Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Computational Calculations in Microwave-Assisted Organic Synthesis (MAOS). Application to Cycloaddition Reactions.

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Table S1. Total electronic energies[a] (E, in a.u.), zero-point correction of energies (ΔZPE, in a.u.), and number of imaginary frequencies[b] (NIMAG) of all stationary points discussed in the main text for the reaction between azidomethylphosphonates and enamines.

Structure	E	ΔZPE	NIMAG(ν)
1	-850.3974439	0.133241	0
2a	-975.6228677	0.274344	0
2b	-517.8723277	0.207064	0
3a	-1826.0274075	0.412519	0
3'a	-1826.0257781	0.412713	0
3b	-1368.2793817	0.345502	0
3'b	-1368.2831273	0.345184	0
4a	-1826.0250033	0.412468	0
4'a	-1826.025381	0.412083	0
4b	-1368.2799814	0.345772	0
4'b	-1368.2908766	0.345352	0

5a	-1613.4717623	0.279899	0
5b	-1155.7118148	0.212119	0
6a	-1613.473035	0.280090	0
6b	-1155.7212268	0.212889	0
TS1a	-1825.9908639	0.409198	1 (-277.2989)
TS1'a	-1825.989622	0.408594	1 (-266.1051)
TS1b	-1368.2425041	0.341660	1 (-308.5172)
TS1'b	-1368.2448407	0.341798	1 (-304.0531)
TS2a	-1825.9687909	0.408061	1 (-390.9736)
TS2'a	-1825.9697716	0.408219	1 (-398.1848)
TS2b	-1368.2300875	0.340572	1 (-443.0743)
TS2'b	-1368.2217031	0.341075	1 (-446.4146)
pyrrolidine	-212.5849119	0.130026	0

[a]Computed at the level of theory B3LYP(L1A1)/6-31G*. [b]The imaginary frequency ν (in parentheses) is given in cm^{-1}.

Table S2. Total electronic energies[a] (E, in a.u.), zero-point correction of energies (ΔZPE, in a.u.), and number of imaginary frequencies[b] (NIMAG) of all stationary points discussed in the main text for the reaction between fulvenes and different dienophiles.

Structure	E	ΔZPE	NIMAG(ν)
7	-310.8308355	0.154663	0
8	-534.3193825	0.138982	0
9	-379.2940655	0.055803	0
10	-845.1564873	0.299612	0
11	-1156.0248735	0.461809	0
12	-1156.0150311	0.461633	0
13	-621.6707131	0.315778	0
14	-621.6770105	0.315636	0
16	-690.1407514	0.216557	0
17	-690.1683901	0.218005	0
18	-310.8208738	0.154384	0
INT2	-690.0801695	0.210294	0
TS3	-845.0808146	0.292401	1 (-317.9248)
TS4	-621.6132528	0.310849	1 (-468.4763)
TS5	-1155.9692712	0.456486	1 (-378.4882)
TS6	-1155.9648876	0.456898	1 (-327.8174)
TS7	-310.7361672	0.149017	1 (-1767.864)
TS8	-621.6020343	0.305740	1 (-646.4656)
TS9	-621.6022775	0.306146	1 (-487.9671)
TS10	-690.0636914	0.204003	1 (-1341.545)
TS11	-690.0579292	0.207338	1 (-343.9382)
TS12	-690.1010398	0.212311	1 (-470.2153)
TS13	-690.0985637	0.212495	1 (-388.8965)

[a]Computed at the level of theory B3LYP(L1A1)/6-31G*. [b]The imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates (optimized at the B3LYP(PCM)/6-31G) of all the stationary points discussed in the main text for the reaction between azidomethylphosphonates and enamines.

1

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	7	-0.000006728	-0.000004384	0.000000035
2	7	0.000006485	0.000005542	-0.000002859
3	7	0.000006818	-0.000010543	-0.000014666
4	6	-0.000001001	0.000007870	0.000018315
5	1	0.000001195	0.000001245	-0.000005896
6	1	0.000001392	-0.000003019	-0.000007481
7	15	0.000016266	-0.000005274	0.000008341
8	8	-0.000004519	-0.000007550	-0.000020640
9	8	-0.000015471	0.000000919	0.000015091
10	6	0.000001932	0.000006827	-0.000005600
11	8	-0.000004200	0.000013264	0.000005087
12	6	0.000000607	-0.000002496	0.000003143
13	1	-0.000000769	0.000000459	0.000001780
14	1	0.000001000	-0.000004319	0.000003947
15	1	-0.000002715	0.000003941	0.000002422
16	1	0.000000608	-0.000001223	-0.000000942
17	1	-0.000001158	-0.000000919	0.000000174
18	1	0.000000258	-0.000000341	-0.000000252

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.523889	-1.273218	0.398128
2	7	0	-2.201014	0.063779	-0.113969
3	6	0	-3.412820	0.840197	-0.420589
4	6	0	-4.528785	0.059088	0.285091
5	6	0	-4.042057	-1.395635	0.204095
6	6	0	-0.922033	0.502049	-0.292887
7	6	0	0.152298	-0.275061	0.069554
8	15	0	1.863234	0.088135	-0.107588
9	8	0	2.400165	-1.138506	-1.027182
10	6	0	3.806156	-1.218528	-1.318995
11	6	0	-0.782577	1.877114	-0.902432
12	8	0	2.557356	-0.351701	1.309829
13	6	0	2.546115	0.597114	2.383804
14	8	0	2.277174	1.451819	-0.560308
15	1	0	-5.504373	0.216888	-0.184319
16	1	0	-4.601657	0.377426	1.332093
17	1	0	-3.330369	1.868045	-0.055292
18	1	0	-3.588001	0.884673	-1.506237
19	1	0	-1.967333	-2.040857	-0.153139
20	1	0	-2.238179	-1.354917	1.457810
21	1	0	-4.260058	-1.811536	-0.786848
22	1	0	-4.503696	-2.048746	0.950385
23	1	0	-0.021232	-1.250654	0.513616

24	1	0	0.265812	2.115894	-1.075583
25	1	0	-1.205182	2.639712	-0.236513
26	1	0	-1.329925	1.935250	-1.850661
27	1	0	3.925542	-2.018881	-2.052264
28	1	0	4.372178	-1.459272	-0.413547
29	1	0	4.167236	-0.275016	-1.739864
30	1	0	3.107862	0.148386	3.206190
31	1	0	1.519056	0.797682	2.713217
32	1	0	3.018893	1.535843	2.079234

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.726082	1.163838	-0.043467
2	7	0	1.348906	-0.253581	-0.068173
3	6	0	2.520358	-1.142961	-0.086486
4	6	0	3.660895	-0.226466	0.372719
5	6	0	3.255795	1.143196	-0.201646
6	6	0	0.078784	-0.690223	-0.055845
7	6	0	-1.055419	0.075201	-0.024953
8	6	0	-2.340043	-0.606999	-0.009083
9	8	0	-2.491900	-1.821601	-0.032610
10	8	0	-3.486376	0.147847	0.035608
11	6	0	-3.433807	1.571980	0.080234
12	1	0	4.638033	-0.568633	0.019778
13	1	0	3.689574	-0.185962	1.468096
14	1	0	2.359955	-2.001447	0.573595
15	1	0	2.701795	-1.522155	-1.102865
16	1	0	1.222555	1.710921	-0.850345
17	1	0	1.414697	1.615098	0.909908
18	1	0	3.522892	1.199959	-1.263495
19	1	0	3.735482	1.982976	0.309070
20	1	0	-0.040055	-1.772187	-0.067483
21	1	0	-0.995073	1.154923	-0.009651
22	1	0	-4.473101	1.905132	0.119807
23	1	0	-2.959349	1.989883	-0.815701
24	1	0	-2.909415	1.931199	0.973672

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.584775	0.204660	-0.695796
2	7	0	-0.024053	0.024827	-1.921160
3	7	0	1.234274	0.077023	-1.903859
4	6	0	1.690155	0.316625	-0.513527
5	6	0	0.423013	0.808021	0.267169
6	6	0	-2.003159	0.521341	-0.692892
7	1	0	-2.341351	0.589085	-1.731306
8	1	0	-2.189846	1.487411	-0.211274
9	15	0	-3.019350	-0.764266	0.144177
10	8	0	-2.933882	-0.815540	1.630821
11	8	0	-2.686598	-2.149995	-0.609637
12	6	0	-1.791711	-3.128068	-0.024308

13	1	0	-0.751000	-2.828940	-0.170443
14	1	0	-2.001825	-3.242675	1.041814
15	1	0	-1.990309	-4.065068	-0.547769
16	8	0	-4.453250	-0.367324	-0.483282
17	6	0	-5.632190	-1.078976	-0.055662
18	1	0	-6.482236	-0.564981	-0.506836
19	1	0	-5.718561	-1.057412	1.034527
20	1	0	-5.595728	-2.114262	-0.407931
21	7	0	0.383787	2.245461	0.288560
22	6	0	-0.241553	3.031547	1.362791
23	1	0	-1.168520	4.503793	-0.849157
24	6	0	0.062087	4.470483	0.936260
25	6	0	-0.106816	4.412568	-0.589698
26	6	0	0.407588	3.009218	-0.971575
27	1	0	1.426953	3.043901	-1.381518
28	1	0	-0.225559	2.555163	-1.747115
29	1	0	0.194856	2.785675	2.334897
30	1	0	-1.332234	2.878669	1.442367
31	1	0	-0.598734	5.198564	1.416875
32	1	0	1.096769	4.721191	1.198752
33	1	0	0.428101	5.208991	-1.115670
34	6	0	0.236223	0.227108	1.669760
35	1	0	0.277683	-0.861059	1.630433
36	1	0	-0.735226	0.505350	2.083251
37	1	0	1.026683	0.588715	2.332867
38	1	0	2.460045	1.094083	-0.510055
39	15	0	2.516388	-1.238575	0.039296
40	8	0	3.594047	-1.598577	-1.105792
41	6	0	4.493728	-0.626684	-1.668037
42	1	0	3.953842	0.017722	-2.367831
43	1	0	4.969247	-0.027828	-0.884053
44	1	0	5.257421	-1.191693	-2.205308
45	8	0	1.665181	-2.420990	0.332989
46	8	0	3.375488	-0.649351	1.283909
47	6	0	4.033695	-1.573549	2.177203
48	1	0	4.833682	-2.106957	1.654173
49	1	0	3.314485	-2.290980	2.580650
50	1	0	4.456921	-0.971210	2.982383

3'a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.558895	2.203191	1.273238
2	6	0	-1.238341	3.572012	1.273654
3	6	0	-1.964565	3.578386	-0.082196
4	6	0	-1.062253	2.734241	-1.011520
5	7	0	-0.072412	2.091655	-0.113170
6	6	0	0.601189	0.885494	-0.529209
7	6	0	1.003232	0.963422	-2.004278
8	6	0	1.756882	0.567461	0.473827
9	15	0	3.384518	-0.007063	-0.181477
10	8	0	4.065796	0.954203	-1.086378
11	8	0	3.019385	-1.453338	-0.815423
12	6	0	3.951654	-2.079586	-1.722265
13	8	0	4.286861	-0.301469	1.123164
14	6	0	4.136052	-1.450085	1.984855
15	7	0	1.216761	-0.458157	1.401229

16	7	0	0.169267	-0.956166	0.901768
17	7	0	-0.184604	-0.384599	-0.261334
18	6	0	-1.302388	-0.934347	-0.994501
19	15	0	-2.942070	-0.880950	-0.146651
20	8	0	-3.358012	0.437384	0.409568
21	8	0	-2.982005	-2.102025	0.911647
22	6	0	-2.798180	-1.871930	2.326075
23	8	0	-3.815051	-1.483293	-1.363140
24	6	0	-5.230768	-1.697571	-1.188362
25	1	0	2.023964	1.471270	1.031418
26	1	0	-1.415822	-0.373686	-1.924677
27	1	0	-1.106804	-1.978435	-1.268671
28	1	0	-0.541075	3.350524	-1.753990
29	1	0	-1.676297	2.006148	-1.558060
30	1	0	-2.935339	3.085728	0.020834
31	1	0	-2.131111	4.586739	-0.473878
32	1	0	-0.480452	4.363337	1.315742
33	1	0	-1.918345	3.702217	2.121300
34	1	0	-1.287502	1.417701	1.522390
35	1	0	0.268944	2.141231	1.986881
36	1	0	1.701600	1.788533	-2.157340
37	1	0	1.484603	0.034540	-2.313574
38	1	0	0.132523	1.125845	-2.645280
39	1	0	4.818395	-2.464386	-1.175086
40	1	0	3.415689	-2.907665	-2.188674
41	1	0	4.284597	-1.367839	-2.482077
42	1	0	-3.333151	-0.972391	2.639929
43	1	0	-1.732079	-1.773322	2.543030
44	1	0	-3.208166	-2.748222	2.831488
45	1	0	-5.404593	-2.481489	-0.445694
46	1	0	-5.721880	-0.770604	-0.878295
47	1	0	-5.614971	-2.013823	-2.159167
48	1	0	5.020864	-1.461404	2.623963
49	1	0	3.227829	-1.354552	2.581735
50	1	0	4.091273	-2.370753	1.396818

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.124431	2.689482	-0.955378
2	7	0	-0.942885	1.785680	-0.136784
3	6	0	-0.549740	1.915145	1.282986
4	6	0	0.307500	3.200799	1.337282
5	6	0	0.064291	3.885834	-0.021448
6	6	0	-1.279640	0.499255	-0.653909
7	7	0	-0.261776	-0.589240	-0.467503
8	7	0	-0.652026	-1.500981	0.434880
9	7	0	-1.832417	-1.330370	0.845819
10	6	0	-2.440403	-0.179844	0.096946
11	6	0	0.989655	-0.774997	-1.168361
12	15	0	2.498654	-0.538647	-0.132203
13	8	0	2.531026	0.696173	0.700043
14	6	0	-3.505070	-0.750241	-0.852472
15	8	0	-4.631956	-1.251947	-0.316907
16	6	0	-4.889508	-1.212372	1.100554
17	8	0	-3.360383	-0.781849	-2.055185
18	8	0	3.593195	-0.678560	-1.307683

19	6	0	4.999312	-0.659237	-0.984427
20	8	0	2.733055	-1.911713	0.687602
21	6	0	2.357730	-2.033221	2.077143
22	1	0	-1.502575	0.586385	-1.719963
23	1	0	-2.905519	0.506380	0.809132
24	1	0	1.037721	-0.043874	-1.979411
25	1	0	1.037173	-1.772696	-1.620307
26	1	0	0.860944	2.267432	-1.214518
27	1	0	-0.649820	2.934408	-1.886567
28	1	0	-0.853357	4.485669	0.001124
29	1	0	0.891635	4.534036	-0.326753
30	1	0	1.360711	2.920534	1.425852
31	1	0	0.049370	3.838816	2.188243
32	1	0	-1.446775	1.991657	1.912159
33	1	0	0.033998	1.052395	1.626764
34	1	0	5.532316	-0.717226	-1.934385
35	1	0	5.254487	-1.520203	-0.360301
36	1	0	5.259192	0.269586	-0.468344
37	1	0	1.297485	-2.288584	2.146715
38	1	0	2.967005	-2.839931	2.488816
39	1	0	2.558240	-1.101443	2.611647
40	1	0	-5.792934	-1.807268	1.240056
41	1	0	-5.081594	-0.185238	1.429221
42	1	0	-4.061455	-1.647202	1.662543

3'b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.012734	0.079448	0.236049
2	6	0	1.280616	0.476304	-0.403072
3	6	0	2.199236	-0.424235	0.440453
4	7	0	1.400909	-0.756515	1.675050
5	7	0	0.203050	-0.440909	1.471644
6	7	0	1.621884	1.863411	-0.345991
7	6	0	1.222637	2.765197	-1.428516
8	6	0	1.775443	4.108890	-0.947047
9	6	0	1.478156	4.069474	0.564599
10	6	0	1.588557	2.572921	0.945266
11	6	0	2.523039	-1.739979	-0.255040
12	8	0	1.891214	-2.217961	-1.176204
13	6	0	-1.285441	0.710557	-0.040921
14	15	0	-2.750740	-0.323600	0.419447
15	8	0	-3.708893	0.138939	-0.818198
16	6	0	-5.131446	-0.047571	-0.688789
17	8	0	-3.329869	-0.126356	1.765351
18	8	0	-2.373069	-1.861138	0.126580
19	6	0	-1.863698	-2.321365	-1.138599
20	8	0	3.592850	-2.322253	0.306654
21	6	0	3.936272	-3.621728	-0.208364
22	1	0	1.264303	0.156734	-1.447145
23	1	0	3.124822	0.070418	0.739935
24	1	0	-1.341533	0.883786	-1.118739
25	1	0	-1.413521	1.679483	0.462565
26	1	0	1.656705	2.432052	-2.378758
27	1	0	0.128076	2.833775	-1.567301
28	1	0	1.314917	4.963679	-1.451605
29	1	0	2.855808	4.146095	-1.126155

30	1	0	2.157380	4.697769	1.147840
31	1	0	0.460497	4.428975	0.754299
32	1	0	2.499878	2.356865	1.517670
33	1	0	-2.045251	-3.397568	-1.166474
34	1	0	-0.788649	-2.131633	-1.204118
35	1	0	-2.389882	-1.844365	-1.972114
36	1	0	-5.593700	0.538871	-1.485156
37	1	0	-5.391856	-1.104130	-0.812684
38	1	0	-5.475299	0.301124	0.288197
39	1	0	4.810989	-3.936834	0.360225
40	1	0	3.108137	-4.319189	-0.060231
41	1	0	4.169074	-3.560927	-1.274644
42	1	0	0.740334	2.260339	1.572147

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.412374	-1.611902	-0.360528
2	6	0	4.509995	-0.789578	0.593920
3	7	0	3.251426	-0.583922	-0.156145
4	6	0	3.087410	-1.778521	-1.002588
5	6	0	4.500069	-1.989690	-1.551613
6	6	0	2.096044	-0.121559	0.590370
7	6	0	0.929110	0.264298	-0.393447
8	15	0	0.380683	2.023710	-0.459417
9	8	0	-0.747636	1.862007	-1.606858
10	6	0	-1.845735	2.798435	-1.696579
11	6	0	2.477167	0.966500	1.598928
12	8	0	1.440818	3.032043	-0.737608
13	8	0	-0.437479	2.260902	0.912414
14	6	0	-0.398202	3.521844	1.608769
15	7	0	-0.137764	-0.640650	0.048346
16	6	0	-1.194907	-1.141292	-0.818259
17	15	0	-2.874322	-0.925939	-0.095482
18	8	0	-3.690752	-1.805082	-1.175304
19	6	0	-5.124216	-1.910680	-1.063291
20	7	0	0.329380	-1.516340	1.002513
21	7	0	1.487130	-1.258690	1.385439
22	8	0	-3.338770	0.471668	0.124170
23	8	0	-2.949224	-1.871151	1.213351
24	6	0	-2.740928	-1.335771	2.537311
25	1	0	1.230080	0.048346	-1.426206
26	1	0	-1.175706	-0.573437	-1.750417
27	1	0	-1.048946	-2.202901	-1.049764
28	1	0	4.953434	0.175632	0.854436
29	1	0	4.339943	-1.346016	1.528685
30	1	0	5.786905	-2.504278	0.150851
31	1	0	6.283830	-1.037871	-0.689121
32	1	0	4.670124	-1.310870	-2.393870
33	1	0	4.659291	-3.013031	-1.905359
34	1	0	2.754137	-2.657233	-0.424766
35	1	0	2.356108	-1.606893	-1.799455
36	1	0	2.961997	1.806412	1.095275
37	1	0	1.579645	1.324361	2.107279
38	1	0	3.146837	0.556231	2.357507
39	1	0	-1.266839	4.121524	1.320747
40	1	0	-0.449293	3.295987	2.675817

41	1	0	0.521504	4.066030	1.380807
42	1	0	-3.360142	-1.926944	3.215336
43	1	0	-3.039110	-0.285360	2.578564
44	1	0	-1.686702	-1.443113	2.803948
45	1	0	-5.465279	-2.432007	-1.958939
46	1	0	-5.390832	-2.488476	-0.173366
47	1	0	-5.579009	-0.917098	-1.014292
48	1	0	-2.293142	2.646892	-2.680375
49	1	0	-2.574022	2.569287	-0.916532
50	1	0	-1.486171	3.829873	-1.623639

4'a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.272947	3.428478	0.147278
2	7	0	1.669825	2.176016	-0.377876
3	6	0	0.445190	2.547375	-1.111490
4	6	0	0.862864	3.841954	-1.807692
5	6	0	1.674007	4.565425	-0.716938
6	6	0	1.606912	1.049407	0.539920
7	6	0	2.946148	0.843639	1.247891
8	6	0	1.028456	-0.207140	-0.208334
9	15	0	1.828610	-1.849528	0.107701
10	8	0	0.968712	-2.724135	-0.950391
11	6	0	1.219266	-4.140122	-1.062811
12	8	0	1.862627	-2.373265	1.501521
13	8	0	3.273262	-1.721958	-0.612955
14	6	0	4.502839	-2.098587	0.041316
15	7	0	-0.350140	-0.165602	0.265742
16	6	0	-1.435234	-1.062704	-0.059952
17	15	0	-3.055360	-0.194753	-0.182402
18	8	0	-3.064423	1.065455	-0.973388
19	7	0	-0.482247	0.656430	1.344478
20	7	0	0.551597	1.313029	1.592853
21	8	0	-3.667778	-0.073943	1.307458
22	6	0	-3.699656	1.186919	2.010973
23	8	0	-3.897042	-1.446645	-0.761664
24	6	0	-5.326988	-1.336713	-0.901533
25	1	0	-1.527746	-1.893689	0.652681
26	1	0	-1.241575	-1.492467	-1.044654
27	1	0	-2.737194	1.354903	2.497929
28	1	0	-3.916116	2.005566	1.320485
29	1	0	-4.495154	1.100441	2.753680
30	1	0	-5.659530	-2.254373	-1.389151
31	1	0	-5.587256	-0.473876	-1.522153
32	1	0	-5.796916	-1.245834	0.081910
33	1	0	0.005127	4.422532	-2.161041
34	1	0	0.157286	1.765567	-1.820677
35	1	0	-0.416639	2.720594	-0.446836
36	1	0	3.364152	3.377123	0.059773
37	1	0	2.030515	3.588407	1.206369
38	1	0	1.011457	5.188074	-0.105993
39	1	0	2.446812	5.221119	-1.129849
40	1	0	1.496812	3.609397	-2.671196
41	1	0	2.905488	-0.041190	1.887500
42	1	0	3.162856	1.700446	1.889285
43	1	0	3.752597	0.737201	0.517462

44	1	0	1.090231	-0.058431	-1.291101
45	1	0	2.212382	-4.314108	-1.489290
46	1	0	1.140250	-4.622079	-0.084376
47	1	0	0.457137	-4.534912	-1.736011
48	1	0	4.967780	-2.893588	-0.547427
49	1	0	4.312596	-2.448071	1.058458
50	1	0	5.159285	-1.225301	0.061936

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.314467	-0.326270	0.603675
2	6	0	-4.409176	0.340103	-0.431647
3	7	0	-3.061120	-0.000330	0.053049
4	6	0	-3.096873	-1.334342	0.700010
5	6	0	-4.599480	-1.668226	0.846966
6	6	0	-1.974959	0.292166	-0.828416
7	6	0	-0.574061	0.334013	-0.132230
8	6	0	-0.059857	1.776203	-0.146140
9	8	0	0.389961	2.279268	-1.152738
10	8	0	-0.232855	2.537044	0.947787
11	6	0	-0.644658	1.975864	2.207563
12	7	0	0.214276	-0.536968	-1.006779
13	7	0	-0.621743	-1.174438	-1.920128
14	7	0	-1.783749	-0.732327	-1.916733
15	6	0	1.235101	-1.418952	-0.460179
16	15	0	2.653957	-0.497376	0.240748
17	8	0	3.506410	-1.759438	0.765261
18	6	0	4.808181	-1.550108	1.351807
19	8	0	2.272878	0.537997	1.244457
20	8	0	3.558177	0.028010	-0.984247
21	6	0	3.523113	1.409287	-1.421572
22	1	0	-2.185251	1.240688	-1.334573
23	1	0	-0.624831	-0.084748	0.875325
24	1	0	0.842839	-2.067163	0.341052
25	1	0	1.587890	-2.061586	-1.271337
26	1	0	-4.525898	1.429342	-0.478968
27	1	0	-4.606214	-0.067958	-1.437036
28	1	0	-6.343347	-0.447096	0.251291
29	1	0	-5.334645	0.273779	1.521204
30	1	0	-4.834593	-2.110302	1.819858
31	1	0	-4.895524	-2.389345	0.076813
32	1	0	-2.582978	-2.097428	0.100574
33	1	0	-2.596150	-1.287666	1.676427
34	1	0	3.545814	2.081641	-0.561380
35	1	0	2.619567	1.592780	-2.004936
36	1	0	4.414375	1.547747	-2.035817
37	1	0	5.135276	-2.521672	1.724449
38	1	0	5.507635	-1.185940	0.594150
39	1	0	4.744716	-0.837260	2.179168
40	1	0	-0.697652	2.824658	2.891142
41	1	0	-1.632073	1.511082	2.128425
42	1	0	0.104293	1.264042	2.563911

4'b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.559129	-0.854689	-1.166427
2	7	0	-3.252576	0.006071	-0.000935
3	6	0	-4.446181	0.119134	0.849959
4	6	0	-5.586144	0.060597	-0.166209
5	6	0	-5.096343	-1.023638	-1.144642
6	6	0	-2.009958	-0.182443	0.667424
7	6	0	-0.749087	0.156026	-0.178697
8	6	0	-0.199139	1.533271	0.173124
9	8	0	-0.111836	2.305612	-0.914563
10	6	0	0.508744	3.591757	-0.716324
11	8	0	0.092003	1.880034	1.299764
12	7	0	0.154670	-0.915548	0.246082
13	6	0	1.259810	-1.368612	-0.581944
14	15	0	2.792519	-0.400401	-0.286144
15	8	0	3.822349	-1.332279	-1.104234
16	6	0	5.213556	-0.958791	-1.179317
17	7	0	-0.581146	-1.937677	0.844926
18	7	0	-1.744106	-1.599105	1.120028
19	8	0	3.213798	-0.690818	1.245704
20	6	0	2.931150	0.276850	2.284131
21	8	0	2.736851	1.040804	-0.659301
22	1	0	-2.005207	0.423526	1.581744
23	1	0	-0.948056	0.102585	-1.256903
24	1	0	1.461399	-2.410576	-0.317095
25	1	0	1.015151	-1.326237	-1.654121
26	1	0	-4.528875	-0.712240	1.571115
27	1	0	-4.415115	1.056718	1.418226
28	1	0	-5.678936	1.026922	-0.675778
29	1	0	-6.550692	-0.179763	0.291472
30	1	0	-5.355370	-2.015479	-0.757133
31	1	0	-5.539197	-0.933654	-2.141233
32	1	0	-3.218049	-0.366854	-2.089253
33	1	0	-3.055595	-1.828956	-1.100950
34	1	0	5.680663	-1.654098	-1.878141
35	1	0	5.680785	-1.051358	-0.194449
36	1	0	5.315679	0.065718	-1.548556
37	1	0	1.854839	0.354159	2.449881
38	1	0	3.429652	-0.096031	3.180438
39	1	0	3.328994	1.256350	2.009390
40	1	0	0.428136	4.103317	-1.675530
41	1	0	1.554969	3.441231	-0.443073
42	1	0	-0.009870	4.150954	0.065983

5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.983490	-1.591842	-0.465630
2	7	0	-0.228897	-1.549493	-0.926230
3	7	0	-0.610313	-0.241073	-0.942372
4	6	0	0.377832	0.569401	-0.477337
5	6	0	1.404488	-0.318877	-0.182027
6	15	0	3.010269	-0.027983	0.568736
7	8	0	3.045320	0.169555	2.038709

8	8	0	3.942128	-1.265883	0.132892
9	8	0	3.501374	1.247436	-0.308842
10	6	0	4.135320	-1.649810	-1.243141
11	1	0	3.252147	-2.180869	-1.605727
12	1	0	4.334782	-0.774503	-1.869013
13	1	0	5.001627	-2.313574	-1.253881
14	6	0	4.658284	1.988183	0.136966
15	1	0	4.540436	2.288991	1.181015
16	1	0	5.564300	1.383580	0.027898
17	1	0	4.723640	2.867803	-0.505279
18	6	0	0.252595	2.051443	-0.360069
19	1	0	0.030373	2.507362	-1.333222
20	1	0	-0.554106	2.313663	0.332311
21	1	0	1.191335	2.472857	0.001201
22	6	0	-1.954678	0.096417	-1.379921
23	1	0	-1.939994	1.043877	-1.925886
24	1	0	-2.292686	-0.693535	-2.054211
25	15	0	-3.121101	0.245117	0.040520
26	8	0	-2.695710	1.217744	1.082275
27	8	0	-4.454835	0.557593	-0.797146
28	6	0	-5.722725	0.691376	-0.114973
29	1	0	-6.443556	0.999688	-0.872868
30	1	0	-6.018932	-0.269198	0.314885
31	1	0	-5.655582	1.452288	0.667532
32	8	0	-3.391147	-1.252581	0.566237
33	6	0	-2.672856	-1.800332	1.698362
34	1	0	-3.335047	-2.537642	2.154883
35	1	0	-2.432941	-1.013683	2.417256
36	1	0	-1.759874	-2.284987	1.343748

5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.040848	0.378286	-0.690743
2	6	0	-2.276834	-0.067537	-0.252399
3	7	0	-2.172971	-1.403857	0.026408
4	7	0	-0.960597	-1.799758	-0.211501
5	7	0	-0.257276	-0.716630	-0.652576
6	6	0	1.146362	-0.866880	-0.993319
7	1	0	1.361527	-1.938418	-0.965561
8	1	0	1.330573	-0.497436	-2.006872
9	15	0	2.287084	-0.017472	0.174684
10	8	0	3.737994	-0.309878	-0.473675
11	6	0	4.616029	-1.310372	0.091884
12	1	0	4.386692	-2.290361	-0.338177
13	1	0	5.631090	-1.018558	-0.181774
14	1	0	4.511348	-1.345807	1.178288
15	8	0	2.143585	-0.366093	1.610342
16	8	0	2.013392	1.508809	-0.252421
17	6	0	2.632081	2.580055	0.499620
18	1	0	3.708675	2.594564	0.307754
19	1	0	2.177480	3.503886	0.141026
20	1	0	2.438815	2.455024	1.567986
21	6	0	-3.466981	0.812775	-0.149065
22	8	0	-3.387554	1.973564	-0.507857
23	8	0	-4.641495	0.366681	0.328996
24	6	0	-4.863988	-0.965143	0.831415

25	1	0	-4.190080	-1.193131	1.659551
26	1	0	-4.734486	-1.710556	0.045036
27	1	0	-5.898269	-0.956557	1.178991
28	1	0	-0.696026	1.349375	-1.010241

6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.667611	3.011321	-0.387315
2	7	0	0.298554	2.270241	-0.862457
3	7	0	-0.076941	0.985670	-0.763592
4	6	0	-1.321908	0.888472	-0.196379
5	6	0	-1.688685	2.210707	0.033700
6	6	0	0.856210	-0.052539	-1.169635
7	15	0	2.235710	-0.249022	0.041071
8	8	0	2.831868	-1.623926	-0.542627
9	6	0	4.054036	-2.166956	0.002591
10	15	0	-2.228972	-0.628739	0.113380
11	8	0	-1.211807	-1.662798	0.815983
12	6	0	-1.021814	-1.657077	2.254199
13	6	0	-2.938930	2.786015	0.619106
14	8	0	1.835792	-0.201597	1.473116
15	8	0	3.380191	0.806397	-0.379336
16	6	0	3.539595	2.062936	0.320954
17	8	0	-3.511869	-0.405507	0.827276
18	8	0	-2.285103	-1.249086	-1.372058
19	6	0	-2.938417	-2.521368	-1.588496
20	1	0	-2.929910	-2.685072	-2.666693
21	1	0	-2.387768	-3.319563	-1.083167
22	1	0	-3.968916	-2.484813	-1.224964
23	1	0	-1.946719	-1.366973	2.758588
24	1	0	-0.755127	-2.679091	2.528936
25	1	0	-0.201183	-0.979597	2.496206
26	1	0	-3.642612	1.995608	0.883422
27	1	0	-3.415579	3.466257	-0.095632
28	1	0	-2.704312	3.368853	1.517084
29	1	0	1.267068	0.207406	-2.148546
30	1	0	0.324289	-1.000003	-1.250485
31	1	0	4.563758	2.387862	0.130184
32	1	0	2.828887	2.791864	-0.074896
33	1	0	3.380990	1.924690	1.392928
34	1	0	4.893575	-1.503590	-0.222438
35	1	0	3.960759	-2.304366	1.083684
36	1	0	4.200624	-3.132690	-0.482510

6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.787664	-2.310988	-0.915113
2	7	0	0.814717	-0.965953	-0.810659
3	6	0	1.914521	-0.567991	-0.101189
4	6	0	2.560058	-1.753504	0.200270
5	7	0	1.850013	-2.786998	-0.311876

6	6	0	-0.323124	-0.209165	-1.309796
7	15	0	-1.517017	0.171596	0.045915
8	8	0	-2.486627	1.151459	-0.779457
9	6	0	-3.679029	1.677154	-0.155119
10	6	0	2.335494	0.797881	0.263935
11	8	0	1.647113	1.752658	-0.385956
12	6	0	1.970919	3.109611	-0.018716
13	8	0	3.231398	1.013824	1.054075
14	8	0	-2.438807	-1.143259	0.213841
15	6	0	-2.172354	-2.116137	1.250168
16	8	0	-0.899617	0.669947	1.303008
17	1	0	0.021134	0.724675	-1.752722
18	1	0	-0.812360	-0.823402	-2.068355
19	1	0	-4.108917	2.382810	-0.866790
20	1	0	-4.386551	0.867409	0.042655
21	1	0	-3.425918	2.193474	0.775101
22	1	0	-1.430110	-2.835155	0.893133
23	1	0	-1.815723	-1.622850	2.157281
24	1	0	1.343018	3.736661	-0.650908
25	1	0	3.029030	3.309421	-0.201708
26	1	0	1.742285	3.273458	1.036696
27	1	0	3.484412	-1.893246	0.743733
28	1	0	-3.118402	-2.623743	1.445292

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.954438	0.246504	1.025006
2	7	0	0.137751	-0.012006	1.974930
3	7	0	-1.069307	-0.048948	2.020537
4	6	0	-1.850329	0.339515	0.287259
5	6	0	-0.941087	0.985765	-0.613525
6	6	0	2.365120	0.165151	1.403525
7	1	0	2.530038	-0.421476	2.315398
8	1	0	2.803613	1.162980	1.558365
9	15	0	3.276696	-0.616168	0.026132
10	8	0	3.121121	0.035689	-1.307797
11	8	0	2.915408	-2.192204	0.059062
12	6	0	1.878588	-2.743416	-0.784888
13	1	0	0.892445	-2.557385	-0.352489
14	1	0	1.935444	-2.311021	-1.787040
15	1	0	2.067302	-3.817831	-0.833417
16	8	0	4.765500	-0.618327	0.655541
17	6	0	5.853061	-1.169512	-0.111046
18	1	0	6.763419	-0.970125	0.456706
19	1	0	5.914234	-0.688590	-1.091939
20	1	0	5.721008	-2.248833	-0.232895
21	7	0	-0.746042	2.306331	-0.514117
22	6	0	0.259376	3.035382	-1.311636
23	1	0	0.547498	4.199790	1.220166
24	6	0	0.077847	4.493727	-0.880759
25	6	0	-0.335596	4.370887	0.593845
26	6	0	-1.234768	3.126155	0.613469
27	1	0	-2.289858	3.385826	0.450175
28	1	0	-1.160708	2.562257	1.547361
29	1	0	0.093724	2.879817	-2.380984
30	1	0	1.259955	2.654634	-1.062087

31	1	0	0.989622	5.079824	-1.025872
32	1	0	-0.722913	4.962703	-1.465156
33	1	0	-0.851554	5.256723	0.974797
34	6	0	-0.321178	0.289070	-1.798692
35	1	0	-0.461538	-0.787503	-1.721054
36	1	0	0.747892	0.494300	-1.882327
37	1	0	-0.820749	0.636717	-2.713911
38	1	0	-2.596254	1.000555	0.719888
39	15	0	-2.556694	-1.269705	-0.091405
40	8	0	-3.384741	-1.741180	1.214415
41	6	0	-4.288499	-0.874900	1.915986
42	1	0	-3.725492	-0.191165	2.558126
43	1	0	-4.921352	-0.311730	1.221002
44	1	0	-4.918247	-1.518345	2.533981
45	8	0	-1.648770	-2.361353	-0.539446
46	8	0	-3.708416	-0.852747	-1.171388
47	6	0	-4.466756	-1.902043	-1.804371
48	1	0	-5.067222	-2.444698	-1.066652
49	1	0	-3.799059	-2.600514	-2.316542
50	1	0	-5.124640	-1.415693	-2.527087

TS1'a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.034754	2.593949	1.197533
2	6	0	-0.858307	3.832238	1.077214
3	6	0	-1.692795	3.538740	-0.177710
4	6	0	-0.714257	2.811452	-1.111625
5	7	0	0.282801	2.201650	-0.202369
6	6	0	1.132655	1.236007	-0.572993
7	6	0	1.385555	1.042949	-2.048085
8	6	0	1.899306	0.531703	0.407999
9	15	0	3.506014	-0.157030	-0.027789
10	8	0	4.446290	0.755431	-0.736390
11	8	0	3.142355	-1.513455	-0.846156
12	6	0	4.170084	-2.134401	-1.642536
13	8	0	4.161845	-0.643881	1.369125
14	6	0	3.743209	-1.804557	2.111137
15	7	0	0.891330	-0.970465	1.180023
16	7	0	-0.048824	-1.269434	0.491185
17	7	0	-0.505794	-0.818082	-0.618928
18	6	0	-1.715340	-1.493135	-1.081853
19	15	0	-3.228864	-0.855716	-0.261042
20	8	0	-3.425814	0.623476	-0.283987
21	8	0	-3.252924	-1.497360	1.230508
22	6	0	-2.895689	-0.723208	2.390141
23	8	0	-4.346401	-1.750029	-1.011926
24	6	0	-5.730199	-1.632436	-0.628344
25	1	0	1.979746	1.016216	1.376091
26	1	0	-1.822273	-1.286506	-2.151913
27	1	0	-1.685325	-2.582981	-0.951096
28	1	0	-0.212978	3.493461	-1.809141
29	1	0	-1.220104	2.026703	-1.681550
30	1	0	-2.519815	2.863018	0.058516
31	1	0	-2.102559	4.441494	-0.640203
32	1	0	-0.238149	4.725224	0.933085
33	1	0	-1.466475	3.985664	1.973454

33	1	0	-1.466475	3.985664	1.973454
34	1	0	-0.470690	1.774983	1.726175
35	1	0	0.979320	2.802883	1.708851
36	1	0	2.137413	1.772426	-2.376936
37	1	0	1.772890	0.042699	-2.232939
38	1	0	0.485228	1.177471	-2.646805
39	1	0	4.931649	-2.591698	-1.001722
40	1	0	3.674840	-2.909053	-2.230789
41	1	0	4.642762	-1.401710	-2.301851
42	1	0	-1.812922	-0.762066	2.542564
43	1	0	-3.402772	-1.183992	3.240710
44	1	0	-3.223173	0.313722	2.279081
45	1	0	-6.299444	-2.236897	-1.336329
46	1	0	-5.874101	-2.015267	0.386465
47	1	0	-6.057470	-0.589892	-0.684213
48	1	0	4.602596	-2.105608	2.714668
49	1	0	2.896684	-1.557384	2.754646
50	1	0	3.454648	-2.616646	1.439602

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.333603	2.917678	-1.427474
2	6	0	-0.493842	3.607688	-0.060956
3	6	0	0.019565	2.549602	0.922436
4	7	0	1.061414	1.839080	0.154303
5	6	0	0.990403	2.152887	-1.287931
6	6	0	1.750333	0.835469	0.671216
7	6	0	2.723204	0.076345	-0.040021
8	6	0	3.626503	-0.734155	0.823659
9	8	0	4.742996	-1.269620	0.269811
10	6	0	5.068263	-1.075245	-1.113884
11	8	0	3.411232	-0.961035	2.000209
12	7	0	1.877224	-1.286944	-1.059116
13	7	0	0.803354	-1.575052	-0.577839
14	7	0	0.186957	-1.121573	0.450214
15	6	0	-1.117678	-1.731799	0.672108
16	15	0	-2.513177	-0.738029	0.000260
17	8	0	-2.819116	0.262315	1.237636
18	6	0	-3.936816	1.167863	1.144510
19	8	0	-3.812042	-1.716296	0.086223
20	6	0	-4.205020	-2.487925	-1.064519
21	8	0	-2.311600	-0.098684	-1.331555
22	1	0	1.628500	0.650442	1.732769
23	1	0	3.167394	0.558595	-0.903015
24	1	0	-1.190033	-2.729872	0.219874
25	1	0	-1.288745	-1.839438	1.748948
26	1	0	-0.765301	1.833012	1.195440
27	1	0	0.446502	2.970055	1.838428
28	1	0	0.129246	4.508715	-0.007774
29	1	0	-1.525880	3.899443	0.153219
30	1	0	-1.146291	2.202093	-1.590409
31	1	0	-0.314467	3.621637	-2.264393
32	1	0	1.853965	2.770320	-1.570768
33	1	0	1.014868	1.227647	-1.869587
34	1	0	-3.867221	1.833928	2.006102
35	1	0	-4.876377	0.609249	1.182550

36	1	0	-3.887895	1.749415	0.218844
37	1	0	-3.542128	-3.351233	-1.191849
38	1	0	-5.220539	-2.837958	-0.870268
39	1	0	-4.185043	-1.873325	-1.968003
40	1	0	5.937773	-1.709341	-1.296121
41	1	0	5.342586	-0.032457	-1.312947
42	1	0	4.244472	-1.382969	-1.761342

TS1'b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.995649	2.231842	1.113114
2	6	0	-0.175590	3.228036	1.126917
3	6	0	-0.119618	3.870484	-0.270340
4	6	0	0.247170	2.684184	-1.165447
5	7	0	1.148061	1.883762	-0.313115
6	6	0	1.787319	0.816632	-0.764958
7	6	0	2.607902	-0.031574	0.031882
8	6	0	3.546775	-0.890736	-0.737642
9	8	0	3.460254	-1.081282	-1.937035
10	8	0	4.548131	-1.517519	-0.068715
11	6	0	4.717279	-1.372691	1.347560
12	7	0	1.528371	-1.395328	0.883089
13	7	0	0.504910	-1.542975	0.257598
14	7	0	0.065858	-0.963570	-0.798083
15	6	0	-1.267364	-1.380271	-1.219124
16	15	0	-2.591046	-0.599508	-0.213246
17	8	0	-2.484573	0.875918	-0.006061
18	8	0	-2.686686	-1.450149	1.165306
19	6	0	-2.163337	-0.945728	2.407811
20	8	0	-3.889924	-1.132914	-1.012119
21	6	0	-5.209021	-0.834973	-0.514724
22	1	0	1.774083	0.655664	-1.836621
23	1	0	2.963089	0.380389	0.968737
24	1	0	-1.406460	-1.045931	-2.252110
25	1	0	-1.409205	-2.468644	-1.196317
26	1	0	0.755851	2.963489	-2.093084
27	1	0	-0.639496	2.081923	-1.398941
28	1	0	-1.068103	4.327092	-0.565605
29	1	0	0.661479	4.639339	-0.315516
30	1	0	-0.088667	3.952849	1.941448
31	1	0	-1.117332	2.681815	1.235394
32	1	0	0.800471	1.329213	1.699885
33	1	0	1.926612	2.686326	1.478600
34	1	0	-1.104369	-1.205505	2.497021
35	1	0	-2.729857	-1.432900	3.204278
36	1	0	-2.290587	0.137987	2.469657
37	1	0	-5.912023	-1.241089	-1.243663
38	1	0	-5.363730	-1.313403	0.456908
39	1	0	-5.349811	0.246481	-0.426342
40	1	0	5.523636	-2.059023	1.612422
41	1	0	5.021407	-0.352088	1.608876
42	1	0	3.807698	-1.648244	1.885938

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.392312	-1.234471	0.788393
2	7	0	3.396923	-0.644558	-0.131352
3	6	0	3.220023	-1.481978	-1.321085
4	6	0	4.503603	-2.316572	-1.368504
5	6	0	4.802492	-2.556670	0.117916
6	6	0	2.409141	0.209096	0.329599
7	6	0	2.822427	1.166892	1.430598
8	6	0	1.309235	0.521150	-0.519048
9	15	0	0.513731	2.131320	-0.551651
10	8	0	1.372575	3.315887	-0.848376
11	8	0	-0.287007	2.277170	0.857316
12	6	0	-0.410456	3.558949	1.502708
13	8	0	-0.616688	1.811448	-1.666928
14	6	0	-1.732604	2.709976	-1.836002
15	7	0	1.269272	-1.127323	1.678173
16	7	0	0.233599	-1.249116	1.113911
17	7	0	-0.278448	-0.595611	0.126356
18	6	0	-1.234207	-1.270496	-0.743380
19	15	0	-2.969665	-1.021335	-0.168097
20	8	0	-3.620090	0.260181	-0.561709
21	8	0	-2.962726	-1.302740	1.425271
22	6	0	-2.940642	-0.190553	2.347105
23	8	0	-3.629768	-2.378206	-0.744259
24	6	0	-5.046234	-2.596443	-0.583511
25	1	0	1.317143	0.100572	-1.519703
26	1	0	-1.158725	-0.784250	-1.720023
27	1	0	-1.032018	-2.341556	-0.858263
28	1	0	5.250988	-0.559129	0.904027
29	1	0	3.957546	-1.404181	1.778308
30	1	0	4.176801	-3.373736	0.496459
31	1	0	5.847153	-2.816140	0.314721
32	1	0	5.308760	-1.735193	-1.833495
33	1	0	4.377374	-3.240087	-1.941518
34	1	0	2.332064	-2.131240	-1.230993
35	1	0	3.094454	-0.864793	-2.218401
36	1	0	3.484447	1.941598	1.024346
37	1	0	1.944739	1.650373	1.860913
38	1	0	3.346681	0.652912	2.238139
39	1	0	-1.363973	4.018984	1.224006
40	1	0	-0.396976	3.374758	2.579385
41	1	0	0.413317	4.219333	1.221933
42	1	0	-2.966407	-0.629621	3.345956
43	1	0	-3.814955	0.446705	2.193022
44	1	0	-2.028252	0.397289	2.218926
45	1	0	-5.293490	-3.471769	-1.186089
46	1	0	-5.278478	-2.791774	0.467754
47	1	0	-5.611187	-1.728997	-0.936698
48	1	0	-2.147801	2.502474	-2.823655
49	1	0	-2.486497	2.497119	-1.075266
50	1	0	-1.404054	3.753649	-1.796447

TS2'a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.344871	0.326838	0.364170
2	6	0	2.150100	-0.602570	-0.364485
3	7	0	0.562091	-1.414563	-1.580975
4	7	0	-0.420821	-0.999702	-1.063163
5	7	0	-0.584939	-0.267622	-0.009232
6	7	0	2.630319	-1.724940	0.292366
7	6	0	2.074312	-2.178752	1.574460
8	6	0	2.785997	-3.512152	1.824327
9	6	0	2.926675	-4.090531	0.409237
10	6	0	3.216852	-2.854917	-0.459564
11	6	0	2.971081	-0.134297	-1.551799
12	6	0	-1.754981	0.603890	0.036060
13	15	0	-3.321747	-0.329711	0.245309
14	8	0	-3.650657	-0.995080	-1.193772
15	6	0	-3.520859	-2.413228	-1.419713
16	15	0	1.298224	2.071560	-0.055303
17	8	0	0.734390	2.475198	-1.376482
18	8	0	-4.333878	0.928516	0.263735
19	6	0	-5.752062	0.692086	0.365432
20	8	0	-3.391988	-1.275786	1.391807
21	8	0	2.802950	2.636675	0.199997
22	6	0	3.504764	3.422775	-0.781766
23	8	0	0.497185	2.609088	1.250407
24	6	0	0.298699	4.027053	1.401456
25	1	0	-1.830016	1.262131	-0.838741
26	1	0	-1.632811	1.228409	0.924039
27	1	0	-2.548639	-2.617752	-1.875506
28	1	0	-3.617814	-2.963912	-0.481138
29	1	0	-4.321106	-2.698695	-2.106198
30	1	0	-6.222789	1.673135	0.446312
31	1	0	-5.978510	0.096585	1.255101
32	1	0	-6.114922	0.179579	-0.530896
33	1	0	2.224609	-4.159761	2.504407
34	1	0	2.278345	-1.448947	2.367059
35	1	0	0.982603	-2.313846	1.516022
36	1	0	4.297012	-2.704072	-0.595378
37	1	0	2.760079	-2.945554	-1.450017
38	1	0	1.979946	-4.547836	0.097849
39	1	0	3.709400	-4.851006	0.325780
40	1	0	3.774378	-3.332169	2.264717
41	1	0	2.442211	0.648390	-2.099001
42	1	0	3.164471	-0.948896	-2.251991
43	1	0	3.937817	0.256397	-1.208564
44	1	0	1.231515	0.172610	1.430737
45	1	0	1.256836	4.526436	1.578567
46	1	0	-0.182947	4.446283	0.512790
47	1	0	-0.348904	4.157878	2.269810
48	1	0	3.779806	4.375490	-0.320013
49	1	0	2.878452	3.599987	-1.658901
50	1	0	4.410558	2.883148	-1.072318

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.897223	0.928965	0.182754
2	6	0	2.253997	0.845440	-0.215495

3	7	0	1.946717	0.081890	-2.177536
4	7	0	0.824260	-0.303972	-2.137661
5	7	0	-0.137991	-0.072206	-1.304645
6	7	0	3.146178	-0.030514	0.344013
7	6	0	4.548468	-0.038713	-0.085491
8	6	0	5.160709	-1.153307	0.767688
9	6	0	4.021966	-2.186379	0.838051
10	6	0	2.743282	-1.327278	0.902561
11	6	0	-1.048085	-1.191851	-1.057304
12	15	0	-2.491195	-0.701265	-0.042087
13	8	0	-3.348021	-2.080586	0.025898
14	6	0	-4.459950	-2.285712	-0.867770
15	6	0	0.213691	2.222256	-0.035527
16	8	0	0.560561	3.082587	-0.826006
17	8	0	-3.268917	0.487010	-0.479253
18	8	0	-1.830289	-0.676159	1.426791
19	6	0	-2.578250	-0.126252	2.530216
20	8	0	-0.871191	2.339937	0.764624
21	6	0	-1.688352	3.497918	0.529923
22	1	0	2.693533	1.742327	-0.641342
23	1	0	0.527572	0.325410	1.003069
24	1	0	-1.457364	-1.551196	-2.009745
25	1	0	-0.559623	-2.044643	-0.562203
26	1	0	4.633804	-0.266956	-1.159255
27	1	0	5.005887	0.942025	0.089584
28	1	0	5.396128	-0.772823	1.768842
29	1	0	6.079377	-1.558006	0.332707
30	1	0	4.015229	-2.793552	-0.074695
31	1	0	4.108224	-2.867415	1.689985
32	1	0	2.385610	-1.203346	1.934643
33	1	0	1.923783	-1.774553	0.322865
34	1	0	-1.903095	-0.130352	3.386886
35	1	0	-3.451076	-0.750569	2.744749
36	1	0	-2.889443	0.895797	2.304470
37	1	0	-4.103079	-2.614418	-1.850293
38	1	0	-5.072479	-3.072631	-0.424028
39	1	0	-5.044218	-1.368865	-0.975692
40	1	0	-2.449672	3.482647	1.310361
41	1	0	-2.159013	3.429511	-0.453784
42	1	0	-1.091641	4.411363	0.590925

TS2'b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.537800	-0.087187	-0.274384
2	7	0	-3.162059	-0.076479	0.234775
3	6	0	-2.802810	-1.355897	0.857996
4	6	0	-4.081099	-2.210061	0.740885
5	6	0	-5.206600	-1.173814	0.572402
6	6	0	-2.236090	0.791541	-0.279267
7	6	0	-0.911870	0.903070	0.228346
8	6	0	-0.263724	2.221775	0.009130
9	8	0	0.469691	2.772661	1.008914
10	6	0	0.431797	2.249954	2.349687
11	8	0	-0.362455	2.839520	-1.035718
12	7	0	0.216344	-0.178975	-1.135401
13	6	0	1.046152	-1.337475	-0.779342

14	15	0	2.545297	-0.784181	0.111109
15	8	0	2.308829	-0.196096	1.459946
16	7	0	-0.681945	-0.400684	-2.040956
17	7	0	-1.786759	0.008834	-2.178877
18	8	0	3.374552	0.145853	-0.911057
19	6	0	3.208575	1.584530	-0.924074
20	8	0	3.379580	-2.160006	0.057407
21	6	0	4.661858	-2.237886	0.715426
22	1	0	-2.653696	1.673982	-0.754473
23	1	0	-0.635143	0.327397	1.103240
24	1	0	0.511246	-2.064685	-0.149346
25	1	0	1.373572	-1.854693	-1.686825
26	1	0	-4.996392	0.900938	-0.152022
27	1	0	-4.563685	-0.343587	-1.344805
28	1	0	-6.100062	-1.586719	0.094911
29	1	0	-5.499029	-0.763160	1.546178
30	1	0	-4.223166	-2.865301	1.605329
31	1	0	-4.023079	-2.843274	-0.152011
32	1	0	-1.952756	-1.827237	0.345118
33	1	0	-2.509600	-1.200936	1.906413
34	1	0	3.109242	1.969256	0.092879
35	1	0	2.324147	1.848740	-1.508085
36	1	0	4.106734	1.988567	-1.394188
37	1	0	4.969655	-3.282978	0.662248
38	1	0	5.389416	-1.608531	0.194849
39	1	0	4.575166	-1.926689	1.760290
40	1	0	0.936208	3.001420	2.960344
41	1	0	-0.600737	2.141576	2.698375
42	1	0	0.971537	1.302997	2.411382

Pyrrolidine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.151290	-0.470341	0.174509
2	7	0	0.022906	-1.173756	-0.359921
3	6	0	1.171364	-0.423777	0.167482
4	6	0	0.756890	1.046517	-0.051007
5	6	0	-0.800667	1.012981	-0.060850
6	1	0	0.042695	-2.144809	-0.053084
7	1	0	2.090836	-0.695616	-0.363609
8	1	0	1.338904	-0.609881	1.245024
9	1	0	1.136602	1.414433	-1.009226
10	1	0	-1.243634	1.656546	0.705082
11	1	0	-1.297684	-0.652320	1.256088
12	1	0	-1.181930	1.345495	-1.031379
13	1	0	-2.064342	-0.785792	-0.342230
14	1	0	1.160433	1.695958	0.731974

Cartesian coordinates (optimized at the B3LYP(L1A1)/6-31G*) of all the stationary points discussed in the main text for the reaction between fulvenes and different dienophiles.

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.973147	-1.173038	-0.000001
2	6	0	2.257143	-0.732518	0.000000
3	6	0	2.257143	0.732518	0.000000
4	6	0	0.973147	1.173038	0.000001
5	6	0	0.082573	0.000000	0.000000
6	6	0	-1.278041	0.000000	0.000000
7	6	0	-2.097475	-1.262525	0.000001
8	6	0	-2.097475	1.262525	-0.000001
9	1	0	0.649139	-2.205528	-0.000001
10	1	0	3.147758	-1.351978	-0.000001
11	1	0	3.147758	1.351978	0.000001
12	1	0	0.649139	2.205528	0.000001
13	1	0	-2.757056	-1.288404	0.878299
14	1	0	-1.493262	-2.170579	-0.000003
15	1	0	-2.757063	-1.288400	-0.878292
16	1	0	-2.757056	1.288404	-0.878299
17	1	0	-1.493262	2.170579	0.000003
18	1	0	-2.757063	1.288400	0.878292

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.449443	-0.040417	0.447460
2	8	0	2.504368	0.284920	-0.588544
3	6	0	1.180608	0.088263	-0.443554
4	8	0	0.433738	0.443139	-1.338296
5	6	0	0.671446	-0.556392	0.799169
6	6	0	-0.632960	-0.812018	0.966982
7	6	0	-1.745769	-0.622275	-0.032328
8	8	0	-2.383906	0.561445	-0.097073
9	6	0	-1.840997	1.718047	0.563260
10	8	0	-2.159863	-1.568256	-0.663934
11	1	0	4.420010	0.261084	0.053685
12	1	0	3.460859	-1.115080	0.653788
13	1	0	3.245293	0.520826	1.364008
14	1	0	-2.607226	2.489051	0.470585
15	1	0	-0.925190	2.038659	0.063155
16	1	0	-1.648467	1.527177	1.622960
17	1	0	-0.953856	-1.304002	1.884107
18	1	0	1.363258	-0.838936	1.584563

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.668558	1.261667	-0.000008
2	6	0	-0.668557	1.261665	0.000012
3	6	0	-1.133575	-0.153655	0.000016
4	8	0	0.000001	-0.970818	0.000042
5	6	0	1.133572	-0.153657	0.000001

6	8	0	2.242841	-0.607758	-0.000023
7	8	0	-2.242842	-0.607758	-0.000036
8	1	0	1.356664	2.097282	-0.000019
9	1	0	-1.356664	2.097278	0.000030

10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651392	0.284644	2.066471
2	6	0	-0.665044	-1.045259	1.906272
3	6	0	-0.951348	0.909770	0.712819
4	6	0	-0.981699	-1.330275	0.445210
5	6	0	0.327759	0.651244	-0.218555
6	6	0	0.276041	-0.913274	-0.408025
7	6	0	-1.885366	-0.143237	0.131130
8	6	0	-3.076859	-0.047865	-0.466885
9	6	0	-3.829972	-1.254905	-0.975324
10	6	0	-3.789468	1.267634	-0.675317
11	6	0	1.596691	1.205614	0.402896
12	8	0	2.363381	0.542132	1.065002
13	8	0	1.867510	2.529491	0.254148
14	6	0	1.099550	3.389164	-0.598101
15	6	0	1.497565	-1.777603	-0.084766
16	8	0	1.506300	-2.596676	0.804587
17	8	0	2.562181	-1.755674	-0.932690
18	6	0	2.687562	-0.814892	-1.997909
19	1	0	-0.369594	0.842854	2.952680
20	1	0	-0.398515	-1.803881	2.630566
21	1	0	-1.279256	1.949162	0.717150
22	1	0	-1.332855	-2.335426	0.214307
23	1	0	0.141165	1.134548	-1.180980
24	1	0	0.030016	-1.099082	-1.460793
25	1	0	-4.802642	-1.344249	-0.472572
26	1	0	-3.286137	-2.190948	-0.824416
27	1	0	-4.044927	-1.155356	-2.047869
28	1	0	-4.763746	1.265199	-0.168276
29	1	0	-3.996611	1.434038	-1.740945
30	1	0	-3.223807	2.126002	-0.304207
31	1	0	1.538279	4.380547	-0.476889
32	1	0	0.046594	3.426630	-0.305760
33	1	0	1.181934	3.090009	-1.648566
34	1	0	3.512886	-1.178565	-2.613350
35	1	0	2.941687	0.179730	-1.619719
36	1	0	1.786424	-0.759949	-2.618223

11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.985657	-0.560122	-2.067877
2	6	0	-1.461668	0.686634	-2.138466
3	6	0	-1.480291	-1.217430	-0.775349
4	6	0	-2.309377	0.998707	-0.908600
5	6	0	-2.766009	-0.415864	-0.550794

6	6	0	-3.981107	-0.855490	-0.194444
7	6	0	-5.183475	0.049759	-0.045966
8	6	0	-4.283219	-2.308731	0.093678
9	6	0	-0.574797	-0.801431	0.370994
10	6	0	-1.430555	1.591715	0.273456
11	6	0	-0.530172	0.477598	0.792751
12	6	0	-2.367124	2.038187	1.420534
13	6	0	-0.635060	2.819566	-0.212951
14	6	0	0.369907	-1.619964	1.241185
15	6	0	0.494185	0.527700	1.922493
16	6	0	0.225902	-0.848837	2.578300
17	6	0	1.859749	-1.262610	0.909543
18	6	0	1.949445	0.254396	1.339847
19	6	0	2.397408	1.316907	0.356332
20	8	0	2.801175	2.407923	0.703562
21	8	0	2.303523	0.935651	-0.932171
22	6	0	2.773579	1.881827	-1.907219
23	6	0	2.284478	-1.714720	-0.483144
24	8	0	1.512115	-2.151517	-1.304853
25	8	0	3.610929	-1.741634	-0.786164
26	6	0	4.616083	-1.336131	0.143221
27	1	0	-0.290546	-1.043453	-2.743358
28	1	0	-1.237597	1.414097	-2.912989
29	1	0	-1.593424	-2.300848	-0.844275
30	1	0	-3.124432	1.700637	-1.114118
31	1	0	-5.568963	0.025912	0.983605
32	1	0	-6.005805	-0.291566	-0.691188
33	1	0	-4.972366	1.091852	-0.295813
34	1	0	-4.659191	-2.431574	1.119609
35	1	0	-3.414180	-2.960549	-0.020397
36	1	0	-5.074815	-2.683064	-0.571473
37	1	0	-1.792564	2.426140	2.269982
38	1	0	-2.980062	1.204313	1.776005
39	1	0	-3.036221	2.839982	1.082771
40	1	0	-0.020320	3.240963	0.590081
41	1	0	-1.319741	3.605946	-0.555855
42	1	0	0.027797	2.562582	-1.043032
43	1	0	0.186785	-2.696724	1.254419
44	1	0	0.478504	1.407405	2.569130
45	1	0	0.963833	-1.131750	3.340993
46	1	0	-0.780685	-0.919083	2.999087
47	1	0	2.491953	-1.822616	1.610816
48	1	0	2.649399	0.353398	2.175240
49	1	0	2.664382	1.382209	-2.869441
50	1	0	2.175443	2.795410	-1.873106
51	1	0	3.819953	2.134443	-1.717287
52	1	0	5.563559	-1.452763	-0.385852
53	1	0	4.628166	-1.974702	1.034033
54	1	0	4.505854	-0.289973	0.444288

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.016761	-0.796541	-0.400298
2	6	0	-0.830107	-1.702324	-0.976002
3	6	0	0.510381	-1.074162	-0.604850
4	6	0	0.597093	0.075829	-1.300609

5	6	0	-0.644679	0.199135	-2.173424
6	6	0	-1.892460	0.506464	-1.277933
7	6	0	1.611103	-1.629286	0.291558
8	6	0	2.857626	-0.649562	0.188064
9	6	0	2.359465	0.793656	0.217537
10	6	0	1.826488	0.963356	-1.206818
11	6	0	3.506235	-0.672278	-1.193944
12	6	0	2.940231	0.246524	-1.983705
13	6	0	-0.911857	-1.298254	-2.467291
14	6	0	2.427265	1.696395	1.204960
15	6	0	1.897826	3.106248	1.082116
16	6	0	1.169994	-1.713133	1.767810
17	6	0	2.004969	-3.044990	-0.187706
18	6	0	-1.818100	1.890012	-0.633368
19	8	0	-2.931091	2.415666	-0.058999
20	6	0	-4.134447	1.672672	0.132574
21	6	0	-1.925736	-0.582099	1.097263
22	8	0	-2.407975	-1.546262	1.925186
23	6	0	-3.143964	-2.681770	1.449535
24	6	0	3.034772	1.397153	2.557416
25	8	0	-0.854260	2.612974	-0.749586
26	8	0	-1.413015	0.393244	1.600266
27	1	0	3.149621	0.417156	-3.036003
28	1	0	4.274941	-1.381480	-1.486296
29	1	0	1.624610	1.986930	-1.520716
30	1	0	3.558979	-0.909880	0.987969
31	1	0	3.807148	2.140668	2.805790
32	1	0	3.491278	0.406509	2.619379
33	1	0	2.274281	1.462534	3.348523
34	1	0	2.714336	3.840026	1.172007
35	1	0	1.194529	3.316893	1.899466
36	1	0	1.359465	3.285228	0.151683
37	1	0	0.290041	-2.356412	1.882681
38	1	0	0.914103	-0.728523	2.165482
39	1	0	1.973203	-2.145567	2.378673
40	1	0	1.179510	-3.752441	-0.048243
41	1	0	2.857898	-3.422764	0.390538
42	1	0	2.280007	-3.052688	-1.247300
43	1	0	-0.560958	0.875484	-3.026598
44	1	0	-0.957063	-2.761920	-0.744383
45	1	0	-0.120407	-1.759846	-3.063630
46	1	0	-1.885881	-1.499055	-2.932627
47	1	0	-2.769837	0.531725	-1.937661
48	1	0	-2.958945	-1.297964	-0.639413
49	1	0	-4.031359	0.954421	0.951041
50	1	0	-4.458558	1.159113	-0.779016
51	1	0	-4.891631	2.410196	0.405467
52	1	0	-4.093897	-2.380158	0.995278
53	1	0	-2.566302	-3.279257	0.739185
54	1	0	-3.350414	-3.282180	2.336468

13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.320230	-0.948536	1.905537
2	6	0	0.236892	-1.377066	0.553965
3	6	0	1.269802	-0.277319	0.325264

4	6	0	0.545285	0.959743	0.845654
5	6	0	-0.135141	0.365119	2.074721
6	6	0	-0.838958	-1.185615	-0.572495
7	6	0	-1.426022	0.218915	-0.490935
8	6	0	-0.544047	1.424984	-0.219734
9	6	0	-2.773963	0.112260	-0.495887
10	6	0	-3.162245	-1.302320	-0.567081
11	6	0	-2.056545	-2.074254	-0.572324
12	6	0	-1.357201	2.599390	0.353357
13	6	0	0.157108	1.900569	-1.512107
14	6	0	2.515670	-0.391514	-0.158849
15	6	0	3.110142	-1.705016	-0.614935
16	6	0	3.467023	0.775622	-0.293809
17	1	0	-0.844306	-1.619282	2.578989
18	1	0	0.629847	-2.397259	0.537713
19	1	0	-0.478188	0.955470	2.918828
20	1	0	1.196325	1.809924	1.072126
21	1	0	3.756213	0.924665	-1.343746
22	1	0	4.397032	0.580028	0.258303
23	1	0	3.051564	1.716803	0.072267
24	1	0	3.417168	-1.645961	-1.668758
25	1	0	2.424528	-2.549642	-0.516536
26	1	0	4.018503	-1.940704	-0.042626
27	1	0	-0.585387	2.233973	-2.246039
28	1	0	0.751340	1.104038	-1.968141
29	1	0	0.826404	2.744531	-1.301196
30	1	0	-2.096870	2.956050	-0.372935
31	1	0	-0.696766	3.442613	0.590168
32	1	0	-1.891589	2.313863	1.264910
33	1	0	-2.014823	-3.155819	-0.645443
34	1	0	-4.190021	-1.650876	-0.606073
35	1	0	-3.483528	0.928917	-0.412063
36	1	0	-0.312847	-1.321093	-1.531801

14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.070854	-0.506969	2.305610
2	6	0	0.357295	-1.220835	0.981800
3	6	0	-0.928276	-1.203243	0.185484
4	6	0	-1.802189	-2.177371	-0.134073
5	6	0	-2.957284	-1.573818	-0.891111
6	6	0	1.287678	-0.200145	0.321964
7	6	0	2.406063	-0.428323	-0.381664
8	6	0	2.918993	-1.816247	-0.691266
9	6	0	0.643248	1.127372	0.717804
10	6	0	-0.616979	1.397455	-0.202223
11	6	0	-1.485481	2.519185	0.403019
12	6	0	0.226070	0.810600	2.149568
13	6	0	3.280370	0.673635	-0.935598
14	6	0	-1.418761	0.100911	-0.336408
15	6	0	-2.599239	-0.110522	-0.956718
16	6	0	-0.132760	1.843918	-1.599723
17	1	0	-0.294890	-1.021075	3.189172
18	1	0	0.761293	-2.229310	1.097085
19	1	0	0.028039	1.570627	2.899018
20	1	0	1.310509	1.993004	0.649752

21	1	0	3.326392	0.623414	-2.032722
22	1	0	4.313304	0.560938	-0.577134
23	1	0	2.937996	1.674277	-0.663817
24	1	0	3.010424	-1.959289	-1.777139
25	1	0	2.275373	-2.610587	-0.307611
26	1	0	3.925496	-1.963075	-0.274172
27	1	0	-0.986548	2.038078	-2.257998
28	1	0	0.485736	1.073651	-2.069804
29	1	0	0.457532	2.766965	-1.529797
30	1	0	-2.322192	2.762878	-0.261141
31	1	0	-0.894520	3.433762	0.543532
32	1	0	-1.903724	2.226529	1.370884
33	1	0	-1.721425	-3.230238	0.114044
34	1	0	-3.917833	-1.742185	-0.378816
35	1	0	-3.073264	-2.011406	-1.895266
36	1	0	-3.215309	0.629425	-1.456850

16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.029669	1.154063	-0.398364
2	6	0	-0.598352	0.772143	-0.717704
3	6	0	-0.598352	-0.772142	-0.717705
4	6	0	-2.029669	-1.154063	-0.398365
5	8	0	-2.792541	0.000000	-0.220934
6	6	0	0.462978	1.134536	0.403712
7	6	0	-0.119647	0.670649	1.733623
8	6	0	-0.119647	-0.670653	1.733622
9	6	0	0.462978	-1.134537	0.403711
10	6	0	1.455571	0.000000	0.140774
11	6	0	2.745199	0.000000	-0.209381
12	6	0	3.534716	-1.270948	-0.414262
13	8	0	-2.524310	-2.240680	-0.289205
14	8	0	-2.524312	2.240680	-0.289204
15	6	0	3.534715	1.270949	-0.414261
16	1	0	0.809662	2.165345	0.354692
17	1	0	-0.524714	1.333092	2.491070
18	1	0	-0.524711	-1.333096	2.491069
19	1	0	0.809662	-2.165345	0.354687
20	1	0	-0.305571	-1.222095	-1.670134
21	1	0	-0.305571	1.222097	-1.670132
22	1	0	4.380332	1.315944	0.284612
23	1	0	2.936715	2.175055	-0.275355
24	1	0	3.965768	1.299709	-1.423708
25	1	0	3.965747	-1.299719	-1.423718
26	1	0	2.936723	-2.175054	-0.275332
27	1	0	4.380347	-1.315931	0.284593

17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.366329	0.931133	-0.783724
2	6	0	-2.980318	-0.420114	-0.493451

3	6	0	-2.317661	-1.100335	0.445811
4	6	0	-1.144551	-0.312779	0.984126
5	6	0	-1.129275	0.928323	0.100365
6	6	0	-0.115989	1.802034	0.166572
7	6	0	-0.007431	3.063792	-0.644335
8	6	0	1.008065	1.477407	1.133856
9	6	0	0.249822	-1.021873	1.021680
10	6	0	1.417622	-0.009790	1.023528
11	6	0	0.511862	-1.886602	-0.202313
12	8	0	1.579735	-1.370105	-0.933029
13	6	0	2.120941	-0.257905	-0.307173
14	8	0	3.019136	0.359779	-0.807049
15	8	0	-0.049932	-2.882351	-0.560244
16	1	0	-3.057828	1.748592	-0.527140
17	1	0	-2.127522	1.061711	-1.849399
18	1	0	-3.879274	-0.767898	-0.993689
19	1	0	-2.584923	-2.083187	0.818985
20	1	0	-1.337180	-0.027064	2.032070
21	1	0	0.041627	3.946032	0.008583
22	1	0	-0.857737	3.196441	-1.319212
23	1	0	0.913399	3.065055	-1.243561
24	1	0	0.705919	1.683523	2.170469
25	1	0	1.891262	2.092329	0.933816
26	1	0	0.277383	-1.688856	1.889538
27	1	0	2.142827	-0.245020	1.812468

18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.863944	-1.132948	-0.216417
2	6	0	-2.281766	-0.642992	-0.119188
3	6	0	-2.270442	0.683368	0.135235
4	6	0	-0.889366	1.150204	0.218379
5	6	0	-0.030445	0.116745	0.003384
6	6	0	1.438488	0.137229	-0.015268
7	6	0	2.149482	-1.171634	0.253992
8	6	0	2.136920	1.258540	-0.267433
9	1	0	-0.655295	-1.601143	-1.190543
10	1	0	-0.650343	-1.905581	0.537693
11	1	0	-3.151393	-1.280066	-0.231372
12	1	0	-3.139485	1.319626	0.269356
13	1	0	-0.602818	2.172346	0.443650
14	1	0	3.235593	-1.046488	0.221561
15	1	0	1.877426	-1.933975	-0.487564
16	1	0	1.881347	-1.578301	1.237736
17	1	0	3.223147	1.264391	-0.247629
18	1	0	1.648265	2.198125	-0.508986

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.857145	1.764350	-0.883598
2	6	0	1.118813	0.852133	0.244856

3	6	0	0.109043	1.073067	1.182775
4	6	0	-0.811443	2.007999	0.635796
5	6	0	-0.275222	2.489954	-0.612693
6	6	0	2.263320	-0.041413	0.397852
7	6	0	2.400796	-0.765975	1.720518
8	6	0	3.165272	-0.242275	-0.587461
9	8	0	-1.037242	-1.561837	0.285971
10	6	0	-0.532042	-1.266172	-0.926449
11	6	0	-1.217861	-0.241529	-1.576860
12	6	0	-2.157028	0.230114	-0.672147
13	6	0	-2.117833	-0.625586	0.503417
14	8	0	0.431807	-2.011222	-1.406997
15	8	0	-2.779761	-0.724896	1.510334
16	1	0	1.482034	1.855895	-1.764382
17	1	0	-0.741941	3.228920	-1.253837
18	1	0	-1.675365	2.413250	1.151198
19	1	0	-0.001268	0.575834	2.138187
20	1	0	0.756547	-2.644545	-0.737548
21	1	0	4.011261	-0.910108	-0.449106
22	1	0	3.092779	0.253172	-1.551112
23	1	0	3.273014	-1.425946	1.723600
24	1	0	2.504948	-0.054967	2.549579
25	1	0	1.510270	-1.370372	1.934179
26	1	0	-0.996059	0.114298	-2.570408
27	1	0	-2.952394	0.940196	-0.840843

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.069586	-0.160719	0.082385
2	6	0	-1.220417	0.954784	0.700731
3	6	0	-0.994452	0.360901	2.087193
4	6	0	-0.937004	-0.984731	1.949848
5	6	0	-1.129034	-1.306228	0.469689
6	6	0	0.477417	0.663767	-0.315473
7	6	0	0.534976	-0.884598	-0.478356
8	6	0	1.651787	1.301186	0.358180
9	8	0	1.924106	2.640107	0.181501
10	6	0	1.123331	3.399208	-0.710443
11	6	0	1.685647	-1.705689	0.022267
12	8	0	2.820274	-1.866561	-0.740394
13	6	0	2.946030	-1.115331	-1.937214
14	6	0	-3.246976	-0.143555	-0.538199
15	6	0	-4.010569	1.105877	-0.783279
16	6	0	-3.910015	-1.375565	-1.035581
17	8	0	2.481377	0.771906	1.096298
18	8	0	1.725439	-2.385810	1.046279
19	1	0	-0.887403	0.974409	2.977841
20	1	0	-0.740993	-1.757504	2.690386
21	1	0	-1.606574	1.988513	0.666524
22	1	0	-1.423760	-2.342904	0.229783
23	1	0	0.364152	1.111879	-1.339921
24	1	0	0.389528	-1.139314	-1.564868
25	1	0	-4.897408	-1.505996	-0.525439
26	1	0	-3.293720	-2.287725	-0.847497
27	1	0	-4.093612	-1.292543	-2.136111
28	1	0	-5.002020	1.050506	-0.267148

29	1	0	-4.194460	1.232150	-1.879661
30	1	0	-3.470081	2.008516	-0.409119
31	1	0	1.506056	4.444910	-0.585041
32	1	0	0.043492	3.344468	-0.432237
33	1	0	1.276951	3.054221	-1.762459
34	1	0	4.003063	-1.297800	-2.259299
35	1	0	2.778922	-0.026672	-1.745876
36	1	0	2.231478	-1.492102	-2.709807

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.401365	-0.705824	2.038901
2	6	0	0.375389	-1.276047	1.012972
3	6	0	1.302781	-0.254710	0.533904
4	6	0	0.687070	1.026433	0.991515
5	6	0	-0.136326	0.660633	2.098627
6	6	0	2.499314	-0.447281	-0.078295
7	6	0	3.025421	-1.817034	-0.422499
8	6	0	3.439484	0.675284	-0.430239
9	6	0	-1.024534	-1.124656	-1.107108
10	6	0	-2.089926	-2.019608	-0.969955
11	6	0	-3.126043	-1.348784	-0.289251
12	6	0	-2.723701	-0.027687	-0.012002
13	6	0	-1.441350	0.177779	-0.563123
14	6	0	-0.639789	1.367690	-0.479560
15	6	0	0.278975	1.672723	-1.659619
16	6	0	-1.348220	2.630648	0.001780
17	1	0	-1.104444	-1.245580	2.660971
18	1	0	0.462495	-2.336167	0.826570
19	1	0	-0.606089	1.360925	2.780540
20	1	0	1.243057	1.958793	0.990746
21	1	0	3.654373	0.676862	-1.507781
22	1	0	4.405212	0.533640	0.074478
23	1	0	3.059177	1.661048	-0.159178
24	1	0	3.292776	-1.865394	-1.487098
25	1	0	2.316901	-2.620466	-0.213206
26	1	0	3.949169	-2.026768	0.134508
27	1	0	-0.326829	2.048487	-2.495146
28	1	0	0.818709	0.792771	-2.013579
29	1	0	1.008256	2.452113	-1.410976
30	1	0	-2.032294	2.993422	-0.776922
31	1	0	-0.628823	3.431784	0.206544
32	1	0	-1.934980	2.459681	0.907329
33	1	0	-2.104640	-3.049461	-1.308458
34	1	0	-4.086296	-1.779354	-0.020032
35	1	0	-3.326107	0.716843	0.493846
36	1	0	-0.122716	-1.300518	-1.679452

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.377519	0.380224	1.213132

2	6	0	-0.024712	0.775112	2.174644
3	6	0	-0.756343	0.597185	1.011157
4	6	0	-0.612093	-0.759196	0.602241
5	6	0	0.258651	-1.429193	1.491529
6	6	0	2.172024	-1.000624	1.016689
7	6	0	-1.666826	1.606616	0.306679
8	6	0	-2.315601	0.904742	-0.955193
9	6	0	-2.686665	-0.535620	-0.602058
10	6	0	-1.322532	-1.234759	-0.644945
11	6	0	-1.280090	0.649334	-2.042457
12	6	0	-0.709275	-0.545383	-1.868185
13	6	0	0.274206	-0.577943	2.753993
14	6	0	-3.891947	-1.074825	-0.368525
15	6	0	-4.096015	-2.539024	-0.052417
16	6	0	-2.792893	2.010997	1.286157
17	6	0	-0.894691	2.874223	-0.105468
18	6	0	2.414293	-1.734544	-0.291328
19	8	0	3.706710	-1.887718	-0.685602
20	6	0	4.805374	-1.270348	-0.009631
21	6	0	2.482004	1.393576	0.172305
22	8	0	2.285868	0.875673	-1.080314
23	6	0	2.480510	1.787436	-2.164443
24	6	0	-5.178451	-0.281512	-0.406828
25	8	0	2.760143	2.568526	0.352816
26	8	0	1.565322	-2.296968	-0.943305
27	1	0	0.112543	-0.978658	-2.423077
28	1	0	-1.016994	1.378848	-2.802325
29	1	0	-1.336243	-2.322446	-0.718403
30	1	0	-3.155694	1.518994	-1.295096
31	1	0	-5.688301	-0.317882	0.566196
32	1	0	-5.876153	-0.714779	-1.137261
33	1	0	-5.030799	0.769258	-0.664786
34	1	0	-4.585936	-2.659270	0.924000
35	1	0	-3.165749	-3.110595	-0.030571
36	1	0	-4.762184	-3.006508	-0.791220
37	1	0	-2.380848	2.492925	2.179756
38	1	0	-3.373410	1.141058	1.608211
39	1	0	-3.477015	2.723418	0.808577
40	1	0	-0.475304	3.383199	0.769099
41	1	0	-1.564987	3.579267	-0.613589
42	1	0	-0.065893	2.640633	-0.776904
43	1	0	0.287700	-2.514559	1.529787
44	1	0	0.055973	1.699464	2.736448
45	1	0	1.171793	-0.645336	3.372632
46	1	0	-0.580542	-0.878085	3.382146
47	1	0	2.557799	-1.610910	1.836172
48	1	0	2.693330	0.738849	2.184987
49	1	0	2.352439	1.195955	-3.072052
50	1	0	1.747260	2.598310	-2.133209
51	1	0	3.483005	2.223823	-2.128348
52	1	0	5.697623	-1.681906	-0.486102
53	1	0	4.822228	-1.513313	1.057496
54	1	0	4.791336	-0.184714	-0.133590

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.234754	1.079278	-0.245366
2	6	0	-0.239047	2.212102	-1.209761
3	6	0	-1.020316	1.191550	-0.715552
4	6	0	-0.628636	-0.021594	-1.371118
5	6	0	0.465258	0.229349	-2.232812
6	6	0	2.172095	0.078801	-1.234691
7	6	0	-2.166163	1.270241	0.297488
8	6	0	-2.937973	-0.112587	0.277268
9	6	0	-1.926075	-1.253482	0.305580
10	6	0	-1.432281	-1.280904	-1.142262
11	6	0	-3.595911	-0.366421	-1.075133
12	6	0	-2.757544	-1.029533	-1.878654
13	6	0	0.484004	1.739276	-2.435455
14	6	0	-1.591326	-2.066172	1.316094
15	6	0	-0.548467	-3.151647	1.205182
16	6	0	-1.624554	1.530327	1.718833
17	6	0	-3.126996	2.415384	-0.087628
18	6	0	2.271916	-1.417767	-0.946722
19	8	0	3.389877	-1.882556	-0.338487
20	6	0	4.390943	-1.056881	0.262760
21	6	0	1.755100	0.795087	1.085327
22	8	0	1.826698	1.749703	2.064401
23	6	0	2.342486	3.046663	1.776203
24	6	0	-2.197671	-1.954167	2.696238
25	8	0	1.500223	-2.244468	-1.381174
26	8	0	1.281796	-0.294543	1.400804
27	1	0	-2.916865	-1.286215	-2.921646
28	1	0	-4.583396	-0.003833	-1.344154
29	1	0	-0.890681	-2.170957	-1.453646
30	1	0	-3.653060	-0.112163	1.106028
31	1	0	-2.588130	-2.927968	3.025114
32	1	0	-3.010556	-1.226997	2.759129
33	1	0	-1.430138	-1.660846	3.425685
34	1	0	-0.976163	-4.128593	1.475914
35	1	0	0.267015	-2.948739	1.911363
36	1	0	-0.097380	-3.226255	0.215511
37	1	0	-1.091203	2.486556	1.761128
38	1	0	-0.932356	0.748354	2.037370
39	1	0	-2.457021	1.583186	2.432136
40	1	0	-2.632211	3.389371	-0.003197
41	1	0	-3.993505	2.428174	0.585370
42	1	0	-3.492555	2.312661	-1.114498
43	1	0	0.678374	-0.454393	-3.048872
44	1	0	-0.294544	3.255075	-0.915636
45	1	0	-0.138521	1.973952	-3.314988
46	1	0	1.463951	2.190827	-2.607645
47	1	0	2.784195	0.301524	-2.112283
48	1	0	2.660387	2.041501	-0.495421
49	1	0	4.033236	-0.645955	1.209224
50	1	0	4.713030	-0.245807	-0.395930
51	1	0	5.232785	-1.727676	0.449574
52	1	0	3.395912	3.007447	1.473689
53	1	0	1.758473	3.548029	0.995670
54	1	0	2.260615	3.613217	2.705748

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.027864	-0.237070	-0.136887
2	6	0	0.916532	-1.260129	0.210229
3	6	0	2.213642	-0.698367	0.243883
4	6	0	2.179866	0.647449	-0.147288
5	6	0	0.830006	0.997466	-0.434350
6	6	0	-1.346988	0.015819	0.030573
7	6	0	-1.577799	1.339892	0.507326
8	6	0	-2.448302	-0.947543	-0.304117
9	1	0	0.644015	-2.234921	0.599588
10	1	0	3.108896	-1.241446	0.534728
11	1	0	3.049978	1.259193	-0.358915
12	1	0	0.642726	1.508516	-1.385185
13	1	0	-2.900318	-1.359169	0.608454
14	1	0	-2.095497	-1.778733	-0.920941
15	1	0	-3.253764	-0.427915	-0.838850
16	1	0	-2.549992	1.807079	0.327064
17	1	0	-0.218434	1.751236	0.113673
18	1	0	-1.196536	1.571055	1.504169

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.733281	-0.916977	0.088786
2	6	0	2.341840	-0.178092	1.179589
3	6	0	3.374198	0.574827	0.670989
4	6	0	3.472331	0.310696	-0.753644
5	6	0	2.489693	-0.586499	-1.100381
6	6	0	0.616313	-1.776135	0.176957
7	6	0	-0.085944	-2.226876	-0.941166
8	6	0	0.093605	-2.158633	1.548895
9	6	0	0.236141	1.948923	-1.336871
10	6	0	-0.593932	1.701049	-0.115485
11	6	0	-0.244183	2.579333	1.052266
12	6	0	-1.645027	0.815846	-0.087693
13	6	0	-2.574806	0.599384	0.981190
14	6	0	-3.596374	-0.245989	0.547556
15	6	0	-3.352696	-0.623273	-0.777483
16	6	0	-2.069531	-0.115172	-1.197157
17	1	0	-2.505900	1.028479	1.972833
18	1	0	-4.449152	-0.552484	1.142810
19	1	0	-3.989098	-1.263350	-1.378144
20	1	0	-1.944334	0.192932	-2.236446
21	1	0	0.806593	2.407795	1.320607
22	1	0	-0.863036	2.407690	1.934261
23	1	0	-0.332625	3.637887	0.771811
24	1	0	0.004754	1.274483	-2.162180
25	1	0	1.304325	1.845921	-1.102983
26	1	0	0.079540	2.983252	-1.677949
27	1	0	2.015809	-0.204200	2.212703
28	1	0	4.022411	1.240330	1.231925
29	1	0	4.215618	0.737715	-1.419650
30	1	0	2.316527	-0.996522	-2.088526
31	1	0	-0.117516	-1.274765	2.159326
32	1	0	0.838884	-2.752499	2.092205
33	1	0	-0.826325	-2.745811	1.478238
34	1	0	-0.807799	-3.034288	-0.834286

35	1	0	0.326633	-2.094604	-1.938444
36	1	0	-1.264755	-1.052439	-1.096200

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.460181	-1.905644	-0.251960
2	6	0	2.470319	-0.698302	0.530394
3	6	0	1.913125	0.365999	-0.285442
4	6	0	1.456098	-0.238417	-1.454114
5	6	0	1.788952	-1.636281	-1.429832
6	6	0	1.783824	1.776762	0.081067
7	6	0	1.324605	2.725739	-1.007251
8	6	0	2.054877	2.252403	1.314096
9	6	0	-1.853124	1.012733	0.874266
10	6	0	-2.912306	1.746494	0.104885
11	6	0	-3.473995	0.911826	-0.805277
12	6	0	-2.835606	-0.382387	-0.720043
13	6	0	-1.855819	-0.370833	0.251259
14	6	0	-1.027568	-1.457913	0.654387
15	6	0	-0.065290	-1.315612	1.696664
16	6	0	-1.223491	-2.820001	0.036234
17	1	0	-3.101259	-1.230611	-1.340635
18	1	0	-4.276278	1.155722	-1.492896
19	1	0	-3.179760	2.781703	0.283357
20	1	0	-2.111722	0.970506	1.943292
21	1	0	-0.328272	-3.433073	0.160435
22	1	0	-1.456104	-2.768915	-1.030365
23	1	0	-2.059467	-3.336381	0.531272
24	1	0	1.036477	-1.045858	1.189306
25	1	0	-0.212831	-0.475393	2.377533
26	1	0	0.177658	-2.240882	2.224870
27	1	0	0.926802	0.256715	-2.260443
28	1	0	1.556781	-2.346968	-2.215959
29	1	0	2.840923	-2.866864	0.075397
30	1	0	3.077120	-0.543026	1.417551
31	1	0	1.993798	2.682921	-1.875569
32	1	0	1.292251	3.758363	-0.646482
33	1	0	0.322242	2.463222	-1.369389
34	1	0	1.966085	3.310555	1.543936
35	1	0	2.377988	1.606764	2.126039
36	1	0	-0.871128	1.502097	0.822750

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.196826	0.559985	-0.732864
2	6	0	-5.360169	-0.054010	-0.278734
3	6	0	-5.006681	-0.930806	0.800561
4	6	0	-3.632778	-0.846860	0.996295
5	6	0	-3.084586	0.086936	0.050385
6	6	0	-1.731345	0.553661	-0.037284
7	6	0	-1.448872	1.694459	-0.998097

8	6	0	-0.638746	0.067255	0.688440
9	8	0	1.401550	-1.096800	-0.706358
10	6	0	2.561588	-0.683806	-0.407499
11	6	0	3.818161	-1.229810	-0.958828
12	6	0	4.842205	-0.550681	-0.417282
13	6	0	4.314413	0.473097	0.513609
14	8	0	2.763494	0.287516	0.435008
15	8	0	4.730668	1.303718	1.222272
16	1	0	-4.126501	1.271457	-1.549816
17	1	0	-6.365341	0.095131	-0.683047
18	1	0	-5.695121	-1.560105	1.367845
19	1	0	-3.059173	-1.377102	1.748792
20	1	0	3.859383	-2.040605	-1.674731
21	1	0	5.911755	-0.666072	-0.577886
22	1	0	-1.629775	1.381345	-2.033964
23	1	0	-2.105060	2.550552	-0.800369
24	1	0	-0.411681	2.031529	-0.930938
25	1	0	-0.809179	-0.680283	1.462995
26	1	0	0.135393	0.797698	0.935169
27	1	0	0.511423	-0.595528	-0.183639

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.633047	-1.608460	-0.057583
2	6	0	-1.905586	-0.229114	0.387211
3	6	0	-0.911430	0.100018	1.302674
4	6	0	-0.044873	-1.019197	1.461368
5	6	0	-0.553565	-2.096166	0.685367
6	6	0	-2.982784	0.635827	-0.083992
7	6	0	-3.021530	2.046860	0.460302
8	6	0	-3.915423	0.217254	-0.962017
9	8	0	0.220961	-0.336995	-1.534839
10	6	0	1.256589	-0.221150	-0.794724
11	6	0	2.241056	-1.210318	-0.397451
12	6	0	3.323772	-0.540977	0.072527
13	6	0	3.042402	0.890563	0.004023
14	8	0	1.728935	1.018386	-0.565398
15	8	0	3.665703	1.870230	0.309735
16	1	0	-2.292003	-2.208451	-0.675068
17	1	0	-0.145745	-3.098800	0.636544
18	1	0	0.788885	-1.079115	2.150756
19	1	0	-0.777531	1.061967	1.780640
20	1	0	-0.518617	-1.001483	-1.102721
21	1	0	-4.708752	0.878664	-1.298080
22	1	0	-3.922431	-0.787789	-1.371552
23	1	0	-3.103799	2.047354	1.554464
24	1	0	-2.103371	2.591831	0.207286
25	1	0	-3.872474	2.602136	0.054825
26	1	0	2.102711	-2.273257	-0.531743
27	1	0	4.254851	-0.936866	0.452426

TS12

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.470839	-0.000004	0.337821
2	6	0	-0.624225	-1.145914	0.731893
3	6	0	0.665554	-0.709956	-0.926721
4	6	0	0.665517	0.709869	-0.926756
5	6	0	-0.624266	1.145940	0.731881
6	6	0	2.002071	1.143458	-0.476151
7	8	0	2.713985	0.000035	-0.080415
8	6	0	2.002141	-1.143444	-0.476117
9	6	0	0.189289	-0.692557	1.808433
10	6	0	0.189271	0.692630	1.808419
11	8	0	2.502199	-2.236794	-0.405303
12	8	0	2.502040	2.236850	-0.405364
13	6	0	-2.705245	-0.000024	-0.216626
14	6	0	-3.457032	-1.266605	-0.528383
15	6	0	-3.457068	1.266533	-0.528393
16	1	0	-0.893666	-2.185370	0.589502
17	1	0	0.805053	-1.331378	2.431030
18	1	0	0.805039	1.331478	2.430986
19	1	0	-0.893720	2.185382	0.589444
20	1	0	0.122958	1.333635	-1.624973
21	1	0	0.123019	-1.333795	-1.624892
22	1	0	-4.376888	-1.320123	0.068714
23	1	0	-2.880567	-2.174194	-0.338755
24	1	0	-3.775219	-1.270569	-1.579051
25	1	0	-3.775198	1.270502	-1.579080
26	1	0	-2.880652	2.174143	-0.338716
27	1	0	-4.376958	1.320003	0.068651

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.116057	-0.491837	-0.283685
2	6	0	1.606824	-0.576157	1.120256
3	6	0	0.517604	-1.458556	1.082839
4	6	0	0.223393	-1.782855	-0.295028
5	8	0	1.184644	-1.084112	-1.104796
6	6	0	1.041938	1.368208	1.368978
7	6	0	0.179057	1.681561	0.298455
8	6	0	-1.067154	1.040113	0.220742
9	6	0	-1.586261	0.151624	1.169274
10	6	0	-1.996184	1.008112	-0.980107
11	6	0	-3.048833	0.016244	-0.578264
12	6	0	-2.798253	-0.455109	0.665814
13	6	0	0.691063	2.543788	-0.830802
14	8	0	-0.603533	-2.482974	-0.824983
15	8	0	3.128732	0.008968	-0.707973
16	1	0	-2.431997	1.996230	-1.189384
17	1	0	-1.478087	0.695792	-1.897666
18	1	0	-3.890028	-0.250917	-1.207509
19	1	0	-3.397112	-1.173599	1.213027
20	1	0	-1.257395	0.070200	2.196134
21	1	0	0.547470	3.606586	-0.593018
22	1	0	0.178101	2.346626	-1.776090
23	1	0	1.763680	2.386492	-0.984604
24	1	0	0.617125	1.165536	2.347092

25	1	0	2.006726	1.869497	1.405294
26	1	0	0.060836	-1.986513	1.907241
27	1	0	2.326424	-0.531809	1.930656