
C	2.304299	-0.790630	-0.902599
C	1.252244	-1.514147	-0.017537
C	1.520278	-0.833711	1.319596
C	0.348789	0.586292	-0.907050
C	-0.040010	-0.872931	-0.628012
C	-0.559896	1.567491	-0.106879
N	-1.474925	0.963476	0.731185
S	-1.482892	-0.663791	0.564380
O	-0.391258	2.773488	-0.194660
C	-2.858519	-1.058226	-0.594950
H	0.274482	0.843530	-1.967730
H	-0.406423	-1.424818	-1.496631
H	1.251739	-2.606356	-0.020892
H	2.399286	1.484222	-0.835524
H	2.026967	1.232368	1.778253
H	1.342488	-1.285659	2.289565
H	-3.782560	-0.754475	-0.098516
H	-2.736133	-0.497028	-1.524506
H	-2.869660	-2.137063	-0.780445
H	2.176424	-0.968441	-1.977453
H	3.329685	-1.034658	-0.607863

Structure *exo*-9. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -877.6520773

C	1.693192	0.911776	-0.020799
C	2.728092	0.032914	-0.714295
C	2.486475	-1.236951	-0.360104
C	1.278207	-1.224676	0.576089
C	1.513878	0.124539	1.300221
C	0.315149	0.615433	-0.720179
C	-0.815223	1.513140	-0.117366
N	-1.766470	0.846490	0.632320
S	-1.582428	-0.777419	0.534988
C	0.077240	-0.859113	-0.357880
O	-0.775838	2.723967	-0.260581
C	-2.664893	-1.352021	-0.840251
H	-0.041158	-1.548679	-1.195457
H	0.358978	0.802358	-1.795598
H	1.903938	1.979393	0.046919
H	3.459365	0.387159	-1.433740
H	2.968060	-2.135218	-0.732446
H	1.125353	-2.116678	1.188225
H	0.670237	0.468214	1.907605
H	2.421087	0.108659	1.909636
H	-3.691814	-1.129048	-0.542937
H	-2.418848	-0.813234	-1.758623

H	-2.537074	-2.431638	-0.967610

Structure *endo*-10. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -913.5414949

C	1.913759	0.399600	1.019665
C	1.859612	0.521122	-0.496042
O	2.202371	-0.816987	-0.915717
C	1.265998	-1.490529	-0.064132
C	1.544770	-0.856066	1.292785
C	0.342428	0.571672	-0.926265
C	-0.065323	-0.875810	-0.639627
C	-0.517080	1.567013	-0.093730
N	-1.416399	0.975282	0.770840
S	-1.478795	-0.647833	0.574734
O	-0.319567	2.769030	-0.174382
C	-2.877619	-0.988500	-0.573011
H	0.272932	0.830825	-1.984909
H	-0.429421	-1.435426	-1.502384
H	1.357782	-2.572441	-0.159160
H	2.497161	1.260667	-0.976105
H	2.100458	1.215954	1.706107
H	1.371811	-1.319102	2.256782
H	-3.786911	-0.669305	-0.059369
H	-2.752069	-0.416439	-1.495339
H	-2.917939	-2.063728	-0.774306

Structure *exo*-10. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -913.5445743

C	-1.660307	0.857320	-0.107555
C	-2.763827	0.080773	0.605212
C	-2.519837	-1.207240	0.346998
C	-1.269932	-1.202750	-0.532672
O	-1.407695	0.023360	-1.255976
C	-0.334372	0.641435	0.706579
C	0.806375	1.532777	0.111735
N	1.778205	0.855615	-0.589134
S	1.558091	-0.760988	-0.524251
C	-0.075742	-0.840924	0.412854
O	0.749401	2.744938	0.236482
C	2.667857	-1.381350	0.808061
H	0.047293	-1.503680	1.270526
H	-0.446715	0.882383	1.765323
H	-1.842755	1.889164	-0.402216
H	-3.514962	0.511529	1.256797
H	-3.016345	-2.089003	0.734118
H	-1.112704	-2.042820	-1.210124
H	3.689933	-1.179222	0.480711
H	2.466027	-0.848991	1.740900
H	2.518392	-2.459499	0.924603

Structure *endo*-TS11. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.175306

C	-1.723002	-1.338680	1.410547
C	-2.734933	-1.154464	0.450091
C	-2.415517	-2.095788	-0.692260
C	-0.917880	-2.183397	-0.541808
C	-0.610879	-1.939840	0.799009
C	-1.943752	0.509754	-0.722077
C	-0.786394	-0.022372	-1.289508
C	0.435992	0.391661	-0.552851
N	0.246771	1.199917	0.504781
S	-1.357636	1.643254	0.563262
O	1.555486	-0.089783	-0.901408
B	2.854505	-0.158059	0.052271
F	3.792259	-0.739862	-0.754485
C	-1.395942	3.255349	-0.313578
F	3.157041	1.119017	0.438592
F	2.451593	-0.974742	1.101191
H	-3.746761	-0.842010	0.691745
H	-1.746648	-0.964552	2.428384
H	0.376901	-2.035363	1.235797
H	-0.262568	-2.694819	-1.237517
H	-2.783104	-1.801416	-1.677962
H	-2.851365	-3.079853	-0.455508
H	-2.863258	0.757188	-1.238675
H	-0.706111	-0.381023	-2.307178
H	-0.821125	3.953980	0.298864
H	-0.936630	3.143587	-1.297152
H	-2.435164	3.588313	-0.389613

Structure *endo*-TS12. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.1843597

C	0.274921	-0.895059	-0.275871
C	-0.214129	-0.104615	0.879474
C	-1.607075	-0.062747	0.924286
S	-2.164999	-1.175397	-0.389200
N	-0.673035	-1.421058	-1.081204
C	-2.119908	1.889253	0.164839
C	-1.011585	2.498228	0.999456
C	0.187902	2.100793	0.182585
C	-0.235955	1.933439	-1.134483
C	-1.637451	1.839343	-1.156886
C	-2.477081	-2.716680	0.559432
O	1.497074	-1.085546	-0.568573
B	2.741246	-0.345987	0.056471
F	2.775947	0.905352	-0.547654
F	2.526733	-0.238449	1.429829
F	3.803905	-1.136244	-0.258393
H	-3.171681	1.994541	0.415801
H	-2.238641	1.640962	-2.037752
H	0.427919	1.780234	-1.976775
H	1.219498	2.225595	0.482255
H	-0.986391	2.216622	2.054504
H	-1.113327	3.594895	0.952625
H	-2.213173	-0.005498	1.820872
H	0.450081	0.081058	1.709597
H	-2.591739	-3.517961	-0.174146
H	-1.627878	-2.916096	1.215357
H	-3.403355	-2.593970	1.128490

Structure *exo*-TS11. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.1702389

C	-1.799871	-1.158678	1.243148
C	-1.451369	-1.986148	0.037443
C	-2.632401	-2.159682	-0.695221
C	-3.575683	-1.210831	-0.276016
C	-2.995646	-0.400881	0.714084
C	-1.702190	0.812151	-0.629581
C	-0.743287	-0.108782	-1.052539
C	0.565346	0.088843	-0.362935
N	0.611464	1.067537	0.562422
S	-0.824149	1.905498	0.521702
O	1.522189	-0.690631	-0.634108
B	3.006972	-0.591424	0.044280
F	2.806420	-0.850378	1.376306
C	-0.466853	3.344335	-0.557354
F	3.689383	-1.573010	-0.618915
F	3.447862	0.679020	-0.225205
H	-3.544830	0.328391	1.301975
H	-4.546356	-1.046616	-0.732207
H	-2.757197	-2.842822	-1.528792
H	-0.572565	-2.618013	-0.023145
H	-2.159698	-1.842340	2.029450
H	-0.983913	-0.579510	1.678125
H	-2.491615	1.249619	-1.225675
H	-0.752346	-0.600809	-2.014171
H	0.254849	3.962344	-0.018402
H	-0.038888	2.988583	-1.496243
H	-1.394926	3.899968	-0.719483

Structure *exo*-TS12. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.1810657

C	0.393440	-0.945432	-0.279861
C	-0.213383	-0.020841	0.710871
C	-1.604869	-0.134976	0.752690
S	-1.998951	-1.487749	-0.391144
N	-0.466929	-1.702632	-0.999614
C	-2.217467	-2.876394	0.787600
O	1.637226	-1.053027	-0.510913
C	-0.065293	2.025313	-0.469693
C	-0.573393	2.798834	0.577842
C	-1.956823	2.592727	0.676728
C	-2.343162	1.631426	-0.274846
C	-1.233113	1.584836	-1.303241
H	-3.378147	1.400527	-0.511300
H	-2.599582	3.002961	1.448900
H	0.026843	3.384330	1.265823
H	0.968485	1.994455	-0.791804
H	-1.436260	2.372167	-2.047598
H	-1.098962	0.653920	-1.857480
H	-2.225603	-0.054703	1.635678
H	0.404246	0.362815	1.506164
H	-2.244604	-3.791733	0.192300
H	-1.375286	-2.892711	1.481819
H	-3.167763	-2.740282	1.311932
B	2.805572	-0.167941	0.089274
F	3.922184	-0.925780	-0.084729
F	2.809738	1.006514	-0.653107
F	2.505529	0.070558	1.426009

Structure *endo*-TS13. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.1810721

C	-0.085156	-0.381555	1.425177
C	1.200781	0.383902	1.379580
C	1.228516	1.372902	0.398059
S	-0.384773	1.398038	-0.409384
N	-0.936074	0.043564	0.389087
C	-1.257492	2.773408	0.428137
O	-0.351453	-1.276847	2.199079
C	2.491113	0.473176	-1.174877
C	1.664259	-0.580913	-1.600514
C	1.655585	-1.578168	-0.615285
C	2.494721	-1.185533	0.434538
C	3.387851	-0.089350	-0.095104
H	2.773040	1.314964	-1.800369
H	1.022109	-0.574669	-2.474015
H	0.979780	-2.424800	-0.607409
H	2.737937	-1.807385	1.288786
H	3.759886	0.625565	0.642264
H	4.261662	-0.552104	-0.581565
H	1.757653	2.316731	0.450532
H	1.817253	0.408941	2.269365
H	-2.306822	2.644697	0.153040
H	-1.123446	2.693484	1.508132
H	-0.872662	3.722000	0.041716
B	-2.142289	-0.752194	-0.386940
F	-2.738129	0.291541	-1.121087
F	-1.542919	-1.679621	-1.224109
F	-2.969564	-1.299970	0.545181

Structure *exo*-TS13. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1202.1795663

C	-0.184750	-0.673322	1.263578
C	1.119333	0.067411	1.308183
C	1.137513	1.205384	0.502861
S	-0.494196	1.388816	-0.240524
N	-1.084183	-0.039587	0.386254
C	-1.281072	2.673813	0.797868
O	-0.434370	-1.698669	1.862046
C	2.338986	-1.361440	0.072925
C	3.569479	-0.705121	0.223052
C	3.581132	0.434708	-0.591719
C	2.349802	0.526426	-1.259875
C	1.719988	-0.845300	-1.198696
H	2.133040	1.246050	-2.043610
H	4.361690	1.188278	-0.607035
H	4.337428	-0.970945	0.942011
H	2.075596	-2.311640	0.523799
H	2.142484	-1.431774	-2.031788
H	0.635008	-0.924246	-1.288452
H	1.673038	2.125517	0.694697
H	1.737209	-0.053968	2.186481
H	-2.340576	2.632583	0.535711
H	-1.126680	2.436045	1.851643
H	-0.855624	3.646759	0.534874
B	-2.324193	-0.663881	-0.486352
F	-2.937427	0.505324	-0.975445
F	-1.752154	-1.397631	-1.514728
F	-3.119612	-1.391381	0.342683

Structure *endo*-TS14. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.08612

S	-1.394710	1.606653	0.576024
C	-1.970581	0.415096	-0.666253
C	-0.789584	-0.097969	-1.242365
C	0.430495	0.415888	-0.551652
N	0.232715	1.257571	0.473051
O	1.559113	-0.041841	-0.904627
B	2.855088	-0.104605	0.055353
F	3.135289	1.165773	0.473534
C	-1.557227	3.195257	-0.322672
F	2.450665	-0.950411	1.084176
F	3.806455	-0.658539	-0.753094
C	-2.673295	-1.291389	0.354669
O	-2.284440	-2.075248	-0.700832
C	-0.917269	-2.107703	-0.581021
C	-0.571005	-1.930279	0.787397
C	-1.698290	-1.422501	1.390467
H	-3.744351	-1.172365	0.462969
H	-1.799332	-1.056605	2.403646
H	0.435005	-1.995274	1.183698
H	-0.395055	-2.683650	-1.332872
H	-2.869949	0.671180	-1.214982
H	-0.716537	-0.378439	-2.286246
H	-1.003779	3.937522	0.257150
H	-1.127321	3.092887	-1.320577
H	-2.616302	3.465237	-0.366585

Structure *endo*-TS14. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31G+(d) Energy = -1238.1365178

S	-1.265867	1.678092	.570036
C	-1.914873	.535887	-.688340
C	-.770530	-.099762	-1.219300
C	.464920	.296753	-.489771
N	.318742	1.153453	.527019
O	1.563692	-.253958	-.819876
B	2.898466	-.233342	.042620
F	3.290611	1.081280	.196496
C	-1.222087	3.264453	-.345590
F	2.560332	-.851839	1.245287
F	3.775926	-.982485	-.712138
C	-2.853347	-1.043112	.287615
O	-2.515444	-1.889430	-.742390
C	-1.173949	-2.105601	-.550677
C	-.878939	-1.953313	.831487
C	-1.958519	-1.293955	1.375085
H	-3.906215	-.794713	.344058
H	-2.061923	-.911055	2.382197
H	.074382	-2.174142	1.296098
H	-.690593	-2.744664	-1.277058
H	-2.752560	.889694	-1.280376
H	-.689434	-.405878	-2.255658
H	-.626312	3.952871	.258909
H	-.754866	3.109550	-1.319967
H	-2.245996	3.637803	-.442751

Structure *exo*-TS14. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.0817727

O	-1.836125	-0.999609	1.190660
C	-1.398768	-1.854838	0.220456
C	-2.511712	-2.232511	-0.579824
C	-3.506071	-1.322448	-0.306268
C	-2.943790	-0.409960	0.633768
C	-1.739515	0.729735	-0.651572
C	-0.747512	-0.199991	-1.018973
C	0.555937	0.059437	-0.332133
N	0.571574	1.055199	0.568287
S	-0.884595	1.847221	0.514185
O	1.530301	-0.704092	-0.589091
B	3.028578	-0.536538	0.040589
F	2.890010	-0.824265	1.373591
C	-0.566270	3.289785	-0.569303
F	3.737833	-1.471386	-0.662378
F	3.394866	0.758854	-0.224771
H	-3.468902	0.275434	1.287842
H	-4.463561	-1.212162	-0.797607
H	-2.503765	-3.008709	-1.333543
H	-0.494474	-2.402537	0.450503
H	-2.455166	1.186715	-1.324530
H	-0.718568	-0.687595	-1.984233
H	0.140335	3.927944	-0.034013
H	-0.129486	2.945586	-1.508620
H	-1.508389	3.821614	-0.731149

Structure *exo*-TS14. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1238.1343436

O	-1.889473	-.981247	1.195878
C	-1.446002	-1.859533	.249555
C	-2.546019	-2.221650	-.577099
C	-3.528478	-1.286990	-.339725
C	-2.970344	-.371971	.603751
C	-1.726382	.728946	-.655179
C	-.736295	-.216408	-.999055
C	.553499	.042601	-.296129
N	.568877	1.042095	.591693
S	-.880258	1.855577	.511168
O	1.537110	-.723821	-.544605
B	3.018145	-.548804	.025709
F	2.941528	-.747399	1.392135
C	-.510554	3.279451	-.580304
F	3.720295	-1.539610	-.628945
F	3.425198	.728959	-.324701
H	-3.499877	.327461	1.239597
H	-4.472248	-1.164218	-.855333
H	-2.535563	-3.008838	-1.320043
H	-.560893	-2.425156	.510088
H	-2.420446	1.189584	-1.348946
H	-.696871	-.716033	-1.958257
H	.186518	3.915803	-.029699
H	-.048672	2.918006	-1.501222
H	-1.441528	3.819830	-.776739

Structure *endo*-TS15. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.096437

O	-0.885779	2.407266	0.983771
C	0.210766	2.012725	0.273003
C	-0.138330	1.914212	-1.097837
C	-1.513083	1.918348	-1.142256
C	-1.943410	1.962242	0.221822
C	-1.623456	0.045260	0.866159
C	-0.216130	-0.062778	0.843496
C	0.248583	-0.935326	-0.266378
N	-0.704918	-1.460780	-1.061185
S	-2.197743	-1.101464	-0.420292
O	1.468598	-1.180716	-0.531022
B	2.701529	-0.398681	0.056823
F	2.526634	-0.303289	1.434715
C	-2.624037	-2.572410	0.587363
F	3.785763	-1.136326	-0.302235
F	2.662215	0.863361	-0.538456
H	-2.918471	2.259714	0.588999
H	-2.153080	1.771326	-2.002045
H	0.571210	1.741237	-1.894173
H	1.177217	2.200842	0.714131
H	-2.211753	0.072531	1.777641
H	0.413829	0.035111	1.715290
H	-2.762272	-3.401263	-0.110506
H	-1.807407	-2.786378	1.279262
H	-3.558088	-2.370578	1.119826

Structure *endo*-TS15. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1238.1441109

O	-.927586	2.455247	.952007
C	.173255	2.113003	.223522
C	-.191879	1.991913	-1.140160
C	-1.568087	1.942024	-1.165478
C	-1.982854	1.964680	.206189
C	-1.612386	.088221	.842891
C	-.201851	-.014625	.807262
C	.253243	-.894388	-.295355
N	-.703143	-1.422403	-1.082671
S	-2.196331	-1.076844	-.427219
O	1.473202	-1.156750	-.563716
B	2.716519	-.497679	.100868
F	2.561513	-.588794	1.489341
C	-2.587249	-2.547981	.594557
F	3.794677	-1.201276	-.366828
F	2.723354	.846128	-.306153
H	-2.961692	2.238372	.582495
H	-2.211613	1.769280	-2.018425
H	.506974	1.852256	-1.953749
H	1.137463	2.329734	.658235
H	-2.185974	.106270	1.764937
H	.429432	.105817	1.677232
H	-2.732352	-3.379703	-.099037
H	-1.755161	-2.752741	1.271047
H	-3.513273	-2.351625	1.143545

Structure *exo*-TS15. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.0948614

C	0.359916	-0.954871	-0.275916
C	-0.195075	0.027937	0.692857
C	-1.602619	-0.026136	0.763491
S	-2.052664	-1.365036	-0.394664
N	-0.531313	-1.681124	-0.977626
C	-2.375184	-2.727305	0.787989
O	1.601189	-1.116635	-0.502387
C	-0.078982	1.829866	-0.610191
C	-0.365191	2.747481	0.434457
C	-1.721116	2.675659	0.652020
C	-2.198720	1.665423	-0.236936
O	-1.247550	1.479490	-1.215978
H	-3.219311	1.513621	-0.568490
H	-2.297906	3.150004	1.434843
H	0.381241	3.291155	0.997684
H	0.833480	1.687926	-1.170911
H	-2.177769	0.013804	1.681777
H	0.441693	0.350378	1.502004
H	-2.440107	-3.645244	0.199777
H	-1.551919	-2.787403	1.502330
H	-3.328347	-2.534215	1.288963
B	2.772504	-0.243466	0.092468
F	3.900441	-0.953019	-0.178884
F	2.714297	0.981965	-0.571316
F	2.528701	-0.089546	1.453309

Structure *exo*-TS15. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1238.143015

O	-1.421721	1.440348	-1.203144
C	-.249754	1.876511	-.665012
C	-.539327	2.760263	.407630
C	-1.872290	2.584107	.703921
C	-2.326955	1.545051	-.166713
C	-1.565787	-.099538	.772818
C	-.166836	.053519	.645208
C	.414085	-.890535	-.340965
N	-.448421	-1.666161	-1.018882
S	-1.971336	-1.460051	-.379908
O	1.661029	-.980065	-.601549
B	2.786070	-.154647	.092622
F	2.634443	-.320710	1.473616
C	-2.144312	-2.856417	.794204
F	3.961651	-.666221	-.388919
F	2.590778	1.190476	-.262640
H	-3.351320	1.323626	-.443455
H	-2.435211	3.008649	1.525270
H	.197736	3.354157	.931986
H	.630311	1.813333	-1.288232
H	-2.100721	-.110625	1.716516
H	.466872	.429438	1.435204
H	-2.181452	-3.767723	.192678
H	-1.283444	-2.874070	1.465813
H	-3.082052	-2.731538	1.344275

Structure *endo*-TS16. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.0917544

C	-0.093139	-0.429068	1.402712
C	1.233640	0.271972	1.339836
C	1.274906	1.309203	0.385800
S	-0.359123	1.400024	-0.384300
N	-0.956766	0.061093	0.409153
C	-1.157869	2.800863	0.478345
O	-0.369984	-1.341486	2.152384
C	2.466631	-1.132571	0.397871
C	1.633049	-1.542606	-0.682801
C	1.709016	-0.538318	-1.617001
C	2.575620	0.448104	-1.057626
O	3.298236	-0.133120	-0.050634
H	3.074211	1.264072	-1.565857
H	1.118167	-0.435096	-2.517071
H	0.938916	-2.371626	-0.674665
H	2.862403	-1.740362	1.200593
H	1.781696	2.257260	0.526666
H	1.822121	0.311928	2.249243
H	-2.215848	2.725488	0.216834
H	-1.013872	2.702314	1.555548
H	-0.734960	3.735405	0.097623
B	-2.161987	-0.712999	-0.394241
F	-2.732922	0.341454	-1.128406
F	-1.554105	-1.640113	-1.227871
F	-3.008163	-1.261457	0.519631

Structure *endo*-TS16. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1238.1416332

C	-.097823	-.575407	1.293023
C	1.214884	.149342	1.334140
C	1.267341	1.254788	.460262
S	-.343924	1.391863	-.351084
N	-.945222	-.014953	.324633
C	-1.155873	2.730539	.598794
O	-.380528	-1.552180	1.958949
C	2.574725	-1.133684	.368799
C	1.821904	-1.508866	-.780675
C	1.887774	-.437439	-1.641768
C	2.668240	.552618	-.972204
O	3.368018	-.060130	.034980
H	3.147779	1.424899	-1.398616
H	1.349066	-.302314	-2.570820
H	1.201377	-2.391274	-.868749
H	2.959550	-1.772178	1.152714
H	1.746428	2.200148	.691630
H	1.758687	.136285	2.271986
H	-2.203620	2.721228	.289104
H	-1.061157	2.530905	1.667806
H	-.684824	3.679075	.321614
B	-2.266466	-.648661	-.394062
F	-2.739750	.447058	-1.159753
F	-1.848737	-1.690472	-1.209629
F	-3.161355	-1.027860	.574369

Structure *exo*-TS16. B3LYP/6-31G(d) Geometry.
B3LYP/6-31G(d) Energy = -1238.0887701

O	1.877248	-0.532117	-1.259485
C	2.331934	-1.294380	-0.218536
C	3.605008	-0.792660	0.176077
C	3.702949	0.467231	-0.366615
C	2.479172	0.681970	-1.061795
C	1.204932	1.050589	0.612753
C	1.156908	-0.229431	1.194458
C	-0.153331	-0.939161	0.966722
N	-0.990170	-0.181060	0.144289
S	-0.393753	1.334670	-0.197977
O	-0.427356	-2.044168	1.388459
C	-1.210379	2.455877	0.999588
B	-2.497023	-0.502738	-0.445429
F	-3.268533	-0.909052	0.607021
F	-2.867878	0.781368	-0.915961
F	-2.393658	-1.411562	-1.460055
H	2.260078	1.427784	-1.815889
H	4.471460	1.209636	-0.197314
H	4.278118	-1.274466	0.872886
H	1.953869	-2.307575	-0.182539
H	1.647227	1.930418	1.064124
H	1.687047	-0.475090	2.105621
H	-2.254314	2.492336	0.684803
H	-1.115789	2.044571	2.006093
H	-0.743018	3.442069	0.920214

Structure *exo*-TS16. B3LYP/6-31+G(d) Geometry.
B3LYP/6-31+G(d) Energy = -1238.13877

O	1.890963	-.531561	-1.263808
C	2.332286	-1.304917	-.224297
C	3.604584	-.809511	.186158
C	3.712606	.454891	-.346906
C	2.494958	.680251	-1.053252
C	1.211260	1.045415	.607660
C	1.152050	-.237856	1.187043
C	-.165482	-.929058	.963636
N	-.996908	-.166688	.137756
S	-.383833	1.348233	-.207026
O	-.458669	-2.025132	1.401115
C	-1.197901	2.468070	.994546
B	-2.491767	-.501565	-.439015
F	-3.320756	-.729095	.639817
F	-2.824741	.716167	-1.091687
F	-2.409989	-1.555298	-1.317283
H	2.287175	1.431161	-1.805793
H	4.484361	1.192509	-.167987
H	4.270445	-1.300310	.884443
H	1.953332	-2.318563	-.203254
H	1.653628	1.921661	1.067148
H	1.676142	-.487089	2.101064
H	-2.241757	2.533589	.680059
H	-1.115999	2.046180	1.998093
H	-.713953	3.447626	.925810

Structure *endo*-TS17. AM1 Geometry.
AM1 Energy = 0.2373646
B3LYP/6-31G(d) Energy = -1108.6266894

C	2.102361	-1.282507	-0.183597
C	1.518893	-0.036061	-0.427719
C	2.284365	1.126287	-0.347300
C	3.637397	1.038475	-0.017763
C	4.231544	-0.203194	0.230941
C	3.451342	-1.364945	0.145561
S	-0.144289	-0.006373	-0.914103
C	-0.934555	-0.631336	0.526612
C	-1.648444	0.427122	1.095479
C	-1.479340	1.713581	0.276356
O	-2.045769	2.766326	0.625739
C	5.670928	-0.293802	0.566090
N	-0.669052	1.562535	-0.827395
H	1.837274	2.116973	-0.541176
H	4.240237	1.957290	0.047434
H	3.909581	-2.346262	0.339601
H	1.501635	-2.202902	-0.249680
H	5.872877	-1.167127	1.234037
H	6.270357	-0.423339	-0.370821
H	6.022145	0.634696	1.080198
H	-1.830191	0.538628	2.172237
H	-0.488544	-1.488140	1.024054
C	-2.570625	-1.914460	-0.206248
H	-2.060587	-2.866710	-0.339248
C	-3.610764	-0.083659	0.779941
H	-4.122916	0.564245	1.493311
C	-3.648477	0.065434	-0.631142
H	-4.012502	0.948576	-1.160297
C	-3.015268	-1.047082	-1.226023
H	-2.830249	-1.169632	-2.293561
C	-3.313325	-1.548562	1.061227
H	-2.735385	-1.726002	1.996077
H	-4.271770	-2.128428	1.124866

Structure *endo*-TS17. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 82.174716

C	.000000	.000000	.000000
C	.000000	.000000	1.512260
C	1.349216	.000000	1.940052
C	2.169784	.369923	.854260
C	1.351895	.633221	-.274724
C	.622885	2.496409	.347575
C	-.199248	2.164359	1.433626
S	.654879	2.680166	2.891911
N	1.862621	3.398548	2.216721
C	1.862505	3.234251	.833204
C	-.453017	3.785142	3.582766
C	-1.691576	3.258400	3.977969
C	-2.615227	4.048894	4.653601
C	-2.324124	5.387011	4.950091
C	-1.089906	5.917021	4.552918
C	-.170416	5.120747	3.874400
C	-3.298962	6.228231	5.681454
O	2.769644	3.653754	.088685
H	.788048	5.563964	3.567953
H	-.843280	6.967823	4.771988
H	-3.586425	3.620305	4.956252
H	-1.938615	2.204779	3.749369
H	-4.347574	5.898631	5.472735
H	-3.116472	6.146200	6.783765
H	-3.198185	7.303191	5.390829
H	.278986	2.721373	-.672482
H	-1.286616	2.057147	1.382609
H	-.868435	-.281991	2.112592
H	1.715250	.859506	-1.279265
H	3.249849	.507702	.893617
H	1.698615	-.209418	2.951529
H	-.859152	.544189	-.458654
H	-.005813	-1.056775	-.383175

Structure *exo*-TS17. AM1 Geometry.
AM1 Energy = 0.2372954
B3LYP/6-31(d) Energy = -1108.6252014

C	-3.763467	-1.085761	1.178992
C	-3.637036	0.098774	0.405453
C	-1.668818	0.435215	0.949704
C	-0.966868	-0.574404	0.288738
C	-2.603087	-1.654904	-0.716534
C	-3.128355	-2.146397	0.498785
C	-1.436496	1.798374	0.285116
N	-0.558008	1.755563	-0.776114
S	-0.079873	0.187128	-1.026174
C	-3.292908	-0.340428	-1.005564
C	1.552811	0.033489	-0.469306
C	2.077643	-1.255406	-0.338653
C	3.404489	-1.428409	0.041370
C	4.220088	-0.315981	0.292603
C	3.684867	0.968929	0.153845
C	2.354151	1.147994	-0.225701
C	5.627674	-0.502447	0.712438
O	-2.020648	2.814435	0.705959
H	1.953372	2.171450	-0.329701
H	4.317109	1.849607	0.345203
H	3.817540	-2.443087	0.144015
H	1.448621	-2.137718	-0.534449
H	6.057463	-1.435196	0.270915
H	6.259062	0.363849	0.395216
H	5.682060	-0.585408	1.827829
H	-1.894824	0.436257	2.022487
H	-0.570082	-1.499923	0.696824
H	-2.076149	-2.231893	-1.473915
H	-4.083239	1.071074	0.625970
H	-4.239439	-0.527886	-1.580922
H	-2.688662	0.394255	-1.582598
H	-2.987690	-3.153450	0.890260
H	-4.194057	-1.142229	2.179049

Structure *exo*-TS17. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 84.393823

C	.000000	.000000	.000000
C	.000000	.000000	1.395221
C	1.229233	.000000	2.071521
C	2.425642	-.004373	1.363147
C	2.421527	-.011812	-.038870
C	1.195590	-.009275	-.715406
S	-1.371188	-.034181	2.417466
C	-1.872019	1.652965	2.412062
C	-3.175215	1.692568	1.899668
C	-3.624864	.289173	1.508630
N	-2.618655	-.652898	1.704618
O	-4.756214	.013588	1.066403
C	3.697703	-.001567	-.789941
C	-4.348981	2.039346	3.586544
C	-3.922897	3.387614	3.720699
C	-2.635925	3.404497	4.300983
C	-2.235211	2.077467	4.563820
C	-3.473899	1.213126	4.509788
H	-.950846	.011118	-.553827
H	1.171400	-.008274	-1.816900
H	3.385942	.000858	1.906536
H	1.247909	.010301	3.176923
H	4.438292	-.695125	-.318245
H	3.545382	-.313149	-1.852594
H	4.131201	1.031711	-.784770
H	-3.618434	2.520949	1.330556
H	-1.159229	2.478781	2.379368
H	-1.299608	1.755482	5.022503
H	-5.327549	1.700830	3.243977
H	-3.949151	1.151360	5.526680
H	-3.295063	.173065	4.162602
H	-2.015978	4.293452	4.438779
H	-4.466080	4.257125	3.343475

Structure *endo*-TS18. AM1 Geometry.
AM1 Energy = 0.2427483
B3LYP/6-31(d) Energy = -1108.6200768

O	-2.238816	2.336669	-.300082
C	-.870537	2.110089	-.322987
C	-1.447613	.137070	-1.323336
C	-2.603864	-.105807	-.564552
C	-2.729745	1.412659	.659142
C	-2.419538	-1.349957	.323548
N	-1.214950	-1.986337	.138858
S	-.398687	-1.238183	-1.100913
C	-.470731	1.523507	.917298
C	-1.639401	1.098083	1.552670
O	-3.321812	-1.704323	1.106206
H	-3.617205	.069545	-.960078
H	-1.372725	.672218	-2.264874
H	-.316937	2.643757	-1.091832
H	-3.790644	1.532014	.889975
H	-1.738756	.534120	2.479481
H	.556642	1.378387	1.246102
C	1.119090	-.676699	-.492768
C	1.629597	-1.111744	.730066
C	2.912515	-.723885	1.117960
C	3.691873	.092117	.290838
C	3.168750	.520300	-.937295
C	1.890463	.135577	-1.329231
H	1.035901	-1.764066	1.393943
H	3.314982	-1.068938	2.082841
C	5.060404	.485019	.697003
H	3.775301	1.159463	-1.596414
H	1.493098	.472880	-2.299302
H	5.328806	1.488594	.284143
H	5.153591	.522569	1.810384
H	5.799041	-.262004	.309101

Structure *endo*-TS18. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 86.170471

C	.000000	.000000	.000000
C	.000000	.000000	1.403295
C	1.224290	.000000	2.072968
C	2.426638	-.015399	1.368938
C	2.423884	-.023148	-.031305
C	1.196719	-.012880	-.708242
S	-1.526785	-.197104	2.142473
C	-2.517954	1.180253	1.746108
C	-2.975829	1.721668	2.957503
C	-2.278362	1.023397	4.127366
N	-1.480481	-.032576	3.699779
O	-2.463194	1.309260	5.325498
C	3.698739	-.046181	-.784263
C	-2.416271	3.642483	2.982884
C	-2.717590	3.813867	1.499782
C	-1.537999	3.093964	.896175
C	-.489151	3.117104	1.830362
C	-1.010577	3.470036	3.095930
H	-4.025749	2.010240	3.147671
H	-3.047280	1.212753	.790242
H	-1.465606	2.833552	-.161239
H	-3.052137	4.063893	3.766906
H	-.441735	3.523206	4.023644
H	.545007	2.830908	1.640151
H	-3.710584	3.414845	1.185091
H	-2.676090	4.905214	1.233750
H	1.254244	.012021	3.171664
H	3.379971	-.016275	1.920105
H	1.181343	-.011052	-1.811754
H	-.960646	.013057	-.547553
H	3.604973	.524109	-1.742425
H	4.529097	.400548	-.183495
H	3.975037	-1.103667	-1.029667

Structure *exo*-TS18. AM1 Geometry.
AM1 Energy = 0.2401852
B3LYP/6-31(d) Energy = -1108.6210171

C	2.535728	-.224831	.438002
C	1.428548	.122208	1.226493
S	.322672	-1.238529	1.158186
N	1.085470	-2.134467	-.013185
C	2.287744	-1.542475	-.316145
O	3.144799	-1.978319	-1.108414
C	2.456422	1.058700	-1.088180
C	2.888447	2.209142	-.326014
C	1.770321	2.668107	.369907
C	.680020	1.815980	-.006794
O	1.046589	1.091958	-1.135891
C	-1.171945	-.660461	.508888
H	3.575453	-.011453	.719898
H	1.413496	.714564	2.136252
H	2.924533	.539019	-1.928594
H	3.915228	2.560356	-.254302
H	1.722260	3.463533	1.109038
H	-.389823	1.868454	.190037
C	-1.636716	-1.041651	-.748961
C	-2.897715	-.619800	-1.173909
C	-3.698148	.177919	-.350207
C	-3.219705	.553805	.913501
C	-1.965162	.134658	1.342820
H	-1.023139	-1.672705	-1.415691
H	-3.263021	-.921121	-2.167804
C	-5.042617	.607932	-.797109
H	-3.843767	1.178557	1.570039
H	-1.605448	.427330	2.341587
H	-5.318896	1.593592	-.347993
H	-5.084417	.700739	-1.910416
H	-5.805938	-.147643	-.480044

Structure *exo*-TS18. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 86.541566

C	.000000	.000000	.000000
C	.000000	.000000	1.403107
C	1.223147	.000000	2.074763
C	2.425918	-.020008	1.371295
C	2.423983	-.029792	-.028889
C	1.197321	-.016099	-.707200
S	-1.537650	-.152621	2.139445
C	-2.388825	1.344810	1.863265
C	-2.722135	1.872315	3.118552
C	-2.079824	1.026328	4.220355
N	-1.447580	-.098629	3.704320
O	-2.174528	1.276090	5.436793
C	3.698801	-.056364	-.781738
C	-1.718648	3.624889	3.273535
C	-2.545312	4.316550	2.345931
C	-2.163129	3.954536	1.033163
C	-1.072215	3.072158	1.105677
C	-.500153	3.154250	2.498916
H	-3.699825	2.308927	3.378003
H	-2.948490	1.494534	.937968
H	-1.697299	3.781439	4.353799
H	-3.400819	4.941744	2.613010
H	-2.688326	4.245612	.120317
H	-.559088	2.578945	.279953
H	.305811	3.935406	2.545821
H	-.065115	2.198206	2.865629
H	1.251643	.018329	3.173885
H	3.379144	-.020833	1.923007
H	1.182744	-.013710	-1.810648
H	-.960057	.014690	-.548348
H	3.613622	.533089	-1.729136
H	4.535484	.366905	-.172738
H	3.959654	-1.112884	-1.047352

Structure *endo*-TS19. AM1 Geometry.
AM1 Energy = 0.1822162
B3LYP/6-31(d) Energy = -1144.5354153

O	-3.270000	-1.490566	1.047631
C	-2.644283	-1.912210	-0.120887
C	-3.051428	-1.059104	-1.199031
C	-3.634351	0.066015	-0.615271
C	-3.549255	-0.121582	0.814837
C	-1.650615	0.409495	1.098965
C	-0.934374	-0.648337	0.518819
S	-0.147576	-0.021126	-0.916208
N	-0.678596	1.547368	-0.828589
C	-1.484509	1.697493	0.277125
C	1.516814	-0.043122	-0.434505
C	2.100756	-1.283492	-0.162518
C	3.451219	-1.358219	0.162401
C	4.231797	-0.194849	0.217157
C	3.637432	1.040351	-0.061554
C	2.282889	1.120669	-0.386663
C	5.665323	-0.274532	0.579074
O	-2.057215	2.747291	0.625439
H	1.835326	2.106406	-0.603083
H	4.241478	1.959962	-0.024615
H	3.910506	-2.334907	0.376456
H	1.499698	-2.205112	-0.202914
H	6.110629	-1.242901	0.241973
H	6.243362	0.562353	0.115145
H	5.779379	-0.204622	1.690849
H	-1.787147	0.519581	2.184154
H	-0.491097	-1.502389	1.023030
H	-2.260242	-2.929652	-0.104402
H	-4.117321	0.363659	1.610284
H	-3.987382	0.973749	-1.104037
H	-2.872575	-1.244949	-2.255663

Structure *endo*-TS19. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 48.698000

C	.000000	.000000	.000000
C	.000000	.000000	1.395580
C	1.229322	.000000	2.071198
C	2.426150	-.003983	1.362716
C	2.421799	-.011235	-.038835
C	1.195226	-.009044	-.715244
S	-1.369373	-.029844	2.420053
C	-1.909092	1.640023	2.366104
C	-3.222185	1.637407	1.856340
C	-3.629163	.210993	1.492404
N	-2.601800	-.695886	1.727092
O	-4.743079	-.103098	1.033097
C	3.694427	.001161	-.795896
C	-4.325634	2.151750	3.468904
O	-3.339512	3.064977	3.903454
C	-2.327620	2.266899	4.432289
C	-2.897199	1.008757	4.827497
C	-4.162607	.944805	4.244867
H	-.950984	.010758	-.553699
H	1.172310	-.008512	-1.816753
H	3.385916	.001506	1.907079
H	1.248665	.009835	3.176673
H	4.505643	-.514169	-.223514
H	3.577741	-.507522	-1.784720
H	4.012394	1.059517	-.982102
H	-3.654513	2.442453	1.241225
H	-1.224113	2.487574	2.283368
H	-1.423112	2.792758	4.751067
H	-5.234336	2.614090	3.073114
H	-4.881436	.129085	4.280696
H	-2.402796	.257092	5.441489

Structure *exo*-TS19. AM1 Geometry.
AM1 Energy = 0.1814185
B3LYP/6-31(d) Energy = -1144.5345199

C	2.344559	1.143245	-0.240346
C	1.545570	0.023910	-0.469280
C	2.073923	-1.261585	-0.320682
C	3.400811	-1.426501	0.062674
C	4.213632	-0.308881	0.299400
C	3.675412	0.972667	0.142663
S	-0.087260	0.166695	-1.031383
C	-0.971093	-0.590707	0.287840
C	-1.677265	0.426314	0.944668
C	-1.438600	1.787814	0.271692
N	-0.568700	1.733598	-0.792077
O	-2.023277	2.803910	0.692479
C	5.621386	-0.486172	0.722629
C	-3.575400	0.113127	0.337668
C	-3.777715	-1.065607	1.150402
C	-3.172026	-2.123629	0.474845
C	-2.638429	-1.576500	-0.741573
O	-3.207087	-0.322228	-0.951263
H	1.941803	2.164356	-0.359065
H	4.305461	1.857403	0.322205
H	3.816257	-2.438682	0.179138
H	1.447565	-2.148088	-0.505299
H	6.052839	-1.425398	0.296759
H	6.251427	0.375773	0.391167
H	5.675667	-0.550446	1.839249
H	-1.890032	0.433718	2.020502
H	-0.572798	-1.509300	0.708572
H	-2.223408	-2.055531	-1.625610
H	-4.051416	1.096800	0.364835
H	-3.048013	-3.149657	0.811249
H	-4.233966	-1.071679	2.137626

Structure *exo*-TS19. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 45.953805

O	.000000	.000000	.000000
C	.000000	.000000	1.411661
C	1.375781	.000000	1.849763
C	2.146515	.364967	.746631
C	1.237611	.551220	-.346950
C	-.223359	2.025115	1.539636
C	.532275	2.490228	.450110
S	-.610673	2.983165	-.798305
N	-1.934234	2.715713	-.023640
C	-1.712172	2.143315	1.225587
C	-.263644	4.652265	-.944491
C	-1.188809	5.678874	-.748121
C	-.856085	7.004699	-1.015526
C	.424058	7.330099	-1.481376
C	1.358339	6.303449	-1.673128
C	1.019559	4.981266	-1.406057
C	.788032	8.740271	-1.749189
O	-2.620853	1.762131	1.986096
H	-2.198040	5.451516	-.375713
H	-1.604854	7.796409	-.855538
H	2.371868	6.547581	-2.035958
H	1.770954	4.184056	-1.558311
H	1.516871	8.810349	-2.595114
H	-.115823	9.346247	-2.005579
H	1.261758	9.187871	-.837745
H	.061477	2.104004	2.598670
H	1.543345	2.897019	.520563
H	1.407302	.702128	-1.414003
H	-.895855	-.422479	1.868644
H	3.220506	.554908	.709296
H	1.697292	-.165318	2.878934

Structure *endo*-TS20. AM1 Geometry.
AM1 Energy = 0.1870086
B3LYP/6-31(d) Energy = -1144.5303648

C	-2.283464	2.402827	-.265759
C	-.812718	2.052592	-.299365
C	-1.459956	.149985	-1.314730
C	-2.605813	-.133014	-.561966
C	-2.774740	1.385912	.755439
C	-2.405358	-1.390953	.297846
N	-1.189925	-2.005627	.102617
S	-.384470	-1.217713	-1.118326
C	-.480574	1.477299	.941023
C	-1.668943	1.074312	1.589542
O	-3.305685	-1.782043	1.064994
H	-3.627644	.056059	-.922619
H	-1.386067	.691749	-2.253088
H	-.120405	2.452783	-1.037572
H	-3.821881	1.312319	1.056576
H	-1.727061	.517781	2.527001
H	.530240	1.283854	1.303255
H	-2.792242	2.340386	-1.254009
H	-2.420367	3.442172	.134296
C	1.130397	-.659418	-.502216
C	1.660523	-1.146804	.692291
C	2.943313	-.762146	1.083678
C	3.702296	.103561	.288797
C	3.158429	.586210	-.909709
C	1.879945	.205469	-1.305016
H	1.081646	-1.836350	1.331159
H	3.361243	-1.147992	2.026220
C	5.070804	.493523	.697956
H	3.747903	1.266836	-1.542155
H	1.463805	.590107	-2.249183
H	5.322129	1.519178	.331206
H	5.176546	.478648	1.810753
H	5.813782	-.224529	.266228

Structure *endo*-TS20. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 51.952263

C	.000000	.000000	.000000
C	.000000	.000000	1.402788
C	1.224650	.000000	2.072461
C	2.426770	-.012118	1.368121
C	2.423835	-.017983	-.032158
C	1.196570	-.009948	-.708786
S	-1.519103	-.205986	2.157360
C	-2.543428	1.096396	1.695089
C	-3.012361	1.716009	2.867073
C	-2.279498	1.113790	4.077255
N	-1.464439	.054500	3.707509
O	-2.459155	1.483060	5.252710
C	3.698771	-.037499	-.785085
C	-2.556184	3.575148	2.741443
O	-2.873736	3.655795	1.357021
C	-1.762358	3.171566	.698815
C	-.631921	3.242670	1.559193
C	-1.116914	3.535881	2.839613
H	-4.084635	1.936067	3.040286
H	-3.055397	1.103665	.731623
H	-1.870598	3.010784	-.377684
H	-3.267591	4.102783	3.388359
H	-.553203	3.639891	3.764056
H	.400578	3.061172	1.267711
H	1.255181	.009032	3.171332
H	3.380277	-.013276	1.919041
H	1.180617	-.008044	-1.812266
H	-.960593	.008175	-.547313
H	3.600093	.520785	-1.749802
H	4.524866	.423804	-.189366
H	3.985241	-1.095048	-1.018210

Structure *exo*-TS20. AM1 Geometry.
AM1 Energy = 0.1838682
B3LYP/6-31(d) Energy = -1144.5324749

C	2.532602	-.259525	.439120
C	1.434673	.121039	1.216676
S	.307378	-1.224391	1.181419
N	1.050717	-2.151837	.020912
C	2.261071	-1.578670	-.298268
O	3.103767	-2.045069	-1.088003
C	2.553365	1.055431	-1.124773
C	2.963432	2.167724	-.341062
C	1.850511	2.657729	.376410
C	.721061	1.883139	.042294
C	1.041728	1.136119	-1.231331
C	-1.184677	-.646173	.524726
H	3.576901	-.057629	.711170
H	1.422986	.732400	2.114390
H	3.164103	.514321	-1.851670
H	3.990076	2.519246	-.234934
H	1.882110	3.445079	1.128962
H	-.292251	2.005335	.422265
H	.758497	1.759925	-2.121074
H	.533284	.150041	-1.331696
C	-1.695261	-1.118225	-.684225
C	-2.954163	-.695454	-1.112412
C	-3.708666	.194282	-.340311
C	-3.185193	.660711	.873762
C	-1.931278	.240985	1.306204
H	-1.122462	-1.828517	-1.305963
H	-3.356511	-1.070107	-2.066251
C	-5.051994	.626048	-.788898
H	-3.772014	1.358916	1.489481
H	-1.534256	.609360	2.265157
H	-5.281010	1.660188	-.431442
H	-5.126812	.611151	-1.904201
H	-5.829105	-.067001	-.376732

Structure *exo*-TS20. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 48.217862

C	.000000	.000000	.000000
C	.000000	.000000	1.403307
C	1.224655	.000000	2.072965
C	2.426915	-.013025	1.368794
C	2.424057	-.019582	-.031464
C	1.196629	-.010760	-.708251
S	-1.518564	-.192553	2.161061
C	-2.529136	1.138133	1.660223
C	-2.990677	1.768865	2.828535
C	-2.284972	1.168606	4.047990
N	-1.472353	.097378	3.697896
O	-2.463635	1.556039	5.217333
C	3.699509	-.044004	-.783266
C	-2.216010	3.599356	2.769884
C	-3.081307	4.087229	1.720230
C	-2.542185	3.633177	.514922
C	-1.344595	2.926271	.843853
O	-1.002047	3.193661	2.165306
H	-4.032442	2.088207	2.999760
H	-3.060649	1.101409	.706771
H	-2.117667	3.916426	3.809971
H	-4.020769	4.616329	1.887229
H	-2.964081	3.724855	-.487310
H	-.563213	2.473675	.232909
H	1.255128	.013090	3.171762
H	3.380178	-.014080	1.920274
H	1.180433	-.009761	-1.812093
H	-.960916	.004884	-.547742
H	3.596428	.488889	-1.761744
H	4.519968	.440103	-.198022
H	3.996672	-1.104391	-.989078

Structure *endo*-17. AM1 Geometry.
AM1 Energy = 0.1490672
B3LYP/6-31(d) Energy = -1108.6917064

C	2.056411	-1.238447	-0.335785
C	1.464391	0.020269	-0.478901
C	2.213195	1.176977	-0.265603
C	3.555507	1.071084	0.100393
C	4.156146	-0.182850	0.253508
C	3.394355	-1.338804	0.030189
S	-0.179373	0.079379	-1.020975
C	-1.024585	-0.736045	0.351498
C	-1.841748	0.394139	1.012803
C	-1.588354	1.709687	0.239214
O	-2.158198	2.756050	0.598885
C	5.576368	-0.291292	0.657700
N	-0.713950	1.617255	-0.815699
H	1.762045	2.177828	-0.384708
H	4.145418	1.985446	0.267961
H	3.859485	-2.329794	0.141998
H	1.471610	-2.154520	-0.513929
H	6.043211	-1.216673	0.238895
H	6.162253	0.592842	0.304284
H	5.649717	-0.336170	1.774203
H	-1.555118	0.549591	2.080893
H	-0.257100	-1.184170	1.018418
C	-2.086365	-1.776456	-0.074819
H	-1.693434	-2.783159	-0.298975
C	-3.302580	-0.117635	0.918418
H	-4.012842	0.395453	1.589680
C	-3.664978	-0.139493	-0.561014
H	-4.369821	0.562786	-1.002365
C	-2.945669	-1.124242	-1.149715
H	-2.933793	-1.446314	-2.187942
C	-3.059292	-1.647048	1.148488
H	-2.575942	-1.874953	2.121514
H	-3.979306	-2.256509	1.026239

Structure *endo*-17. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 28.559412

C	.000000	.000000	.000000
C	.000000	.000000	1.566499
C	1.526256	.000000	1.817227
C	2.091857	-.896017	.688752
C	.825595	-1.327263	-.101557
C	2.844067	-2.066472	1.345924
N	2.829614	-2.025093	2.731271
S	2.029234	-.866375	3.347573
C	-.481495	-1.422779	1.822897
C	.004769	-2.207367	.831242
C	3.050681	.312630	4.051875
C	2.433011	1.518423	4.417957
C	3.141901	2.496068	5.107297
C	4.487424	2.294770	5.443744
C	5.107571	1.094185	5.074942
C	4.392592	.118594	4.384410
C	5.250349	3.341438	6.161375
O	3.415010	-2.963328	.699699
H	4.905114	-.812437	4.101653
H	6.165007	.917579	5.327729
H	2.642200	3.439021	5.389329
H	1.372770	1.694370	4.156408
H	4.579717	3.938878	6.828464
H	6.062328	2.890376	6.783641
H	5.722940	4.037995	5.421759
H	2.805920	-.354329	.018503
H	1.928509	1.038510	1.781190
H	-.556386	.810367	2.074227
H	1.030587	-1.733480	-1.107983
H	-.124733	-3.274687	.666760
H	-1.126192	-1.690557	2.658149
H	.523116	.875229	-.441716
H	-1.020217	-.099455	-.428292

Structure *exo*-17. AM1 Geometry.
AM1 Energy = 0.1464498
B3LYP/6-31(d) Energy = -1108.6928644

C	-3.534694	-1.341012	1.241455
C	-3.352913	0.016742	0.569769
C	-1.875647	0.404595	0.838162
C	-1.078416	-0.651054	0.046468
C	-2.164724	-1.516127	-0.632600
C	-2.830017	-2.251778	0.529785
C	-1.539039	1.806368	0.272656
N	-0.610376	1.833621	-0.738718
S	-0.113058	0.320063	-1.133958
C	-3.265871	-0.443737	-0.921174
C	1.489387	0.111006	-0.514342
C	2.027951	-1.179373	-0.526249
C	3.335640	-1.389196	-0.101824
C	4.119980	-0.312131	0.335355
C	3.572945	0.975302	0.336069
C	2.261180	1.191076	-0.087615
C	5.506894	-0.539155	0.801257
O	-2.108486	2.808759	0.741300
H	1.852360	2.216853	-0.082180
H	4.181342	1.829092	0.672300
H	3.758881	-2.404938	-0.111634
H	1.425338	-2.033832	-0.872134
H	5.966904	-1.414970	0.280681
H	6.144609	0.359863	0.614273
H	5.507250	-0.745747	1.901862
H	-1.642881	0.392475	1.928956
H	-0.376395	-1.253195	0.660830
H	-1.827049	-2.138492	-1.478718
H	-4.084152	0.806874	0.815764
H	-4.212022	-0.895842	-1.287991
H	-2.941242	0.362177	-1.612993
H	-2.706166	-3.318717	0.692890
H	-4.133255	-1.477183	2.139020

Structure *exo*-17. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 28.544193

C	.000000	.000000	.000000
C	.000000	.000000	1.396193
C	1.230544	.000000	2.071011
C	2.426518	-.008157	1.361428
C	2.422147	-.013174	-.040132
C	1.194728	-.009705	-.715571
S	-1.392305	-.138619	2.379498
C	-1.288075	1.420686	3.333625
C	-2.548436	2.203488	2.894163
C	-3.319388	1.327990	1.887361
N	-2.685665	.131733	1.593245
C	-1.484789	1.222686	4.854632
C	-1.365808	2.632297	5.433685
C	-2.463151	3.327696	5.054831
C	-3.337064	2.396944	4.217942
C	-3.034224	1.043178	4.935872
O	-4.410696	1.660849	1.392123
C	3.693336	-.004054	-.799459
H	-.949467	.009512	-.555281
H	1.169975	-.011906	-1.816790
H	3.386663	-.007690	1.905859
H	1.251383	.007233	3.176742
H	4.505477	-.517664	-.226530
H	3.574433	-.515899	-1.786341
H	4.011385	1.053306	-.990274
H	-2.318188	3.180160	2.403170
H	-.341549	1.964697	3.115403
H	-.855788	.441769	5.319927
H	-4.395603	2.678988	4.084692
H	-3.413135	1.016763	5.980779
H	-3.412810	.159160	4.383395
H	-.508991	2.947574	6.027156
H	-2.743588	4.359923	5.255658

Structure *endo*-18. AM1 Geometry.
AM1 Energy = 0.153974
B3LYP/6-31(d) Energy = -1108.6850383

C	-2.468175	2.316315	-.030956
C	-1.043333	1.775377	-.408860
C	-1.471465	.483826	-1.140134
C	-2.664620	-.039332	-.310052
C	-2.842634	1.036324	.790224
C	-2.322264	-1.451339	.219628
N	-1.128024	-1.972966	-.211997
S	-.371889	-.943739	-1.247668
C	-.552124	1.385732	.978468
C	-1.617434	.946944	1.689200
O	-3.130666	-2.047428	.955174
H	-3.594379	-.116555	-.925722
H	-1.732670	.697734	-2.200721
H	-.388099	2.447021	-.990608
H	-3.824061	1.020334	1.295112
H	-1.663004	.564428	2.706931
H	.490637	1.470635	1.274888
H	-3.124123	2.484091	-.910569
H	-2.421473	3.233951	.592213
C	1.156609	-.517995	-.565666
C	1.659442	-1.141960	.576041
C	2.949783	-.840998	1.013429
C	3.743204	.076950	.317288
C	3.227395	.695858	-.830298
C	1.942721	.397990	-1.272349
H	1.054562	-1.875661	1.137365
H	3.345504	-1.334912	1.914266
C	5.118328	.380609	.774381
H	3.844354	1.418346	-1.385478
H	1.552051	.887837	-2.177837
H	5.400967	1.432695	.523548
H	5.214149	.241031	1.879391
H	5.844709	-.306774	.270453

Structure *endo*-18. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 31.711659

C	.000000	.000000	.000000
C	.000000	.000000	1.403975
C	1.225502	.000000	2.072806
C	2.427400	-.009895	1.369094
C	2.424263	-.013524	-.031641
C	1.196721	-.006130	-.708058
S	-1.532825	-.179746	2.128117
C	-2.459689	1.373358	1.856567
C	-2.865572	1.794201	3.292064
C	-2.156295	.856987	4.281842
N	-1.478317	-.183600	3.665174
C	-2.456638	3.287113	3.374697
C	-2.802177	3.719785	1.908593
C	-1.841538	2.659488	1.264344
C	-.937758	3.336849	3.301101
C	-.573935	2.965941	2.050716
O	-2.246860	.966698	5.518068
C	3.699053	-.031147	-.784480
H	-3.968153	1.690500	3.470321
H	-3.345003	1.069775	1.239468
H	-1.748681	2.664996	.162035
H	-2.926638	3.846241	4.203363
H	-.317801	3.631827	4.144121
H	.421736	2.889629	1.620107
H	-3.871038	3.567403	1.646192
H	-2.493568	4.763859	1.689666
H	1.253980	.008755	3.171785
H	3.381092	-.008499	1.919856
H	1.180193	-.001402	-1.811709
H	-.960420	.006796	-.548602
H	3.593424	.503822	-1.761584
H	4.518173	.454784	-.198648
H	4.000193	-1.089745	-.993531

Structure *exo*-18. AM1 Geometry.
AM1 Energy = 0.1489573
B3LYP/6-31(d) Energy = -1108.6890385

C	2.544982	-.215949	.155917
C	1.427315	.392726	1.027301
S	.284845	-.986033	1.286102
N	.971032	-2.118579	.313260
C	2.141778	-1.657522	-.235595
O	2.884343	-2.320162	-.983247
C	2.612860	.734162	-1.066011
C	3.100672	2.066502	-.503953
C	2.105729	2.584256	.254294
C	.933075	1.605783	.209593
C	1.099959	1.074137	-1.252273
C	-1.218536	-.516425	.573941
H	3.524705	-.259556	.689561
H	1.753410	.678657	2.050441
H	3.153191	.322448	-1.936587
H	4.091533	2.463906	-.710490
H	2.072504	3.509612	.822566
H	-.056950	2.004425	.493115
H	.924610	1.863468	-2.013737
H	.470996	.185771	-1.477922
C	-1.691150	-1.069813	-.615938
C	-2.953092	-.710131	-1.089968
C	-3.748467	.197775	-.382758
C	-3.263767	.745390	.813580
C	-2.007401	.388386	1.291949
H	-1.086766	-1.797056	-1.186257
H	-3.324907	-1.148963	-2.028759
C	-5.094118	.564109	-.879920
H	-3.882941	1.458608	1.378343
H	-1.643218	.819576	2.237584
H	-5.359704	1.609232	-.585177
H	-5.145692	.485307	-1.993870
H	-5.859288	-.127879	-.444242

Structure *exo*-18. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 29.894902

C	.000000	.000000	.000000
C	.000000	.000000	1.403608
C	1.224351	.000000	2.074735
C	2.426537	-.014099	1.371799
C	2.424176	-.019360	-.028994
C	1.197414	-.009261	-.706972
S	-1.544509	-.116504	2.122376
C	-2.228290	1.582357	2.075249
C	-2.460447	1.918656	3.568269
C	-1.903452	.756246	4.408166
N	-1.467217	-.315252	3.645797
C	-1.362522	2.756651	1.570020
C	-2.284015	3.973740	1.640439
C	-2.479150	4.268793	2.946624
C	-1.695078	3.251792	3.773653
C	-.474378	3.036724	2.825507
O	-1.906312	.749950	5.652417
C	3.699856	-.039104	-.780266
H	-3.543747	2.029256	3.828215
H	-3.178352	1.506884	1.491521
H	-1.486903	3.507414	4.826613
H	-3.075120	5.054141	3.407509
H	-2.681567	4.454824	.748197
H	-.841595	2.580154	.611311
H	.153764	3.947393	2.717486
H	.165429	2.177382	3.115936
H	1.250991	.015074	3.174347
H	3.380482	-.011827	1.922477
H	1.182238	-.004323	-1.810514
H	-.959682	.010563	-.549566
H	3.594313	.488877	-1.761111
H	4.516985	.452737	-.196417
H	4.003661	-1.098348	-.981829

Structure *endo*-19. AM1 Geometry.
AM1 Energy = 0.1125039
B3LYP/6-31(d) Energy = -1144.5817833

O	-3.016874	-1.593418	1.139905
C	-2.128109	-1.771061	-0.010478
C	-1.016972	-0.746800	0.370776
C	-1.824958	0.393567	1.028488
C	-3.279852	-0.157449	0.947025
C	-1.593512	1.692777	0.223069
N	-0.732136	1.581496	-0.840560
S	-0.184925	0.042882	-1.016256
C	-2.969471	-1.136339	-1.120719
C	-3.679305	-0.145610	-0.531400
C	1.460219	0.005352	-0.479100
C	2.061611	-1.246229	-0.313048
C	3.401231	-1.329240	0.050655
C	4.155148	-0.163354	0.248738
C	3.544883	1.082910	0.072555
C	2.200731	1.171812	-0.291121
C	5.577096	-0.253550	0.651145
O	-2.170353	2.740905	0.564583
H	1.742252	2.166994	-0.428361
H	4.128450	2.004826	0.220259
H	3.873881	-2.314455	0.181385
H	1.483575	-2.170313	-0.470497
H	6.050362	-1.182160	0.246888
H	6.155118	0.629197	0.281662
H	5.653083	-0.279165	1.768142
H	-1.535728	0.563195	2.092395
H	-0.257715	-1.204729	1.039090
H	-1.831435	-2.829638	-0.098509
H	-4.001212	0.202705	1.699157
H	-4.380630	0.571331	-0.950959
H	-2.950875	-1.474984	-2.152043

Structure *endo*-19. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 5.969956

C	.000000	.000000	.000000
C	.000000	.000000	1.396500
C	1.230987	.000000	2.070602
C	2.426574	-.010494	1.360842
C	2.421897	-.016748	-.040588
C	1.194334	-.011584	-.715765
S	-1.391360	-.140967	2.377094
C	-1.302076	1.421627	3.311546
C	-2.578097	2.185627	2.875464
C	-3.333856	1.306820	1.864176
N	-2.681473	.118715	1.584119
C	-3.319119	2.385155	4.235578
O	-2.161671	2.581271	5.117044
C	-1.500336	1.299348	4.850400
C	-3.784107	1.001102	4.697646
C	-2.667345	.331533	5.069550
O	-4.415666	1.635004	1.347863
C	3.692934	-.010430	-.799936
H	-.949512	.010946	-.555571
H	1.169750	-.014092	-1.817059
H	3.386998	-.011196	1.904679
H	1.253133	.008450	3.176270
H	4.502478	-.531708	-.230222
H	3.571342	-.515740	-1.789871
H	4.016898	1.046283	-.984475
H	-2.359649	3.174430	2.402053
H	-.368774	1.989321	3.093779
H	-.591019	1.199842	5.472902
H	-4.013544	3.240882	4.309983
H	-4.827466	.696174	4.691208
H	-2.546722	-.670405	5.476016

Structure *exo*-19. AM1 Geometry.
AM1 Energy = 0.1097342
B3LYP/6-31(d) Energy = -1144.5845654

C	2.257820	1.192321	-0.070313
C	1.487412	0.116627	-0.510434
C	2.027408	-1.173160	-0.534564
C	3.333715	-1.387015	-0.108441
C	4.116286	-0.314159	0.342493
C	3.568503	0.972824	0.355014
S	-0.113670	0.329500	-1.134387
C	-1.073495	-0.640614	0.047790
C	-1.893908	0.415144	0.816594
C	-1.552202	1.818009	0.255725
N	-0.603993	1.842361	-0.735024
C	-2.181667	-1.499029	-0.627104
C	-2.844091	-2.252246	0.535738
C	-3.572591	-1.331237	1.207955
C	-3.355913	-0.000735	0.474788
O	-3.195040	-0.483139	-0.903242
O	-2.134325	2.815054	0.718429
C	5.502066	-0.545482	0.809584
H	1.849490	2.218279	-0.056302
H	4.175601	1.823566	0.701343
H	3.757926	-2.402234	-0.128504
H	1.427199	-2.024137	-0.892743
H	5.964736	-1.413865	0.278979
H	6.139222	0.356678	0.636242
H	5.499403	-0.766423	1.907402
H	-1.709907	0.405880	1.915038
H	-0.382155	-1.243318	0.670388
H	-1.933059	-2.051039	-1.548560
H	-4.128326	0.786315	0.515633
H	-2.702009	-3.313363	0.711815
H	-4.192598	-1.427669	2.094196

Structure *exo*-19. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 1.257431

O	.000000	.000000	.000000
C	.000000	.000000	1.469157
C	1.526457	.000000	1.763381
C	2.084978	.852396	.597506
C	.786448	1.228577	-.183096
C	2.999309	-.050132	-.251340
N	3.110724	-1.337194	.247562
S	2.303969	-1.638784	1.513653
C	-.451608	1.438132	1.754064
C	.029807	2.190585	.738816
C	3.294227	-1.720859	2.906539
C	4.686190	-1.827993	2.903874
C	5.392343	-2.012567	4.089922
C	4.711584	-2.090988	5.311733
C	3.314153	-1.983232	5.319248
C	2.614218	-1.798978	4.132035
C	5.461792	-2.266164	6.576157
O	3.560365	.333891	-1.291620
H	5.246552	-1.765737	1.959474
H	6.490528	-2.093689	4.063066
H	2.765878	-2.041703	6.275449
H	1.511773	-1.714461	4.156934
H	4.848858	-2.817339	7.332559
H	6.410147	-2.832874	6.404448
H	5.726019	-1.263149	7.000175
H	2.656530	1.755678	.919508
H	1.750321	.418903	2.769824
H	-.605474	-.839854	1.855090
H	.892575	1.463833	-1.255285
H	-1.030845	1.709757	2.634818
H	-.038688	3.257865	.539375

Structure *endo*-20. AM1 Geometry.
AM1 Energy = 0.1173553
B3LYP/6-31(d) Energy = -1144.5753667

O	-2.400954	2.272700	-.086987
C	-1.058297	1.781808	-.411751
C	-1.454423	.475866	-1.162079
C	-2.671405	-.015734	-.344873
C	-2.829479	1.113343	.714215
C	-2.347389	-1.410811	.235857
N	-1.148487	-1.950300	-.159495
S	-.377853	-.963591	-1.226559
C	-.556668	1.395877	.981327
C	-1.645085	.988684	1.675089
O	-3.168659	-1.975078	.981413
H	-3.594960	-.090181	-.967691
H	-1.696258	.697765	-2.224702
H	-.506176	2.544916	-.986005
H	-3.837443	1.286530	1.126300
H	-1.740954	.611779	2.689979
H	.485743	1.465501	1.277823
C	1.152076	-.531215	-.553051
C	1.625316	-1.080848	.638451
C	2.916666	-.777930	1.071460
C	3.740864	.067396	.321118
C	3.255437	.609905	-.877526
C	1.970291	.309142	-1.315651
H	.997124	-1.758993	1.242447
H	3.289091	-1.213542	2.011581
C	5.116597	.373145	.774746
H	3.897421	1.273670	-1.476234
H	1.606316	.734407	-2.264009
H	5.425051	1.399200	.455614
H	5.196351	.308368	1.887927
H	5.833651	-.362612	.328977

Structure *endo*-20. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 8.745460

C	.000000	.000000	.000000
C	.000000	.000000	1.404407
C	1.225541	.000000	2.074025
C	2.427004	-.012494	1.370246
C	2.424125	-.016729	-.030727
C	1.196547	-.005810	-.707862
S	-1.536979	-.174912	2.116254
C	-2.369797	1.441712	2.027466
C	-2.752885	1.725653	3.503657
C	-2.079516	.659906	4.381956
N	-1.471624	-.341531	3.643014
C	-2.253047	3.187945	3.705056
O	-2.522648	3.721959	2.363643
C	-1.685784	2.774587	1.613382
C	-.723693	3.149500	3.680572
C	-.376251	2.893060	2.397701
O	-2.141320	.653311	5.623545
C	3.698505	-.037590	-.783948
H	-3.857369	1.672806	3.683538
H	-3.270938	1.281512	1.381249
H	-1.692493	3.031982	.537407
H	-2.764559	3.794209	4.474055
H	-.113101	3.307619	4.565434
H	.604475	2.784504	1.942062
H	1.252233	.013415	3.173389
H	3.381187	-.011483	1.920559
H	1.180533	.000557	-1.811438
H	-.960130	.007763	-.549148
H	3.595463	.502012	-1.758769
H	4.520626	.441312	-.196398
H	3.993863	-1.096822	-.998085

Structure *exo*-20. AM1 Geometry.
AM1 Energy = 0.1115461
B3LYP/6-31(d) Energy = -1144.5833962

C	2.533244	-.261867	.144148
C	1.418496	.215213	1.098700
S	.257197	-1.166502	1.122776
N	.934608	-2.139454	-.016412
C	2.120517	-1.623576	-.468413
O	2.874162	-2.167049	-1.296407
C	2.558440	.872496	-.921012
C	3.110813	2.100799	-.186642
C	2.130325	2.508774	.651952
C	.958039	1.542070	.433370
O	1.132935	1.222394	-.983861
C	-1.229835	-.566909	.485757
H	3.521629	-.377053	.645668
H	1.735951	.355174	2.152185
H	2.933681	.615265	-1.926318
H	4.109333	2.493757	-.353203
H	2.096445	3.329314	1.361125
H	-.070938	1.893569	.619472
C	-1.457715	-.396841	-.879546
C	-2.711741	.025538	-1.321254
C	-3.740394	.275953	-.406739
C	-3.498537	.101548	.963837
C	-2.251181	-.322314	1.409453
H	-.651689	-.581429	-1.611704
H	-2.890141	.160048	-2.399193
C	-5.076493	.704539	-.879373
H	-4.302899	.295352	1.689292
H	-2.078321	-.470497	2.486915
H	-5.584604	1.347093	-.118774
H	-4.998504	1.279206	-1.835139
H	-5.717988	-.194894	-1.063134

Structure *exo*-20. AM1 Geometry in CH_2Cl_2.
AM1 HF+ΔGsol (kcal/mol) = 2.872672

C	.000000	.000000	.000000
C	.000000	.000000	1.403884
C	1.224425	.000000	2.075829
C	2.425701	-.028762	1.372147
C	2.423022	-.046421	-.028621
C	1.196411	-.019236	-.707592
S	-1.555373	-.052335	2.095653
C	-1.770142	1.533607	2.973854
C	-2.096101	1.100997	4.426513
C	-1.922115	-.424860	4.513112
N	-1.638000	-1.012061	3.292354
C	-.554694	2.476369	3.187395
C	-1.133967	3.719243	3.874764
C	-1.419233	3.347105	5.143443
C	-1.021709	1.870264	5.252699
O	.113884	1.824573	4.322790
O	-2.073643	-1.070045	5.564756
C	3.697961	-.094316	-.780050
H	-3.133631	1.358059	4.754533
H	-2.607136	2.070758	2.466293
H	-.739691	1.449844	6.232479
H	-1.854335	3.899382	5.973517
H	-1.269723	4.667245	3.358259
H	.155278	2.601220	2.351208
H	1.242805	.050172	3.176948
H	3.380563	-.028950	1.921942
H	1.181644	-.009931	-1.810587
H	-.959460	.026029	-.548144
H	3.597601	.410966	-1.773160
H	4.519938	.402764	-.207245
H	3.991005	-1.160990	-.956613

Structure 21. AM1 Geometry.
AM1 Energy = -0.1638818
B3LYP/6-31(d) Energy = -1239.1324773

N	1.005463	0.433412	-0.735918
S	-0.344554	1.422301	-0.825552
C	-0.042246	2.344904	0.645092
C	1.124174	1.945715	1.157087
C	1.740788	0.810708	0.340729
C	-1.716453	0.470878	-0.394229
C	-2.929146	1.143717	-0.209436
C	-4.080997	0.420883	0.077990
C	-4.034071	-0.977911	0.179420
C	-2.815814	-1.637512	-0.015058
C	-1.654137	-0.919581	-0.302049
C	-5.259592	-1.743787	0.500496
O	2.857699	0.341732	0.737933
H	-0.707059	-1.467911	-0.455867
H	-2.767875	-2.735703	0.056886
H	-5.036320	0.947911	0.224049
H	-2.980212	2.240836	-0.290483
H	-6.170962	-1.223331	0.115333
H	-5.220388	-2.768406	0.054645
H	-5.358672	-1.848940	1.611199
H	-0.753655	3.105011	0.953787
H	1.657493	2.317441	2.037844
B	3.685195	-1.048849	-0.045709
F	4.730834	-1.092975	0.849249
F	2.719231	-2.029146	0.063407
F	3.942120	-0.544021	-1.301800

Structure 22. AM1 Geometry.
AM1 Energy = -0.1626819
B3LYP/6-31(d) Energy = -1239.1375512

N	-0.632489	-0.415439	-1.412339
S	0.493734	-1.460202	-0.740913
C	-0.286391	-1.651099	0.825614
C	-1.440009	-0.979779	0.802242
C	-1.648195	-0.252091	-0.521254
C	1.897916	-0.539284	-0.349025
C	2.881000	-1.169177	0.421704
C	4.060954	-0.496287	0.717312
C	4.271702	0.807835	0.244672
C	3.282656	1.422446	-0.530991
C	2.094906	0.754659	-0.830711
C	5.522127	1.527966	0.575296
O	-2.679926	0.449659	-0.792275
H	1.333292	1.262215	-1.448181
H	3.439299	2.444323	-0.911052
H	4.835473	-0.989749	1.324372
H	2.729158	-2.193487	0.796917
H	6.375590	0.815976	0.695908
H	5.784198	2.264780	-0.223760
H	5.392570	2.086368	1.537611
H	0.184977	-2.265695	1.586765
H	-2.210445	-0.904222	1.581623
B	-4.029214	0.709027	0.340994
F	-4.775396	1.508299	-0.487666
F	-4.463199	-0.587369	0.558135
F	-3.380399	1.307653	1.407849

Structure 23. AM1 Geometry.
AM1 Energy = -0.1531043
B3LYP/6-31(d) Energy = -1239.1315982

N	1.479816	0.119939	0.181276
S	0.412086	0.707593	-0.962117
C	0.502278	2.393806	-0.476840
C	1.379682	2.514848	0.519267
C	1.987639	1.181099	0.943113
C	-1.170819	0.270517	-0.418988
C	-2.243800	1.112403	-0.731349
C	-3.534880	0.741504	-0.376353
C	-3.768111	-0.470841	0.291981
C	-2.686908	-1.306052	0.589952
C	-1.386899	-0.942159	0.235802
C	-5.143952	-0.851311	0.684026
O	2.790835	1.103417	1.874417
H	-0.547731	-1.626749	0.467836
H	-2.856488	-2.264080	1.106678
H	-4.381099	1.401349	-0.621767
H	-2.080030	2.065968	-1.256858
H	-5.891475	-0.465982	-0.052667
H	-5.250296	-1.962336	0.750162
H	-5.384139	-0.416008	1.687708
H	-0.094277	3.128081	-1.012153
H	1.704181	3.423968	1.037095
B	2.387002	-1.332589	-0.237985
F	3.194610	-1.660407	0.853690
F	1.436047	-2.341532	-0.500156
F	3.142921	-1.050565	-1.392443

Structure *endo*-TS24. AM1 Geometry.
AM1 Energy = -0.0611613
B3LYP/6-31(d) Energy = -1433.2079254

C	1.933883	3.293169	1.042562
C	1.123216	3.350184	-0.234090
C	1.840908	2.649560	-1.226742
C	2.809124	1.835941	-0.599403
C	2.715060	2.010907	0.806577
C	1.023835	0.874607	1.139563
C	-0.001369	1.613023	0.535379
S	-0.520012	0.726748	-0.889921
N	0.525964	-0.574541	-0.748036
C	1.299551	-0.396074	0.349189
C	-2.087197	0.171298	-0.419812
C	-3.069553	1.135514	-0.173064
C	-4.363865	0.738309	0.143103
C	-4.689902	-0.624225	0.213609
C	-3.699280	-1.578286	-0.041419
C	-2.397762	-1.187051	-0.358439
C	-6.064707	-1.045426	0.566334
O	2.224390	-1.170490	0.791779
H	-1.635742	-1.962313	-0.557501
H	-3.944302	-2.650986	0.007141
H	-5.137896	1.496264	0.336911
H	-2.828111	2.208402	-0.228509
H	-6.814994	-0.285151	0.236652
H	-6.318259	-2.024551	0.089769
H	-6.150215	-1.164260	1.676669
H	1.226696	0.856822	2.218787
H	-0.710801	2.284072	1.012905
H	0.324146	4.071692	-0.396686
H	3.406514	1.590721	1.540012
H	3.458932	1.114037	-1.102274
H	1.637550	2.672478	-2.298422
H	1.322774	3.292737	1.973384
H	2.638919	4.165799	1.086219
B	2.684326	-2.657845	-0.005139
F	3.643217	-3.034236	0.916829
F	1.509725	-3.389123	-0.009305
F	3.148705	-2.206364	-1.228490

Structure *exo*-TS24. AM1 Geometry.
AM1 Energy = -0.0605956
B3LYP/6-31(d) Energy = -1433.2046016

C	2.421543	-1.235217	0.282717
C	2.089485	0.106981	0.466063
C	3.047467	1.108103	0.276991
C	4.339665	0.764037	-0.103570
C	4.687544	-0.581184	-0.296579
C	3.720924	-1.572674	-0.098289
S	0.525943	0.588693	1.019420
C	-0.045126	1.582826	-0.313988
C	-1.072235	0.878939	-0.951391
C	-1.322415	-0.447789	-0.250686
N	-0.503281	-0.715819	0.795643
O	-2.274023	-1.179236	-0.706514
C	6.059701	-0.944071	-0.717732
C	-2.797184	1.915307	-0.396927
C	-2.491910	3.043629	-1.204211
C	-1.503852	3.815293	-0.557018
C	-1.176764	3.196700	0.670600
C	-2.292398	2.230166	0.997553
H	1.678600	-2.039097	0.434439
H	3.983361	-2.632510	-0.243195
H	5.094826	1.550704	-0.252422
H	2.788699	2.167750	0.427799
H	6.805296	-0.201170	-0.341096
H	6.341866	-1.955921	-0.334816
H	6.118606	-0.964231	-1.835966
H	-1.305600	0.936162	-2.021672
H	0.649272	2.295574	-0.751896
H	-0.467728	3.563708	1.410693
H	-3.566226	1.163232	-0.591629
H	-3.097958	2.763999	1.572452
H	-1.992431	1.341047	1.595488
H	-1.014031	4.694613	-0.975524
H	-2.890232	3.230380	-2.202447
B	-2.681814	-2.748576	-0.036086
F	-3.696788	-3.031925	-0.930117
F	-1.505718	-3.461182	-0.186456
F	-3.064589	-2.430459	1.254453

Structure *endo*-TS25. AM1 Geometry.
AM1 Energy = -0.0559216
B3LYP/6-31(d) Energy = -1433.2026472

C	-2.973555	.314627	1.034782
C	-1.790630	-.388893	.785818
C	-1.790008	-1.493375	-.066802
C	-2.981644	-1.888446	-.676010
C	-4.171648	-1.192664	-.436853
C	-4.157053	-.085224	.423670
S	-.393054	.061262	1.688499
C	.068231	1.696093	1.269514
C	1.397903	1.641781	.825542
C	1.836295	.192538	.650083
N	.927617	-.736398	1.025158
O	3.016479	-.006796	.179803
C	-5.436585	-1.629349	-1.070178
C	1.377327	2.391850	-1.057031
C	.322172	3.425272	-.691817
C	-.897376	2.537903	-.593125
C	-.678212	1.413178	-1.409518
C	.701633	1.319628	-1.698967
H	2.171750	2.368000	1.116357
H	-.420943	2.496041	1.818206
H	-1.851060	2.875940	-.191400
H	2.428596	2.646962	-1.212040
H	1.189784	.500921	-2.236633
H	-1.431994	.679626	-1.701455
H	.547023	4.002060	.233741
H	.195867	4.154080	-1.536444
H	-.866024	-2.065678	-.265944
H	-2.981618	-2.760659	-1.348574
H	-5.088641	.467111	.619551
H	-2.975412	1.183471	1.711410
H	-5.953526	-2.370776	-.408745
H	-6.125532	-.763769	-1.230639
H	-5.243096	-2.117445	-2.057267
B	3.578741	-1.582213	-.320377
F	4.815494	-1.168162	-.778956
F	3.561781	-2.327807	.842161
F	2.646473	-1.913517	-1.293583

Structure *exo*-TS25. AM1 Geometry.
AM1 Energy = -0.0578349
B3LYP/6-31(d) Energy = -1433.2015450

C	-2.972348	.109031	1.097253
C	-1.757519	-.502719	.769923
C	-1.711955	-1.517665	-.186418
C	-2.889864	-1.914273	-.821001
C	-4.110675	-1.308285	-.505592
C	-4.141525	-.290721	.459397
S	-.371414	-.044800	1.689126
C	.052364	1.603097	1.255738
C	1.359343	1.565857	.752380
C	1.819611	.126183	.571373
N	.954368	-.818246	1.010824
O	2.971272	-.056350	.032765
C	-5.359958	-1.746974	-1.167829
C	1.183514	2.163638	-1.215045
C	.898070	3.517072	-.888769
C	-.447333	3.613991	-.472396
C	-1.037721	2.335072	-.547817
C	-.152633	1.476589	-1.420289
H	2.134120	2.312052	.973751
H	-.414034	2.388463	1.845052
H	2.115017	1.780396	-1.641007
H	1.627126	4.328470	-.873001
H	-.923171	4.512340	-.078896
H	-2.066522	2.074090	-.301985
H	-.464471	1.577786	-2.495281
H	-.160453	.391238	-1.169138
H	-.764048	-2.022749	-.447396
H	-2.853791	-2.716681	-1.574732
H	-5.097855	.189538	.716911
H	-3.011595	.902723	1.859878
H	-6.092659	-.905896	-1.241294
H	-5.154630	-2.130750	-2.197668
H	-5.831621	-2.571821	-.574779
B	3.601562	-1.646062	-.355056
F	4.765015	-1.202087	-.954418
F	3.724396	-2.245608	.883075
F	2.627748	-2.148185	-1.203600

Structure *endo*-TS26. AM1 Geometry.
AM1 Energy = -0.0590483
B3LYP/6-31(d) Energy = -1433.2152148

C	-2.635614	-0.988065	-0.848480
C	-2.237807	0.281166	-0.430065
C	-3.084825	1.064550	0.360536
C	-4.329675	0.572963	0.736861
C	-4.741972	-0.703256	0.325627
C	-3.886657	-1.475081	-0.467635
S	-0.738580	0.982923	-0.925681
C	0.092903	1.195712	0.609725
C	1.158236	0.284774	0.634650
C	1.174984	-0.557599	-0.624898
N	0.210103	-0.256473	-1.533385
O	2.023396	-1.494960	-0.867081
B	2.964878	-2.295020	0.357073
F	2.040742	-2.540149	1.364692
C	-6.073474	-1.218368	0.717588
F	3.358155	-3.369699	-0.408348
F	3.940148	-1.358942	0.672950
C	2.827469	1.534839	0.455800
C	2.171153	2.561679	1.361743
C	1.113837	3.106725	0.425217
C	1.582068	2.921910	-0.896117
C	2.617797	1.965136	-0.880341
H	-1.981108	-1.618265	-1.475772
H	-4.198455	-2.479387	-0.794800
H	-4.995792	1.187305	1.361505
H	-2.774663	2.068805	0.688987
H	-6.370802	-0.833794	1.724376
H	-6.841762	-0.884966	-0.025892
H	-6.078623	-2.335922	0.748918
H	1.577328	-0.159496	1.550663
H	-0.478700	1.570102	1.456488
H	0.343034	3.805980	0.745897
H	3.626912	0.866185	0.790073
H	3.120385	1.554358	-1.759189
H	1.165922	3.387267	-1.790546
H	1.770417	2.143348	2.312867
H	2.908975	3.368405	1.617381

Structure *exo*-TS26. AM1 Geometry.
AM1 Energy = -0.0578557
B3LYP/6-31(d) Energy = -1433.2117699

C	2.068815	2.330407	-1.052683
C	2.811971	1.527154	-0.005316
C	2.737557	2.266061	1.205560
C	1.697533	3.212388	1.101176
C	1.098908	3.089349	-0.174334
C	1.142672	0.328202	0.473223
C	0.080746	1.232619	0.350372
S	-0.789649	0.822723	-1.121855
N	0.139401	-0.493616	-1.581404
C	1.137132	-0.664987	-0.671735
C	-2.279827	0.207404	-0.501538
C	-2.699153	-1.099144	-0.750032
C	-3.943033	-1.520782	-0.279078
C	-4.768800	-0.647787	0.437296
C	-4.335798	0.664954	0.675152
C	-3.097820	1.092338	0.208029
C	-6.079058	-1.106899	0.951319
O	1.990405	-1.613112	-0.826134
B	3.040786	-2.247086	0.420818
F	2.237491	-2.267613	1.552220
F	3.297457	-3.455129	-0.186039
F	4.069470	-1.317680	0.437399
H	-2.067566	-1.808560	-1.312899
H	-4.273912	-2.552955	-0.473981
H	-4.980098	1.360402	1.234290
H	-2.770953	2.126060	0.401112
H	-6.801103	-0.257014	1.028493
H	-6.519702	-1.887972	0.283616
H	-5.949639	-1.551112	1.971308
H	1.579013	0.000453	1.427843
H	-0.473448	1.720548	1.149209
H	0.291527	3.703705	-0.569234
H	3.558744	0.766209	-0.252788
H	2.779502	3.051555	-1.541314
H	1.603159	1.722821	-1.859782
H	1.354947	3.867678	1.902058
H	3.330113	2.066366	2.099885

Structure *endo*-TS27. AM1 Geometry.
AM1 Energy = -0.0531068
B3LYP/6-31(d) Energy = -1433.2085433

C	-2.414306	-1.387299	-.540110
C	-2.090135	-.627991	.584589
C	-3.047446	.199179	1.180801
C	-4.329180	.270731	.645446
C	-4.668434	-.485373	-.485857
C	-3.701941	-1.310470	-1.071568
S	-.572440	-.794948	1.382876
C	.247992	.753405	1.426127
C	1.497796	.563209	.813511
C	1.586256	-.819880	.193435
N	.481338	-1.594279	.352424
O	2.608036	-1.275993	-.441220
B	4.232474	-.655273	-.301793
F	4.211926	.446273	-1.144721
C	-6.039180	-.422881	-1.041688
F	4.359024	-.360224	1.049303
F	4.877310	-1.780909	-.761019
C	1.501589	1.908050	-.743825
C	.532416	1.276034	-1.566853
C	-.750762	1.532539	-1.040169
C	-.617062	2.322753	.120397
C	.764684	2.937268	.097904
H	2.436193	1.003396	1.191030
H	.019604	1.392336	2.276466
H	-1.425850	2.695131	.747101
H	2.570051	1.980527	-.972424
H	.757633	.627978	-2.416837
H	-1.684321	1.115885	-1.421820
H	1.209495	3.109887	1.104086
H	.737272	3.919682	-.445035
H	-1.672575	-2.053028	-1.014828
H	-3.958160	-1.910092	-1.959034
H	-5.083173	.921188	1.114376
H	-2.793919	.795860	2.071133
H	-6.683918	-1.191434	-.543618
H	-6.496816	.582385	-.869114
H	-6.036561	-.628176	-2.140669

Structure *exo*-TS27. AM1 Geometry.
AM1 Energy = -0.054551
B3LYP/6-31(d) Energy = -1433.2076641

C	-.138505	1.327760	-1.239782
C	1.334008	1.618088	-1.033596
C	1.414517	2.883049	-.390710
C	.158700	3.191363	.173091
C	-.736012	2.136894	-.111922
C	1.449512	.544112	.749746
C	.208853	.786279	1.358042
S	-.612898	-.762199	1.463628
N	.448222	-1.658128	.526383
C	1.541215	-.891059	.266268
C	-2.106341	-.644834	.609271
C	-3.108677	.145206	1.182002
C	-4.368065	.198817	.594055
C	-4.640800	-.539472	-.566546
C	-3.631635	-1.331517	-1.125465
C	-2.365439	-1.388139	-.542505
C	-5.978408	-.474605	-1.197718
O	2.549906	-1.397072	-.346617
B	4.184670	-.758784	-.352431
F	4.346280	-.241534	.924441
F	4.815940	-1.948195	-.632404
F	4.118867	.177174	-1.372448
H	2.389868	1.033357	1.047330
H	-.012966	1.497180	2.150889
H	2.123254	1.147131	-1.628571
H	2.326646	3.470632	-.273884
H	-.058845	4.057413	.798225
H	-1.786586	2.079346	.170648
H	-.468568	1.750207	-2.227371
H	-.404151	.246317	-1.229418
H	-1.591023	-2.030088	-.997710
H	-3.837575	-1.921907	-2.032028
H	-5.157223	.818951	1.046187
H	-2.910356	.722962	2.098664
H	-6.766923	-.224555	-.445795
H	-5.985175	.317095	-1.989775
H	-6.241480	-1.450140	-1.676715

Structure *endo*-TS28. AM1 Geometry.
AM1 Energy = -0.0509428
B3LYP/6-31(d) Energy = -1433.2096431

C	-3.504686	-0.618237	-0.281239
C	-3.344760	-1.491811	0.827891
C	-2.949774	-2.849250	0.266475
C	-2.305746	-2.423677	-1.033632
C	-2.865728	-1.185714	-1.406284
C	-1.406681	-1.052519	1.297151
C	-0.667170	-1.571900	0.229620
S	-0.010428	-0.236143	-0.689440
N	-0.651559	0.986059	0.232909
C	-1.386139	0.467944	1.306209
C	1.671023	-0.352096	-0.285349
C	2.375660	0.711660	0.276668
C	3.745802	0.579059	0.509263
C	4.415290	-0.603276	0.179631
C	3.694327	-1.662649	-0.392580
C	2.330075	-1.538614	-0.625783
C	5.871455	-0.733069	0.413083
O	-1.935525	1.130160	2.192992
B	-0.755782	2.586080	-0.412587
F	-0.590073	2.519566	-1.817368
F	-2.017746	3.116923	-0.099894
F	0.289147	3.343203	0.155991
H	1.875157	1.666488	0.532804
H	4.300561	1.420123	0.954370
H	4.213654	-2.595431	-0.659655
H	1.780191	-2.376486	-1.081927
H	6.152006	-1.795237	0.619743
H	6.431033	-0.392854	-0.495511
H	6.196148	-0.104666	1.278940
H	-1.501207	-1.551165	2.272788
H	-0.151041	-2.527534	0.178867
H	-1.750734	-3.108088	-1.673238
H	-3.841313	-1.374211	1.793531
H	-3.960585	0.375451	-0.243629
H	-2.765674	-0.703143	-2.380514
H	-2.286230	-3.445638	0.932786
H	-3.870745	-3.455732	0.055009

Structure *exo*-TS28. AM1 Geometry.
AM1 Energy = -0.0512215
B3LYP/6-31(d) Energy = -1433.2067366

C	2.500862	0.741800	0.135915
C	1.718057	-0.331600	-0.290749
C	2.290694	-1.591061	-0.492937
C	3.646437	-1.779149	-0.249427
C	4.443575	-0.712995	0.193671
C	3.860409	0.544332	0.380398
S	0.050641	-0.093351	-0.694712
C	-0.727937	-1.443417	0.093653
C	-1.449487	-0.961069	1.189129
C	-1.335148	0.547705	1.318789
N	-0.502536	1.106713	0.332618
O	-1.886123	1.171046	2.231787
C	5.889063	-0.915059	0.441605
C	-3.420149	-1.112787	0.596262
C	-3.435266	-2.533469	0.665361
C	-2.797215	-3.053562	-0.480687
C	-2.389307	-1.977916	-1.299090
C	-3.152080	-0.753800	-0.852738
H	2.065109	1.750715	0.269900
H	4.476128	1.391501	0.721410
H	4.097969	-2.770552	-0.405977
H	1.685284	-2.439011	-0.848562
H	6.099118	-1.965857	0.759927
H	6.465307	-0.710836	-0.496798
H	6.259536	-0.222007	1.236929
H	-1.604351	-1.523502	2.119825
H	-0.288767	-2.430694	-0.026289
H	-1.879784	-2.049536	-2.258747
H	-3.912749	-0.426683	1.289925
H	-4.129741	-0.698386	-1.407188
H	-2.635382	0.221471	-1.010676
H	-2.583658	-4.107162	-0.661625
H	-3.798763	-3.119720	1.510445
B	-0.770907	2.652340	-0.392456
F	0.443764	3.068976	-0.986023
F	-1.176495	3.557565	0.597234
F	-1.769413	2.507804	-1.388143

Structure *endo*-TS29. AM1 Geometry.
AM1 Energy = -0.0434667
B3LYP/6-31(d) Energy = -1433.1970461

C	-.633414	2.212867	1.625466
C	-1.466572	2.997794	.783326
C	-.546895	3.748419	-.170042
C	.642840	2.818472	-.180395
C	.642261	2.099768	1.027311
C	-1.910161	1.608675	-.594591
C	-.733148	1.386966	-1.318801
S	-.346925	-.308498	-1.207088
N	-1.450442	-.709733	-.014971
C	-2.312788	.376317	.205138
C	1.242021	-.423286	-.537098
C	2.273281	.194585	-1.254745
C	3.591544	.036584	-.844452
C	3.894863	-.740430	.284258
C	2.855862	-1.354824	.989818
C	1.529271	-1.204870	.580908
C	5.301949	-.923223	.706617
O	-3.277657	.386699	.977177
B	-1.983022	-2.366285	.046794
F	-2.792858	-2.524106	1.179420
F	-.833477	-3.185098	.142308
F	-2.686510	-2.658169	-1.141336
H	-2.738447	2.231109	-.971072
H	-.389505	1.895206	-2.215982
H	1.467292	2.907962	-.886040
H	-2.454564	3.372127	1.063502
H	-.960309	1.700562	2.533700
H	1.459917	1.481567	1.402974
H	.728004	-1.731054	1.134005
H	3.081077	-1.974955	1.871799
H	4.403543	.517640	-1.410507
H	2.047664	.804319	-2.143789
H	5.918231	-.026600	.449968
H	5.370721	-1.098791	1.808596
H	5.740117	-1.811222	.183080
H	-.987401	3.942809	-1.174171
H	-.255965	4.734733	.280916

Structure *exo*-TS29. AM1 Geometry.
AM1 Energy = -0.0456928
B3LYP/6-31(d) Energy = -1433.2013302

C	.161729	2.083158	-1.265989
C	1.585144	2.591177	-1.131211
C	1.514890	3.797639	-.381451
C	.277006	3.843976	.297055
C	-.463261	2.692618	-.034883
C	2.033435	1.420235	.475867
C	.857719	1.358282	1.230279
S	.333234	-.310730	1.267548
N	1.413968	-.900109	.150488
C	2.326845	.095207	-.213859
C	-1.243569	-.339950	.555524
C	-2.269258	.242666	1.310107
C	-3.582398	.174918	.860378
C	-3.887347	-.480447	-.342572
C	-2.854571	-1.063110	-1.083501
C	-1.532845	-.999701	-.638137
C	-5.290067	-.571727	-.806856
O	3.259954	-.035862	-1.013461
B	1.641680	-2.615540	-.037421
F	3.015616	-2.890098	-.006968
F	1.056938	-2.975464	-1.268827
F	.977571	-3.273468	1.023017
H	2.910777	2.020063	.758681
H	.579990	1.957190	2.094004
H	2.374931	2.314294	-1.835127
H	2.324787	4.520602	-.273189
H	-.018092	4.605329	1.019453
H	-1.455089	2.423667	.327374
H	-.740813	-1.498204	-1.231150
H	-3.081376	-1.589460	-2.024221
H	-4.389532	.629796	1.454595
H	-2.045227	.749816	2.261883
H	-5.882692	.315280	-.472778
H	-5.340555	-.634278	-1.921964
H	-5.767626	-1.492143	-.383119
H	.069000	.974905	-1.335318
H	-.307877	2.521815	-2.188026

Structure *endo*-TS30. AM1 Geometry.
AM1 Energy = -0.1158889
B3LYP/6-31(d) Energy = -1469.1165213

C	-2.445020	-1.219204	-0.387459
C	-2.127127	0.138601	-0.416969
C	-3.103080	1.101863	-0.143782
C	-4.398751	0.703984	0.166548
C	-4.732142	-0.657942	0.205206
C	-3.747527	-1.611043	-0.076029
S	-0.556491	0.688824	-0.881860
C	-0.051300	1.611268	0.516484
C	0.965303	0.887325	1.164161
C	1.255716	-0.400168	0.400255
N	0.492386	-0.606964	-0.697463
O	2.190009	-1.152096	0.861637
C	-6.107994	-1.080051	0.552655
C	2.594974	1.997393	0.850788
O	1.873007	3.206854	0.986692
C	1.177906	3.327838	-0.209833
C	1.863438	2.580829	-1.224668
C	2.767297	1.748924	-0.563781
H	-1.687483	-1.992849	-0.607096
H	-3.998427	-2.683195	-0.052258
H	-5.167755	1.461344	0.381771
H	-2.856126	2.174537	-0.172294
H	-6.855380	-0.308876	0.242230
H	-6.367974	-2.047114	0.055405
H	-6.190754	-1.222886	1.660396
H	1.108229	0.879000	2.254695
H	-0.754206	2.303308	0.972245
H	0.480611	4.161586	-0.264529
H	3.271074	1.776840	1.679835
H	3.408942	0.971428	-0.986281
H	1.662874	2.631077	-2.293237
B	2.826016	-2.526295	-0.017430
F	3.758407	-2.898554	0.932049
F	1.731873	-3.355182	-0.174137
F	3.320736	-1.908588	-1.155669

Structure *exo*-TS30. AM1 Geometry.
AM1 Energy = -0.1162165
B3LYP/6-31(d) Energy = -1469.1143828

O	2.226507	2.184152	-0.941194
C	2.760961	1.877225	0.323876
C	2.538187	3.022277	1.179322
C	1.577563	3.809572	0.548605
C	1.251209	3.144615	-0.684043
C	1.091464	0.887165	0.939657
C	0.059186	1.604473	0.312482
S	-0.516835	0.625054	-1.030438
N	0.513936	-0.679877	-0.829640
C	1.327754	-0.436608	0.223350
C	-2.074532	0.132090	-0.469015
C	-2.401172	-1.212694	-0.294720
C	-3.696696	-1.557924	0.092552
C	-4.665294	-0.571619	0.306074
C	-4.323288	0.776408	0.122107
C	-3.035003	1.127888	-0.264599
C	-6.033229	-0.943008	0.733488
O	2.273311	-1.178149	0.676351
H	-1.656945	-2.013169	-0.458657
H	-3.954449	-2.619913	0.230094
H	-5.080114	1.559128	0.282708
H	-2.781183	2.189607	-0.408497
H	-6.783374	-0.196264	0.373913
H	-6.316696	-1.949794	0.338326
H	-6.082667	-0.979541	1.851760
H	1.315573	0.925991	2.013166
H	-0.632927	2.306478	0.770052
H	0.678263	3.472779	-1.549402
H	3.557753	1.127330	0.314015
H	1.101616	4.713638	0.920884
H	2.987066	3.163572	2.160627
B	2.633881	-2.773875	0.037046
F	3.634186	-3.069393	0.943791
F	1.433291	-3.442268	0.199497
F	3.031333	-2.497158	-1.257266

Structure *endo*-TS31. AM1 Geometry.
AM1 Energy = -0.1113741
B3LYP/6-31(d) Energy = -1469.1136859

C	-2.983754	.350811	1.042678
C	-1.792708	-.343792	.807336
C	-1.776182	-1.452953	-.038851
C	-2.958612	-1.859252	-.658603
C	-4.155838	-1.170576	-.435381
C	-4.157933	-.059612	.420779
S	-.408932	.130332	1.720418
C	.059781	1.736518	1.238033
C	1.400404	1.669799	.815764
C	1.834763	.209309	.705247
N	.918811	-.698282	1.108159
O	3.016801	-.012299	.248668
C	-5.411127	-1.619104	-1.079459
C	1.389223	2.329706	-1.028189
O	.384651	3.296077	-.764522
C	-.794144	2.570317	-.734187
C	-.621568	1.357290	-1.469742
C	.751354	1.205907	-1.677005
H	2.164728	2.400185	1.127881
H	-.435996	2.571935	1.722948
H	-1.679950	3.120473	-.423493
H	2.381413	2.751891	-1.208305
H	1.283327	.362270	-2.125693
H	-1.415908	.665739	-1.746440
H	-.847135	-2.021741	-.223988
H	-2.945844	-2.735607	-1.325724
H	-5.095786	.485875	.606050
H	-3.000280	1.219037	1.720025
H	-6.103668	-.758888	-1.252850
H	-5.204216	-2.112576	-2.061135
H	-5.930550	-2.359357	-.418586
B	3.523577	-1.585274	-.319244
F	4.780692	-1.201909	-.745758
F	3.458506	-2.394492	.796558
F	2.584097	-1.812113	-1.317684

Structure *exo*-TS31. AM1 Geometry.
AM1 Energy = -0.1139393
B3LYP/6-31(d) Energy = -1469.1129073

C	-2.984415	.038274	1.154888
C	-1.761122	-.513606	.757174
C	-1.711432	-1.460988	-.265117
C	-2.894607	-1.850053	-.896113
C	-4.122852	-1.303487	-.511468
C	-4.157501	-.352926	.520398
S	-.368454	-.066116	1.670230
C	.038160	1.591037	1.255957
C	1.343999	1.568429	.734626
C	1.816794	.131297	.547833
N	.958313	-.821412	.975498
O	2.970435	-.031191	.006572
C	-5.376289	-1.734223	-1.171092
C	1.092464	2.097493	-1.196585
C	.832893	3.491852	-.912292
C	-.496489	3.573725	-.501590
C	-1.026853	2.241195	-.572258
O	-.154183	1.451573	-1.312672
H	2.113146	2.319435	.960979
H	-.418118	2.367715	1.863897
H	1.908882	1.614226	-1.742323
H	1.580091	4.282714	-.937379
H	-1.031598	4.445824	-.133416
H	-2.039861	1.852702	-.470890
H	-.755761	-1.913597	-.586762
H	-2.854698	-2.598008	-1.703735
H	-5.120358	.079070	.832959
H	-3.026554	.774946	1.972405
H	-6.137958	-.916098	-1.160947
H	-5.188679	-2.032387	-2.232224
H	-5.803061	-2.617142	-.629938
B	3.651527	-1.609934	-.346719
F	4.808642	-1.138392	-.937737
F	3.776303	-2.179708	.905360
F	2.705883	-2.156696	-1.197460

Structure *endo*-TS32. AM1 Geometry.
AM1 Energy = -0.1138825
B3LYP/6-31(d) Energy = -1469.1245274

C	2.601242	1.934261	-0.859518
C	2.750851	1.513677	0.516192
O	2.125466	2.483168	1.328774
C	1.181164	3.073536	0.492644
C	1.609409	2.912219	-0.870889
C	1.143112	0.284320	0.643875
C	0.072924	1.199441	0.605550
S	-0.752626	0.977899	-0.926071
N	0.199379	-0.263707	-1.526728
C	1.163271	-0.560695	-0.616894
C	-2.253148	0.276748	-0.433806
C	-2.656783	-0.984773	-0.869957
C	-3.908745	-1.472223	-0.493264
C	-4.758436	-0.709382	0.314911
C	-4.341145	0.559948	0.741750
C	-3.095158	1.052168	0.369612
C	-6.077545	-1.239463	0.728074
O	2.016736	-1.493045	-0.857750
B	3.017436	-2.240089	0.355581
F	3.946880	-1.250513	0.649471
F	2.121081	-2.523953	1.376598
F	3.454209	-3.295049	-0.412607
H	-2.006466	-1.607884	-1.508474
H	-4.226741	-2.469277	-0.836258
H	-5.004233	1.169199	1.374635
H	-2.780792	2.050553	0.711586
H	-5.973646	-1.800521	1.691870
H	-6.812759	-0.411611	0.882385
H	-6.487153	-1.939653	-0.041303
H	1.512899	-0.179188	1.573739
H	-0.499324	1.563831	1.456334
H	0.539173	3.814631	0.965156
H	3.567781	0.963476	0.995374
H	3.120579	1.485367	-1.706648
H	1.186636	3.427045	-1.731092

Structure *exo*-TS32. AM1 Geometry.
AM1 Energy = -0.114752
B3LYP/6-31(d) Energy = -1469.1239551

C	-3.099898	1.092642	0.214307
C	-2.283200	0.209230	-0.498796
C	-2.704159	-1.096466	-0.749241
C	-3.947177	-1.518816	-0.276526
C	-4.771121	-0.647170	0.443430
C	-4.337020	0.664958	0.683102
S	-0.794891	0.826018	-1.123156
C	0.074995	1.240148	0.348781
C	1.136181	0.325859	0.476125
C	1.122617	-0.670769	-0.667637
N	0.132384	-0.491078	-1.579436
O	1.971169	-1.626574	-0.816542
B	3.055426	-2.197344	0.415981
F	4.036274	-1.213747	0.425530
C	-6.080710	-1.106197	0.959197
F	2.267824	-2.255213	1.558144
F	3.379130	-3.394121	-0.181705
C	2.747096	1.490617	-0.069241
O	2.007917	2.225208	-1.011377
C	1.154988	3.017846	-0.242848
C	1.748518	3.199547	1.055957
C	2.755051	2.244172	1.165672
H	-2.074751	-1.804937	-1.315801
H	-4.278846	-2.550407	-0.473321
H	-4.980176	1.359499	1.244663
H	-2.772758	2.125982	0.408539
H	-6.806687	-0.258568	1.023687
H	-6.516033	-1.897443	0.300066
H	-5.952325	-1.536991	1.985052
H	1.555311	-0.008923	1.436534
H	-0.476745	1.724515	1.151077
H	0.462298	3.639383	-0.807217
H	3.483300	0.796019	-0.488723
H	1.407932	3.905666	1.809350
H	3.385218	2.019216	2.024670

Structure *endo*-TS33. AM1 Geometry.
AM1 Energy = -0.1083860
B3LYP/6-31(d) Energy = -1469.1191846

C	.516083	1.216019	-1.498354
C	1.437376	1.879611	-.602545
O	.690901	2.801775	.168499
C	-.602492	2.298293	.149280
C	-.764687	1.474733	-1.012648
C	1.480001	.541093	.863568
C	.221641	.688461	1.482901
S	-.564667	-.867409	1.425442
N	.504984	-1.634683	.385670
C	1.591209	-.835885	.224639
C	-2.071412	-.678299	.609204
C	-3.030982	.142931	1.210450
C	-4.292190	.266480	.637674
C	-4.609056	-.432020	-.536600
C	-3.646581	-1.265290	-1.117130
C	-2.379376	-1.394390	-.547554
C	-5.943357	-.275467	-1.158553
O	2.614749	-1.259955	-.428318
B	4.208733	-.549822	-.370147
F	4.400927	-.298932	.980905
F	4.883866	-1.615061	-.919146
F	4.068257	.580573	-1.164030
H	2.406267	.971649	1.285902
H	-.011949	1.329420	2.329782
H	-1.322523	2.819348	.776717
H	2.481330	2.165627	-.774146
H	.812264	.574234	-2.328410
H	-1.711212	1.085083	-1.383791
H	-1.639707	-2.064114	-1.019833
H	-3.889086	-1.829398	-2.031370
H	-5.047845	.912778	1.109829
H	-2.794550	.694561	2.134076
H	-6.732040	-.124885	-.380535
H	-5.942632	.618283	-1.833626
H	-6.211907	-1.173539	-1.767632

Structure *exo*-TS33. AM1 Geometry.
AM1 Energy = -0.1121006
B3LYP/6-31(d) Energy = -1469.1221449

C	-2.316844	-1.266095	-.625648
C	-2.103803	-.637245	.600569
C	-3.143262	.055961	1.231589
C	-4.393460	.126226	.627915
C	-4.621450	-.500303	-.606743
C	-3.575564	-1.193280	-1.224657
S	-.621822	-.774946	1.470534
C	.208108	.771325	1.383933
C	1.452831	.526299	.772581
C	1.542243	-.911149	.293497
N	.445628	-1.671992	.542261
O	2.557185	-1.421653	-.309847
B	4.151260	-.724913	-.377660
F	4.003436	.236563	-1.368939
C	-5.959752	-.441584	-1.236977
F	4.361644	-.227011	.900957
F	4.823585	-1.875186	-.721022
C	1.271398	1.530437	-.999578
O	-.102755	1.255800	-1.118094
C	-.701130	2.045011	-.138339
C	.164987	3.155782	.148995
C	1.405027	2.840724	-.401319
H	2.392658	1.012402	1.078017
H	-.001335	1.473977	2.187233
H	1.916373	1.001854	-1.710467
H	2.336534	3.400808	-.336787
H	-.104262	4.026264	.742275
H	-1.777536	1.917395	-.028623
H	-1.509831	-1.822535	-1.133677
H	-3.742912	-1.689817	-2.193356
H	-5.211749	.670570	1.123580
H	-2.981353	.540796	2.207168
H	-6.490695	.503921	-.965273
H	-5.881469	-.497867	-2.350850
H	-6.580371	-1.305258	-.885665

Structure *endo*-TS34. AM1 Geometry.
AM1 Energy = -0.1057849
B3LYP/6-31(d) Energy = -1469.1165728

C	2.439019	0.819366	0.039619
C	1.721383	-0.330681	-0.291298
C	2.375351	-1.558727	-0.427949
C	3.747120	-1.637543	-0.215651
C	4.479262	-0.492724	0.132873
C	3.815104	0.732169	0.253227
S	0.030215	-0.229519	-0.657409
C	-0.627432	-1.592416	0.197396
C	-1.381823	-1.123349	1.284061
C	-1.339947	0.396885	1.371646
N	-0.583059	0.965616	0.337296
O	-1.888115	1.014225	2.290780
C	5.936215	-0.584823	0.378912
C	-3.238021	-1.520217	0.780418
O	-2.893536	-2.777953	0.217697
C	-2.357631	-2.468647	-1.020150
C	-2.841618	-1.189704	-1.439880
C	-3.419027	-0.594187	-0.316505
H	1.937328	1.802624	0.121645
H	4.379306	1.640824	0.516030
H	4.262582	-2.603967	-0.323134
H	1.821692	-2.468287	-0.707138
H	6.394962	-1.405527	-0.225756
H	6.447467	0.375345	0.120418
H	6.123123	-0.800299	1.461952
H	-1.448789	-1.671504	2.238079
H	-0.139171	-2.558776	0.112009
H	-1.915255	-3.300979	-1.564676
H	-3.797278	-1.590887	1.716799
H	-3.823874	0.417619	-0.233185
H	-2.729066	-0.758361	-2.433836
B	-0.916723	2.505612	-0.370628
F	0.170794	2.848854	-1.209289
F	-1.061167	3.449556	0.655973
F	-2.101401	2.399870	-1.137431

Structure *exo*-TS34. AM1 Geometry.
AM1 Energy = -0.1053524
B3LYP/6-31(d) Energy = -1469.1160092

O	-3.124408	-0.799448	-0.825815
C	-3.447869	-1.014791	0.528735
C	-3.534082	-2.445384	0.730433
C	-2.911651	-3.040232	-0.365281
C	-2.489551	-1.969225	-1.224542
C	-1.542731	-0.861084	1.169445
C	-0.808896	-1.421547	0.113543
S	-0.017956	-0.120894	-0.753691
N	-0.590687	1.130685	0.172790
C	-1.419145	0.656961	1.192675
C	1.632072	-0.389931	-0.297821
C	2.400510	0.584459	0.337484
C	3.745295	0.326510	0.609990
C	4.326714	-0.892277	0.248001
C	3.542599	-1.860900	-0.397610
C	2.203296	-1.611951	-0.671055
C	5.757325	-1.154700	0.524004
O	-1.989700	1.342723	2.047975
H	1.972189	1.566587	0.620240
H	4.350487	1.097656	1.112413
H	3.992774	-2.821475	-0.690513
H	1.603630	-2.379609	-1.184424
H	6.376368	-0.827107	-0.350033
H	6.101434	-0.591456	1.426427
H	5.940290	-2.244338	0.693844
H	-1.693854	-1.354792	2.139228
H	-0.350841	-2.406914	0.076078
H	-2.095837	-1.967689	-2.239697
H	-3.989518	-0.189387	1.000144
H	-2.714459	-4.096630	-0.532318
H	-3.934574	-2.926820	1.620464
B	-0.498284	2.762426	-0.419256
F	-1.707111	3.411773	-0.133787
F	-0.272172	2.718548	-1.814531
F	0.595391	3.377200	0.224836

Structure *endo*-TS35. AM1 Geometry.
AM1 Energy = -0.0986962
B3LYP/6-31(d) Energy = -1469.1073637

C	2.266343	.191713	-1.235585
C	1.227853	-.444954	-.545544
C	1.505055	-1.265835	.546450
C	2.828534	-1.436408	.957552
C	3.874666	-.804116	.278884
C	3.581510	.012816	-.824169
S	-.358793	-.302985	-1.218058
C	-.695854	1.394689	-1.324958
C	-1.863330	1.659495	-.592766
C	-2.297394	.433708	.207201
N	-1.468071	-.673960	-.020731
O	-3.255147	.473768	.987280
C	5.278464	-1.009346	.701795
C	-1.362008	2.997192	.724435
O	-.474762	3.667459	-.159831
C	.668058	2.890017	-.160119
C	.711931	2.106994	1.032977
C	-.556551	2.189703	1.612527
H	-2.677750	2.288528	-.993695
H	-.339871	1.912578	-2.211107
H	1.430053	3.164262	-.887246
H	-2.270487	3.561810	.951833
H	-.930929	1.673662	2.497424
H	1.561729	1.515704	1.371166
H	.697700	-1.805787	1.077250
H	3.045616	-2.087426	1.819157
H	4.399319	.507535	-1.369817
H	2.048074	.832614	-2.104428
H	5.901691	-.108886	.477362
H	5.340727	-1.221249	1.797769
H	5.713674	-1.882639	.151655
B	-2.046978	-2.317049	.053574
F	-.918773	-3.169395	.089657
F	-2.812736	-2.575551	-1.102141
F	-2.805365	-2.457699	1.223281

Structure *exo*-TS35. AM1 Geometry.
AM1 Energy = -0.1016280
B3LYP/6-31(d) Energy = -1469.1128468

C	-2.274795	.163125	1.331193
C	-1.231686	-.358831	.555110
C	-1.500159	-.980047	-.663123
C	-2.820089	-1.064833	-1.112728
C	-3.869316	-.542286	-.351688
C	-3.584461	.074653	.877108
S	.342760	-.301185	1.268934
C	.827562	1.378796	1.236070
C	1.999040	1.471595	.470018
C	2.326198	.146995	-.211984
N	1.442182	-.866419	.159731
O	3.262173	.043788	-1.012835
C	-5.268678	-.655803	-.821231
C	1.466638	2.557279	-1.112344
C	1.389310	3.815182	-.400816
C	.156771	3.828534	.251360
C	-.505834	2.608840	-.107350
O	.158358	2.031767	-1.178854
H	2.862524	2.091619	.753711
H	.548099	1.971043	2.103282
H	2.121865	2.237894	-1.928643
H	2.194613	4.544059	-.332431
H	-.225169	4.572954	.946209
H	-1.515702	2.241518	.075698
H	-.692473	-1.425442	-1.276733
H	-3.030002	-1.558817	-2.074694
H	-4.405489	.480560	1.487441
H	-2.066389	.635384	2.304070
H	-5.888788	.195929	-.447695
H	-5.317161	-.668670	-1.938141
H	-5.717106	-1.609192	-.440819
B	1.694131	-2.579126	-.044798
F	1.097135	-2.941421	-1.268585
F	1.058029	-3.251650	1.023360
F	3.073041	-2.828370	-.036150