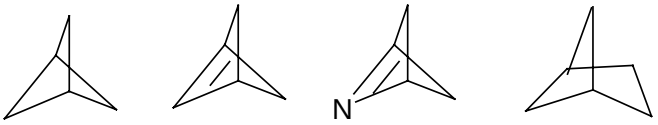
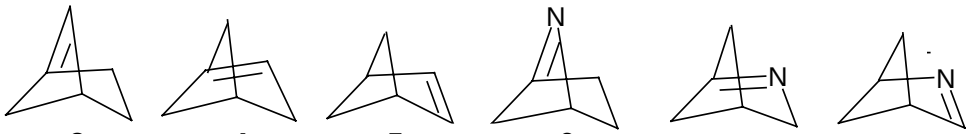
Supporting Information:

- **scheme listing structural formulas for compounds 1-40**
- **optimized geometries, G3B3 enthalpies and ZPE for closed shell alkenes and imines**
- **isodesmic reactions used to determine strain energies and enthalpies**
- **DFT optimized geometries of bridgehead alkenes and imines with diradical character**
- **all structures listed have NIMAG=0**

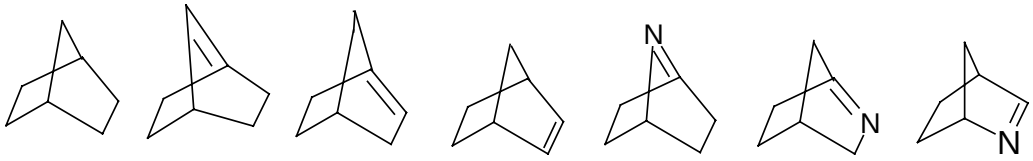
(x,y,z, in Angstroms; energies in a.u.)



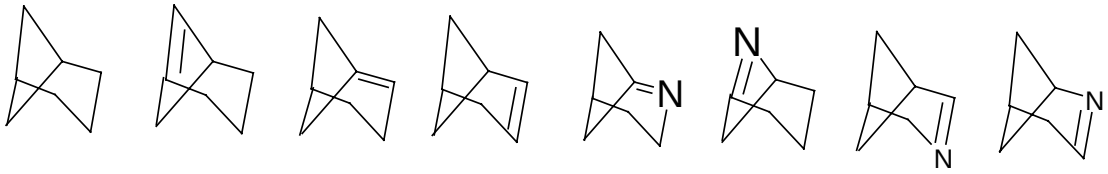
1 **1a** **1b** **2**



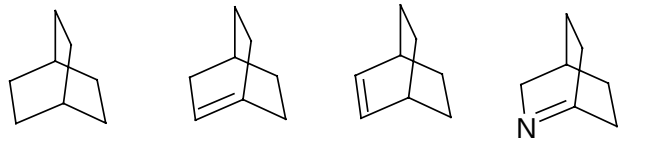
3 **4** **5** **6** **7** **8**



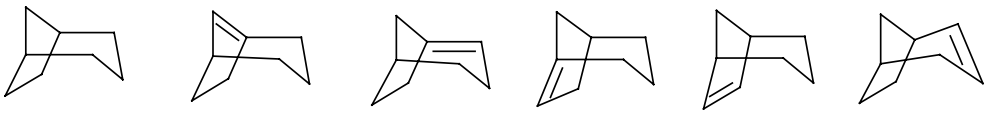
9 **10** **11** **12** **13** **14** **15**



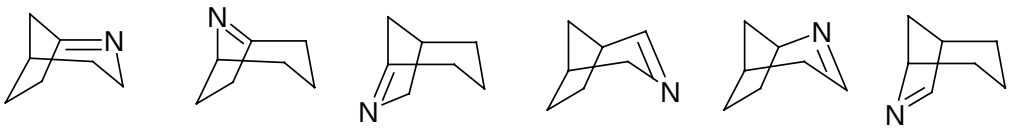
16 **17** **18** **19** **20** **21** **22** **23**



24 **25** **26** **27** **28**



29 **30** **31** **32** **33** **34**



35 **36** **37** **38** **39** **40**

Scheme 1

Compound **1**

	x	y	z
c	0.422083	0.095236	-0.279010
c	-0.537323	-0.859914	-1.047065
c	-0.557820	-0.009182	0.925427
c	1.124245	-1.177763	0.276989
c	-0.402785	-1.459758	0.382943
h	0.902045	0.999659	-0.664202
h	-0.101361	-1.440872	-1.867512
h	-1.518365	-0.456399	-1.321591
h	-0.140986	0.192934	1.918450
h	-1.540359	0.459994	0.802594
h	1.687818	-1.782810	-0.441962
h	1.671106	-1.066541	1.219992
h	-0.882691	-2.364179	0.768194

total energy = -195.071974; ZPE=0.113009

Compound **2**

	x	y	z
c	-1.224021	0.721388	0.027239
c	-0.563913	-0.643445	0.380860
c	0.258032	1.163216	-0.151532
c	0.070121	-1.051390	-0.964992
c	0.697482	0.326433	-1.370823
c	0.571586	0.200627	1.031098
h	-1.705060	1.194120	0.889243
h	-1.887524	0.765976	-0.845361
h	-1.099730	-1.416373	0.938339
h	0.552751	2.215878	-0.132609
h	0.822199	-1.839683	-0.848188
h	-0.676196	-1.403854	-1.685759
h	1.787615	0.280286	-1.471733
h	0.289992	0.715613	-2.310632
h	1.575275	-0.238238	1.090335
h	0.285860	0.616900	2.002286

total energy = -234.389055; ZPE=0.141979

Compound **3**

	x	y	z
c	-1.496135	0.565336	-0.175246
c	-0.801932	-0.902666	-0.155571
c	-0.139781	1.239704	-0.145768
c	0.725553	-0.450140	-0.110918
c	0.679424	0.713937	-1.136585
c	0.644366	0.628051	1.009396
h	-2.141389	0.753958	0.687928
h	-2.061236	0.722923	-1.097089
h	-1.102735	-1.547207	0.682310
h	-1.049240	-1.426102	-1.086872
h	1.486142	-1.243732	-0.122557
h	0.370490	0.633097	-2.180527

h	1.591527	1.123918	1.212298
h	0.117514	0.359229	1.929564

total energy = -233.065589; ZPE=0.116314

Compound **3 (DFT, diradical, triplet)**

	x	y	z
c	-1.256604	-0.546465	-0.301932
c	-0.938866	0.958368	0.050963
c	0.171595	-1.091467	-0.145102
c	0.593882	0.822436	0.303637
c	0.676732	-0.455188	1.133327
c	1.046598	-0.067962	-0.909547
h	-1.642896	-0.671196	-1.316157
h	-1.960038	-1.002784	0.396212
h	-1.158481	1.638021	-0.776505
h	-1.474525	1.307604	0.935886
h	1.147784	1.722651	0.579389
h	0.492657	-0.645865	2.185146
h	2.111631	-0.293291	-0.880954
h	0.723850	0.226527	-1.911094

total energy = -233.316802; ZPE=0.119285

Compound **4**

	x	y	z
c	-1.242848	0.857837	-0.032332
c	-0.879732	-0.533765	0.510274
c	0.273670	1.296070	-0.249134
c	0.466100	-0.401364	0.797418
c	1.044681	-0.058934	-0.626861
c	0.732804	1.046664	1.209959
h	-1.771311	1.582905	0.598675
h	-1.829938	0.727734	-0.949455
h	-1.216525	-1.392297	-0.072106
h	0.520799	2.239521	-0.763296
h	2.130205	0.085928	-0.679037
h	0.682645	-0.639833	-1.477801
h	1.795977	1.257633	1.364965
h	0.130991	1.480052	2.014594

total energy = -233.059581; ZPE=0.116353

Compound **4 (DFT, diradical, triplet)**

	x	y	z
c	1.195553	0.696866	0.038486
c	1.148390	-0.816426	-0.098407
c	-0.341284	0.937662	0.077938
c	-0.314441	-1.058596	-0.084504
c	-0.828279	-0.162374	1.079576
c	-0.866509	0.008139	-1.068905
h	1.677886	1.199777	-0.808910
h	1.694318	1.041929	0.952908

h	1.959158	-1.523169	-0.018126
h	-0.693520	1.967781	0.165390
h	-1.913430	-0.175150	1.188530
h	-0.328687	-0.240656	2.045465
h	-1.954684	0.012699	-1.138469
h	-0.401623	0.085162	-2.051891

total energy = -233.3271493; ZPE=0.118417

Compound **5**

	x	y	z
c	-1.069840	0.399665	1.162042
c	-1.002559	-0.800576	0.571456
c	0.285469	1.038294	0.818364
c	0.388400	-0.793894	-0.082822
c	0.403166	0.649515	-0.697007
c	1.242844	-0.176828	1.079011
h	-1.864793	0.847495	1.746602
h	-1.727527	-1.605310	0.539544
h	0.501426	2.044393	1.184635
h	0.710116	-1.673827	-0.644272
h	1.365780	0.924121	-1.145375
h	-0.426358	0.926794	-1.355175
h	2.284941	0.019551	0.798615
h	1.187917	-0.661935	2.058724

total energy = -233.160243; ZPE=0.118236

Compound **6**

	x	y	z
c	-1.152048	0.017447	-0.520940
c	-0.289150	-1.053872	0.317987
c	0.109968	0.854785	-0.594163
c	1.080044	-0.240614	0.316765
n	1.136777	0.228998	-1.172752
c	0.630817	1.178102	0.782180
h	-1.991349	0.445579	0.031287
h	-1.467053	-0.377007	-1.486246
h	-0.693446	-1.286994	1.310291
h	-0.189980	-1.974275	-0.263168
h	1.996644	-0.711121	0.685890
h	1.454415	1.886653	0.778816
h	-0.034269	1.266742	1.646651

total energy = -249.114661; ZPE=0.104018

Compound **6 (DFT, diradical, triplet)**

	x	y	z
c	1.257506	-0.404468	0.473212
c	0.964458	0.805502	-0.487541
c	-0.187461	-0.906209	0.560861
c	-0.562584	0.595013	-0.627616
n	-0.688880	-0.900140	-0.798819
c	-1.053228	0.356357	0.825604

h	1.657088	-0.108277	1.443933
h	1.922397	-1.144263	0.027202
h	1.211455	1.776895	-0.053704
h	1.474032	0.711880	-1.447679
h	-1.113984	1.202709	-1.346245
h	-2.119256	0.151020	0.885364
h	-0.721712	1.033841	1.615735

total energy = -249.3744926; ZPE=0. 0.108267

Compound **7**

	x	y	z
c	-1.216540	-0.307291	0.667607
n	-0.949297	-1.423973	-0.317991
c	0.107644	0.534837	0.391195
c	0.322950	-1.105530	-0.450251
c	0.451211	0.223169	-1.180696
c	1.105788	-0.600899	0.772299
h	-2.140730	0.168824	0.323075
h	-1.319764	-0.546355	1.737456
h	0.274885	1.556448	0.759411
h	1.441600	0.605540	-1.443607
h	-0.319875	0.431406	-1.920281
h	2.150262	-0.349196	0.580819
h	0.958993	-1.107761	1.726362

total energy = -249.093994; ZPE=0.103723

Compound **7 (DFT, diradical, triplet)**

	x	y	z
c	1.205968	0.002398	0.582918
n	1.096100	-0.004622	-0.907075
c	-0.291513	0.004163	0.964279
c	-0.303619	-0.004382	-1.036125
c	-0.818407	-1.081385	-0.028228
c	-0.817331	1.081684	-0.037360
h	1.758980	-0.881957	0.917804
h	1.759224	0.889683	0.909572
h	-0.577894	0.008768	2.018118
h	-1.903825	-1.175866	-0.031780
h	-0.329570	-2.055870	-0.039111
h	-1.902654	1.177158	-0.041463
h	-0.327555	2.055573	-0.056517

total energy = -249.3760272; ZPE= 0.108199

Compound **8**

	x	y	z
c	-1.213758	-0.115988	0.756164
n	-0.965019	-1.110792	-0.014880
c	-0.052525	0.867905	0.661090
c	0.375751	-0.685785	-0.566292
c	0.131954	0.816946	-0.898544

c	1.112460	-0.185258	0.712333
h	-2.116219	-0.030486	1.358710
h	-0.059419	1.792571	1.240569
h	0.802351	-1.400315	-1.270521
h	1.025978	1.345583	-1.245199
h	-0.733622	1.057073	-1.523605
h	2.097463	0.250416	0.515197
h	1.148236	-0.866432	1.568081

total energy = -249.214116; ZPE=0.107481

Compound **9**

	x	y	z
c	-1.534370	0.336163	-0.126047
c	-1.128353	-0.183624	1.293124
c	-0.172212	0.665865	-0.781935
c	0.415957	-0.087176	1.273653
c	0.965470	-1.182302	0.328718
c	0.634685	1.187025	0.427935
c	0.558367	-0.663112	-1.090361
h	-2.098765	-0.405017	-0.703198
h	-2.159221	1.233899	-0.053297
h	-1.473561	-1.205852	1.484971
h	-1.547778	0.452684	2.081053
h	-0.246831	1.339146	-1.641439
h	0.871938	-0.092280	2.268527
h	0.545881	-2.168855	0.555665
h	2.054669	-1.264694	0.421093
h	1.689355	1.378672	0.196245
h	0.204514	2.088199	0.881473
h	-0.082787	-1.367912	-1.631769
h	1.442247	-0.485604	-1.713989

total energy = -273.695296; ZPE=0.170871

Compound **10**

	x	y	z
c	-1.092868	1.139107	-0.566153
c	-1.473473	-0.072613	0.457281
c	0.414791	1.064281	-0.341303
c	-0.069997	-0.408792	1.173480
c	0.487254	1.010389	1.038743
c	1.025003	-0.203419	-0.941372
c	0.790103	-1.237878	0.205737
h	-1.554248	2.068522	-0.218705
h	-1.410085	0.952156	-1.598107
h	-2.204583	0.303293	1.184055
h	-1.921463	-0.959929	-0.014641
h	-0.194961	-0.842438	2.171643
h	-0.024718	1.787329	1.614050
h	2.088234	-0.065401	-1.161471
h	0.534773	-0.491781	-1.876968
h	1.725302	-1.544531	0.684119
h	0.278308	-2.141549	-0.140780

total energy = -272.362990; ZPE=0.145116

Compound **10 (DFT, diradical, triplet)**

	x	y	z
c	-1.094750	0.858166	-0.730661
c	-1.463751	-0.205246	0.381618
c	0.415227	0.972579	-0.528176
c	-0.081820	-0.510872	1.049056
c	0.580708	0.850065	0.952584
c	1.149078	-0.244947	-1.069075
c	0.777743	-1.322081	0.031813
h	-1.602680	1.807431	-0.544330
h	-1.359375	0.525314	-1.737368
h	-2.159881	0.216315	1.110451
h	-1.922819	-1.104589	-0.038169
h	-0.159325	-0.969062	2.035658
h	0.561197	1.637651	1.695638
h	2.229389	-0.087484	-1.103253
h	0.812981	-0.531194	-2.068141
h	1.678770	-1.710597	0.511449
h	0.227132	-2.169765	-0.384882

total energy = -272.681817; ZPE=0.149040

Compound **11**

	x	y	z
c	-0.972735	-0.121922	1.084590
c	-1.284080	-0.952610	-0.256442
c	0.454071	0.539524	0.875793
c	0.120425	-0.797051	-0.811254
c	0.421682	0.701470	-0.651994
c	1.627229	-0.513343	0.932480
c	1.063994	-1.483927	-0.116170
h	-0.998565	-0.782166	1.959081
h	-1.717258	0.667855	1.238835
h	-2.077792	-0.488004	-0.852217
h	-1.564318	-1.985024	-0.030146
h	0.599164	1.433245	1.498077
h	1.375851	1.011322	-1.089236
h	-0.376636	1.352397	-1.024854
h	1.728327	-1.039385	1.890206
h	2.592221	-0.025908	0.727917
h	0.940979	-2.537026	0.132895

total energy = -272.404350; ZPE=0.146193

Compound **12**

	x	y	z
c	-0.777506	0.635539	-1.217933
c	-1.184951	-0.446601	-0.539774
c	0.628838	0.972255	-0.741270
c	-0.058108	-0.848279	0.402412

c	1.563237	-0.159456	-1.295183
c	0.523957	0.544676	0.742549
c	1.089097	-1.418804	-0.502771
h	-1.284243	1.123144	-2.045350
h	-2.091881	-1.021709	-0.700638
h	0.980127	1.986654	-0.946544
h	-0.333874	-1.493993	1.239984
h	2.612981	0.072324	-1.080875
h	1.464593	-0.275490	-2.378609
h	1.493666	0.500543	1.254446
h	-0.168423	1.167293	1.317791
h	0.733383	-2.222942	-1.153829
h	1.897418	-1.826530	0.115330

total energy = -272.479666; ZPE=0.147494

Compound **13**

	x	y	z
c	-1.095397	1.123499	-0.750656
c	-1.455859	-0.061540	0.284650
c	0.357105	0.937303	-0.392581
c	-0.026812	-0.329064	0.989943
n	0.573102	1.055473	0.890079
c	1.072820	-0.248821	-1.097988
c	0.837217	-1.247129	0.068661
h	-1.507811	2.072928	-0.409738
h	-1.380192	0.908327	-1.783800
h	-2.167737	0.329022	1.015903
h	-1.894380	-0.942657	-0.199453
h	-0.106733	-0.635567	2.035067
h	2.125892	-0.013345	-1.269856
h	0.614490	-0.549418	-2.044486
h	1.764276	-1.525914	0.574561
h	0.324214	-2.159264	-0.252513

total energy = -288.394583; ZPE=0.132577

Compound **13 (DFT, diradical, triplet)**

	x	y	z
c	1.276980	-0.872429	-0.317960
c	1.275656	0.693996	-0.500841
c	-0.000008	-1.035652	0.499083
c	0.000005	1.098072	0.293876
n	0.000000	0.085046	1.379620
c	-1.276960	-0.872448	-0.317979
c	-1.275673	0.694001	-0.500821
h	2.157560	-1.202763	0.235670
h	1.238594	-1.422788	-1.259407
h	2.166180	1.143836	-0.058244
h	1.224279	1.006636	-1.546186
h	0.000003	2.121634	0.666868
h	-2.157578	-1.202822	0.235569
h	-1.238510	-1.422763	-1.259450
h	-2.166182	1.143795	-0.058151

h	-1.224339	1.006671	-1.546157

total energy = -288.7372461; ZPE= 0.138177

Compound **14**

	x	y	z
c	-1.268433	0.200110	0.726046
n	-0.935118	-1.236585	0.447380
c	0.001016	0.873432	0.086216
c	-0.091592	-1.139445	-0.534714
c	1.347439	-1.315772	-0.116033
c	-0.148830	0.203686	-1.287541
c	1.348948	0.158771	0.554273
h	-2.196507	0.595436	0.283564
h	-1.351300	0.290633	1.814762
h	0.050203	1.967447	0.142003
h	1.485791	-2.092390	0.636903
h	2.081048	-1.412560	-0.921234
h	0.679339	0.370118	-1.982291
h	-1.105000	0.392591	-1.783589
h	2.207210	0.739238	0.199213
h	1.412055	0.070850	1.643056

total energy = -288.450996; ZPE=0.134824

Compound **15**

	x	y	z
c	1.207925	-0.756375	-0.452292
c	1.209133	0.803003	-0.409768
c	-0.121313	-1.107691	0.281892
c	-0.138854	1.119649	0.328265
c	-0.169820	-0.018350	1.372955
n	-1.215642	-0.704301	-0.647844
c	-1.211088	0.577089	-0.599057
h	2.067701	-1.178090	0.079009
h	1.208889	-1.156181	-1.469794
h	2.053331	1.190647	0.170521
h	1.252399	1.259437	-1.403131
h	-0.218413	-2.149841	0.590551
h	-0.250519	2.150021	0.671362
h	0.693574	-0.023080	2.047821
h	-1.095626	-0.044433	1.956684
h	-1.857737	1.177676	-1.240083

total energy = -288.532630; ZPE=0.136616

Compound **16**

	x	y	z
c	-1.541419	0.491522	-0.510873
c	-1.474980	-0.978043	-0.025190
c	-0.167331	0.964785	-1.021698
c	-0.086446	-1.361286	0.545112
c	1.033216	-0.564113	-0.150346

c	0.849230	0.948185	0.152502
c	0.644803	-0.223138	-1.621250
h	-2.297888	0.578212	-1.301916
h	-1.863163	1.158208	0.301140
h	-1.683878	-1.630165	-0.881369
h	-2.265910	-1.182653	0.705646
h	-0.250188	1.883352	-1.613124
h	-0.038930	-1.165238	1.625238
h	0.072089	-2.440297	0.418250
h	2.018740	-1.005937	0.033802
h	1.751599	1.525866	-0.076959
h	0.484283	1.229404	1.148870
h	0.118302	-0.976656	-2.218255
h	1.511163	0.134267	-2.187696

total energy = -273.667522; ZPE=0.170255

Compound **17**

	x	y	z
c	-1.024323	1.240240	-0.904962
c	-0.776468	-0.217292	-1.543476
c	0.128789	1.296849	0.031855
c	0.090393	-1.193745	-0.678180
c	1.101911	-0.437302	0.282632
c	0.168995	0.441372	1.096147
c	1.496451	0.855844	-0.497060
h	-1.981597	1.263694	-0.372865
h	-1.047258	1.990011	-1.704909
h	-0.291508	-0.076065	-2.514063
h	-1.750997	-0.673570	-1.747128
h	-0.557679	-1.833120	-0.065741
h	0.645508	-1.865089	-1.347242
h	1.858936	-1.107704	0.718866
h	-0.641092	0.154314	1.765995
h	1.652882	0.770326	-1.577289
h	2.328963	1.396360	-0.043334

total energy = -272.392515; ZPE=0.145808

Compound **18**

	x	y	z
c	0.135108	0.577085	0.528704
c	-0.905941	-0.325811	1.329977
c	-0.873207	0.532211	-0.664446
c	1.418566	-0.168816	0.056604
c	-1.106425	-0.855114	-0.100480
c	-0.231986	-1.841731	-0.422022
c	1.058371	-1.306036	-1.001327
h	0.355512	1.556184	0.975162
h	-1.710442	0.288344	1.756015
h	-0.516558	-1.026950	2.072625
h	-0.494759	0.660140	-1.680807
h	-1.721452	1.203211	-0.493534
h	1.935780	-0.619695	0.912797

h	2.111562	0.558179	-0.386870
h	-0.128319	-2.668900	0.283147
h	0.962338	-0.868054	-1.998806
h	1.851735	-2.058236	-1.055847

total energy = -272.393575; ZPE=0.145936

Compound **19**

	x	y	z
c	0.698129	1.044246	-0.000004
c	1.016746	-0.049328	-1.067118
c	1.016747	-0.049321	1.067119
c	-0.799741	1.284661	-0.000001
c	0.537278	-1.077638	0.000004
c	-1.608946	0.219914	0.000000
c	-1.001677	-1.167973	0.000001
h	1.283503	1.967876	-0.000008
h	2.092498	-0.139295	-1.252801
h	0.478735	0.002356	-2.019802
h	0.478737	0.002370	2.019803
h	2.092500	-0.139287	1.252800
h	-1.185336	2.301978	0.000001
h	0.996054	-2.072323	0.000007
h	-2.692747	0.319061	0.000002
h	-1.347583	-1.735050	0.877999
h	-1.347575	-1.735049	-0.878001

total energy = -272.461915; ZPE=0.146896

Compound **20**

	x	y	z
c	-0.001415	0.984390	0.277946
c	-1.052350	0.217762	1.149583
c	-1.029873	0.864922	-0.951997
c	1.238942	0.045843	0.181416
c	-1.206763	-0.460057	-0.209836
n	-0.429511	-1.390562	-0.655420
c	0.750350	-1.466027	0.208405
h	0.239528	2.011725	0.574615
h	-1.905197	0.853102	1.399974
h	-0.708872	-0.336536	2.022798
h	-0.621793	0.781037	-1.959168
h	-1.815311	1.625077	-0.874779
h	1.916784	0.249733	1.019783
h	1.793263	0.232370	-0.744907
h	1.495142	-2.137386	-0.228474
h	0.576798	-1.793400	1.243666

total energy = -288.442420; ZPE=0.134510

Compound **21**

	x	y	z
c	-1.179478	0.855034	-0.107979
c	-1.220085	-0.621113	0.413019

c	0.241764	1.228329	-0.679810
c	0.203098	-1.203369	0.913025
c	1.055111	-0.279147	0.130138
c	0.800245	-0.063876	-1.346148
n	1.094466	0.979236	0.527522
h	-1.953237	0.996293	-0.873598
h	-1.396983	1.549713	0.709919
h	-1.585397	-1.278482	-0.381661
h	-1.927320	-0.702442	1.244001
h	0.289189	2.208023	-1.176941
h	0.325226	-1.034043	1.985953
h	0.276144	-2.270549	0.680818
h	0.132254	-0.718305	-1.916543
h	1.718118	0.132248	-1.903002

total energy = -288.449625; ZPE=0.134585

Compound **22**

	x	y	z
c	0.605831	1.077712	-0.057808
c	0.640394	0.155481	-1.314806
c	1.285520	-0.098707	0.707580
c	-0.837302	1.133820	0.409562
n	0.540133	-1.019115	-0.300389
c	-1.574753	0.098307	0.514708
c	-0.924143	-1.170789	0.147661
h	1.086589	2.058955	-0.087837
h	1.615321	0.184403	-1.811636
h	-0.157531	0.273747	-2.056148
h	1.064595	-0.207785	1.775080
h	2.368611	-0.112419	0.549840
h	-1.275965	2.101541	0.671212
h	0.984786	-1.985005	-0.563628
h	-0.997731	-1.840461	1.015808
h	-1.528002	-1.631543	-0.646452

total energy = -288.507448; ZPE=0.135910

Compound **23**

	x	y	z
c	-0.685589	-1.013072	-0.000001
c	-0.987850	0.075383	-1.068481
c	-0.987848	0.075380	1.068481
n	0.753674	-1.340693	-0.000001
c	-0.497826	1.097294	0.000001
c	1.528227	-0.327685	0.000001
c	1.037762	1.108817	0.000000
h	-1.266232	-1.938111	-0.000002
h	-2.061128	0.171347	-1.260996
h	-0.444493	0.006990	-2.017393
h	-0.444490	0.006986	2.017393
h	-2.061126	0.171346	1.261000
h	-0.922660	2.106056	0.000002
h	2.607705	-0.507778	-0.000003
h	1.437726	1.635658	0.879341
h	1.437725	1.635659	-0.879341

total energy = -288.509794; ZPE=0.135742

Compound **24**

	x	y	z
c	-1.023072	0.928399	0.775317
c	-1.515380	-0.484872	0.340453
c	0.443325	1.126193	0.340354
c	-0.381484	-1.226402	-0.395437
c	1.318486	0.039295	0.996881
c	0.828578	-1.371239	0.549962
c	0.038090	-0.410403	-1.634995
c	0.540094	0.997271	-1.193238
h	-1.103524	1.050287	1.862822
h	-1.647874	1.712082	0.328722
h	-2.390777	-0.406534	-0.316352
h	-1.832843	-1.070852	1.212110
h	0.791093	2.119496	0.651211
h	-0.729159	-2.219718	-0.706336
h	2.368025	0.193099	0.716288
h	1.271561	0.139407	2.088572
h	1.631128	-1.916909	0.037958
h	0.546464	-1.978089	1.419399
h	0.822587	-0.948725	-2.181498
h	-0.813386	-0.321832	-2.321312
h	1.578334	1.156472	-1.510506
h	-0.054050	1.788519	-1.667426

total energy = -312.686445; ZPE=0.199234

Compound **25**

	x	y	z
c	-1.123264	1.208482	0.797196
c	-1.485424	-0.300104	0.528368
c	0.336161	1.381480	0.438057
c	-0.340925	-0.857527	-0.324015
c	1.241247	0.517607	1.284310
c	0.918098	-0.911968	0.611885
c	-0.168546	0.163989	-1.538530
c	0.661312	1.248959	-0.877163
h	-1.313248	1.477737	1.842262
h	-1.743037	1.860254	0.174024
h	-2.450954	-0.382975	0.014300
h	-1.565055	-0.851040	1.472810
h	-0.565534	-1.864056	-0.699885
h	2.306995	0.737697	1.162568
h	1.003465	0.532549	2.355706
h	1.798106	-1.229118	0.038736
h	0.741521	-1.670173	1.385655
h	0.379371	-0.269943	-2.381946
h	-1.165914	0.438483	-1.908310
h	1.727068	1.209560	-1.118095

total energy = -311.405312; ZPE=0.174706

Compound **26**

	x	y	z
c	-1.252953	0.720014	-0.015837
c	-1.269527	-0.772558	-0.452645
c	0.218561	1.217745	0.055168
c	0.190359	-1.259938	-0.673870
c	0.866861	0.956493	-1.285692
c	0.954322	0.359303	1.123032
c	0.851998	-0.327798	-1.663895
c	0.939107	-1.132296	0.683350
h	-1.726540	0.846502	0.966051
h	-1.815587	1.339048	-0.722858
h	-1.843353	-0.901565	-1.376592
h	-1.748270	-1.399178	0.310539
h	0.249741	2.277278	0.330519
h	0.197083	-2.300063	-1.016659
h	1.302233	1.759172	-1.876273
h	0.458294	0.486769	2.093593
h	1.981629	0.720551	1.240334
h	1.274004	-0.691486	-2.597834
h	1.958759	-1.518201	0.578094
h	0.437401	-1.756958	1.433336

total energy = -311.477245; ZPE=0.176103

Compound **27**

	x	y	z
c	-1.053627	1.210715	0.718809
c	-1.427792	-0.296887	0.472882
c	0.433198	1.296210	0.404340
c	-0.235625	-0.880372	-0.295047
c	1.289997	0.525302	1.368091
c	0.966794	-0.927048	0.716948
c	0.027393	0.155649	-1.478709
n	0.882666	1.134627	-0.801601
h	-1.272472	1.524264	1.743998
h	-1.612534	1.859084	0.037360
h	-2.358892	-0.376858	-0.100565
h	-1.572911	-0.816119	1.427028
h	-0.439468	-1.885246	-0.684155
h	2.356953	0.729180	1.260139
h	0.991893	0.593925	2.420650
h	1.872880	-1.265991	0.205866
h	0.729476	-1.647943	1.508995
h	0.594647	-0.266829	-2.314573
h	-0.946843	0.491736	-1.878279

total energy = -327.449626; ZPE=0.163195

Compound **28**

	x	y	z
c	-1.271587	0.763063	-0.658946
c	-1.248138	-0.788310	-0.643643
c	-0.021799	1.279784	0.105147
c	0.021439	-1.262793	0.108685

c	-0.009119	0.572862	1.438703
n	0.012651	-0.706162	1.471806
c	1.273565	-0.745744	-0.644968
c	1.244563	0.805582	-0.659416
h	-2.179588	1.146875	-0.182365
h	-1.259015	1.155095	-1.683069
h	-1.238107	-1.200753	-1.659422
h	-2.134796	-1.189396	-0.142588
h	-0.040302	2.368913	0.207436
h	0.040037	-2.354573	0.175275
h	-0.018185	1.127850	2.381007
h	2.174093	-1.117029	-0.145725
h	1.275568	-1.157550	-1.661055
h	2.139019	1.219376	-0.182255
h	1.219183	1.197675	-1.683258

total energy = -327.815400; ZPE=0.165204

Compound **29 (exo)**

	x	y	z
c	-1.211855	-0.504673	-1.133389
c	-1.307338	-1.317866	0.192599
c	-0.618788	0.870125	-0.727734
c	-0.764180	-0.368809	1.292989
c	-1.140348	1.015041	0.719364
c	0.940647	0.865962	-0.735451
c	0.782731	-0.478790	1.453964
c	1.542102	0.603279	0.660181
h	-2.208856	-0.368029	-1.568712
h	-0.601878	-1.004483	-1.894085
h	-2.350864	-1.579312	0.404344
h	-0.748222	-2.259406	0.153362
h	-0.987074	1.663723	-1.387440
h	-1.248727	-0.569910	2.255011
h	-0.705397	1.858115	1.267360
h	-2.229919	1.149258	0.723558
h	1.316802	1.828252	-1.105325
h	1.297515	0.108998	-1.446529
h	1.057410	-0.396492	2.513215
h	1.109704	-1.477190	1.134180
h	1.518241	1.538720	1.233088
h	2.602273	0.335789	0.572474

total energy = -312.679295; ZPE=0.199189

Compound **29 (endo)**

	x	y	z
c	-1.428742	-0.401650	-1.521837
c	-1.542014	-1.209044	-0.188955
c	-0.702167	0.916315	-1.140580
c	-0.873598	-0.313930	0.888728
c	-1.125465	1.100767	0.330442
c	0.833160	0.771023	-1.205033
c	0.648471	-0.554508	0.980310
c	1.328499	-0.445688	-0.398545

h	-2.425275	-0.178763	-1.919998
h	-0.893673	-0.954442	-2.302790
h	-2.594160	-1.380039	0.066069
h	-1.069117	-2.195916	-0.254639
h	-1.017398	1.751756	-1.777105
h	-1.326687	-0.462611	1.876282
h	-0.552801	1.879030	0.850328
h	-2.189418	1.364326	0.400401
h	1.290002	1.690643	-0.812244
h	1.163235	0.680277	-2.248737
h	1.079898	0.185179	1.669930
h	0.851927	-1.542307	1.415397
h	2.418988	-0.407016	-0.283174
h	1.119541	-1.359613	-0.970168

total energy = -312.689226; ZPE=0.199088

Compound **30**

	x	y	z
c	-1.097306	-0.909880	-1.571768
c	-1.608261	-1.396630	-0.181090
c	-0.749696	0.554606	-1.312616
c	-1.302309	-0.197578	0.738327
c	-1.374041	0.992072	-0.185422
c	0.701612	0.934638	-1.333230
c	0.249528	-0.104598	1.096964
c	1.222309	0.023738	-0.120979
h	-1.871119	-0.996937	-2.343398
h	-0.237134	-1.486291	-1.929441
h	-2.685058	-1.593571	-0.194914
h	-1.111774	-2.315298	0.151135
h	-1.892671	-0.195433	1.663792
h	-1.157317	1.981560	0.220247
h	0.853744	1.991562	-1.087532
h	1.267604	0.700651	-2.243969
h	0.379404	0.767294	1.751349
h	0.538867	-0.984208	1.690454
h	2.181604	0.422857	0.231219
h	1.435399	-0.974937	-0.517937

total energy = -311.409249; ZPE=0.174826

Compound **31 (exo)**

	x	y	z
c	-1.744306	-0.066942	0.284118
c	-1.109246	-1.152946	1.249189
c	-0.579280	0.936522	-0.096873
c	0.333499	-0.815796	0.945538
c	0.406027	0.691281	1.070253
c	0.199629	0.610051	-1.414205
c	0.931392	-1.354105	-0.134012
c	1.419021	-0.365445	-1.167357
h	-2.157648	-0.547501	-0.609555
h	-2.562173	0.472477	0.776600
h	-1.390546	-2.171814	0.969535
h	-1.405505	-0.979787	2.290673

h	-0.964328	1.961967	-0.147293
h	1.395076	1.130590	0.920589
h	0.008669	1.047563	2.027713
h	-0.478316	0.153983	-2.146183
h	0.565612	1.542930	-1.863274
h	0.679063	-2.364740	-0.454817
h	2.287362	0.215941	-0.836030
h	1.713017	-0.857668	-2.099844

total energy = -311.722433; ZPE=0.175392

Compound **31 (endo)**

	x	y	z
c	-1.694265	0.141054	0.272964
c	-1.075211	-1.069397	1.047543
c	-0.451291	0.821436	-0.356320
c	0.415693	-0.857748	0.831617
c	0.621008	0.643839	0.815582
c	-0.049852	0.073306	-1.666718
c	1.055850	-1.424718	-0.224510
c	0.214957	-1.485424	-1.474529
h	-2.419977	-0.171779	-0.486358
h	-2.207457	0.827876	0.955453
h	-1.421685	-2.041504	0.685373
h	-1.318175	-1.020275	2.116462
h	-0.618689	1.880927	-0.587195
h	1.626022	0.960209	0.523540
h	0.301528	1.204596	1.706121
h	-0.845972	0.218725	-2.410839
h	0.858246	0.532249	-2.080604
h	2.071784	-1.066983	-0.417350
h	0.718842	-1.900430	-2.354896
h	-0.733671	-2.014723	-1.351929

total energy = -311.691999; ZPE=0.174915

Compound **32 (exo)**

	x	y	z
c	-1.836298	-0.010739	-0.465025
c	-0.863172	-1.173671	-0.656507
c	-0.894844	0.929160	0.358124
c	0.098939	-1.093798	0.282301
c	1.551057	-0.976377	-0.060006
c	-0.361309	-0.107144	1.359196
c	0.360987	1.375574	-0.500668
c	1.695988	0.599699	-0.211923
h	-2.137438	0.411315	-1.432260
h	-2.759723	-0.239791	0.090345
h	-0.749616	-1.690744	-1.606141
h	-1.409392	1.795224	0.798016
h	2.253077	-1.336392	0.703026
h	1.782121	-1.482719	-1.003703
h	0.439471	0.254126	2.010939
h	-1.156242	-0.519085	1.993206
h	0.561860	2.439669	-0.323733

h	0.116336	1.289951	-1.566322
h	2.134449	0.994997	0.711226
h	2.416286	0.826520	-1.007135

total energy = -311.715888; ZPE=0.175134

Compound 32 (endo)

	x	y	z
c	-1.726204	0.462283	-0.858531
c	-1.495531	-0.894952	-0.196682
c	-0.454580	1.214503	-0.342806
c	-0.583756	-0.746540	0.785969
c	0.742191	-1.446067	0.737009
c	-0.463521	0.738414	1.116982
c	0.918693	0.700232	-0.890635
c	1.330019	-0.787786	-0.579796
h	-1.762036	0.353313	-1.950896
h	-2.640235	1.002524	-0.562833
h	-1.678578	-1.829961	-0.721508
h	-0.515269	2.303198	-0.487995
h	1.367801	-1.249791	1.615352
h	0.683743	-2.531011	0.595017
h	0.445106	0.997361	1.671594
h	-1.328735	1.111829	1.679406
h	1.676042	1.369089	-0.459925
h	0.977287	0.843083	-1.978169
h	2.426468	-0.860970	-0.601346
h	0.955034	-1.413867	-1.397346

total energy = -311.715074; ZPE=0.175029

Compound **33 (exo)**

	x	y	z
c	-1.072547	0.820816	1.725897
c	-1.134081	-0.511116	1.662691
c	0.246784	1.307518	1.136722
c	0.137436	-1.059265	1.024402
c	1.135413	0.065734	1.392627
c	0.074543	1.519109	-0.399991
c	-0.046829	-1.107939	-0.524666
c	0.362039	0.224911	-1.208508
h	-1.867020	1.489249	2.047229
h	-1.988072	-1.130987	1.922891
h	0.624634	2.219361	1.612946
h	0.427711	-2.042911	1.410665
h	2.058740	0.051068	0.802753
h	1.405086	0.002975	2.452561
h	-0.940827	1.882226	-0.601586
h	0.756833	2.302645	-0.754352
h	-1.090410	-1.355422	-0.755238
h	0.562025	-1.913912	-0.954459
h	-0.105332	0.293479	-2.198333
h	1.441608	0.183997	-1.397361

total energy = -311.753742; ZPE=0.176144

Compound **33 (endo)**

	x	y	z
c	-1.110501	0.707818	1.567932
c	-1.172599	-0.627160	1.504061
c	0.214912	1.191832	0.986374
c	0.104856	-1.174242	0.873182
c	1.097578	-0.049813	1.243144
c	0.097130	1.383243	-0.550904
c	-0.023326	-1.206616	-0.674802
c	-0.526939	0.144440	-1.237896
h	-1.907696	1.371753	1.891828
h	-2.029287	-1.242228	1.766766
h	0.597910	2.105562	1.455767
h	0.399493	-2.160056	1.251706
h	2.012711	-0.063452	0.638473
h	1.377046	-0.113424	2.301112
h	-0.504784	2.270342	-0.787703
h	1.103263	1.573529	-0.949710
h	-0.703746	-2.007555	-0.992362
h	0.962622	-1.450399	-1.094367
h	-1.613491	0.188686	-1.106393
h	-0.347135	0.187807	-2.319208

total energy = -311.762314; ZPE=0.175932

Compound **34**

	x	y	z
c	-1.524871	0.515099	-0.650983
c	-1.060869	-0.968249	-0.798817
c	-0.584343	1.091785	0.440876
c	-0.039647	-1.211283	0.352177
c	0.767807	1.432248	-0.159139
c	1.415100	-0.976184	-0.109108
c	1.676093	0.482352	-0.407679
c	-0.421015	-0.122176	1.375777
h	-1.461997	1.071153	-1.591851
h	-2.567058	0.564409	-0.310732
h	-0.608852	-1.159579	-1.778214
h	-1.914162	-1.649300	-0.705280
h	-1.017088	1.966656	0.938697
h	-0.130481	-2.224591	0.759808
h	0.973337	2.471792	-0.410757
h	2.120304	-1.329670	0.660319
h	1.625542	-1.584063	-1.002100
h	2.641946	0.743067	-0.839155
h	0.339847	0.030939	2.149554
h	-1.370873	-0.362359	1.871083

total energy = -311.767382; ZPE=0.175807

Compound **35 (endo)**

	x	y	z
c	-1.242870	0.091758	0.333005
c	-0.558469	-1.085577	1.093310
c	-0.034118	0.968694	-0.098805
c	0.909798	-0.634692	1.027768
c	0.906834	0.863280	1.205987
c	0.627142	0.356333	-1.374181
n	1.769344	-0.972066	0.126071
c	1.108551	-1.140444	-1.160142
h	-1.827360	-0.248772	-0.528710
h	-1.913631	0.653819	0.992010
h	-0.726974	-2.065176	0.640915
h	-0.882531	-1.139762	2.138462
h	-0.307158	2.012224	-0.292363
h	1.890621	1.309329	1.062482
h	0.388160	1.288736	2.075178
h	-0.094690	0.400648	-2.202230
h	1.496836	0.959130	-1.658146
h	1.817525	-1.439842	-1.938056
h	0.250441	-1.829410	-1.197142

total energy = -327.738818; ZPE=0.163230

Compound **35 (exo)**

	x	y	z
c	-1.640430	0.048016	0.273216
c	-0.980549	-1.106219	1.137722
c	-0.470338	1.047243	-0.125847
c	0.432426	-0.754495	0.726100
c	0.567071	0.738384	0.981297
c	0.252111	0.736649	-1.477680
n	0.881286	-1.300902	-0.345547
c	1.419031	-0.296908	-1.269000
h	-2.116979	-0.370920	-0.618468
h	-2.406956	0.579786	0.847585
h	-1.273281	-2.102362	0.804559
h	-1.193794	-0.985857	2.204425
h	-0.831605	2.081077	-0.121745
h	1.554784	1.168987	0.808292
h	0.217247	1.024388	1.977669
h	-0.461299	0.331682	-2.204399
h	0.657339	1.663038	-1.904129
h	2.317461	0.219450	-0.901967
h	1.690028	-0.780794	-2.211828

total energy = -327.772447; ZPE=0.164272

Compound **36**

	x	y	z
c	-0.835615	-0.748534	-1.340534
c	-1.331660	-1.227003	0.044751
c	-0.442661	0.701976	-1.010239
c	-0.944424	-0.022855	0.934121

n	-0.959968	1.174475	0.084496
c	0.983163	1.110554	-1.158788
c	0.610289	0.009984	1.271392
c	1.546595	0.165961	0.025904
h	-1.626124	-0.751525	-2.099912
h	-0.007199	-1.342499	-1.740374
h	-2.415671	-1.374842	0.062332
h	-0.860734	-2.161578	0.366541
h	-1.534803	0.064788	1.852940
h	1.128933	2.159012	-0.890208
h	1.488802	0.876910	-2.102273
h	0.765337	0.864468	1.937947
h	0.894870	-0.895191	1.826833
h	2.508012	0.579337	0.351191
h	1.760359	-0.818732	-0.403282

total energy = -327.460332; ZPE=0.163317

Compound **37 (exo)**

	x	y	z
c	-1.768585	-0.054072	-0.513733
n	-0.765514	-1.128021	-0.777413
c	-0.919555	0.908425	0.365203
c	0.062754	-1.057260	0.206527
c	1.526248	-0.994449	-0.081282
c	-0.405410	-0.153368	1.349084
c	0.360709	1.404822	-0.429553
c	1.684862	0.590636	-0.171539
h	-2.077872	0.367614	-1.476660
h	-2.673377	-0.403274	0.008023
h	-1.483458	1.741054	0.803710
h	2.187615	-1.391092	0.696624
h	1.749913	-1.472715	-1.037987
h	0.382255	0.173191	2.032442
h	-1.215168	-0.609451	1.931709
h	0.570430	2.448027	-0.164872
h	0.137273	1.400407	-1.502544
h	2.131028	0.941492	0.765297
h	2.403823	0.832491	-0.962091

total energy = -327.768352; ZPE=0.164136

Compound **37 (endo)**

	x	y	z
c	-1.625085	-0.129553	-0.723282
n	-0.566593	-1.174073	-0.820006
c	-1.003786	0.848557	0.318667
c	0.109665	-1.062724	0.272269
c	1.590269	-0.872240	0.177550
c	-0.565688	-0.209006	1.341152
c	0.344524	1.520815	-0.111354
c	1.545710	0.571303	-0.493063
h	-1.765489	0.298144	-1.723054
h	-2.603694	-0.504176	-0.382663
h	-1.707355	1.608986	0.682032

h	2.095999	-0.875642	1.147990
h	2.092456	-1.565003	-0.502675
h	0.102581	0.158316	2.125611
h	-1.412525	-0.730646	1.804725
h	0.646703	2.149725	0.736328
h	0.182728	2.204784	-0.954572
h	2.488102	1.106887	-0.320591
h	1.472995	0.364229	-1.564722

total energy = -327.768037; ZPE=0.164008

Compound **38**

	x	y	z
c	-1.487633	0.577541	-0.636704
c	-1.135538	-0.938937	-0.746386
c	-0.500418	1.107739	0.438173
c	-0.074899	-1.196307	0.359477
c	0.864786	1.331890	-0.196527
c	1.360534	-0.966454	-0.157936
n	1.714729	0.423425	-0.471522
c	-0.385383	-0.095310	1.390922
h	-1.388848	1.104298	-1.591590
h	-2.519246	0.719458	-0.293202
h	-0.753553	-1.202217	-1.738935
h	-2.025993	-1.553896	-0.575051
h	-0.850554	2.030246	0.913094
h	-0.150437	-2.210159	0.769606
h	1.139475	2.360962	-0.453554
h	2.096431	-1.323881	0.577059
h	1.536010	-1.555807	-1.068402
h	0.399706	0.025549	2.146419
h	-1.334786	-0.279508	1.909104

total energy = -327.811361; ZPE=0.164722

Compound **39**

	x	y	z
c	1.432229	-0.605236	-0.667113
c	1.157254	0.930797	-0.735372
c	0.463861	-1.118126	0.425016
c	0.104782	1.211275	0.371803
n	-0.846310	-1.426744	-0.185343
c	-1.330009	1.020689	-0.154194
c	-1.618985	-0.442382	-0.425934
c	0.376985	0.081197	1.383610
h	1.257058	-1.114774	-1.618998
h	2.469034	-0.805695	-0.372935
h	0.803013	1.248276	-1.722455
h	2.076085	1.492811	-0.533613
h	0.824111	-2.034623	0.901785
h	0.217550	2.214336	0.797358
h	-2.071291	1.397318	0.567969
h	-1.495505	1.597065	-1.076265
h	-2.591612	-0.674038	-0.874858
h	-0.411447	-0.033196	2.136698
h	1.330471	0.230443	1.905826

total energy = -327.814636; ZPE=0.164559

Compound **40 (endo)**

	x	y	z
c	-1.114951	0.599975	-0.947694
n	-1.149451	-0.677345	-0.983587
c	-0.499480	1.189053	0.317533
c	-0.552482	-1.145267	0.302719
c	-0.813044	0.023268	1.274151
c	1.041674	1.278250	0.138798
c	0.972672	-1.312969	0.111557
c	1.618550	-0.027968	-0.459148
h	-1.441073	1.193337	-1.804174
h	-0.920481	2.155199	0.614668
h	-1.012951	-2.091509	0.602528
h	-0.179106	0.005325	2.167303
h	-1.862860	0.040972	1.589348
h	1.309967	2.124976	-0.505520
h	1.484857	1.480325	1.123005
h	1.180995	-2.154796	-0.558882
h	1.409915	-1.565109	1.086724
h	1.454232	-0.015624	-1.542328
h	2.705033	-0.057732	-0.315056

total energy = -327.814298; ZPE=0.165086

Compound **40 (exo)**

c	-1.370316	0.599189	-0.716598
n	-1.409177	-0.675041	-0.758799
c	-0.453261	1.180934	0.351014
c	-0.495339	-1.154157	0.324612
c	-0.506813	0.002653	1.347431
c	0.975548	1.306906	-0.260388
c	0.919673	-1.314474	-0.290787
c	1.768918	-0.023076	-0.157699
h	-1.903459	1.205208	-1.452123
h	-0.800494	2.138359	0.752491
h	-0.867311	-2.105438	0.715360
h	0.322966	-0.020483	2.060711
h	-1.447108	0.011698	1.909673
h	0.894697	1.629330	-1.306432
h	1.537826	2.092722	0.258466
h	0.800132	-1.604162	-1.340890
h	1.454388	-2.135737	0.201872
h	2.580314	-0.030520	-0.894789
h	2.261826	-0.043547	0.821736

total energy = -327.807045; ZPE=0.165163

Compound **Cyclobutane**

c	0.000000	1.084272	0.124765
c	1.084272	0.000000	-0.124765

```
c      -1.084272    0.000000   -0.124765
c       0.000000   -1.084272    0.124765
h       0.000000    1.965711   -0.524987
h       0.000000    1.422793    1.166792
h       1.422793    0.000000   -1.166792
h       1.965711    0.000000    0.524987
h      -1.422793    0.000000   -1.166792
h      -1.965711    0.000000    0.524987
h       0.000000   -1.422793    1.166792
h       0.000000   -1.965711   -0.524987

total energy = -157.038606;    ZPE= 0.106976
```

Compound **Cyclobutene**

```
c      -0.000244    0.786728   -0.699674
c       0.000244    0.670134    0.814766
c       0.000244   -0.786728   -0.699674
c      -0.000244   -0.670134    0.814766
h       0.889212    1.247367   -1.146227
h      -0.891051    1.246291   -1.145753
h       0.000383    1.420571    1.601429
h       0.891051   -1.246291   -1.145753
h      -0.889212   -1.247367   -1.146227
h      -0.000383   -1.420571    1.601429

total energy = -155.823621;   ZPE= 0.083459
```

Compound **Azetidine**

```
c       -0.084710    1.080765    0.000000
c       -0.084710   -0.053659    1.053828
c       -0.084710   -0.053659   -1.053828
n        0.383800   -0.988208    0.000000
h        0.847493    1.651563    0.000000
h       -0.933183    1.769291    0.000000
h        0.593565    0.041383    1.910373
h       -1.098445   -0.262510    1.431257
h        0.593565    0.041383   -1.910373
h       -1.098445   -0.262510   -1.431257
h       -0.066375   -1.901821    0.000000

total energy = -173.073212;   ZPE= 0.096242
```

Compound **1-azetine**

```
c        0.516666    0.917675   -0.000136
c       -0.901064    0.408010    0.000463
c        0.793025   -0.618456    0.000033
n       -0.687629   -0.862539   -0.000277
h        0.836761    1.468949    0.891133
h        0.835145    1.467303   -0.893068
h       -1.878145    0.897025   -0.000294
h        1.283094   -1.018460    0.893730
h        1.284790   -1.020417   -0.891725

total energy = -171.873898;   ZPE= 0.072458
```

Compound **Cyclopentane**

c	0.328124	0.694861	-1.031129
c	-0.328124	-0.694861	-1.031129
c	0.000000	1.243110	0.371796
c	0.000000	-1.243110	0.371796
c	0.000000	0.000000	1.308299
h	-0.027716	1.344949	-1.838415
h	1.415147	0.589461	-1.152559
h	0.027716	-1.344949	-1.838415
h	-1.415147	-0.589461	-1.152559
h	0.702572	2.017450	0.698232
h	-0.995850	1.703481	0.359737
h	-0.702572	-2.017450	0.698232
h	0.995850	-1.703481	0.359737
h	-0.877463	0.006536	1.964106
h	0.877463	-0.006536	1.964106

total energy = -196.340085; ZPE= 0.135853

Compound **Cyclopentene**

c	1.236643	-0.318150	0.100940
c	-0.000311	-1.227487	-0.132354
c	0.667946	1.075841	-0.045676
c	-1.236813	-0.317556	0.100924
c	-0.667391	1.076159	-0.045687
h	2.048595	-0.527330	-0.607343
h	1.663439	-0.456933	1.106355
h	-0.000488	-2.114703	0.508565
h	-0.000338	-1.577907	-1.170689
h	1.293580	1.962894	-0.102397
h	-2.048804	-0.526275	-0.607477
h	-1.663850	-0.456119	1.106257
h	-1.292578	1.963539	-0.102159

total energy = -195.134482; ZPE= 0.112613

Compound **Pyrrolidine**

c	-1.156234	-0.454091	0.193245
n	0.000708	-1.273887	-0.200237
c	-0.778390	1.029995	-0.070484
c	1.156844	-0.452786	0.193005
c	0.777127	1.030947	-0.070156
h	-1.334465	-0.612075	1.265155
h	-2.055924	-0.778812	-0.338715
h	0.000650	-1.354698	-1.217986
h	-1.165951	1.361036	-1.040694
h	-1.198469	1.700236	0.687107
h	1.335673	-0.610888	1.264795
h	2.056733	-0.776241	-0.339391
h	1.196078	1.701411	0.687845
h	1.164631	1.362858	-1.040107

total energy = -212.374403; ZPE= 0.125173

Compound **1-azacylopentene**

c	-1.134526	0.552788	0.079922
c	0.257670	1.201928	-0.098945
c	-0.794897	-0.918775	-0.040952
c	1.233938	0.005894	0.077090
n	0.440207	-1.231107	-0.044823
h	-1.871062	0.875094	-0.665631
h	-1.576720	0.756989	1.065765
h	0.445369	2.008346	0.615464
h	0.352516	1.626063	-1.104115
h	-1.559763	-1.695540	-0.097450
h	2.038404	-0.004615	-0.666548
h	1.716700	0.000399	1.063584

total energy = -211.184048; ZPE= 0.101582

Compound **Cyclohexane**

c	-1.453350	0.215783	-0.225189
c	-0.539804	1.366419	0.225256
c	-0.913501	-1.150751	0.225235
c	0.913560	1.150662	-0.225353
c	0.539875	-1.366344	-0.225399
c	1.453272	-0.215779	0.225452
h	-1.533648	0.227632	-1.322873
h	-2.470143	0.366649	0.160651
h	-0.917535	2.322415	-0.160649
h	-0.569582	1.442049	1.322903
h	-1.552483	-1.956033	-0.160486
h	-0.963945	-1.214326	1.322913
h	1.552598	1.956028	0.160096
h	0.963937	1.213885	-1.323055
h	0.917652	-2.322462	0.160159
h	0.569662	-1.441566	-1.323076
h	2.470287	-0.366680	-0.159780
h	1.532886	-0.227538	1.323190

total energy = -235.620686; ZPE= 0.164262

Compound **Cyclohexene**

c	0.698173	-1.192189	-0.319101
c	1.498923	0.047550	0.111315
c	-0.698510	-1.192368	0.318233
c	0.666397	1.305923	0.057045
c	-1.499069	0.048283	-0.110115
c	-0.665724	1.306139	-0.057441
h	1.244326	-2.106120	-0.054905
h	0.593198	-1.191649	-1.413089
h	2.387004	0.163335	-0.525618
h	1.888279	-0.090853	1.132880
h	-1.245062	-2.105681	0.052737
h	-0.593368	-1.193636	1.412203
h	1.199956	2.254485	0.111790
h	-2.385556	0.164556	0.528987

```
h       -1.891063   -0.089306   -1.130770
h       -1.198858    2.254855   -0.113829

total energy = -234.412225;   ZPE= 0.141107
```

Compound **Piperidine**

```
c       -0.008316   -0.791553    1.216650
n       -0.605669   -1.355187    0.000000
c       -0.008316    0.746945    1.265910
c       -0.008316   -0.791553   -1.216650
c        0.639782    1.330709    0.000000
c       -0.008316    0.746945   -1.265910
h       -0.534873   -1.209083    2.083226
h        1.028082   -1.155929    1.271265
h       -1.604765   -1.147012    0.000000
h        0.514396    1.097809    2.166084
h       -1.046455    1.103757    1.344523
h       -0.534873   -1.209083   -2.083226
h        1.028082   -1.155929   -1.271265
h        0.570571    2.425823    0.000000
h        1.712483    1.085434    0.000000
h       -1.046455    1.103757   -1.344523
h        0.514396    1.097809   -2.166084

total energy = -251.653477;   ZPE= 0.153384
```

Compound **1-piperideine**

```
c       -0.724276    1.155207   -0.321111
c       -1.441397   -0.125830    0.125839
c        0.674770    1.218832    0.302025
n       -0.654151   -1.361142    0.055176
c        1.465876   -0.031400   -0.103493
c        0.611463   -1.282280   -0.054658
h       -1.322183    2.033228   -0.047422
h       -0.635495    1.159744   -1.416611
h       -2.346870   -0.288391   -0.471935
h       -1.785322   -0.028445    1.166274
h        1.206473    2.128257   -0.000760
h        0.583037    1.254220    1.396183
h        2.344120   -0.177907    0.539535
h        1.863334    0.073311   -1.125303
h        1.153346   -2.233196   -0.117802

total energy = -250.456073;   ZPE= 0.129884
```

Compound **Cycloheptane**

```
c        0.970806    1.252181   -0.402632
c        1.776850   -0.000554   -0.000164
c       -0.313850    1.529996    0.401363
c        0.970012   -1.252561    0.402821
c       -1.543191    0.760004   -0.114462
c       -0.314708   -1.529906   -0.401239
c       -1.543689   -0.759177    0.114326
h        1.641395    2.118537   -0.330601
```

```
h         0.694864    1.183801   -1.464239
 h        2.441388    0.253128    0.837003
 h        2.440608   -0.254841   -0.837769
 h       -0.152828    1.321210    1.469251
 h       -0.539633    2.602626    0.336218
 h        1.640089   -2.119357    0.331280
 h        0.694002   -1.183507    1.464368
 h       -2.447110    1.175007    0.352479
 h       -1.641511    0.960597   -1.192094
 h       -0.541059   -2.602407   -0.335956
 h       -0.153461   -1.321361   -1.469143
 h       -2.447767   -1.173622   -0.352805
 h       -1.642363   -0.959703    1.191937

total energy = -274.881120;   ZPE= 0.192145
```

Compound **Cycloheptene**

```
c         0.794384    1.028607    0.867733
c         0.000000    0.000000    1.691278
c         0.054645    1.600671   -0.354830
c        -0.794384   -1.028607    0.867733
c         0.000000    0.669396   -1.548086
c        -0.054645   -1.600671   -0.354830
c         0.000000   -0.669396   -1.548086
h         1.088400    1.853121    1.530589
h         1.729768    0.576237    0.513882
h        -0.701949    0.526110    2.353048
h         0.701949   -0.526110    2.353048
h        -0.960826    1.919202   -0.068053
h         0.562595    2.520742   -0.673321
h        -1.088400   -1.853121    1.530589
h        -1.729768   -0.576237    0.513882
h        -0.010609    1.165952   -2.518886
h        -0.562595   -2.520742   -0.673321
h         0.960826   -1.919202   -0.068053
h         0.010609   -1.165952   -2.518886

total energy = -273.675178;   ZPE= 0.168917
```

Compound **Azacycloheptane**

```
c        -1.029671   -1.202055   -0.374944
c        -1.761099    0.112342   -0.021180
c         0.267439   -1.509215    0.404138
c        -0.882485    1.314643    0.383185
n         1.481991   -0.851021   -0.080633
c         0.434682    1.490888   -0.392608
h        -1.734363   -2.034487   -0.239766
h        -0.773094   -1.207086   -1.444357
h        -2.463591   -0.078549    0.801165
h        -2.384181    0.395074   -0.880330
h         0.150257   -1.263143    1.468575
h         0.451799   -2.590684    0.358970
h        -1.490455    2.223449    0.284723
h        -0.634707    1.242604    1.451824
h         1.594400   -1.061356   -1.071389
```

```
h         0.766482    2.534276   -0.291817
h         0.279031    1.323881   -1.468801
c         1.579663    0.592183    0.122868
h         2.523452    0.912865   -0.336708
h         1.689857    0.767598    1.203585

total energy = -290.914237;   ZPE= 0.181100
```

Compound **Tetrahydroazepine**

```
c        0.764374   -1.217499    0.523375
c        1.691271   -0.102533    0.010858
c       -0.486267   -1.476010   -0.334269
c        0.942303    1.130079   -0.521188
n       -1.625363   -0.570193   -0.164749
c       -0.272590    1.535966    0.327409
c       -1.503798    0.658441    0.139238
h        1.335464   -2.152013    0.600574
h        0.426799   -0.988811    1.543050
h        2.335148   -0.494889   -0.787578
h        2.364722    0.197566    0.825060
h       -0.227870   -1.504910   -1.403697
h       -0.869240   -2.477086   -0.100775
h        1.636844    1.976615   -0.590384
h        0.595851    0.939185   -1.545141
h       -0.573124    2.560865    0.073714
h       -0.007433    1.567650    1.395817
h       -2.451382    1.196519    0.270069

total energy = -289.718032;   ZPE= 0.157663
```

*Isodesmic reactions used in determination of strain energy for **1-40**. Conformations of acyclic alkene and imine products are indicated where appropriate.*

1 + $6C_2H_6 = 2(CH_3)_3CH + 3CH_3CH_2CH_3$

2 + $6C_2H_6 = 2(CH_3)_3CH + CH_3CH_2CH_2CH_3 + 2CH_3CH_2CH_3$

3 + $5C_2H_6 = (CH_3)_3CH + (CH_3)_2C{=}CHCH_3 + CH_3CH_2CH_2CH_3 + CH_3CH_2CH_3$

4 + $6C_2H_6 = (CH_3)_3CH + 3CH_3CH_2CH_3 + (CH_3)_2C{=}CHCH_3$

5 + $6C_2H_6 = 2(CH_3)_3CH + 2CH_3CH_2CH_3 + (Z\text{-})CH_3CH{=}CHCH_3$

6 + $5C_2H_6 = (CH_3)_3CH + CH_3N{=}C(CH_3)_2 + CH_3CH_2CH_2CH_3 + CH_3CH_2CH_3$

7 + $6C_2H_6 = (CH_3)_3CH + CH_3N{=}C(CH_3)_2 + 3CH_3CH_2CH_3$

8 + $6C_2H_6 = 2(CH_3)_3CH + 2CH_3CH_2CH_3 + (Z\text{-})CH_3CH{=}NCH_3$

9 + $6C_2H_6$ = $2(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$

10 + $5C_2H_6$ = $(CH_3)_3CH$ + $(CH_3)_2C{=}CHCH_3$ + $2CH_3CH_2CH_2CH_3$

11 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$

12 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + (Z-)$CH_3CH{=}CHCH_3$

13 + $5C_2H_6$ = $(CH_3)_3CH$ + $CH_3N{=}C(CH_3)_2$ + $2CH_3CH_2CH_2CH_3$

14 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$

15 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_3$ + $CH_3CH_2CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_3$

16 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$

17 + $5C_2H_6$ = $(CH_3)_3CH$ + $(CH_3)_2C{=}CHCH_3$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3CH_2CH_3$

18 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$

19 + $7C_2H_6$ = $2(CH_3)_3CH$ + $3CH_3CH_2CH_3$ + (Z-)$CH_3CH{=}CHCH_3$

20 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$

21 + $5C_2H_6$ = $(CH_3)_3CH$ + $CH_3N{=}C(CH_3)_2$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3CH_2CH_3$

22 + $6C_2H_6$ = $2(CH_3)_3CH$ + $2CH_3CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_2CH_3$

23 + $6C_2H_6$ = $2(CH_3)_3CH$ + $2CH_3CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_2CH_3$

24 + $6C_2H_6$ = $2(CH_3)_3CH$ + $3CH_3CH_2CH_2CH_3$

25 + $6C_2H_6$ = $(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$ + $CH_3CH_2CH_3$

26 + $6C_2H_6$ = $2(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + (Z-)$CH_3CH{=}CHCH_3$

27 + $6C_2H_6$ = $(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$ + $CH_3CH_2CH_3$

28 + $6C_2H_6$ = $2(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_3$

29 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + $CH_3CH_2CH_2CH_3$

30 + $5C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_2CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$

31 + $6C_2H_6$ = $(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$

32 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $(CH_3)_2C{=}CHCH_3$

33 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + (Z-)$CH_3CH{=}CHCH_3$

34 + $7C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + (Z-)$CH_3CH{=}CHCH_3$

35 + $6C_2H_6$ = $(CH_3)_3CH$ + $2CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$

36 + $5C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$

37 + $6C_2H_6$ = $(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $2CH_3CH_2CH_3$ + $CH_3N{=}C(CH_3)_2$

38 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_2CH_3$

39 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_2CH_3$

40 + $6C_2H_6$ = $2(CH_3)_3CH$ + $CH_3CH_2CH_2CH_2CH_3$ + $CH_3CH_2CH_3$ + (Z-)$CH_3N{=}CHCH_3$

*Isodesmic reactions used in determination of enthalpies of formation for **1-40** and **H,L,P**.*

Symbols and letters in the equations designate compounds depicted in Schemes 1 and 2.

2 (cyclo-$[(CH_2)_4]$) → **1** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_5]$ + cyclo-$[(CH_2)_4]$ → **2** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_3CH{=}CH]$ + cyclo-$[(CH_2)_4]$ → **3,4,5** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_3CH{=}N]$ + cyclo-$[(CH_2)_4]$ → **6,7,8** + $CH_3CH_2CH_3$

2 (cyclo-$[(CH_2)_5]$) → **9** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_3CH{=}CH]$ + cyclo-$[(CH_2)_5]$ → **10,11,12** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_3CH{=}N]$ + cyclo-$[(CH_2)_5]$ → **13,14,15** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_6]$ + cyclo-$[(CH_2)_4]$ → **16** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_4CH{=}CH]$ + cyclo-$[(CH_2)_4]$ → **17,18,19** + $CH_3CH_2CH_3$

cyclo-$[(CH_2)_3CH{=}N]$ + cyclo-$[(CH_2)_4]$ → **20,21,22,23** + C_2H_6

2 (cyclo-$[(CH_2)_6]$) → **24** + $CH_3CH_2CH_2CH_3$

cyclo-$[(CH_2)_4CH{=}CH]$ + cyclo-$[(CH_2)_6]$ → **25,26** + $CH_3CH_2CH_2CH_3$

cyclo-[$(CH_2)_3CH{=}N$] + cyclo-[$(CH_2)_5$] → **27,28** + C_2H_6

cyclo-[$(CH_2)_5$] + cyclo-[$(CH_2)_6$] → **29** + $CH_3CH_2CH_3$

cyclo-[$(CH_2)_3CH{=}N$] + cyclo-[$(CH_2)_5$] → **30,31,34** + $CH_3CH_2CH_3$

cyclo-[$(CH_2)_3CH{=}CH$] + cyclo-[$(CH_2)_6$] → **32,33** + $CH_3CH_2CH_3$

cyclo-[$(CH_2)_3CH{=}N$] + cyclo-[$(CH_2)_6$] → **35,36,37,38,39,40** + $CH_3CH_2CH_3$

cyclo-[$(CH_2)_3CH{=}CH$] + cyclo-[$(CH_2)_4NH$] → cyclo-[$(CH_2)_3CH{=}N$] + cyclo-[$(CH_2)_5$]

cyclo-[$(CH_2)_4CH{=}CH$] + cyclo-[$(CH_2)_5NH$] → cyclo-[$(CH_2)_4CH{=}N$] + cyclo-[$(CH_2)_6$]

cyclo-[$(CH_2)_5CH{=}CH$] + cyclo-[$(CH_2)_6NH$] → cyclo-[$(CH_2)_5CH{=}N$] + cyclo-[$(CH_2)_7$]