Electronic Supplementary Information

The Importance of Chain Conformational Mobility During *5-Exo*-Cyclizations of *C-*, *N-* and *O*-Centred Radicals

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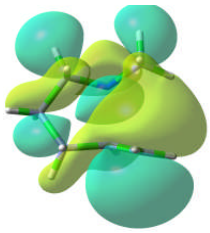
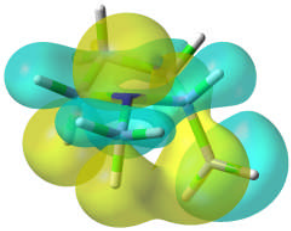
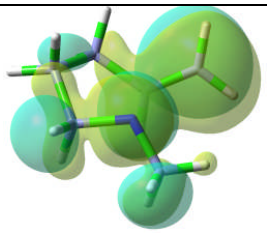
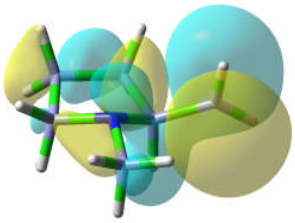
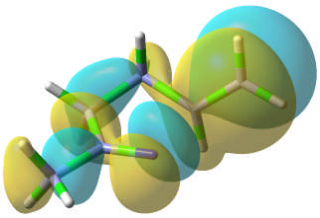
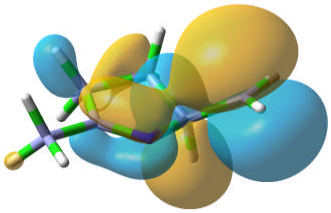
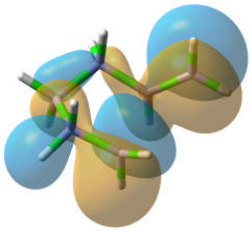
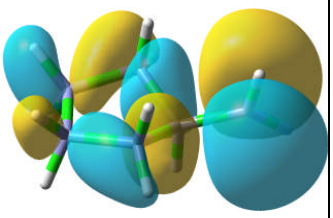
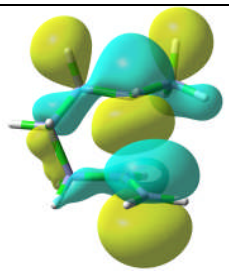
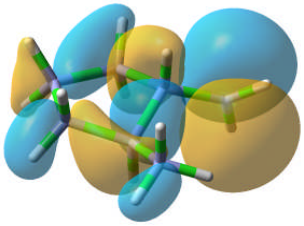
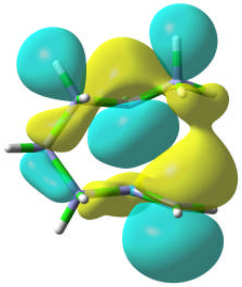
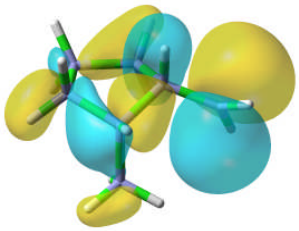
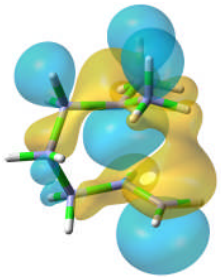
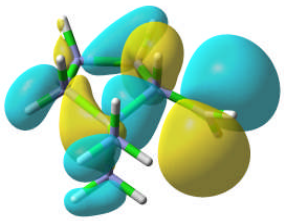
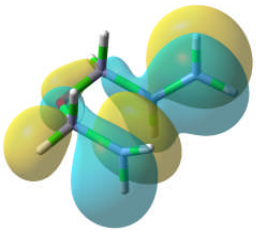
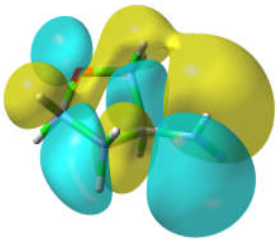
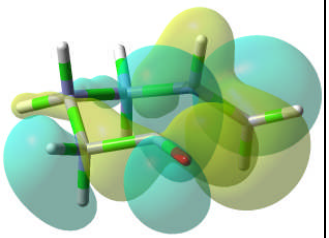
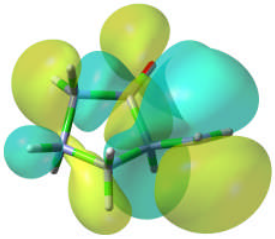
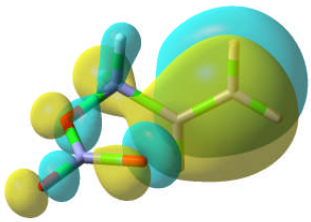
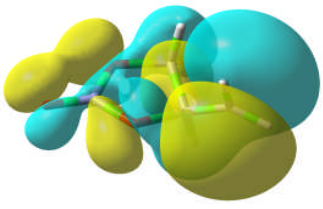
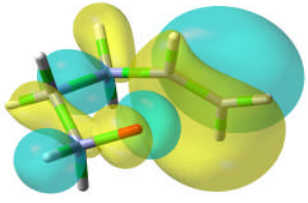
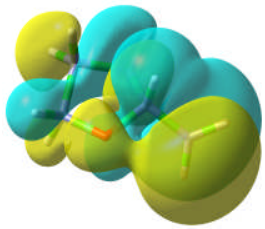
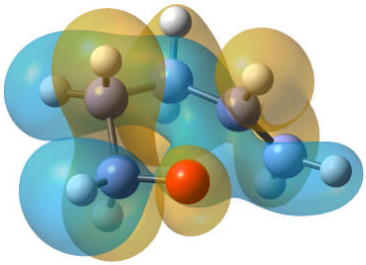
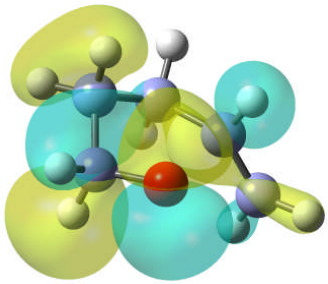
SOMOs of TSs and cyclised radicals computed at the G4 level

 5TSCis	 5cCis		
 5TS	 5c	 6TS	 6c
 7TS	 7c	 8TS	 8c
 9TS	 9c	 10TS	 10c
 11TS	 11c	 12TS	 12c
 13TS	 13C	 14TS	 14C

Penultimate Occupied MOs for Pentenyloxyl Cyclization TS computed at the G4 level.

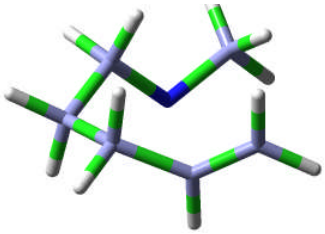
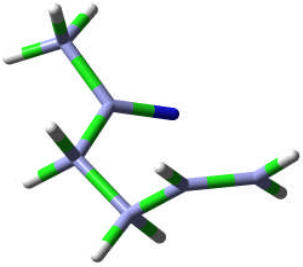
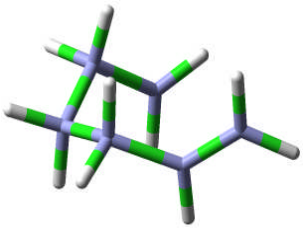
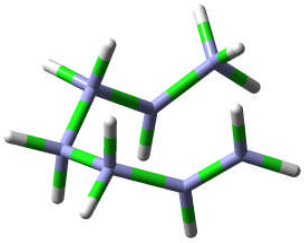
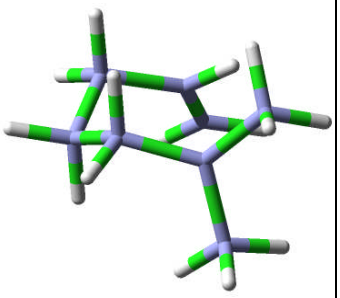
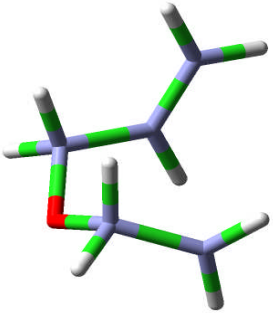
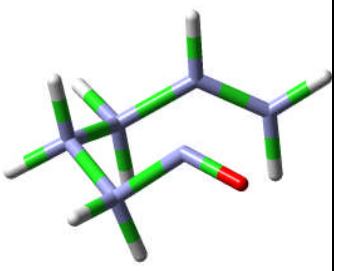
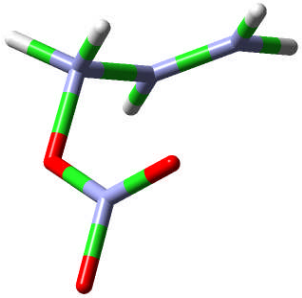
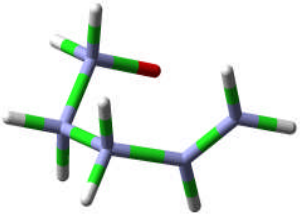


14TS POMO(α)



14TS POMO(β)

Structures of reactive chair-like precursor conformations computed at the um062x/6-311+(2d,p) level.

 **5PRcis**	 **6PR**	 **7PR**	 **8PRcis**
 **10PR**	 **11PR**	 **12PR**	 **13PR**
 **14PR**			

Cartesian coordinates of GS and TS geometries optimized with the G4 method

5e

E(UHF) = -288.70275897

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.644597	0.036935	-0.481069
2	1	0	3.605162	0.850941	-1.200018
3	1	0	4.565899	-0.535096	-0.449450
4	6	0	2.619012	-0.238707	0.318191
5	1	0	2.703208	-1.067222	1.022009
6	6	0	1.306908	0.491817	0.337133
7	1	0	1.155149	0.939331	1.331165
8	1	0	1.338588	1.325028	-0.376263
9	6	0	0.111222	-0.422750	0.023556
10	1	0	0.090721	-1.266601	0.723719
11	1	0	0.226688	-0.855282	-0.976453
12	6	0	-1.229463	0.308193	0.099956
13	1	0	-1.239579	1.162984	-0.603316
14	1	0	-1.357144	0.764525	1.100521
15	7	0	-2.336496	-0.569749	-0.177985
16	6	0	-3.601432	0.113909	-0.128211
17	1	0	-4.421798	-0.582770	-0.320458
18	1	0	-3.767581	0.591431	0.852758
19	1	0	-3.648902	0.924588	-0.875654

5TS(Cis) Chair

E(UHF) = -288.66681284 AU

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659675	-0.805254	-0.069741
2	6	0	1.472342	0.703324	0.142066
3	6	0	0.144086	1.153375	-0.440042
4	6	0	0.308600	-1.423284	0.281988
5	1	0	1.888130	-1.015041	-1.120554
6	1	0	2.475653	-1.207627	0.537992
7	1	0	2.289722	1.274394	-0.313028
8	1	0	1.486235	0.929920	1.215143
9	1	0	0.109619	1.214787	-1.523410
10	1	0	0.137208	-1.384100	1.374135
11	1	0	0.260757	-2.485433	-0.006671
12	6	0	-0.682683	2.008103	0.263866
13	1	0	-1.514244	2.516172	-0.211515
14	1	0	-0.594637	2.113849	1.340825
15	7	0	-0.675402	-0.685616	-0.479146
16	6	0	-2.011624	-0.761793	0.066954
17	1	0	-2.659979	-0.026199	-0.418183
18	1	0	-2.420182	-1.761097	-0.149264
19	1	0	-2.072843	-0.617138	1.158007

5c Cis

E(UHF) **= -288.69789199 AU**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.791565	-0.584036	0.000099
2	6	0	1.372736	0.890089	-0.172047

3	6	0	-0.167840	0.864092	-0.449025
4	6	0	0.493692	-1.249047	0.460117
5	1	0	2.099934	-1.013793	-0.957571
6	1	0	2.614372	-0.708431	0.708919
7	1	0	1.915667	1.396314	-0.973498
8	1	0	1.565790	1.449804	0.748012
9	1	0	-0.380953	1.192048	-1.474260
10	1	0	0.338538	-1.099100	1.548042
11	1	0	0.471606	-2.330441	0.279998
12	6	0	-0.922545	1.742134	0.495235
13	1	0	-1.629731	2.485180	0.145959
14	1	0	-0.832336	1.598653	1.567871
15	7	0	-0.500284	-0.583983	-0.363102
16	6	0	-1.881015	-0.948314	-0.132764
17	1	0	-2.527672	-0.422752	-0.843416
18	1	0	-2.003347	-2.024406	-0.302146
19	1	0	-2.249441	-0.724702	0.884114

6e

E(UHF) = -287.55083960 H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.273462	-0.139431	-0.440901
2	1	0	-3.235596	0.456004	-1.349089
3	1	0	-4.199622	-0.670875	-0.249151
4	6	0	-2.240992	-0.203342	0.393886
5	1	0	-2.324535	-0.812475	1.294625
6	6	0	-0.927110	0.498511	0.203519
7	1	0	-0.958378	1.124578	-0.693824
8	1	0	-0.736497	1.174623	1.046748
9	6	0	0.244097	-0.490405	0.100533
10	1	0	0.103867	-1.155494	-0.761829
11	1	0	0.268187	-1.149310	0.979781
12	7	0	1.775455	1.401553	-0.014988
13	6	0	1.617797	0.159947	-0.024422
14	6	0	2.807146	-0.777959	-0.161812
15	1	0	2.692184	-1.400726	-1.055430
16	1	0	3.737973	-0.214382	-0.235756
17	1	0	2.859371	-1.446738	0.704029

6c

E(UHF) = -287.54673983

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.675911	1.306888	-0.013309
2	6	0	-0.858505	1.260301	-0.107662
3	6	0	-1.190964	-0.184227	0.384053
4	1	0	1.157658	1.836435	-0.841887
5	1	0	1.026319	1.789132	0.909893
6	1	0	-1.180156	1.373077	-1.147411
7	1	0	-1.357246	2.032845	0.481840
8	1	0	-1.400861	-0.145700	1.470802
9	6	0	-2.337946	-0.833618	-0.303278
10	1	0	-3.283830	-0.312230	-0.396463
11	1	0	-2.278405	-1.875583	-0.590023
12	7	0	0.053316	-0.964686	0.232638
13	6	0	1.028686	-0.173118	0.022390
14	6	0	2.437852	-0.652035	-0.142086
15	1	0	2.839622	-0.345069	-1.115215
16	1	0	3.088796	-0.206297	0.620022
17	1	0	2.484692	-1.738960	-0.060679

6TS

E(UHF) = -287.51622971

1 imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632266	1.226568	-0.102653
2	6	0	0.877372	1.196169	0.155321
3	6	0	1.454554	-0.092370	-0.387769
4	1	0	-1.173029	1.877044	0.593698
5	1	0	-0.862407	1.598183	-1.111251
6	1	0	1.073840	1.245337	1.231981
7	1	0	1.369985	2.062494	-0.301410
8	1	0	1.366617	-0.228500	-1.464242
9	6	0	2.501825	-0.730765	0.240373
10	1	0	2.754332	-0.509989	1.272792
11	1	0	3.028705	-1.552209	-0.230737
12	7	0	-0.264359	-1.158611	-0.107963
13	6	0	-1.098366	-0.218145	-0.013956
14	6	0	-2.577804	-0.499418	0.143923
15	1	0	-2.946794	-0.070826	1.082921
16	1	0	-3.143024	-0.030449	-0.670042
17	1	0	-2.769602	-1.573043	0.140598

7e

E(UHF) =-233.64490022 H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.013749	-0.162292	0.437287
2	1	0	3.018992	0.482889	1.311814
3	1	0	3.903608	-0.760939	0.273297
4	6	0	1.972913	-0.208832	-0.388538
5	1	0	2.011881	-0.872722	-1.252691
6	6	0	0.701077	0.573640	-0.232672
7	1	0	0.782833	1.246507	0.629819
8	1	0	0.553611	1.212778	-1.115786
9	6	0	-0.536381	-0.328212	-0.072148
10	1	0	-0.419399	-0.952389	0.821403
11	1	0	-0.603351	-1.017864	-0.923010
12	6	0	-1.853743	0.481509	0.031220
13	1	0	-1.941152	1.104851	-0.869379
14	1	0	-1.766598	1.171709	0.880888
15	6	0	-3.065545	-0.370648	0.184842
16	1	0	-3.540378	-0.821589	-0.679805
17	1	0	-3.392464	-0.704222	1.163508

7TS

E(UHF) = -233.62405637 H

1 imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.302927	-0.875793	0.168183
2	6	0	0.166351	-1.235040	-0.081908
3	6	0	1.094760	-0.145655	0.410899
4	6	0	-0.487396	1.456537	0.187890
5	6	0	-1.532520	0.543855	-0.378880
6	1	0	-1.980272	-1.605264	-0.289410
7	1	0	-1.505089	-0.885954	1.247659
8	1	0	0.333270	-1.391321	-1.155192
9	1	0	0.416405	-2.181327	0.415227

10	1	0	1.071510	0.030004	1.484841
11	1	0	-0.580426	1.741449	1.233358
12	1	0	-0.036576	2.213304	-0.444773
13	1	0	-2.549591	0.885090	-0.134002
14	1	0	-1.463445	0.525004	-1.473233
15	6	0	2.221607	0.228217	-0.265805
16	1	0	2.963463	0.881913	0.179143
17	1	0	2.371503	-0.045626	-1.305886

7c

E(UHF) = -233.66316928 H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.467530	-0.787380	-0.053475
2	6	0	0.002462	-1.193330	0.199541
3	6	0	-0.826577	-0.003654	-0.361144
4	6	0	0.007579	1.206400	0.128569
5	6	0	1.485186	0.769724	-0.012567
6	1	0	2.148397	-1.232769	0.677341
7	1	0	1.789319	-1.142875	-1.037926
8	1	0	-0.193802	-1.282901	1.275260
9	1	0	-0.268076	-2.148169	-0.259636
10	1	0	-0.763925	-0.046143	-1.457382
11	1	0	-0.224680	2.122584	-0.421186
12	1	0	-0.236615	1.395596	1.181355
13	1	0	1.922797	1.171941	-0.931289
14	1	0	2.092808	1.151218	0.812882
15	6	0	-2.252512	0.016835	0.050122
16	1	0	-3.054001	-0.228817	-0.635782
17	1	0	-2.514228	0.188764	1.090089

8TS

E(UHF) = -272.67698981

1 imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.872500	-0.689231	0.449974
2	6	0	-0.138863	-1.539187	-0.265160
3	6	0	-1.546698	-1.028644	0.072802
4	6	0	-1.561620	0.478808	-0.207578
5	1	0	0.023326	-1.474725	-1.349430
6	1	0	-0.036835	-2.602068	0.003138
7	1	0	-2.321665	-1.553498	-0.496168
8	1	0	-1.754460	-1.209544	1.135956
9	1	0	-1.540226	0.652560	-1.291001
10	1	0	-2.491198	0.929645	0.162911
11	1	0	0.878187	-0.809104	1.533695
12	6	0	2.214930	-0.431776	-0.163183
13	1	0	2.767961	0.337878	0.384364
14	1	0	2.838156	-1.340011	-0.165791
15	1	0	2.122884	-0.100288	-1.203183
16	6	0	-0.370167	1.167530	0.427176
17	1	0	-0.359412	1.158455	1.515805
18	6	0	0.303616	2.185182	-0.196659
19	1	0	0.205552	2.355300	-1.264667
20	1	0	1.025550	2.799314	0.330134

8e = 9e

E(UHF) = -272.69854268

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.603515	0.116741	-0.410218
2	1	0	3.747865	-0.914614	-0.720965
3	1	0	4.416036	0.803522	-0.623035
4	6	0	2.491510	0.511124	0.202559
5	1	0	2.390725	1.556959	0.494457
6	6	0	1.315694	-0.365156	0.524589
7	1	0	1.538455	-1.402402	0.245424
8	1	0	1.144419	-0.363588	1.611241
9	6	0	0.021897	0.092733	-0.173078
10	1	0	0.168249	0.071862	-1.259623
11	1	0	-0.186231	1.137756	0.089829
12	6	0	-1.201037	-0.782669	0.199863
13	1	0	-1.329016	-0.747483	1.291318
14	1	0	-0.962255	-1.825071	-0.052959
15	6	0	-2.468075	-0.369865	-0.473343
16	6	0	-3.352354	0.694583	0.082944
17	1	0	-2.980284	1.711314	-0.135786
18	1	0	-4.364697	0.641228	-0.331359
19	1	0	-3.427710	0.625267	1.175603
20	1	0	-2.622463	-0.679697	-1.504046

8TS

E(UHF) = -272.67424864 AU

1 Imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.776274	-1.365163	-0.104308
2	6	0	1.092301	0.065890	-0.427298
3	6	0	-0.829630	0.850608	0.412709
4	6	0	-1.473129	-0.525120	0.542913
5	6	0	-0.729655	-1.586084	-0.288912
6	1	0	1.346319	-2.060288	-0.740969
7	1	0	1.062694	-1.588727	0.932466
8	1	0	-0.246357	1.186325	1.267013
9	1	0	-1.465041	-0.824806	1.597901
10	1	0	-2.524361	-0.475859	0.240595
11	1	0	-1.034799	-2.600901	-0.010501
12	1	0	-0.981965	-1.455782	-1.349217
13	6	0	-1.340752	1.816264	-0.412371
14	1	0	-0.969042	2.834984	-0.396961
15	1	0	-2.074961	1.576989	-1.176290
16	6	0	2.227491	0.773858	0.247841
17	1	0	3.204930	0.421946	-0.120120
18	1	0	2.192715	1.853933	0.068704
19	1	0	2.221633	0.608034	1.331882
20	1	0	0.930835	0.342629	-1.467961

8c

E(UHF) **= -272.71475258 AU**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.780934	-1.357349	0.024674
2	6	0	0.504017	-0.592530	-0.338102
3	6	0	0.276306	0.797117	0.333967
4	6	0	-1.212949	1.079131	0.008679
5	6	0	-1.918675	-0.304596	-0.009166
6	1	0	-0.964746	-2.204339	-0.643458
7	1	0	-0.675221	-1.770520	1.035684
8	1	0	0.377573	0.643025	1.418113
9	1	0	-1.659626	1.778823	0.720157
10	1	0	-1.276006	1.552841	-0.977942
11	1	0	-2.592557	-0.424897	0.843825

12	1	0	-2.533886	-0.412790	-0.907200
13	6	0	1.209212	1.867813	-0.096618
14	1	0	2.015795	2.220676	0.534330
15	1	0	1.147667	2.267629	-1.104646
16	6	0	1.797491	-1.290832	0.070972
17	1	0	1.897724	-2.264388	-0.420890
18	1	0	2.673684	-0.689988	-0.193126
19	1	0	1.822948	-1.463024	1.153969
20	1	0	0.519841	-0.425566	-1.425252

9c

E(UHF) = -272.71125202 H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.451752	0.442366	-0.609251
2	6	0	0.030134	0.854438	-0.523781
3	6	0	0.741835	-0.543927	-0.464675
4	6	0	-0.162655	-1.362040	0.491972
5	6	0	-1.595288	-0.782838	0.331180
6	1	0	-2.130531	1.259346	-0.344909
7	1	0	-1.689134	0.151463	-1.638800
8	1	0	0.633281	-0.963389	-1.475390
9	1	0	-0.110809	-2.430932	0.268083
10	1	0	0.189618	-1.244744	1.522567
11	1	0	-2.290314	-1.519099	-0.081826
12	1	0	-2.002468	-0.486251	1.302272
13	6	0	2.182955	-0.541795	-0.111710
14	1	0	2.947678	-0.417569	-0.870196
15	1	0	2.503374	-0.543466	0.924993
16	6	0	0.323993	1.745093	0.689138
17	1	0	1.391322	1.973129	0.765448
18	1	0	-0.219251	2.692621	0.608984
19	1	0	0.018641	1.272063	1.629059
20	1	0	0.343257	1.389049	-1.427524

9TS

E(UHF) = -272.67274291 H

1 imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.135294	-1.141990	0.286167
2	6	0	1.074112	0.332245	0.590416
3	6	0	-1.154081	0.443541	0.524320
4	6	0	-1.328151	-0.991159	0.037315
5	6	0	-0.045553	-1.520725	-0.621659
6	1	0	2.087482	-1.409243	-0.196664
7	1	0	1.077146	-1.723541	1.214111
8	1	0	-1.130525	0.580776	1.602401
9	1	0	-1.585327	-1.631830	0.889603
10	1	0	-2.167983	-1.049600	-0.663017
11	1	0	-0.095652	-2.601666	-0.794609
12	1	0	0.081382	-1.046799	-1.602961
13	6	0	-1.557966	1.515116	-0.229945
14	1	0	-1.577872	2.521653	0.173067
15	1	0	-1.790620	1.409838	-1.285720
16	6	0	1.629556	1.303753	-0.409769
17	1	0	1.288555	2.324605	-0.212529
18	1	0	2.730278	1.313527	-0.380626
19	1	0	1.335730	1.050512	-1.433690
20	1	0	1.228132	0.617080	1.629567

10e

E(UHF) = -311.75197739 AU

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.912474	0.485713	-0.376020
2	1	0	-3.970373	1.348327	0.282540
3	1	0	-4.726938	0.362081	-1.082100
4	6	0	-2.899510	-0.373168	-0.313671
5	1	0	-2.884263	-1.223305	-0.996502
6	6	0	-1.727429	-0.274234	0.619243
7	1	0	-1.865649	0.575072	1.299691
8	1	0	-1.683057	-1.175180	1.249017
9	6	0	-0.385288	-0.132229	-0.121082
10	1	0	-0.404052	0.779064	-0.730771
11	1	0	-0.263622	-0.969310	-0.820690
12	6	0	0.827959	-0.089585	0.842467
13	1	0	0.816306	-1.010986	1.442263
14	1	0	0.676222	0.743085	1.543803
15	6	0	2.152365	0.056651	0.158255
16	6	0	2.627965	1.413233	-0.255841
17	1	0	3.723744	1.465836	-0.282539
18	1	0	2.286960	1.690895	-1.269440
19	1	0	2.266101	2.195679	0.420512
20	6	0	2.819615	-1.146312	-0.429933
21	1	0	2.517438	-1.329466	-1.476810
22	1	0	3.911065	-1.033774	-0.447894
23	1	0	2.580904	-2.058427	0.128413

10TS

E(UHF) = -311.72522233 AU

1 imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.387958	-1.512943	-0.017522
2	6	0	-0.970146	-0.117675	0.006456
3	6	0	0.929316	0.860540	-0.562751
4	6	0	1.785203	-0.395576	-0.425796
5	6	0	1.080503	-1.466362	0.422960
6	1	0	-0.963774	-2.191888	0.630397
7	1	0	-0.446622	-1.924617	-1.033158
8	1	0	0.501820	1.034121	-1.547381
9	1	0	1.984804	-0.802856	-1.424390
10	1	0	2.758334	-0.143662	0.008427
11	1	0	1.565247	-2.443957	0.323963
12	1	0	1.140467	-1.191066	1.482959
13	6	0	1.157835	1.972683	0.212244
14	1	0	0.670389	2.919888	0.008456
15	1	0	1.760385	1.920671	1.114543
16	6	0	-1.931254	0.246644	-1.094195
17	1	0	-2.909840	-0.237628	-0.942362
18	1	0	-2.116422	1.326301	-1.127630
19	1	0	-1.568050	-0.069104	-2.078111
20	6	0	-1.337250	0.427838	1.362089
21	1	0	-1.446648	1.516647	1.339152
22	1	0	-2.297901	0.008197	1.701065
23	1	0	-0.589681	0.188060	2.123153

10c

E(UHF) = -311.76184929 AU

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

1	6	0	0.622165	-1.402861	-0.349975
2	6	0	-0.547993	-0.457559	0.000717
3	6	0	0.039213	0.928051	-0.477907
4	6	0	1.520573	0.876096	-0.028158
5	6	0	1.915874	-0.626301	-0.009071
6	1	0	0.551933	-2.361602	0.174529
7	1	0	0.590429	-1.625386	-1.423410
8	1	0	0.013297	0.879218	-1.576409
9	1	0	2.153602	1.470572	-0.692532
10	1	0	1.621558	1.317876	0.969063
11	1	0	2.713350	-0.849860	-0.723006
12	1	0	2.296131	-0.911933	0.976174
13	6	0	-0.693354	2.143878	-0.047286
14	1	0	-1.506013	2.554001	-0.635676
15	1	0	-0.498420	2.596569	0.919388
16	6	0	-1.833163	-0.816821	-0.749940
17	1	0	-2.192869	-1.811469	-0.462694
18	1	0	-2.633206	-0.101064	-0.531410
19	1	0	-1.671576	-0.821106	-1.833844
20	6	0	-0.817239	-0.464527	1.515630
21	1	0	-1.593074	0.260157	1.781517
22	1	0	-1.158456	-1.455064	1.836276
23	1	0	0.076862	-0.220645	2.097969

11e

E(UHF) = -269.47431083

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.948552	-0.110383	-0.360742
2	1	0	-3.054576	0.741820	-1.026354
3	1	0	-3.813804	-0.757003	-0.261487
4	6	0	-1.820801	-0.342170	0.300786
5	1	0	-1.730538	-1.206942	0.954947
6	6	0	-0.606710	0.533199	0.243685
7	1	0	-0.725236	1.309854	-0.530254
8	1	0	-0.474604	1.058547	1.208314
9	6	0	1.736070	0.453795	0.011354
10	1	0	1.830892	0.988586	0.982397
11	1	0	1.730747	1.251259	-0.757575
12	6	0	2.876130	-0.468010	-0.198724
13	1	0	2.743935	-1.529823	-0.036823
14	1	0	3.866164	-0.074604	-0.391043
15	8	0	0.526276	-0.272535	-0.015035

11TS

E(UHF) = -269.45693490

1 Imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150392	-1.183852	0.044848
2	6	0	-1.081750	-0.089090	-0.425878
3	6	0	0.605119	1.428565	-0.161451
4	6	0	1.534363	0.374739	0.348097
5	1	0	-0.321042	-1.366114	1.120144
6	1	0	-0.360287	-2.116267	-0.491255
7	1	0	-1.053373	0.116147	-1.493160
8	1	0	0.697471	1.734039	-1.199294
9	1	0	0.222704	2.180476	0.519512
10	1	0	2.577277	0.558597	0.058882
11	1	0	1.494344	0.329273	1.448784
12	6	0	-2.186922	0.275971	0.280320
13	1	0	-2.946706	0.924631	-0.140545

14	1	0	-2.316102	-0.020027	1.317239
15	8	0	1.210400	-0.897344	-0.206991

11c

E(UHF) = -269.49802155

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.027611	-1.167815	0.147701
2	6	0	-0.807832	0.024397	-0.378108
3	6	0	0.085654	1.193261	0.113291
4	6	0	1.508722	0.618352	-0.000720
5	1	0	-0.195203	-1.340233	1.214125
6	1	0	-0.160587	-2.097993	-0.396298
7	1	0	-0.775448	-0.006235	-1.473390
8	1	0	-0.053811	2.105828	-0.470452
9	1	0	-0.160085	1.424148	1.155525
10	1	0	2.011934	0.945077	-0.919653
11	1	0	2.139289	0.911957	0.848716
12	6	0	-2.213334	0.062431	0.090469
13	1	0	-3.048631	-0.031045	-0.591496
14	1	0	-2.430780	0.149244	1.150512
15	8	0	1.383548	-0.805562	-0.044173

12e

E(UHF) = -307.38068128

Number	Number	Type	X	Y	Z
1	6	0	-3.512475	-0.145944	-0.417811
2	1	0	-3.542380	0.590049	-1.216784
3	1	0	-4.392272	-0.769989	-0.302485
4	6	0	-2.455381	-0.268644	0.378271
5	1	0	-2.467978	-1.021072	1.166998
6	6	0	-1.198353	0.548458	0.283707
7	1	0	-1.305815	1.304462	-0.504037
8	1	0	-1.046602	1.097009	1.224865
9	6	0	0.047135	-0.312269	0.010897
10	1	0	-0.071750	-0.845569	-0.938393
11	1	0	0.137905	-1.081971	0.787285
12	6	0	1.333793	0.519721	-0.032201
13	1	0	1.512877	1.054601	0.910336
14	1	0	1.268639	1.270333	-0.831747
15	6	0	2.561736	-0.318240	-0.365547
16	8	0	3.656081	-0.217043	0.070008

12TS

E(UHF) = -307.35907133

1 Imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.442111	0.549043	0.368086
2	6	0	-1.222193	-0.153215	-0.419763
3	6	0	-0.925031	1.258219	0.048181
4	6	0	0.543818	1.655906	-0.183421

5	1	0	1.411138	0.521221	1.466208
6	1	0	2.492500	0.635165	0.070538
7	1	0	-1.134908	-0.318395	-1.492816
8	1	0	-1.582388	1.965975	-0.471350
9	1	0	-1.163573	1.336301	1.116442
10	1	0	0.730624	1.769297	-1.258378
11	1	0	0.766523	2.619911	0.282781
12	6	0	-2.012769	-1.009953	0.295278
13	1	0	-2.355847	-1.949308	-0.122108
14	1	0	-2.242212	-0.824543	1.340160
15	6	0	0.886819	-0.775849	-0.121685
16	8	0	1.350202	-1.862566	-0.106441

12c

E(UHF) = -307.39996881

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.221000	0.947817	0.300096
2	6	0	0.639030	-0.599745	-0.365424
3	6	0	-0.616339	-1.386026	0.054211
4	6	0	-1.788634	-0.404627	-0.151127
5	1	0	-1.292145	1.058627	1.390808
6	1	0	-1.688627	1.830166	-0.142713
7	1	0	0.712832	-0.598542	-1.466908
8	1	0	-0.737103	-2.316048	-0.506216
9	1	0	-0.536402	-1.653890	1.115579
10	1	0	-2.057902	-0.361923	-1.213078
11	1	0	-2.685806	-0.698810	0.398595
12	6	0	1.925442	-1.041891	0.218725
13	1	0	2.861291	-0.649496	-0.159209
14	1	0	1.940147	-1.581587	1.159109
15	6	0	0.269973	0.888984	-0.044078
16	8	0	1.029110	1.818054	-0.081298

13e

E(UHF) = -379.06498923

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.178923	0.019459	-0.279261
2	1	0	3.244186	0.925982	-0.874074
3	1	0	4.092237	-0.554503	-0.168857
4	6	0	2.042391	-0.361681	0.291723
5	1	0	1.992773	-1.274882	0.879906
6	6	0	0.774327	0.423117	0.214007
7	1	0	0.457313	0.782051	1.199018
8	1	0	0.868239	1.282732	-0.455266
9	6	0	-1.504769	-0.035311	-0.187498
10	8	0	-1.847643	1.058130	0.302356
11	8	0	-2.453465	-0.755745	-0.596119
12	8	0	-0.263278	-0.465017	-0.299458

13TS

E(UHF) = -379.07066236

I imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651705	1.191625	-0.131945
2	6	0	-1.379728	0.011150	0.451196
3	1	0	-0.877623	1.287382	-1.200725
4	1	0	-0.946911	2.118414	0.369996
5	1	0	-1.207730	-0.185981	1.505014
6	6	0	-2.407462	-0.607234	-0.185663
7	1	0	-2.989217	-1.382131	0.299295
8	1	0	-2.649448	-0.379208	-1.218810
9	8	0	0.328949	-1.131452	-0.070549
10	8	0	0.759450	1.083081	0.051734
11	6	0	1.222955	-0.187776	-0.023259
12	8	0	2.407422	-0.439762	-0.033278

13c

E(UHF) = -379.11296835

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569199	1.262146	-0.058587
2	6	0	-1.091536	-0.119218	0.407632
3	1	0	-0.883886	1.488425	-1.083234
4	1	0	-0.866759	2.075989	0.604087
5	1	0	-1.231325	-0.123596	1.494716
6	6	0	-2.303359	-0.603166	-0.283881
7	1	0	-3.239150	-0.724997	0.244334
8	1	0	-2.254235	-0.844617	-1.339269
9	8	0	0.049386	-0.963893	0.112573
10	8	0	0.848728	1.115857	-0.018451
11	6	0	1.167776	-0.206918	-0.026142
12	8	0	2.270302	-0.635942	-0.137038

14e

E(UHF) = -269.49205403

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.990382	-0.022802	-0.434068
2	1	0	-2.983294	0.777243	-1.169500
3	1	0	-3.897721	-0.614214	-0.372840
4	6	0	-1.944010	-0.259182	0.350508
5	1	0	-1.994647	-1.073874	1.073079
6	6	0	-0.649566	0.502061	0.326073
7	1	0	-0.719361	1.323041	-0.398571
8	1	0	-0.482271	0.968027	1.309137
9	6	0	0.559033	-0.389316	-0.006037
10	1	0	0.421102	-0.848571	-0.991516
11	1	0	0.637778	-1.210677	0.715892
12	6	0	1.879550	0.389030	-0.003600
13	1	0	2.042014	0.865512	0.990024
14	1	0	1.845579	1.256734	-0.693945
15	8	0	3.000552	-0.349292	-0.230309

14TS

E(UHF) = -269.46626960

1 Imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.290174	-0.754142	0.344716
2	6	0	-1.026770	0.271145	-0.442122
3	6	0	-0.027854	1.271992	0.081384
4	6	0	1.395671	0.711584	-0.088554
5	1	0	1.210280	-0.828507	1.445664
6	1	0	2.195374	-1.315875	0.053973
7	1	0	-1.077059	0.156397	-1.519888
8	1	0	-0.138459	2.225023	-0.449047
9	1	0	-0.229192	1.465366	1.141364
10	1	0	1.689465	0.751497	-1.143287
11	1	0	2.131073	1.280133	0.490895
12	6	0	-2.068038	-0.197531	0.313270
13	1	0	-2.834524	-0.835416	-0.110977
14	1	0	-2.110275	-0.016903	1.382557
15	8	0	0.223028	-1.337501	-0.317927

14c

E(UHF) = -269.50054163

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.308230	-0.831179	0.172809
2	6	0	-0.800817	0.052196	-0.389660
3	6	0	0.067919	1.201105	0.184245
4	6	0	1.483576	0.673873	-0.075624
5	1	0	1.516918	-1.088297	1.221459
6	1	0	1.962502	-1.444320	-0.458205
7	1	0	-0.872579	0.194141	-1.483047
8	1	0	-0.145448	2.159612	-0.294074
9	1	0	-0.120288	1.303636	1.258323
10	1	0	1.773717	0.860573	-1.115120
11	1	0	2.242387	1.121734	0.570850
12	6	0	-2.163103	-0.067232	0.179730
13	1	0	-2.991718	0.486051	-0.244760
14	1	0	-2.312845	-0.633235	1.091141
15	8	0	-0.053435	-1.141559	-0.121946

References and Notes

1. Gaussian 09, Revision C 1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.