

# Cyclization cascade of allenyl azides: A dual mechanism

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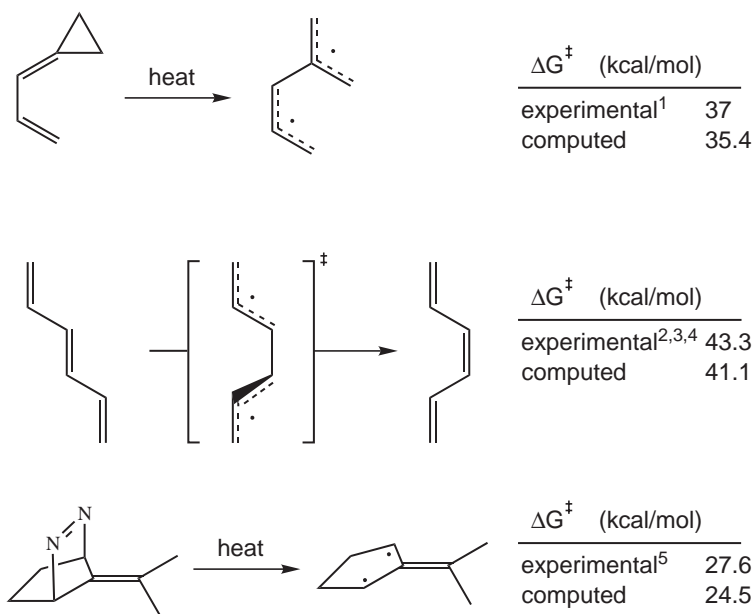
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## 1 Gaussian reference

See References section at the end of this document (cite 1)

## 2 Method Validation

The combination of the B3LYP density functional and pople basis set chosen in this work has shown to be highly accurate in several diyl forming reactions.<sup>2-6</sup> A summary is given in Figure S1.



**Figure S1:** Reference systems used to validate the level of theory employed.

### 3 Cartesian Coordinates

Geometries: B3LYP/6-31G(d,p)

SCF energies: B3LYP/6-311+G(d,p)

C-1

SCF Energy: -588.856325523

Num. Imaginary Frequencies: 0

C	0.865385	-1.051709	-0.107096
C	1.059282	0.348026	-0.062839
C	2.337102	0.884196	0.140121
C	3.436685	0.046847	0.304178
C	3.266300	-1.338007	0.269330
C	1.995578	-1.867689	0.067908
N	-0.091687	1.155580	-0.223030
H	2.466089	1.962221	0.171287
H	4.420655	0.477963	0.460442
H	4.116476	-2.000116	0.398672
H	1.859914	-2.945424	0.040402
C	-0.436779	-1.705547	-0.313315
C	-1.609868	-1.180807	-0.594096
H	-0.402047	-2.793720	-0.222897
N	0.026950	2.384869	-0.194021
N	-0.017226	3.525965	-0.191670
C	-2.825589	-0.773204	-0.883805
C	-3.860013	-0.370151	0.083804
H	-3.099667	-0.707769	-1.937817
C	-3.681785	-0.170150	1.395264
H	-4.849723	-0.221193	-0.344133
H	-4.507798	0.118751	2.036437
H	-2.707950	-0.286448	1.861925

C-3

SCF Energy: -588.901834753

Num. Imaginary Frequencies: 0

C	1.230911	-0.879144	-0.287877
C	1.112783	0.505122	0.034426
C	2.198714	1.297522	0.402407
C	3.443888	0.677303	0.448794
C	3.593007	-0.687509	0.136593
C	2.502570	-1.469383	-0.230001
N	-0.233320	0.793791	-0.113885
H	2.072641	2.347847	0.640593
H	4.316299	1.258267	0.731389
H	4.580585	-1.136319	0.183666
H	2.631794	-2.521005	-0.468787
C	-0.089301	-1.380771	-0.624840
C	-0.950002	-0.327614	-0.504108
H	-0.335457	-2.390472	-0.920273
N	-1.022176	1.915935	0.032044
N	-2.212081	1.635267	-0.237916
C	-2.355418	0.167648	-0.615238
C	-3.410980	-0.463405	0.263731
H	-2.713820	0.174454	-1.655319
C	-3.213053	-1.489434	1.087517
H	-4.390744	0.001293	0.181272
H	-4.026108	-1.889704	1.684598
H	-2.240878	-1.961319	1.192727

C-5a

SCF Energy: -479.393886062

Num. Imaginary Frequencies: 0

C	-0.754219	0.668525	-0.106457
C	-0.981969	-0.785454	0.041780
C	-2.324246	-1.275992	0.166911
C	-3.349859	-0.376714	0.133999
C	-3.126860	1.045689	-0.019572
C	-1.871825	1.566233	-0.138502
H	-2.494081	-2.341506	0.281458
H	-4.374961	-0.725422	0.223896
H	-3.991684	1.702400	-0.037715
H	-1.715454	2.635304	-0.251096
C	0.604981	0.818791	-0.205829
C	1.152921	-0.532472	-0.105098
N	0.133700	-1.490552	0.025878
C	2.457380	-0.938086	-0.145906
H	1.167114	1.724925	-0.380056
C	3.650779	-0.112566	-0.171131
H	2.604130	-2.016245	-0.177298
C	3.808443	1.069227	0.449851
H	4.505795	-0.542167	-0.692460
H	4.745234	1.613626	0.387697
H	3.024845	1.499874	1.064151

C-5b

SCF Energy: -479.397793949

Num. Imaginary Frequencies: 0

C	-1.359156	0.277585	0.000000
C	0.000000	0.853874	0.000000
C	0.155157	2.276171	0.000000
C	-0.969546	3.053231	0.000000
C	-2.300254	2.490018	0.000000
C	-2.502556	1.140038	0.000000
H	1.151394	2.706189	0.000000
H	-0.873302	4.135611	0.000000
H	-3.148000	3.168601	0.000000
H	-3.505429	0.722451	0.000000
C	-1.171638	-1.081706	0.000000
C	0.275659	-1.279927	0.000000
N	0.956867	-0.064536	0.000000
C	0.869198	-2.518031	0.000000
H	-1.916924	-1.866967	0.000000
H	0.183256	-3.363147	0.000000
C	2.274712	-2.860574	0.000000
C	3.305929	-1.991746	0.000000
H	2.488932	-3.927808	0.000000
H	4.329494	-2.354591	0.000000
H	3.127491	-0.922191	0.000000

C-7a

SCF Energy: -479.425619335

Num. Imaginary Frequencies: 0

C	0.521239	0.535840	0.168332
C	0.804475	-0.848634	0.034700
C	2.108740	-1.298724	-0.149198
C	3.134405	-0.348562	-0.203045
C	2.861101	1.015702	-0.069116
C	1.548079	1.467230	0.132186
H	2.310442	-2.359684	-0.254241
H	4.159214	-0.676085	-0.352849
H	3.673526	1.734474	-0.121289
H	1.347181	2.529305	0.245777
C	-0.951745	0.620895	0.467296
C	-1.338281	-0.830854	0.249265
N	-0.364962	-1.660012	0.055141
C	-2.773024	-0.897969	0.008483
H	-1.074292	0.848556	1.537528
C	-3.197626	0.345542	-0.298482
H	-3.363103	-1.805901	-0.014615
C	-2.074691	1.376067	-0.291845
H	-4.216390	0.603296	-0.571649
H	-2.367012	2.322213	0.175090
H	-1.770865	1.604714	-1.321192



C-7b

SCF Energy: -479.443179317

Num. Imaginary Frequencies: 0

C	-1.286847	0.002709	0.000000
C	0.000000	0.633104	0.000000
C	0.150250	2.023001	0.000000
C	-1.006654	2.795585	0.000000
C	-2.283769	2.199434	0.000000
C	-2.432042	0.818056	0.000000
H	1.133417	2.484225	0.000000
H	-0.923440	3.878409	0.000000
H	-3.165100	2.834023	0.000000
H	-3.421787	0.369749	0.000000
C	-1.079225	-1.420422	0.000000
C	0.283459	-1.609708	0.000000
N	0.930454	-0.379066	0.000000
C	1.319668	-2.628273	0.000000
H	-1.839914	-2.187475	0.000000
H	1.132173	-3.694202	0.000000
C	2.527055	-2.028643	0.000000
C	2.376906	-0.519004	0.000000
H	3.493476	-2.516284	0.000000
H	2.832596	-0.055009	0.886198
H	2.832596	-0.055009	-0.886198

C-2

SCF Energy: -588.819442087

Num. Imaginary Frequencies: 1

C	1.150765	-0.854073	-0.323373
C	1.149809	0.546613	-0.129958
C	2.287006	1.234495	0.282055
C	3.452424	0.499883	0.516805
C	3.479727	-0.883967	0.316073
C	2.335321	-1.562169	-0.108144
N	-0.100809	1.055391	-0.496685
H	2.260274	2.310835	0.415483
H	4.347387	1.015678	0.850714
H	4.397477	-1.435788	0.493509
H	2.355738	-2.638327	-0.254217
C	-0.153615	-1.382318	-0.721278
C	-1.193324	-0.546381	-0.773659
H	-0.267184	-2.427202	-0.999283
N	-0.768562	1.976635	0.049894
N	-1.861045	2.328150	0.235785
C	-2.503381	-0.188366	-0.766247
C	-3.467162	-0.595528	0.257627
H	-2.893991	0.372075	-1.613084
C	-3.253492	-1.433065	1.284545
H	-4.458663	-0.163552	0.134746
H	-4.047218	-1.672193	1.983691
H	-2.285371	-1.893506	1.458818

C-4a

SCF Energy: -588.867939904

Num. Imaginary Frequencies: 1

C	1.366655	-0.860714	-0.293414
C	1.049804	0.448410	0.200265
C	2.057647	1.333190	0.587587
C	3.379307	0.895689	0.504811
C	3.700383	-0.398045	0.051949
C	2.702955	-1.284681	-0.343281
N	-0.324837	0.615051	0.205315
H	1.813463	2.330154	0.940347
H	4.180044	1.566485	0.802982
H	4.740450	-0.708585	0.020729
H	2.954608	-2.289648	-0.672029
C	0.115393	-1.430629	-0.705214
C	-0.854706	-0.487229	-0.384274
H	-0.051784	-2.417460	-1.117798
N	-1.642501	1.927082	-0.705377
N	-2.477507	1.207078	-1.037676
C	-2.302821	-0.472250	-0.625141
C	-3.276447	-0.651660	0.483239
H	-2.615865	-0.969416	-1.543989
C	-2.937384	-0.689299	1.775607
H	-4.316599	-0.759379	0.183665
H	-3.688563	-0.841025	2.544080
H	-1.906550	-0.572295	2.093393

C-4b

SCF Energy: -588.869714286

Num. Imaginary Frequencies: 1

C	-1.234023	-0.859914	-0.227987
C	-1.185243	0.569461	-0.130866
C	-2.331605	1.315023	0.154066
C	-3.531886	0.625852	0.313307
C	-3.600379	-0.775843	0.187318
C	-2.461942	-1.525614	-0.088152
N	0.112712	0.985140	-0.361671
H	-2.283193	2.395440	0.244224
H	-4.438664	1.182686	0.531587
H	-4.558991	-1.273568	0.299152
H	-2.524294	-2.604531	-0.204055
C	0.124732	-1.285376	-0.413601
C	0.887332	-0.121519	-0.461340
H	0.483709	-2.291374	-0.584655
N	1.484256	2.205133	0.412618
N	2.467033	1.644445	0.184873
C	2.327816	0.094460	-0.644405
C	3.297776	-0.871219	-0.091892
H	2.622327	0.486087	-1.621302
C	3.054064	-1.643762	0.974934
H	4.263904	-0.921844	-0.587470
H	3.795952	-2.350075	1.333740
H	2.111398	-1.595133	1.509741

C-6a

SCF Energy: -479.369103796

Num. Imaginary Frequencies: 1

C	-0.611975	0.580458	-0.228538
C	-0.848203	-0.822192	0.032911
C	-2.159825	-1.272720	0.288971
C	-3.190642	-0.351421	0.256741
C	-2.965300	1.023590	-0.025885
C	-1.691625	1.493064	-0.273196
H	-2.339169	-2.322433	0.497139
H	-4.207874	-0.684210	0.445124
H	-3.810129	1.705261	-0.043658
H	-1.517284	2.545374	-0.481363
C	0.771620	0.677336	-0.480517
C	1.268633	-0.713168	-0.274392
N	0.291644	-1.585511	-0.014967
C	2.665770	-0.924055	-0.264168
H	1.233506	1.400004	-1.138464
C	3.390550	0.211688	0.077787
H	3.108864	-1.886141	-0.501050
C	2.701637	1.224885	0.761455
H	4.428202	0.351070	-0.220784
H	3.076170	2.246639	0.773031
H	2.002357	0.978227	1.547785

C-6b

SCF Energy: -479.370245123

Num. Imaginary Frequencies: 1

C	-0.948483	0.910964	0.049735
C	-0.528468	-0.472974	-0.142319
C	-1.494809	-1.513701	-0.212614
C	-2.818797	-1.184614	-0.056086
C	-3.236783	0.169770	0.150539
C	-2.332603	1.203102	0.198608
H	-1.176344	-2.539584	-0.370414
H	-3.575355	-1.963316	-0.091027
H	-4.297147	0.374979	0.266712
H	-2.663523	2.225820	0.357358
C	0.214579	1.687321	-0.015411
C	1.279570	0.768861	-0.174581
N	0.795489	-0.543950	-0.330960
C	2.672406	0.922815	-0.114602
H	0.309189	2.754781	0.132566
H	3.140879	1.890782	-0.268739
C	3.391130	-0.264572	0.021183
C	2.681323	-1.373881	0.481507
H	4.392094	-0.370973	-0.389602
H	2.991452	-2.383776	0.219088
H	2.035925	-1.299604	1.345016

C-8

SCF Energy: -479.355701499

Num. Imaginary Frequencies: 1

C	-0.940217	0.784129	-0.078903
C	-0.832212	-0.633867	-0.224825
C	-1.934793	-1.449506	-0.073467
C	-3.174931	-0.842497	0.228069
C	-3.292644	0.542082	0.373348
C	-2.174671	1.373994	0.222273
H	-1.847072	-2.525478	-0.184043
H	-4.054651	-1.467785	0.348748
H	-4.259688	0.977346	0.604776
H	-2.268797	2.450332	0.336637
C	0.378320	1.268165	-0.292057
C	1.193901	0.096058	-0.559253
N	0.493148	-1.024704	-0.521553
C	2.637431	0.129888	-0.881132
H	0.725155	2.293862	-0.263058
H	2.908418	0.298949	-1.921191
C	3.650079	-0.028972	0.060527
C	3.469297	-0.264990	1.411811
H	4.672560	0.038363	-0.308888
H	4.316732	-0.374180	2.079037
H	2.477954	-0.365390	1.840498

N<sub>2</sub>  
SCF Energy: -109.559421709  
Num. Imaginary Frequencies: 0  
N 0.447250 0.000000 0.000000  
N 1.552750 0.000000 0.000000  
N 0.000000 0.000000 0.552750  
N 0.000000 0.000000 -0.552750



NC-1

SCF Energy: -436.390235639

Num. Imaginary Frequencies: 0

C	3.247083	-1.289191	1.055987
C	3.178070	-1.130404	-0.271218
C	2.436411	-0.078821	-0.990042
C	1.664480	0.839167	-0.445525
C	0.902754	1.752988	0.098427
C	-0.583032	1.632492	0.360980
C	-1.171951	0.288394	-0.049670
N	-2.620371	0.312744	0.264421
N	-3.247315	-0.712943	-0.014547
N	-3.937307	-1.599655	-0.224944
H	1.358066	2.699722	0.395778
H	2.545967	-0.071148	-2.074961
H	3.713031	-1.827358	-0.913457
H	3.819569	-2.098782	1.495680
H	2.737354	-0.615258	1.739008
H	-0.675745	-0.526864	0.492145
H	-1.016033	0.115502	-1.122089
H	-0.777347	1.800231	1.428175
H	-1.112800	2.435188	-0.168411

NC-3

SCF Energy: -436.418906761

Num. Imaginary Frequencies: 0

C	0.148396	-0.275939	-0.470110
C	0.814412	-1.437247	-0.464439
C	2.257787	-1.169666	-0.048093
C	2.207538	0.276792	0.536306
N	0.980038	0.789117	-0.079149
C	-1.191057	0.371196	-0.645476
C	-2.401882	-0.280829	-0.026901
C	-2.407617	-1.404245	0.686515
H	-1.397789	0.572844	-1.708258
H	-3.327180	0.266300	-0.194041
H	-3.330831	-1.799816	1.097701
H	-1.497121	-1.960255	0.887010
N	-0.964855	1.740418	-0.007464
N	0.242555	1.870540	0.315177
H	0.434223	-2.404029	-0.763226
H	2.632796	-1.888146	0.687977
H	2.935514	-1.215173	-0.911941
H	2.106327	0.263428	1.629140
H	3.074435	0.883951	0.268880

NC-5a

SCF Energy: -326.886172051

Num. Imaginary Frequencies: 0

C	-0.128999	-0.405108	-0.112393
C	-0.497843	0.930430	-0.371708
C	-1.964919	1.080760	-0.133552
C	-2.355045	-0.365950	0.279945
N	-1.146086	-1.188919	0.244557
C	1.210758	-0.994021	-0.271568
C	2.440980	-0.365119	-0.085707
C	2.684326	0.911371	0.390533
H	1.205870	-2.048239	-0.531636
H	3.314657	-0.970413	-0.325013
H	3.698518	1.285662	0.474007
H	1.887675	1.562021	0.731800
H	0.155190	1.707776	-0.747147
H	-2.185395	1.821507	0.648807
H	-2.495671	1.425660	-1.032274
H	-2.788124	-0.412133	1.287990
H	-3.105663	-0.803586	-0.391735

NC-5b

SCF Energy: -326.890495751

Num. Imaginary Frequencies: 0

C	0.122765	0.393214	-0.000140
C	1.314532	1.150979	0.000167
C	2.480637	0.222025	0.000172
C	1.765640	-1.160106	-0.000092
N	0.321778	-0.923068	-0.000253
C	-1.192021	1.039786	-0.000140
C	-2.441544	0.419695	-0.000007
C	-2.696290	-0.939659	0.000219
H	-1.168284	2.126064	-0.000370
H	-3.299334	1.091853	-0.000137
H	-3.719225	-1.302272	0.000318
H	-1.883072	-1.654238	0.000324
H	1.374948	2.233588	0.000243
H	3.126814	0.369772	-0.877087
H	3.126652	0.369474	0.877596
H	2.033520	-1.764106	-0.877503
H	2.033224	-1.764262	0.877303

NC-7a

SCF Energy: -326.963532724

Num. Imaginary Frequencies: 0

C	0.010472	-0.757994	0.142856
C	-0.000943	0.736238	0.426785
C	1.348582	1.126555	-0.190765
C	2.141184	-0.209101	-0.038111
N	1.142153	-1.303985	-0.095324
C	-1.372684	-1.214704	0.013527
C	-2.161091	-0.130745	-0.121833
C	-1.388815	1.181436	-0.082391
H	-1.683473	-2.250369	-0.052717
H	-3.232158	-0.164928	-0.299502
H	-1.871343	1.934072	0.550506
H	-1.332883	1.611177	-1.093568
H	0.033567	0.875194	1.517792
H	1.227350	1.363814	-1.254765
H	1.839781	1.975634	0.292674
H	2.894149	-0.354495	-0.819301
H	2.669710	-0.252318	0.925742

NC-7b

SCF Energy: -326.950701091

Num. Imaginary Frequencies: 0

C	0.019090	0.768826	-0.102892
C	-1.223385	1.253115	0.081892
C	-2.191572	0.086108	-0.027884
C	-1.252474	-1.142168	0.142915
N	0.029587	-0.625309	-0.338734
C	1.408260	1.195928	0.001179
C	2.183795	0.099244	0.071885
C	1.338759	-1.156846	0.020215
H	1.736506	2.226351	0.052746
H	3.262158	0.079977	0.181721
H	1.333367	-1.663135	1.006365
H	1.703544	-1.891776	-0.711024
H	-1.503218	2.287420	0.223493
H	-2.988302	0.098467	0.723473
H	-2.681063	0.058684	-1.013818
H	-1.183350	-1.426104	1.208928
H	-1.581586	-2.017963	-0.424602

NC-2

SCF Energy: -436.350322610

Num. Imaginary Frequencies: 1

C	2.107095	0.176485	0.676197
C	2.163548	-1.246569	0.088859
N	1.215600	0.888895	-0.245594
N	0.458640	1.820035	0.177452
N	-0.641461	2.192547	0.097166
C	0.795884	-1.555337	-0.481335
C	-0.067916	-0.578196	-0.692995
C	-1.289831	-0.017878	-0.919593
C	-2.466787	-0.242090	-0.073992
C	-2.565297	-1.077803	0.970203
H	0.556363	-2.577152	-0.770070
H	-1.452706	0.504153	-1.859763
H	-3.339516	0.343177	-0.358096
H	-3.489899	-1.166186	1.530113
H	-1.728407	-1.688459	1.296652
H	1.687080	0.155797	1.688971
H	3.098126	0.640171	0.708916
H	2.921002	-1.307561	-0.704460
H	2.458333	-1.965963	0.860507

NC-4a

SCF Energy: -436.387941269

Num. Imaginary Frequencies: 1

C	0.193904	-0.176568	-0.468952
C	0.651118	-1.423849	-0.170814
C	2.117867	-1.344219	0.143762
C	2.336307	0.199813	0.227658
N	1.168220	0.787950	-0.442612
C	-1.167766	0.260039	-0.773955
C	-2.321428	-0.521145	-0.350191
C	-2.389635	-1.234674	0.788563
H	-1.279580	0.793421	-1.715466
H	-3.193825	-0.485705	-0.999763
H	-3.271827	-1.817537	1.032886
H	-1.578095	-1.241343	1.508545
N	-1.000173	1.864711	0.293223
N	0.112878	2.082445	0.532135
H	0.080527	-2.339482	-0.265096
H	2.391860	-1.906279	1.045327
H	2.719602	-1.758279	-0.677628
H	2.379475	0.535237	1.273597
H	3.263186	0.517844	-0.258049



NC-4b

SCF Energy: -436.385810535

Num. Imaginary Frequencies: 1

C	-0.275605	-0.374616	-0.370231
C	-1.360415	-0.983265	-0.915703
C	-2.562316	-0.683401	-0.067380
C	-2.006390	0.442830	0.864955
N	-0.542887	0.364180	0.757030
C	1.093259	-0.305497	-0.889922
C	2.237795	-0.798269	-0.114523
C	2.266594	-0.940367	1.220501
H	1.180239	-0.464295	-1.962223
H	3.120052	-1.054682	-0.697720
H	3.145302	-1.342520	1.714950
H	1.417733	-0.654604	1.832890
N	1.169872	1.562667	-0.742718
N	0.388716	1.960929	0.016437
H	-1.355013	-1.641569	-1.776938
H	-3.439429	-0.399948	-0.662231
H	-2.859930	-1.553716	0.534891
H	-2.352174	1.430954	0.530227
H	-2.324218	0.321469	1.904724

NC-6a

SCF Energy: -326.873697958

Num. Imaginary Frequencies: 1

C	-0.053131	-0.599393	-0.139754
C	-0.276079	0.759779	-0.568249
C	-1.689455	1.103742	-0.208883
C	-2.229722	-0.277803	0.287196
N	-1.094682	-1.210445	0.357585
C	1.309359	-1.116847	-0.284059
C	2.303920	-0.208439	-0.040402
C	2.010075	1.049799	0.552916
H	1.494631	-2.140821	-0.589046
H	3.329765	-0.424175	-0.339082
H	2.682260	1.893760	0.424241
H	1.287532	1.132254	1.353942
H	0.297098	1.255391	-1.339625
H	-1.731999	1.866810	0.581902
H	-2.248262	1.512574	-1.059046
H	-2.708163	-0.213164	1.271394
H	-2.989891	-0.674546	-0.400366

NC-6b

SCF Energy: -326.865002946

Num. Imaginary Frequencies: 1

C	-0.073571	0.573172	-0.203151
C	-1.290356	1.170027	0.063710
C	-2.342217	0.104640	0.136378
C	-1.467268	-1.188865	0.112259
N	-0.156923	-0.769964	-0.399217
C	1.240568	1.186492	-0.115088
C	2.273991	0.346878	0.152758
C	2.120872	-1.082316	0.076785
H	1.336130	2.265954	-0.062848
H	3.209356	0.754337	0.540424
H	2.603983	-1.699223	0.835519
H	1.902840	-1.575710	-0.856912
H	-1.474226	2.236167	0.132589
H	-3.003531	0.200144	1.006458
H	-2.989448	0.127252	-0.753552
H	-1.367335	-1.600833	1.127457
H	-1.891430	-1.978503	-0.516519

NC-8

SCF Energy: -326.882955991

Num. Imaginary Frequencies: 1

C	-0.087597	0.247378	-0.378400
C	-0.889716	1.093898	0.403995
C	-2.224767	0.448412	0.603730
C	-2.030790	-0.885145	-0.170312
N	-0.675303	-0.896218	-0.732418
C	1.289991	0.571527	-0.829692
C	2.443264	0.146761	-0.178723
C	2.488355	-0.636161	0.961572
H	1.382329	1.176351	-1.728274
H	3.391480	0.463286	-0.611413
H	3.434079	-0.922187	1.407705
H	1.582021	-0.999891	1.433326
H	-0.591619	2.057224	0.800517
H	-2.454955	0.292928	1.667072
H	-3.046285	1.057684	0.201002
H	-2.150862	-1.766219	0.473159
H	-2.751506	-1.005664	-0.989195

phenyl-22

SCF Energy: -672.413769228

Num. Imaginary Frequencies: 0

C	2.208519	0.862093	-0.107358
C	1.516638	-0.379768	0.082912
C	2.195258	-1.597482	0.202350
C	3.583491	-1.572910	0.122359
C	4.284429	-0.365775	-0.075975
C	3.612413	0.843973	-0.191142
H	1.660956	-2.529485	0.358927
H	4.137816	-2.502233	0.214373
H	5.368546	-0.386104	-0.136456
H	4.162677	1.769402	-0.336980
C	1.225310	1.906784	-0.164682
C	-0.001114	1.292566	-0.021916
N	0.174482	-0.083186	0.098057
C	-1.419824	1.580808	0.068112
H	1.410160	2.964637	-0.283727
C	-2.073524	0.398157	0.277288
C	-2.003212	2.948124	-0.101203
C	-1.076276	-0.743673	0.449587
C	-3.471716	0.057891	0.226957
C	-1.505457	-1.989645	-0.285417
H	-1.028874	-1.008521	1.524097
H	-3.089743	2.942984	0.009975
H	-1.588410	3.644032	0.637421
H	-1.765006	3.354341	-1.091238
C	-2.823929	-2.214635	-0.445460
H	-0.758290	-2.725135	-0.566777
H	-3.166398	-3.151555	-0.876557
C	-3.828102	-1.215776	-0.089772
H	-4.225343	0.830186	0.351657
H	-4.876889	-1.484645	-0.170950

phenyl-21  
SCF Energy: -672.401713830  
Num. Imaginary Frequencies: 0

C	-1.598443	-0.533048	0.185242
C	-2.158526	0.759432	0.001803
C	-3.524923	0.921345	-0.219082
C	-4.329693	-0.221429	-0.253772
C	-3.783681	-1.495595	-0.067811
C	-2.410523	-1.657983	0.165633
H	-3.939819	1.913241	-0.365531
H	-5.396850	-0.118365	-0.428894
H	-4.429343	-2.368026	-0.103753
H	-1.997744	-2.651805	0.318754
C	-0.145488	-0.305137	0.495117
C	-0.061650	1.193059	0.259436
N	-1.188428	1.793880	0.021708
C	1.320971	1.593953	0.087556
H	0.044802	-0.518869	1.556151
C	2.033293	0.448524	-0.161354
C	1.790290	3.014359	0.109416
C	1.114775	-0.776025	-0.298987
C	3.455773	0.259999	-0.276067
C	1.787467	-2.069390	0.055857
H	0.809025	-0.846192	-1.356655
H	2.823102	3.114885	-0.233070
H	1.148381	3.628200	-0.531798
H	1.723501	3.438082	1.118501
C	3.131986	-2.154644	0.075596
H	1.169585	-2.948649	0.220331
H	3.617134	-3.106733	0.272511
C	3.976011	-0.991009	-0.167069
H	4.109290	1.123302	-0.364091
H	5.052094	-1.134701	-0.203494

(Z)-18→phenyl-22

SCF Energy: -672.377929291

Num. Imaginary Frequencies: 1

C	2.316031	0.795514	0.020206
C	1.614749	-0.465866	-0.125047
C	2.329298	-1.683594	-0.228924
C	3.704395	-1.639285	-0.158389
C	4.403496	-0.404914	-0.007941
C	3.733818	0.795907	0.074514
H	1.797291	-2.622414	-0.349012
H	4.276051	-2.560709	-0.222194
H	5.488660	-0.421045	0.038557
H	4.278437	1.728997	0.190879
C	1.332538	1.803570	0.045279
C	0.097458	1.136934	-0.044957
N	0.286295	-0.244355	-0.225930
C	-1.252676	1.534155	0.091008
H	1.483202	2.864017	0.195251
C	-2.097172	0.428092	0.272370
C	-1.697259	2.956048	-0.077090
C	-1.400866	-0.799382	0.661085
C	-3.449633	0.359309	-0.168890
C	-2.046854	-2.047201	0.374692
H	-0.797996	-0.762295	1.563020
H	-2.698959	3.123093	0.324742
H	-1.006794	3.632431	0.436398
H	-1.696411	3.245826	-1.134908
C	-3.323683	-2.060444	-0.126795
H	-1.546057	-2.975253	0.631261
H	-3.817918	-3.013816	-0.295578
C	-4.051707	-0.857649	-0.371296
H	-3.967008	1.278109	-0.429101
H	-5.068146	-0.913617	-0.746735

(E)-18→phenyl-21

SCF Energy: -672.375910819

Num. Imaginary Frequencies: 1

C	1.684296	-0.560958	-0.314220
C	2.202101	0.714343	0.103062
C	3.573585	0.855921	0.386722
C	4.397503	-0.246542	0.225082
C	3.894901	-1.495739	-0.213462
C	2.546997	-1.658505	-0.488842
H	3.961830	1.813812	0.717501
H	5.459942	-0.153213	0.433533
H	4.578028	-2.331453	-0.331636
H	2.161828	-2.619482	-0.819966
C	0.285966	-0.346467	-0.537851
C	0.104627	1.086940	-0.163669
N	1.235374	1.697861	0.180700
C	-1.234619	1.543007	-0.046588
H	-0.233023	-0.789573	-1.379132
C	-2.085550	0.450656	0.178422
C	-1.614037	2.987663	-0.138360
C	-1.399718	-0.758700	0.647900
C	-3.469274	0.375963	-0.162147
C	-2.091796	-2.011973	0.531330
H	-0.736260	-0.655603	1.499243
H	-2.599426	3.187844	0.289214
H	-0.865890	3.585243	0.392444
H	-1.611740	3.335504	-1.178909
C	-3.387903	-2.045680	0.089256
H	-1.595389	-2.922919	0.852639
H	-3.913244	-2.994573	0.026044
C	-4.095460	-0.842463	-0.224305
H	-3.991669	1.280505	-0.459749
H	-5.132318	-0.905908	-0.540108



phenyl-(Z)-18

SCF Energy: -672.414957160

Num. Imaginary Frequencies: 0

C	2.566829	0.713487	0.066587
C	1.990196	-0.629269	-0.097184
C	2.862332	-1.756577	-0.233848
C	4.211561	-1.541760	-0.199733
C	4.778164	-0.223115	-0.034455
C	3.988004	0.883197	0.095953
H	2.440309	-2.748539	-0.358728
H	4.892718	-2.382515	-0.299143
H	5.859608	-0.124706	-0.016315
H	4.422319	1.871386	0.219644
C	1.490485	1.562326	0.156405
C	0.303069	0.717328	0.053036
N	0.666939	-0.625753	-0.105136
C	-1.011565	1.151109	0.080002
H	1.522757	2.633902	0.290370
C	-2.180182	0.254145	0.035308
C	-1.303805	2.631543	0.133316
C	-2.123142	-1.091642	0.462995
C	-3.428142	0.748317	-0.406581
C	-3.257768	-1.895863	0.436216
H	-1.175688	-1.488179	0.799883
C	-4.477620	-1.391857	-0.019570
H	-3.188602	-2.924656	0.777154
H	-5.359522	-2.025588	-0.040116
C	-4.556248	-0.064812	-0.444854
H	-3.517359	1.773709	-0.746318
H	-5.497839	0.339308	-0.804606
H	-2.074606	2.850319	0.878497
H	-0.420937	3.222046	0.367354
H	-1.684744	2.984446	-0.833280

phenyl-(E)-18

SCF Energy: -672.417118706

Num. Imaginary Frequencies: 0

C	2.059523	-0.768051	-0.187935
C	2.446617	0.621076	0.112626
C	3.835566	0.954821	0.221448
C	4.758561	-0.033539	0.027497
C	4.378910	-1.393918	-0.278757
C	3.069126	-1.763866	-0.388093
H	4.124044	1.975748	0.449747
H	5.817778	0.197403	0.101526
H	5.165592	-2.128974	-0.421726
H	2.793030	-2.789374	-0.617193
C	0.685780	-0.767083	-0.215476
C	0.288102	0.610557	0.060384
N	1.409097	1.431138	0.245113
C	-0.986765	1.133881	0.089159
H	0.026605	-1.587993	-0.457380
C	-2.193320	0.287581	0.045048
C	-1.173838	2.623262	0.168795
C	-2.273060	-0.912383	0.780142
C	-3.325326	0.689478	-0.691956
C	-3.427290	-1.691868	0.753091
H	-1.434730	-1.206883	1.401178
C	-4.528296	-1.292706	-0.005986
H	-3.470432	-2.606757	1.336592
H	-5.427644	-1.900935	-0.026269
C	-4.472130	-0.098352	-0.727974
H	-3.295283	1.612101	-1.262117
H	-5.325329	0.221278	-1.318905
H	-1.900381	2.884700	0.945487
H	-0.217712	3.108515	0.359854
H	-1.572182	3.009859	-0.778667

phenyl-tau-14  
SCF Energy: -672.430536982  
Num. Imaginary Frequencies: 0

C	2.113166	-0.715698	-0.303882
C	2.467437	0.557059	0.185100
C	3.796220	0.893622	0.435835
C	4.773863	-0.073028	0.184841
C	4.427050	-1.339144	-0.300436
C	3.088152	-1.672420	-0.548063
H	4.051281	1.878636	0.812705
H	5.818493	0.160662	0.368901
H	5.205274	-2.073207	-0.487387
H	2.829569	-2.658670	-0.924272
C	0.616730	-0.712721	-0.441974
C	0.292778	0.702802	0.028690
N	1.342046	1.386913	0.374077
C	-1.065722	1.286109	0.018160
H	0.268625	-0.868566	-1.471791
C	-2.247377	0.376139	0.046135
C	-1.217911	2.621365	-0.046663
C	-2.371871	-0.620974	1.028153
C	-3.281749	0.521165	-0.891452
C	-3.496857	-1.443015	1.072665
H	-1.594201	-0.732123	1.778735
H	-0.351995	3.272103	-0.092972
H	-2.202950	3.076075	-0.034636
C	-4.517657	-1.288038	0.132613
H	-3.579475	-2.200833	1.846441
H	-5.392072	-1.931238	0.165138
C	-4.406789	-0.302190	-0.848564
H	-3.190122	1.277821	-1.664967
H	-5.193926	-0.177122	-1.586573
H	0.120403	-1.478124	0.165184

phenyl-14  
SCF Energy: -672.447326082  
Num. Imaginary Frequencies: 0

C	2.082144	-0.683480	-0.337120
C	2.505716	0.569797	0.189647
C	3.847460	0.845542	0.472732
C	4.776377	-0.154316	0.209176
C	4.381730	-1.399225	-0.324537
C	3.048857	-1.671382	-0.599604
H	4.154188	1.805070	0.879245
H	5.826880	0.027637	0.415633
H	5.136788	-2.154532	-0.521093
H	2.753257	-2.633124	-1.009228
C	0.658784	-0.615078	-0.472609
C	0.253296	0.636282	-0.051309
N	1.381881	1.354517	0.331700
C	-1.081225	1.242534	-0.029724
H	0.006482	-1.381331	-0.864417
C	-2.262738	0.334210	0.025152
C	-1.245696	2.581514	-0.058001
C	-2.286239	-0.784531	0.874733
C	-3.398678	0.602679	-0.756056
C	-3.416280	-1.597400	0.950987
H	-1.416727	-1.007674	1.483956
H	1.346689	2.235591	0.818070
H	-0.409375	3.262880	-0.177651
H	-2.229657	3.028514	0.023424
C	-4.541237	-1.314433	0.174361
H	-3.418381	-2.452248	1.621166
H	-5.418969	-1.951587	0.230989
C	-4.527226	-0.211950	-0.681464
H	-3.382281	1.445556	-1.440109
H	-5.392334	0.009042	-1.300063

phenyl-(Z)-18→tau-14  
SCF Energy: -672.343949778  
Num. Imaginary Frequencies: 1

C	-1.037107	0.944840	-0.256170
C	-0.879060	2.344955	-0.479549
C	-2.296704	0.240792	-0.071082
C	-3.531374	0.859526	-0.360741
C	-4.729623	0.184426	-0.155935
C	-4.721775	-1.129637	0.319793
C	-3.506241	-1.765308	0.588305
C	-2.305900	-1.089310	0.402066
H	-1.694781	3.028339	-0.239359
H	-0.352916	2.631729	-1.392205
H	0.421602	2.343027	0.074289
H	-3.543534	1.865260	-0.767476
H	-5.671176	0.675942	-0.381802
H	-5.658120	-1.658976	0.469853
H	-3.496458	-2.789341	0.949164
H	-1.361117	-1.580584	0.606537
C	0.265971	0.352024	-0.102401
C	1.233130	1.263325	0.578012
N	0.809521	-0.737460	-0.615031
C	2.491245	0.596740	0.357143
C	2.165498	-0.610310	-0.348510
C	3.818782	0.852447	0.742846
C	4.802881	-0.056121	0.385725
C	4.481642	-1.228615	-0.337981
C	3.177433	-1.517336	-0.708484
H	1.003418	1.643575	1.575572
H	4.072096	1.754376	1.293594
H	5.836863	0.131324	0.659934
H	5.278154	-1.918798	-0.602042
H	2.926542	-2.418282	-1.259071

phenyl-(E)-18→14

SCF Energy: -672.371222127

Num. Imaginary Frequencies: 1

C	2.203606	-0.762230	-0.336252
C	2.422884	0.559640	0.219894
C	3.723875	0.989719	0.570369
C	4.775834	0.132662	0.329210
C	4.575881	-1.160447	-0.238594
C	3.316752	-1.611548	-0.566170
H	3.878888	1.973287	1.002673
H	5.786945	0.444281	0.575642
H	5.439607	-1.796021	-0.410539
H	3.174323	-2.596983	-1.001395
C	0.811378	-0.905137	-0.502485
C	0.252292	0.319422	-0.089679
N	1.234933	1.181507	0.380593
C	-1.016693	0.964664	-0.145833
H	0.283783	-1.729407	-0.962111
C	-2.290465	0.259736	-0.019792
C	-0.860250	2.388347	-0.161650
C	-2.360573	-1.025514	0.556475
C	-3.481491	0.859550	-0.475685
C	-3.579170	-1.687621	0.663811
H	-1.453418	-1.481420	0.938021
H	0.394254	2.242169	0.431672
H	-0.356925	2.808516	-1.035089
H	-1.692249	3.000638	0.180298
C	-4.750902	-1.079244	0.205500
H	-3.619638	-2.673970	1.115988
H	-5.701900	-1.596442	0.293180
C	-4.699057	0.196007	-0.363594
H	-3.434033	1.839013	-0.940105
H	-5.607576	0.667750	-0.725544

phenyl-(E)-18→phenyl-(Z)-18

SCF Energy: -672.371274039

Num. Imaginary Frequencies: 1

C	2.362216	0.153128	0.751136
C	2.235031	-0.035917	-0.660604
C	3.296174	-0.494328	-1.414021
C	4.513075	-0.770301	-0.750542
C	4.649199	-0.590358	0.628603
C	3.573717	-0.126531	1.397848
H	3.194129	-0.637309	-2.484902
H	5.360110	-1.130261	-1.327127
H	5.597653	-0.811734	1.107765
H	3.681647	0.011793	2.470060
C	1.086258	0.615668	1.167872
C	0.271535	0.677114	-0.036202
N	0.937660	0.295836	-1.112700
C	-1.129156	1.162936	-0.085762
H	0.763835	0.869373	2.170413
C	-2.224062	0.250237	-0.025748
C	-1.334106	2.650382	-0.212868
C	-2.014785	-1.156149	0.070962
C	-3.574811	0.702493	-0.055017
C	-3.081552	-2.038969	0.141943
H	-0.999613	-1.537674	0.074863
C	-4.400339	-1.567799	0.116646
H	-2.889111	-3.105836	0.213387
H	-5.232762	-2.262694	0.171170
C	-4.633954	-0.191118	0.015032
H	-3.781644	1.764096	-0.135679
H	-5.653221	0.184439	-0.010155
H	-1.806505	2.910303	-1.170612
H	-1.982747	3.048218	0.578922
H	-0.382033	3.183504	-0.164872

22

SCF Energy: -518.774131145

Num. Imaginary Frequencies: 0

C	1.068291	-0.945830	0.000104
C	0.902312	0.477560	-0.000025
C	1.990006	1.355970	-0.000079
C	3.265651	0.800919	-0.000058
C	3.455152	-0.595626	0.000020
C	2.373451	-1.467828	0.000082
H	1.846066	2.432387	-0.000146
H	4.131341	1.456733	-0.000112
H	4.465676	-0.993554	0.000024
H	2.532041	-2.542786	0.000141
C	-0.242138	-1.540159	-0.000005
C	-1.136821	-0.495223	-0.000118
N	-0.452260	0.711758	-0.000134
C	-2.564732	-0.187816	-0.000189
H	-0.475222	-2.595112	-0.000016
C	-2.700771	1.156403	-0.000152
C	-3.642876	-1.225879	0.000054
C	-1.354312	1.851245	0.000244
H	-3.635883	1.703208	0.000088
H	-1.208607	2.484681	0.886775
H	-1.208601	2.485761	-0.885477
H	-4.635491	-0.769056	0.000092
H	-3.562490	-1.873635	-0.880489
H	-3.562289	-1.873349	0.880793



21

SCF Energy: -518.757119144

Num. Imaginary Frequencies: 0

C	0.967345	0.584588	0.170160
C	0.996053	-0.828056	0.034777
C	2.197289	-1.505994	-0.151286
C	3.377713	-0.756558	-0.205321
C	3.355347	0.634432	-0.069634
C	2.145541	1.315237	0.133467
H	2.204400	-2.585905	-0.257199
H	4.326409	-1.263639	-0.356512
H	4.284178	1.194767	-0.121993
H	2.139666	2.396051	0.247938
C	-0.466645	0.934158	0.469955
C	-1.107512	-0.420988	0.255363
N	-0.301772	-1.413620	0.057873
C	-2.539537	-0.249592	0.011872
H	-0.544643	1.187836	1.538457
C	-2.722766	1.053808	-0.300243
C	-3.534244	-1.367033	-0.002811
C	-1.438178	1.871279	-0.296602
H	-3.678987	1.485135	-0.583828
H	-1.559086	2.856157	0.166795
H	-1.091667	2.039447	-1.324199
H	-4.517978	-1.027507	-0.336872
H	-3.191742	-2.166415	-0.668785
H	-3.640585	-1.812269	0.992915

(Z)-18→22

SCF Energy: -518.701721584

Num. Imaginary Frequencies: 1

C	-1.120722	-0.890683	0.085825
C	-0.936579	0.534874	-0.150979
C	-2.061958	1.395195	-0.267449
C	-3.315250	0.853694	-0.113451
C	-3.502341	-0.543232	0.135787
C	-2.437091	-1.407279	0.229703
H	-1.917514	2.454358	-0.457882
H	-4.190940	1.492691	-0.183502
H	-4.514658	-0.921302	0.247334
H	-2.594487	-2.465689	0.419209
C	0.160254	-1.459851	0.066789
C	1.056561	-0.381416	-0.114996
N	0.361188	0.823123	-0.324440
C	2.464252	-0.309227	-0.044386
H	0.426194	-2.490067	0.261786
C	2.948889	1.000783	0.067371
C	3.347562	-1.515025	-0.172268
C	2.059537	1.979563	0.500643
H	3.914474	1.272341	-0.353498
H	2.202411	3.022340	0.222522
H	1.417646	1.815119	1.354036
H	4.328874	-1.239800	-0.569690
H	3.516918	-1.968823	0.812624
H	2.904072	-2.277411	-0.817392

(E)-18→21

SCF Energy: -518.701737643

Num. Imaginary Frequencies: 1

C	-1.020743	0.625534	-0.257356
C	-1.035011	-0.771853	0.106177
C	-2.261633	-1.412928	0.370607
C	-3.428573	-0.678939	0.247947
C	-3.419999	0.688780	-0.134121
C	-2.230870	1.342383	-0.391937
H	-2.274434	-2.460061	0.655308
H	-4.383415	-1.160406	0.441632
H	-4.362902	1.220187	-0.220636
H	-2.223844	2.391071	-0.677432
C	0.341035	0.933213	-0.479692
C	1.045808	-0.331815	-0.161115
N	0.219216	-1.334956	0.143263
C	2.466569	-0.334076	-0.108902
H	0.701546	1.677199	-1.176282
C	2.972803	0.934470	0.172196
C	3.276081	-1.576010	-0.313994
C	2.106595	1.863309	0.766189
H	3.984396	1.222742	-0.111279
H	2.314060	2.930614	0.711868
H	1.429808	1.564559	1.553887
H	4.348754	-1.380286	-0.242966
H	3.001833	-2.313925	0.448830
H	3.057324	-2.039401	-1.281768

(Z)-18

SCF Energy: -518.724414059

Num. Imaginary Frequencies: 0

C	-1.250350	-0.833340	-0.000006
C	-1.001322	0.616456	0.000019
C	-2.111797	1.518635	0.000030
C	-3.374742	0.994847	0.000012
C	-3.619923	-0.428333	-0.000014
C	-2.593080	-1.329091	-0.000021
H	-1.933449	2.589096	0.000052
H	-4.232692	1.661738	0.000019
H	-4.649022	-0.775254	-0.000026
H	-2.784836	-2.398523	-0.000036
C	-0.005300	-1.414790	-0.000015
C	0.950524	-0.310865	-0.000002
N	0.288611	0.918720	0.000026
C	2.329369	-0.425615	-0.000009
H	0.218092	-2.472079	-0.000071
C	3.274314	0.688850	0.000034
C	2.996809	-1.777324	0.000015
C	3.010343	2.008668	-0.000064
H	4.319446	0.379715	0.000121
H	3.829575	2.722255	-0.000022
H	1.990290	2.372719	-0.000188
H	2.298085	-2.611469	-0.000132
H	3.647722	-1.873862	-0.877970
H	3.647448	-1.873953	0.878197

(E)-18

SCF Energy: -518.725074466

Num. Imaginary Frequencies: 0

C	1.093835	-0.742376	-0.135467
C	1.151462	0.714563	0.079085
C	2.425717	1.351793	0.227800
C	3.550803	0.580403	0.153167
C	3.494784	-0.846946	-0.067012
C	2.305685	-1.502176	-0.210627
H	2.471902	2.423409	0.392368
H	4.528134	1.043176	0.260076
H	4.429303	-1.398139	-0.115949
H	2.272761	-2.575800	-0.373746
C	-0.242335	-1.043789	-0.239998
C	-0.943523	0.226927	-0.078827
N	-0.042871	1.284443	0.096012
C	-2.302175	0.449557	-0.116768
H	-0.694404	-1.999499	-0.460774
C	-3.292015	-0.626942	-0.160485
C	-2.844428	1.850505	-0.133111
C	-3.241815	-1.772568	0.536569
H	-4.183659	-0.417431	-0.752485
H	-4.040643	-2.504474	0.467725
H	-2.424078	-1.992481	1.214439
H	-2.034766	2.575851	-0.071315
H	-3.416084	2.017503	-1.055905
H	-3.544333	2.003066	0.697520

tau-14

SCF Energy: -518.741355790

Num. Imaginary Frequencies: 0

C	-1.307125	-0.807291	0.000031
C	-1.013448	0.568626	-0.000032
C	-2.022800	1.528162	-0.000066
C	-3.347495	1.081693	-0.000038
C	-3.645542	-0.285333	0.000023
C	-2.623316	-1.245284	0.000058
H	-1.777149	2.585026	-0.000112
H	-4.157324	1.805341	-0.000063
H	-4.682547	-0.607799	0.000044
H	-2.866737	-2.304392	0.000106
C	0.015652	-1.522403	0.000051
C	0.982816	-0.335543	-0.000008
N	0.376591	0.813465	-0.000051
C	2.449886	-0.489830	-0.000028
H	0.158681	-2.159441	0.881351
C	3.378867	0.656993	-0.000025
C	2.975798	-1.735710	-0.000060
C	3.103968	1.966971	0.000127
H	4.425219	0.352275	-0.000168
H	3.917952	2.686255	0.000115
H	2.088586	2.339195	0.000245
H	0.158664	-2.159522	-0.881197
H	4.050311	-1.886999	-0.000079
H	2.364638	-2.630489	-0.000074

14

SCF Energy: -518.755389437

Num. Imaginary Frequencies: 0

C	-1.093629	0.680514	-0.271416
C	-1.194746	-0.668610	0.170966
C	-2.423235	-1.268705	0.466093
C	-3.568436	-0.499005	0.299034
C	-3.494142	0.835655	-0.151771
C	-2.272670	1.429624	-0.437848
H	-2.482204	-2.297976	0.808404
H	-4.539056	-0.934621	0.516698
H	-4.410739	1.404945	-0.274471
H	-2.225228	2.458725	-0.782659
C	0.301482	0.956202	-0.446604
C	1.000555	-0.190954	-0.130478
N	0.085479	-1.176587	0.223743
C	2.437143	-0.499161	-0.199504
H	0.738821	1.873194	-0.812160
C	3.432887	0.533494	0.138578
C	2.858331	-1.730665	-0.561628
C	3.212770	1.694259	0.767965
H	4.453562	0.278079	-0.142250
H	4.033571	2.371467	0.981410
H	2.224740	1.995353	1.097230
H	0.348077	-2.060974	0.628314
H	3.915136	-1.975565	-0.588811
H	2.167111	-2.512403	-0.858241

(Z)-18→tau-14

SCF Energy: -518.651365043

Num. Imaginary Frequencies: 1

C	-1.199247	0.712785	-0.223234
C	-1.040947	-0.649172	0.200034
C	-2.166874	-1.456897	0.429188
C	-3.423245	-0.912151	0.208189
C	-3.583523	0.419941	-0.238014
C	-2.482715	1.232495	-0.463687
H	-2.040309	-2.480801	0.765900
H	-4.307196	-1.521541	0.374783
H	-4.584472	0.807881	-0.402255
H	-2.611506	2.257206	-0.801765
C	0.139650	1.222658	-0.385117
C	0.974939	0.059709	0.035172
N	0.290161	-1.022593	0.349363
C	2.359587	0.415290	0.200461
H	0.392041	1.764899	-1.298526
C	3.492314	-0.388131	-0.199654
C	2.442606	1.742210	0.710299
C	3.392315	-1.668316	-0.604640
H	4.471045	0.079691	-0.112348
H	4.276534	-2.248843	-0.846421
H	2.427791	-2.162239	-0.665344
H	2.009173	1.908066	1.698697
H	3.360985	2.314267	0.563467
H	1.145627	2.057038	0.264276



(E)-18→14

SCF Energy: -518.676340880

Num. Imaginary Frequencies: 1

C	1.105535	-0.770921	-0.220757
C	1.116505	0.632860	0.144787
C	2.333838	1.299991	0.414847
C	3.506039	0.587921	0.279002
C	3.509892	-0.786357	-0.102664
C	2.336701	-1.464644	-0.347348
H	2.333843	2.345838	0.705527
H	4.455958	1.080731	0.465932
H	4.461714	-1.300647	-0.197780
H	2.349449	-2.510784	-0.640978
C	-0.247647	-1.145350	-0.347459
C	-0.988999	0.024780	-0.098322
N	-0.153785	1.084319	0.232656
C	-2.340906	0.458054	-0.215037
H	-0.639103	-2.093124	-0.690412
C	-3.498635	-0.383897	0.048720
C	-2.408032	1.867397	-0.444574
C	-3.444313	-1.582284	0.654910
H	-4.460811	0.013205	-0.267042
H	-4.338940	-2.178988	0.801825
H	-2.508240	-1.986528	1.026451
H	-1.157219	2.006942	0.146794
H	-1.963210	2.227347	-1.374776
H	-3.336820	2.380472	-0.200763

(E)-18→(Z)-18

SCF Energy: -518.685436609

Num. Imaginary Frequencies: 1

C	1.194167	-0.558442	-0.535943
C	1.096130	0.375174	0.542705
C	2.223870	0.964728	1.075897
C	3.478877	0.618596	0.525920
C	3.587212	-0.292185	-0.528306
C	2.444341	-0.892440	-1.073600
H	2.144295	1.673504	1.893792
H	4.377922	1.072068	0.932832
H	4.566248	-0.536356	-0.928352
H	2.530906	-1.599885	-1.893653
C	-0.147472	-0.937130	-0.806287
C	-0.967985	-0.195941	0.138019
N	-0.247439	0.574596	0.934072
C	-2.445105	-0.306111	0.246135
H	-0.506046	-1.626462	-1.561088
C	-3.289241	0.581204	-0.424764
C	-2.976235	-1.411695	1.115128
C	-2.900568	1.643744	-1.218654
H	-4.359005	0.409118	-0.303391
H	-3.636720	2.274859	-1.703305
H	-1.855021	1.891029	-1.366523
H	-2.650055	-1.278237	2.155515
H	-4.069433	-1.444931	1.099734
H	-2.598966	-2.393888	0.798429

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