Theoretical studies involving Two Diels-Alder reactions under solvent-free conditions

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Appendix 1. Supplementary Material

Cartesian co-ordinates and example computer program output (e.g. energy data) for selected transition states. Atom numbering differs to the discussion.

1. TS1 (ENDO): Semi-empirical (MNDO); Spartan 14.

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	-0.2686287	-1.5963611	-0.8280099
2 C C2	1.0929222	-1.4726183	-0.4183267
3 C C3	1.8866995	-0.3236884	-0.1853612
4 C C4	1.7299351	0.2574216	1.4660493
5 C C5	0.4498260	0.7652616	1.7688437
6 C C6	-1.1821185	-0.6940072	-1.3213704
7 O O1	-0.8660430	0.5770630	-1.6343358
8 C C7	-1.8662473	1.5070954	-1.9733272
9 C C8	-0.6289192	0.0177422	2.4095051
10 O O2	-1.7814286	0.4280924	2.5438839
11 H H1	-0.3562745	-0.9891747	2.8011776
12 H H11	-0.6680419	-2.6151615	-0.7201816
13 H H12	1.5678269	-2.4338507	-0.1762869
14 H H13	2.9754021	-0.5271343	-0.2150062
15 H H14	1.6651194	0.5879867	-0.7646987
16 H H15	2.0718987	-0.6218088	2.0441415
17 H H16	2.5305457	1.0231167	1.4322961
18 H H17	0.2354932	1.8005360	1.4937968
19 H H18	-2.2150778	-1.0259508	-1.5096715
20 H H19	-2.4399319	1.1931888	-2.8789423
21 H H20	-1.3474147	2.4681462	-2.1974033
22 H H21	-2.5855615	1.6741055	-1.1367725

Atomic Charges:

	Electrostatic	Mulliken	Natural
1 C1 :	-0.422	-0.160	-0.160
2 C2 :	+0.163	+0.021	+0.021
3 C3 :	-0.120	-0.046	-0.046
4 C4 :	-0.006	+0.093	+0.093
5 C5 :	-0.428	-0.304	-0.304
6 C6 :	+0.492	+0.171	+0.171
7 O1 :	-0.385	-0.268	-0.268
8 C7 :	+0.141	+0.203	+0.203
9 C8 :	+0.664	+0.295	+0.295

10 O2	:	-0.559	-0.352	-0.352
11 H1	:	-0.074	-0.011	-0.011
12 H11	:	+0.094	+0.058	+0.058
13 H12	:	+0.033	+0.045	+0.045
14 H13	:	+0.038	+0.026	+0.026
15 H14	:	+0.066	+0.046	+0.046
16 H15	:	+0.030	+0.009	+0.009
17 H16	:	+0.057	+0.020	+0.020
18 H17	:	+0.114	+0.066	+0.066
19 H18	:	+0.013	+0.065	+0.065
20 H19	:	+0.014	-0.011	-0.011
21 H20	:	+0.040	+0.027	+0.027
22 H21	:	+0.034	+0.007	+0.007

Bond Orders Mulliken

1 C1	C2	:	1.187
2 C1	C6	:	1.632
3 C1	O1	:	0.070
4 C1	H11	:	0.962
5 C2	C3	:	1.373
6 C2	C5	:	0.275
7 C2	O2	:	0.031
8 C2	H12	:	0.963
9 C3	C4	:	0.535
10 C3	C6	:	0.052
11 C3	H13	:	0.958
12 C3	H14	:	0.957
13 C4	C5	:	1.393
14 C4	O2	:	0.027
15 C4	H15	:	0.957
16 C4	H16	:	0.952
17 C5	C6	:	0.091
18 C5	C8	:	1.029
19 C5	O2	:	0.056
20 C5	H1	:	0.035
21 C5	H17	:	0.963
22 C6	O1	:	1.076
23 C6	H18	:	0.943
24 O1	C7	:	0.942
25 C7	H19	:	0.956
26 C7	H20	:	0.965
27 C7	H21	:	0.957
28 C8	O2	:	1.857
29 C8	H1	:	0.903
30 O2	H1	:	0.054

Heat of Formation: 35.451 kJ/mol

Energy Due to Solvation
Solvation Energy SM5.4/A -28.809

A A A A A

1	C1	S1	0.06134	-0.33501	0.24790	0.00718	-0.02687
2	C1	PX	-0.07545	0.43591	0.23990	-0.00126	-0.01555
3	C1	PY	0.05207	-0.19138	-0.17004	0.00070	0.01587
4	C1	PZ	-0.03329	0.18355	0.10706	-0.00418	-0.00992
5	C2	S1	-0.00597	-0.22717	0.01071	-0.00089	-0.01779
6	C2	PX	-0.01430	-0.10576	0.47227	0.00008	-0.06411
7	C2	PY	-0.04474	0.07573	0.38546	-0.00503	-0.03853
8	C2	PZ	-0.00479	-0.05986	0.11685	0.01879	-0.00578
9	C3	S1	-0.01005	0.04095	-0.44739	-0.02165	0.03991
10	C3	PX	-0.04790	-0.06848	0.02885	-0.01041	0.03824
11	C3	PY	-0.05619	-0.19291	0.18132	-0.01182	-0.07196
12	C3	PZ	0.03084	0.01228	0.08815	-0.05272	-0.07201
13	C4	S1	-0.16224	-0.02797	0.08613	0.11048	0.45430
14	C4	PX	0.18372	0.04417	-0.04739	0.16329	-0.35391
15	C4	PY	0.24380	0.03889	-0.01099	-0.05648	0.26170
16	C4	PZ	-0.18623	-0.04181	-0.08874	0.00895	0.11827
17	C5	S1	0.15963	0.03501	-0.04733	0.45334	-0.35447
18	C5	PX	-0.07459	0.00426	-0.05694	-0.34309	-0.52905
19	C5	PY	-0.57074	-0.07453	-0.00858	0.17250	0.00445
20	C5	PZ	0.22722	0.03126	0.05786	0.05241	0.18092
21	C6	S1	-0.05692	0.30300	0.05100	-0.00060	-0.00386
22	C6	PX	-0.05348	0.28458	-0.03268	-0.00036	0.00166
23	C6	PY	0.07671	-0.37240	-0.01729	0.00998	-0.00821
24	C6	PZ	-0.03612	0.17420	-0.00213	-0.00642	0.00545
25	O1	S1	-0.01121	0.05841	-0.00173	-0.00089	0.00110
26	O1	PX	0.02445	-0.14729	0.00241	-0.00054	0.00063
27	O1	PY	0.00352	0.02624	0.00743	0.00895	-0.00906
28	O1	PZ	0.00262	-0.02788	-0.00196	-0.00042	0.00143
29	C7	S1	0.00259	-0.03939	0.00005	-0.00306	0.00298
30	C7	PX	0.01272	-0.10106	-0.00456	-0.00446	0.00470
31	C7	PY	-0.01789	0.10733	0.00319	0.00109	-0.00160
32	C7	PZ	0.00492	-0.03473	-0.00121	-0.00093	0.00109
33	C8	S1	-0.34307	-0.04567	-0.01174	-0.15743	-0.01447
34	C8	PX	-0.17635	-0.02264	-0.01610	-0.23129	-0.11087
35	C8	PY	-0.13510	-0.02120	-0.00407	-0.39595	-0.02134
36	C8	PZ	0.11625	0.01505	-0.00162	0.23699	0.03408
37	O2	S1	0.03772	0.00568	-0.00177	0.00372	-0.02888
38	O2	PX	0.14011	0.02042	-0.00318	0.05079	-0.07240
39	O2	PY	0.00961	0.00143	0.00322	0.11358	0.03499
40	O2	PZ	-0.04487	-0.00658	0.00212	-0.06184	0.00638
41	H1	S	0.15219	0.01844	0.00891	-0.13025	0.01568
42	H11	S	-0.02383	0.19180	-0.20596	-0.00416	0.02195
43	H12	S	-0.01696	0.22412	0.06030	-0.00390	0.00741
44	H13	S	0.03013	0.00130	0.27745	0.01292	-0.05141
45	H14	S	0.04101	0.07855	0.23194	0.00091	-0.01530
46	H15	S	0.24767	0.03979	-0.01580	-0.13567	-0.11905
47	H16	S	-0.08706	-0.01701	-0.02672	-0.12506	-0.21695
48	H17	S	0.31831	0.03204	0.04214	-0.48598	0.20075
49	H18	S	0.01430	-0.06811	-0.05336	0.00114	0.00258
50	H19	S	0.00116	-0.00321	-0.00155	0.00021	-0.00006
51	H20	S	0.00411	-0.00604	-0.00135	0.00241	-0.00188
52	H21	S	0.00223	-0.00729	-0.00187	0.00055	-0.00038

MO:	51	52
Eigenvalues:	0.23190	0.30204
(ev):	6.31032	8.21884

TS2 (ENDO): **START** (PM3 GEOMETRY)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.253657	0.44650000	-0.78860000	-0.68310000	12.01100
2	6	-0.476066	-0.73760000	-0.82970000	-0.04660000	12.01100
3	6	-0.234418	-0.86060000	-1.04699900	1.38250000	12.01100
4	6	-0.426874	0.16220000	-1.12820000	2.23300000	12.01100
5	8	-0.666388	0.42720000	-0.54060000	-2.03790000	15.99900
6	6	-0.265090	1.62760000	-0.85190000	-2.70700000	12.01100
15	6	0.385387	-0.82031973	1.03032093	-0.44622105	12.01100
16	6	-0.466688	0.32699817	0.90037583	0.47790055	12.01100
17	6	-0.460512	0.20002637	0.68135983	1.78334755	12.01100
18	8	-0.641001	-1.97954573	0.95415793	-0.10237485	15.99900
11	1	0.244879	1.20180000	-1.03160000	1.92879900	1.00800
12	1	0.210694	1.82660000	-1.92920000	-2.69470000	1.00800
13	1	0.192602	2.49090000	-0.31660000	-2.29480000	1.00800
14	1	0.238194	1.43160000	-0.51810000	-3.72890000	1.00800
7	1	0.261837	1.41849900	-0.91290000	-0.18580000	1.00800
8	1	0.350361	-1.67590000	-0.69950000	-0.60040000	1.00800
9	1	0.258667	-1.88910000	-1.14940000	1.75030000	1.00800
10	1	0.251367	0.02350000	-1.29770000	3.29580000	1.00800
19	1	0.237837	-0.57546943	1.20667593	-1.50623045	1.00800
20	1	0.223243	1.31653927	0.99657493	0.01568607	1.00800
21	1	0.231920	1.05551227	0.58857963	2.44638455	1.00800
22	1	0.296393	-0.76425643	0.58000373	2.27669855	1.00800

TS2: FINAL (HF 3-21G) Eigenvector Following Method

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.237001	0.32361598	-1.08275522	-0.68089153	12.01100
2	6	-0.331947	-0.84862116	-1.45459342	-0.09635738	12.01100
3	6	-0.169716	-0.99928758	-1.45352103	1.28452210	12.01100
4	6	-0.487507	0.03077235	-1.13688492	2.14911643	12.01100
5	8	-0.681809	0.36531096	-0.89796421	-2.03751622	15.99900
6	6	-0.274452	1.65607727	-0.79044782	-2.67018655	12.01100
15	6	0.390741	-0.75534810	1.43930779	-0.28895403	12.01100
16	6	-0.476457	0.46754459	1.07213938	0.39472963	12.01100
17	6	-0.369351	0.39007260	0.84943669	1.75962986	12.01100
18	8	-0.599631	-1.84870353	1.47660802	0.25672631	15.99900
11	1	0.226248	1.03889525	-1.40896347	1.89902172	1.00800
12	1	0.202592	2.23351217	-1.69590152	-2.53015474	1.00800
13	1	0.199123	2.21044920	0.05408261	-2.27964685	1.00800
14	1	0.238681	1.46075473	-0.64234970	-3.71912418	1.00800

7	1	0.244498	1.26707074	-1.17741120	-0.18734273	1.00800
8	1	0.264277	-1.70858955	-1.54193789	-0.72842652	1.00800
9	1	0.252397	-1.99543742	-1.53071319	1.67507675	1.00800
10	1	0.227752	-0.16750177	-1.12385770	3.20498600	1.00800
19	1	0.187591	-0.64892285	1.65881214	-1.34578711	1.00800
20	1	0.219665	1.40332010	1.21577216	-0.10659860	1.00800
21	1	0.224723	1.28286940	0.89066387	2.35529198	1.00800
22	1	0.275583	-0.50515597	1.17753969	2.24828533	1.00800

ENERGIES AND GRADIENT

Total Energy = -286742.0722835 (kcal/mol)
Total Energy = -456.952522177 (a.u.)
Electronic Kinetic Energy = 286117.0995739 (kcal/mol)
Electronic Kinetic Energy = 455.956564892 (a.u.)
The Virial (-V/T) = 2.0022
eK, ee and eN Energy = -624892.0245458 (kcal/mol)
Nuclear Repulsion Energy = 338149.9522623 (kcal/mol)
RMS Gradient = 0.0096692 (kcal/mol/Ang)

TS3 (**EXO**): **START** (PM3 GEOMETRY)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.187858	0.44545854	-0.79220454	-0.66185667	12.01100
2	6	-0.349356	-0.73864146	-0.83330454	-0.02535667	12.01100
3	6	-0.289118	-0.86164146	-1.05060354	1.40374333	12.01100
4	6	-0.425975	0.16115854	-1.13180454	2.25424333	12.01100
5	8	-0.672152	0.42615854	-0.54420454	-2.01665667	15.99900
6	6	-0.291004	1.62655854	-0.85550454	-2.68575667	12.01100
15	6	0.329895	1.65835297	1.01393215	-0.36997355	12.01100
16	6	-0.494327	0.35850833	0.89164169	0.32470700	12.01100
17	6	-0.438661	0.23871872	0.71512518	1.63720521	12.01100
18	8	-0.600552	2.73254310	0.96076895	0.18772128	15.99900
11	1	0.264548	1.20075854	-1.03520454	1.95004233	1.00800
12	1	0.215441	1.82555854	-1.93280454	-2.67345667	1.00800
13	1	0.217116	2.48985854	-0.32020454	-2.27355667	1.00800
14	1	0.235822	1.43055854	-0.52170454	-3.70765667	1.00800
7	1	0.306688	1.41745754	-0.91650454	-0.16455667	1.00800
8	1	0.254122	-1.67694146	-0.70310454	-0.57915667	1.00800
9	1	0.241997	-1.89014146	-1.15300454	1.77154333	1.00800
10	1	0.248123	0.02245854	-1.30130454	3.31704333	1.00800
19	1	0.224824	1.61634162	1.16168860	-1.46132458	1.00800
20	1	0.299349	-0.52671197	0.95668005	-0.31883676	1.00800
21	1	0.278304	-0.72567242	0.62767623	2.12964414	1.00800
22	1	0.257056	1.09332815	0.64644421	2.30692579	1.00800

TS3: FINAL (**HF 3-21G**) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)	Mass

		(Mulliken)	x	y	z	
1	6	0.261901	0.27176810	-1.08109706	-0.75605540	12.01100
2	6	-0.350107	-0.85853381	-1.40074750	-0.06518493	12.01100
3	6	-0.169172	-0.89954787	-1.39399274	1.32163698	12.01100
4	6	-0.516542	0.15327261	-0.96967891	2.11413019	12.01100
5	8	-0.687801	0.19965138	-0.98445493	-2.10871553	15.99900
6	6	-0.276634	1.41363410	-0.83575766	-2.87599891	12.01100
15	6	0.337908	1.99330909	1.09809866	0.05667711	12.01100
16	6	-0.454502	0.60141699	1.18338671	0.38096880	12.01100
17	6	-0.367895	0.22562118	0.97075214	1.70796214	12.01100
18	8	-0.621784	2.82891042	0.51103237	0.74522527	15.99900
11	1	0.275246	1.17243288	-1.09297309	1.79566975	1.00800
12	1	0.208543	2.16439214	-1.54823018	-2.55815241	1.00800
13	1	0.213610	1.80472117	0.16690605	-2.77855674	1.00800
14	1	0.236816	1.13958997	-1.02448050	-3.90036133	1.00800
7	1	0.279264	1.24808805	-1.14855532	-0.32617122	1.00800
8	1	0.255155	-1.75692033	-1.54251495	-0.63185141	1.00800
9	1	0.240412	-1.85051046	-1.56878349	1.78989643	1.00800
10	1	0.226036	0.02276387	-0.99871993	3.18099057	1.00800
19	1	0.174326	2.28589671	1.55936667	-0.88409283	1.00800
20	1	0.234751	-0.07551003	1.59822146	-0.33538456	1.00800
21	1	0.230577	-0.75175454	1.28304556	2.02046279	1.00800
22	1	0.269889	0.99135806	1.10169098	2.45159575	1.00800

ENERGIES AND GRADIENT

Total Energy = -286742.8864776 (kcal/mol)
Total Energy = -456.953819678 (a.u.)
Electronic Kinetic Energy = 286112.2953801 (kcal/mol)
Electronic Kinetic Energy = 455.948908923 (a.u.)
The Virial (-V/T) = 2.0022
eK, ee and eN Energy = -621301.0084869 (kcal/mol)
Nuclear Repulsion Energy = 334558.1220093 (kcal/mol)
RMS Gradient = 0.0041544 (kcal/mol/Ang)

TS4 (ENDO): **START**

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
		(Mulliken)	x	y	z	
1	6	0.182193	0.44650000	-0.78860000	-0.68310000	12.01100
2	6	-0.361652	-0.73760000	-0.82970000	-0.04660000	12.01100
3	6	-0.218191	-0.86060000	-1.04699900	1.38250000	12.01100
4	6	-0.363432	0.16220000	-1.12820000	2.23300000	12.01100
5	8	-0.610173	0.42720000	-0.54060000	-2.03790000	15.99900
6	6	-0.190233	1.62760000	-0.85190000	-2.70700000	12.01100
15	6	0.310156	-0.81200000	0.91520000	-0.59100000	12.01100
16	6	-0.312855	0.33530000	0.78530000	0.33310000	12.01100
17	6	-0.445683	0.20830000	0.56630000	1.63850000	12.01100
18	8	-0.617056	-1.97120000	0.83910000	-0.24720000	15.99900
11	1	0.204434	1.20180000	-1.03160000	1.92879900	1.00800
12	1	0.176920	1.82660000	-1.92920000	-2.69470000	1.00800
13	1	0.159288	2.49090000	-0.31660000	-2.29480000	1.00800

14	1	0.200148	1.43160000	-0.51810000	-3.72890000	1.00800
7	1	0.229069	1.41849900	-0.91290000	-0.18580000	1.00800
8	1	0.330655	-1.67590000	-0.69950000	-0.60040000	1.00800
9	1	0.220254	-1.88910000	-1.14940000	1.75030000	1.00800
10	1	0.222248	0.02350000	-1.29770000	3.29580000	1.00800
19	1	0.218198	-0.56720000	1.09160000	-1.65100000	1.00800
20	1	0.209202	1.32480000	0.88150000	-0.12909900	1.00800
21	1	0.190567	1.06380000	0.47350000	2.30160000	1.00800
22	1	0.265944	-0.75600000	0.46490000	2.13190000	1.00800

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S	C 1 S	C 1 Px	C 1 Py	C 1 Pz
1.997319	0.677069	0.798762	0.514221	0.586410
C 1 S	C 1 Px	C 1 Py	C 1 Pz	C 1 Dx2
0.458598	0.269859	0.346789	0.066201	0.036292
C 1 Dy2	C 1 Dz2	C 1 Dxy	C 1 Dxz	C 1 Dyz
-0.013514	0.028772	0.010097	0.022620	0.018311
C 2 S	C 2 S	C 2 Px	C 2 Py	C 2 Pz
1.997608	0.650057	0.740907	0.599571	0.726641
C 2 S	C 2 Px	C 2 Py	C 2 Pz	C 2 Dx2
0.555487	0.245177	0.459696	0.308788	0.025831
C 2 Dy2	C 2 Dz2	C 2 Dxy	C 2 Dxz	C 2 Dyz
-0.007831	0.024254	0.011992	0.017098	0.006374
C 3 S	C 3 S	C 3 Px	C 3 Py	C 3 Pz
1.997032	0.649144	0.715925	0.612247	0.701554
C 3 S	C 3 Px	C 3 Py	C 3 Pz	C 3 Dx2
0.508760	0.257466	0.483757	0.223191	0.029196
C 3 Dy2	C 3 Dz2	C 3 Dxy	C 3 Dxz	C 3 Dyz
-0.012961	0.019713	0.007360	0.016034	0.009775
C 4 S	C 4 S	C 4 Px	C 4 Py	C 4 Pz
1.996957	0.659300	0.756256	0.501328	0.744809
C 4 S	C 4 Px	C 4 Py	C 4 Pz	C 4 Dx2
0.631995	0.290679	0.345119	0.359261	0.032839
C 4 Dy2	C 4 Dz2	C 4 Dxy	C 4 Dxz	C 4 Dyz
-0.010689	0.031913	0.007643	0.010327	0.005695
O 5 S	O 5 S	O 5 Px	O 5 Py	O 5 Pz
1.995371	0.892280	0.957599	1.111030	0.828373
O 5 S	O 5 Px	O 5 Py	O 5 Pz	O 5 Dx2
0.949250	0.606918	0.722821	0.488806	0.013914
O 5 Dy2	O 5 Dz2	O 5 Dxy	O 5 Dxz	O 5 Dyz
0.001358	0.026672	0.004417	0.006231	0.005132
C 6 S	C 6 S	C 6 Px	C 6 Py	C 6 Pz
1.996634	0.638317	0.587320	0.720266	0.675696
C 6 S	C 6 Px	C 6 Py	C 6 Pz	C 6 Dx2
0.593594	0.180415	0.355063	0.335549	0.022025
C 6 Dy2	C 6 Dz2	C 6 Dxy	C 6 Dxz	C 6 Dyz
0.024771	0.021779	0.015366	0.016902	0.006535
C 15 S	C 15 S	C 15 Px	C 15 Py	C 15 Pz
1.997444	0.694828	0.740737	0.358765	0.758403
C 15 S	C 15 Px	C 15 Py	C 15 Pz	C 15 Dx2
0.504007	0.075904	0.180949	0.250325	0.040469
C 15 Dy2	C 15 Dz2	C 15 Dxy	C 15 Dxz	C 15 Dyz

-0.013480 0.029148 0.027631 0.040055 0.004659
C 16 S C 16 S C 16 Px C 16 Py C 16 Pz
1.997403 0.642348 0.687861 0.653590 0.725461
C 16 S C 16 Px C 16 Py C 16 Pz C 16 Dx2
0.538094 0.317130 0.494806 0.182216 0.023905
C 16 Dy2 C 16 Dz2 C 16 Dxy C 16 Dxz C 16 Dyz
-0.009725 0.022443 0.004316 0.018706 0.014302
C 17 S C 17 S C 17 Px C 17 Py C 17 Pz
1.997121 0.645426 0.714051 0.582063 0.750098
C 17 S C 17 Px C 17 Py C 17 Pz C 17 Dx2
0.634750 0.389108 0.416315 0.235985 0.029074
C 17 Dy2 C 17 Dz2 C 17 Dxy C 17 Dxz C 17 Dyz
-0.008743 0.028923 0.005857 0.017582 0.008073
O 18 S O 18 S O 18 Px O 18 Py O 18 Pz
1.995537 0.891012 0.888990 0.917889 1.075018
O 18 S O 18 Px O 18 Py O 18 Pz O 18 Dx2
0.970155 0.469370 0.654772 0.717504 0.013218
O 18 Dy2 O 18 Dz2 O 18 Dxy O 18 Dxz O 18 Dyz
0.005234 -0.000701 0.010234 0.007549 0.001276
H 11 S H 11 S H 12 S H 12 S H 13 S
0.526975 0.268591 0.529771 0.293309 0.531758
H 13 S H 14 S H 14 S H 7 S H 7 S
0.308955 0.527623 0.272230 0.522059 0.248873
H 8 S H 8 S H 9 S H 9 S H 10 S
0.487016 0.182330 0.511632 0.268114 0.520038
H 10 S H 19 S H 19 S H 20 S H 20 S
0.257714 0.528182 0.253620 0.513653 0.277145
H 21 S H 21 S H 22 S H 22 S
0.517881 0.291552 0.518982 0.215073

TS4: FINAL (HF 6-31G*) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.222568	0.32392041	-1.23672065	-0.78090457	12.01100
2	6	-0.262967	-0.83719658	-1.57819635	-0.14413311	12.01100
3	6	-0.061486	-0.95526477	-1.51810153	1.23951280	12.01100
4	6	-0.470881	0.07462130	-1.12000674	2.08958330	12.01100
5	8	-0.578942	0.35681286	-1.16823581	-2.10761824	15.99900
6	6	-0.193247	1.59632714	-0.88652676	-2.70652504	12.01100
15	6	0.349705	-0.68494407	1.51705174	-0.38436315	12.01100
16	6	-0.381460	0.47187655	1.09058067	0.36808349	12.01100
17	6	-0.328482	0.32275485	0.80390720	1.73019181	12.01100
18	8	-0.574579	-1.81473026	1.51608642	0.03544005	15.99900
11	1	0.190062	1.08297626	-1.40384173	1.84542441	1.00800
12	1	0.164618	2.33826384	-1.62831442	-2.43025335	1.00800
13	1	0.170885	1.94574374	0.09945444	-2.42222980	1.00800
14	1	0.202073	1.43912006	-0.91847705	-3.77328744	1.00800
7	1	0.208145	1.27388890	-1.23952369	-0.28731055	1.00800
8	1	0.220463	-1.71305500	-1.72174714	-0.74902531	1.00800
9	1	0.212795	-1.94482344	-1.61475999	1.65009355	1.00800

10	1	0.193116	-0.12177501	-1.14415692	3.14830914	1.00800
19	1	0.120691	-0.48689478	1.84975077	-1.40955197	1.00800
20	1	0.169907	1.44742259	1.23797479	-0.06019781	1.00800
21	1	0.191462	1.19134622	0.89719279	2.36000685	1.00800
22	1	0.235552	-0.58723273	1.14314470	2.18687010	1.00800

ENERGIES AND GRADIENT

Total Energy = -288340.1661600 (kcal/mol)
Total Energy = -459.499246562 (a.u.)
Electronic Kinetic Energy = 287991.6953584 (kcal/mol)
Electronic Kinetic Energy = 458.943923060 (a.u.)
The Virial (-V/T) = 2.0012
eK, ee and eN Energy = -623818.4230481 (kcal/mol)
Nuclear Repulsion Energy = 335478.2568880 (kcal/mol)
RMS Gradient = 0.0089781 (kcal/mol/Ang)

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S C 1 S C 1 Px C 1 Py C 1 Pz
1.996945 0.690150 0.796616 0.460822 0.621084
C 1 S C 1 Px C 1 Py C 1 Pz C 1 Dx2
0.420071 0.260073 0.379229 0.062991 0.032135
C 1 Dy2 C 1 Dz2 C 1 Dxy C 1 Dxz C 1 Dyz
-0.020697 0.030910 0.005546 0.024031 0.017525
C 2 S C 2 S C 2 Px C 2 Py C 2 Pz
1.996630 0.658493 0.719924 0.590737 0.741237
C 2 S C 2 Px C 2 Py C 2 Pz C 2 Dx2
0.497688 0.277000 0.494305 0.230099 0.022571
C 2 Dy2 C 2 Dz2 C 2 Dxy C 2 Dxz C 2 Dyz
-0.016252 0.023360 0.004553 0.017356 0.005264
C 3 S C 3 S C 3 Px C 3 Py C 3 Pz
1.996774 0.680412 0.740245 0.471365 0.756131
C 3 S C 3 Px C 3 Py C 3 Pz C 3 Dx2
0.483807 0.296859 0.378831 0.197335 0.027831
C 3 Dy2 C 3 Dz2 C 3 Dxy C 3 Dxz C 3 Dyz
-0.017616 0.022380 0.003625 0.014928 0.008580
C 4 S C 4 S C 4 Px C 4 Py C 4 Pz
1.997013 0.640047 0.719672 0.557502 0.715651
C 4 S C 4 Px C 4 Py C 4 Pz C 4 Dx2
0.654598 0.304099 0.461519 0.356294 0.026514
C 4 Dy2 C 4 Dz2 C 4 Dxy C 4 Dxz C 4 Dyz
-0.009352 0.027949 0.006446 0.009373 0.003557
O 5 S O 5 S O 5 Px O 5 Py O 5 Pz
1.995278 0.889734 0.954289 1.098065 0.866611
O 5 S O 5 Px O 5 Py O 5 Pz O 5 Dx2
0.924678 0.590323 0.718503 0.481493 0.016783
O 5 Dy2 O 5 Dz2 O 5 Dxy O 5 Dxz O 5 Dyz
0.002029 0.026303 0.003673 0.006126 0.005055
C 6 S C 6 S C 6 Px C 6 Py C 6 Pz
1.996627 0.641027 0.573993 0.726831 0.701070
C 6 S C 6 Px C 6 Py C 6 Pz C 6 Dx2
0.583314 0.166710 0.341816 0.353472 0.019416
C 6 Dy2 C 6 Dz2 C 6 Dxy C 6 Dxz C 6 Dyz

0.022240 0.026271 0.021549 0.014329 0.004584
C 15 S C 15 S C 15 Px C 15 Py C 15 Pz
1.996882 0.694164 0.735851 0.440583 0.694250
C 15 S C 15 Px C 15 Py C 15 Pz C 15 Dx2
0.418439 0.066884 0.261967 0.230690 0.040105
C 15 Dy2 C 15 Dz2 C 15 Dxy C 15 Dxz C 15 Dyz
-0.019588 0.024827 0.025024 0.034245 0.005972
C 16 S C 16 S C 16 Px C 16 Py C 16 Pz
1.996873 0.643625 0.702449 0.600788 0.710995
C 16 S C 16 Px C 16 Py C 16 Pz C 16 Dx2
0.571759 0.317493 0.558187 0.227642 0.026182
C 16 Dy2 C 16 Dz2 C 16 Dxy C 16 Dxz C 16 Dyz
-0.014327 0.016229 0.003701 0.014791 0.005074
C 17 S C 17 S C 17 Px C 17 Py C 17 Pz
1.997049 0.653876 0.731480 0.471910 0.746335
C 17 S C 17 Px C 17 Py C 17 Pz C 17 Dx2
0.637611 0.387520 0.370476 0.266546 0.026217
C 17 Dy2 C 17 Dz2 C 17 Dxy C 17 Dxz C 17 Dyz
-0.009892 0.021457 0.003883 0.016163 0.007850
O 18 S O 18 S O 18 Px O 18 Py O 18 Pz
1.995541 0.902561 0.932374 0.846923 1.068783
O 18 S O 18 Px O 18 Py O 18 Pz O 18 Dx2
0.963008 0.496467 0.645494 0.685202 0.014760
O 18 Dy2 O 18 Dz2 O 18 Dxy O 18 Dxz O 18 Dyz
0.000305 0.003169 0.010633 0.007931 0.001428
H 11 S H 11 S H 12 S H 12 S H 13 S
0.527864 0.282074 0.535564 0.299818 0.534871
H 13 S H 14 S H 14 S H 7 S H 7 S
0.294244 0.532650 0.265276 0.534191 0.257664
H 8 S H 8 S H 9 S H 9 S H 10 S
0.523144 0.256393 0.529100 0.258105 0.526052
H 10 S H 19 S H 19 S H 20 S H 20 S
0.280832 0.543699 0.335609 0.526980 0.303113
H 21 S H 21 S H 22 S H 22 S
0.528001 0.280537 0.522652 0.241796

TS5 (EXO): **START**

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.174625	0.00000000	0.00000000	0.00000000	12.01100
2	6	-0.310999	1.34490000	0.00000000	0.00000000	12.01100
3	6	-0.204668	2.13610000	1.21590000	0.00000000	12.01100
4	6	-0.395361	1.64070000	2.44890000	0.10080000	12.01100
5	8	-0.613437	-0.63170000	-1.22350000	0.03480000	15.99900
6	6	-0.220630	-1.99570000	-1.18810000	-0.31720000	12.01100
15	6	0.269004	-0.98480000	0.53840000	1.88640000	12.01100
16	6	-0.303048	0.49190000	0.54720000	1.80960000	12.01100
17	6	-0.439703	1.22390000	1.65700000	1.83199900	12.01100
18	8	-0.567730	-1.66500000	1.53730000	1.97220000	15.99900
11	1	0.234481	0.57860000	2.66010000	0.19980000	1.00800

12	1	0.180264	-2.13210000	-0.91250000	-1.36860000	1.00800
13	1	0.190753	-2.57700000	-0.50839900	0.31670000	1.00800
14	1	0.196850	-2.31690000	-2.21980000	-0.15490000	1.00800
7	1	0.281755	-0.61660000	0.90950000	0.00130000	1.00800
8	1	0.216628	1.90490000	-0.94350000	-0.00260000	1.00800
9	1	0.206399	3.21870000	1.06600000	-0.09440000	1.00800
10	1	0.213993	2.27090000	3.33210000	0.09070000	1.00800
19	1	0.187030	-1.46879900	-0.45140000	1.86180000	1.00800
20	1	0.244479	0.96470000	-0.43890000	1.73140000	1.00800
21	1	0.230236	2.30860000	1.64310000	1.77470000	1.00800
22	1	0.229079	0.79060000	2.65190000	1.90910000	1.00800

TS5 (EXO): **FINAL** (HF 6-31G*) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.235615	0.09889196	-0.16285138	-0.38403507	12.01100
2	6	-0.294659	1.44534588	-0.04503815	-0.60447645	12.01100
3	6	-0.071167	2.13816727	1.13390977	-0.35096019	12.01100
4	6	-0.480398	1.58056285	2.26799183	0.23573824	12.01100
5	8	-0.578051	-0.48164492	-1.33848324	-0.53964489	15.99900
6	6	-0.195668	-1.88157098	-1.41089267	-0.38750830	12.01100
15	6	0.301377	-1.09189110	1.00496568	2.16596189	12.01100
16	6	-0.361956	0.30858648	0.70523712	2.18512667	12.01100
17	6	-0.326167	1.24460601	1.74768358	2.06920921	12.01100
18	8	-0.598175	-1.58530843	2.02821380	1.74379534	15.99900
11	1	0.234143	0.55532782	2.52100636	0.03224524	1.00800
12	1	0.177516	-2.37465517	-0.63952940	-0.96686314	1.00800
13	1	0.181648	-2.15436970	-1.31180783	0.65498737	1.00800
14	1	0.198315	-2.17856923	-2.38237641	-0.74991958	1.00800
7	1	0.251568	-0.54939440	0.68349734	-0.27894460	1.00800
8	1	0.210818	1.98211611	-0.93396160	-0.88245305	1.00800
9	1	0.202275	3.20902255	1.10093009	-0.46228105	1.00800
10	1	0.190249	2.21970149	3.13081855	0.32562231	1.00800
19	1	0.117979	-1.74786327	0.21168047	2.54610049	1.00800
20	1	0.182212	0.61828473	-0.27619986	2.49190515	1.00800
21	1	0.190801	2.24230451	1.55439359	2.42151144	1.00800
22	1	0.231724	0.88826600	2.73212641	2.31849276	1.00800

ENERGIES AND GRADIENT

Total Energy = -288341.5181991 (kcal/mol)
Total Energy = -459.501401173 (a.u.)
Electronic Kinetic Energy = 287995.5603279 (kcal/mol)
Electronic Kinetic Energy = 458.950082280 (a.u.)
The Virial (-V/T) = 2.0012
eK, ee and eN Energy = -620817.5955624 (kcal/mol)
Nuclear Repulsion Energy = 332476.0773634 (kcal/mol)
RMS Gradient = 0.0068992 (kcal/mol/Ang)

TS6 (ENDO): **START**; Geometry Optimised Reactants (HF 3-21G* **S-TRANS** ACROLEIN)

NET CHARGES AND COORDINATES (START)

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.520520	7.05126623	0.20137832	-4.30922189	12.01100
2	6	-0.408381	8.32701010	0.25412563	-3.98453131	12.01100
3	6	0.261084	9.37082353	-0.17740365	-4.93097326	12.01100
4	8	-0.725815	10.55736425	-0.15608132	-4.69418772	15.99900
9	6	0.449636	9.14338248	-1.68397474	-3.08723780	12.01100
10	6	-0.584121	8.71787138	-1.42515237	-4.30618194	12.01100
11	6	-0.294236	7.30510294	-1.51694456	-4.70733797	12.01100
12	6	-0.407399	6.27512141	-1.14837989	-3.96751027	12.01100
13	8	-0.616909	10.46307243	-1.51160084	-2.72525131	15.99900
14	6	-0.274796	11.00346173	-2.45153979	-1.77539043	12.01100
7	1	0.263443	8.66174254	0.60822263	-3.02970784	1.00800
8	1	0.162336	8.98899468	-0.52749974	-5.88726084	1.00800
5	1	0.254859	6.27696332	0.51004443	-3.63541527	1.00800
6	1	0.293789	6.72975568	-0.15630848	-5.27093148	1.00800
15	1	0.253242	8.48431458	-2.02745614	-2.30984663	1.00800
16	1	0.422699	9.43854675	-1.14441161	-5.05001535	1.00800
17	1	0.261300	7.12837394	-1.91619863	-5.69068840	1.00800
18	1	0.283372	5.26577100	-1.27395409	-4.30914424	1.00800
19	1	0.287899	6.40322978	-0.69161761	-3.00439452	1.00800
20	1	0.207906	11.06677110	-3.44430694	-2.20289465	1.00800
21	1	0.184734	10.39676945	-2.48945671	-0.87698296	1.00800
22	1	0.245882	11.99038898	-2.09594357	-1.52859334	1.00800

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S	C 1 S	C 1 Px	C 1 Py	C 1 Pz
1.991486	0.360601	0.639034	0.467280	0.581472
C 1 S	C 1 Px	C 1 Py	C 1 Pz	C 2 S
1.140774	0.300916	0.446893	0.592064	1.991032
C 2 S	C 2 Px	C 2 Py	C 2 Pz	C 2 S
0.349354	0.587845	0.562799	0.544986	1.011550
C 2 Px	C 2 Py	C 2 Pz	C 3 S	C 3 S
0.176010	0.612404	0.572401	1.991361	0.411955
C 3 Px	C 3 Py	C 3 Pz	C 3 S	C 3 Px
0.677236	0.450772	0.580678	0.917474	0.081150
C 3 Py	C 3 Pz	O 4 S	O 4 S	O 4 Px
0.221297	0.406994	1.987471	0.412378	0.609638
O 4 Py	O 4 Pz	O 4 S	O 4 Px	O 4 Py
0.743651	0.768491	1.583754	0.716139	0.954450
O 4 Pz	C 9 S	C 9 S	C 9 Px	C 9 Py
0.949843	1.988048	0.420180	0.498616	0.427844
C 9 Pz	C 9 S	C 9 Px	C 9 Py	C 9 Pz
0.610640	0.698610	0.156377	0.437580	0.312467
C 10 S	C 10 S	C 10 Px	C 10 Py	C 10 Pz
1.993188	0.359426	0.595011	0.494043	0.619410
C 10 S	C 10 Px	C 10 Py	C 10 Pz	C 11 S
1.141397	0.401920	0.526880	0.452846	1.990678
C 11 S	C 11 Px	C 11 Py	C 11 Pz	C 11 S
0.369237	0.570907	0.503962	0.575739	0.973299

C 11 Px C 11 Py C 11 Pz C 12 S C 12 S
0.190617 0.570727 0.549070 1.990019 0.374941
C 12 Px C 12 Py C 12 Pz C 12 S C 12 Px
0.618959 0.443877 0.603546 1.097199 0.383843
C 12 Py C 12 Pz O 13 S O 13 S O 13 Px
0.375602 0.519413 1.986481 0.415384 0.619152
O 13 Py O 13 Pz O 13 S O 13 Px O 13 Py
0.717939 0.748709 1.523981 0.785953 0.919706
O 13 Pz C 14 S C 14 S C 14 Px C 14 Py
0.899604 1.987465 0.370718 0.559213 0.511496
C 14 Pz C 14 S C 14 Px C 14 Py C 14 Pz
0.498381 1.038781 0.519843 0.402669 0.386230
H 7 S H 7 S H 8 S H 8 S H 5 S
0.458649 0.277909 0.510835 0.326830 0.464960
H 5 S H 6 S H 6 S H 15 S H 15 S
0.280181 0.479366 0.226845 0.481133 0.265626
H 16 S H 16 S H 17 S H 17 S H 18 S
0.561689 0.015612 0.460742 0.277958 0.467907
H 18 S H 19 S H 19 S H 20 S H 20 S
0.248721 0.472562 0.239539 0.484833 0.307262
H 21 S H 21 S H 22 S H 22 S
0.485781 0.329485 0.482010 0.272108

TS6 (ENDO): **FINAL** (HF 3-21G*) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.427616	6.94888018	0.31512270	-4.40771653	12.01100
2	6	-0.425728	8.37855925	0.51083195	-4.26529756	12.01100
3	6	0.377688	9.18761770	0.84532385	-5.40400013	12.01100
4	8	-0.624292	10.31432048	1.32682918	-5.39815128	15.99900
9	6	0.386552	9.24097914	-1.99492783	-3.06253886	12.01100
10	6	-0.331217	8.83532535	-1.65127985	-4.33352222	12.01100
11	6	-0.255361	7.48790302	-2.09160084	-4.48390503	12.01100
12	6	-0.453638	6.52759124	-1.25891874	-3.82351603	12.01100
13	8	-0.664772	10.48850924	-2.35145091	-2.79275769	15.99900
14	6	-0.287451	10.85731821	-2.82401946	-1.46707761	12.01100
7	1	0.203546	8.75513964	0.84796603	-3.31619269	1.00800
8	1	0.137295	8.70412809	0.59872803	-6.35504597	1.00800
5	1	0.231319	6.34001325	0.95827715	-3.78734637	1.00800
6	1	0.216018	6.60096549	0.35037204	-5.43030579	1.00800
15	1	0.262965	8.54334091	-1.99820276	-2.24960707	1.00800
16	1	0.281586	9.55907481	-1.78551996	-5.11403242	1.00800
17	1	0.238595	7.21622312	-2.66652776	-5.34708560	1.00800
18	1	0.216291	5.48911538	-1.48795771	-4.01054874	1.00800
19	1	0.210662	6.68817376	-1.10408945	-2.76151997	1.00800
20	1	0.228073	10.49726892	-3.83258652	-1.32549790	1.00800
21	1	0.218313	10.45191752	-2.17063227	-0.70656450	1.00800
22	1	0.261171	11.93223028	-2.80144076	-1.44254087	1.00800

ENERGIES AND GRADIENT

Total Energy = -286695.8243203 (kcal/mol)
Total Energy = -456.878821366 (a.u.)
Electronic Kinetic Energy = 286114.8841885 (kcal/mol)
Electronic Kinetic Energy = 455.953034451 (a.u.)
The Virial (-V/T) = 2.0020
eK, ee and eN Energy = -612775.4492266 (kcal/mol)
Nuclear Repulsion Energy = 326079.6249064 (kcal/mol)
RMS Gradient = 0.0107675 (kcal/mol/Ang)

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S C 1 S C 1 Px C 1 Py C 1 Pz
1.989361 0.351774 0.570694 0.448393 0.547233
C 1 S C 1 Px C 1 Py C 1 Pz C 2 S
1.104374 0.374353 0.474762 0.566671 1.989746
C 2 S C 2 Px C 2 Py C 2 Pz C 2 S
0.358990 0.560255 0.476746 0.558237 1.024447
C 2 Px C 2 Py C 2 Pz C 3 S C 3 S
0.324395 0.676029 0.456883 1.987587 0.424498
C 3 Px C 3 Py C 3 Pz C 3 S C 3 Px
0.577774 0.374254 0.586363 0.723573 0.142670
C 3 Py C 3 Pz O 4 S O 4 S O 4 Px
0.403558 0.402036 1.986979 0.425343 0.640281
O 4 Py O 4 Pz O 4 S O 4 Px O 4 Py
0.588046 0.846208 1.547967 0.784352 0.808991
O 4 Pz C 9 S C 9 S C 9 Px C 9 Py
0.996125 1.987473 0.432809 0.500913 0.354521
C 9 Pz C 9 S C 9 Px C 9 Py C 9 Pz
0.642132 0.739113 0.151860 0.433802 0.370825
C 10 S C 10 S C 10 Px C 10 Py C 10 Pz
1.990233 0.374559 0.612916 0.403885 0.580370
C 10 S C 10 Px C 10 Py C 10 Pz C 11 S
1.076861 0.376941 0.577553 0.337899 1.988507
C 11 S C 11 Px C 11 Py C 11 Pz C 11 S
0.375478 0.564627 0.492892 0.514035 0.958025
C 11 Px C 11 Py C 11 Pz C 12 S C 12 S
0.237672 0.532846 0.591279 1.989553 0.353586
C 12 Px C 12 Py C 12 Pz C 12 S C 12 Px
0.567532 0.460379 0.544184 1.109833 0.473986
C 12 Py C 12 Pz O 13 S O 13 S O 13 Px
0.438991 0.515594 1.986217 0.411490 0.666476
O 13 Py O 13 Pz O 13 S O 13 Px O 13 Py
0.765977 0.673868 1.512070 0.827862 0.955803
O 13 Pz C 14 S C 14 S C 14 Px C 14 Py
0.865008 1.987451 0.371520 0.584059 0.568216
C 14 Pz C 14 S C 14 Px C 14 Py C 14 Pz
0.412710 1.050714 0.557734 0.500539 0.254507
H 7 S H 7 S H 8 S H 8 S H 5 S
0.472529 0.323925 0.491228 0.371477 0.469163
H 5 S H 6 S H 6 S H 15 S H 15 S
0.299517 0.474477 0.309504 0.486068 0.250967

H 16 S H 16 S H 17 S H 17 S H 18 S
0.467456 0.250958 0.471813 0.289593 0.475334
H 18 S H 19 S H 19 S H 20 S H 20 S
0.308375 0.472018 0.317320 0.483957 0.287969
H 21 S H 21 S H 22 S H 22 S
0.483422 0.298265 0.481229 0.257601

TS7 (EXO): **START** (HF 3-21G* geometry optimised reactants)

NET CHARGES AND COORDINATES (START)

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.449926	1.72060842	2.80481763	0.22648979	12.01100
2	6	-0.221582	0.57302571	2.43265033	-0.37431837	12.01100
3	6	-0.237846	0.41425034	1.00403152	-0.41448087	12.01100
4	6	-0.421151	1.44849110	0.35639680	0.15765716	12.01100
5	16	0.392812	2.63768203	1.44764721	0.75823613	32.06400
10	6	0.871609	3.86711923	2.62545934	-0.73865874	12.01100
11	6	-0.415020	2.58706898	2.28120862	-1.43636467	12.01100
12	6	-0.398149	2.46648785	0.97159403	-1.47911857	12.01100
13	6	0.857220	3.65810000	0.35525712	-0.81277267	12.01100
14	8	-0.683479	4.45548628	1.41408798	-0.39333349	15.99900
15	8	-0.563899	4.34985791	3.68043749	-0.49216867	15.99900
16	8	-0.571200	3.93885825	-0.78375816	-0.63790390	15.99900
9	1	0.327813	1.57144934	-0.69906965	0.25620317	1.00800
6	1	0.330771	2.07152614	3.80045152	0.38270013	1.00800
7	1	0.272055	-0.13980990	3.12025389	-0.77618255	1.00800
8	1	0.270279	-0.42958233	0.51296083	-0.84948161	1.00800
17	1	0.320429	1.68465414	0.38264049	-1.89845450	1.00800
18	1	0.319263	1.92828010	3.02874604	-1.81207506	1.00800

TS7 (EXO): **FINAL** (HF 3-21G*) Eigenvector Following Method

NET CHARGES AND COORDINATES (TS7) Eigenvector Following Method

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.461095	1.54857482	2.81289527	0.35263542	12.01100
2	6	-0.201383	0.31949883	2.42840929	-0.23325611	12.01100
3	6	-0.201334	0.20067989	1.06978350	-0.29135706	12.01100
4	6	-0.461203	1.34021196	0.42991720	0.25064613	12.01100
5	16	0.415776	2.17194487	1.51398469	1.32523464	32.06400
10	6	0.911141	4.05712096	2.59365110	-0.88876271	12.01100
11	6	-0.374110	2.69909115	2.28256949	-1.40702075	12.01100
12	6	-0.374172	2.57774644	0.89975160	-1.46621497	12.01100
13	6	0.911184	3.85712679	0.31447065	-0.98639919	12.01100
14	8	-0.706795	4.66347417	1.37723067	-0.59114978	15.99900
15	8	-0.578606	4.60092442	3.63886116	-0.71424865	15.99900
16	8	-0.578628	4.20954637	-0.82038493	-0.90524051	15.99900
9	1	0.296762	1.43492892	-0.62873452	0.37459024	1.00800
6	1	0.296732	1.82437686	3.82475740	0.56513294	1.00800
7	1	0.265053	-0.34617527	3.12670604	-0.69342297	1.00800

8	1	0.265061	-0.57250539	0.53892239	-0.80407202	1.00800
17	1	0.287817	1.99309277	0.35089553	-2.16689865	1.00800
18	1	0.287801	2.22392411	2.98215106	-2.05420161	1.00800

ENERGIES AND GRADIENT

Total Energy = -579594.3158332 (kcal/mol)
Total Energy = -923.642220866 (a.u.)
Electronic Kinetic Energy = 576982.9944548 (kcal/mol)
Electronic Kinetic Energy = 919.480815877 (a.u.)
The Virial (-V/T) = 2.0045
eK, ee and eN Energy = -1091144.4663749 (kcal/mol)
Nuclear Repulsion Energy = 511550.1505418 (kcal/mol)
RMS Gradient = 0.0042732 (kcal/mol/Ang)

TS8 (ENDO): **START** (HF 3-21G* geometry optimised reactants)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.340539	1.49844440	2.67814307	0.10651292	12.01100
2	6	-0.386338	0.23794197	2.20111731	0.10874703	12.01100
3	6	-0.356926	0.19641024	0.76375712	0.11535899	12.01100
4	6	-0.358683	1.42726408	0.21473992	0.11784519	12.01100
5	16	0.384925	2.66539283	1.41169630	0.11230061	32.06400
10	6	0.888976	0.00255611	0.28762594	-1.75520370	12.01100
11	6	-0.424563	1.43214639	0.73455939	-1.73642019	12.01100
12	6	-0.420827	1.46505684	2.04999328	-1.73346726	12.01100
13	6	0.887071	0.05960035	2.56791541	-1.75008865	12.01100
14	8	-0.679956	-0.76366511	1.44766763	-1.76257109	15.99900
15	8	-0.606647	-0.46287136	-0.80328525	-1.76313884	15.99900
16	8	-0.614473	-0.35071935	3.68074464	-1.75308731	15.99900
9	1	0.329379	1.66800060	-0.82490547	0.12261905	1.00800
6	1	0.330040	1.79881305	3.70214960	0.10179471	1.00800
7	1	0.362901	-0.63368056	2.81974090	0.10592901	1.00800
8	1	0.358963	-0.70947846	0.19649320	0.11799566	1.00800
17	1	0.324679	2.30805535	2.70052117	-1.72164312	1.00800
18	1	0.322021	2.24157136	0.04265846	-1.72760921	1.00800

TS8 (ENDO): **FINAL** (HF 3-21G*) Eigenvector Following Method

NET CHARGES AND COORDINATES (TS8) Eigenvector Following Method

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.445542	1.52808099	2.63008486	0.24274241	12.01100
2	6	-0.220169	0.24730106	2.15315677	0.59922387	12.01100
3	6	-0.220171	0.21150445	0.78770505	0.61719685	12.01100
4	6	-0.445497	1.46529089	0.23511434	0.27421549	12.01100
5	16	0.393187	2.73065596	1.40422156	0.56228181	32.06400
10	6	0.909039	-0.00467013	0.29340136	-2.13060593	12.01100
11	6	-0.377289	1.38457638	0.71282124	-1.82513088	12.01100
12	6	-0.377365	1.42104936	2.10254133	-1.84323180	12.01100

13	6	0.909082	0.05547987	2.58616532	-2.16038464	12.01100
14	8	-0.711702	-0.76353841	1.45973916	-2.20386529	15.99900
15	8	-0.581764	-0.48254269	-0.78740715	-2.28081256	15.99900
16	8	-0.581775	-0.36516455	3.68631122	-2.33876123	15.99900
9	1	0.290459	1.67757622	-0.81289250	0.30843416	1.00800
6	1	0.290466	1.79499956	3.66606777	0.24966599	1.00800
7	1	0.288390	-0.60461726	2.79222149	0.68709982	1.00800
8	1	0.288374	-0.67263858	0.19666881	0.72133263	1.00800
17	1	0.296147	2.26336550	2.70148116	-2.10394028	1.00800
18	1	0.296130	2.19415274	0.06394856	-2.06957116	1.00800

ENERGIES AND GRADIENT

Total Energy = -579595.6687811 (kcal/mol)
Total Energy = -923.644376925 (a.u.)
Electronic Kinetic Energy = 576995.5542961 (kcal/mol)
Electronic Kinetic Energy = 919.500831256 (a.u.)
The Virial (-V/T) = 2.0045
eK, ee and eN Energy = -1090552.5956787 (kcal/mol)
Nuclear Repulsion Energy = 510956.9268975 (kcal/mol)
RMS Gradient = 0.0077332 (kcal/mol/Ang)

TS9 (EXO): **START** (HF 6-31G* geometry optimised reactants)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.347186	1.75146407	2.65619043	-0.00505576	12.01100
2	6	-0.195013	0.49456857	2.17706813	0.00635813	12.01100
3	6	-0.195301	0.45294388	0.74075209	0.00631396	12.01100
4	6	-0.349070	1.67998088	0.18963523	-0.00513189	12.01100
5	16	0.290191	2.92179021	1.38795994	-0.01619274	12.01100
10	6	0.757445	3.16017804	2.48545926	-1.88784032	12.01100
11	6	-0.367123	1.72812732	2.07283289	-1.84592139	12.01100
12	6	-0.364636	1.68871596	0.75637542	-1.83974767	12.01100
13	6	0.756822	3.09357845	0.25847855	-1.87740464	12.01100
14	8	-0.585713	3.90645427	1.34857024	-1.90448949	15.99900
15	8	-0.527542	3.62499685	3.56165522	-1.90507179	15.99900
16	8	-0.527021	3.49327407	-0.84364202	-1.88442838	15.99900
9	1	0.306706	1.93158885	-0.85133911	-0.00775665	12.01100
6	1	0.305651	2.06293452	3.68084678	-0.00761677	12.01100
7	1	0.238049	-0.37987053	2.79981237	0.01458124	12.01100
8	1	0.238496	-0.45609260	0.16968857	0.01450048	12.01100
17	1	0.282910	0.84890130	0.09282257	-1.81354466	1.00800
18	1	0.282337	0.92953183	2.78563105	-1.82616943	1.00800

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S C 1 S C 1 Px C 1 Py C 1 Pz
1.997385 0.664469 0.734711 0.729596 0.510837
C 1 S C 1 Px C 1 Py C 1 Pz C 1 Dx2
0.638268 0.224628 0.389261 0.383113 0.020694
C 1 Dy2 C 1 Dz2 C 1 Dxy C 1 Dxz C 1 Dyz
0.036567 -0.013784 0.016946 0.009890 0.004603

C 2 S C 2 S C 2 Px C 2 Py C 2 Pz
1.996981 0.659911 0.736848 0.720545 0.564093
C 2 S C 2 Px C 2 Py C 2 Pz C 2 Dx2
0.513301 0.230010 0.250705 0.460343 0.029103
C 2 Dy2 C 2 Dz2 C 2 Dxy C 2 Dxz C 2 Dyz
0.021844 -0.017302 0.016515 0.006260 0.005855
C 3 S C 3 S C 3 Px C 3 Py C 3 Pz
1.996988 0.660023 0.737506 0.720395 0.563343
C 3 S C 3 Px C 3 Py C 3 Pz C 3 Dx2
0.513862 0.239589 0.241645 0.459579 0.030075
C 3 Dy2 C 3 Dz2 C 3 Dxy C 3 Dxz C 3 Dyz
0.020861 -0.017278 0.016536 0.006027 0.006150
C 4 S C 4 S C 4 Px C 4 Py C 4 Pz
1.997393 0.663999 0.727123 0.737165 0.512649
C 4 S C 4 Px C 4 Py C 4 Pz C 4 Dx2
0.639021 0.223555 0.390566 0.382226 0.020218
C 4 Dy2 C 4 Dz2 C 4 Dxy C 4 Dxz C 4 Dyz
0.037581 -0.013464 0.016455 0.009892 0.004688
S 5 S S 5 S S 5 Px S 5 Py S 5 Pz
1.998882 2.000109 1.991829 1.989528 1.994234
S 5 S S 5 Px S 5 Py S 5 Pz S 5 S
1.261361 1.007814 0.748042 1.237032 0.498196
S 5 Px S 5 Py S 5 Pz S 5 Dx2 S 5 Dy2
0.158680 0.039241 0.602323 0.021082 0.036002
S 5 Dz2 S 5 Dxy S 5 Dxz S 5 Dyz C 10 S
0.022323 0.057533 0.019567 0.026033 1.997580
C 10 S C 10 Px C 10 Py C 10 Pz C 10 S
0.684811 0.704644 0.695579 0.433615 0.298911
C 10 Px C 10 Py C 10 Pz C 10 Dx2 C 10 Dy2
0.077828 -0.027255 0.229143 0.022858 0.050427
C 10 Dz2 C 10 Dxy C 10 Dxz C 10 Dyz C 11 S
-0.023853 0.053806 0.012795 0.031667 1.997588
C 11 S C 11 Px C 11 Py C 11 Pz C 11 S
0.640767 0.696580 0.758259 0.613422 0.592031
C 11 Px C 11 Py C 11 Pz C 11 Dx2 C 11 Dy2
0.293287 0.222435 0.480692 0.025334 0.028214
C 11 Dz2 C 11 Dxy C 11 Dxz C 11 Dyz C 12 S
-0.012037 0.015406 0.004988 0.010158 1.997597
C 12 S C 12 Px C 12 Py C 12 Pz C 12 S
0.641266 0.699683 0.756836 0.611536 0.591334
C 12 Px C 12 Py C 12 Pz C 12 Dx2 C 12 Dy2
0.303676 0.213502 0.476662 0.026487 0.026370
C 12 Dz2 C 12 Dxy C 12 Dxz C 12 Dyz C 13 S
-0.011799 0.016306 0.005252 0.009928 1.997580
C 13 S C 13 Px C 13 Py C 13 Pz C 13 S
0.684798 0.694605 0.705744 0.433654 0.299425
C 13 Px C 13 Py C 13 Pz C 13 Dx2 C 13 Dy2
0.075927 -0.025242 0.228962 0.019538 0.049361
C 13 Dz2 C 13 Dxy C 13 Dxz C 13 Dyz O 14 S
-0.023923 0.058240 0.012145 0.032363 1.995455
O 14 S O 14 Px O 14 Py O 14 Pz O 14 S
0.896351 0.998100 0.816072 1.113838 0.940169

O 14 Px O 14 Py O 14 Pz O 14 Dx2 O 14 Dy2
0.591468 0.463490 0.712795 0.004879 0.020519
O 14 Dz2 O 14 Dxy O 14 Dxz O 14 Dyz O 15 S
0.004862 0.018781 0.006208 0.002727 1.995554
O 15 S O 15 Px O 15 Py O 15 Pz O 15 S
0.900370 1.090698 0.944645 0.828684 0.981193
O 15 Px O 15 Py O 15 Pz O 15 Dx2 O 15 Dy2
0.660040 0.485400 0.602286 0.002453 0.012934
O 15 Dz2 O 15 Dxy O 15 Dxz O 15 Dyz O 16 S
-0.000433 0.008780 0.002517 0.012420 1.995554
O 16 S O 16 Px O 16 Py O 16 Pz O 16 S
0.900406 1.097969 0.937301 0.828733 0.981320
O 16 Px O 16 Py O 16 Pz O 16 Dx2 O 16 Dy2
0.671391 0.473346 0.602306 0.001978 0.013650
O 16 Dz2 O 16 Dxy O 16 Dxz O 16 Dyz H 9 S
-0.000442 0.008558 0.001900 0.013053 0.511267
H 9 S H 6 S H 6 S H 7 S H 7 S
0.182028 0.511343 0.183006 0.519969 0.241983
H 8 S H 8 S H 17 S H 17 S H 18 S
0.519932 0.241571 0.519221 0.197869 0.518988
H 18 S
0.198675

TS9 (EXO): **FINAL** (HF 6-31G*) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.397068	1.65623266	2.61963206	0.19226750	12.01100
2	6	-0.137667	0.32401339	2.14459094	0.28617203	12.01100
3	6	-0.137665	0.28380120	0.78307221	0.29021243	12.01100
4	6	-0.397123	1.58564563	0.22965416	0.19929849	12.01100
5	16	0.298755	2.74705956	1.39309985	0.77998523	12.01100
10	6	0.826329	3.28268425	2.48746900	-2.16911479	12.01100
11	6	-0.344759	1.87173885	2.11030602	-1.89891631	12.01100
12	6	-0.344731	1.83003915	0.71272797	-1.89468996	12.01100
13	6	0.826308	3.21582914	0.25043227	-2.16270368	12.01100
14	8	-0.608965	4.02118348	1.34570699	-2.22884353	15.99900
15	8	-0.531644	3.75961899	3.55378229	-2.31450477	15.99900
16	8	-0.531649	3.62815333	-0.84328461	-2.30208018	15.99900
9	1	0.266849	1.80209816	-0.81769476	0.28757436	12.01100
6	1	0.266839	1.93414813	3.65287332	0.27428974	12.01100
7	1	0.225621	-0.53005497	2.78821481	0.19358416	12.01100
8	1	0.225626	-0.60677717	0.19041813	0.20132397	12.01100
17	1	0.247478	1.02424555	0.10893734	-2.25511198	1.00800
18	1	0.247467	1.10341144	2.75886086	-2.26335996	1.00800

ENERGIES

Total Energy = -582608.4124728 (kcal/mol)
Total Energy = -928.445489011 (a.u.)
Electronic Kinetic Energy = 582026.2297469 (kcal/mol)
Electronic Kinetic Energy = 927.517721896 (a.u.)

The Virial (-V/T) = 2.0010
eK, ee and eN Energy = -1092767.5996921 (kcal/mol)
Nuclear Repulsion Energy = 510159.1872194 (kcal/mol)
RMS Gradient = 0.0075161 (kcal/mol/Ang)

ATOMIC ORBITAL ELECTRON POPULATIONS
C 1 S C 1 S C 1 Px C 1 Py C 1 Pz
1.997366 0.658490 0.701141 0.721992 0.483132
C 1 S C 1 Px C 1 Py C 1 Pz C 1 Dx2
0.667769 0.265684 0.394046 0.441689 0.018382
C 1 Dy2 C 1 Dz2 C 1 Dxy C 1 Dxz C 1 Dyz
0.034345 -0.013284 0.013874 0.007857 0.004585
C 2 S C 2 S C 2 Px C 2 Py C 2 Pz
1.996802 0.667938 0.718595 0.751674 0.535224
C 2 S C 2 Px C 2 Py C 2 Pz C 2 Dx2
0.489524 0.241760 0.226543 0.449715 0.026630
C 2 Dy2 C 2 Dz2 C 2 Dxy C 2 Dxz C 2 Dyz
0.023822 -0.018696 0.016697 0.004306 0.007134
C 3 S C 3 S C 3 Px C 3 Py C 3 Pz
1.996804 0.667941 0.719928 0.750291 0.535245
C 3 S C 3 Px C 3 Py C 3 Pz C 3 Dx2
0.489560 0.250334 0.217919 0.449750 0.027707
C 3 Dy2 C 3 Dz2 C 3 Dxy C 3 Dxz C 3 Dyz
0.022684 -0.018726 0.016798 0.004192 0.007238
C 4 S C 4 S C 4 Px C 4 Py C 4 Pz
1.997367 0.658476 0.694759 0.728383 0.483136
C 4 S C 4 Px C 4 Py C 4 Pz C 4 Dx2
0.667795 0.264612 0.394744 0.442091 0.017848
C 4 Dy2 C 4 Dz2 C 4 Dxy C 4 Dxz C 4 Dyz
0.035270 -0.013308 0.013514 0.007929 0.004508
S 5 S S 5 S S 5 Px S 5 Py S 5 Pz
1.998886 1.998817 1.992781 1.990348 1.993660
S 5 S S 5 Px S 5 Py S 5 Pz S 5 S
1.269124 1.059817 0.761216 1.129251 0.552268
S 5 Px S 5 Py S 5 Pz S 5 Dx2 S 5 Dy2
0.265851 0.073129 0.489163 0.018076 0.023538
S 5 Dz2 S 5 Dxy S 5 Dxz S 5 Dyz C 10 S
0.005123 0.044765 0.012612 0.022821 1.997204
C 10 S C 10 Px C 10 Py C 10 Pz C 10 S
0.694515 0.697447 0.685393 0.441658 0.241037
C 10 Px C 10 Py C 10 Pz C 10 Dx2 C 10 Dy2
0.077310 -0.022668 0.221314 0.022668 0.048535
C 10 Dz2 C 10 Dxy C 10 Dxz C 10 Dyz C 11 S
-0.024943 0.052507 0.011152 0.030541 1.997287
C 11 S C 11 Px C 11 Py C 11 Pz C 11 S
0.644827 0.703217 0.736742 0.550571 0.625132
C 11 Px C 11 Py C 11 Pz C 11 Dx2 C 11 Dy2
0.308831 0.233256 0.486152 0.022662 0.022123
C 11 Dz2 C 11 Dxy C 11 Dxz C 11 Dyz C 12 S
-0.011694 0.012464 0.005070 0.008120 1.997287
C 12 S C 12 Px C 12 Py C 12 Pz C 12 S

0.644830 0.705588 0.734761 0.550185 0.625132
C 12 Px C 12 Py C 12 Pz C 12 Dx2 C 12 Dy2
0.315521 0.226454 0.486224 0.023434 0.020801
C 12 Dz2 C 12 Dxy C 12 Dxz C 12 Dyz C 13 S
-0.011771 0.013185 0.005289 0.007810 1.997204
C 13 S C 13 Px C 13 Py C 13 Pz C 13 S
0.694515 0.687925 0.695226 0.441341 0.241041
C 13 Px C 13 Py C 13 Pz C 13 Dx2 C 13 Dy2
0.076293 -0.021867 0.221556 0.019481 0.047517
C 13 Dz2 C 13 Dxy C 13 Dxz C 13 Dyz O 14 S
-0.025034 0.056778 0.010709 0.031006 1.995405
O 14 S O 14 Px O 14 Py O 14 Pz O 14 S
0.900135 1.021973 0.835463 1.055866 0.940590
O 14 Px O 14 Py O 14 Pz O 14 Dx2 O 14 Dy2
0.600730 0.466353 0.735296 0.006251 0.022704
O 14 Dz2 O 14 Dxy O 14 Dxz O 14 Dyz O 15 S
0.001549 0.017987 0.005936 0.002727 1.995545
O 15 S O 15 Px O 15 Py O 15 Pz O 15 S
0.904103 1.079790 0.950659 0.826697 0.964464
O 15 Px O 15 Py O 15 Pz O 15 Dx2 O 15 Dy2
0.658060 0.501524 0.610297 0.003517 0.013197
O 15 Dz2 O 15 Dxy O 15 Dxz O 15 Dyz O 16 S
0.000501 0.008792 0.002585 0.011915 1.995544
O 16 S O 16 Px O 16 Py O 16 Pz O 16 S
0.904106 1.087820 0.942546 0.826773 0.964453
O 16 Px O 16 Py O 16 Pz O 16 Dx2 O 16 Dy2
0.669648 0.489678 0.610574 0.003026 0.013952
O 16 Dz2 O 16 Dxy O 16 Dxz O 16 Dyz H 9 S
0.000471 0.008547 0.001980 0.012531 0.516675
H 9 S H 6 S H 6 S H 7 S H 7 S
0.216476 0.516682 0.216479 0.522876 0.251503
H 8 S H 8 S H 17 S H 17 S H 18 S
0.522875 0.251499 0.519937 0.232585 0.519929
H 18 S
0.232604

TS10 (ENDO): **START** (HF 6-31G* geometry optimised reactants)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.294773	1.76832534	2.65547458	-0.05072490	12.01100
2	6	-0.284297	0.51138284	2.17633858	-0.05072548	12.01100
3	6	-0.286124	0.46977554	0.74002208	-0.05072526	12.01100
4	6	-0.297479	1.69687134	0.18891828	-0.05072482	12.01100
5	16	0.279141	2.93871734	1.38725658	-0.05072378	32.06400
10	6	0.806931	0.25351878	0.33410148	-1.94764518	12.01100
11	6	-0.375464	1.68562609	0.74839404	-1.93291086	12.01100
12	6	-0.380069	1.72369376	2.06490353	-1.93523015	12.01100
13	6	0.808519	0.31784519	2.56117008	-1.95157546	12.01100
14	8	-0.616831	-0.49418053	1.47012857	-1.95815049	15.99900

15	8	-0.573420	-0.21034717	-0.74263976	-1.95046131	15.99900
16	8	-0.575180	-0.08312106	3.66283132	-1.95823553	15.99900
9	1	0.293777	1.94850434	-0.85205342	-0.05072653	1.00800
6	1	0.293496	2.07979534	3.68013358	-0.05072669	1.00800
7	1	0.318519	-0.36310156	2.79907358	-0.05072788	1.00800
8	1	0.318903	-0.43929166	0.16894888	-0.05072737	1.00800
17	1	0.282128	2.56310705	2.72943549	-1.92747107	1.00800
18	1	0.282222	2.48522510	0.03652061	-1.92272316	1.00800

TS10 (ENDO): **FINAL** (HF 6-31G*) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.380475	1.79911174	2.61276560	0.08089386	12.01100
2	6	-0.161074	0.53396185	2.13698853	0.50222606	12.01100
3	6	-0.161080	0.49468466	0.77391696	0.50785440	12.01100
4	6	-0.380503	1.73026554	0.22261725	0.09076095	12.01100
5	16	0.294564	3.00807632	1.38306174	0.37504911	32.06400
10	6	0.825833	0.24373507	0.32949475	-2.38577534	12.01100
11	6	-0.351566	1.62219412	0.71362307	-1.99862777	12.01100
12	6	-0.351679	1.66222941	2.11162566	-2.00437727	12.01100
13	6	0.825867	0.30787798	2.57078828	-2.39490925	12.01100
14	8	-0.618441	-0.49373701	1.47177060	-2.48509921	15.99900
15	8	-0.533067	-0.22076622	-0.73510766	-2.57732143	15.99900
16	8	-0.533067	-0.09506856	3.65859423	-2.59520326	15.99900
9	1	0.260276	1.95117233	-0.82671104	0.12707265	1.00800
6	1	0.260266	2.08011152	3.64788541	0.10867460	1.00800
7	1	0.245527	-0.31542141	2.78056026	0.62810254	1.00800
8	1	0.245524	-0.39033784	0.18141163	0.63884699	1.00800
17	1	0.256547	2.50497847	2.70852492	-2.28496047	1.00800
18	1	0.256547	2.42937098	0.06722499	-2.27407808	1.00800

ENERGIES AND GRADIENT

Total Energy = -582610.0410347 (kcal/mol)
Total Energy = -928.448084289 (a.u.)
Electronic Kinetic Energy = 582028.5518890 (kcal/mol)
Electronic Kinetic Energy = 927.521422465 (a.u.)
The Virial (-V/T) = 2.0010
eK, ee and eN Energy = -1091723.7737940 (kcal/mol)
Nuclear Repulsion Energy = 509113.7327593 (kcal/mol)
RMS Gradient = 0.0060894 (kcal/mol/Ang)

HF 3-21G EXO TS (FINAL) Synchronous Transit Method (Thiophene and Maleic Anhydride) Not displayed in manuscript

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.461282	-0.35247561	1.11717903	1.15492039	12.01100
2	6	-0.201290	-1.62214526	0.49300316	1.14239658	12.01100

3	6	-0.201423	-1.50684155	-0.86560137	1.07694942	12.01100
4	6	-0.461059	-0.15029476	-1.26574079	1.04039910	12.01100
5	16	0.415800	0.85489635	-0.00936027	1.69809169	32.06400
10	6	0.911240	1.36081302	1.31673026	-1.05898022	12.01100
11	6	-0.374238	-0.00664227	0.74366769	-0.95204389	12.01100
12	6	-0.374070	0.11017054	-0.63914770	-1.01943093	12.01100
13	6	0.911139	1.55308722	-0.96248211	-1.17049440	12.01100
14	8	-0.706813	2.24460240	0.24351985	-1.11320638	15.99900
15	8	-0.578611	1.72790303	2.44949545	-1.08626606	15.99900
16	8	-0.578653	2.10413078	-2.00983593	-1.30495115	15.99900
9	1	0.296773	0.17850624	-2.28386063	1.06003305	1.00800
6	1	0.296770	-0.19949772	2.16947628	1.27473670	1.00800
7	1	0.265044	-2.53561288	1.04034164	1.04999717	1.00800
8	1	0.265056	-2.31592981	-1.54738995	0.92529039	1.00800
17	1	0.287777	-0.61135069	-1.31073571	-1.42244181	1.00800
18	1	0.287840	-0.83335480	1.32071249	-1.29502309	1.00800

ENERGIES AND GRADIENT

Total Energy = -579594.3158941 (kcal/mol)
Total Energy = -923.642220963 (a.u.)
Electronic Kinetic Energy = 576983.0490138 (kcal/mol)
Electronic Kinetic Energy = 919.480902823 (a.u.)
The Virial (-V/T) = 2.0045
eK, ee and eN Energy = -1091156.1644992 (kcal/mol)
Nuclear Repulsion Energy = 511561.8486051 (kcal/mol)
RMS Gradient = 0.0100480 (kcal/mol/Ang)

ENDO TS: START (s-trans acrolein and 1-methoxybutadiene, PM3 geometry)

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.313496	-0.71890000	0.06880000	-0.02890000	12.01100
2	6	-0.473302	0.00929999	0.07640000	-1.15980000	12.01100
3	6	-0.251483	1.45960000	0.10980000	-1.16690000	12.01100
4	6	-0.422053	2.23000000	0.03580000	-0.08200000	12.01100
5	8	-0.611347	-2.08840000	0.00110000	-0.15980000	15.99900
6	6	-0.268892	-2.80510000	0.34610000	1.00330000	12.01100
15	6	-0.468880	1.52383130	-1.70611056	-0.18826535	12.01100
16	6	-0.460279	0.19615245	-1.76234724	-0.17156622	12.01100
17	6	0.350583	-0.58982524	-1.74922025	-1.42769595	12.01100
18	8	-0.593849	-1.79933868	-1.79939683	-1.43649094	15.99900
11	1	0.243262	1.83490000	-0.06400000	0.92620000	1.00800
12	1	0.203757	-2.67170000	1.40320000	1.25860000	1.00800
13	1	0.192771	-2.53380000	-0.27450000	1.86530000	1.00800
14	1	0.249459	-3.84250000	0.15750000	0.71630000	1.00800
7	1	0.265999	-0.28810000	0.08570000	0.98190000	1.00800
8	1	0.310997	-0.48080000	0.05950000	-2.14140000	1.00800
9	1	0.238722	1.91740000	0.20680000	-2.15920000	1.00800
10	1	0.249804	3.31340000	0.07049990	-0.13390000	1.00800
19	1	0.234229	2.12318002	-1.71418675	0.71766561	1.00800
20	1	0.265602	2.10616650	-1.64829514	-1.10534389	1.00800

21	1	0.243271	-0.36414823	-1.82022589	0.76982950	1.00800
22	1	0.188135	-0.02921019	-1.69095973	-2.37615675	1.00800

ENDO TS HF 3-21G (s-trans acrolein and 1-methoxybutadiene) (separate single-point energy calculation after TS search) Eigenvector Following Method

NET CHARGES AND COORDINATES

Atom	Z	Charge (Mulliken)	Coordinates(Angstrom) x	y	z	Mass
1	6	0.288137	-0.60351331	0.48504372	-0.18993244	12.01100
2	6	-0.349811	0.18823303	0.79518109	-1.26286259	12.01100
3	6	-0.185648	1.56112109	0.61653108	-1.24275492	12.01100
4	6	-0.486315	2.23912997	0.06581530	-0.17040099	12.01100
5	8	-0.682481	-1.94561161	0.54876564	-0.33237877	15.99900
6	6	-0.297875	-2.79879659	0.09629637	0.75307496	12.01100
15	6	-0.392004	1.48838343	-1.83935149	-0.13650660	12.01100
16	6	-0.459686	0.11980058	-1.83141728	0.08767916	12.01100
17	6	0.396313	-0.81914264	-2.18311692	-0.95580458	12.01100
18	8	-0.603475	-2.00387565	-2.43280066	-0.79288724	15.99900
11	1	0.230775	1.90897035	0.26188176	0.83196753	1.00800
12	1	0.178716	-2.46854466	0.51712757	1.69615252	1.00800
13	1	0.266475	-2.79204792	-0.97849707	0.77882694	1.00800
14	1	0.232567	-3.78388220	0.46145781	0.51630324	1.00800
7	1	0.250880	-0.22541633	0.46458927	0.81020626	1.00800
8	1	0.261247	-0.31170382	1.04441148	-2.17724174	1.00800
9	1	0.239204	2.08912043	0.73421012	-2.17095001	1.00800
10	1	0.224369	3.30010295	-0.08419746	-0.25567719	1.00800
19	1	0.245342	2.14087699	-2.10803669	0.67346913	1.00800
20	1	0.234480	1.84810685	-2.14292267	-1.10187456	1.00800
21	1	0.232006	-0.25101239	-1.87990656	1.09407495	1.00800
22	1	0.176784	-0.37818133	-2.21909998	-1.95080034	1.00800

ENERGIES AND GRADIENT

Total Energy = -286742.5483308 (kcal/mol)
Total Energy = -456.953280807 (a.u.)
Electronic Kinetic Energy = 286107.9509350 (kcal/mol)
Electronic Kinetic Energy = 455.941985610 (a.u.)
The Virial (-V/T) = 2.0022
eK, ee and eN Energy = -623883.3488146 (kcal/mol)
Nuclear Repulsion Energy = 337140.8004838 (kcal/mol)
RMS Gradient = 0.0099711 (kcal/mol/Ang)

ATOMIC ORBITAL ELECTRON POPULATIONS

C 1 S C 1 S C 1 Px C 1 Py C 1 Pz
1.988032 0.414924 0.510981 0.355698 0.641340
C 1 S C 1 Px C 1 Py C 1 Pz C 2 S
0.784038 0.094469 0.482876 0.439505 1.988021
C 2 S C 2 Px C 2 Py C 2 Pz C 2 S

0.392554 0.612628 0.466185 0.579528 0.904864
C 2 Px C 2 Py C 2 Pz C 3 S C 3 S
0.306018 0.646964 0.453049 1.988217 0.398205
C 3 Px C 3 Py C 3 Pz C 3 S C 3 Px
0.613992 0.404745 0.587476 0.899284 0.318522
C 3 Py C 3 Pz C 4 S C 4 S C 4 Px
0.510900 0.464306 1.989010 0.369625 0.559389
C 4 Py C 4 Pz C 4 S C 4 Px C 4 Py
0.427207 0.585689 1.061121 0.504974 0.560810
C 4 Pz O 5 S O 5 S O 5 Px O 5 Py
0.428489 1.986253 0.408991 0.578119 0.798161
O 5 Pz O 5 S O 5 Px O 5 Py O 5 Pz
0.726665 1.522040 0.746399 0.987797 0.928055
C 6 S C 6 S C 6 Px C 6 Py C 6 Pz
1.987559 0.370109 0.509899 0.590951 0.466981
C 6 S C 6 Px C 6 Py C 6 Pz C 15 S
1.053569 0.445128 0.538646 0.335033 1.988927
C 15 S C 15 Px C 15 Py C 15 Pz C 15 S
0.376276 0.602108 0.370511 0.574709 1.054819
C 15 Px C 15 Py C 15 Pz C 16 S C 16 S
0.342730 0.518350 0.563573 1.988936 0.373333
C 16 Px C 16 Py C 16 Pz C 16 S C 16 Px
0.599802 0.455804 0.562353 0.990529 0.304094
C 16 Py C 16 Pz C 17 S C 17 S C 17 Px
0.696677 0.488157 1.987633 0.427180 0.609308
C 17 Py C 17 Pz C 17 S C 17 Px C 17 Py
0.342707 0.588550 0.723803 0.092118 0.416988
C 17 Pz O 18 S O 18 S O 18 Px O 18 Py
0.415400 1.987041 0.426354 0.655002 0.579031
O 18 Pz O 18 S O 18 Px O 18 Py O 18 Pz
0.839543 1.553888 0.773193 0.805999 0.983423
H 11 S H 11 S H 12 S H 12 S H 13 S
0.474881 0.294344 0.486640 0.334644 0.478667
H 13 S H 14 S H 14 S H 7 S H 7 S
0.254858 0.484046 0.283387 0.485893 0.263227
H 8 S H 8 S H 9 S H 9 S H 10 S
0.470968 0.267785 0.478617 0.282180 0.475379
H 10 S H 19 S H 19 S H 20 S H 20 S
0.300252 0.473687 0.280972 0.476751 0.288769
H 21 S H 21 S H 22 S H 22 S
0.471601 0.296394 0.490727 0.332488

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