Supporting Information

For

A Procedure for Computing Hydrocarbon Strain Energies Using Computational Group Equivalents, with Numerous Examples

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Table S1. Definitions of strain-free reference states.

Compound	Constituent Atom Types for Strain-Free Reference
cyclopropene	2 x C_d-(H)(C) + C-(C_d)$_2$(H)$_2$
cyclopropane	3 x C-(H)$_2$(C)$_2$
tetrahedrane	4 x C-(H)(C)$_3$
methylenecyclopropene	2 x C_d-(C_d)(H) + C_d-(C)$_2$ + C_d-(H)$_2$
bicyclo[1.1.0]but-1(3)-ene	2 x C-(H)$_2$(C)$_2$ + 2 x C_d-(C)$_2$
cyclobutene	2 x C-(C_d)(C)(H)$_2$ + 2 x C_d-(H)(C)
bicyclobutane	2 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
methylenecyclopropane	2 x C-(C_d)(C)(H)$_2$ + C_d-(H)$_2$ + C_d-(C_d)$_2$
cyclobutane	4 x C-(H)$_2$(C)$_2$
[1.1.1]propellane	3 x C-(H)$_2$(C)$_2$ + 2 x C-(C)$_4$
cyclopentadiene	C-(C_d)$_2$(H)$_2$ + 2 x C_d-(H)(C) + 2 x C_d-(C_d)(H)
bicyclo[2.1.0]pent-1-ene	2 x C-(C_d)(C)(H)$_2$ + C-(C_d)(C)$_2$(H) + C_d-(H)(C) + C_d-(C)$_2$
bicyclo[2.1.0]pent-1(4)-ene	2 x C-(C_d)(C)(H)$_2$ + C-(C_d)$_2$(H)$_2$ + 2 x C_d-(C)$_2$
bicyclo[2.1.0]pent-2-ene	C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)$_2$(H) + 2 x C_d-(H)(C)
bicyclo[2.1.0]pent-4-ene	C-(H)$_2$(C)$_2$ + C-(C_d)(C)(H)$_2$ + C-(C_d)(C)$_2$(H) + C_d-(H)(C) + C_d-(C)$_2$
cyclopentene	C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)(H)$_2$ + 2 x C_d-(H)(C)
bicyclo[2.1.0]pentane	3 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
spiropentane	4 x C-(H)$_2$(C)$_2$ + C-(C)$_4$
bicyclo[1.1.1]pentane	3 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
methylenecyclobutane	C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)(H)$_2$ + C_d-(C)$_2$ + C_d-(H)$_2$
cyclopentane	5 x C-(H)$_2$(C)$_2$
prismane	6 x C-(H)(C)$_3$
benzvalene	2 x C_d-(H)(C) + 2 x C-(C_d)(C)$_2$(H) + 2 x C-(H)(C)$_3$
[2.1.1]propellane	4 x C-(H)$_2$(C)$_2$ + 2 x C-(C)$_4$
bicyclo[2.1.1]hexene	2 x C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)$_2$(H) + 2 x C_d-(H)(C)
bicyclo[2.2.0]hex-1-ene	C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)(H)$_2$ + C-(C_d)(C)$_2$(H) + C_d-(H)(C) + C_d-(C)$_2$
Bicyclo[2.2.0]hex-1(4)-ene	4 x C-(C_d)(C)(H)$_2$ + 2 x C_d-(C)$_2$
Bicyclo[2.2.0]hex-2-ene	2 x C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)$_2$(H) + 2 x C_d-(H)(C)
cyclohexene	2 x C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)(H)$_2$ + 2 x C_d-(H)(C)
methylenecyclopentane	2 x C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)(H)$_2$ + C_d-(C)$_2$ + C_d-(H)$_2$
bicyclo[2.1.1]hexane	4 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
bicyclo[3.1.0]hexane	4 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
spirohexane	5 x C-(H)$_2$(C)$_2$ + C-(C)$_4$
cis-bicyclo[2.2.0]hexane	4 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
trans-bicyclo[2.2.0]hexane	4 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
cyclohexane	6 x C-(H)$_2$(C)$_2$
bicyclo[4.1.0]hepta-1,3,5-triene	C-(C_d)$_2$(H)$_2$ + 2 x C_B-(C) + 4 x C_B-(H)
norbornadiene[a]	C-(H)$_2$(C)$_2$ + 2 x C-(C_d)$_2$(C)(H) + 4 x C_d-(H)(C)
quadricycane	C-(H)$_2$(C)$_2$ + 6 x C-(H)(C)$_3$
bicyclo[3.2.0]hept-1(5)-ene	C-(H)$_2$(C)$_2$ + 4 x C-(C_d)(C)(H)$_2$ + 2 x C_d-(C)$_2$
bicyclo[3.2.0]hept-2-ene	2xC-(H)$_2$(C)$_2$+C-(H)(C)$_3$+C-(C_d)(C)$_2$(H)+C-(C_d)(C)(H)$_2$+2xC_d-(H)(C)
bicyclo[3.2.0]hept-6-ene	3 x C-(H)$_2$(C)$_2$ + 2 x C-(C_d)(C)$_2$(H) + 2 x C_d-(H)(C)
[2.2.1]propellane	5 x C-(H)$_2$(C)$_2$ + 2 x C-(C)$_4$
norbornene	3 x C-(H)$_2$(C)$_2$ + 2 x C_d-(H)(C) + 2 x C-(C_d)(C)$_2$(H)
norbornane	5 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
bicyclo[3.2.0]heptane	5 x C-(H)$_2$(C)$_2$ + 2 x C-(H)(C)$_3$
spiro[3.3]heptane	6 x C-(H)$_2$(C)$_2$ + C-(C)$_4$

methylcyclohexane[b]	5 x C-$(H)_2(C)_2$ + C-$(H)(C)_3$ + C-$(H)_3(C)$
cubane	8 x C-$(H)(C)_3$
[3.4.4.4]fenestrane	3 x C-$(H)_2(C)_2$ + 4 x C-$(H)(C)_3$ + C-$(C)_4$
[2.2.2]propellane	6 x C-$(H)_2(C)_2$ + 2 x C-$(C)_4$
bicyclo[2.2.2]octene	4 x C-$(H)_2(C)_2$ + 2 x C-$(C_d)(C)_2(H)$ + 2 x C_d-$(H)(C)$
bicyclo[2.2.2]octane	6 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$
cis-1,3-dimethylcyclohexane[b]	4 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$ + 2 x C-$(H)_3(C)$
trans-1,4-dimethylcyclohexane[b]	4 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$ + 2 x C-$(H)_3(C)$
[4.4.4.4]fenestrane	4 x C-$(H)_2(C)_2$ + 4 x C-$(H)(C)_3$ + C-$(C)_4$
cis-1,3,5-trimethylcyclohexane[b]	3 x C-$(H)_2(C)_2$ + 3 x C-$(H)(C)_3$ + 3 x C-$(H)_3(C)$
[4.4.4.5]fenestrane	5 x C-$(H)_2(C)_2$ + 4 x C-$(H)(C)_3$ + C-$(C)_4$
adamantane	6 x C-$(H)_2(C)_2$ + 4 x C-$(H)(C)_3$
trans-decalin	8 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$
cis-decalin	8 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$
1-methyladamantane	6 x C-$(H)_2(C)_2$ + 3 x C-$(H)(C)_3$ + C-$(C)_4$ + C-$(H)_3(C)$
spiro[5.5]undecane	10 x C-$(H)_2(C)_2$ + C-$(C)_4$
1,3-dimethyladamantane	6 x C-$(H)_2(C)_2$ + 2 x C-$(H)(C)_3$ + 2 x C-$(C)_4$ + 2 x C-$(H)_3(C)$
1,3,5-trimethyladamantane	6 x C-$(H)_2(C)_2$ + C-$(H)(C)_3$ + 3 x C-$(C)_4$ + 3 x C-$(H)_3(C)$
1,3,5,7-tetramethyladamantane	6 x C-$(H)_2(C)_2$ + 4 x C-$(C)_4$ + 4 x C-$(H)_3(C)$

Notes:

a. Here, 2 x C-$(C_d)(C)_2(H)$ is used instead of 2 x C-$(C_d)_2(C)(H)$, only because the latter atom type has not been defined; the resulting strain energy is thus not as well defined as in the other cases.

b. All equatorial.

Table S2. Calculated enthalpies (0 K) of compounds in Figure 1 (hartrees).

Compound	PG[a]	W1BD	G4	CBS-APNO	CBS-QB3	M062X[b]
ethyne	D*H	-77.325151	-77.290352	-77.301555	-77.187430	-77.276323
ethene	D2H	-78.554639	-78.521873	-78.532205	-78.416641	-78.498270
ethane	D3D	-79.769187	-79.738111	-79.747981	-79.630571	-79.707199
propyne	C3V	-116.628275	-116.576744	-116.595044	-116.421713	-116.554447
propene	CS	-117.853578	-117.803858	-117.820506	-117.646210	-117.771138
propane	C2V	-119.063722	-119.015782	-119.031778	-118.855866	-118.975051
1-butyne	CS	-155.921899	-155.853608	-155.877663	-155.646162	-155.821269
2-butyne	D3H	-155.929934	-155.861543	-155.886097	-155.654661	-155.830857
1,3-butadiene	C2H	-155.942692	-155.874489	-155.897881	-155.666934	-155.839719
isobutene	C2V	-157.154275	-157.087980	-157.110621	-156.877857	-157.045435
trans-2-butene	C2H	-157.152252	-157.085741	-157.108624	-156.875767	-157.043494
1-butene	C1	-157.147661	-157.081325	-157.104024	-156.871268	-157.038459
isobutane	C3V	-158.361278	-158.297004	-158.318908	-158.084516	-158.245904
1,4-pentadiene	C2	-195.231526	-195.146736	-195.176260	-194.886589	-195.101687
2-methyl-1,3-butadiene	CS	-195.242673	-195.157846	-195.187474	-194.897942	-195.113373
2-pentyne	CS	-195.223732	-195.138675	-195.168880	-194.879333	-195.097624
3-methyl-1-butyne	CS	-195.218701	-195.134164	-195.164236	-194.874209	-195.091147
3-methyl-1-butene	CS	-196.445017	-196.362533	-196.391002	-196.099856	-196.308999
neopentane	TD	-197.659693	-197.579721	-197.607992	-197.314715	-197.518331
benzene	D6H	-232.201357	-232.093991	-232.136548	-231.789656	-232.061879
3-methylenepenta-1,4-diene	C2	-233.324518	-233.221324	-233.257161	-232.911696	-233.174681
3-methylpenta-1,4-diene	CS		-234.427345	-234.462490	-234.114525	-234.371431
4-methyl-2-pentyne	CS	-234.520655	-234.419436	-234.455527	-234.107584	-234.367679
3,3-dimethyl-1-butyne	C3V	-234.517271	-234.417191	-234.453462	-234.104700	-234.362896
3,3-dimethyl-1-	CS	-235.743173	-235.644896	-235.679040	-235.329773	-235.580627
hexane	C2H	-236.948301	-236.850364	-236.884309	-236.533041	-236.779383
toluene	CS	-271.500755	-271.377411	-271.425767	-271.020463	-271.334886
4,4-dimethyl-2-pentyne	C3V	-273.819324	-273.702683	-273.744859	-273.338211	-273.639378
heptane	C2V	-276.243107	-276.128553	-276.168559	-275.758727	-276.047347
styrene	CS	-309.587406	-309.445521	-309.500582	-309.039037	-309.400972
ethylbenzene	CS	-310.795291	-310.655778	-310.710090	-310.246276	-310.602597
alpha-methylstyrene	C1		-348.727881	-348.789410	-348.268896	-348.672906
allylbenzene	C1		-348.721238	-348.782537	-348.261698	-348.665946
isopropylbenzene	CS		-349.936410	-349.996662	-349.474282	-349.872185
naphthalene	D2H		-385.655807	-385.728620	-385.150897	-385.611013
t-butylbenzene	CS		-389.217121	-389.283328	-388.702422	-389.141475

Notes:

[a] Point group.

[b] M062X/6-31+G(2df,p).

Table S3. Calculated enthalpies (298 K) of compounds in Figure 1 (hartrees).

Compound	PG[a]	W1BD	G4	CBS-APNO	CBS-QB3	M062X[b]
ethyne	D*H	-77.321387	-77.286491	-77.297912	-77.183664	-77.272648
ethene	D2H	-78.550644	-78.517874	-78.528224	-78.412647	-78.494285
ethane	D3D	-79.764732	-79.733661	-79.743538	-79.626126	-79.702764
propyne	C3V	-116.623357	-116.571773	-116.590255	-116.416794	-116.549626
propene	CS	-117.848524	-117.798805	-117.815456	-117.641158	-117.766094
propane	C2V	-119.058189	-119.010253	-119.026271	-118.850348	-118.969578
1-butyne	CS	-155.915909	-155.847570	-155.871807	-155.640186	-155.815387
2-butyne	D3H	-155.923220	-155.854800	-155.879471	-155.647930	-155.824189
1,3-butadiene	C2H	-155.937066	-155.868858	-155.892254	-155.661312	-155.834114
isobutene	C2V	-157.147962	-157.081678	-157.104323	-156.871544	-157.039179
trans-2-butene	C2H	-157.145784	-157.079280	-157.102153	-156.869301	-157.037088
1-butene	C1	-157.141400	-157.075059	-157.097797	-156.865019	-157.032252
isobutane	C3V	-158.354563	-158.290273	-158.312204	-158.077822	-158.239279
1,4-pentadiene	C2	-195.224523	-195.139715	-195.169290	-194.879594	-195.094709
2-methyl-1,3-butadiene	CS	-195.235820	-195.150999	-195.180643	-194.891087	-195.106615
2-pentyne	CS	-195.215919	-195.130821	-195.161145	-194.871515	-195.089950
3-methyl-1-butyne	CS	-195.211413	-195.126825	-195.157110	-194.866944	-195.084009
3-methyl-1-butene	CS	-196.437437	-196.354937	-196.383494	-196.092293	-196.301550
neopentane	TD	-197.651981	-197.571947	-197.600059	-197.307018	-197.510550
benzene	D6H	-232.195982	-232.088593	-232.131210	-231.784285	-232.056561
3-methylenepenta-1,4-diene	C2	-233.316935	-233.213765	-233.249571	-232.904109	-233.167199
3-methylpenta-1,4-diene	CS		-234.418914	-234.454146	-234.106134	-234.363083
4-methyl-2-pentyne	CS	-234.511499	-234.410247	-234.446492	-234.098439	-234.358659
3,3-dimethyl-1-butyne	C3V	-234.508627	-234.408466	-234.445031	-234.096091	-234.354496
3,3-dimethyl-1-	CS	-235.734377	-235.636075	-235.670371	-235.321008	-235.572082
hexane	C2H	-236.938821	-236.840895	-236.874862	-236.523584	-236.770011
toluene	CS	-271.493508	-271.370152	-271.418555	-271.013230	-271.327718
4,4-dimethyl-2-pentyne	C3V	-273.808783	-273.692074	-273.734506	-273.327697	-273.629094
heptane	C2V	-276.232297	-276.117753	-276.157750	-275.747940	-276.036642
styrene	CS	-309.579570	-309.437694	-309.492851	-309.031180	-309.393227
ethylbenzene	CS	-310.786920	-310.647390	-310.701793	-310.237925	-310.594332
alpha-methylstyrene	C1		-348.718798	-348.780297	-348.259792	-348.663965
allylbenzene	C1		-348.712052	-348.773453	-348.252561	-348.656897
isopropylbenzene	CS		-349.926699	-349.987024	-349.464565	-349.862616
naphthalene	D2H		-385.647935	-385.720834	-385.143061	-385.603286
t-butylbenzene	CS		-389.206195	-389.272559	-388.691557	-389.130856

Notes:

[a] Point group.

[b] M062X/6-31+G(2df,p).

Table S4. Calculated enthalpies (0 K) of compounds in Figure 2 (hartrees).

Compound	PG[a]	W1BD	G4	CBS-APNO	CBS-QB3	M062X[b]
cyclopropene	C2V	-116.59057	-116.53835	-116.55666	-116.38356	-116.52249
cyclopropane	C2V	-117.84005	-117.79018	-117.80744	-117.63237	-117.76382
tetrahedrane	C2V	-154.61783	-154.54738	-154.57291	-154.34202	-154.54692
methylenecyclopropene	C2V	-154.67526	-154.60436	-154.62993	-154.39977	-154.59131
bicyclo[1.1.0]but-1(3)-ene	C2V	-154.60471	-154.53603	-154.56296	-154.33003	-154.51797
cyclobutene	D2D	-155.92348	-155.85402	-155.87862	-155.64679	-155.82273
bicyclobutane	D3H	-155.89922	-155.83084	-155.85554	-155.62337	-155.80904
methylenecyclopropane	C2V	-155.91139	-155.84305	-155.86747	-155.63586	-155.81697
cyclobutane	C1	-157.13675	-157.06960	-157.09331	-156.85982	-157.02981
[1.1.1]propellane	CS	-193.96982	-193.88422	-193.91695	-193.62685	-193.85940
cyclopentadiene	CS	-194.05791	-193.96936	-194.00205	-193.71277	-193.93544
bicyclo[2.1.0]pent-1-ene	C1	-193.91955	-193.83306	-193.86436	-193.57476	-193.80230
bicyclo[2.1.0]pent-1(4)-ene	CS	-193.90803	-193.82171	(fails)	-193.56357	-193.79114
bicyclo[2.1.0]pent-2-ene	CS	-193.98336	-193.89601	-193.92741	-193.63872	-193.86720
bicyclo[2.1.0]pent-4-ene	D2D	-193.91674	-193.83006	-193.86157	-193.57211	-193.80119
cyclopentene	D3H	-195.25789	-195.17136	-195.20246	-194.91231	-195.12872
bicyclo[2.1.0]pentane	CS	-195.21158	-195.12588	-195.15691	-194.86630	-195.08983
spiropentane	C2	-195.20085	-195.11594	-195.14698	-194.85618	-195.08479
bicyclo[1.1.1]pentane	D3H	-195.19346	-195.10877	-195.13923	-194.85010	-195.07032
methylenecyclobutane	C2V	-195.22474	-195.13938	-195.16993	-194.87969	-195.09835
cyclopentane	C2V	-196.46229	-196.37794	-196.40852	-196.11638	-196.32721
prismane	C2V	-232.02048	-231.91389	-231.95401	-231.60693	-231.89217
benzvalene	C1	-232.08540	-231.97951	-232.01893	-231.67290	-231.95425
[2.1.1]propellane	D2H	-233.26413	-233.16162	-233.20035	-232.85193	-233.12329
bicyclo[2.1.1]hexene	CS	-233.30652	-233.20310	-233.24075	-232.89436	-233.15786
bicyclo[2.2.0]hex-1-ene	D3D	-233.26274	-233.15876	-233.19671	-232.84917	-233.11734
Bicyclo[2.2.0]hex-1(4)-ene	C2	-233.25077	-233.14601	-233.18419	-232.83699	-233.10474
Bicyclo[2.2.0]hex-2-ene	C2V	-233.29654	-233.19177	-233.22944	-232.88242	-233.14989
cyclohexene	CS	-234.55894	-234.45629	-234.49337	-234.14461	-234.40407
methylenecyclopentane	CS	-234.55317	-234.45093	-234.48809	-234.13915	-234.39835
bicyclo[2.1.1]hexane	C2	-234.53447	-234.43253	-234.46979	-234.12160	-234.38026
bicyclo[3.1.0]hexane	C2H	-234.54338	-234.44100	-234.47870	-234.12940	-234.39335
spirohexane	D3D	-234.50847	-234.40673	-234.44379	-234.09453	-234.36073
cis-bicyclo[2.2.0]hexane	C2V	-234.50875	-234.40581	-234.44319	-234.09383	-234.35610
trans-bicyclo[2.2.0]hexane	C2V	-234.44588	-234.34413	-234.38097	-234.03291	-234.29340
cyclohexane	C2V	-235.76621	-235.66587	-235.70196	-235.35163	-235.60491
bicyclo[4.1.0]hepta-1,3,5-triene	CS	-270.21241	-270.08738	-270.13772	-269.73369	-270.06168
norbornadiene	C1	-271.42699	-271.30476	-271.34968	-270.94631	-271.25537
quadricycane	CS	-271.39146	-271.26837	-271.31486	-270.90966	-271.23387
bicyclo[3.2.0]hept-1(5)-ene	C2V	-272.61338	-272.49150	-272.53660	-272.13074	-272.43924
bicyclo[3.2.0]hept-2-ene	CS	-272.63577	-272.51449	-272.55880	-272.15296	-272.46089
bicyclo[3.2.0]hept-6-ene	C2V	-272.62842	-272.50733	-272.55206	-272.14598	-272.45368
[2.2.1]propellane	CS	-272.55869	-272.43874	-272.48287	-272.07684	-272.39081
norbornene	C2	-272.64993	-272.52940	-272.57401	-272.16858	-272.47286
bicyclo[2.2.1]heptane	CS	-273.86445	-273.74561	-273.78962	-273.38233	-273.68164
bicyclo[3.2.0]heptane	D4H	-273.84124	-273.72207	-273.76563	-273.35801	-273.66062
spiro[3.3]heptane	C2	-273.80947	-273.69135	-273.73420	-273.32683	-273.63083
methylcyclohexane[c]	D3H	-275.06494	-274.94855	-274.99028	-274.58166	-274.87672
cubane	C2V	-309.41137	-309.26907	-309.32097	-308.85997	-309.22723
[3.4.4.4]fenestrane	D3H	-310.50040	-310.36264	-310.41404	-309.95135	-310.31843
[2.2.2]propellane	CS	-311.86287	-311.72597	-311.77497	-311.31133	-311.66490

bicyclo[2.2.2]octene	C2H	-311.95858	-311.82157	-311.87306	-311.40796	-311.75536
bicyclo[2.2.2]octane	D2D	-313.16617	-313.03086	-313.08158	-312.61482	-312.95690
cis-1,3-dimethylcyclohexane[c]	C3V	-314.36336	-314.23123	-314.27867	-313.81140	-314.14831
trans-1,4-dimethylcyclohexane[c]	C2	-314.36352	-314.23105	-314.27856	-313.81152	-314.14837
[4.4.4.4]fenestrane	TD	-349.86976	-349.71442	-349.77092	-349.25056	-349.65322
cis-1,3,5-trimethylcyclohexane[c]	C2H	-353.66219	-353.51385	-353.56714	-353.04160	-353.41994
[4.4.4.5]fenestrane	C2	-389.25994	-389.08827	-389.15185	-388.57233	-389.01529
adamantane	C3V		-390.42101	-390.48551	-389.90263	-390.33493
trans-decalin	C2		-391.60460	-391.66631	-391.08310	-391.51101
cis-decalin	C2V		-391.60025	-391.66196	-391.07868	-391.50628
1-methyladamantane	C3V		-429.70903	-429.77806	-429.13783	-429.61018
spiro[5.5]undecane	TD		-430.88038	-430.94820	-430.30615	-430.77556
1,3-dimethyladamantane	C2V		-468.99522	-469.07139	-468.37113	-468.88505
1,3,5-trimethyladamantane	C2V		-508.28257	-508.36565	-507.60558	-508.16000
1,3,5,7-tetramethyladamantane	C2V		-547.56640	-547.65695	-546.83665	-547.43450

Notes:

[a] Point group.

[b] M062X/6-31+G(2df,p).

[c] All methyl groups equatorial.

Table S5. Calculated enthalpies (298 K) of compounds in Figure 2 (hartrees).

Compound	PG[a]	W1BD	G4	CBS-APNO	CBS-QB3	M062X[b]
cyclopropene	C2V	-116.586274	-116.534083	-116.552433	-116.379268	-116.518268
cyclopropane	C2V	-117.835706	-117.785829	-117.803121	-117.628035	-117.759514
tetrahedrane	C2V	-154.613038	-154.542614	-154.568279	-154.337232	-154.542244
methylenecyclopropene	C2V	-154.670221	-154.599350	-154.624995	-154.394739	-154.586374
bicyclo[1.1.0]but-1(3)-ene	C2V	-154.599903	-154.531222	-154.557873	-154.325231	-154.513255
cyclobutene	D2D	-155.918675	-155.849216	-155.873854	-155.641994	-155.817960
bicyclobutane	D3H	-155.894485	-155.826116	-155.850871	-155.618645	-155.804401
methylenecyclopropane	C2V	-155.906137	-155.837811	-155.862277	-155.630606	-155.811777
cyclobutane	C1	-157.131621	-157.064467	-157.088204	-156.854705	-157.024777
[1.1.1]propellane	CS	-193.964844	-193.879243	-193.911995	-193.621881	-193.854552
cyclopentadiene	CS	-194.052773	-193.964217	-193.996962	-193.707640	-193.930359
bicyclo[2.1.0]pent-1-ene	C1	-193.913806	-193.827286	-193.858769	-193.569070	-193.796696
bicyclo[2.1.0]pent-1(4)-ene	CS	-193.902269	-193.815924	(fails)	-193.557817	-193.785344
bicyclo[2.1.0]pent-2-ene	CS	-193.978243	-193.890904	-193.922376	-193.633613	-193.862176
bicyclo[2.1.0]pent-4-ene	D2D	-193.911147	-193.824457	-193.856076	-193.566538	-193.795682
cyclopentene	D3H	-195.252233	-195.165703	-195.196869	-194.906672	-195.123175
bicyclo[2.1.0]pentane	CS	-195.206175	-195.120482	-195.151558	-194.860914	-195.084500
spiropentane	C2	-195.194935	-195.110027	-195.141114	-194.850278	-195.078948
bicyclo[1.1.1]pentane	D3H	-195.188499	-195.103809	-195.134330	-194.845149	-195.065464
methylenecyclobutane	C2V	-195.218630	-195.133275	-195.163877	-194.873591	-195.092355
cyclopentane	C2V	-196.456118	-196.371766	-196.402312	-196.110218	-196.321970
prismane	C2V	-232.015385	-231.908849	-231.949037	-231.601859	-231.887190
benzvalene	C1	-232.080092	-231.974220	-232.013728	-231.667598	-231.949080
[2.1.1]propellane	D2H	-233.258227	-233.155705	-233.194460	-232.846046	-233.117502
bicyclo[2.1.1]hexene	CS	-233.301082	-233.197664	-233.235405	-232.888937	-233.152536
bicyclo[2.2.0]hex-1-ene	D3D	-233.256655	-233.152678	-233.190700	-232.843103	-233.111350
Bicyclo[2.2.0]hex-1(4)-ene	C2	-233.244202	-233.139486	-233.177758	-232.830437	-233.098302
Bicyclo[2.2.0]hex-2-ene	C2V	-233.290528	-233.185764	-233.223515	-232.876430	-233.143955
cyclohexene	CS	-234.552425	-234.449764	-234.486890	-234.138117	-234.397636
methylenecyclopentane	CS	-234.546298	-234.444043	-234.481241	-234.132287	-234.391543
bicyclo[2.1.1]hexane	C2	-234.528734	-234.426789	-234.464101	-234.115887	-234.374616
bicyclo[3.1.0]hexane	C2H	-234.537186	-234.434805	-234.472553	-234.123225	-234.387264
spirohexane	D3D	-234.501608	-234.399862	-234.436980	-234.087687	-234.353981
cis-bicyclo[2.2.0]hexane	C2V	-234.502267	-234.399334	-234.436775	-234.087370	-234.349822
trans-bicyclo[2.2.0]hexane	C2V	-234.439671	-234.337935	-234.374867	-234.026736	-234.287347
cyclohexane	C2V	-235.759432	-235.659083	-235.695219	-235.344878	-235.598274
bicyclo[4.1.0]hepta-1,3,5-triene	CS	-270.206141	-270.081133	-270.131523	-269.727418	-270.055539
norbornadiene	C1	-271.421092	-271.298867	-271.343891	-270.940430	-271.249604
quadricycane	CS	-271.385825	-271.262754	-271.309330	-270.904052	-271.228357
bicyclo[3.2.0]hept-1(5)-ene	C2V	-272.605984	-272.484141	-272.529338	-272.123380	-272.432043
bicyclo[3.2.0]hept-2-ene	CS	-272.628955	-272.507674	-272.552074	-272.146173	-272.454209
bicyclo[3.2.0]hept-6-ene	C2V	-272.621633	-272.500545	-272.545351	-272.139222	-272.447010
[2.2.1]propellane	CS	-272.551730	-272.431763	-272.476007	-272.069890	-272.383957
norbornene	C2	-272.643676	-272.523134	-272.567828	-272.162346	-272.466719
bicyclo[2.2.1]heptane	CS	-273.857816	-273.738958	-273.782980	-273.375716	-273.675051
bicyclo[3.2.0]heptane	D4H	-273.834076	-273.714896	-273.758502	-273.350869	-273.653628
spiro[3.3]heptane	C2	-273.801733	-273.683599	-273.726544	-273.319124	-273.623297
methylcyclohexane[c]	D3H	-275.056691	-274.940282	-274.982108	-274.573439	-274.868669
cubane	C2V	-309.405779	-309.263504	-309.315507	-308.854407	-309.221791
[3.4.4.4]fenestrane	D3H	-310.492465	-310.354745	-310.406277	-309.943456	-310.310608
[2.2.2]propellane	CS	-311.854781	-311.717896	-311.767020	-311.303270	-311.657029

bicyclo[2.2.2]octene	C2H	-311.951236	-311.814218	-311.865759	-311.400641	-311.748083
bicyclo[2.2.2]octane	D2D	-313.158191	-313.022882	-313.073711	-312.606859	-312.949279
cis-1,3-dimethylcyclohexane[c]	C3V	-314.353696	-314.221468	-314.269035	-313.801769	-314.138821
trans-1,4-dimethylcyclohexane[c]	C2	-314.353830	-314.221336	-314.268913	-313.801858	-314.138880
[4.4.4.4]fenestrane	TD	-349.861202	-349.705879	-349.762546	-349.242042	-349.644737
cis-1,3,5-trimethylcyclohexane[c]	C2H	-353.650998	-353.502629	-353.556014	-353.030442	-353.408988
[4.4.4.5]fenestrane	C2	-389.250955	-389.079277	-389.142963	-388.563382	-389.006384
adamantane	C3V		-390.413082	-390.477448	-389.894758	-390.327067
trans-decalin	C2		-391.594591	-391.656348	-391.073148	-391.501233
cis-decalin	C2V		-391.590306	-391.652108	-391.068795	-391.496593
1-methyladamantane	C3V		-429.699314	-429.768501	-429.128184	-429.600811
spiro[5.5]undecane	TD		-430.869249	-430.937132	-430.295086	-430.764707
1,3-dimethyladamantane	C2V		-468.984078	-469.060313	-468.360072	-468.874203
1,3,5-trimethyladamantane	C2V		-508.269728	-508.353047	-507.592847	-508.147677
1,3,5,7-tetramethyladamantane	C2V		-547.552647	-547.642804	-546.823027	-547.420767

Notes:

[a] Point group.

[b] M062X/6-31+G(2df,p).

[c] All methyl groups equatorial.

List S1: G-4 optimized geometries & abbreviated calculation results.

Ethyne

Species name: ethyne
Full file name: ethyne_g4.log
Method: G4 calculation
Point group: D*H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026454	E(Thermal)=	0.029370
E(CCSD(T))=	-77.092977	E(Empiric)=	-0.034735
DE(Plus)=	-0.006117	DE(2DF)=	-0.061580
E(Delta-G3XP)=	-0.113843	DE(HF)=	-0.007552
G4(0 K)=	-77.290352	G4 Energy=	-77.287435
G4 Enthalpy=	-77.286491	G4 Free Energy=	-77.309361

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.599454
2	6	0	0.000000	0.000000	-0.599454
3	1	0	0.000000	0.000000	1.661640
4	1	0	0.000000	0.000000	-1.661640

Ethene

Species name: ethene
Full file name: ethene_g4.log
Method: G4 calculation
Point group: D2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.050245	E(Thermal)=	0.053300
E(CCSD(T))=	-78.321716	E(Empiric)=	-0.041682
DE(Plus)=	-0.005929	DE(2DF)=	-0.076975
E(Delta-G3XP)=	-0.117562	DE(HF)=	-0.008254
G4(0 K)=	-78.521873	G4 Energy=	-78.518818
G4 Enthalpy=	-78.517874	G4 Free Energy=	-78.542745

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.663591
2	6	0	0.000000	0.000000	-0.663591

3	1	0	0.000000	0.921292	1.238172
4	1	0	0.000000	-0.921292	1.238172
5	1	0	0.000000	-0.921292	-1.238172
6	1	0	0.000000	0.921292	-1.238172

Ethane

Species name: ethane
Full file name: ethane_g4.log
Method: G4 calculation
Point group: D3D
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073450	E(Thermal)=	0.076956
E(CCSD(T))=	-79.534464	E(Empiric)=	-0.048629
DE(Plus)=	-0.003249	DE(2DF)=	-0.095322
E(Delta-G3XP)=	-0.121101	DE(HF)=	-0.008797
G4(0 K)=	-79.738111	G4 Energy=	-79.734605
G4 Enthalpy=	-79.733661	G4 Free Energy=	-79.759546

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.765033
2	6	0	0.000000	0.000000	-0.765033
3	1	0	0.000000	1.019540	1.164045
4	1	0	0.882947	-0.509770	1.164045
5	1	0	-0.882947	-0.509770	1.164045
6	1	0	0.000000	-1.019540	-1.164045
7	1	0	-0.882947	0.509770	-1.164045
8	1	0	0.882947	0.509770	-1.164045

Propyne

Species name: propyne
Full file name: propyne_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054602	E(Thermal)=	0.058629
E(CCSD(T))=	-116.283304	E(Empiric)=	-0.055576
DE(Plus)=	-0.007173	DE(2DF)=	-0.101015
E(Delta-G3XP)=	-0.172787	DE(HF)=	-0.011491
G4(0 K)=	-116.576744	G4 Energy=	-116.572717
G4 Enthalpy=	-116.571773	G4 Free Energy=	-116.599950

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.420141
2	6	0	0.000000	0.000000	0.218682
3	6	0	0.000000	0.000000	-1.236297
4	1	0	0.000000	0.000000	2.481619
5	1	0	0.000000	1.021183	-1.632258
6	1	0	-0.884370	-0.510592	-1.632258
7	1	0	0.884370	-0.510592	-1.632258

Propene

Species name: propene
Full file name: propene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.078400	E(Thermal)=	0.082509
E(CCSD(T))=	-117.507708	E(Empiric)=	-0.062523
DE(Plus)=	-0.007387	DE(2DF)=	-0.116414
E(Delta-G3XP)=	-0.175993	DE(HF)=	-0.012234
G4(0 K)=	-117.803858	G4 Energy=	-117.799749
G4 Enthalpy=	-117.798805	G4 Free Energy=	-117.828869

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.290426	0.153943	0.000000
2	6	0	0.000000	0.472767	0.000000
3	6	0	-1.136024	-0.506462	0.000000
4	1	0	1.622258	-0.880961	0.000000
5	1	0	2.067951	0.910466	0.000000
6	1	0	-0.283621	1.524854	0.000000
7	1	0	-0.776592	-1.539589	0.000000
8	1	0	-1.778205	-0.368130	0.878760
9	1	0	-1.778205	-0.368130	-0.878760

Propane

Species name: propane
Full file name: propane_g4.log

Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.101676	E(Thermal)=	0.106261
E(CCSD(T))=	-118.716169	E(Empiric)=	-0.069470
DE(Plus)=	-0.005081	DE(2DF)=	-0.134712
E(Delta-G3XP)=	-0.179312	DE(HF)=	-0.012714
G4(0 K)=	-119.015782	G4 Energy=	-119.011197
G4 Enthalpy=	-119.010253	G4 Free Energy=	-119.040836

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.276122	-0.259763
2	6	0	0.000000	0.000000	0.586561
3	6	0	0.000000	-1.276122	-0.259763
4	1	0	0.000000	2.174431	0.365815
5	1	0	0.883312	1.320660	-0.906945
6	1	0	-0.883312	1.320660	-0.906945
7	1	0	-0.876276	0.000000	1.246969
8	1	0	0.876276	0.000000	1.246969
9	1	0	0.000000	-2.174431	0.365815
10	1	0	0.883312	-1.320660	-0.906945
11	1	0	-0.883312	-1.320660	-0.906945

1-Butyne

Species name: 1butyne
Full file name: 1butyne_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.083153	E(Thermal)=	0.088246
E(CCSD(T))=	-155.464709	E(Empiric)=	-0.076417
DE(Plus)=	-0.009152	DE(2DF)=	-0.140438
E(Delta-G3XP)=	-0.230627	DE(HF)=	-0.015417
G4(0 K)=	-155.853608	G4 Energy=	-155.848514
G4 Enthalpy=	-155.847570	G4 Free Energy=	-155.880513

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.330886	-1.457835	0.000000
2	6	0	-0.741597	-0.410091	0.000000

3	6	0	0.000000	0.845799	0.000000
4	6	0	1.526084	0.642758	0.000000
5	1	0	-1.861666	-2.377202	0.000000
6	1	0	-0.292444	1.438463	0.876044
7	1	0	-0.292444	1.438463	-0.876044
8	1	0	2.038347	1.609343	0.000000
9	1	0	1.843299	0.083571	0.884223
10	1	0	1.843299	0.083571	-0.884223

2-Butyne

Species name: 2butyne
Full file name: 2butyne_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.082677	E(Thermal)=	0.088476
E(CCSD(T))=	-155.472484	E(Empiric)=	-0.076417
DE(Plus)=	-0.007855	DE(2DF)=	-0.140421
E(Delta-G3XP)=	-0.231608	DE(HF)=	-0.015437
G4(0 K)=	-155.861543	G4 Energy=	-155.855744
G4 Enthalpy=	-155.854800	G4 Free Energy=	-155.888581

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.601793
2	6	0	0.000000	0.000000	-0.601793
3	6	0	0.000000	0.000000	2.058000
4	6	0	0.000000	0.000000	-2.058000
5	1	0	0.000000	1.020281	2.457860
6	1	0	0.000000	1.020281	-2.457860
7	1	0	0.883589	-0.510140	2.457860
8	1	0	-0.883589	-0.510140	2.457860
9	1	0	0.883589	-0.510140	-2.457860
10	1	0	-0.883589	-0.510140	-2.457860

1,3-Butadiene (s-trans)

Species name: 13butadiene
Full file name: 13butadiene_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.083879	E(Thermal)=	0.088566
E(CCSD(T))=	-155.486660	E(Empiric)=	-0.076417
DE(Plus)=	-0.010861	DE(2DF)=	-0.138090
E(Delta-G3XP)=	-0.230639	DE(HF)=	-0.015701
G4(0 K)=	-155.874489	G4 Energy=	-155.869803
G4 Enthalpy=	-155.868858	G4 Free Energy=	-155.900298

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.324488	0.650691	0.000000
2	6	0	0.324488	-0.650691	0.000000
3	6	0	0.324488	1.818881	0.000000
4	6	0	-0.324488	-1.818881	0.000000
5	1	0	-1.413602	0.642140	0.000000
6	1	0	1.413602	-0.642140	0.000000
7	1	0	1.409756	1.864440	0.000000
8	1	0	-0.201323	2.766799	0.000000
9	1	0	-1.409756	-1.864440	0.000000
10	1	0	0.201323	-2.766799	0.000000

Isobutylene

Species name: isobutylene
Full file name: isobutylene_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.106071	E(Thermal)=	0.111428
E(CCSD(T))=	-156.694791	E(Empiric)=	-0.083364
DE(Plus)=	-0.008841	DE(2DF)=	-0.156287
E(Delta-G3XP)=	-0.234691	DE(HF)=	-0.016076
G4(0 K)=	-157.087980	G4 Energy=	-157.082622
G4 Enthalpy=	-157.081678	G4 Free Energy=	-157.114654

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.124495
2	6	0	0.000000	0.000000	1.456901
3	6	0	0.000000	1.275057	-0.677920
4	6	0	0.000000	-1.275057	-0.677920
5	1	0	0.000000	0.923221	2.027801
6	1	0	0.000000	-0.923221	2.027801
7	1	0	0.000000	2.159642	-0.036201
8	1	0	0.878411	1.327351	-1.334134

9	1	0	-0.878411	1.327351	-1.334134
10	1	0	0.000000	-2.159642	-0.036201
11	1	0	-0.878411	-1.327351	-1.334134
12	1	0	0.878411	-1.327351	-1.334134

Trans-2-butene

Species name: trans2butene
Full file name: trans2butene_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.106109	E(Thermal)=	0.111626
E(CCSD(T))=	-156.693574	E(Empiric)=	-0.083364
DE(Plus)=	-0.008599	DE(2DF)=	-0.155713
E(Delta-G3XP)=	-0.234399	DE(HF)=	-0.016201
G4(0 K)=	-157.085741	G4 Energy=	-157.080224
G4 Enthalpy=	-157.079280	G4 Free Energy=	-157.112502

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.323605	0.581631	0.000000
2	6	0	0.323605	-0.581631	0.000000
3	6	0	0.323605	1.934777	0.000000
4	6	0	-0.323605	-1.934777	0.000000
5	1	0	-1.414172	0.573704	0.000000
6	1	0	1.414172	-0.573704	0.000000
7	1	0	0.025349	2.520627	0.878747
8	1	0	0.025349	2.520627	-0.878747
9	1	0	1.415004	1.857664	0.000000
10	1	0	-0.025349	-2.520627	0.878747
11	1	0	-1.415004	-1.857664	0.000000
12	1	0	-0.025349	-2.520627	-0.878747

1-Butene C1

Species name: 1butene
Full file name: 1butene_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.106646	E(Thermal)=	0.111968
E(CCSD(T))=	-156.689143	E(Empiric)=	-0.083364

DE(Plus)= -0.009343 DE(2DF)= -0.155973
E(Delta-G3XP)= -0.234017 DE(HF)= -0.016131
G4(0 K)= -157.081325 G4 Energy= -157.076003
G4 Enthalpy= -157.075059 G4 Free Energy= -157.108860

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.859404	0.014603	-0.277265
2	6	0	0.722315	-0.292889	0.338735
3	6	0	-0.538335	0.523411	0.303061
4	6	0	-1.727837	-0.248320	-0.291317
5	1	0	1.960711	0.922387	-0.866257
6	1	0	2.735852	-0.622106	-0.217462
7	1	0	0.665583	-1.216216	0.916531
8	1	0	-0.796856	0.835356	1.324873
9	1	0	-0.365071	1.442251	-0.269025
10	1	0	-2.638707	0.358107	-0.273710
11	1	0	-1.528764	-0.535277	-1.328531
12	1	0	-1.926031	-1.165335	0.274291

Butane

Species name: butane
Full file name: butane_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.129709 E(Thermal)= 0.135563
E(CCSD(T))= -157.897982 E(Empiric)= -0.090311
DE(Plus)= -0.006825 DE(2DF)= -0.174199
E(Delta-G3XP)= -0.237705 DE(HF)= -0.016624
G4(0 K)= -158.293938 G4 Energy= -158.288084
G4 Enthalpy= -158.287140 G4 Free Energy= -158.321367

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704164	1.833178	0.000000
2	6	0	-0.704164	0.302308	0.000000
3	6	0	0.704164	-0.302308	0.000000
4	6	0	0.704164	-1.833178	0.000000
5	1	0	-1.722110	2.235537	0.000000
6	1	0	-0.190081	2.228569	0.883359
7	1	0	-0.190081	2.228569	-0.883359
8	1	0	-1.254392	-0.065309	-0.876582

9	1	0	-1.254392	-0.065309	0.876582
10	1	0	1.254392	0.065309	0.876582
11	1	0	1.254392	0.065309	-0.876582
12	1	0	1.722110	-2.235537	0.000000
13	1	0	0.190081	-2.228569	-0.883359
14	1	0	0.190081	-2.228569	0.883359

Isobutane

Species name: isobutane
Full file name: isobutane_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.129273	E(Thermal)=	0.135060
E(CCSD(T))=	-157.900274	E(Empiric)=	-0.090311
DE(Plus)=	-0.007281	DE(2DF)=	-0.174412
E(Delta-G3XP)=	-0.237523	DE(HF)=	-0.016476
G4(0 K)=	-158.297004	G4 Energy=	-158.291217
G4 Enthalpy=	-158.290273	G4 Free Energy=	-158.323661

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.372646
2	1	0	0.000000	0.000000	1.471935
3	6	0	0.000000	1.460975	-0.095682
4	6	0	1.265242	-0.730488	-0.095682
5	6	0	-1.265242	-0.730488	-0.095682
6	1	0	0.000000	1.519796	-1.190990
7	1	0	-0.885156	1.995967	0.264572
8	1	0	0.885156	1.995967	0.264572
9	1	0	1.316182	-0.759898	-1.190990
10	1	0	1.285980	-1.764551	0.264572
11	1	0	2.171136	-0.231416	0.264572
12	1	0	-1.316182	-0.759898	-1.190990
13	1	0	-1.285980	-1.764551	0.264572
14	1	0	-2.171136	-0.231416	0.264572

1,4-Pentadiene

Species name: 14pentadiene
Full file name: 14pentadiene_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.111606	E(Thermal)=	0.117682
E(CCSD(T))=	-194.662186	E(Empiric)=	-0.097258
DE(Plus)=	-0.013544	DE(2DF)=	-0.177145
E(Delta-G3XP)=	-0.288672	DE(HF)=	-0.019537
G4(0 K)=	-195.146736	G4 Energy=	-195.140659
G4 Enthalpy=	-195.139715	G4 Free Energy=	-195.175364

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.662379
2	6	0	0.000000	1.251777	-0.179218
3	6	0	-0.954231	2.176790	-0.174569
4	6	0	0.000000	-1.251777	-0.179218
5	6	0	0.954231	-2.176790	-0.174569
6	1	0	0.882934	-0.009715	1.315224
7	1	0	-0.882934	0.009715	1.315224
8	1	0	0.857396	1.366523	-0.841108
9	1	0	-1.826284	2.093004	0.468504
10	1	0	-0.902610	3.056750	-0.807037
11	1	0	-0.857396	-1.366523	-0.841108
12	1	0	1.826284	-2.093004	0.468504
13	1	0	0.902610	-3.056750	-0.807037

2-Methylbuta-1,3-diene

Species name:	2m13butadiene
Full file name:	2m13butadiene_g4.log
Method:	G4 calculation
Point group:	CS
NImag:	0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.111748	E(Thermal)=	0.117651
E(CCSD(T))=	-194.672734	E(Empiric)=	-0.097258
DE(Plus)=	-0.012255	DE(2DF)=	-0.178335
E(Delta-G3XP)=	-0.289464	DE(HF)=	-0.019548
G4(0 K)=	-195.157846	G4 Energy=	-195.151943
G4 Enthalpy=	-195.150999	G4 Free Energy=	-195.186365

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.377926	-1.944683	0.000000
2	6	0	-0.824818	-0.685658	0.000000
3	6	0	0.000000	0.525085	0.000000

4	6	0	-0.584846	1.730697	0.000000
5	6	0	1.500173	0.375941	0.000000
6	1	0	0.679612	-2.185576	0.000000
7	1	0	-1.062621	-2.785370	0.000000
8	1	0	-1.899368	-0.510341	0.000000
9	1	0	-0.006390	2.648286	0.000000
10	1	0	-1.665167	1.835794	0.000000
11	1	0	1.993624	1.350410	0.000000
12	1	0	1.842409	-0.180745	0.880113
13	1	0	1.842409	-0.180745	-0.880113

2-Pentyne

Species name: 2pentyne
Full file name: 2pentyne_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.111139	E(Thermal)=	0.118049
E(CCSD(T))=	-194.654014	E(Empiric)=	-0.097258
DE(Plus)=	-0.009862	DE(2DF)=	-0.179833
E(Delta-G3XP)=	-0.289500	DE(HF)=	-0.019346
G4(0 K)=	-195.138675	G4 Energy=	-195.131765
G4 Enthalpy=	-195.130821	G4 Free Energy=	-195.169801

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.650810	0.122116	0.000000
2	6	0	-1.199381	0.241516	0.000000
3	6	0	0.000000	0.349717	0.000000
4	6	0	1.456135	0.450977	0.000000
5	6	0	2.157709	-0.919414	0.000000
6	1	0	-3.091296	0.597380	0.883728
7	1	0	-3.091296	0.597380	-0.883728
8	1	0	-2.965069	-0.927711	0.000000
9	1	0	1.782723	1.027425	0.875439
10	1	0	1.782723	1.027425	-0.875439
11	1	0	3.244733	-0.793495	0.000000
12	1	0	1.877781	-1.498937	0.884028
13	1	0	1.877781	-1.498937	-0.884028

3-Methyl-1-butyne

Species name: 3m1butyne
Full file name: 3m1butyne_g4.log

Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.110823	E(Thermal)=	0.117218
E(CCSD(T))=	-194.648533	E(Empiric)=	-0.097258
DE(Plus)=	-0.011496	DE(2DF)=	-0.180069
E(Delta-G3XP)=	-0.288470	DE(HF)=	-0.019160
G4(0 K)=	-195.134164	G4 Energy=	-195.127770
G4 Enthalpy=	-195.126825	G4 Free Energy=	-195.163107

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.142667	-2.223233	0.000000
2	6	0	0.115175	-1.048773	0.000000
3	6	0	0.404869	0.384889	0.000000
4	6	0	-0.142667	1.058751	1.273838
5	6	0	-0.142667	1.058751	-1.273838
6	1	0	1.497305	0.504194	0.000000
7	1	0	-0.359833	-3.262481	0.000000
8	1	0	0.118031	2.121852	1.281044
9	1	0	-1.232673	0.971751	1.316748
10	1	0	0.269775	0.594385	2.173252
11	1	0	0.118031	2.121852	-1.281044
12	1	0	-1.232673	0.971751	-1.316748
13	1	0	0.269775	0.594385	-2.173252

3-Methyl-1-butene CS

Species name: 3m1butene
Full file name: 3m1butene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.134200	E(Thermal)=	0.140851
E(CCSD(T))=	-195.873121	E(Empiric)=	-0.104205
DE(Plus)=	-0.011633	DE(2DF)=	-0.195836
E(Delta-G3XP)=	-0.292069	DE(HF)=	-0.019869
G4(0 K)=	-196.362533	G4 Energy=	-196.355881
G4 Enthalpy=	-196.354937	G4 Free Energy=	-196.392077

Standard orientation:

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

1	6	0	-0.038197	-2.155253	0.000000
2	6	0	0.465784	-0.925606	0.000000
3	6	0	-0.330587	0.352588	0.000000
4	6	0	-0.038197	1.176242	1.266987
5	6	0	-0.038197	1.176242	-1.266987
6	1	0	-1.110605	-2.331712	0.000000
7	1	0	0.595718	-3.035834	0.000000
8	1	0	1.549455	-0.794813	0.000000
9	1	0	-1.396263	0.088379	0.000000
10	1	0	1.022335	1.449533	1.319236
11	1	0	-0.620866	2.103611	1.273731
12	1	0	-0.282437	0.611206	2.171358
13	1	0	1.022335	1.449533	-1.319236
14	1	0	-0.620866	2.103611	-1.273731
15	1	0	-0.282437	0.611206	-2.171358

Pentane

Species name: pentane
Full file name: pentane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.157799	E(Thermal)=	0.164963
E(CCSD(T))=	-197.079787	E(Empiric)=	-0.111152
DE(Plus)=	-0.008659	DE(2DF)=	-0.213684
E(Delta-G3XP)=	-0.296033	DE(HF)=	-0.020532
G4(0 K)=	-197.572047	G4 Energy=	-197.564884
G4 Enthalpy=	-197.563940	G4 Free Energy=	-197.601763

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.557724	0.323989
2	6	0	0.000000	1.282379	-0.523214
3	6	0	0.000000	0.000000	0.315511
4	6	0	0.000000	-1.282379	-0.523214
5	6	0	0.000000	-2.557724	0.323989
6	1	0	0.000000	3.455728	-0.301926
7	1	0	-0.883384	2.602939	0.970841
8	1	0	0.883384	2.602939	0.970841
9	1	0	0.876627	1.281437	-1.184740
10	1	0	-0.876627	1.281437	-1.184740
11	1	0	-0.876906	0.000000	0.978542
12	1	0	0.876906	0.000000	0.978542
13	1	0	0.876627	-1.281437	-1.184740
14	1	0	-0.876627	-1.281437	-1.184740
15	1	0	0.000000	-3.455728	-0.301926
16	1	0	-0.883384	-2.602939	0.970841

17	1	0	0.883384	-2.602939	0.970841

Neopentane

Species name: neopentane
Full file name: neopentane_g4.log
Method: G4 calculation
Point group: TD
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.157141	E(Thermal)=	0.163970
E(CCSD(T))=	-197.085880	E(Empiric)=	-0.111152
DE(Plus)=	-0.009894	DE(2DF)=	-0.214356
E(Delta-G3XP)=	-0.295439	DE(HF)=	-0.020141
G4(0 K)=	-197.579721	G4 Energy=	-197.572891
G4 Enthalpy=	-197.571947	G4 Free Energy=	-197.606335

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.888543	0.888543	0.888543
3	6	0	-0.888543	-0.888543	0.888543
4	6	0	0.888543	-0.888543	-0.888543
5	6	0	-0.888543	0.888543	-0.888543
6	1	0	1.534256	1.534256	0.282943
7	1	0	0.282943	1.534256	1.534256
8	1	0	1.534256	0.282943	1.534256
9	1	0	-1.534256	-1.534256	0.282943
10	1	0	-1.534256	-0.282943	1.534256
11	1	0	-0.282943	-1.534256	1.534256
12	1	0	0.282943	-1.534256	-1.534256
13	1	0	1.534256	-0.282943	-1.534256
14	1	0	1.534256	-1.534256	-0.282943
15	1	0	-1.534256	0.282943	-1.534256
16	1	0	-0.282943	1.534256	-1.534256
17	1	0	-1.534256	1.534256	-0.282943

Benzene

Species name: benzene
Full file name: benzene_g4.log
Method: G4 calculation
Point group: D6H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.098705	E(Thermal)=	0.103160
E(CCSD(T))=	-231.530418	E(Empiric)=	-0.104205
DE(Plus)=	-0.014014	DE(2DF)=	-0.182003
E(Delta-G3XP)=	-0.339214	DE(HF)=	-0.022842
G4(0 K)=	-232.093991	G4 Energy=	-232.089537
G4 Enthalpy=	-232.088593	G4 Free Energy=	-232.119128

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.393554	0.000000
2	6	0	1.206853	0.696777	0.000000
3	6	0	-1.206853	0.696777	0.000000
4	6	0	1.206853	-0.696777	0.000000
5	6	0	-1.206853	-0.696777	0.000000
6	6	0	0.000000	-1.393554	0.000000
7	1	0	0.000000	2.478745	0.000000
8	1	0	2.146656	1.239372	0.000000
9	1	0	-2.146656	1.239372	0.000000
10	1	0	2.146656	-1.239372	0.000000
11	1	0	-2.146656	-1.239372	0.000000
12	1	0	0.000000	-2.478745	0.000000

3-Methylenepenta-1,4-diene

Species name: 3methylenepenta14diene
Full file name: 3methylenepenta14diene_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.117058	E(Thermal)=	0.123673
E(CCSD(T))=	-232.644949	E(Empiric)=	-0.111152
DE(Plus)=	-0.015718	DE(2DF)=	-0.200083
E(Delta-G3XP)=	-0.343530	DE(HF)=	-0.022950
G4(0 K)=	-233.221324	G4 Energy=	-233.214709
G4 Enthalpy=	-233.213765	G4 Free Energy=	-233.250603

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.681572
2	6	0	0.000000	0.000000	2.027875
3	6	0	0.000000	1.294343	-0.022141
4	6	0	0.000000	-1.294343	-0.022141
5	6	0	-0.406990	1.551567	-1.267177
6	6	0	0.406990	-1.551567	-1.267177

7	1	0	0.029570	0.923099	2.596542
8	1	0	-0.029570	-0.923099	2.596542
9	1	0	0.324279	2.131760	0.593537
10	1	0	-0.324279	-2.131760	0.593537
11	1	0	-0.399893	2.565393	-1.652563
12	1	0	-0.784130	0.782688	-1.929952
13	1	0	0.399893	-2.565393	-1.652563
14	1	0	0.784130	-0.782688	-1.929952

3-Methyl-1,4-pentadiene, Cs conformation

Species name: 3m14pentadiene
Full file name: 3m14pentadiene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.139116	E(Thermal)=	0.146603
E(CCSD(T))=	-233.845323	E(Empiric)=	-0.118099
DE(Plus)=	-0.015833	DE(2DF)=	-0.217283
E(Delta-G3XP)=	-0.346649	DE(HF)=	-0.023276
G4(0 K)=	-234.427345	G4 Energy=	-234.419858
G4 Enthalpy=	-234.418914	G4 Free Energy=	-234.458630

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.373713	0.076882	0.000000
2	6	0	1.334293	1.286699	0.000000
3	1	0	0.970239	-0.843531	0.000000
4	6	0	-0.487399	0.089128	1.240517
5	6	0	-0.487399	0.089128	-1.240517
6	6	0	-0.487399	-0.842725	2.187399
7	6	0	-0.487399	-0.842725	-2.187399
8	1	0	0.775557	2.229530	0.000000
9	1	0	1.971417	1.274587	-0.889371
10	1	0	1.971417	1.274587	0.889371
11	1	0	-1.146123	0.952833	1.339126
12	1	0	-1.146123	0.952833	-1.339126
13	1	0	0.152286	-1.718857	2.125591
14	1	0	-1.125708	-0.770724	3.061703
15	1	0	0.152286	-1.718857	-2.125591
16	1	0	-1.125708	-0.770724	-3.061703

4-Methyl-2-pentyne

Species name: 4m2pentyne

Full file name: 4m2pentyne_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.138772	E(Thermal)=	0.147017
E(CCSD(T))=	-233.837975	E(Empiric)=	-0.118099
DE(Plus)=	-0.012295	DE(2DF)=	-0.219442
E(Delta-G3XP)=	-0.347317	DE(HF)=	-0.023080
G4(0 K)=	-234.419436	G4 Energy=	-234.411191
G4 Enthalpy=	-234.410247	G4 Free Energy=	-234.452682

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168355	-3.000498	0.000000
2	6	0	0.041743	-1.559223	0.000000
3	6	0	0.223591	-0.368419	0.000000
4	6	0	0.420569	1.082059	0.000000
5	6	0	-0.168355	1.723190	1.272329
6	6	0	-0.168355	1.723190	-1.272329
7	1	0	-0.730856	-3.322399	-0.883645
8	1	0	-0.730856	-3.322399	0.883645
9	1	0	0.783737	-3.543100	0.000000
10	1	0	1.502678	1.276229	0.000000
11	1	0	0.024586	2.800977	1.280434
12	1	0	-1.250969	1.567965	1.315264
13	1	0	0.271524	1.285994	2.172555
14	1	0	0.024586	2.800977	-1.280434
15	1	0	-1.250969	1.567965	-1.315264
16	1	0	0.271524	1.285994	-2.172555

3,3-Dimethyl-1-butyne

Species name: 33dm1butyne
Full file name: 33dm1butyne_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.137929	E(Thermal)=	0.145710
E(CCSD(T))=	-233.833995	E(Empiric)=	-0.118099
DE(Plus)=	-0.014231	DE(2DF)=	-0.219877
E(Delta-G3XP)=	-0.346150	DE(HF)=	-0.022769
G4(0 K)=	-234.417191	G4 Energy=	-234.409410
G4 Enthalpy=	-234.408466	G4 Free Energy=	-234.446701

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.373478
2	6	0	0.000000	0.000000	1.170933
3	6	0	0.000000	0.000000	-0.296705
4	6	0	0.000000	1.459284	-0.805563
5	6	0	-1.263777	-0.729642	-0.805563
6	6	0	1.263777	-0.729642	-0.805563
7	1	0	0.000000	0.000000	3.435273
8	1	0	0.000000	1.475213	-1.900733
9	1	0	0.885300	1.995966	-0.453195
10	1	0	-0.885300	1.995966	-0.453195
11	1	0	-1.277572	-0.737607	-1.900733
12	1	0	-2.171207	-0.231291	-0.453195
13	1	0	-1.285908	-1.764675	-0.453195
14	1	0	1.277572	-0.737607	-1.900733
15	1	0	2.171207	-0.231291	-0.453195
16	1	0	1.285908	-1.764675	-0.453195

3,3-Dimethyl-1-butene CS

Species name: tbuethylene
Full file name: tbuethylene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.161559	E(Thermal)=	0.169436
E(CCSD(T))=	-235.057399	E(Empiric)=	-0.125046
DE(Plus)=	-0.014041	DE(2DF)=	-0.236268
E(Delta-G3XP)=	-0.350184	DE(HF)=	-0.023518
G4(0 K)=	-235.644896	G4 Energy=	-235.637019
G4 Enthalpy=	-235.636075	G4 Free Energy=	-235.675695

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.121921	-2.202200	0.000000
2	6	0	0.567330	-1.065782	0.000000
3	6	0	0.030766	0.350499	0.000000
4	6	0	-1.504341	0.397737	0.000000
5	6	0	0.567330	1.070912	1.257264
6	6	0	0.567330	1.070912	-1.257264
7	1	0	-1.206279	-2.229211	0.000000
8	1	0	0.380222	-3.164093	0.000000
9	1	0	1.657148	-1.121384	0.000000
10	1	0	-1.851964	1.436052	0.000000
11	1	0	-1.919767	-0.093137	-0.885871

12	1	0	-1.919767	-0.093137	0.885871
13	1	0	0.249891	2.119594	1.266996
14	1	0	0.198644	0.594058	2.170882
15	1	0	1.662185	1.052571	1.287500
16	1	0	0.249891	2.119594	-1.266996
17	1	0	0.198644	0.594058	-2.170882
18	1	0	1.662185	1.052571	-1.287500

Hexane

Species name: hexane
Full file name: hexane_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.185735	E(Thermal)=	0.194260
E(CCSD(T))=	-236.261615	E(Empiric)=	-0.131993
DE(Plus)=	-0.010447	DE(2DF)=	-0.253147
E(Delta-G3XP)=	-0.354456	DE(HF)=	-0.024441
G4(0 K)=	-236.850364	G4 Energy=	-236.841839
G4 Enthalpy=	-236.840895	G4 Free Energy=	-236.882430

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.413694	2.900961	0.000000
2	6	0	-1.413694	1.369860	0.000000
3	6	0	-0.005189	0.765970	0.000000
4	6	0	0.005189	-0.765970	0.000000
5	6	0	1.413694	-1.369860	0.000000
6	6	0	1.413694	-2.900961	0.000000
7	1	0	-2.431866	3.302802	0.000000
8	1	0	-0.899688	3.296399	0.883351
9	1	0	-0.899688	3.296399	-0.883351
10	1	0	-1.964202	1.003074	-0.876595
11	1	0	-1.964202	1.003074	0.876595
12	1	0	0.546433	1.133405	0.876983
13	1	0	0.546433	1.133405	-0.876983
14	1	0	-0.546433	-1.133405	-0.876983
15	1	0	-0.546433	-1.133405	0.876983
16	1	0	1.964202	-1.003074	0.876595
17	1	0	1.964202	-1.003074	-0.876595
18	1	0	2.431866	-3.302802	0.000000
19	1	0	0.899688	-3.296399	-0.883351
20	1	0	0.899688	-3.296399	0.883351

Toluene

Species name: toluene
Full file name: toluene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.125560	E(Thermal)=	0.131875
E(CCSD(T))=	-270.716165	E(Empiric)=	-0.125046
DE(Plus)=	-0.015723	DE(2DF)=	-0.221807
E(Delta-G3XP)=	-0.397692	DE(HF)=	-0.026537
G4(0 K)=	-271.377411	G4 Energy=	-271.371096
G4 Enthalpy=	-271.370152	G4 Free Energy=	-271.408351

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003648	0.911383	0.000000
2	6	0	0.026817	2.420506	0.000000
3	6	0	-0.007003	0.193801	1.199775
4	6	0	-0.007003	0.193801	-1.199775
5	6	0	-0.007003	-1.198540	1.202697
6	6	0	-0.007003	-1.198540	-1.202697
7	6	0	-0.006217	-1.900935	0.000000
8	1	0	1.057276	2.797365	0.000000
9	1	0	-0.467112	2.831085	0.885585
10	1	0	-0.467112	2.831085	-0.885585
11	1	0	-0.011655	0.733759	2.142448
12	1	0	-0.011655	0.733759	-2.142448
13	1	0	-0.011956	-1.735043	2.146173
14	1	0	-0.011956	-1.735043	-2.146173
15	1	0	-0.009457	-2.985827	0.000000

4,4-Dimethyl-2-pentyne

Species name: 44dm2pentyne
Full file name: 44dm2pentyne_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.165825	E(Thermal)=	0.175491
E(CCSD(T))=	-273.023556	E(Empiric)=	-0.138940
DE(Plus)=	-0.015134	DE(2DF)=	-0.259223
E(Delta-G3XP)=	-0.404993	DE(HF)=	-0.026662
G4(0 K)=	-273.702683	G4 Energy=	-273.693018
G4 Enthalpy=	-273.692074	G4 Free Energy=	-273.736505

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	3.237840
2	6	0	0.000000	0.000000	1.781113
3	6	0	0.000000	0.000000	0.576391
4	6	0	0.000000	0.000000	-0.892504
5	6	0	0.000000	1.457847	-1.405710
6	6	0	-1.262533	-0.728924	-1.405710
7	6	0	1.262533	-0.728924	-1.405710
8	1	0	0.883696	-0.510202	3.637383
9	1	0	0.000000	1.020405	3.637383
10	1	0	-0.883696	-0.510202	3.637383
11	1	0	0.000000	1.473940	-2.501176
12	1	0	0.885185	1.995341	-1.053814
13	1	0	-0.885185	1.995341	-1.053814
14	1	0	-1.276469	-0.736970	-2.501176
15	1	0	-2.170608	-0.231078	-1.053814
16	1	0	-1.285423	-1.764263	-1.053814
17	1	0	1.276469	-0.736970	-2.501176
18	1	0	2.170608	-0.231078	-1.053814
19	1	0	1.285423	-1.764263	-1.053814

Heptane

Species name: heptane
Full file name: heptane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.213813	E(Thermal)=	0.223669
E(CCSD(T))=	-275.443445	E(Empiric)=	-0.152834
DE(Plus)=	-0.012290	DE(2DF)=	-0.292606
E(Delta-G3XP)=	-0.412838	DE(HF)=	-0.028353
G4(0 K)=	-276.128553	G4 Energy=	-276.118697
G4 Enthalpy=	-276.117753	G4 Free Energy=	-276.162746

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.839663	-0.353025
2	6	0	0.000000	2.564530	0.494536
3	6	0	0.000000	1.281801	-0.344096
4	6	0	0.000000	0.000000	0.495416
5	6	0	0.000000	-1.281801	-0.344096
6	6	0	0.000000	-2.564530	0.494536

7	6	0	0.000000	-3.839663	-0.353025
8	1	0	0.000000	4.737783	0.272738
9	1	0	0.883393	3.884716	-0.999883
10	1	0	-0.883393	3.884716	-0.999883
11	1	0	-0.876606	2.563732	1.156052
12	1	0	0.876606	2.563732	1.156052
13	1	0	0.876932	1.282530	-1.006875
14	1	0	-0.876932	1.282530	-1.006875
15	1	0	-0.877025	0.000000	1.157940
16	1	0	0.877025	0.000000	1.157940
17	1	0	0.876932	-1.282530	-1.006875
18	1	0	-0.876932	-1.282530	-1.006875
19	1	0	-0.876606	-2.563732	1.156052
20	1	0	0.876606	-2.563732	1.156052
21	1	0	0.000000	-4.737783	0.272738
22	1	0	0.883393	-3.884716	-0.999883
23	1	0	-0.883393	-3.884716	-0.999883

Styrene

Species name: styrene
Full file name: styrene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.131057	E(Thermal)=	0.137940
E(CCSD(T))=	-308.692275	E(Empiric)=	-0.138940
DE(Plus)=	-0.018734	DE(2DF)=	-0.244029
E(Delta-G3XP)=	-0.452618	DE(HF)=	-0.029982
G4(0 K)=	-309.445521	G4 Energy=	-309.438638
G4 Enthalpy=	-309.437694	G4 Free Energy=	-309.477261

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.277974	2.001030	0.000000
2	6	0	0.000000	0.558613	0.000000
3	6	0	-1.007321	-0.419816	0.000000
4	6	0	-0.688762	-1.771014	0.000000
5	6	0	0.644552	-2.182543	0.000000
6	6	0	1.655776	-1.226447	0.000000
7	6	0	1.334119	0.127093	0.000000
8	6	0	-1.467682	2.605933	0.000000
9	1	0	0.613094	2.627144	0.000000
10	1	0	-2.049803	-0.120411	0.000000
11	1	0	-1.483867	-2.509649	0.000000
12	1	0	0.889827	-3.239283	0.000000
13	1	0	2.696663	-1.533164	0.000000
14	1	0	2.127033	0.869381	0.000000

15	1	0	-2.406037	2.061603	0.000000
16	1	0	-1.543159	3.687285	0.000000

Ethylbenzene

Species name: ethylbenzene
Full file name: ethylbenzene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.153970	E(Thermal)=	0.161413
E(CCSD(T))=	-309.898360	E(Empiric)=	-0.145887
DE(Plus)=	-0.017824	DE(2DF)=	-0.261576
E(Delta-G3XP)=	-0.455796	DE(HF)=	-0.030306
G4(0 K)=	-310.655778	G4 Energy=	-310.648334
G4 Enthalpy=	-310.647390	G4 Free Energy=	-310.688040

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.232962	0.490660	0.000000
2	6	0	-0.193538	2.002297	0.000000
3	6	0	1.240894	2.559552	0.000000
4	6	0	-0.235114	-0.227034	1.199962
5	6	0	-0.235114	-0.227034	-1.199962
6	6	0	-0.235114	-1.619380	1.203151
7	6	0	-0.235114	-1.619380	-1.203151
8	6	0	-0.234458	-2.321239	0.000000
9	1	0	-0.727369	2.382827	0.878509
10	1	0	-0.727369	2.382827	-0.878509
11	1	0	1.236777	3.654273	0.000000
12	1	0	1.791862	2.220849	-0.883155
13	1	0	1.791862	2.220849	0.883155
14	1	0	-0.241500	0.313430	2.142605
15	1	0	-0.241500	0.313430	-2.142605
16	1	0	-0.240865	-2.156487	2.146290
17	1	0	-0.240865	-2.156487	-2.146290
18	1	0	-0.237909	-3.406161	0.000000

Methyl styrene

Species name: mstyrene
Full file name: mstyrene_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.158848	E(Thermal)=	0.166988
E(CCSD(T))=	-347.877888	E(Empiric)=	-0.159781
DE(Plus)=	-0.021222	DE(2DF)=	-0.283600
E(Delta-G3XP)=	-0.510554	DE(HF)=	-0.033685
G4(0 K)=	-348.727881	G4 Energy=	-348.719742
G4 Enthalpy=	-348.718798	G4 Free Energy=	-348.760794

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.690230	0.124018	-0.028295
2	6	0	0.206393	0.055618	-0.011165
3	6	0	-0.572847	1.202969	0.208826
4	6	0	-1.960820	1.142406	0.209412
5	6	0	-2.612165	-0.071452	-0.002720
6	6	0	-1.857024	-1.222258	-0.206775
7	6	0	-0.466486	-1.159948	-0.204091
8	6	0	2.344010	1.233588	-0.390764
9	6	0	2.453459	-1.119062	0.366605
10	1	0	-0.080411	2.148147	0.408222
11	1	0	-2.536688	2.044871	0.387748
12	1	0	-3.695912	-0.120074	0.001854
13	1	0	-2.349972	-2.175632	-0.367728
14	1	0	0.100098	-2.069224	-0.368478
15	1	0	1.829961	2.126184	-0.727927
16	1	0	3.427899	1.275941	-0.379821
17	1	0	2.325665	-1.922040	-0.369164
18	1	0	3.523168	-0.910324	0.440415
19	1	0	2.107693	-1.513126	1.328683

Allylbenzene

Species name:	allylbenzene
Full file name:	allylbenzene_g4.log
Method:	G4 calculation
Point group:	C1
NImag:	0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.158834	E(Thermal)=	0.167076
E(CCSD(T))=	-347.871577	E(Empiric)=	-0.159781
DE(Plus)=	-0.022013	DE(2DF)=	-0.282869
E(Delta-G3XP)=	-0.510153	DE(HF)=	-0.033679
G4(0 K)=	-348.721238	G4 Energy=	-348.712996
G4 Enthalpy=	-348.712052	G4 Free Energy=	-348.755348

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.007206	-0.361427	-0.206705
2	6	0	-1.423202	-0.827787	-0.421465
3	6	0	-2.413212	-0.161573	0.497208
4	6	0	-3.468095	0.544707	0.102475
5	6	0	1.038163	-1.279274	0.003725
6	6	0	0.322648	1.001378	-0.230507
7	6	0	2.352727	-0.852047	0.180081
8	6	0	1.633872	1.432331	-0.055800
9	6	0	2.655111	0.506174	0.149785
10	1	0	-1.461595	-1.914710	-0.272298
11	1	0	-1.722548	-0.647255	-1.461947
12	1	0	-2.216339	-0.282473	1.561680
13	1	0	-4.150767	0.999860	0.812238
14	1	0	-3.694713	0.690806	-0.950280
15	1	0	0.809671	-2.341023	0.027698
16	1	0	-0.471257	1.726277	-0.381305
17	1	0	3.139273	-1.582101	0.342103
18	1	0	1.859450	2.493758	-0.078537
19	1	0	3.677514	0.841970	0.287867

Isopropylbenzene

Species name: iprbenzene
Full file name: iprbenzene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.181668	E(Thermal)=	0.190435
E(CCSD(T))=	-349.081845	E(Empiric)=	-0.166728
DE(Plus)=	-0.020165	DE(2DF)=	-0.301489
E(Delta-G3XP)=	-0.513840	DE(HF)=	-0.034012
G4(0 K)=	-349.936410	G4 Energy=	-349.927643
G4 Enthalpy=	-349.926699	G4 Free Energy=	-349.970015

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.214493	0.106263	0.000000
2	6	0	-1.148119	-0.933121	0.000000
3	6	0	-0.744549	-2.266751	0.000000
4	6	0	0.609919	-2.585802	0.000000
5	6	0	1.553931	-1.560604	0.000000
6	6	0	1.144556	-0.230828	0.000000
7	6	0	-0.670073	1.556877	0.000000
8	6	0	-0.214493	2.299917	1.268738
9	6	0	-0.214493	2.299917	-1.268738

10	1	0	-2.207874	-0.693689	0.000000
11	1	0	-1.490550	-3.055112	0.000000
12	1	0	0.928703	-3.622863	0.000000
13	1	0	2.613177	-1.797616	0.000000
14	1	0	1.893873	0.555036	0.000000
15	1	0	-1.767395	1.548294	0.000000
16	1	0	-0.603067	3.323880	1.277477
17	1	0	0.877813	2.358721	1.323596
18	1	0	-0.566273	1.792772	2.172112
19	1	0	-0.603067	3.323880	-1.277477
20	1	0	0.877813	2.358721	-1.323596
21	1	0	-0.566273	1.792772	-2.172112

Naphthalene

Species name: naphthalene
Full file name: naphthalene_g4.log
Method: G4 calculation
Point group: D2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.144791	E(Thermal)=	0.151719
E(CCSD(T))=	-384.724648	E(Empiric)=	-0.166728
DE(Plus)=	-0.021902	DE(2DF)=	-0.288890
E(Delta-G3XP)=	-0.561673	DE(HF)=	-0.036759
G4(0 K)=	-385.655807	G4 Energy=	-385.648879
G4 Enthalpy=	-385.647935	G4 Free Energy=	-385.685761

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.715603
2	6	0	0.000000	0.000000	-0.715603
3	6	0	0.000000	1.242527	1.399280
4	6	0	0.000000	-1.242527	1.399280
5	6	0	0.000000	1.242527	-1.399280
6	6	0	0.000000	-1.242527	-1.399280
7	6	0	0.000000	2.428345	0.707081
8	6	0	0.000000	-2.428345	0.707081
9	6	0	0.000000	2.428345	-0.707081
10	6	0	0.000000	-2.428345	-0.707081
11	1	0	0.000000	1.238699	2.485339
12	1	0	0.000000	-1.238699	2.485339
13	1	0	0.000000	1.238699	-2.485339
14	1	0	0.000000	-1.238699	-2.485339
15	1	0	0.000000	3.371855	1.242885
16	1	0	0.000000	-3.371855	1.242885
17	1	0	0.000000	3.371855	-1.242885
18	1	0	0.000000	-3.371855	-1.242885

t-Butylbenzene

Species name: tbubenzene
Full file name: tbubenzene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.209132	E(Thermal)=	0.219114
E(CCSD(T))=	-388.264381	E(Empiric)=	-0.187569
DE(Plus)=	-0.022699	DE(2DF)=	-0.342072
E(Delta-G3XP)=	-0.571905	DE(HF)=	-0.037626
G4(0 K)=	-389.217121	G4 Energy=	-389.207139
G4 Enthalpy=	-389.206195	G4 Free Energy=	-389.251714

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000395	0.082542	0.000000
2	6	0	0.516502	-1.364982	0.000000
3	6	0	0.000395	-2.095176	1.261160
4	6	0	0.851611	1.191877	0.000000
5	6	0	-1.380157	0.332455	0.000000
6	6	0	0.349488	2.493188	0.000000
7	6	0	-1.886843	1.626958	0.000000
8	6	0	-1.021685	2.719105	0.000000
9	6	0	2.053867	-1.438128	0.000000
10	6	0	0.000395	-2.095176	-1.261160
11	1	0	0.357464	-3.131031	1.275046
12	1	0	-1.092192	-2.119409	1.299319
13	1	0	0.355069	-1.601475	2.171557
14	1	0	1.925535	1.053594	0.000000
15	1	0	-2.077469	-0.498758	0.000000
16	1	0	1.039945	3.330784	0.000000
17	1	0	-2.961075	1.782518	0.000000
18	1	0	-1.413228	3.730871	0.000000
19	1	0	2.371978	-2.485623	0.000000
20	1	0	2.484910	-0.962763	-0.886750
21	1	0	2.484910	-0.962763	0.886750
22	1	0	0.357464	-3.131031	-1.275046
23	1	0	0.355069	-1.601475	-2.171557
24	1	0	-1.092192	-2.119409	-1.299319

Cyclopropene

Species name: cp2
Full file name: cp2_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.055396	E(Thermal)=	0.058717
E(CCSD(T))=	-116.247976	E(Empiric)=	-0.055576
DE(Plus)=	-0.006521	DE(2DF)=	-0.100247
E(Delta-G3XP)=	-0.172140	DE(HF)=	-0.011285
G4(0 K)=	-116.538348	G4 Energy=	-116.535028
G4 Enthalpy=	-116.534083	G4 Free Energy=	-116.561631

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.860503
2	6	0	0.000000	0.645285	-0.500753
3	6	0	0.000000	-0.645285	-0.500753
4	1	0	0.911919	0.000000	1.462173
5	1	0	-0.911919	0.000000	1.462173
6	1	0	0.000000	1.576517	-1.039161
7	1	0	0.000000	-1.576517	-1.039161

Cyclopropane

Species name: cp
Full file name: cp_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.080028	E(Thermal)=	0.083430
E(CCSD(T))=	-117.496300	E(Empiric)=	-0.062523
DE(Plus)=	-0.006841	DE(2DF)=	-0.117019
E(Delta-G3XP)=	-0.175631	DE(HF)=	-0.011889
G4(0 K)=	-117.790175	G4 Energy=	-117.786773
G4 Enthalpy=	-117.785829	G4 Free Energy=	-117.812781

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.870150	0.000000
2	6	0	0.753572	-0.435075	0.000000
3	6	0	-0.753572	-0.435075	0.000000

4	1	0	0.000000	1.460853	0.909432
5	1	0	0.000000	1.460853	-0.909432
6	1	0	1.265135	-0.730426	0.909432
7	1	0	1.265135	-0.730426	-0.909432
8	1	0	-1.265135	-0.730426	0.909432
9	1	0	-1.265135	-0.730426	-0.909432

Tetrahedrane

Species name: tetrahedrane
Full file name: tetrahedrane_g4.log
Method: G4 calculation
Point group: TD
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.058964	E(Thermal)=	0.062782
E(CCSD(T))=	-154.156207	E(Empiric)=	-0.069470
DE(Plus)=	-0.009614	DE(2DF)=	-0.129737
E(Delta-G3XP)=	-0.227461	DE(HF)=	-0.013851
G4(0 K)=	-154.547376	G4 Energy=	-154.543558
G4 Enthalpy=	-154.542614	G4 Free Energy=	-154.570084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.522086	0.522086	0.522086
2	6	0	-0.522086	-0.522086	0.522086
3	6	0	-0.522086	0.522086	-0.522086
4	6	0	0.522086	-0.522086	-0.522086
5	1	0	1.139334	1.139334	1.139334
6	1	0	-1.139334	-1.139334	1.139334
7	1	0	-1.139334	1.139334	-1.139334
8	1	0	1.139334	-1.139334	-1.139334

Methylenecyclopropene

Species name: mcp2
Full file name: mcp2_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.060001	E(Thermal)=	0.064062
E(CCSD(T))=	-154.220024	E(Empiric)=	-0.069470
DE(Plus)=	-0.009856	DE(2DF)=	-0.123958
E(Delta-G3XP)=	-0.226352	DE(HF)=	-0.014696

G4(0 K)= -154.604355 G4 Energy= -154.600294
G4 Enthalpy= -154.599350 G4 Free Energy= -154.629297

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.263020
2	6	0	0.000000	0.000000	1.587795
3	6	0	0.000000	0.658310	-1.018446
4	6	0	0.000000	-0.658310	-1.018446
5	1	0	0.000000	0.927478	2.147015
6	1	0	0.000000	-0.927478	2.147015
7	1	0	0.000000	1.572443	-1.588784
8	1	0	0.000000	-1.572443	-1.588784

Bicyclo[1.1.0]but-1(3)-ene

Species name: bcb2
Full file name: bcb2_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.060957 E(Thermal)= 0.064819
E(CCSD(T))= -154.154920 E(Empiric)= -0.069470
DE(Plus)= -0.011792 DE(2DF)= -0.120910
E(Delta-G3XP)= -0.225605 DE(HF)= -0.014290
G4(0 K)= -154.536029 G4 Energy= -154.532167
G4 Enthalpy= -154.531222 G4 Free Energy= -154.560678

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.686928	0.000000	-0.304807
2	6	0	0.686928	0.000000	-0.304807
3	6	0	0.000000	1.231426	0.184801
4	6	0	0.000000	-1.231426	0.184801
5	1	0	0.000000	1.538065	1.237167
6	1	0	0.000000	2.058182	-0.517135
7	1	0	0.000000	-1.538065	1.237167
8	1	0	0.000000	-2.058182	-0.517135

Cyclobutene

Species name: cb2
Full file name: cb2_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.085124	E(Thermal)=	0.088979
E(CCSD(T))=	-155.470113	E(Empiric)=	-0.076417
DE(Plus)=	-0.008073	DE(2DF)=	-0.139490
E(Delta-G3XP)=	-0.229718	DE(HF)=	-0.015329
G4(0 K)=	-155.854015	G4 Energy=	-155.850161
G4 Enthalpy=	-155.849216	G4 Free Energy=	-155.878988

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.668844	0.814546
2	6	0	0.000000	-0.668844	0.814546
3	6	0	0.000000	-0.785987	-0.699262
4	6	0	0.000000	0.785987	-0.699262
5	1	0	0.000000	1.418102	1.598244
6	1	0	0.000000	-1.418102	1.598244
7	1	0	-0.888290	-1.246484	-1.144973
8	1	0	0.888290	-1.246484	-1.144973
9	1	0	-0.888290	1.246484	-1.144973
10	1	0	0.888290	1.246484	-1.144973

Bicyclobutane

Species name: bcb
Full file name: bcb_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.085008	E(Thermal)=	0.088791
E(CCSD(T))=	-155.444513	E(Empiric)=	-0.076417
DE(Plus)=	-0.008914	DE(2DF)=	-0.140679
E(Delta-G3XP)=	-0.230437	DE(HF)=	-0.014890
G4(0 K)=	-155.830843	G4 Energy=	-155.827060
G4 Enthalpy=	-155.826116	G4 Free Energy=	-155.855623

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.743163	0.000000	-0.321441

2	6	0	0.743163	0.000000	-0.321441
3	6	0	0.000000	1.135302	0.314648
4	6	0	0.000000	-1.135302	0.314648
5	1	0	-1.440708	0.000000	-1.143284
6	1	0	1.440708	0.000000	-1.143284
7	1	0	0.000000	1.236237	1.402360
8	1	0	0.000000	2.083549	-0.218321
9	1	0	0.000000	-1.236237	1.402360
10	1	0	0.000000	-2.083549	-0.218321

Methylenecyclopropane

Species name: mcp
Full file name: mcp_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.083870	E(Thermal)=	0.088165
E(CCSD(T))=	-155.456591	E(Empiric)=	-0.076417
DE(Plus)=	-0.009471	DE(2DF)=	-0.139450
E(Delta-G3XP)=	-0.229794	DE(HF)=	-0.015197
G4(0 K)=	-155.843050	G4 Energy=	-155.838755
G4 Enthalpy=	-155.837811	G4 Free Energy=	-155.868446

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.317187
2	6	0	0.000000	0.000000	1.633588
3	6	0	0.000000	0.769296	-0.930505
4	6	0	0.000000	-0.769296	-0.930505
5	1	0	0.000000	0.925127	2.202168
6	1	0	0.000000	-0.925127	2.202168
7	1	0	0.911177	1.277329	-1.235730
8	1	0	-0.911177	1.277329	-1.235730
9	1	0	-0.911177	-1.277329	-1.235730
10	1	0	0.911177	-1.277329	-1.235730

Cyclobutane

Species name: cb
Full file name: cb_g4.log
Method: G4 calculation
Point group: D2D
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.108940	E(Thermal)=	0.113130
E(CCSD(T))=	-156.682512	E(Empiric)=	-0.083364
DE(Plus)=	-0.006950	DE(2DF)=	-0.157473
E(Delta-G3XP)=	-0.232586	DE(HF)=	-0.015655
G4(0 K)=	-157.069601	G4 Energy=	-157.065411
G4 Enthalpy=	-157.064467	G4 Free Energy=	-157.094462

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.084373	0.124868
2	6	0	-1.084373	0.000000	-0.124868
3	6	0	0.000000	-1.084373	0.124868
4	6	0	1.084373	0.000000	-0.124868
5	1	0	0.000000	1.965391	-0.521788
6	1	0	0.000000	1.421089	1.165992
7	1	0	-1.421089	0.000000	-1.165992
8	1	0	-1.965391	0.000000	0.521788
9	1	0	0.000000	-1.965391	-0.521788
10	1	0	0.000000	-1.421089	1.165992
11	1	0	1.421089	0.000000	-1.165992
12	1	0	1.965391	0.000000	0.521788

[1.1.1]Propellane

Species name: 111propellane
Full file name: 111propellane_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091659	E(Thermal)=	0.095690
E(CCSD(T))=	-193.408919	E(Empiric)=	-0.090311
DE(Plus)=	-0.011515	DE(2DF)=	-0.163804
E(Delta-G3XP)=	-0.283772	DE(HF)=	-0.017556
G4(0 K)=	-193.884218	G4 Energy=	-193.880187
G4 Enthalpy=	-193.879243	G4 Free Energy=	-193.908852

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.789403
2	6	0	0.000000	0.000000	-0.789403
3	6	0	0.000000	1.298215	0.000000
4	6	0	1.124287	-0.649108	0.000000
5	6	0	-1.124287	-0.649108	0.000000

6	1	0	-0.915102	1.882690	0.000000
7	1	0	0.915102	1.882690	0.000000
8	1	0	2.088008	-0.148844	0.000000
9	1	0	1.172907	-1.733846	0.000000
10	1	0	-1.172907	-1.733846	0.000000
11	1	0	-2.088008	-0.148844	0.000000

Cyclopentadiene

Species name: cpd
Full file name: cpd_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091042	E(Thermal)=	0.095237
E(CCSD(T))=	-193.494305	E(Empiric)=	-0.090311
DE(Plus)=	-0.011736	DE(2DF)=	-0.160662
E(Delta-G3XP)=	-0.284341	DE(HF)=	-0.019044
G4(0 K)=	-193.969357	G4 Energy=	-193.965161
G4 Enthalpy=	-193.964217	G4 Free Energy=	-193.995315

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.215366
2	6	0	0.000000	1.179506	0.280400
3	6	0	0.000000	-1.179506	0.280400
4	6	0	0.000000	0.734255	-0.989306
5	6	0	0.000000	-0.734255	-0.989306
6	1	0	0.875868	0.000000	1.880575
7	1	0	-0.875868	0.000000	1.880575
8	1	0	0.000000	2.209401	0.611114
9	1	0	0.000000	-2.209401	0.611114
10	1	0	0.000000	1.344124	-1.884352
11	1	0	0.000000	-1.344124	-1.884352

Bicyclo[2.1.0]pent-1-ene

Species name: bcp6
Full file name: bcp6_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.088297	E(Thermal)=	0.093124

E(CCSD(T))= -193.353584 E(Empiric)= -0.090311
DE(Plus)= -0.012506 DE(2DF)= -0.162623
E(Delta-G3XP)= -0.284122 DE(HF)= -0.018208
G4(0 K)= -193.833058 G4 Energy= -193.828230
G4 Enthalpy= -193.827286 G4 Free Energy= -193.860176

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448817	0.092610	0.308471
2	6	0	-0.347231	0.708712	-0.442920
3	6	0	-0.331563	-0.814124	-0.210082
4	6	0	1.147593	-0.607721	0.213668
5	6	0	0.949278	0.864232	-0.072441
6	1	0	-2.388584	-0.096100	-0.204727
7	1	0	-1.573042	0.365740	1.356213
8	1	0	-0.602993	-1.503813	-1.003187
9	1	0	1.850464	-1.179255	-0.402729
10	1	0	1.383902	-0.798948	1.270580
11	1	0	1.514698	1.750130	0.203678

Bicyclo[2.1.0]pent-1(4)-ene

Species name: bcp4
Full file name: bcp4_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.088993 E(Thermal)= 0.093833
E(CCSD(T))= -193.343644 E(Empiric)= -0.090311
DE(Plus)= -0.012631 DE(2DF)= -0.162189
E(Delta-G3XP)= -0.283872 DE(HF)= -0.018055
G4(0 K)= -193.821708 G4 Energy= -193.816869
G4 Enthalpy= -193.815924 G4 Free Energy= -193.848859

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.760695	1.393470	0.000000
2	6	0	0.250684	0.513708	0.678282
3	6	0	0.250684	0.513708	-0.678282
4	6	0	0.250684	-1.032303	-0.773271
5	6	0	0.250684	-1.032303	0.773271
6	1	0	-0.542005	2.456214	0.000000
7	1	0	-1.831104	1.165115	0.000000
8	1	0	1.119016	-1.452101	-1.283725

9	1	0	-0.658588	-1.427402	-1.235707
10	1	0	1.119016	-1.452101	1.283725
11	1	0	-0.658588	-1.427402	1.235707

[2.1.0]Bicyclopent-2-ene

Species name: bcp3
Full file name: bcp3_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.090393	E(Thermal)=	0.094552
E(CCSD(T))=	-193.419470	E(Empiric)=	-0.090311
DE(Plus)=	-0.011743	DE(2DF)=	-0.162632
E(Delta-G3XP)=	-0.284120	DE(HF)=	-0.018123
G4(0 K)=	-193.896006	G4 Energy=	-193.891848
G4 Enthalpy=	-193.890904	G4 Free Energy=	-193.922477

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.926630	-1.010967	0.000000
2	6	0	-0.268120	-0.462167	0.760665
3	6	0	-0.268120	-0.462167	-0.760665
4	6	0	-0.268120	1.056770	-0.670572
5	6	0	-0.268120	1.056770	0.670572
6	1	0	1.035505	-2.094544	0.000000
7	1	0	1.861965	-0.458039	0.000000
8	1	0	-0.878340	-1.082766	1.403632
9	1	0	-0.878340	-1.082766	-1.403632
10	1	0	-0.132842	1.824337	-1.423443
11	1	0	-0.132842	1.824337	1.423443

Bicyclo[2.1.0]pent-4-ene

Species name: bcp5
Full file name: bcp5_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.088797	E(Thermal)=	0.093450
E(CCSD(T))=	-193.352081	E(Empiric)=	-0.090311
DE(Plus)=	-0.011420	DE(2DF)=	-0.162461
E(Delta-G3XP)=	-0.284488	DE(HF)=	-0.018091

G4(0 K)= -193.830055 G4 Energy= -193.825401
G4 Enthalpy= -193.824457 G4 Free Energy= -193.856982

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.466291	-0.219972	0.266915
2	6	0	0.421966	-0.716707	-0.345320
3	6	0	0.507797	0.778885	-0.357444
4	6	0	-0.888898	0.776083	0.327160
5	6	0	-1.049387	-0.781410	-0.052876
6	1	0	2.091831	-0.391807	1.133989
7	1	0	0.741495	1.392712	-1.221386
8	1	0	-1.647487	1.426459	-0.118082
9	1	0	-0.873933	0.924192	1.413119
10	1	0	-1.672487	-0.878710	-0.945291
11	1	0	-1.386027	-1.494120	0.707043

Cyclopentene

Species name: cyclopentene
Full file name: cyclopentene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.114770 E(Thermal)= 0.119486
E(CCSD(T))= -194.693544 E(Empiric)= -0.097258
DE(Plus)= -0.010059 DE(2DF)= -0.178534
E(Delta-G3XP)= -0.287380 DE(HF)= -0.019359
G4(0 K)= -195.171363 G4 Energy= -195.166647
G4 Enthalpy= -195.165703 G4 Free Energy= -195.198814

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.248383	-1.209276	0.000000
2	6	0	-0.064168	-0.324751	1.236639
3	6	0	-0.064168	-0.324751	-1.236639
4	6	0	-0.064168	1.074364	0.665812
5	6	0	-0.064168	1.074364	-0.665812
6	1	0	-0.310864	-2.148191	0.000000
7	1	0	1.311675	-1.468636	0.000000
8	1	0	-1.044271	-0.562491	1.674792
9	1	0	0.667761	-0.458634	2.041521
10	1	0	-1.044271	-0.562491	-1.674792
11	1	0	0.667761	-0.458634	-2.041521

12	1	0	-0.099026	1.959682	1.291610
13	1	0	-0.099026	1.959682	-1.291610

[2.1.0]Bicyclopentane

Species name: bcp2
Full file name: bcp2_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.114418	E(Thermal)=	0.118875
E(CCSD(T))=	-194.646312	E(Empiric)=	-0.097258
DE(Plus)=	-0.009679	DE(2DF)=	-0.180911
E(Delta-G3XP)=	-0.287470	DE(HF)=	-0.018671
G4(0 K)=	-195.125883	G4 Energy=	-195.121426
G4 Enthalpy=	-195.120482	G4 Free Energy=	-195.152776

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.943393	-1.046970	0.000000
2	6	0	-0.246055	-0.539058	0.765750
3	6	0	-0.246055	-0.539058	-0.765750
4	6	0	-0.246055	0.994729	-0.783026
5	6	0	-0.246055	0.994729	0.783026
6	1	0	1.071290	-2.124880	0.000000
7	1	0	1.877965	-0.488408	0.000000
8	1	0	-0.795161	-1.175555	1.449302
9	1	0	-0.795161	-1.175555	-1.449302
10	1	0	-1.164559	1.421265	-1.192280
11	1	0	0.607567	1.467819	-1.280439
12	1	0	-1.164559	1.421265	1.192280
13	1	0	0.607567	1.467819	1.280439

Spiropentane

Species name: spiropentane
Full file name: spiropentane_g4.log
Method: G4 calculation
Point group: D2D
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.113164	E(Thermal)=	0.118136
E(CCSD(T))=	-194.635921	E(Empiric)=	-0.097258
DE(Plus)=	-0.010621	DE(2DF)=	-0.178650

E(Delta-G3XP)= -0.287886 DE(HF)= -0.018771
G4(0 K)= -195.115943 G4 Energy= -195.110971
G4 Enthalpy= -195.110027 G4 Free Energy= -195.142029

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.764077	1.269258
3	6	0	0.000000	-0.764077	1.269258
4	6	0	0.764077	0.000000	-1.269258
5	6	0	-0.764077	0.000000	-1.269258
6	1	0	0.912110	1.268690	1.573605
7	1	0	-0.912110	1.268690	1.573605
8	1	0	-0.912110	-1.268690	1.573605
9	1	0	0.912110	-1.268690	1.573605
10	1	0	1.268690	-0.912110	-1.573605
11	1	0	1.268690	0.912110	-1.573605
12	1	0	-1.268690	0.912110	-1.573605
13	1	0	-1.268690	-0.912110	-1.573605

[1.1.1]Bicyclopentane

Species name: bcp
Full file name: bcp_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.115129 E(Thermal)= 0.119142
E(CCSD(T))= -194.628723 E(Empiric)= -0.097258
DE(Plus)= -0.008738 DE(2DF)= -0.183945
E(Delta-G3XP)= -0.287059 DE(HF)= -0.018171
G4(0 K)= -195.108766 G4 Energy= -195.104753
G4 Enthalpy= -195.103809 G4 Free Energy= -195.133546

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.939623
2	6	0	0.000000	0.000000	-0.939623
3	6	0	0.000000	1.241017	0.000000
4	6	0	1.074752	-0.620509	0.000000
5	6	0	-1.074752	-0.620509	0.000000
6	1	0	0.000000	0.000000	2.030686
7	1	0	0.000000	0.000000	-2.030686
8	1	0	-0.903780	1.857132	0.000000

9	1	0	0.903780	1.857132	0.000000
10	1	0	2.060214	-0.145870	0.000000
11	1	0	1.156434	-1.711263	0.000000
12	1	0	-1.156434	-1.711263	0.000000
13	1	0	-2.060214	-0.145870	0.000000

Methylenecyclobutane

Species name: mcb
Full file name: mcb_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.112934	E(Thermal)=	0.118091
E(CCSD(T))=	-194.658778	E(Empiric)=	-0.097258
DE(Plus)=	-0.010630	DE(2DF)=	-0.179288
E(Delta-G3XP)=	-0.287319	DE(HF)=	-0.019038
G4(0 K)=	-195.139377	G4 Energy=	-195.134219
G4 Enthalpy=	-195.133275	G4 Free Energy=	-195.167348

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.103993	0.614926	0.000000
2	6	0	-0.624273	1.832336	0.000000
3	6	0	0.232673	-0.389521	1.093617
4	6	0	0.232673	-0.389521	-1.093617
5	6	0	0.232673	-1.502372	0.000000
6	1	0	-0.849898	2.355497	0.924325
7	1	0	-0.849898	2.355497	-0.924325
8	1	0	-0.479487	-0.488578	1.917662
9	1	0	1.228391	-0.227289	1.522235
10	1	0	-0.479487	-0.488578	-1.917662
11	1	0	1.228391	-0.227289	-1.522235
12	1	0	-0.694157	-2.080592	0.000000
13	1	0	1.077618	-2.193747	0.000000

Cyclopentane

Species name: cyclopentane
Full file name: cyclopentane_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)= 0.138351 E(Thermal)= 0.143585
E(CCSD(T))= -195.895987 E(Empiric)= -0.104205
DE(Plus)= -0.008454 DE(2DF)= -0.197370
E(Delta-G3XP)= -0.290626 DE(HF)= -0.019653
G4(0 K)= -196.377944 G4 Energy= -196.372710
G4 Enthalpy= -196.371766 G4 Free Energy= -196.406166

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.307343
2	6	0	0.000000	1.242296	0.371470
3	6	0	0.000000	-1.242296	0.371470
4	6	0	-0.328041	0.694450	-1.030513
5	6	0	0.328041	-0.694450	-1.030513
6	1	0	0.875877	0.006655	1.962623
7	1	0	-0.875877	-0.006655	1.962623
8	1	0	-0.700784	2.015754	0.698029
9	1	0	0.994571	1.702214	0.359812
10	1	0	-1.413851	0.588798	-1.151592
11	1	0	0.026175	1.343819	-1.836646
12	1	0	1.413851	-0.588798	-1.151592
13	1	0	-0.026175	-1.343819	-1.836646
14	1	0	0.700784	-2.015754	0.698029
15	1	0	-0.994571	-1.702214	0.359812

Prismane

Species name: prismane
Full file name: prismane_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.095984 E(Thermal)= 0.100085
E(CCSD(T))= -231.343248 E(Empiric)= -0.104205
DE(Plus)= -0.011680 DE(2DF)= -0.192914
E(Delta-G3XP)= -0.337415 DE(HF)= -0.020415
G4(0 K)= -231.913893 G4 Energy= -231.909793
G4 Enthalpy= -231.908849 G4 Free Energy= -231.939083

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.878860	0.779396
2	6	0	0.000000	0.878860	-0.779396
3	6	0	-0.761115	-0.439430	0.779396

4	6	0	-0.761115	-0.439430	-0.779396
5	6	0	0.761115	-0.439430	0.779396
6	6	0	0.761115	-0.439430	-0.779396
7	1	0	0.000000	1.674883	1.511732
8	1	0	0.000000	1.674883	-1.511732
9	1	0	-1.450491	-0.837441	1.511732
10	1	0	-1.450491	-0.837441	-1.511732
11	1	0	1.450491	-0.837441	1.511732
12	1	0	1.450491	-0.837441	-1.511732

Benzvalene

Species name: benzvalene
Full file name: benzvalene_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.096141	E(Thermal)=	0.100488
E(CCSD(T))=	-231.410934	E(Empiric)=	-0.104205
DE(Plus)=	-0.013807	DE(2DF)=	-0.187145
E(Delta-G3XP)=	-0.338424	DE(HF)=	-0.021137
G4(0 K)=	-231.979511	G4 Energy=	-231.975164
G4 Enthalpy=	-231.974220	G4 Free Energy=	-232.005989

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.074421	-0.200950
2	6	0	0.000000	-1.074421	-0.200950
3	6	0	-0.721987	0.000000	-1.013978
4	6	0	0.721987	0.000000	-1.013978
5	6	0	0.000000	0.667849	1.252664
6	6	0	0.000000	-0.667849	1.252664
7	1	0	0.000000	2.104816	-0.536801
8	1	0	0.000000	-2.104816	-0.536801
9	1	0	-1.483998	0.000000	-1.780205
10	1	0	1.483998	0.000000	-1.780205
11	1	0	0.000000	1.349896	2.090590
12	1	0	0.000000	-1.349896	2.090590

[2.1.1]Propellane

Species name: 211propellane
Full file name: 211propellane_g4.log
Method: G4 calculation
Point group: C2V

NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.119798	E(Thermal)=	0.124771
E(CCSD(T))=	-232.590241	E(Empiric)=	-0.111152
DE(Plus)=	-0.012281	DE(2DF)=	-0.204390
E(Delta-G3XP)=	-0.341951	DE(HF)=	-0.021406
G4(0 K)=	-233.161622	G4 Energy=	-233.156649
G4 Enthalpy=	-233.155705	G4 Free Energy=	-233.188723

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.124492	-0.945741
2	6	0	-0.823879	0.000000	-0.371451
3	6	0	0.823879	0.000000	-0.371451
4	6	0	0.000000	-1.124492	-0.945741
5	6	0	-0.771177	0.000000	1.186502
6	6	0	0.771177	0.000000	1.186502
7	1	0	0.000000	1.211198	-2.029979
8	1	0	0.000000	2.080758	-0.429056
9	1	0	0.000000	-2.080758	-0.429056
10	1	0	0.000000	-1.211198	-2.029979
11	1	0	-1.242180	-0.883760	1.621589
12	1	0	-1.242180	0.883760	1.621589
13	1	0	1.242180	-0.883760	1.621589
14	1	0	1.242180	0.883760	1.621589

[2.1.1]Bicyclohexene

Species name: bchx4
Full file name: bchx4_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.120689	E(Thermal)=	0.125179
E(CCSD(T))=	-232.632918	E(Empiric)=	-0.111152
DE(Plus)=	-0.012274	DE(2DF)=	-0.204593
E(Delta-G3XP)=	-0.341350	DE(HF)=	-0.021499
G4(0 K)=	-233.203098	G4 Energy=	-233.198608
G4 Enthalpy=	-233.197664	G4 Free Energy=	-233.229804

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.065846	0.000000	-0.809335

2	6	0	0.000000	1.021941	-0.279804
3	6	0	0.000000	-1.021941	-0.279804
4	6	0	-1.065846	0.000000	-0.809335
5	6	0	0.000000	0.667774	1.215537
6	6	0	0.000000	-0.667774	1.215537
7	1	0	1.164263	0.000000	-1.899901
8	1	0	2.046373	0.000000	-0.327412
9	1	0	0.000000	2.072118	-0.570556
10	1	0	0.000000	-2.072118	-0.570556
11	1	0	-2.046373	0.000000	-0.327412
12	1	0	-1.164263	0.000000	-1.899901
13	1	0	0.000000	1.367015	2.039480
14	1	0	0.000000	-1.367015	2.039480

Bicyclo[2.2.0]hex-1-ene

Species name: bchx5
Full file name: bchx5_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.118821	E(Thermal)=	0.123962
E(CCSD(T))=	-232.587958	E(Empiric)=	-0.111152
DE(Plus)=	-0.012690	DE(2DF)=	-0.202707
E(Delta-G3XP)=	-0.341258	DE(HF)=	-0.021820
G4(0 K)=	-233.158763	G4 Energy=	-233.153622
G4 Enthalpy=	-233.152678	G4 Free Energy=	-233.186812

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.162263	-0.783368	-0.457988
2	6	0	-0.049635	0.704495	-0.403874
3	6	0	1.149324	0.990994	0.137326
4	6	0	1.585253	-0.484516	0.125434
5	6	0	-1.514913	0.657299	-0.048108
6	6	0	-1.150209	-0.816939	0.419619
7	1	0	0.090974	-1.349961	-1.388526
8	1	0	1.539037	1.849003	0.674162
9	1	0	1.736638	-0.881367	1.136167
10	1	0	2.437079	-0.785535	-0.495860
11	1	0	-1.895235	1.358409	0.698259
12	1	0	-2.186551	0.641574	-0.912229
13	1	0	-0.937317	-0.847843	1.490670
14	1	0	-1.877122	-1.592069	0.162896

Bicyclo[2.2.0]hex-1(4)-ene

Species name: bchx6
Full file name: bchx6_g4.log
Method: G4 calculation
Point group: D2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.118494	E(Thermal)=	0.124069
E(CCSD(T))=	-232.574362	E(Empiric)=	-0.111152
DE(Plus)=	-0.010752	DE(2DF)=	-0.204101
E(Delta-G3XP)=	-0.341824	DE(HF)=	-0.022309
G4(0 K)=	-233.146006	G4 Energy=	-233.140430
G4 Enthalpy=	-233.139486	G4 Free Energy=	-233.173535

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.659222	0.000000
2	6	0	0.000000	-0.659222	0.000000
3	6	0	-1.523213	0.803156	0.000000
4	6	0	-1.523213	-0.803156	0.000000
5	6	0	1.523213	0.803156	0.000000
6	6	0	1.523213	-0.803156	0.000000
7	1	0	-1.976815	1.255496	0.888472
8	1	0	-1.976815	1.255496	-0.888472
9	1	0	-1.976815	-1.255496	0.888472
10	1	0	-1.976815	-1.255496	-0.888472
11	1	0	1.976815	1.255496	0.888472
12	1	0	1.976815	1.255496	-0.888472
13	1	0	1.976815	-1.255496	0.888472
14	1	0	1.976815	-1.255496	-0.888472

Bicyclo[2.2.0]hex-2-ene (cis)

Species name: bchx7
Full file name: bchx7_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.119524	E(Thermal)=	0.124583
E(CCSD(T))=	-232.621983	E(Empiric)=	-0.111152
DE(Plus)=	-0.011884	DE(2DF)=	-0.202941
E(Delta-G3XP)=	-0.341480	DE(HF)=	-0.021851
G4(0 K)=	-233.191767	G4 Energy=	-233.186708
G4 Enthalpy=	-233.185764	G4 Free Energy=	-233.219831

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.565506	0.089599	0.789085
2	6	0	0.565506	0.089599	-0.789085
3	6	0	-0.263355	1.349891	0.670619
4	6	0	-0.263355	1.349891	-0.670619
5	6	0	-0.263355	-1.239766	0.777659
6	6	0	-0.263355	-1.239766	-0.777659
7	1	0	1.479398	0.107862	1.384799
8	1	0	1.479398	0.107862	-1.384799
9	1	0	-0.758769	1.962591	1.417083
10	1	0	-0.758769	1.962591	-1.417083
11	1	0	-1.238411	-1.183771	1.267007
12	1	0	0.285011	-2.085028	1.200621
13	1	0	-1.238411	-1.183771	-1.267007
14	1	0	0.285011	-2.085028	-1.200621

Cyclohexene

Species name: cyclohexene
Full file name: cyclohexene_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.143793	E(Thermal)=	0.149373
E(CCSD(T))=	-233.883053	E(Empiric)=	-0.118099
DE(Plus)=	-0.011824	DE(2DF)=	-0.217983
E(Delta-G3XP)=	-0.345953	DE(HF)=	-0.023170
G4(0 K)=	-234.456288	G4 Energy=	-234.450708
G4 Enthalpy=	-234.449764	G4 Free Energy=	-234.484308

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005456	0.666403	1.304270
2	6	0	-0.005456	-0.666403	1.304270
3	6	0	-0.005456	1.500866	0.048614
4	6	0	0.005456	-1.500866	0.048614
5	6	0	-0.371196	0.671118	-1.191580
6	6	0	0.371196	-0.671118	-1.191580
7	1	0	0.020030	1.203498	2.250233
8	1	0	-0.020030	-1.203498	2.250233
9	1	0	-0.708039	2.335924	0.165823
10	1	0	0.708039	-2.335924	0.165823
11	1	0	0.981004	1.969776	-0.087846
12	1	0	-0.981004	-1.969776	-0.087846

13	1	0	-1.452813	0.482659	-1.192276
14	1	0	1.452813	-0.482659	-1.192276
15	1	0	-0.150187	1.235871	-2.103760
16	1	0	0.150187	-1.235871	-2.103760

Methylenecyclopentane

Species name: methylenecyclopentane
Full file name: methylenecyclopentane_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.142574	E(Thermal)=	0.148512
E(CCSD(T))=	-233.875860	E(Empiric)=	-0.118099
DE(Plus)=	-0.012314	DE(2DF)=	-0.218771
E(Delta-G3XP)=	-0.345427	DE(HF)=	-0.023028
G4(0 K)=	-234.450925	G4 Energy=	-234.444987
G4 Enthalpy=	-234.444043	G4 Free Energy=	-234.479721

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.879672
2	6	0	0.000000	0.000000	2.208390
3	6	0	0.000000	1.235379	-0.011186
4	6	0	0.000000	-1.235379	-0.011186
5	6	0	0.317326	0.701246	-1.421853
6	6	0	-0.317326	-0.701246	-1.421853
7	1	0	0.019788	0.922498	2.780661
8	1	0	-0.019788	-0.922498	2.780661
9	1	0	0.698084	2.004061	0.332927
10	1	0	-0.999410	1.691220	-0.004859
11	1	0	-0.698084	-2.004061	0.332927
12	1	0	0.999410	-1.691220	-0.004859
13	1	0	1.402814	0.615442	-1.554702
14	1	0	-0.058862	1.346939	-2.219979
15	1	0	-1.402814	-0.615442	-1.554702
16	1	0	0.058862	-1.346939	-2.219979

[2.1.1]Bicyclohexane

Species name: bchx
Full file name: bchx_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.144655	E(Thermal)=	0.149454
E(CCSD(T))=	-233.859874	E(Empiric)=	-0.118099
DE(Plus)=	-0.010014	DE(2DF)=	-0.222268
E(Delta-G3XP)=	-0.344790	DE(HF)=	-0.022142
G4(0 K)=	-234.432532	G4 Energy=	-234.427733
G4 Enthalpy=	-234.426789	G4 Free Energy=	-234.459600

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.061490	0.000000	-0.851926
2	6	0	0.000000	1.027033	-0.359615
3	6	0	0.000000	-1.027033	-0.359615
4	6	0	-1.061490	0.000000	-0.851926
5	6	0	0.000000	0.783257	1.162793
6	6	0	0.000000	-0.783257	1.162793
7	1	0	1.174379	0.000000	-1.938702
8	1	0	2.044726	0.000000	-0.370352
9	1	0	0.000000	2.063156	-0.700115
10	1	0	0.000000	-2.063156	-0.700115
11	1	0	-2.044726	0.000000	-0.370352
12	1	0	-1.174379	0.000000	-1.938702
13	1	0	-0.883948	1.204388	1.650828
14	1	0	0.883948	1.204388	1.650828
15	1	0	-0.883948	-1.204388	1.650828
16	1	0	0.883948	-1.204388	1.650828

Bicyclo[3.1.0]hexane

Species name:	bchx3
Full file name:	bchx3_g4.log
Method:	G4 calculation
Point group:	CS
NImag:	0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.144025	E(Thermal)=	0.149280
E(CCSD(T))=	-233.868143	E(Empiric)=	-0.118099
DE(Plus)=	-0.011068	DE(2DF)=	-0.219424
E(Delta-G3XP)=	-0.345658	DE(HF)=	-0.022638
G4(0 K)=	-234.441004	G4 Energy=	-234.435749
G4 Enthalpy=	-234.434805	G4 Free Energy=	-234.469223

Standard orientation:

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

1	6	0	0.923387	-1.304246	0.000000
2	6	0	-0.287830	-0.814619	0.757084
3	6	0	-0.287830	-0.814619	-0.757084
4	6	0	-0.287830	0.633055	-1.229608
5	6	0	-0.287830	0.633055	1.229608
6	6	0	0.174482	1.451224	0.000000
7	1	0	1.830287	-0.707167	0.000000
8	1	0	1.105625	-2.373522	0.000000
9	1	0	-0.867800	-1.540535	1.316619
10	1	0	-0.867800	-1.540535	-1.316619
11	1	0	0.349572	0.805449	-2.104018
12	1	0	-1.308490	0.916115	-1.515104
13	1	0	0.349572	0.805449	2.104018
14	1	0	-1.308490	0.916115	1.515104
15	1	0	1.264695	1.547315	0.000000
16	1	0	-0.226456	2.468221	0.000000

Spirohexane

Species name: spirohexane
Full file name: spirohexane_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.141882	E(Thermal)=	0.147810
E(CCSD(T))=	-233.831788	E(Empiric)=	-0.118099
DE(Plus)=	-0.012069	DE(2DF)=	-0.219200
E(Delta-G3XP)=	-0.344938	DE(HF)=	-0.022522
G4(0 K)=	-234.406734	G4 Energy=	-234.400806
G4 Enthalpy=	-234.399862	G4 Free Energy=	-234.435943

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.096023	0.296094	0.000000
2	6	0	-0.271384	-1.825409	0.000000
3	6	0	0.096023	-0.780585	1.095316
4	6	0	0.096023	-0.780585	-1.095316
5	6	0	0.759356	1.638318	0.000000
6	6	0	-0.751141	1.535914	0.000000
7	1	0	0.294394	-2.759465	0.000000
8	1	0	-1.337506	-2.065179	0.000000
9	1	0	1.091509	-0.951006	1.518771
10	1	0	-0.613197	-0.653177	1.918205
11	1	0	1.091509	-0.951006	-1.518771
12	1	0	-0.613197	-0.653177	-1.918205
13	1	0	1.248798	1.968675	0.911234
14	1	0	1.248798	1.968675	-0.911234
15	1	0	-1.280257	1.796587	0.911685

16	1	0	-1.280257	1.796587	-0.911685

cis-bicyclo[2.2.0]hexane

Species name: cis_bchx5
Full file name: cis_bchx5_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.142883	E(Thermal)=	0.148413
E(CCSD(T))=	-233.832259	E(Empiric)=	-0.118099
DE(Plus)=	-0.010404	DE(2DF)=	-0.221069
E(Delta-G3XP)=	-0.344518	DE(HF)=	-0.022342
G4(0 K)=	-234.405808	G4 Energy=	-234.400278
G4 Enthalpy=	-234.399334	G4 Free Energy=	-234.434344

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505309	0.603778	0.580503
2	6	0	0.505309	-0.603778	0.580503
3	6	0	0.505309	1.442533	-0.245417
4	6	0	1.499365	0.240156	-0.262475
5	6	0	-1.499365	-0.240156	-0.262475
6	6	0	-0.505309	-1.442533	-0.245417
7	1	0	-0.898788	1.060836	1.489887
8	1	0	0.898788	-1.060836	1.489887
9	1	0	0.141768	1.784617	-1.219467
10	1	0	0.893192	2.311547	0.292409
11	1	0	1.737189	-0.173132	-1.247649
12	1	0	2.441971	0.450881	0.249155
13	1	0	-1.737189	0.173132	-1.247649
14	1	0	-2.441971	-0.450881	0.249155
15	1	0	-0.141768	-1.784617	-1.219467
16	1	0	-0.893192	-2.311547	0.292409

trans-Bicyclo[2.2.0]hexane

Species name: trans_bchx5
Full file name: trans_bchx5_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.142885	E(Thermal)=	0.148132

E(CCSD(T))= -233.768779 E(Empiric)= -0.118099
DE(Plus)= -0.011204 DE(2DF)= -0.222550
E(Delta-G3XP)= -0.344090 DE(HF)= -0.022289
G4(0 K)= -234.344126 G4 Energy= -234.338879
G4 Enthalpy= -234.337935 G4 Free Energy= -234.371660

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196752	0.721119	0.000000
2	6	0	0.196752	-0.721119	0.000000
3	6	0	0.196752	0.773942	1.515485
4	6	0	-0.196752	-0.773942	1.515485
5	6	0	0.196752	0.773942	-1.515485
6	6	0	-0.196752	-0.773942	-1.515485
7	1	0	-1.296403	0.752710	0.000000
8	1	0	1.296403	-0.752710	0.000000
9	1	0	1.269659	0.898418	1.685659
10	1	0	-0.360017	1.443076	2.177050
11	1	0	0.360017	-1.443076	2.177050
12	1	0	-1.269659	-0.898418	1.685659
13	1	0	1.269659	0.898418	-1.685659
14	1	0	-0.360017	1.443076	-2.177050
15	1	0	0.360017	-1.443076	-2.177050
16	1	0	-1.269659	-0.898418	-1.685659

Cyclohexane

Species name: cyclohexane
Full file name: cyclohexane_g4.log
Method: G4 calculation
Point group: D3D
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.167213 E(Thermal)= 0.173056
E(CCSD(T))= -235.088394 E(Empiric)= -0.125046
DE(Plus)= -0.009671 DE(2DF)= -0.236715
E(Delta-G3XP)= -0.349780 DE(HF)= -0.023478
G4(0 K)= -235.665870 G4 Energy= -235.660027
G4 Enthalpy= -235.659083 G4 Free Energy= -235.693046

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269300	0.732831	0.229812
2	6	0	0.000000	1.465662	-0.229812
3	6	0	1.269300	0.732831	0.229812

4	6	0	1.269300	-0.732831	-0.229812
5	6	0	0.000000	-1.465662	0.229812
6	6	0	-1.269300	-0.732831	-0.229812
7	1	0	-1.326930	0.766104	1.327076
8	1	0	-2.161922	1.248186	-0.143090
9	1	0	0.000000	2.496372	0.143090
10	1	0	0.000000	1.532207	-1.327076
11	1	0	1.326930	0.766104	1.327076
12	1	0	2.161922	1.248186	-0.143090
13	1	0	2.161922	-1.248186	0.143090
14	1	0	1.326930	-0.766104	-1.327076
15	1	0	0.000000	-1.532207	1.327076
16	1	0	0.000000	-2.496372	-0.143090
17	1	0	-2.161922	-1.248186	0.143090
18	1	0	-1.326930	-0.766104	-1.327076

Bicyclo[4.1.0]hepta-1,3,5-triene

Species name: bcheptatriene
Full file name: bcheptatriene_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.102937	E(Thermal)=	0.108239
E(CCSD(T))=	-269.431981	E(Empiric)=	-0.118099
DE(Plus)=	-0.014953	DE(2DF)=	-0.206260
E(Delta-G3XP)=	-0.393486	DE(HF)=	-0.025538
G4(0 K)=	-270.087380	G4 Energy=	-270.082078
G4 Enthalpy=	-270.081133	G4 Free Energy=	-270.115445

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.139880
2	6	0	0.000000	0.674345	0.800416
3	6	0	0.000000	-0.674345	0.800416
4	6	0	0.000000	1.453227	-0.332666
5	6	0	0.000000	-1.453227	-0.332666
6	6	0	0.000000	0.699914	-1.524242
7	6	0	0.000000	-0.699914	-1.524242
8	1	0	0.909112	0.000000	2.744980
9	1	0	-0.909112	0.000000	2.744980
10	1	0	0.000000	2.537934	-0.348353
11	1	0	0.000000	-2.537934	-0.348353
12	1	0	0.000000	1.219886	-2.477318
13	1	0	0.000000	-1.219886	-2.477318

Norbornadiene

Species name: norbornadiene
Full file name: norbornadiene_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.126464	E(Thermal)=	0.131409
E(CCSD(T))=	-270.644259	E(Empiric)=	-0.125046
DE(Plus)=	-0.015241	DE(2DF)=	-0.225486
E(Delta-G3XP)=	-0.396278	DE(HF)=	-0.024911
G4(0 K)=	-271.304757	G4 Energy=	-271.299811
G4 Enthalpy=	-271.298867	G4 Free Energy=	-271.332252

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.354892
2	6	0	0.000000	1.121522	0.271535
3	6	0	0.000000	-1.121522	0.271535
4	6	0	1.244181	0.666179	-0.520788
5	6	0	1.244181	-0.666179	-0.520788
6	6	0	-1.244181	0.666179	-0.520788
7	6	0	-1.244181	-0.666179	-0.520788
8	1	0	0.899842	0.000000	1.976377
9	1	0	-0.899842	0.000000	1.976377
10	1	0	0.000000	2.157611	0.608874
11	1	0	0.000000	-2.157611	0.608874
12	1	0	1.933179	1.337913	-1.014841
13	1	0	1.933179	-1.337913	-1.014841
14	1	0	-1.933179	1.337913	-1.014841
15	1	0	-1.933179	-1.337913	-1.014841

Quadricyclane

Species name: quadricyclane
Full file name: quadricyclane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.126301	E(Thermal)=	0.130969
E(CCSD(T))=	-270.606762	E(Empiric)=	-0.125046
DE(Plus)=	-0.013168	DE(2DF)=	-0.229363
E(Delta-G3XP)=	-0.395776	DE(HF)=	-0.024551
G4(0 K)=	-271.268366	G4 Energy=	-271.263698
G4 Enthalpy=	-271.262754	G4 Free Energy=	-271.295616

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.539262
2	6	0	0.000000	1.150870	0.550625
3	6	0	0.000000	-1.150870	0.550625
4	6	0	0.757493	0.775012	-0.710174
5	6	0	0.757493	-0.775012	-0.710174
6	6	0	-0.757493	0.775012	-0.710174
7	6	0	-0.757493	-0.775012	-0.710174
8	1	0	0.889599	0.000000	2.179676
9	1	0	-0.889599	0.000000	2.179676
10	1	0	0.000000	2.184608	0.875814
11	1	0	0.000000	-2.184608	0.875814
12	1	0	1.450035	1.424356	-1.227472
13	1	0	1.450035	-1.424356	-1.227472
14	1	0	-1.450035	1.424356	-1.227472
15	1	0	-1.450035	-1.424356	-1.227472

Bicyclo[3.2.0]hept-1(5)-ene

Species name: bchp2
Full file name: bchp2_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.148403	E(Thermal)=	0.154818
E(CCSD(T))=	-271.827556	E(Empiric)=	-0.131993
DE(Plus)=	-0.012410	DE(2DF)=	-0.242339
E(Delta-G3XP)=	-0.399288	DE(HF)=	-0.026318
G4(0 K)=	-272.491501	G4 Energy=	-272.485085
G4 Enthalpy=	-272.484141	G4 Free Energy=	-272.521849

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.104272	1.962072	0.000000
2	1	0	0.609639	2.789525	0.000000
3	1	0	-1.103461	2.406328	0.000000
4	6	0	0.058886	1.057690	1.280557
5	6	0	0.058886	1.057690	-1.280557
6	6	0	-0.006488	-0.305871	0.664336
7	6	0	-0.006488	-0.305871	-0.664336
8	6	0	-0.006488	-1.823902	0.792326
9	6	0	-0.006488	-1.823902	-0.792326

10	1	0	1.015891	1.237171	1.788998
11	1	0	-0.724575	1.259245	2.020413
12	1	0	1.015891	1.237171	-1.788998
13	1	0	-0.724575	1.259245	-2.020413
14	1	0	0.884626	-2.272612	1.244962
15	1	0	-0.891670	-2.275450	1.253368
16	1	0	0.884626	-2.272612	-1.244962
17	1	0	-0.891670	-2.275450	-1.253368

Bicyclo[3.2.0]hept-2-ene

Species name: bchp4
Full file name: bchp4_g4.log
Method: G4 calculation
Point group: C1
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.148991	E(Thermal)=	0.154862
E(CCSD(T))=	-271.851063	E(Empiric)=	-0.131993
DE(Plus)=	-0.013665	DE(2DF)=	-0.241344
E(Delta-G3XP)=	-0.399573	DE(HF)=	-0.025844
G4(0 K)=	-272.514490	G4 Energy=	-272.508619
G4 Enthalpy=	-272.507674	G4 Free Energy=	-272.543957

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.391742	0.741160	0.640939
2	6	0	0.813681	1.277488	-0.083359
3	6	0	1.698821	0.327025	-0.387663
4	6	0	1.273902	-1.045913	0.087466
5	6	0	-0.172646	-0.809472	0.563481
6	6	0	-1.288166	-0.876355	-0.523159
7	6	0	-1.689169	0.592789	-0.210851
8	1	0	-0.528141	1.205248	1.623915
9	1	0	0.926777	2.330451	-0.322183
10	1	0	2.637162	0.496217	-0.906074
11	1	0	1.930314	-1.407395	0.891503
12	1	0	1.324336	-1.799915	-0.709579
13	1	0	-0.425938	-1.363228	1.469244
14	1	0	-2.064716	-1.630519	-0.374220
15	1	0	-0.878119	-1.002086	-1.529190
16	1	0	-2.594001	0.662576	0.399491
17	1	0	-1.795763	1.268309	-1.064021

Bicyclo[3.2.0]hept-6-ene

Species name: bchp3
Full file name: bchp3_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.149006	E(Thermal)=	0.154844
E(CCSD(T))=	-271.843869	E(Empiric)=	-0.131993
DE(Plus)=	-0.013013	DE(2DF)=	-0.241813
E(Delta-G3XP)=	-0.399906	DE(HF)=	-0.025741
G4(0 K)=	-272.507328	G4 Energy=	-272.501490
G4 Enthalpy=	-272.500545	G4 Free Energy=	-272.536535

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.964732	1.305133	0.000000
2	1	0	-1.306288	2.343977	0.000000
3	1	0	-1.857287	0.671126	0.000000
4	6	0	-0.077831	0.966450	1.216409
5	6	0	-0.077831	0.966450	-1.216409
6	6	0	0.709082	-0.286395	0.793452
7	6	0	0.709082	-0.286395	-0.793452
8	6	0	-0.077831	-1.582517	0.668564
9	6	0	-0.077831	-1.582517	-0.668564
10	1	0	0.625891	1.787370	1.402410
11	1	0	-0.653706	0.820298	2.136087
12	1	0	0.625891	1.787370	-1.402410
13	1	0	-0.653706	0.820298	-2.136087
14	1	0	1.683708	-0.370954	1.283411
15	1	0	1.683708	-0.370954	-1.283411
16	1	0	-0.500430	-2.244891	1.417230
17	1	0	-0.500430	-2.244891	-1.417230

[2.2.1]Propellane

Species name: 221propellane
Full file name: 221propellane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.147686	E(Thermal)=	0.153714
E(CCSD(T))=	-271.770781	E(Empiric)=	-0.131993
DE(Plus)=	-0.013358	DE(2DF)=	-0.245305
E(Delta-G3XP)=	-0.399724	DE(HF)=	-0.025261
G4(0 K)=	-272.438736	G4 Energy=	-272.432707
G4 Enthalpy=	-272.431763	G4 Free Energy=	-272.467327

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.519300
2	6	0	0.000000	0.792580	0.254218
3	6	0	0.000000	-0.792580	0.254218
4	6	0	1.373145	0.782707	-0.453854
5	6	0	1.373145	-0.782707	-0.453854
6	6	0	-1.373145	0.782707	-0.453854
7	6	0	-1.373145	-0.782707	-0.453854
8	1	0	0.909969	0.000000	2.112145
9	1	0	-0.909969	0.000000	2.112145
10	1	0	1.331514	1.205475	-1.460454
11	1	0	2.185897	1.281341	0.085905
12	1	0	1.331514	-1.205475	-1.460454
13	1	0	2.185897	-1.281341	0.085905
14	1	0	-1.331514	1.205475	-1.460454
15	1	0	-2.185897	1.281341	0.085905
16	1	0	-1.331514	-1.205475	-1.460454
17	1	0	-2.185897	-1.281341	0.085905

Norbornene

Species name: norbornene
Full file name: norbornene_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.150411	E(Thermal)=	0.155728
E(CCSD(T))=	-271.865598	E(Empiric)=	-0.131993
DE(Plus)=	-0.013414	DE(2DF)=	-0.243616
E(Delta-G3XP)=	-0.399678	DE(HF)=	-0.025507
G4(0 K)=	-272.529395	G4 Energy=	-272.524078
G4 Enthalpy=	-272.523134	G4 Free Energy=	-272.557970

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.131677	0.792339	0.000000
2	6	0	0.221533	0.250253	1.127328
3	6	0	0.221533	0.250253	-1.127328
4	6	0	-1.125467	0.789637	0.668489
5	6	0	-1.125467	0.789637	-0.668489
6	6	0	0.221533	-1.278322	0.779945
7	6	0	0.221533	-1.278322	-0.779945
8	1	0	1.204889	1.882669	0.000000

9	1	0	2.135423	0.352955	0.000000
10	1	0	0.508193	0.476307	2.154969
11	1	0	0.508193	0.476307	-2.154969
12	1	0	-1.955988	1.011929	1.327444
13	1	0	-1.955988	1.011929	-1.327444
14	1	0	-0.643563	-1.792265	1.205291
15	1	0	1.120577	-1.760208	1.176642
16	1	0	-0.643563	-1.792265	-1.205291
17	1	0	1.120577	-1.760208	-1.176642

Norbornane

Species name: norbornane
Full file name: norbornane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.174093	E(Thermal)=	0.179798
E(CCSD(T))=	-273.078381	E(Empiric)=	-0.138940
DE(Plus)=	-0.011404	DE(2DF)=	-0.261807
E(Delta-G3XP)=	-0.403046	DE(HF)=	-0.026121
G4(0 K)=	-273.745607	G4 Energy=	-273.739902
G4 Enthalpy=	-273.738958	G4 Free Energy=	-273.774028

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.389069
2	6	0	0.000000	1.132421	0.340306
3	6	0	0.000000	-1.132421	0.340306
4	6	0	1.254502	0.782334	-0.493472
5	6	0	1.254502	-0.782334	-0.493472
6	6	0	-1.254502	0.782334	-0.493472
7	6	0	-1.254502	-0.782334	-0.493472
8	1	0	0.890048	0.000000	2.026873
9	1	0	-0.890048	0.000000	2.026873
10	1	0	0.000000	2.152655	0.729601
11	1	0	0.000000	-2.152655	0.729601
12	1	0	1.207361	1.205033	-1.501636
13	1	0	2.159561	1.175829	-0.020287
14	1	0	1.207361	-1.205033	-1.501636
15	1	0	2.159561	-1.175829	-0.020287
16	1	0	-1.207361	1.205033	-1.501636
17	1	0	-2.159561	1.175829	-0.020287
18	1	0	-1.207361	-1.205033	-1.501636
19	1	0	-2.159561	-1.175829	-0.020287

Bicyclo[3.2.0]heptane

Species name: bchp
Full file name: bchp_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.172507	E(Thermal)=	0.178736
E(CCSD(T))=	-273.054326	E(Empiric)=	-0.138940
DE(Plus)=	-0.011900	DE(2DF)=	-0.260229
E(Delta-G3XP)=	-0.402945	DE(HF)=	-0.026235
G4(0 K)=	-273.722069	G4 Energy=	-273.715840
G4 Enthalpy=	-273.714896	G4 Free Energy=	-273.751981

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.967585	1.371068	0.000000
2	1	0	-1.324335	2.405048	0.000000
3	1	0	-1.856263	0.727990	0.000000
4	6	0	-0.072992	1.041314	1.212001
5	6	0	-0.072992	1.041314	-1.212001
6	6	0	0.716416	-0.206646	0.786806
7	6	0	0.716416	-0.206646	-0.786806
8	6	0	-0.072992	-1.549291	0.777429
9	6	0	-0.072992	-1.549291	-0.777429
10	1	0	0.620334	1.872201	1.393051
11	1	0	-0.641323	0.888237	2.135721
12	1	0	0.620334	1.872201	-1.393051
13	1	0	-0.641323	0.888237	-2.135721
14	1	0	1.691102	-0.267613	1.275734
15	1	0	1.691102	-0.267613	-1.275734
16	1	0	0.463440	-2.387773	1.228583
17	1	0	-1.063098	-1.497038	1.241145
18	1	0	0.463440	-2.387773	-1.228583
19	1	0	-1.063098	-1.497038	-1.241145

Spiro[3.3]heptane

Species name: spiroheptane
Full file name: spiroheptane_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.170581	E(Thermal)=	0.177387
E(CCSD(T))=	-273.021465	E(Empiric)=	-0.138940

DE(Plus)= -0.013251 DE(2DF)= -0.260016
E(Delta-G3XP)= -0.402159 DE(HF)= -0.026099
G4(0 K)= -273.691349 G4 Energy= -273.684543
G4 Enthalpy= -273.683599 G4 Free Energy= -273.721223

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.168716
2	6	0	0.000000	2.123689	-0.279693
3	6	0	0.000000	-2.123689	-0.279693
4	6	0	0.926605	0.937060	-0.658062
5	6	0	-0.572326	1.253214	0.872048
6	6	0	-0.926605	-0.937060	-0.658062
7	6	0	0.572326	-1.253214	0.872048
8	1	0	-0.748448	2.319414	-1.052583
9	1	0	0.475527	3.070229	-0.012589
10	1	0	0.748448	-2.319414	-1.052583
11	1	0	-0.475527	-3.070229	-0.012589
12	1	0	1.060776	0.709151	-1.719680
13	1	0	1.914851	1.032531	-0.195648
14	1	0	-1.652211	1.277596	1.046810
15	1	0	-0.062984	1.449795	1.821782
16	1	0	-1.060776	-0.709151	-1.719680
17	1	0	-1.914851	-1.032531	-0.195648
18	1	0	1.652211	-1.277596	1.046810
19	1	0	0.062984	-1.449795	1.821782

Equatorial methylcyclohexane

Species name: eq_mcyclohex
Full file name: eq_mcyclohex_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.194492 E(Thermal)= 0.201810
E(CCSD(T))= -274.273383 E(Empiric)= -0.145887
DE(Plus)= -0.012078 DE(2DF)= -0.276487
E(Delta-G3XP)= -0.407927 DE(HF)= -0.027275
G4(0 K)= -274.948545 G4 Energy= -274.941227
G4 Enthalpy= -274.940282 G4 Free Energy= -274.979289

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570871	0.904745	0.000000

2	6	0	-0.548471	2.435972	0.000000
3	6	0	0.091755	0.326485	1.262760
4	6	0	0.091755	0.326485	-1.262760
5	6	0	0.091755	-1.208883	1.267170
6	6	0	0.091755	-1.208883	-1.267170
7	6	0	0.749128	-1.773545	0.000000
8	1	0	-1.622906	0.579630	0.000000
9	1	0	0.481564	2.812569	0.000000
10	1	0	-1.049577	2.842601	-0.885214
11	1	0	-1.049577	2.842601	0.885214
12	1	0	-0.414579	0.708634	2.157652
13	1	0	1.128802	0.689702	1.316451
14	1	0	-0.414579	0.708634	-2.157652
15	1	0	1.128802	0.689702	-1.316451
16	1	0	-0.944597	-1.569814	1.327844
17	1	0	0.602717	-1.584496	2.161205
18	1	0	-0.944597	-1.569814	-1.327844
19	1	0	0.602717	-1.584496	-2.161205
20	1	0	0.698477	-2.868403	0.000000
21	1	0	1.816509	-1.511310	0.000000

Cubane

Species name: cubane
Full file name: cubane_g4.log
Method: G4 calculation
Point group: D4H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.131465	E(Thermal)=	0.136084
E(CCSD(T))=	-308.515107	E(Empiric)=	-0.138940
DE(Plus)=	-0.011688	DE(2DF)=	-0.259207
E(Delta-G3XP)=	-0.448943	DE(HF)=	-0.026647
G4(0 K)=	-309.269067	G4 Energy=	-309.264449
G4 Enthalpy=	-309.263504	G4 Free Energy=	-309.295325

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.110790	0.785466
2	6	0	1.110790	0.000000	0.785466
3	6	0	0.000000	-1.110790	0.785466
4	6	0	-1.110790	0.000000	0.785466
5	6	0	0.000000	1.110790	-0.785466
6	6	0	1.110790	0.000000	-0.785466
7	6	0	0.000000	-1.110790	-0.785466
8	6	0	-1.110790	0.000000	-0.785466
9	1	0	0.000000	1.999855	1.414322
10	1	0	1.999855	0.000000	1.414322
11	1	0	0.000000	-1.999855	1.414322

12	1	0	-1.999855	0.000000	1.414322
13	1	0	0.000000	1.999855	-1.414322
14	1	0	1.999855	0.000000	-1.414322
15	1	0	0.000000	-1.999855	-1.414322
16	1	0	-1.999855	0.000000	-1.414322

[3.4.4.4]Fenestrane

Species name: 3444fenestrane
Full file name: 3444fenestrane_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.150175	E(Thermal)=	0.157124
E(CCSD(T))=	-309.600485	E(Empiric)=	-0.145887
DE(Plus)=	-0.017607	DE(2DF)=	-0.269229
E(Delta-G3XP)=	-0.451307	DE(HF)=	-0.028298
G4(0 K)=	-310.362638	G4 Energy=	-310.355689
G4 Enthalpy=	-310.354745	G4 Free Energy=	-310.392466

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.112166
2	6	0	0.000000	0.785378	-1.338141
3	6	0	1.074298	0.460611	0.754164
4	6	0	-1.074298	-0.460611	0.754164
5	6	0	0.000000	-0.785378	-1.338141
6	6	0	1.144122	1.555281	-0.416866
7	6	0	0.000000	0.000000	1.902703
8	6	0	-1.144122	-1.555281	-0.416866
9	1	0	-0.828375	1.379297	-1.706646
10	1	0	1.985063	-0.134382	0.816881
11	1	0	-1.985063	0.134382	0.816881
12	1	0	0.828375	-1.379297	-1.706646
13	1	0	0.715687	2.530419	-0.182152
14	1	0	2.150060	1.677270	-0.829050
15	1	0	-0.460326	0.762762	2.534413
16	1	0	0.460326	-0.762762	2.534413
17	1	0	-2.150060	-1.677270	-0.829050
18	1	0	-0.715687	-2.530419	-0.182152

[2.2.2]Propellane

Species name: 222propellane
Full file name: 222propellane_g4.log

Method: G4 calculation
Point group: D3H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.175562	E(Thermal)=	0.182696
E(CCSD(T))=	-310.963677	E(Empiric)=	-0.152834
DE(Plus)=	-0.015119	DE(2DF)=	-0.284630
E(Delta-G3XP)=	-0.456319	DE(HF)=	-0.028957
G4(0 K)=	-311.725974	G4 Energy=	-311.718840
G4 Enthalpy=	-311.717896	G4 Free Energy=	-311.755637

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.769359
2	6	0	0.000000	0.000000	-0.769359
3	6	0	0.000000	1.553740	0.787917
4	6	0	0.000000	1.553740	-0.787917
5	6	0	1.345578	-0.776870	0.787917
6	6	0	1.345578	-0.776870	-0.787917
7	6	0	-1.345578	-0.776870	0.787917
8	6	0	-1.345578	-0.776870	-0.787917
9	1	0	0.884069	2.007191	1.246120
10	1	0	-0.884069	2.007191	1.246120
11	1	0	0.884069	2.007191	-1.246120
12	1	0	-0.884069	2.007191	-1.246120
13	1	0	1.296244	-1.769222	1.246120
14	1	0	2.180313	-0.237969	1.246120
15	1	0	1.296244	-1.769222	-1.246120
16	1	0	2.180313	-0.237969	-1.246120
17	1	0	-2.180313	-0.237969	1.246120
18	1	0	-1.296244	-1.769222	1.246120
19	1	0	-2.180313	-0.237969	-1.246120
20	1	0	-1.296244	-1.769222	-1.246120

[2.2.2]Bicyclooctene

Species name: bce
Full file name: bce_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.179588	E(Thermal)=	0.185999
E(CCSD(T))=	-311.062903	E(Empiric)=	-0.152834
DE(Plus)=	-0.014875	DE(2DF)=	-0.282471
E(Delta-G3XP)=	-0.458547	DE(HF)=	-0.029531
G4(0 K)=	-311.821573	G4 Energy=	-311.815162
G4 Enthalpy=	-311.814218	G4 Free Energy=	-311.850947

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.288902	0.090272
2	6	0	0.000000	-1.288902	0.090272
3	6	0	0.000000	0.667564	1.466667
4	6	0	0.000000	-0.667564	1.466667
5	6	0	-1.253527	0.777047	-0.671460
6	6	0	-1.253527	-0.777047	-0.671460
7	6	0	1.253527	0.777047	-0.671460
8	6	0	1.253527	-0.777047	-0.671460
9	1	0	0.000000	2.381273	0.130691
10	1	0	0.000000	-2.381273	0.130691
11	1	0	0.000000	1.276334	2.364832
12	1	0	0.000000	-1.276334	2.364832
13	1	0	-1.238449	1.168188	-1.695013
14	1	0	-2.157709	1.166087	-0.194805
15	1	0	-1.238449	-1.168188	-1.695013
16	1	0	-2.157709	-1.166087	-0.194805
17	1	0	2.157709	1.166087	-0.194805
18	1	0	1.238449	1.168188	-1.695013
19	1	0	2.157709	-1.166087	-0.194805
20	1	0	1.238449	-1.168188	-1.695013

[2.2.2]Bicyclooctane

Species name: bco
Full file name: bco_g4.log
Method: G4 calculation
Point group: D3H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.202693	E(Thermal)=	0.209726
E(CCSD(T))=	-312.268345	E(Empiric)=	-0.159781
DE(Plus)=	-0.012607	DE(2DF)=	-0.300896
E(Delta-G3XP)=	-0.461794	DE(HF)=	-0.030130
G4(0 K)=	-313.030859	G4 Energy=	-313.023826
G4 Enthalpy=	-313.022882	G4 Free Energy=	-313.060579

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.297430
2	6	0	0.000000	0.000000	-1.297430
3	6	0	0.000000	1.450616	0.778983
4	6	0	0.000000	1.450616	-0.778983

5	6	0	1.256270	-0.725308	0.778983
6	6	0	1.256270	-0.725308	-0.778983
7	6	0	-1.256270	-0.725308	0.778983
8	6	0	-1.256270	-0.725308	-0.778983
9	1	0	0.000000	0.000000	2.392958
10	1	0	0.000000	0.000000	-2.392958
11	1	0	0.877480	1.980012	1.166546
12	1	0	-0.877480	1.980012	1.166546
13	1	0	0.877480	1.980012	-1.166546
14	1	0	-0.877480	1.980012	-1.166546
15	1	0	1.276001	-1.749926	1.166546
16	1	0	2.153481	-0.230086	1.166546
17	1	0	1.276001	-1.749926	-1.166546
18	1	0	2.153481	-0.230086	-1.166546
19	1	0	-2.153481	-0.230086	1.166546
20	1	0	-1.276001	-1.749926	1.166546
21	1	0	-2.153481	-0.230086	-1.166546
22	1	0	-1.276001	-1.749926	-1.166546

Equatorial cis-1,3-dimethylcyclohexane

Species name: eq_cis13dmcyclohex
Full file name: eq_cis13dmcyclohex_g4.log
Method: G4 calculation
Point group: CS
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.221806	E(Thermal)=	0.230621
E(CCSD(T))=	-313.458382	E(Empiric)=	-0.166728
DE(Plus)=	-0.014468	DE(2DF)=	-0.316230
E(Delta-G3XP)=	-0.466162	DE(HF)=	-0.031064
G4(0 K)=	-314.231227	G4 Energy=	-314.222412
G4 Enthalpy=	-314.221468	G4 Free Energy=	-314.263812

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.461227	-0.966295	0.000000
2	1	0	0.423636	-2.063390	0.000000
3	1	0	1.528665	-0.696479	0.000000
4	6	0	-0.190581	-0.422416	1.282689
5	6	0	-0.190581	-0.422416	-1.282689
6	6	0	-0.190581	1.115415	1.268403
7	6	0	-0.190581	1.115415	-1.268403
8	6	0	-0.845442	1.678322	0.000000
9	6	0	0.486096	-0.977645	2.539499
10	6	0	0.486096	-0.977645	-2.539499
11	1	0	-1.240616	-0.753584	1.287383
12	1	0	-1.240616	-0.753584	-1.287383
13	1	0	-0.700780	1.497360	2.161084

14	1	0	0.848722	1.470620	1.330532
15	1	0	-0.700780	1.497360	-2.161084
16	1	0	0.848722	1.470620	-1.330532
17	1	0	-1.913678	1.420388	0.000000
18	1	0	-0.792666	2.773170	0.000000
19	1	0	1.538967	-0.674073	2.584382
20	1	0	-0.002570	-0.612865	3.449518
21	1	0	0.456335	-2.072505	2.558729
22	1	0	1.538967	-0.674073	-2.584382
23	1	0	-0.002570	-0.612865	-3.449518
24	1	0	0.456335	-2.072505	-2.558729

Equatorial trans-1,4-dimethylcyclohexane

Species name: eq_trans14dmcyclohex
Full file name: eq_trans14dmcyclohex_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.221904	E(Thermal)=	0.230671
E(CCSD(T))=	-313.458342	E(Empiric)=	-0.166728
DE(Plus)=	-0.014367	DE(2DF)=	-0.316218
E(Delta-G3XP)=	-0.466225	DE(HF)=	-0.031070
G4(0 K)=	-314.231047	G4 Energy=	-314.222280
G4 Enthalpy=	-314.221336	G4 Free Energy=	-314.262898

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.229282	1.485575	0.000000
2	6	0	0.252749	2.939119	0.000000
3	6	0	0.229282	0.732380	1.259721
4	6	0	0.229282	0.732380	-1.259721
5	6	0	-0.229282	-0.732380	1.259721
6	6	0	-0.229282	-0.732380	-1.259721
7	6	0	0.229282	-1.485575	0.000000
8	6	0	-0.252749	-2.939119	0.000000
9	1	0	-1.330407	1.492667	0.000000
10	1	0	1.348380	2.989363	0.000000
11	1	0	-0.102997	3.477671	-0.885124
12	1	0	-0.102997	3.477671	0.885124
13	1	0	-0.140826	1.243824	2.156704
14	1	0	1.327345	0.769662	1.314891
15	1	0	-0.140826	1.243824	-2.156704
16	1	0	1.327345	0.769662	-1.314891
17	1	0	-1.327345	-0.769662	1.314891
18	1	0	0.140826	-1.243824	2.156704
19	1	0	-1.327345	-0.769662	-1.314891
20	1	0	0.140826	-1.243824	-2.156704

21	1	0	1.330407	-1.492667	0.000000
22	1	0	-1.348380	-2.989363	0.000000
23	1	0	0.102997	-3.477671	-0.885124
24	1	0	0.102997	-3.477671	0.885124

[4.4.4.4]Fenestrane

Species name: 4444fenestrane
Full file name: 4444fenestrane_g4.log
Method: G4 calculation
Point group: D2D
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.180171	E(Thermal)=	0.187766
E(CCSD(T))=	-348.862078	E(Empiric)=	-0.166728
DE(Plus)=	-0.018526	DE(2DF)=	-0.307740
E(Delta-G3XP)=	-0.507621	DE(HF)=	-0.031896
G4(0 K)=	-349.714418	G4 Energy=	-349.706823
G4 Enthalpy=	-349.705879	G4 Free Energy=	-349.744677

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	1.356655	0.623154
3	6	0	1.356655	0.000000	-0.623154
4	6	0	0.000000	-1.356655	0.623154
5	6	0	-1.356655	0.000000	-0.623154
6	6	0	1.477085	1.477085	0.000000
7	6	0	1.477085	-1.477085	0.000000
8	6	0	-1.477085	-1.477085	0.000000
9	6	0	-1.477085	1.477085	0.000000
10	1	0	0.000000	1.466174	1.709021
11	1	0	1.466174	0.000000	-1.709021
12	1	0	0.000000	-1.466174	1.709021
13	1	0	-1.466174	0.000000	-1.709021
14	1	0	2.220062	1.642397	0.785706
15	1	0	1.642397	2.220062	-0.785706
16	1	0	2.220062	-1.642397	0.785706
17	1	0	1.642397	-2.220062	-0.785706
18	1	0	-2.220062	-1.642397	0.785706
19	1	0	-1.642397	-2.220062	-0.785706
20	1	0	-2.220062	1.642397	0.785706
21	1	0	-1.642397	2.220062	-0.785706

Equatorial cis-1,3,5-trimethylcyclohexane

Species name: eq_cis135tmcyclohex
Full file name: eq_cis135tmcyclohex_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.249219	E(Thermal)=	0.259492
E(CCSD(T))=	-352.643376	E(Empiric)=	-0.187569
DE(Plus)=	-0.016924	DE(2DF)=	-0.355951
E(Delta-G3XP)=	-0.524398	DE(HF)=	-0.034847
G4(0 K)=	-353.513845	G4 Energy=	-353.503573
G4 Enthalpy=	-353.502629	G4 Free Energy=	-353.547093

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.280258	0.739158	-0.334129
2	6	0	0.000000	1.456097	0.123714
3	6	0	-1.280258	0.739158	-0.334129
4	6	0	-1.261017	-0.728048	0.123714
5	6	0	0.000000	-1.478315	-0.334129
6	6	0	1.261017	-0.728048	0.123714
7	6	0	2.539420	1.466135	0.148337
8	6	0	-2.539420	1.466135	0.148337
9	6	0	0.000000	-2.932269	0.148337
10	1	0	1.288263	0.743779	-1.435006
11	1	0	0.000000	2.490301	-0.243931
12	1	0	0.000000	1.520853	1.222914
13	1	0	-1.288263	0.743779	-1.435006
14	1	0	-2.156664	-1.245150	-0.243931
15	1	0	-1.317098	-0.760427	1.222914
16	1	0	0.000000	-1.487557	-1.435006
17	1	0	2.156664	-1.245150	-0.243931
18	1	0	1.317098	-0.760427	1.222914
19	1	0	2.582883	1.491228	1.243896
20	1	0	3.448170	0.968739	-0.207703
21	1	0	2.563037	2.501833	-0.207703
22	1	0	-2.582883	1.491228	1.243896
23	1	0	-2.563037	2.501833	-0.207703
24	1	0	-3.448170	0.968739	-0.207703
25	1	0	0.000000	-2.982457	1.243896
26	1	0	-0.885132	-3.470572	-0.207703
27	1	0	0.885132	-3.470572	-0.207703

[4.4.4.5]Fenestrane

Species name: 4445fenestrane
Full file name: 4445fenestrane_g4.log
Method: G4 calculation
Point group: C2

NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.211075	E(Thermal)=	0.219121
E(CCSD(T))=	-388.143053	E(Empiric)=	-0.187569
DE(Plus)=	-0.020165	DE(2DF)=	-0.347426
E(Delta-G3XP)=	-0.565440	DE(HF)=	-0.035689
G4(0 K)=	-389.088267	G4 Energy=	-389.080221
G4 Enthalpy=	-389.079277	G4 Free Energy=	-389.119859

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.138353
2	6	0	0.000000	0.000000	2.287105
3	6	0	0.599788	1.124447	-0.668113
4	6	0	-0.599788	-1.124447	-0.668113
5	6	0	0.000000	0.788197	-2.059636
6	6	0	0.000000	-0.788197	-2.059636
7	6	0	0.015824	2.108475	0.429713
8	6	0	-0.015824	-2.108475	0.429713
9	6	0	-0.671523	0.895896	1.175289
10	6	0	0.671523	-0.895896	1.175289
11	1	0	0.732045	0.497253	2.931581
12	1	0	-0.732045	-0.497253	2.931581
13	1	0	1.692869	1.143073	-0.730322
14	1	0	-1.692869	-1.143073	-0.730322
15	1	0	0.556408	1.208402	-2.902713
16	1	0	-1.034859	1.144469	-2.139855
17	1	0	1.034859	-1.144469	-2.139855
18	1	0	-0.556408	-1.208402	-2.902713
19	1	0	0.795726	2.635602	0.986994
20	1	0	-0.704734	2.849632	0.071923
21	1	0	-0.795726	-2.635602	0.986994
22	1	0	0.704734	-2.849632	0.071923
23	1	0	-1.758599	0.976206	1.242496
24	1	0	1.758599	-0.976206	1.242496

Adamantane

Species name: adamantane
Full file name: adamantane_g4.log
Method: G4 calculation
Point group: TD
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.240250	E(Thermal)=	0.247232
E(CCSD(T))=	-389.476350	E(Empiric)=	-0.194516
DE(Plus)=	-0.015399	DE(2DF)=	-0.363752
E(Delta-G3XP)=	-0.574525	DE(HF)=	-0.036715

G4(0 K)= -390.421007 G4 Energy= -390.414026
G4 Enthalpy= -390.413082 G4 Free Energy= -390.449425

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891578	0.891578	0.891578
2	1	0	-1.524484	1.524484	1.524484
3	6	0	0.000000	0.000000	1.779667
4	6	0	0.000000	1.779667	0.000000
5	6	0	-1.779667	0.000000	0.000000
6	6	0	0.891578	-0.891578	0.891578
7	6	0	0.891578	0.891578	-0.891578
8	6	0	-0.891578	-0.891578	-0.891578
9	6	0	1.779667	0.000000	0.000000
10	6	0	0.000000	0.000000	-1.779667
11	6	0	0.000000	-1.779667	0.000000
12	1	0	-0.623016	-0.623016	2.433964
13	1	0	0.623016	0.623016	2.433964
14	1	0	0.623016	2.433964	0.623016
15	1	0	-0.623016	2.433964	-0.623016
16	1	0	-2.433964	0.623016	-0.623016
17	1	0	-2.433964	-0.623016	0.623016
18	1	0	1.524484	-1.524484	1.524484
19	1	0	1.524484	1.524484	-1.524484
20	1	0	-1.524484	-1.524484	-1.524484
21	1	0	2.433964	-0.623016	-0.623016
22	1	0	2.433964	0.623016	0.623016
23	1	0	0.623016	-0.623016	-2.433964
24	1	0	-0.623016	0.623016	-2.433964
25	1	0	0.623016	-2.433964	-0.623016
26	1	0	-0.623016	-2.433964	0.623016

Trans-decalin

Species name: trans_decalin
Full file name: trans_decalin_g4.log
Method: G4 calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.259276 E(Thermal)= 0.268342
E(CCSD(T))= -390.649793 E(Empiric)= -0.201463
DE(Plus)= -0.017649 DE(2DF)= -0.379018
E(Delta-G3XP)= -0.577965 DE(HF)= -0.037989
G4(0 K)= -391.604601 G4 Energy= -391.595536
G4 Enthalpy= -391.594591 G4 Free Energy= -391.637234

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.231884	0.736742	0.000000
2	6	0	-0.231884	-0.736742	0.000000
3	6	0	-0.228542	1.459223	1.275157
4	6	0	0.228542	0.732725	2.547282
5	6	0	-0.228542	-0.732725	2.547282
6	6	0	0.228542	-1.459223	1.275157
7	6	0	-0.228542	1.459223	-1.275157
8	6	0	0.228542	0.732725	-2.547282
9	6	0	-0.228542	-0.732725	-2.547282
10	6	0	0.228542	-1.459223	-1.275157
11	1	0	1.334885	0.729196	0.000000
12	1	0	-1.334885	-0.729196	0.000000
13	1	0	-1.326305	1.527891	1.270237
14	1	0	0.143473	2.491381	1.271905
15	1	0	1.325245	0.768909	2.609337
16	1	0	-0.149384	1.250070	3.436599
17	1	0	-1.325245	-0.768909	2.609337
18	1	0	0.149384	-1.250070	3.436599
19	1	0	1.326305	-1.527891	1.270237
20	1	0	-0.143473	-2.491381	1.271905
21	1	0	-1.326305	1.527891	-1.270237
22	1	0	0.143473	2.491381	-1.271905
23	1	0	1.325245	0.768909	-2.609337
24	1	0	-0.149384	1.250070	-3.436599
25	1	0	-1.325245	-0.768909	-2.609337
26	1	0	0.149384	-1.250070	-3.436599
27	1	0	1.326305	-1.527891	-1.270237
28	1	0	-0.143473	-2.491381	-1.271905

Cis-decalin

Species name: cis_decalin
Full file name: cis_decalin_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.259595	E(Thermal)=	0.268591
E(CCSD(T))=	-390.645477	E(Empiric)=	-0.201463
DE(Plus)=	-0.017238	DE(2DF)=	-0.379417
E(Delta-G3XP)=	-0.578358	DE(HF)=	-0.037889
G4(0 K)=	-391.600247	G4 Energy=	-391.591251
G4 Enthalpy=	-391.590306	G4 Free Energy=	-391.632710

Standard orientation:

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

1	6	0	0.724604	0.276284	0.689114
2	6	0	-0.724604	-0.276284	0.689114
3	6	0	0.724604	1.817353	0.679681
4	6	0	-0.131262	2.414383	-0.447859
5	6	0	-1.563567	1.864739	-0.405275
6	6	0	-1.571734	0.330301	-0.446624
7	6	0	1.571734	-0.330301	-0.446624
8	6	0	1.563567	-1.864739	-0.405275
9	6	0	0.131262	-2.414383	-0.447859
10	6	0	-0.724604	-1.817353	0.679681
11	1	0	1.191348	-0.048103	1.630934
12	1	0	-1.191348	0.048103	1.630934
13	1	0	1.755174	2.187453	0.611694
14	1	0	0.331232	2.173480	1.641787
15	1	0	-0.140174	3.507464	-0.367580
16	1	0	0.317432	2.183127	-1.422694
17	1	0	-2.153779	2.270561	-1.234981
18	1	0	-2.052124	2.203833	0.519258
19	1	0	-2.599604	-0.045296	-0.369203
20	1	0	-1.199169	-0.002849	-1.423437
21	1	0	1.199169	0.002849	-1.423437
22	1	0	2.599604	0.045296	-0.369203
23	1	0	2.052124	-2.203833	0.519258
24	1	0	2.153779	-2.270561	-1.234981
25	1	0	-0.317432	-2.183127	-1.422694
26	1	0	0.140174	-3.507464	-0.367580
27	1	0	-0.331232	-2.173480	1.641787
28	1	0	-1.755174	-2.187453	0.611694

1-Methyladamantane

Species name: 1madamantane
Full file name: 1madamantane_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.265807	E(Thermal)=	0.274578
E(CCSD(T))=	-428.664565	E(Empiric)=	-0.215357
DE(Plus)=	-0.018778	DE(2DF)=	-0.403539
E(Delta-G3XP)=	-0.632146	DE(HF)=	-0.040453
G4(0 K)=	-429.709029	G4 Energy=	-429.700258
G4 Enthalpy=	-429.699314	G4 Free Energy=	-429.740438

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.252878
2	6	0	0.000000	0.000000	2.783407

3	6	0	0.000000	1.448451	0.709976
4	6	0	1.254396	-0.724226	0.709976
5	6	0	-1.254396	-0.724226	0.709976
6	6	0	0.000000	1.453675	-0.830831
7	6	0	1.258919	-0.726837	-0.830831
8	6	0	-1.258919	-0.726837	-0.830831
9	6	0	1.258388	0.726531	-1.344664
10	6	0	0.000000	-1.453061	-1.344664
11	6	0	-1.258388	0.726531	-1.344664
12	1	0	-0.885321	0.511140	3.179230
13	1	0	0.885321	0.511140	3.179230
14	1	0	0.000000	-1.022280	3.179230
15	1	0	-0.880875	1.984091	1.088296
16	1	0	0.880875	1.984091	1.088296
17	1	0	2.158711	-0.229186	1.088296
18	1	0	1.277836	-1.754906	1.088296
19	1	0	-1.277836	-1.754906	1.088296
20	1	0	-2.158711	-0.229186	1.088296
21	1	0	0.000000	2.488817	-1.191822
22	1	0	2.155379	-1.244409	-1.191822
23	1	0	-2.155379	-1.244409	-1.191822
24	1	0	1.280506	0.739301	-2.441698
25	1	0	2.161206	1.247773	-1.001757
26	1	0	0.000000	-1.478601	-2.441698
27	1	0	0.000000	-2.495545	-1.001757
28	1	0	-1.280506	0.739301	-2.441698
29	1	0	-2.161206	1.247773	-1.001757

Spiro[5.5]undecane

Species name: spiroundecane
Full file name: spiroundecane_g4.log
Method: G4 calculation
Point group: C2
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.287652	E(Thermal)=	0.297835
E(CCSD(T))=	-429.828086	E(Empiric)=	-0.222304
DE(Plus)=	-0.020120	DE(2DF)=	-0.419627
E(Delta-G3XP)=	-0.636244	DE(HF)=	-0.041646
G4(0 K)=	-430.880377	G4 Energy=	-430.870193
G4 Enthalpy=	-430.869249	G4 Free Energy=	-430.914212

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.390053
2	6	0	0.000000	1.253484	1.298482
3	6	0	0.000000	-1.253484	1.298482
4	6	0	-1.286509	0.032307	-0.476312

5	6	0	1.286509	-0.032307	-0.476312
6	6	0	-0.192876	2.579128	0.547074
7	6	0	0.192876	-2.579128	0.547074
8	6	0	-1.494290	1.350598	-1.238697
9	6	0	1.494290	-1.350598	-1.238697
10	6	0	-1.475556	2.558839	-0.293860
11	6	0	1.475556	-2.558839	-0.293860
12	1	0	-0.813420	1.146948	2.031031
13	1	0	0.931003	1.280837	1.878892
14	1	0	0.813420	-1.146948	2.031031
15	1	0	-0.931003	-1.280837	1.878892
16	1	0	-2.146388	-0.122099	0.191257
17	1	0	-1.301262	-0.804175	-1.182259
18	1	0	2.146388	0.122099	0.191257
19	1	0	1.301262	0.804175	-1.182259
20	1	0	-0.221378	3.407004	1.265017
21	1	0	0.668841	2.771089	-0.105201
22	1	0	0.221378	-3.407004	1.265017
23	1	0	-0.668841	-2.771089	-0.105201
24	1	0	-2.444477	1.309555	-1.783964
25	1	0	-0.713302	1.472102	-2.000684
26	1	0	2.444477	-1.309555	-1.783964
27	1	0	0.713302	-1.472102	-2.000684
28	1	0	-2.344831	2.504550	0.376913
29	1	0	-1.577983	3.490922	-0.861283
30	1	0	2.344831	-2.504550	0.376913
31	1	0	1.577983	-3.490922	-0.861283

1,3-Dimethyladamantane

Species name: 13dmadamantane
Full file name: 13dmadamantane_g4.log
Method: G4 calculation
Point group: C2V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.293177	E(Thermal)=	0.303379
E(CCSD(T))=	-467.852760	E(Empiric)=	-0.236198
DE(Plus)=	-0.022205	DE(2DF)=	-0.443251
E(Delta-G3XP)=	-0.689806	DE(HF)=	-0.044181
G4(0 K)=	-468.995224	G4 Energy=	-468.985022
G4 Enthalpy=	-468.984078	G4 Free Energy=	-469.028362

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.435177
2	6	0	0.000000	1.280791	-0.570017
3	6	0	0.000000	-1.280791	-0.570017
4	6	0	1.254260	1.257382	0.333857

5	6	0	-1.254260	1.257382	0.333857
6	6	0	-1.254260	-1.257382	0.333857
7	6	0	1.254260	-1.257382	0.333857
8	6	0	1.256754	0.000000	1.223127
9	6	0	-1.256754	0.000000	1.223127
10	6	0	0.000000	0.000000	2.113755
11	6	0	0.000000	2.526857	-1.459425
12	6	0	0.000000	-2.526857	-1.459425
13	1	0	0.880113	0.000000	-2.093233
14	1	0	-0.880113	0.000000	-2.093233
15	1	0	2.158396	1.281075	-0.288815
16	1	0	1.277125	2.160772	0.957522
17	1	0	-2.158396	1.281075	-0.288815
18	1	0	-1.277125	2.160772	0.957522
19	1	0	-2.158396	-1.281075	-0.288815
20	1	0	-1.277125	-2.160772	0.957522
21	1	0	2.158396	-1.281075	-0.288815
22	1	0	1.277125	-2.160772	0.957522
23	1	0	2.154448	0.000000	1.852541
24	1	0	-2.154448	0.000000	1.852541
25	1	0	0.000000	-0.881243	2.767711
26	1	0	0.000000	0.881243	2.767711
27	1	0	0.000000	3.442872	-0.857401
28	1	0	-0.885158	2.552241	-2.105582
29	1	0	0.885158	2.552241	-2.105582
30	1	0	0.000000	-3.442872	-0.857401
31	1	0	0.885158	-2.552241	-2.105582
32	1	0	-0.885158	-2.552241	-2.105582

1,3,5-trimethyladamantane

Species name: 135tmadamantane
Full file name: 135tmadamantane_g4.log
Method: G4 calculation
Point group: C3V
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.319435	E(Thermal)=	0.331333
E(CCSD(T))=	-507.040957	E(Empiric)=	-0.257039
DE(Plus)=	-0.025633	DE(2DF)=	-0.482912
E(Delta-G3XP)=	-0.747562	DE(HF)=	-0.047902
G4(0 K)=	-508.282570	G4 Energy=	-508.270672
G4 Enthalpy=	-508.269728	G4 Free Energy=	-508.316902

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.802408
2	1	0	0.000000	0.000000	2.898790
3	6	0	0.000000	1.451255	1.289932

4	6	0	1.256823	-0.725627	1.289932
5	6	0	-1.256823	-0.725627	1.289932
6	6	0	0.000000	1.476329	-0.254455
7	6	0	1.278538	-0.738164	-0.254455
8	6	0	-1.278538	-0.738164	-0.254455
9	6	0	1.252919	0.723373	-0.754287
10	6	0	0.000000	-1.446747	-0.754287
11	6	0	-1.252919	0.723373	-0.754287
12	6	0	0.000000	2.918320	-0.769986
13	6	0	2.527339	-1.459160	-0.769986
14	6	0	-2.527339	-1.459160	-0.769986
15	1	0	-0.881146	1.986033	1.668164
16	1	0	0.881146	1.986033	1.668164
17	1	0	2.160528	-0.229921	1.668164
18	1	0	1.279382	-1.756111	1.668164
19	1	0	-1.279382	-1.756111	1.668164
20	1	0	-2.160528	-0.229921	1.668164
21	1	0	1.279049	0.738459	-1.852680
22	1	0	2.157406	1.245579	-0.413016
23	1	0	0.000000	-1.476918	-1.852680
24	1	0	0.000000	-2.491158	-0.413016
25	1	0	-1.279049	0.738459	-1.852680
26	1	0	-2.157406	1.245579	-0.413016
27	1	0	0.000000	2.948024	-1.865746
28	1	0	-0.885151	3.462998	-0.421595
29	1	0	0.885151	3.462998	-0.421595
30	1	0	2.553064	-1.474012	-1.865746
31	1	0	3.441620	-0.964936	-0.421595
32	1	0	2.556468	-2.498062	-0.421595
33	1	0	-2.553064	-1.474012	-1.865746
34	1	0	-2.556468	-2.498062	-0.421595
35	1	0	-3.441620	-0.964936	-0.421595

1,3,5,7-Tetramethyladamantane

Species name: 1357tmadamantane
Full file name: 1357tmadamantane_g4.log
Method: G4 calculation
Point group: TD
NImag: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.348943	E(Thermal)=	0.361755
E(CCSD(T))=	-546.229126	E(Empiric)=	-0.277880
DE(Plus)=	-0.029050	DE(2DF)=	-0.522537
E(Delta-G3XP)=	-0.805103	DE(HF)=	-0.051650
G4(0 K)=	-547.566403	G4 Energy=	-547.553591
G4 Enthalpy=	-547.552647	G4 Free Energy=	-547.600121

Standard orientation:

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

1	6	0	-0.902271	0.902271	0.902271
2	6	0	-1.786586	1.786586	1.786586
3	6	0	0.000000	0.000000	1.770879
4	6	0	0.000000	1.770879	0.000000
5	6	0	-1.770879	0.000000	0.000000
6	6	0	0.902271	-0.902271	0.902271
7	6	0	0.902271	0.902271	-0.902271
8	6	0	-0.902271	-0.902271	-0.902271
9	6	0	1.770879	0.000000	0.000000
10	6	0	0.000000	0.000000	-1.770879
11	6	0	0.000000	-1.770879	0.000000
12	6	0	1.786586	-1.786586	1.786586
13	6	0	1.786586	1.786586	-1.786586
14	6	0	-1.786586	-1.786586	-1.786586
15	1	0	-2.432503	1.180736	2.432503
16	1	0	-1.180736	2.432503	2.432503
17	1	0	-2.432503	2.432503	1.180736
18	1	0	-0.622546	-0.622546	2.428036
19	1	0	0.622546	0.622546	2.428036
20	1	0	0.622546	2.428036	0.622546
21	1	0	-0.622546	2.428036	-0.622546
22	1	0	-2.428036	0.622546	-0.622546
23	1	0	-2.428036	-0.622546	0.622546
24	1	0	2.428036	-0.622546	-0.622546
25	1	0	2.428036	0.622546	0.622546
26	1	0	0.622546	-0.622546	-2.428036
27	1	0	-0.622546	0.622546	-2.428036
28	1	0	0.622546	-2.428036	-0.622546
29	1	0	-0.622546	-2.428036	0.622546
30	1	0	2.432503	-2.432503	1.180736
31	1	0	2.432503	-1.180736	2.432503
32	1	0	1.180736	-2.432503	2.432503
33	1	0	2.432503	1.180736	-2.432503
34	1	0	2.432503	2.432503	-1.180736
35	1	0	1.180736	2.432503	-2.432503
36	1	0	-1.180736	-2.432503	-2.432503
37	1	0	-2.432503	-1.180736	-2.432503
38	1	0	-2.432503	-2.432503	-1.180736

List S2: W1BD optimized geometries & abbreviated calculation results.

Ethyne

Species name: ethyne
Full file name: ethyne_w1bd.log
Method: W1BD calculation
Point group: D*H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.026585 E(Thermal)= 0.029405
W1BD (0 K)= -77.325151 W1BD Energy= -77.322331
W1BD Enthalpy= -77.321387 W1BD Free Energy= -77.344106
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C2H2\RABLENP\26-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Ethyne\\0,1\C,0,0.,0.,0.5980128454\C,0,0.,0.,-0.598
0128454\H,0,0.,0.,1.6596171763\H,0,0.,0.,-1.6596171763\\Version=AM64L-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.598013
2	6	0	0.000000	0.000000	-0.598013
3	1	0	0.000000	0.000000	1.659617
4	1	0	0.000000	0.000000	-1.659617

Ethene

Species name: ethene
Full file name: ethene_w1bd.log
Method: W1BD calculation
Point group: D2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.050157 E(Thermal)= 0.053207
W1BD (0 K)= -78.554639 W1BD Energy= -78.551588
W1BD Enthalpy= -78.550644 W1BD Free Energy= -78.575503
1\1\GINC-NODE53\Mixed\W1BD\W1BD\C2H4\RABLENP\12-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Ethene\\0,1\C,0,-0.6620535521,0.,0.\C,0,0.662053552
1,0.,0.\H,0,-1.2315912921,0.9206726093,0.\H,0,-1.2315912921,-0.9206726

Standard orientation:

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

1	6	0	0.000000	0.000000	0.662054
2	6	0	0.000000	0.000000	-0.662054
3	1	0	0.000000	0.920673	1.231591
4	1	0	0.000000	-0.920673	1.231591
5	1	0	0.000000	-0.920673	-1.231591
6	1	0	0.000000	0.920673	-1.231591

Ethane

Species name: ethane
Full file name: ethane_w1bd.log
Method: W1BD calculation
Point group: D3D
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.073258 E(Thermal)= 0.076770
W1BD (0 K)= -79.769187 W1BD Energy= -79.765676
W1BD Enthalpy= -79.764732 W1BD Free Energy= -79.790622
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C2H6\RABLENP\24-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Ethane\\0,1\C,0,0.,0.,0.763584694\C,0,0.,0.,-0.7635
84694\H,0,0.,1.0161138848,1.1609766738\H,0,0.8799804374,-0.5080569424,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.763585
2	6	0	0.000000	0.000000	-0.763585
3	1	0	0.000000	1.016114	1.160977
4	1	0	0.879980	-0.508057	1.160977
5	1	0	-0.879980	-0.508057	1.160977
6	1	0	0.000000	-1.016114	-1.160977
7	1	0	-0.879980	0.508057	-1.160977
8	1	0	0.879980	0.508057	-1.160977

Propyne

Species name: propyne
Full file name: propyne_w1bd.log
Method: W1BD calculation
Point group: C3V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.054657 E(Thermal)= 0.058631
W1BD (0 K)= -116.628275 W1BD Energy= -116.624301
W1BD Enthalpy= -116.623357 W1BD Free Energy= -116.651446
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C3H4\RABLENP\26-Nov-2019\0\\#n W1BD fo

pt=(calcfc,tight)\\Propyne\\0,1\C,0,0.,0.,-1.4139255644\C,0,0.,0.,-0.2
150129843\C,0,0.,0.,1.2399002901\H,0,0.,0.,-2.4746578692\H,0,0.,1.0188

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.417678
2	6	0	0.000000	0.000000	0.218765
3	6	0	0.000000	0.000000	-1.236148
4	1	0	0.000000	0.000000	2.478410
5	1	0	0.000000	1.018890	-1.626726
6	1	0	-0.882384	-0.509445	-1.626726
7	1	0	0.882384	-0.509445	-1.626726

Propene

Species name: propene
Full file name: propene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.078242 E(Thermal)= 0.082353
W1BD (0 K)= -117.853578 W1BD Energy= -117.849468
W1BD Enthalpy= -117.848524 W1BD Free Energy= -117.878590
1\1\GINC-NODE75\Mixed\W1BD\W1BD\C3H6\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Propene\\0,1\C,0,0.0021824059,0.,0.0048245903\C,0,0
.0041298759,0.,1.3312844702\C,0,1.225974575,0.,2.1959390595\H,0,0.9245

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.287726	0.153159	0.000000
2	6	0	0.000000	0.471375	0.000000
3	6	0	-1.133959	-0.505696	0.000000
4	1	0	1.617465	-0.879298	0.000000
5	1	0	2.059398	0.911247	0.000000
6	1	0	-0.278311	1.521537	0.000000
7	1	0	-0.775969	-1.535326	0.000000
8	1	0	-1.772591	-0.365595	0.876199
9	1	0	-1.772591	-0.365595	-0.876199

Propane

Species name: propane
Full file name: propane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.101456 E(Thermal)= 0.106045
W1BD (0 K)= -119.063722 W1BD Energy= -119.059134
W1BD Enthalpy= -119.058189 W1BD Free Energy= -119.088778
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C3H8\RABLENP\24-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Propane\\0,1\C,0,0.,1.2739640972,0.2587164957\C,0,0
.,0.,-0.5849932047\C,0,0.,-1.2739640972,0.2587164957\H,0,0.,2.16865265

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.273964	-0.259078
2	6	0	0.000000	0.000000	0.584632
3	6	0	0.000000	-1.273964	-0.259078
4	1	0	0.000000	2.168653	0.365346
5	1	0	0.880668	1.318655	-0.903521
6	1	0	-0.880668	1.318655	-0.903521
7	1	0	-0.873415	0.000000	1.242268
8	1	0	0.873415	0.000000	1.242268
9	1	0	0.000000	-2.168653	0.365346
10	1	0	0.880668	-1.318655	-0.903521
11	1	0	-0.880668	-1.318655	-0.903521

1-Butyne

Species name: 1butyne
Full file name: 1butyne_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.083162 E(Thermal)= 0.088207
W1BD (0 K)= -155.921899 W1BD Energy= -155.916853
W1BD Enthalpy= -155.915909 W1BD Free Energy= -155.948773
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C4H6\RABLENP\27-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\1-Butyne\\0,1\C,0,-1.9599642068,0.2200124095,0.\C,0
,-0.8280392496,-0.1774302345,0.\C,0,0.5564676999,-0.6370063782,0.\C,0,

Standard orientation:

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

1	6	0	-1.328759	-1.459273	0.000000
2	6	0	-0.738933	-0.414611	0.000000
3	6	0	0.000000	0.843184	0.000000
4	6	0	1.523496	0.649799	0.000000
5	1	0	-1.855659	-2.379957	0.000000
6	1	0	-0.297287	1.428914	0.873968
7	1	0	-0.297287	1.428914	-0.873968
8	1	0	2.027322	1.616708	0.000000
9	1	0	1.844042	0.095412	0.881363
10	1	0	1.844042	0.095412	-0.881363

2-Butyne

Species name: 2butyne
Full file name: 2butyne_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.082620 E(Thermal)= 0.088390
W1BD (0 K)= -155.929934 W1BD Energy= -155.924164
W1BD Enthalpy= -155.923220 W1BD Free Energy= -155.956813
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C4H6\RABLENP\27-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\2-Butyne\\0,1\C,0,0.,0.0000000001,-0.6004814876\C,0
,0.,0.0000000001,0.6004814876\C,0,0.,0.0000000001,-2.0570722079\C,0,0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.600481
2	6	0	0.000000	0.000000	-0.600481
3	6	0	0.000000	0.000000	2.057072
4	6	0	0.000000	0.000000	-2.057072
5	1	0	0.000000	1.017872	2.451760
6	1	0	0.000000	1.017872	-2.451760
7	1	0	0.881503	-0.508936	2.451760
8	1	0	-0.881503	-0.508936	2.451760
9	1	0	0.881503	-0.508936	-2.451760
10	1	0	-0.881503	-0.508936	-2.451760

1,3-Butadiene (s-trans)

Species name: 13butadiene
Full file name: 13butadiene_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.083702 E(Thermal)= 0.088384
W1BD (0 K)= -155.942692 W1BD Energy= -155.938010
W1BD Enthalpy= -155.937066 W1BD Free Energy= -155.968494
1\1\GINC-NODE55\Mixed\W1BD\W1BD\C4H6\RABLENP\03-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\1,3-Butadiene (s-trans)\\0,1\C,0,-0.6103028952,-0.3
938955947,0.\C,0,0.6103028952,0.3938955947,0.\C,0,-1.8398308547,0.1233

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.324532	0.649848	0.000000
2	6	0	0.324532	-0.649848	0.000000
3	6	0	0.324532	1.815178	0.000000
4	6	0	-0.324532	-1.815178	0.000000
5	1	0	-1.410431	0.645187	0.000000
6	1	0	1.410431	-0.645187	0.000000
7	1	0	1.406881	1.858500	0.000000
8	1	0	-0.202710	2.758789	0.000000
9	1	0	-1.406881	-1.858500	0.000000
10	1	0	0.202710	-2.758789	0.000000

Isobutylene

Species name: isobutylene
Full file name: isobutylene_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.105811 E(Thermal)= 0.111180
W1BD (0 K)= -157.154275 W1BD Energy= -157.148906
W1BD Enthalpy= -157.147962 W1BD Free Energy= -157.180970
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C4H8\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Isobutylene\\0,1\C,0,0.,0.,0.\C,0,0.,0.,1.33012251\
C,0,1.2727757469,0.,-0.8006389093\C,0,-1.2727757469,0.,-0.8006389093\H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.123998
2	6	0	0.000000	0.000000	1.454120
3	6	0	0.000000	1.272776	-0.676641
4	6	0	0.000000	-1.272776	-0.676641
5	1	0	0.000000	0.922059	2.021178
6	1	0	0.000000	-0.922059	2.021178

7	1	0	0.000000	2.153978	-0.036777
8	1	0	0.876262	1.322427	-1.329453
9	1	0	-0.876262	1.322427	-1.329453
10	1	0	0.000000	-2.153978	-0.036777
11	1	0	-0.876262	-1.322427	-1.329453
12	1	0	0.876262	-1.322427	-1.329453

Trans-2-butene

Species name: trans2butene
Full file name: trans2butene_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.105885 E(Thermal)= 0.111409
W1BD (0 K)= -157.152252 W1BD Energy= -157.146728
W1BD Enthalpy= -157.145784 W1BD Free Energy= -157.179024
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C4H8\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Trans-2-butene\\0,1\C,0,-0.5355763024,0.3928043143,
0.\C,0,0.5355763024,-0.3928043143,0.\C,0,-1.9564829433,-0.0801560282,0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.323079	0.580308	0.000000
2	6	0	0.323079	-0.580308	0.000000
3	6	0	0.323079	1.931287	0.000000
4	6	0	-0.323079	-1.931287	0.000000
5	1	0	-1.410582	0.569836	0.000000
6	1	0	1.410582	-0.569836	0.000000
7	1	0	0.024829	2.513466	0.876293
8	1	0	0.024829	2.513466	-0.876293
9	1	0	1.410695	1.853955	0.000000
10	1	0	-0.024829	-2.513466	0.876293
11	1	0	-1.410695	-1.853955	0.000000
12	1	0	-0.024829	-2.513466	-0.876293

1-Butene C1

Species name: 1butene
Full file name: 1butene_w1bd.log
Method: W1BD calculation
Point group: C1
NImag: 0

Temperature= 298.150000 Pressure= 1.000000

E(ZPE)= 0.106458 E(Thermal)= 0.111775
W1BD (0 K)= -157.147661 W1BD Energy= -157.142345
W1BD Enthalpy= -157.141400 W1BD Free Energy= -157.175193
1\1\GINC-D209\Mixed\W1BD\W1BD\C4H8\RABLEN\10-Nov-2011\0\\#n W1BD\\1-Bu
tene C1\\0,1\C,0,0.0020050744,-0.0018919395,0.0056673332\C,0,0.0044686
73,0.0039991797,1.3323948451\C,0,1.2269740542,0.0043591975,2.200565931

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.855780	0.018119	-0.277809
2	6	0	0.721997	-0.295374	0.335790
3	6	0	-0.537242	0.518083	0.306698
4	6	0	-1.725730	-0.244725	-0.292315
5	1	0	1.952673	0.927249	-0.859948
6	1	0	2.728606	-0.618507	-0.220239
7	1	0	0.672644	-1.220114	0.905822
8	1	0	-0.792296	0.817928	1.328745
9	1	0	-0.363840	1.438819	-0.254762
10	1	0	-2.632581	0.360895	-0.265917
11	1	0	-1.530499	-0.518678	-1.329827
12	1	0	-1.923538	-1.164205	0.261945

Butane

Species name: butane
Full file name: butane_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.129447 E(Thermal)= 0.135308
W1BD (0 K)= -158.358582 W1BD Energy= -158.352721
W1BD Enthalpy= -158.351777 W1BD Free Energy= -158.386025
1\1\GINC-NODE39\Mixed\W1BD\W1BD\C4H10\RABLENP\24-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Butane\\0,1\C,0,-0.1201951797,1.9569583563,0.\C,0,
0.5132952829,0.5668007789,0.\C,0,-0.5132952829,-0.5668007789,0.\C,0,0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.702120	1.830618	0.000000
2	6	0	-0.702120	0.302924	0.000000
3	6	0	0.702120	-0.302924	0.000000
4	6	0	0.702120	-1.830618	0.000000
5	1	0	-1.716893	2.231119	0.000000
6	1	0	-0.190301	2.224543	0.880657

7	1	0	-0.190301	2.224543	-0.880657
8	1	0	-1.250157	-0.062528	-0.873957
9	1	0	-1.250157	-0.062528	0.873957
10	1	0	1.250157	0.062528	0.873957
11	1	0	1.250157	0.062528	-0.873957
12	1	0	1.716893	-2.231119	0.000000
13	1	0	0.190301	-2.224543	-0.880657
14	1	0	0.190301	-2.224543	0.880657

Isobutane

Species name: isobutane
Full file name: isobutane_w1bd.log
Method: W1BD calculation
Point group: C3V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.129048 E(Thermal)= 0.134819
W1BD (0 K)= -158.361278 W1BD Energy= -158.355507
W1BD Enthalpy= -158.354563 W1BD Free Energy= -158.387914
1\1\GINC-NODE74\Mixed\W1BD\W1BD\C4H10\RABLENP\13-Oct-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Isobutane\\0,1\C,0,0.,-0.0000000011,-0.372324648\H
,0,0.,-0.0000000011,-1.4676153793\C,0,0.,1.4581224538,0.0941234628\C,0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.371013
2	1	0	0.000000	0.000000	1.466304
3	6	0	0.000000	1.458122	-0.095435
4	6	0	1.262771	-0.729061	-0.095435
5	6	0	-1.262771	-0.729061	-0.095435
6	1	0	0.000000	1.516433	-1.187050
7	1	0	-0.882124	1.990817	0.264433
8	1	0	0.882124	1.990817	0.264433
9	1	0	1.313269	-0.758216	-1.187050
10	1	0	1.283035	-1.759350	0.264433
11	1	0	2.165160	-0.231466	0.264433
12	1	0	-1.313269	-0.758216	-1.187050
13	1	0	-1.283035	-1.759350	0.264433
14	1	0	-2.165160	-0.231466	0.264433

1,4-Pentadiene

Species name: 14pentadiene
Full file name: 14pentadiene_w1bd.log
Method: W1BD calculation

Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.111459 E(Thermal)= 0.117517
W1BD (0 K)= -195.231526 W1BD Energy= -195.225468
W1BD Enthalpy= -195.224523 W1BD Free Energy= -195.260127
1\1\GINC-NODE39\Mixed\W1BD\W1BD\C5H8\RABLENP\25-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\1,4-Pentadiene\\0,1\C,0,0.,0.,0.6591768322\C,0,0.43
07744064,1.1744635881,-0.1785131777\C,0,-0.1477322785,2.3680593328,-0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.659354
2	6	0	0.000000	1.250972	-0.178336
3	6	0	-0.954142	2.172359	-0.173710
4	6	0	0.000000	-1.250972	-0.178336
5	6	0	0.954142	-2.172359	-0.173710
6	1	0	0.880489	-0.008182	1.308905
7	1	0	-0.880489	0.008182	1.308905
8	1	0	0.855597	1.374016	-0.835749
9	1	0	-1.825564	2.083252	0.464417
10	1	0	-0.898434	3.050270	-0.803359
11	1	0	-0.855597	-1.374016	-0.835749
12	1	0	1.825564	-2.083252	0.464417
13	1	0	0.898434	-3.050270	-0.803359

2-Methylbuta-1,3-diene

Species name: 2m13butadiene
Full file name: 2m13butadiene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.111508 E(Thermal)= 0.117417
W1BD (0 K)= -195.242673 W1BD Energy= -195.236764
W1BD Enthalpy= -195.235820 W1BD Free Energy= -195.271206
1\1\GINC-NODE66\Mixed\W1BD\W1BD\C5H8\RABLENP\12-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\2-Methylbuta-1,3-diene\\0,1\C,0,-1.9793113114,-0.07
35931581,0.\C,0,-0.8043624689,-0.7049068543,0.\C,0,0.5158406501,-0.072

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.371860	-1.943469	0.000000

2	6	0	-0.821658	-0.687785	0.000000
3	6	0	0.000000	0.523818	0.000000
4	6	0	-0.589833	1.724843	0.000000
5	6	0	1.497610	0.382464	0.000000
6	1	0	0.683428	-2.180624	0.000000
7	1	0	-1.055625	-2.780886	0.000000
8	1	0	-1.893854	-0.518978	0.000000
9	1	0	-0.015273	2.641316	0.000000
10	1	0	-1.667827	1.822157	0.000000
11	1	0	1.982185	1.357092	0.000000
12	1	0	1.840706	-0.169651	0.877852
13	1	0	1.840706	-0.169651	-0.877852

2-Pentyne

Species name: 2pentyne
Full file name: 2pentyne_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.111059 E(Thermal)= 0.117928
W1BD (0 K)= -195.223732 W1BD Energy= -195.216863
W1BD Enthalpy= -195.215919 W1BD Free Energy= -195.254519
1\1\GINC-NODE79\Mixed\W1BD\W1BD\C5H8\RABLENP\14-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\2-Pentyne\\0,1\C,0,2.6449101966,-0.2245948362,0.\C,
0,1.2207577813,0.081134729,0.\C,0,0.0472733119,0.3400208863,0.\C,0,-1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.650537	0.141711	0.000000
2	6	0	-1.197906	0.249156	0.000000
3	6	0	0.000000	0.344592	0.000000
4	6	0	1.457284	0.437978	0.000000
5	6	0	2.154784	-0.930138	0.000000
6	1	0	-3.081850	0.619830	0.881616
7	1	0	-3.081850	0.619830	-0.881616
8	1	0	-2.968730	-0.902608	0.000000
9	1	0	1.780059	1.011859	0.873343
10	1	0	1.780059	1.011859	-0.873343
11	1	0	3.238328	-0.805557	0.000000
12	1	0	1.876117	-1.507504	0.881206
13	1	0	1.876117	-1.507504	-0.881206

3-Methyl-1-butyne

Species name: 3m1butyne
Full file name: 3m1butyne_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.110779 E(Thermal)= 0.117122
W1BD (0 K)= -195.218701 W1BD Energy= -195.212358
W1BD Enthalpy= -195.211413 W1BD Free Energy= -195.247609
1\1\GINC-NODE44\Mixed\W1BD\W1BD\C5H8\RABLENP\14-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\3-Methyl-1-butyne\\0,1\C,0,-0.1172897386,-2.2217032
776,0.\C,0,0.1230230455,-1.0459151547,0.\C,0,0.3965047051,0.3916240775

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.141203	-2.222392	0.000000
2	6	0	0.112116	-1.049337	0.000000
3	6	0	0.401501	0.385085	0.000000
4	6	0	-0.141203	1.058862	1.271756
5	6	0	-0.141203	1.058862	-1.271756
6	1	0	1.490775	0.496319	0.000000
7	1	0	-0.360235	-3.260387	0.000000
8	1	0	0.121741	2.117557	1.277633
9	1	0	-1.227603	0.975073	1.316281
10	1	0	0.270570	0.596163	2.167790
11	1	0	0.121741	2.117557	-1.277633
12	1	0	-1.227603	0.975073	-1.316281
13	1	0	0.270570	0.596163	-2.167790

3-Methyl-1-butene CS

Species name: 3m1butene
Full file name: 3m1butene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.133965 E(Thermal)= 0.140602
W1BD (0 K)= -196.445017 W1BD Energy= -196.438381
W1BD Enthalpy= -196.437437 W1BD Free Energy= -196.474537
1\1\GINC-NODE79\Mixed\W1BD\W1BD\C5H10\RABLENP\11-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\3-Methyl-1-butene CS\\0,1\C,0,0.0034233492,0.,0.00
74780008\C,0,0.0031607095,0.,1.3340391106\C,0,1.2241379242,0.,2.211490

Standard orientation:

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

1	6	0	-0.038837	-2.151004	0.000000
2	6	0	0.466539	-0.924480	0.000000
3	6	0	-0.328335	0.351796	0.000000
4	6	0	-0.038837	1.174344	1.264463
5	6	0	-0.038837	1.174344	-1.264463
6	1	0	-1.108923	-2.323347	0.000000
7	1	0	0.595191	-3.027706	0.000000
8	1	0	1.547683	-0.800133	0.000000
9	1	0	-1.389768	0.086565	0.000000
10	1	0	1.017556	1.448506	1.316753
11	1	0	-0.621871	2.097114	1.269645
12	1	0	-0.282859	0.611691	2.165878
13	1	0	1.017556	1.448506	-1.316753
14	1	0	-0.621871	2.097114	-1.269645
15	1	0	-0.282859	0.611691	-2.165878

Pentane

Species name: pentane
Full file name: pentane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.157509 E(Thermal)= 0.164680
W1BD (0 K)= -197.653348 W1BD Energy= -197.646177
W1BD Enthalpy= -197.645233 W1BD Free Energy= -197.683082
1\1\GINC-NODE44\Mixed\W1BD\W1BD\C5H12\RABLENP\23-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Pentane\\0,1\C,0,0.,2.5536654676,0.3233285624\C,0,
0.,1.2807243324,-0.5217615068\C,0,0.,0.,0.3136745768\C,0,0.,-1.2807243

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.553665	0.323450
2	6	0	0.000000	1.280724	-0.521640
3	6	0	0.000000	0.000000	0.313796
4	6	0	0.000000	-1.280724	-0.521640
5	6	0	0.000000	-2.553665	0.323450
6	1	0	0.000000	3.448369	-0.300862
7	1	0	-0.880662	2.599085	0.967629
8	1	0	0.880662	2.599085	0.967629
9	1	0	0.873971	1.280277	-1.180126
10	1	0	-0.873971	1.280277	-1.180126
11	1	0	-0.874480	0.000000	0.973606
12	1	0	0.874480	0.000000	0.973606
13	1	0	0.873971	-1.280277	-1.180126
14	1	0	-0.873971	-1.280277	-1.180126

15	1	0	0.000000	-3.448369	-0.300862
16	1	0	-0.880662	-2.599085	0.967629
17	1	0	0.880662	-2.599085	0.967629

Neopentane

Species name: neopentane
Full file name: neopentane_w1bd.log
Method: W1BD calculation
Point group: TD
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.157008 E(Thermal)= 0.163776
W1BD (0 K)= -197.659693 W1BD Energy= -197.652925
W1BD Enthalpy= -197.651981 W1BD Free Energy= -197.686234
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C5H12\RABLENP\13-Oct-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Neopentane\\0,1\C,0,0.,-0.0000000005,-0.0000000015
\C,0,-0.0000000004,0.,1.5359208886\C,0,-0.0000000003,-1.448080103,-0.5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.886764	0.886764	0.886764
3	6	0	-0.886764	-0.886764	0.886764
4	6	0	0.886764	-0.886764	-0.886764
5	6	0	-0.886764	0.886764	-0.886764
6	1	0	1.529866	1.529866	0.282366
7	1	0	0.282366	1.529866	1.529866
8	1	0	1.529866	0.282366	1.529866
9	1	0	-1.529866	-1.529866	0.282366
10	1	0	-1.529866	-0.282366	1.529866
11	1	0	-0.282366	-1.529866	1.529866
12	1	0	0.282366	-1.529866	-1.529866
13	1	0	1.529866	-0.282366	-1.529866
14	1	0	1.529866	-1.529866	-0.282366
15	1	0	-1.529866	0.282366	-1.529866
16	1	0	-0.282366	1.529866	-1.529866
17	1	0	-1.529866	1.529866	-0.282366

Benzene

Species name: benzene
Full file name: benzene_w1bd.log
Method: W1BD calculation
Point group: D6H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.098920 E(Thermal)= 0.103351
W1BD (0 K)= -232.201357 W1BD Energy= -232.196926
W1BD Enthalpy= -232.195982 W1BD Free Energy= -232.226479
1\1\GINC-NODE74\Mixed\W1BD\W1BD\C6H6\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Benzene\\0,1\C,0,0.,0.,0.\C,0,0.,0.,1.39074086\C,0,
1.2044169148,0.,-0.69537043\C,0,1.2044169148,0.,2.08611129\C,0,2.40883

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.390741	0.000000
2	6	0	1.204417	0.695370	0.000000
3	6	0	-1.204417	0.695370	0.000000
4	6	0	1.204417	-0.695370	0.000000
5	6	0	-1.204417	-0.695370	0.000000
6	6	0	0.000000	-1.390741	0.000000
7	1	0	0.000000	2.472801	0.000000
8	1	0	2.141508	1.236400	0.000000
9	1	0	-2.141508	1.236400	0.000000
10	1	0	2.141508	-1.236400	0.000000
11	1	0	-2.141508	-1.236400	0.000000
12	1	0	0.000000	-2.472801	0.000000

3-Methylenepenta-1,4-diene

Species name: 3methylenepenta14diene
Full file name: 3methylenepenta14diene_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.116780 E(Thermal)= 0.123419
W1BD (0 K)= -233.324518 W1BD Energy= -233.317879
W1BD Enthalpy= -233.316935 W1BD Free Energy= -233.353852
1\1\GINC-NODE62\Mixed\W1BD\W1BD\C6H8\RABLENP\12-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\3-Methylenepenta-1,4-diene\\0,1\C,0,0.,0.,0.6786051
763\C,0,0.,0.,2.0228804232\C,0,0.1669633336,1.2839686865,-0.0220346338

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.679250
2	6	0	0.000000	0.000000	2.023525
3	6	0	0.000000	1.294779	-0.021390
4	6	0	0.000000	-1.294779	-0.021390

5	6	0	-0.400757	1.555243	-1.264974
6	6	0	0.400757	-1.555243	-1.264974
7	1	0	0.031585	0.921574	2.588696
8	1	0	-0.031585	-0.921574	2.588696
9	1	0	0.318699	2.130047	0.594075
10	1	0	-0.318699	-2.130047	0.594075
11	1	0	-0.393755	2.569312	-1.640720
12	1	0	-0.770724	0.791019	-1.932188
13	1	0	0.393755	-2.569312	-1.640720
14	1	0	0.770724	-0.791019	-1.932188

3-Methyl-1,4-pentadiene, Cs conformation

Species name: 3m14pentadiene
Full file name: 3m14pentadiene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.138903 E(Thermal)= 0.146359
W1BD (0 K)= -234.528034 W1BD Energy= -234.520577
W1BD Enthalpy= -234.519633 W1BD Free Energy= -234.559260
1\1\GINC-NODE37\Mixed\W1BD\W1BD\C6H10\RABLENP\21-Apr-2020\0\\#n W1BD f
opt=(calcfc,tight)\\3-Methyl-1,4-pentadiene, Cs conformation\\0,1\C,0,-0.233531
9095,-0.2958563468,0.\C,0,-0.1953772084,-1.8371180094,0.\H,0,-1.277968

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.372323	0.080109	0.000000
2	6	0	1.333730	1.285364	0.000000
3	1	0	0.965226	-0.838182	0.000000
4	6	0	-0.486854	0.090708	1.239061
5	6	0	-0.486854	0.090708	-1.239061
6	6	0	-0.486854	-0.844234	2.179396
7	6	0	-0.486854	-0.844234	-2.179396
8	1	0	0.779170	2.226190	0.000000
9	1	0	1.969219	1.270846	-0.885900
10	1	0	1.969219	1.270846	0.885900
11	1	0	-1.143631	0.950726	1.345798
12	1	0	-1.143631	0.950726	-1.345798
13	1	0	0.149920	-1.718302	2.110583
14	1	0	-1.123613	-0.772536	3.051005
15	1	0	0.149920	-1.718302	-2.110583
16	1	0	-1.123613	-0.772536	-3.051005

4-Methyl-2-pentyne

Species name: 4m2pentyne
Full file name: 4m2pentyne_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.138631 E(Thermal)= 0.146842
W1BD (0 K)= -234.520655 W1BD Energy= -234.512444
W1BD Enthalpy= -234.511499 W1BD Free Energy= -234.553763
1\1\GINC-NODE82\Mixed\W1BD\W1BD\C6H10\RABLENP\14-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight) scf=(conver=10) integral=(grid=ultrafine)\\4-Methyl
-2-pentyne\\0,1\C,0,-0.1669111296,-3.0003689119,0.\C,0,0.0412042869,-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.166879	-3.000345	0.000000
2	6	0	0.041418	-1.558631	0.000000
3	6	0	0.219485	-0.369809	0.000000
4	6	0	0.417029	1.081541	0.000000
5	6	0	-0.166879	1.723167	1.270093
6	6	0	-0.166879	1.723167	-1.270093
7	1	0	-0.726966	-3.318324	-0.881484
8	1	0	-0.726966	-3.318324	0.881484
9	1	0	0.784227	-3.536361	0.000000
10	1	0	1.496490	1.267309	0.000000
11	1	0	0.028684	2.796706	1.276954
12	1	0	-1.246139	1.571417	1.314583
13	1	0	0.272181	1.287457	2.166927
14	1	0	0.028684	2.796706	-1.276954
15	1	0	-1.246139	1.571417	-1.314583
16	1	0	0.272181	1.287457	-2.166927

3,3-Dimethyl-1-butyne

Species name: 33dm1butyne
Full file name: 33dm1butyne_w1bd.log
Method: W1BD calculation
Point group: C3V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.137908 E(Thermal)= 0.145608
W1BD (0 K)= -234.517271 W1BD Energy= -234.509571
W1BD Enthalpy= -234.508627 W1BD Free Energy= -234.546704
1\1\GINC-NODE49\Mixed\W1BD\W1BD\C6H10\RABLENP\15-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\3,3-Dimethyl-1-butyne\\0,1\C,0,0.,0.,2.3696620937\

C,0,0.,0.,1.1694061869\C,0,0.,0.,-0.2993133179\C,0,0.,1.4565726002,-0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.371671
2	6	0	0.000000	0.000000	1.171415
3	6	0	0.000000	0.000000	-0.297305
4	6	0	0.000000	1.456573	-0.805165
5	6	0	-1.261429	-0.728286	-0.805165
6	6	0	1.261429	-0.728286	-0.805165
7	1	0	0.000000	0.000000	3.432558
8	1	0	0.000000	1.471037	-1.896503
9	1	0	0.882459	1.991087	-0.454127
10	1	0	-0.882459	1.991087	-0.454127
11	1	0	-1.273955	-0.735518	-1.896503
12	1	0	-2.165561	-0.231312	-0.454127
13	1	0	-1.283102	-1.759775	-0.454127
14	1	0	1.273955	-0.735518	-1.896503
15	1	0	2.165561	-0.231312	-0.454127
16	1	0	1.283102	-1.759775	-0.454127

3,3-Dimethyl-1-butene CS

Species name: tbuethylene
Full file name: tbuethylene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.161319 E(Thermal)= 0.169172
W1BD (0 K)= -235.743173 W1BD Energy= -235.735321
W1BD Enthalpy= -235.734377 W1BD Free Energy= -235.773938
1\1\GINC-NODE81\Mixed\W1BD\W1BD\C6H12\RABLENP\12-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\3,3-Dimethyl-1-butene CS\\0,1\C,0,0.0022873115,0.,
0.0077215766\C,0,0.0037498824,0.,1.3345692299\C,0,1.1968397678,0.,2.26

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.121847	-2.199644	0.000000
2	6	0	0.566326	-1.065208	0.000000
3	6	0	0.030379	0.349684	0.000000
4	6	0	-1.501533	0.399795	0.000000
5	6	0	0.566326	1.068678	1.254976
6	6	0	0.566326	1.068678	-1.254976
7	1	0	-1.203255	-2.225933	0.000000

8	1	0	0.382983	-3.156591	0.000000
9	1	0	1.652514	-1.124517	0.000000
10	1	0	-1.843076	1.436119	0.000000
11	1	0	-1.917129	-0.087663	-0.883004
12	1	0	-1.917129	-0.087663	0.883004
13	1	0	0.249938	2.113730	1.262538
14	1	0	0.197330	0.594261	2.165220
15	1	0	1.657344	1.049182	1.284815
16	1	0	0.249938	2.113730	-1.262538
17	1	0	0.197330	0.594261	-2.165220
18	1	0	1.657344	1.049182	-1.284815

Hexane

Species name: hexane
Full file name: hexane_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.185411 E(Thermal)= 0.193947
W1BD (0 K)= -236.948301 W1BD Energy= -236.939766
W1BD Enthalpy= -236.938821 W1BD Free Energy= -236.980401
1\1\GINC-NODE33\Mixed\W1BD\W1BD\C6H14\RABLENP\24-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Hexane\\0,1\C,0,0.2159293605,3.2147943205,0.\C,0,-
0.5434595283,1.8889669144,0.\C,0,0.3749069153,0.6661539144,0.\C,0,-0.3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.410425	2.896934	0.000000
2	6	0	-1.410425	1.369031	0.000000
3	6	0	-0.005765	0.764384	0.000000
4	6	0	0.005765	-0.764384	0.000000
5	6	0	1.410425	-1.369031	0.000000
6	6	0	1.410425	-2.896934	0.000000
7	1	0	-2.425265	3.297343	0.000000
8	1	0	-0.898602	3.290916	0.880612
9	1	0	-0.898602	3.290916	-0.880612
10	1	0	-1.958838	1.004531	-0.873918
11	1	0	-1.958838	1.004531	0.873918
12	1	0	0.543223	1.130022	0.874502
13	1	0	0.543223	1.130022	-0.874502
14	1	0	-0.543223	-1.130022	-0.874502
15	1	0	-0.543223	-1.130022	0.874502
16	1	0	1.958838	-1.004531	0.873918
17	1	0	1.958838	-1.004531	-0.873918
18	1	0	2.425265	-3.297343	0.000000
19	1	0	0.898602	-3.290916	-0.880612
20	1	0	0.898602	-3.290916	0.880612

Toluene

Species name: toluene
Full file name: toluene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.125636 E(Thermal)= 0.131938
W1BD (0 K)= -271.500755 W1BD Energy= -271.494453
W1BD Enthalpy= -271.493508 W1BD Free Energy= -271.531770
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C7H8\RABLENP\12-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Toluene\\0,1\C,0,-0.0115281216,-0.9115187372,0.\C,0
,0.0086130352,-2.4182111143,0.\C,0,-0.0089079086,-0.1944537338,-1.1971

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004237	0.910461	0.000000
2	6	0	0.027787	2.416948	0.000000
3	6	0	-0.007272	0.193398	1.197171
4	6	0	-0.007272	0.193398	-1.197171
5	6	0	-0.007272	-1.196396	1.200081
6	6	0	-0.007272	-1.196396	-1.200081
7	6	0	-0.006228	-1.897574	0.000000
8	1	0	1.056304	2.787478	0.000000
9	1	0	-0.464284	2.825854	0.882584
10	1	0	-0.464284	2.825854	-0.882584
11	1	0	-0.012149	0.730213	2.138083
12	1	0	-0.012149	0.730213	-2.138083
13	1	0	-0.011883	-1.731650	2.140663
14	1	0	-0.011883	-1.731650	-2.140663
15	1	0	-0.009081	-2.979353	0.000000

4,4-Dimethyl-2-pentyne

Species name: 44dm2pentyne
Full file name: 44dm2pentyne_w1bd.log
Method: W1BD calculation
Point group: C3V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.165702 E(Thermal)= 0.175298
W1BD (0 K)= -273.819324 W1BD Energy= -273.809727
W1BD Enthalpy= -273.808783 W1BD Free Energy= -273.852868

1\1\GINC-NODE33\Mixed\W1BD\W1BD\C7H12\RABLENP\17-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\4,4-Dimethyl-2-pentyne\\0,1\C,0,0.,-0.0000000001,-
3.2364941734\C,0,0.,-0.0000000001,-1.7796773828\C,0,0.,-0.0000000001,-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	3.236713
2	6	0	0.000000	0.000000	1.779896
3	6	0	0.000000	0.000000	0.577704
4	6	0	0.000000	0.000000	-0.892506
5	6	0	0.000000	1.454980	-1.404954
6	6	0	-1.260049	-0.727490	-1.404954
7	6	0	1.260049	-0.727490	-1.404954
8	1	0	0.881502	-0.508935	3.631404
9	1	0	0.000000	1.017870	3.631404
10	1	0	-0.881502	-0.508935	3.631404
11	1	0	0.000000	1.469642	-2.496606
12	1	0	0.882377	1.990261	-1.054344
13	1	0	-0.882377	1.990261	-1.054344
14	1	0	-1.272747	-0.734821	-2.496606
15	1	0	-2.164805	-0.230969	-1.054344
16	1	0	-1.282428	-1.759292	-1.054344
17	1	0	1.272747	-0.734821	-2.496606
18	1	0	2.164805	-0.230969	-1.054344
19	1	0	1.282428	-1.759292	-1.054344

Heptane

Species name: heptane
Full file name: heptane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.213461 E(Thermal)= 0.223327
W1BD (0 K)= -276.243107 W1BD Energy= -276.233241
W1BD Enthalpy= -276.232297 W1BD Free Energy= -276.277330
1\1\GINC-NODE03\Mixed\W1BD\W1BD\C7H16\RABLENP\28-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Heptane\\0,1\C,0,3.8336546518,0.,0.3553060945\C,0,
2.5610133518,0.,-0.4902292491\C,0,1.2799753048,0.,0.3451058286\C,0,0.,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.833655	-0.352598
2	6	0	0.000000	2.561013	0.492937

3	6	0	0.000000	1.279975	-0.342398
4	6	0	0.000000	0.000000	0.494097
5	6	0	0.000000	-1.279975	-0.342398
6	6	0	0.000000	-2.561013	0.492937
7	6	0	0.000000	-3.833655	-0.352598
8	1	0	0.000000	4.728610	0.271370
9	1	0	0.880660	3.878854	-0.996810
10	1	0	-0.880660	3.878854	-0.996810
11	1	0	-0.873940	2.560803	1.151430
12	1	0	0.873940	2.560803	1.151430
13	1	0	0.874440	1.280911	-1.001998
14	1	0	-0.874440	1.280911	-1.001998
15	1	0	-0.874496	0.000000	1.153449
16	1	0	0.874496	0.000000	1.153449
17	1	0	0.874440	-1.280911	-1.001998
18	1	0	-0.874440	-1.280911	-1.001998
19	1	0	-0.873940	-2.560803	1.151430
20	1	0	0.873940	-2.560803	1.151430
21	1	0	0.000000	-4.728610	0.271370
22	1	0	0.880660	-3.878854	-0.996810
23	1	0	-0.880660	-3.878854	-0.996810

Styrene

Species name: styrene
Full file name: styrene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.131086 E(Thermal)= 0.137978
W1BD (0 K)= -309.587406 W1BD Energy= -309.580514
W1BD Enthalpy= -309.579570 W1BD Free Energy= -309.619502
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C8H8\RABLENP\16-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Styrene\\0,1\C,0,-1.9482632103,-0.5263555937,0.\C,0
,-0.5124401818,-0.2179128279,0.\C,0,-0.0076634847,1.0895538775,0.\C,0,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.279911	1.999131	0.000000
2	6	0	0.000000	0.557474	0.000000
3	6	0	-1.004392	-0.420005	0.000000
4	6	0	-0.685163	-1.768219	0.000000
5	6	0	0.646095	-2.177791	0.000000
6	6	0	1.654193	-1.222843	0.000000
7	6	0	1.331921	0.128214	0.000000
8	6	0	-1.469722	2.598470	0.000000
9	1	0	0.605224	2.627748	0.000000
10	1	0	-2.044528	-0.124076	0.000000

11	1	0	-1.476880	-2.505871	0.000000
12	1	0	0.891528	-3.231296	0.000000
13	1	0	2.692145	-1.528373	0.000000
14	1	0	2.122803	0.868023	0.000000
15	1	0	-2.402551	2.050638	0.000000
16	1	0	-1.545865	3.676629	0.000000

Ethylbenzene

Species name: ethylbenzene
Full file name: ethylbenzene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.154006 E(Thermal)= 0.161433
W1BD (0 K)= -310.795291 W1BD Energy= -310.787864
W1BD Enthalpy= -310.786920 W1BD Free Energy= -310.827516
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C8H10\RABLENP\19-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Ethylbenzene\\0,1\C,0,0.3252315577,-0.4292738335,0
.\C,0,0.5833647477,-1.9168958602,0.\C,0,-0.7060796201,-2.7504886847,0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.231804	0.488974	0.000000
2	6	0	-0.192524	1.998314	0.000000
3	6	0	1.235605	2.562220	0.000000
4	6	0	-0.234062	-0.228268	1.197318
5	6	0	-0.234062	-0.228268	-1.197318
6	6	0	-0.234062	-1.618074	1.200500
7	6	0	-0.234062	-1.618074	-1.200500
8	6	0	-0.232912	-2.318763	0.000000
9	1	0	-0.726441	2.374830	0.875323
10	1	0	-0.726441	2.374830	-0.875323
11	1	0	1.223863	3.653354	0.000000
12	1	0	1.787179	2.229689	-0.880393
13	1	0	1.787179	2.229689	0.880393
14	1	0	-0.241096	0.308798	2.138329
15	1	0	-0.241096	0.308798	-2.138329
16	1	0	-0.239792	-2.153890	2.140774
17	1	0	-0.239792	-2.153890	-2.140774
18	1	0	-0.236254	-3.400572	0.000000

Cyclopropene

Species name: cp2
Full file name: cp2_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.055017 E(Thermal)= 0.058368
W1BD (0 K)= -116.590570 W1BD Energy= -116.587218
W1BD Enthalpy= -116.586274 W1BD Free Energy= -116.613860
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C3H4\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclopropene\\0,1\C,0,0.,0.,0.8632277002\C,0,-0.643
2705374,0.,-0.4982039629\C,0,0.6432705374,0.,-0.4982039629\H,0,0.,0.91

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.861445
2	6	0	0.000000	0.643271	-0.499987
3	6	0	0.000000	-0.643271	-0.499987
4	1	0	0.910750	0.000000	1.456855
5	1	0	-0.910750	0.000000	1.456855
6	1	0	0.000000	1.571112	-1.041269
7	1	0	0.000000	-1.571112	-1.041269

Cyclopropane

Species name: cp
Full file name: cp_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.079908 E(Thermal)= 0.083306
W1BD (0 K)= -117.840049 W1BD Energy= -117.836650
W1BD Enthalpy= -117.835706 W1BD Free Energy= -117.862646
1\1\GINC-NODE47\Mixed\W1BD\W1BD\C3H6\RABLENP\24-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclopropane\\0,1\C,0,-0.0000000019,0.8683404878,0.
\C,0,-0.752004923,-0.4341702497,0.\C,0,0.7520049249,-0.4341702464,0.\H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.868340	0.000000
2	6	0	0.752005	-0.434170	0.000000
3	6	0	-0.752005	-0.434170	0.000000
4	1	0	0.000000	1.455424	0.907496

5	1	0	0.000000	1.455424	-0.907496
6	1	0	1.260434	-0.727712	0.907496
7	1	0	1.260434	-0.727712	-0.907496
8	1	0	-1.260434	-0.727712	0.907496
9	1	0	-1.260434	-0.727712	-0.907496

Tetrahedrane

Species name: tetrahedrane
Full file name: tetrahedrane_w1bd.log
Method: W1BD calculation
Point group: TD
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.058612 E(Thermal)= 0.062458
W1BD (0 K)= -154.617828 W1BD Energy= -154.613982
W1BD Enthalpy= -154.613038 W1BD Free Energy= -154.640543
1\1\GINC-NODE47\Mixed\W1BD\W1BD\C4H4\RABLENP\24-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Tetrahedrane\\0,1\C,0,-0.0000000002,-0.0000000004,0
.902846575\C,0,0.0000000003,-0.8512119135,-0.300948856\C,0,-0.73717114

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521259	0.521259	0.521259
2	6	0	-0.521259	-0.521259	0.521259
3	6	0	-0.521259	0.521259	-0.521259
4	6	0	0.521259	-0.521259	-0.521259
5	1	0	1.137756	1.137756	1.137756
6	1	0	-1.137756	-1.137756	1.137756
7	1	0	-1.137756	1.137756	-1.137756
8	1	0	1.137756	-1.137756	-1.137756

Methylenecyclopropene

Species name: mcp2
Full file name: mcp2_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.059614 E(Thermal)= 0.063705
W1BD (0 K)= -154.675256 W1BD Energy= -154.671165
W1BD Enthalpy= -154.670221 W1BD Free Energy= -154.700212
1\1\GINC-NODE75\Mixed\W1BD\W1BD\C4H4\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Methylenecyclopropene\\0,1\C,0,0.,0.,0.2630879103\C

,0,0.,0.,1.5881846785\C,0,0.,-0.6567545808,-1.0153862142\C,0,0.,0.6567

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.261875
2	6	0	0.000000	0.000000	1.586972
3	6	0	0.000000	0.656755	-1.016599
4	6	0	0.000000	-0.656755	-1.016599
5	1	0	0.000000	0.926299	2.142973
6	1	0	0.000000	-0.926299	2.142973
7	1	0	0.000000	1.567131	-1.589918
8	1	0	0.000000	-1.567131	-1.589918

Bicyclo[1.1.0]but-1(3)-ene

Species name: bcb2
Full file name: bcb2_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.060968 E(Thermal)= 0.064827
W1BD (0 K)= -154.604706 W1BD Energy= -154.600847
W1BD Enthalpy= -154.599903 W1BD Free Energy= -154.629342
1\1\GINC-NODE41\Mixed\W1BD\W1BD\C4H4\RABLENP\19-Feb-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[1.1.0]but-1(3)-ene\\0,1\C,0,-0.6818735005,0
.,-0.1635821538\C,0,0.6818735005,0.,-0.1635821538\C,0,0.,1.2286519764,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.681874	0.000000	-0.306671
2	6	0	0.681874	0.000000	-0.306671
3	6	0	0.000000	1.228652	0.185693
4	6	0	0.000000	-1.228652	0.185693
5	1	0	0.000000	1.523892	1.237234
6	1	0	0.000000	2.053834	-0.511365
7	1	0	0.000000	-1.523892	1.237234
8	1	0	0.000000	-2.053834	-0.511365

Cyclobutene

Species name: cb2

Full file name: cb2_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature=   298.150000 Pressure=   1.000000
E(ZPE)=   0.084905 E(Thermal)=   0.088765
W1BD (0 K)=   -155.923480 W1BD Energy=   -155.919619
W1BD Enthalpy=   -155.918675 W1BD Free Energy=   -155.948446
1\1\GINC-NODE74\Mixed\W1BD\W1BD\C4H6\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclobutene\\0,1\C,0,0.,0.6672007106,-0.8037857085\
C,0,0.,-0.6672007106,-0.8037857085\C,0,0.,-0.7848016461,0.7070345698\C

                        Standard orientation:

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

     1   6   0   0.000000   0.667201   0.812426
     2   6   0   0.000000   -0.667201   0.812426
     3   6   0   0.000000   -0.784802   -0.698394
     4   6   0   0.000000   0.784802   -0.698394
     5   1   0   0.000000   1.411028   1.598029
     6   1   0   0.000000   -1.411028   1.598029
     7   1   0   -0.886368   -1.242733   -1.141109
     8   1   0   0.886368   -1.242733   -1.141109
     9   1   0   -0.886368   1.242733   -1.141109
    10   1   0   0.886368   1.242733   -1.141109

Bicyclobutane

Species name: bcb
Full file name: bcb_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature=   298.150000 Pressure=   1.000000
E(ZPE)=   0.084823 E(Thermal)=   0.088610
W1BD (0 K)=   -155.899216 W1BD Energy=   -155.895429
W1BD Enthalpy=   -155.894485 W1BD Free Energy=   -155.923989
1\1\GINC-NODE33\Mixed\W1BD\W1BD\C4H6\RABLENP\23-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclobutane\\0,1\C,0,0.,0.7422612159,0.3198259427
\C,0,0.,-0.7422612159,0.3198259427\C,0,-1.1342873181,0.,-0.3116696733\

                        Standard orientation:

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

     1   6   0   -0.742261   0.000000   -0.318322
     2   6   0   0.742261   0.000000   -0.318322

3	6	0	0.000000	1.134287	0.313174
4	6	0	0.000000	-1.134287	0.313174
5	1	0	-1.427272	0.000000	-1.147515
6	1	0	1.427272	0.000000	-1.147515
7	1	0	0.000000	1.232043	1.397522
8	1	0	0.000000	2.078606	-0.219117
9	1	0	0.000000	-1.232043	1.397522
10	1	0	0.000000	-2.078606	-0.219117

Methylenecyclopropane

Species name: mcp
Full file name: mcp_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.083604 E(Thermal)= 0.087916
W1BD (0 K)= -155.911392 W1BD Energy= -155.907081
W1BD Enthalpy= -155.906137 W1BD Free Energy= -155.936797
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C4H6\RABLENP\12-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Methylenecyclopropane\\0,1\C,0,0.,0.,-0.3082543941\
C,0,0.,0.,-1.6238288696\C,0,0.,-0.7688314856,0.936322578\C,0,0.,0.7688

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.315795
2	6	0	0.000000	0.000000	1.631370
3	6	0	0.000000	0.768831	-0.928782
4	6	0	0.000000	-0.768831	-0.928782
5	1	0	0.000000	0.924618	2.195194
6	1	0	0.000000	-0.924618	2.195194
7	1	0	0.909967	1.272557	-1.231999
8	1	0	-0.909967	1.272557	-1.231999
9	1	0	-0.909967	-1.272557	-1.231999
10	1	0	0.909967	-1.272557	-1.231999

Cyclobutane

Species name: cb
Full file name: cb_w1bd.log
Method: W1BD calculation
Point group: D2D
NImag: 0

Temperature= 298.150000 Pressure= 1.000000

E(ZPE)= 0.108760 E(Thermal)= 0.112946
W1BD (0 K)= -157.136752 W1BD Energy= -157.132566
W1BD Enthalpy= -157.131621 W1BD Free Energy= -157.161601
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C4H8\RABLENP\24-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclobutane\\0,1\C,0,0.,1.0825762932,0.1231942903\C
,0,-1.0825762932,0.,-0.1231942903\C,0,0.,-1.0825762932,0.1231942903\C,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.082576	0.123194
2	6	0	-1.082576	0.000000	-0.123194
3	6	0	0.000000	-1.082576	0.123194
4	6	0	1.082576	0.000000	-0.123194
5	1	0	0.000000	1.957028	-0.526364
6	1	0	0.000000	1.422059	1.159329
7	1	0	-1.422059	0.000000	-1.159329
8	1	0	-1.957028	0.000000	0.526364
9	1	0	0.000000	-1.957028	-0.526364
10	1	0	0.000000	-1.422059	1.159329
11	1	0	1.422059	0.000000	-1.159329
12	1	0	1.957028	0.000000	0.526364

[1.1.1]Propellane

Species name: 111propellane
Full file name: 111propellane_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.091593 E(Thermal)= 0.095628
W1BD (0 K)= -193.969823 W1BD Energy= -193.965788
W1BD Enthalpy= -193.964844 W1BD Free Energy= -193.994451
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C5H6\RABLENP\23-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\[1.1.1]Propellane\\0,1\C,0,0.,0.0000000013,0.783913
1323\C,0,0.,0.0000000013,-0.7839131323\C,0,-0.0000000007,1.2967633599,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.783913
2	6	0	0.000000	0.000000	-0.783913
3	6	0	0.000000	1.296763	0.000000
4	6	0	1.123030	-0.648382	0.000000
5	6	0	-1.123030	-0.648382	0.000000
6	1	0	-0.913095	1.877341	0.000000

7	1	0	0.913095	1.877341	0.000000
8	1	0	2.082372	-0.147907	0.000000
9	1	0	1.169277	-1.729434	0.000000
10	1	0	-1.169277	-1.729434	0.000000
11	1	0	-2.082372	-0.147907	0.000000

Cyclopentadiene

Species name: cpd
Full file name: cpd_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.090930 E(Thermal)= 0.095119
W1BD (0 K)= -194.057907 W1BD Energy= -194.053718
W1BD Enthalpy= -194.052773 W1BD Free Energy= -194.083855
1\1\GINC-NODE56\Mixed\W1BD\W1BD\C5H6\RABLENP\03-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclopentadiene\\0,1\C,0,0.,0.,1.2144597266\C,0,1.1
764870593,0.,0.2816706257\C,0,-1.1764870593,0.,0.2816706257\C,0,0.7326

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.213156
2	6	0	0.000000	1.176487	0.280367
3	6	0	0.000000	-1.176487	0.280367
4	6	0	0.000000	0.732629	-0.987414
5	6	0	0.000000	-0.732629	-0.987414
6	1	0	0.874432	0.000000	1.874180
7	1	0	-0.874432	0.000000	1.874180
8	1	0	0.000000	2.205193	0.606041
9	1	0	0.000000	-2.205193	0.606041
10	1	0	0.000000	1.344890	-1.877401
11	1	0	0.000000	-1.344890	-1.877401

Bicyclo[2.1.0]pent-1-ene

Species name: bcp6
Full file name: bcp6_w1bd.log
Method: W1BD calculation
Point group: C1
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.088195 E(Thermal)= 0.092992
W1BD (0 K)= -193.919547 W1BD Energy= -193.914750

W1BD Enthalpy=   -193.913806 W1BD Free Energy=   -193.946611
1\1\GINC-NODE06\Mixed\W1BD\W1BD\C5H6\RABLENP\20-Feb-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.1.0]pent-1-ene\\0,1\C,0,1.0175916608,-1.1
846716443,-0.0383467983\C,0,0.0491815433,-0.3731431193,0.7029517847\C,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.443607	0.095661	0.310206
2	6	0	-0.345943	0.701550	-0.447390
3	6	0	-0.330464	-0.813721	-0.210918
4	6	0	1.144568	-0.605015	0.215049
5	6	0	0.946125	0.862762	-0.075331
6	1	0	-2.381854	-0.093113	-0.196796
7	1	0	-1.557062	0.368580	1.355455
8	1	0	-0.605884	-1.507706	-0.994050
9	1	0	1.847763	-1.173438	-0.396362
10	1	0	1.373978	-0.791751	1.270535
11	1	0	1.498990	1.750004	0.211523

Bicyclo[2.1.0]pent-1(4)-ene

Species name: bcp4
Full file name: bcp4_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.088941 E(Thermal)= 0.093758
W1BD (0 K)= -193.908031 W1BD Energy= -193.903213
W1BD Enthalpy= -193.902269 W1BD Free Energy= -193.935142
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C5H6\RABLENP\19-Feb-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.1.0]pent-1(4)-ene\\0,1\C,0,0.250816329,1.
5634153635,0.\C,0,-0.4084688662,0.3978980474,-0.6747874086\C,0,-0.4084

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762616	1.388024	0.000000
2	6	0	0.251102	0.513117	0.674787
3	6	0	0.251102	0.513117	-0.674787
4	6	0	0.251102	-1.029045	-0.771972
5	6	0	0.251102	-1.029045	0.771972
6	1	0	-0.549341	2.447155	0.000000
7	1	0	-1.826823	1.148646	0.000000
8	1	0	1.117645	-1.445838	-1.279196
9	1	0	-0.654942	-1.420570	-1.234737

```
    10          1           0        1.117645   -1.445838    1.279196
    11          1           0       -0.654942   -1.420570    1.234737
---------------------------------------------------------------------



[2.1.0]Bicyclopent-2-ene

Species name:    bcp3
Full file name:  bcp3_w1bd.log
Method:          W1BD calculation
Point group:     CS
NImag:           0

Temperature=                298.150000 Pressure=                        1.000000
E(ZPE)=                       0.090159 E(Thermal)=                      0.094328
W1BD (0 K)=                -193.983355 W1BD  Energy=                 -193.979187
W1BD  Enthalpy=            -193.978243 W1BD  Free Energy=            -194.009824
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C5H6\RABLENP\27-Nov-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\[2.1.0]Bicyclopent-2-ene\\0,1\C,0,0.5334075083,-1.2
631729374,0.\C,0,-0.4031164937,-0.3463496258,0.7598969814\C,0,-0.40311

                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------

     1          6           0        0.922418   -1.012427    0.000000
     2          6           0       -0.266204   -0.460320    0.759897
     3          6           0       -0.266204   -0.460320   -0.759897
     4          6           0       -0.266204    1.055417   -0.668864
     5          6           0       -0.266204    1.055417    0.668864
     6          1           0        1.025753   -2.092654    0.000000
     7          1           0        1.855921   -0.463052    0.000000
     8          1           0       -0.878958   -1.079716    1.396810
     9          1           0       -0.878958   -1.079716   -1.396810
    10          1           0       -0.134691    1.824266   -1.417599
    11          1           0       -0.134691    1.824266    1.417599
---------------------------------------------------------------------



Bicyclo[2.1.0]pent-4-ene

Species name:    bcp5
Full file name:  bcp5_w1bd.log
Method:          W1BD calculation
Point group:     C1
NImag:           0

Temperature=                298.150000 Pressure=                        1.000000
E(ZPE)=                       0.088585 E(Thermal)=                      0.093231
W1BD (0 K)=                -193.916737 W1BD  Energy=                 -193.912091
W1BD  Enthalpy=            -193.911147 W1BD  Free Energy=            -193.943644
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C5H6\RABLENP\19-Feb-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.1.0]pent-4-ene\\0,1\C,0,1.0076369148,-1.0
```

058259792,-0.0200895974\C,0,0.104840673,-0.3681334109,0.6720343123\C,0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.461445	-0.223862	0.267671
2	6	0	0.422133	-0.708290	-0.353527
3	6	0	0.505585	0.781773	-0.354083
4	6	0	-0.888132	0.772626	0.327576
5	6	0	-1.044291	-0.782809	-0.053938
6	1	0	2.066542	-0.400824	1.145778
7	1	0	0.747335	1.401136	-1.207431
8	1	0	-1.643029	1.419712	-0.118761
9	1	0	-0.873878	0.918459	1.410218
10	1	0	-1.670219	-0.880853	-0.939275
11	1	0	-1.367190	-1.494259	0.707275

Cyclopentene

Species name: cyclopentene
Full file name: cyclopentene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.114633 E(Thermal)= 0.119346
W1BD (0 K)= -195.257891 W1BD Energy= -195.253177
W1BD Enthalpy= -195.252233 W1BD Free Energy= -195.285335
1\1\GINC-NODE65\Mixed\W1BD\W1BD\C5H8\RABLENP\19-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cyclopentene\\0,1\C,0,0.1238213431,1.2280385584,0.\
C,0,-0.0938597876,0.31715626,-1.2340871821\C,0,-0.0938597876,0.3171562

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.246257	-1.208068	0.000000
2	6	0	-0.063499	-0.324245	1.234087
3	6	0	-0.063499	-0.324245	-1.234087
4	6	0	-0.063499	1.072131	0.664249
5	6	0	-0.063499	1.072131	-0.664249
6	1	0	-0.316416	-2.140617	0.000000
7	1	0	1.304874	-1.470318	0.000000
8	1	0	-1.040461	-0.559821	1.670591
9	1	0	0.668081	-0.456022	2.034150
10	1	0	-1.040461	-0.559821	-1.670591
11	1	0	0.668081	-0.456022	-2.034150
12	1	0	-0.098626	1.958199	1.284094

```
    13          1           0       -0.098626    1.958199   -1.284094
---------------------------------------------------------------------
```

[2.1.0]Bicyclopentane

```
Species name:    bcp2
Full file name:  bcp2_w1bd.log
Method:          W1BD calculation
Point group:     CS
NImag:           0

Temperature=                298.150000 Pressure=                        1.000000
E(ZPE)=                       0.114202 E(Thermal)=                      0.118660
W1BD (0 K)=                -195.211577 W1BD  Energy=                 -195.207119
W1BD  Enthalpy=            -195.206175 W1BD  Free Energy=            -195.238460
1\1\GINC-NODE39\Mixed\W1BD\W1BD\C5H8\RABLENP\25-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\[2.1.0]Bicyclopentane\\0,1\C,0,0.4889965377,-1.3199
969328,0.\C,0,-0.4238789541,-0.4094479374,0.7647825336\C,0,-0.42387895

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------

     1          6           0        0.938884   -1.048799    0.000000
     2          6           0       -0.244380   -0.536622    0.764783
     3          6           0       -0.244380   -0.536622   -0.764783
     4          6           0       -0.244380    0.994014   -0.781470
     5          6           0       -0.244380    0.994014    0.781470
     6          1           0        1.062447   -2.123577    0.000000
     7          1           0        1.871234   -0.492990    0.000000
     8          1           0       -0.797369   -1.171745    1.441969
     9          1           0       -0.797369   -1.171745   -1.441969
    10          1           0       -1.160656    1.417625   -1.188403
    11          1           0        0.607093    1.464451   -1.277055
    12          1           0       -1.160656    1.417625    1.188403
    13          1           0        0.607093    1.464451    1.277055
---------------------------------------------------------------------
```

Spiropentane

```
Species name:    spiropentane
Full file name:  spiropentane_w1bd.log
Method:          W1BD calculation
Point group:     D2D
NImag:           0

Temperature=                298.150000 Pressure=                        1.000000
E(ZPE)=                       0.112945 E(Thermal)=                      0.117913
W1BD (0 K)=                -195.200847 W1BD  Energy=                 -195.195879
W1BD  Enthalpy=            -195.194935 W1BD  Free Energy=            -195.226919
1\1\GINC-NODE39\Mixed\W1BD\W1BD\C5H8\RABLENP\25-Sep-2018\0\\#n W1BD fo
```

pt=(calcfc,tight)\\Spiropentane\\0,1\C,0,0.,0.,0.\C,0,0.,0.7633121256,
-1.2665379311\C,0,0.,-0.7633121256,-1.2665379311\C,0,-0.7633121256,0.,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.763312	1.266538
3	6	0	0.000000	-0.763312	1.266538
4	6	0	0.763312	0.000000	-1.266538
5	6	0	-0.763312	0.000000	-1.266538
6	1	0	0.910481	1.264155	1.569367
7	1	0	-0.910481	1.264155	1.569367
8	1	0	-0.910481	-1.264155	1.569367
9	1	0	0.910481	-1.264155	1.569367
10	1	0	1.264155	-0.910481	-1.569367
11	1	0	1.264155	0.910481	-1.569367
12	1	0	-1.264155	0.910481	-1.569367
13	1	0	-1.264155	-0.910481	-1.569367

[1.1.1]Bicyclopentane

Species name: bcp
Full file name: bcp_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.114881 E(Thermal)= 0.118902
W1BD (0 K)= -195.193464 W1BD Energy= -195.189443
W1BD Enthalpy= -195.188499 W1BD Free Energy= -195.218242
1\1\GINC-NODE06\Mixed\W1BD\W1BD\C5H8\RABLENP\25-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\[1.1.1]Bicyclopentane\\0,1\C,0,0.,0.0000000011,0.93
81171121\C,0,0.,0.0000000011,-0.9381171121\C,0,-0.0000000007,1.2392092

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.938117
2	6	0	0.000000	0.000000	-0.938117
3	6	0	0.000000	1.239209	0.000000
4	6	0	1.073187	-0.619605	0.000000
5	6	0	-1.073187	-0.619605	0.000000
6	1	0	0.000000	0.000000	2.026612
7	1	0	0.000000	0.000000	-2.026612
8	1	0	-0.901495	1.852213	0.000000
9	1	0	0.901495	1.852213	0.000000

10	1	0	2.054811	-0.145389	0.000000
11	1	0	1.153316	-1.706824	0.000000
12	1	0	-1.153316	-1.706824	0.000000
13	1	0	-2.054811	-0.145389	0.000000

Methylenecyclobutane

Species name: mcb
Full file name: mcb_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.112691 E(Thermal)= 0.117852
W1BD (0 K)= -195.224735 W1BD Energy= -195.219574
W1BD Enthalpy= -195.218630 W1BD Free Energy= -195.252703
1\1\GINC-NODE75\Mixed\W1BD\W1BD\C5H8\RABLENP\13-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Methylenecyclobutane\\0,1\C,0,-0.0721361554,0.61744
77034,0.\C,0,0.0862891263,1.9302167933,0.\C,0,-0.1122364757,-0.4386362

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101363	0.613854	0.000000
2	6	0	-0.617333	1.831326	0.000000
3	6	0	0.229791	-0.389768	1.091838
4	6	0	0.229791	-0.389768	-1.091838
5	6	0	0.229791	-1.500425	0.000000
6	1	0	-0.839604	2.351497	0.923496
7	1	0	-0.839604	2.351497	-0.923496
8	1	0	-0.484702	-0.486316	1.909109
9	1	0	1.221778	-0.228609	1.519679
10	1	0	-0.484702	-0.486316	-1.909109
11	1	0	1.221778	-0.228609	-1.519679
12	1	0	-0.693156	-2.077689	0.000000
13	1	0	1.074138	-2.186767	0.000000

Cyclopentane

Species name: cyclopentane
Full file name: cyclopentane_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.138192 E(Thermal)= 0.143416

W1BD (0 K)= -196.462286 W1BD Energy= -196.457062
W1BD Enthalpy= -196.456118 W1BD Free Energy= -196.490439
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C5H10\RABLENP\25-Nov-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Cyclopentane\\0,1\C,0,0.,1.3037017336,0.\C,0,-1.23
25313263,0.3703150757,-0.136676873\C,0,1.2325313263,0.3703150757,0.136

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.304790
2	6	0	0.000000	1.240086	0.371404
3	6	0	0.000000	-1.240086	0.371404
4	6	0	-0.323609	0.694648	-1.028868
5	6	0	0.323609	-0.694648	-1.028868
6	1	0	0.873564	0.005811	1.956864
7	1	0	-0.873564	-0.005811	1.956864
8	1	0	-0.702787	2.007434	0.695948
9	1	0	0.989726	1.701185	0.362552
10	1	0	-1.405517	0.595648	-1.155155
11	1	0	0.038161	1.340285	-1.829793
12	1	0	1.405517	-0.595648	-1.155155
13	1	0	-0.038161	-1.340285	-1.829793
14	1	0	0.702787	-2.007434	0.695948
15	1	0	-0.989726	-1.701185	0.362552

Prismane

Species name: prismane
Full file name: prismane_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.095379 E(Thermal)= 0.099526
W1BD (0 K)= -232.020476 W1BD Energy= -232.016329
W1BD Enthalpy= -232.015385 W1BD Free Energy= -232.045676
1\1\GINC-NODE37\Mixed\W1BD\W1BD\C6H6\RABLENP\04-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Prismane\\0,1\C,0,0.,0.8768035487,0.7781266271\C,0,
0.,0.8768035487,-0.7781266271\C,0,-0.7593341473,-0.4384017743,0.778126

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.876804	0.778127
2	6	0	0.000000	0.876804	-0.778127
3	6	0	-0.759334	-0.438402	0.778127
4	6	0	-0.759334	-0.438402	-0.778127

5	6	0	0.759334	-0.438402	0.778127
6	6	0	0.759334	-0.438402	-0.778127
7	1	0	0.000000	1.669593	1.510201
8	1	0	0.000000	1.669593	-1.510201
9	1	0	-1.445910	-0.834796	1.510201
10	1	0	-1.445910	-0.834796	-1.510201
11	1	0	1.445910	-0.834796	1.510201
12	1	0	1.445910	-0.834796	-1.510201

Benzvalene

Species name: benzvalene
Full file name: benzvalene_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.095880 E(Thermal)= 0.100241
W1BD (0 K)= -232.085398 W1BD Energy= -232.081036
W1BD Enthalpy= -232.080092 W1BD Free Energy= -232.111876
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C6H6\RABLENP\29-Jan-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Benzvalene\\0,1\C,0,0.,1.0735697663,-0.0465053262\C
,0,0.,-1.0735697663,-0.0465053262\C,0,-0.7206555897,0.,-0.8555599028\C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.073570	-0.201207
2	6	0	0.000000	-1.073570	-0.201207
3	6	0	-0.720656	0.000000	-1.010261
4	6	0	0.720656	0.000000	-1.010261
5	6	0	0.000000	0.666504	1.249362
6	6	0	0.000000	-0.666504	1.249362
7	1	0	0.000000	2.100947	-0.535659
8	1	0	0.000000	-2.100947	-0.535659
9	1	0	-1.475984	0.000000	-1.780215
10	1	0	1.475984	0.000000	-1.780215
11	1	0	0.000000	1.343152	2.088513
12	1	0	0.000000	-1.343152	2.088513

[2.1.1]Propellane

Species name: 211propellane
Full file name: 211propellane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.119715 E(Thermal)= 0.124675
W1BD (0 K)= -233.264131 W1BD Energy= -233.259171
W1BD Enthalpy= -233.258227 W1BD Free Energy= -233.291210
1\1\GINC-NODE49\Mixed\W1BD\W1BD\C6H8\RABLENP\23-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\[2.1.1]Propellane\\0,1\C,0,0.,1.1226546627,-0.94346
06067\C,0,-0.8192615931,0.,-0.3687632873\C,0,0.8192615931,0.,-0.368763

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.122655	-0.944460
2	6	0	-0.819262	0.000000	-0.369762
3	6	0	0.819262	0.000000	-0.369762
4	6	0	0.000000	-1.122655	-0.944460
5	6	0	-0.769683	0.000000	1.184382
6	6	0	0.769683	0.000000	1.184382
7	1	0	0.000000	1.206449	-2.024897
8	1	0	0.000000	2.075449	-0.429042
9	1	0	0.000000	-2.075449	-0.429042
10	1	0	0.000000	-1.206449	-2.024897
11	1	0	-1.239350	-0.881063	1.616489
12	1	0	-1.239350	0.881063	1.616489
13	1	0	1.239350	-0.881063	1.616489
14	1	0	1.239350	0.881063	1.616489

[2.1.1]Bicyclohexene

Species name: bchx4
Full file name: bchx4_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.120451 E(Thermal)= 0.124948
W1BD (0 K)= -233.306523 W1BD Energy= -233.302026
W1BD Enthalpy= -233.301082 W1BD Free Energy= -233.333226
1\1\GINC-NODE65\Mixed\W1BD\W1BD\C6H8\RABLENP\19-Oct-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\[2.1.1]Bicyclohexene\\0,1\C,0,1.0633485797,0.,-0.81
32020105\C,0,0.,1.0207224077,-0.283196103\C,0,0.,-1.0207224077,-0.2831

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.063349	0.000000	-0.808626
2	6	0	0.000000	1.020722	-0.278620

3	6	0	0.000000	-1.020722	-0.278620
4	6	0	-1.063349	0.000000	-0.808626
5	6	0	0.000000	0.666364	1.212984
6	6	0	0.000000	-0.666364	1.212984
7	1	0	1.158008	0.000000	-1.895454
8	1	0	2.041181	0.000000	-0.329436
9	1	0	0.000000	2.067980	-0.568050
10	1	0	0.000000	-2.067980	-0.568050
11	1	0	-2.041181	0.000000	-0.329436
12	1	0	-1.158008	0.000000	-1.895454
13	1	0	0.000000	1.360172	2.038510
14	1	0	0.000000	-1.360172	2.038510

Bicyclo[2.2.0]hex-1-ene

Species name: bchx5
Full file name: bchx5_w1bd.log
Method: W1BD calculation
Point group: C1
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.118575 E(Thermal)= 0.123717
W1BD (0 K)= -233.262741 W1BD Energy= -233.257599
W1BD Enthalpy= -233.256655 W1BD Free Energy= -233.290779
1\1\GINC-NODE41\Mixed\W1BD\W1BD\C6H8\RABLENP\20-Feb-2020\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.2.0]hex-1-ene\\0,1\C,0,-0.7711756885,-0.0
06765156,0.4943560877\C,0,0.6820590907,0.0182185389,0.1227444429\C,0,0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.163384	-0.783489	-0.456835
2	6	0	-0.049471	0.700728	-0.407794
3	6	0	1.144672	0.989779	0.136151
4	6	0	1.582584	-0.482013	0.127795
5	6	0	-1.511085	0.656496	-0.046618
6	6	0	-1.148401	-0.815307	0.418586
7	1	0	0.094802	-1.352037	-1.382425
8	1	0	1.525585	1.847872	0.674468
9	1	0	1.731824	-0.877278	1.135346
10	1	0	2.431358	-0.778682	-0.492560
11	1	0	-1.881056	1.356307	0.700608
12	1	0	-2.183126	0.643138	-0.905466
13	1	0	-0.937401	-0.850356	1.486006
14	1	0	-1.872084	-1.586126	0.156313

Bicyclo[2.2.0]hex-1(4)-ene

Species name: bchx6
Full file name: bchx6_w1bd.log
Method: W1BD calculation
Point group: D2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.118178 E(Thermal)= 0.123805
W1BD (0 K)= -233.250773 W1BD Energy= -233.245146
W1BD Enthalpy= -233.244202 W1BD Free Energy= -233.278453
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C6H8\RABLENP\04-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.2.0]hex-1(4)-ene\\0,1\C,0,0.6566000132,0.
,0.\C,0,-0.6566000132,0.,0.\C,0,0.8016165361,1.5222528347,0.\C,0,-0.80

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.656600	0.000000
2	6	0	0.000000	-0.656600	0.000000
3	6	0	-1.522253	0.801617	0.000000
4	6	0	-1.522253	-0.801617	0.000000
5	6	0	1.522253	0.801617	0.000000
6	6	0	1.522253	-0.801617	0.000000
7	1	0	-1.971592	1.251551	0.886849
8	1	0	-1.971592	1.251551	-0.886849
9	1	0	-1.971592	-1.251551	0.886849
10	1	0	-1.971592	-1.251551	-0.886849
11	1	0	1.971592	1.251551	0.886849
12	1	0	1.971592	1.251551	-0.886849
13	1	0	1.971592	-1.251551	0.886849
14	1	0	1.971592	-1.251551	-0.886849

Bicyclo[2.2.0]hex-2-ene (cis)

Species name: bchx7
Full file name: bchx7_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.119240 E(Thermal)= 0.124304
W1BD (0 K)= -233.296537 W1BD Energy= -233.291472
W1BD Enthalpy= -233.290528 W1BD Free Energy= -233.324590
1\1\GINC-NODE49\Mixed\W1BD\W1BD\C6H8\RABLENP\04-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[2.2.0]hex-2-ene (cis)\\0,1\C,0,-0.563807178
6,0.0800316367,-0.7882425255\C,0,-0.5638071786,0.0800316367,0.78824252

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.562723	0.089185	0.788243
2	6	0	0.562723	0.089185	-0.788243
3	6	0	-0.262365	1.347942	0.668909
4	6	0	-0.262365	1.347942	-0.668909
5	6	0	-0.262365	-1.238506	0.776051
6	6	0	-0.262365	-1.238506	-0.776051
7	1	0	1.475502	0.107717	1.379714
8	1	0	1.475502	0.107717	-1.379714
9	1	0	-0.755587	1.963826	1.410790
10	1	0	-0.755587	1.963826	-1.410790
11	1	0	-1.234395	-1.183697	1.263666
12	1	0	0.286528	-2.079572	1.197074
13	1	0	-1.234395	-1.183697	-1.263666
14	1	0	0.286528	-2.079572	-1.197074

Cyclohexene

Species name: cyclohexene
Full file name: cyclohexene_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.143699 E(Thermal)= 0.149267
W1BD (0 K)= -234.558937 W1BD Energy= -234.553369
W1BD Enthalpy= -234.552425 W1BD Free Energy= -234.586941
1\1\GINC-NODE37\Mixed\W1BD\W1BD\C6H10\RABLENP\26-Nov-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Cyclohexene\\0,1\C,0,0.6650295373,0.0018220655,0.9
997606794\C,0,-0.6650295373,-0.0018220655,0.9997606794\C,0,1.497472579

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005618	0.665008	1.302159
2	6	0	-0.005618	-0.665008	1.302159
3	6	0	-0.005618	1.497529	0.048640
4	6	0	0.005618	-1.497529	0.048640
5	6	0	-0.367973	0.670887	-1.189995
6	6	0	0.367973	-0.670887	-1.189995
7	1	0	0.020401	1.196988	2.247307
8	1	0	-0.020401	-1.196988	2.247307
9	1	0	-0.708286	2.327252	0.166667
10	1	0	0.708286	-2.327252	0.166667
11	1	0	0.977133	1.965675	-0.085400
12	1	0	-0.977133	-1.965675	-0.085400
13	1	0	-1.446545	0.486804	-1.195457

14	1	0	1.446545	-0.486804	-1.195457
15	1	0	-0.141929	1.233405	-2.097940
16	1	0	0.141929	-1.233405	-2.097940

Methylenecyclopentane

Species name: methylenecyclopentane
Full file name: methylenecyclopentane_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.142405 E(Thermal)= 0.148332
W1BD (0 K)= -234.553169 W1BD Energy= -234.547242
W1BD Enthalpy= -234.546298 W1BD Free Energy= -234.581937
1\1\GINC-NODE06\Mixed\W1BD\W1BD\C6H10\RABLENP\21-Feb-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Methylenecyclopentane\\0,1\C,0,0.,0.,-0.8779715772
\C,0,0.,0.,-2.2049611004\C,0,0.1222271953,1.2269875964,0.0111198558\C,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.878211
2	6	0	0.000000	0.000000	2.205200
3	6	0	0.000000	1.233060	-0.010881
4	6	0	0.000000	-1.233060	-0.010881
5	6	0	0.312335	0.701743	-1.419927
6	6	0	-0.312335	-0.701743	-1.419927
7	1	0	0.018921	0.921346	2.773848
8	1	0	-0.018921	-0.921346	2.773848
9	1	0	0.700109	1.995037	0.331966
10	1	0	-0.995428	1.687802	0.000185
11	1	0	-0.700109	-1.995037	0.331966
12	1	0	0.995428	-1.687802	0.000185
13	1	0	1.393715	0.623459	-1.558689
14	1	0	-0.072060	1.343112	-2.212699
15	1	0	-1.393715	-0.623459	-1.558689
16	1	0	0.072060	-1.343112	-2.212699

[2.1.1]Bicyclohexane

Species name: bchx
Full file name: bchx_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.144433 E(Thermal)= 0.149228
W1BD (0 K)= -234.534473 W1BD Energy= -234.529679
W1BD Enthalpy= -234.528734 W1BD Free Energy= -234.561526
1\1\GINC-NODE06\Mixed\W1BD\W1BD\C6H10\RABLENP\26-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\[2.1.1]Bicyclohexane\\0,1\C,0,0.,1.0591494712,-0.8
926402076\C,0,-1.0251166612,0.,-0.4003527589\C,0,1.0251166612,0.,-0.40

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.059149	0.000000	-0.850686
2	6	0	0.000000	1.025117	-0.358399
3	6	0	0.000000	-1.025117	-0.358399
4	6	0	-1.059149	0.000000	-0.850686
5	6	0	0.000000	0.781797	1.160753
6	6	0	0.000000	-0.781797	1.160753
7	1	0	1.170116	0.000000	-1.933859
8	1	0	2.039031	0.000000	-0.370243
9	1	0	0.000000	2.058258	-0.698516
10	1	0	0.000000	-2.058258	-0.698516
11	1	0	-2.039031	0.000000	-0.370243
12	1	0	-1.170116	0.000000	-1.933859
13	1	0	-0.881470	1.201248	1.646306
14	1	0	0.881470	1.201248	1.646306
15	1	0	-0.881470	-1.201248	1.646306
16	1	0	0.881470	-1.201248	1.646306

Bicyclo[3.1.0]hexane

Species name: bchx3
Full file name: bchx3_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.143879 E(Thermal)= 0.149132
W1BD (0 K)= -234.543383 W1BD Energy= -234.538130
W1BD Enthalpy= -234.537186 W1BD Free Energy= -234.571600
1\1\GINC-NODE72\Mixed\W1BD\W1BD\C6H10\RABLENP\19-Oct-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Bicyclo[3.1.0]hexane\\0,1\C,0,-0.5950997198,-1.454
1015172,0.\C,0,0.4779929047,-0.7142481014,-0.7552995996\C,0,0.47799290

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.921967	-1.303619	0.000000

2	6	0	-0.285571	-0.812943	0.755300
3	6	0	-0.285571	-0.812943	-0.755300
4	6	0	-0.285571	0.631450	-1.227636
5	6	0	-0.285571	0.631450	1.227636
6	6	0	0.168257	1.451379	0.000000
7	1	0	1.825232	-0.707089	0.000000
8	1	0	1.101824	-2.369655	0.000000
9	1	0	-0.866181	-1.537453	1.309840
10	1	0	-0.866181	-1.537453	-1.309840
11	1	0	0.355185	0.801929	-2.095345
12	1	0	-1.301731	0.910715	-1.517825
13	1	0	0.355185	0.801929	2.095345
14	1	0	-1.301731	0.910715	1.517825
15	1	0	1.253366	1.557222	0.000000
16	1	0	-0.242615	2.460494	0.000000

Spirohexane

Species name: spirohexane
Full file name: spirohexane_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.141637 E(Thermal)= 0.147555
W1BD (0 K)= -234.508471 W1BD Energy= -234.502553
W1BD Enthalpy= -234.501608 W1BD Free Energy= -234.537647
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C6H10\RABLENP\21-Feb-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Spirohexane\\0,1\C,0,0.0776411971,-0.3007999891,0.
\C,0,-0.1678430634,1.835049991,0.\C,0,0.1365515866,0.7725831681,-1.093

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.094226	0.296266	0.000000
2	6	0	-0.267934	-1.822922	0.000000
3	6	0	0.094226	-0.778733	1.093336
4	6	0	0.094226	-0.778733	-1.093336
5	6	0	0.759091	1.633805	0.000000
6	6	0	-0.749641	1.533693	0.000000
7	1	0	0.303251	-2.749445	0.000000
8	1	0	-1.328863	-2.068145	0.000000
9	1	0	1.086248	-0.945587	1.516642
10	1	0	-0.616740	-0.652409	1.910026
11	1	0	1.086248	-0.945587	-1.516642
12	1	0	-0.616740	-0.652409	-1.910026
13	1	0	1.245559	1.962221	0.909380
14	1	0	1.245559	1.962221	-0.909380
15	1	0	-1.274847	1.794440	0.909736
16	1	0	-1.274847	1.794440	-0.909736

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cis-bicyclo[2.2.0]hexane

Species name: cis_bchx5
Full file name: cis_bchx5_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.142608 E(Thermal)= 0.148145
W1BD (0 K)= -234.508748 W1BD Energy= -234.503211
W1BD Enthalpy= -234.502267 W1BD Free Energy= -234.537308
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C6H10\RABLENP\04-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\cis-bicyclo[2.2.0]hexane\\0,1\C,0,0.0088490119,0.7
859784338,0.5769866957\C,0,-0.0088490119,-0.7859784338,0.5769866957\C,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.504702	0.602591	0.577333
2	6	0	0.504702	-0.602591	0.577333
3	6	0	0.504702	1.441109	-0.243460
4	6	0	1.496488	0.240678	-0.262574
5	6	0	-1.496488	-0.240678	-0.262574
6	6	0	-0.504702	-1.441109	-0.243460
7	1	0	-0.896158	1.055274	1.486088
8	1	0	0.896158	-1.055274	1.486088
9	1	0	0.143017	1.784190	-1.213790
10	1	0	0.891421	2.304497	0.296732
11	1	0	1.731988	-0.170159	-1.245308
12	1	0	2.435414	0.449951	0.248486
13	1	0	-1.731988	0.170159	-1.245308
14	1	0	-2.435414	-0.449951	0.248486
15	1	0	-0.143017	-1.784190	-1.213790
16	1	0	-0.891421	-2.304497	0.296732

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trans-Bicyclo[2.2.0]hexane

Species name: trans_bchx5
Full file name: trans_bchx5_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.142531 E(Thermal)= 0.147798
W1BD (0 K)= -234.445882 W1BD Energy= -234.440615

W1BD Enthalpy=   -234.439671 W1BD Free Energy=   -234.473421
1\1\GINC-NODE01\Mixed\W1BD\W1BD\C6H10\RABLENP\04-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\trans-Bicyclo[2.2.0]hexane\\0,1\C,0,0.2753086061,-
0.6918545359,0.\C,0,-0.2753086061,0.6918545359,0.\C,0,-0.1083549225,-0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196096	0.718334	0.000000
2	6	0	0.196096	-0.718334	0.000000
3	6	0	0.196096	0.772464	1.514942
4	6	0	-0.196096	-0.772464	1.514942
5	6	0	0.196096	0.772464	-1.514942
6	6	0	-0.196096	-0.772464	-1.514942
7	1	0	-1.291474	0.752987	0.000000
8	1	0	1.291474	-0.752987	0.000000
9	1	0	1.264686	0.897845	1.685661
10	1	0	-0.362772	1.438949	2.171253
11	1	0	0.362772	-1.438949	2.171253
12	1	0	-1.264686	-0.897845	1.685661
13	1	0	1.264686	0.897845	-1.685661
14	1	0	-0.362772	1.438949	-2.171253
15	1	0	0.362772	-1.438949	-2.171253
16	1	0	-1.264686	-0.897845	-1.685661

Cyclohexane

Species name: cyclohexane
Full file name: cyclohexane_w1bd.log
Method: W1BD calculation
Point group: D3D
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.167052 E(Thermal)= 0.172881
W1BD (0 K)= -235.766206 W1BD Energy= -235.760376
W1BD Enthalpy= -235.759432 W1BD Free Energy= -235.793365
1\1\GINC-NODE03\Mixed\W1BD\W1BD\C6H12\RABLENP\23-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Cyclohexane\\0,1\C,0,-0.0000000002,1.4633382001,-0
.227435547\C,0,-1.2672880557,0.7316690999,0.227435547\C,0,-1.267288055

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.267288	0.731669	0.227436
2	6	0	0.000000	1.463338	-0.227436
3	6	0	1.267288	0.731669	0.227436
4	6	0	1.267288	-0.731669	-0.227436

5	6	0	0.000000	-1.463338	0.227436
6	6	0	-1.267288	-0.731669	-0.227436
7	1	0	-1.329504	0.767590	1.320521
8	1	0	-2.155213	1.244313	-0.149702
9	1	0	0.000000	2.488626	0.149702
10	1	0	0.000000	1.535179	-1.320521
11	1	0	1.329504	0.767590	1.320521
12	1	0	2.155213	1.244313	-0.149702
13	1	0	2.155213	-1.244313	0.149702
14	1	0	1.329504	-0.767590	-1.320521
15	1	0	0.000000	-1.535179	1.320521
16	1	0	0.000000	-2.488626	-0.149702
17	1	0	-2.155213	-1.244313	0.149702
18	1	0	-1.329504	-0.767590	-1.320521

Bicyclo[4.1.0]hepta-1,3,5-triene

Species name: bcheptatriene
Full file name: bcheptatriene_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.102858 E(Thermal)= 0.108184
W1BD (0 K)= -270.212412 W1BD Energy= -270.207085
W1BD Enthalpy= -270.206141 W1BD Free Energy= -270.240524
1\1\GINC-NODE01\Mixed\W1BD\W1BD\C7H6\RABLENP\12-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Bicyclo[4.1.0]hepta-1,3,5-trien
e)\\0,1\C,0,0.,0.,2.1408837466\C,0,0.,-0.6719084015,0.8002740176\C,0,0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.140829
2	6	0	0.000000	0.671908	0.800219
3	6	0	0.000000	-0.671908	0.800219
4	6	0	0.000000	1.448504	-0.333455
5	6	0	0.000000	-1.448504	-0.333455
6	6	0	0.000000	0.698719	-1.523467
7	6	0	0.000000	-0.698719	-1.523467
8	1	0	0.908129	0.000000	2.739540
9	1	0	-0.908129	0.000000	2.739540
10	1	0	0.000000	2.530281	-0.348319
11	1	0	0.000000	-2.530281	-0.348319
12	1	0	0.000000	1.217357	-2.473494
13	1	0	0.000000	-1.217357	-2.473494

Norbornadiene

Species name: norbornadiene
Full file name: norbornadiene_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.126254 E(Thermal)= 0.131208
W1BD (0 K)= -271.426990 W1BD Energy= -271.422036
W1BD Enthalpy= -271.421092 W1BD Free Energy= -271.454482
1\1\GINC-NODE37\Mixed\W1BD\W1BD\C7H8\RABLENP\04-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Norbornadiene\\0,1\C,0,0.,0.,1.347130683\C,0,-1.120
2316471,0.,0.2657978997\C,0,1.1202316471,0.,0.2657978997\C,0,-0.664545

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.353712
2	6	0	0.000000	1.120232	0.272379
3	6	0	0.000000	-1.120232	0.272379
4	6	0	1.240354	0.664545	-0.520015
5	6	0	1.240354	-0.664545	-0.520015
6	6	0	-1.240354	0.664545	-0.520015
7	6	0	-1.240354	-0.664545	-0.520015
8	1	0	0.896714	0.000000	1.972559
9	1	0	-0.896714	0.000000	1.972559
10	1	0	0.000000	2.152856	0.609117
11	1	0	0.000000	-2.152856	0.609117
12	1	0	1.927746	1.330728	-1.018453
13	1	0	1.927746	-1.330728	-1.018453
14	1	0	-1.927746	1.330728	-1.018453
15	1	0	-1.927746	-1.330728	-1.018453

Quadricyclane

Species name: quadricyclane
Full file name: quadricyclane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.125948 E(Thermal)= 0.130633
W1BD (0 K)= -271.391455 W1BD Energy= -271.386769
W1BD Enthalpy= -271.385825 W1BD Free Energy= -271.418702
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C7H8\RABLENP\04-Dec-2019\0\\#n W1BD fo
pt=(calcfc,tight)\\Quadricyclane\\0,1\C,0,0.,0.,-1.535191951\C,0,0.,1.
1495511681,-0.5497574331\C,0,0.,-1.1495511681,-0.5497574331\C,0,-0.756

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.534600
2	6	0	0.000000	1.149551	0.549165
3	6	0	0.000000	-1.149551	0.549165
4	6	0	0.756311	0.773443	-0.707493
5	6	0	0.756311	-0.773443	-0.707493
6	6	0	-0.756311	0.773443	-0.707493
7	6	0	-0.756311	-0.773443	-0.707493
8	1	0	0.887244	0.000000	2.171875
9	1	0	-0.887244	0.000000	2.171875
10	1	0	0.000000	2.180488	0.872999
11	1	0	0.000000	-2.180488	0.872999
12	1	0	1.443338	1.422561	-1.226875
13	1	0	1.443338	-1.422561	-1.226875
14	1	0	-1.443338	1.422561	-1.226875
15	1	0	-1.443338	-1.422561	-1.226875

Bicyclo[3.2.0]hept-1(5)-ene

Species name: bchp2
Full file name: bchp2_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.148124 E(Thermal)= 0.154571
W1BD (0 K)= -272.613375 W1BD Energy= -272.606928
W1BD Enthalpy= -272.605984 W1BD Free Energy= -272.643796
1\1\GINC-NODE37\Mixed\W1BD\W1BD\C7H10\RABLENP\07-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Bicyclo[3.2.0]hept-1(5)-ene\\0,1\C,0,-0.0908834995
,1.9613807283,0.\H,0,0.6360671471,2.7723321238,0.\H,0,-1.0791075617,2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088962	1.961483	0.000000
2	1	0	0.638693	2.771803	0.000000
3	1	0	-1.076787	2.421102	0.000000
4	6	0	0.059745	1.055900	1.277961
5	6	0	0.059745	1.055900	-1.277961
6	6	0	-0.011833	-0.305565	0.661931
7	6	0	-0.011833	-0.305565	-0.661931
8	6	0	-0.011833	-1.821950	0.790918
9	6	0	-0.011833	-1.821950	-0.790918
10	1	0	1.012209	1.226581	1.789390

11	1	0	-0.725840	1.259043	2.009257
12	1	0	1.012209	1.226581	-1.789390
13	1	0	-0.725840	1.259043	-2.009257
14	1	0	0.878098	-2.266571	1.240591
15	1	0	-0.895012	-2.270266	1.249647
16	1	0	0.878098	-2.266571	-1.240591
17	1	0	-0.895012	-2.270266	-1.249647

Bicyclo[3.2.0]hept-2-ene

Species name: bchp4
Full file name: bchp4_w1bd.log
Method: W1BD calculation
Point group: C1
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.148779 E(Thermal)= 0.154651
W1BD (0 K)= -272.635771 W1BD Energy= -272.629899
W1BD Enthalpy= -272.628955 W1BD Free Energy= -272.665244
1\1\GINC-NODE38\Mixed\W1BD\W1BD\C7H10\RABLENP\12-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Bicyclo[3.2.0]hept-2-ene\\0,1\C,0,0.6133402977,-0.
2266045374,0.8246022023\C,0,-0.3618559287,0.8822070858,1.0995636781\C,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.385634	0.742611	0.636098
2	6	0	0.823550	1.271343	-0.081114
3	6	0	1.700711	0.317509	-0.384229
4	6	0	1.263706	-1.051299	0.082127
5	6	0	-0.177300	-0.806985	0.561665
6	6	0	-1.298133	-0.871028	-0.514681
7	6	0	-1.680933	0.602356	-0.214465
8	1	0	-0.520771	1.203818	1.616749
9	1	0	0.950294	2.320881	-0.315349
10	1	0	2.638472	0.485383	-0.898060
11	1	0	1.914854	-1.420622	0.881456
12	1	0	1.306754	-1.797156	-0.717738
13	1	0	-0.427076	-1.353223	1.469015
14	1	0	-2.080049	-1.610986	-0.349221
15	1	0	-0.900168	-1.013018	-1.519357
16	1	0	-2.582977	0.688238	0.391136
17	1	0	-1.775127	1.269645	-1.071032

Bicyclo[3.2.0]hept-6-ene

Species name: bchp3

Full file name: bchp3_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature=   298.150000 Pressure=   1.000000
E(ZPE)=   0.148772 E(Thermal)=   0.154614
W1BD (0 K)=   -272.628419 W1BD Energy=   -272.622577
W1BD Enthalpy=   -272.621633 W1BD Free Energy=   -272.657624
1\1\GINC-NODE12\Mixed\W1BD\W1BD\C7H10\RABLENP\07-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Bicyclo[3.2.0]hept-6-ene\\0,1\C,0,-0.9659485633,1.
2495683056,0.\H,0,-1.4032916874,2.2480071594,0.\H,0,-1.7918700171,0.53

                        Standard orientation:

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

     1   6   0   -0.957421   1.312651   0.000000
     2   1   0   -1.280844   2.353587   0.000000
     3   1   0   -1.857566   0.696495   0.000000
     4   6   0   -0.077935   0.963662   1.215078
     5   6   0   -0.077935   0.963662   -1.215078
     6   6   0   0.704793   -0.287321   0.792381
     7   6   0   0.704793   -0.287321   -0.792381
     8   6   0   -0.077935   -1.582299   0.666764
     9   6   0   -0.077935   -1.582299   -0.666764
    10   1   0   0.625428   1.778118   1.407954
    11   1   0   -0.657161   0.814879   2.127986
    12   1   0   0.625428   1.778118   -1.407954
    13   1   0   -0.657161   0.814879   -2.127986
    14   1   0   1.677768   -0.372251   1.277937
    15   1   0   1.677768   -0.372251   -1.277937
    16   1   0   -0.498104   -2.247992   1.410489
    17   1   0   -0.498104   -2.247992   -1.410489

[2.2.1]Propellane

Species name: 221propellane
Full file name: 221propellane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature=   298.150000 Pressure=   1.000000
E(ZPE)=   0.147483 E(Thermal)=   0.153501
W1BD (0 K)=   -272.558693 W1BD Energy=   -272.552674
W1BD Enthalpy=   -272.551730 W1BD Free Energy=   -272.587258
1\1\GINC-NODE43\Mixed\W1BD\W1BD\C7H10\RABLENP\24-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\[2.2.1]Propellane\\0,1\C,0,0.,0.,1.4897819012\C,0,
0.,-0.7912148719,0.2285313233\C,0,0.,0.7912148719,0.2285313233\C,0,-1.

                        Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.517147
2	6	0	0.000000	0.791215	0.255897
3	6	0	0.000000	-0.791215	0.255897
4	6	0	1.368936	0.780747	-0.454201
5	6	0	1.368936	-0.780747	-0.454201
6	6	0	-1.368936	0.780747	-0.454201
7	6	0	-1.368936	-0.780747	-0.454201
8	1	0	0.907237	0.000000	2.107656
9	1	0	-0.907237	0.000000	2.107656
10	1	0	1.324930	1.203175	-1.456624
11	1	0	2.178938	1.276353	0.084594
12	1	0	1.324930	-1.203175	-1.456624
13	1	0	2.178938	-1.276353	0.084594
14	1	0	-1.324930	1.203175	-1.456624
15	1	0	-2.178938	1.276353	0.084594
16	1	0	-1.324930	-1.203175	-1.456624
17	1	0	-2.178938	-1.276353	0.084594

Norbornene

Species name: norbornene
Full file name: norbornene_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.150199 E(Thermal)= 0.155509
W1BD (0 K)= -272.649930 W1BD Energy= -272.644620
W1BD Enthalpy= -272.643676 W1BD Free Energy= -272.678486
1\1\GINC-NODE64\Mixed\W1BD\W1BD\C7H10\RABLENP\21-Oct-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Norbornene\\0,1\C,0,-1.4716363251,-0.0982263045,0.
\C,0,-0.4150690856,-0.1251790144,1.1255268297\C,0,-0.4150690856,-0.125

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.129678	0.790234	0.000000
2	6	0	0.221187	0.250136	1.125527
3	6	0	0.221187	0.250136	-1.125527
4	6	0	-1.123025	0.787789	0.666983
5	6	0	-1.123025	0.787789	-0.666983
6	6	0	0.221187	-1.275730	0.778363
7	6	0	0.221187	-1.275730	-0.778363
8	1	0	1.203584	1.876869	0.000000
9	1	0	2.129157	0.350884	0.000000

10	1	0	0.506870	0.476964	2.149749
11	1	0	0.506870	0.476964	-2.149749
12	1	0	-1.955191	1.008124	1.320432
13	1	0	-1.955191	1.008124	-1.320432
14	1	0	-0.641023	-1.788073	1.201920
15	1	0	1.117837	-1.754771	1.173591
16	1	0	-0.641023	-1.788073	-1.201920
17	1	0	1.117837	-1.754771	-1.173591

Norbornane

Species name: norbornane
Full file name: norbornane_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.173904 E(Thermal)= 0.179595
W1BD (0 K)= -273.864451 W1BD Energy= -273.858760
W1BD Enthalpy= -273.857816 W1BD Free Energy= -273.892849
1\1\GINC-NODE33\Mixed\W1BD\W1BD\C7H12\RABLENP\27-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\Norbornane\\0,1\C,0,0.,0.,1.3841018362\C,0,0.,1.13
02868554,0.3380973315\C,0,0.,-1.1302868554,0.3380973315\C,0,1.25223210

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.385320
2	6	0	0.000000	1.130287	0.339316
3	6	0	0.000000	-1.130287	0.339316
4	6	0	1.252232	0.780987	-0.492282
5	6	0	1.252232	-0.780987	-0.492282
6	6	0	-1.252232	0.780987	-0.492282
7	6	0	-1.252232	-0.780987	-0.492282
8	1	0	0.887382	0.000000	2.020602
9	1	0	-0.887382	0.000000	2.020602
10	1	0	0.000000	2.146942	0.729221
11	1	0	0.000000	-2.146942	0.729221
12	1	0	1.204347	1.201487	-1.497268
13	1	0	2.153881	1.172975	-0.019881
14	1	0	1.204347	-1.201487	-1.497268
15	1	0	2.153881	-1.172975	-0.019881
16	1	0	-1.204347	1.201487	-1.497268
17	1	0	-2.153881	1.172975	-0.019881
18	1	0	-1.204347	-1.201487	-1.497268
19	1	0	-2.153881	-1.172975	-0.019881

Bicyclo[3.2.0]heptane

Species name: bchp
Full file name: bchp_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.172312 E(Thermal)= 0.178530
W1BD (0 K)= -273.841239 W1BD Energy= -273.835020
W1BD Enthalpy= -273.834076 W1BD Free Energy= -273.871132
1\1\GINC-NODE08\Mixed\W1BD\W1BD\C7H12\RABLENP\08-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Bicyclo[3.2.0]heptane\\0,1\C,0,-0.6620613783,1.543
2702266,0.\H,0,-0.7865917069,2.6263284242,0.\H,0,-1.6645053081,1.10807

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.961738	1.376220	0.000000
2	1	0	-1.304186	2.411234	0.000000
3	1	0	-1.854569	0.746025	0.000000
4	6	0	-0.073004	1.038812	1.210231
5	6	0	-0.073004	1.038812	-1.210231
6	6	0	0.712137	-0.207565	0.785351
7	6	0	0.712137	-0.207565	-0.785351
8	6	0	-0.073004	-1.548760	0.775799
9	6	0	-0.073004	-1.548760	-0.775799
10	1	0	0.620311	1.863658	1.395864
11	1	0	-0.643124	0.884146	2.128316
12	1	0	0.620311	1.863658	-1.395864
13	1	0	-0.643124	0.884146	-2.128316
14	1	0	1.685480	-0.268507	1.269667
15	1	0	1.685480	-0.268507	-1.269667
16	1	0	0.465203	-2.382741	1.224338
17	1	0	-1.060058	-1.498768	1.237678
18	1	0	0.465203	-2.382741	-1.224338
19	1	0	-1.060058	-1.498768	-1.237678

Spiro[3.3]heptane

Species name: spiroheptane
Full file name: spiroheptane_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.170297 E(Thermal)= 0.177088
W1BD (0 K)= -273.809468 W1BD Energy= -273.802677
W1BD Enthalpy= -273.801733 W1BD Free Energy= -273.839297

1\1\GINC-NODE41\Mixed\W1BD\W1BD\C7H12\RABLENP\24-Feb-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Spiro[3.3]heptane\\0,1\C,0,0.,0.,-0.1674687507\C,0
,0.0530572257,2.1206571318,0.2777430561\C,0,-0.0530572257,-2.120657131

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.167514
2	6	0	0.000000	2.121321	-0.277698
3	6	0	0.000000	-2.121321	-0.277698
4	6	0	0.923740	0.936864	-0.656936
5	6	0	-0.572595	1.250521	0.869291
6	6	0	-0.923740	-0.936864	-0.656936
7	6	0	0.572595	-1.250521	0.869291
8	1	0	-0.744618	2.321049	-1.047730
9	1	0	0.477143	3.061802	-0.006527
10	1	0	0.744618	-2.321049	-1.047730
11	1	0	-0.477143	-3.061802	-0.006527
12	1	0	1.054321	0.710780	-1.715772
13	1	0	1.908778	1.031780	-0.196451
14	1	0	-1.649746	1.273427	1.039116
15	1	0	-0.066633	1.445501	1.816879
16	1	0	-1.054321	-0.710780	-1.715772
17	1	0	-1.908778	-1.031780	-0.196451
18	1	0	1.649746	-1.273427	1.039116
19	1	0	0.066633	-1.445501	1.816879

Equatorial methylcyclohexane

Species name: eq_mcyclohex
Full file name: eq_mcyclohex_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.194280 E(Thermal)= 0.201580
W1BD (0 K)= -275.064936 W1BD Energy= -275.057635
W1BD Enthalpy= -275.056691 W1BD Free Energy= -275.095655
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C7H14\RABLENP\17-Nov-2019\0\\#n W1BD f
opt=(calcfc,tight)\\Equatorial methylcyclohexane\\0,1\C,0,-0.328101682
8,1.0152337039,0.\C,0,0.0763042834,2.4891079051,0.\C,0,0.1662434965,0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566925	0.906270	0.000000
2	6	0	-0.534690	2.434279	0.000000

3	6	0	0.089248	0.324946	1.260535
4	6	0	0.089248	0.324946	-1.260535
5	6	0	0.089248	-1.206844	1.264911
6	6	0	0.089248	-1.206844	-1.264911
7	6	0	0.740415	-1.773602	0.000000
8	1	0	-1.617636	0.590247	0.000000
9	1	0	0.494523	2.802019	0.000000
10	1	0	-1.031906	2.842528	-0.882108
11	1	0	-1.031906	2.842528	0.882108
12	1	0	-0.419502	0.704177	2.150787
13	1	0	1.122558	0.686611	1.318307
14	1	0	-0.419502	0.704177	-2.150787
15	1	0	1.122558	0.686611	-1.318307
16	1	0	-0.943115	-1.566672	1.330204
17	1	0	0.602471	-1.579819	2.154273
18	1	0	-0.943115	-1.566672	-1.330204
19	1	0	0.602471	-1.579819	-2.154273
20	1	0	0.681324	-2.864426	0.000000
21	1	0	1.806027	-1.520399	0.000000

Cubane

Species name: cubane
Full file name: cubane_w1bd.log
Method: W1BD calculation
Point group: D4H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.131050 E(Thermal)= 0.135695
W1BD (0 K)= -309.411369 W1BD Energy= -309.406724
W1BD Enthalpy= -309.405779 W1BD Free Energy= -309.437630
1\1\GINC-NODE11\Mixed\W1BD\W1BD\C8H8\RABLENP\28-Sep-2018\0\\#n W1BD fo
pt=(calcfc,tight)\\Cubane\\0,1\C,0,-1.1084879087,0.,0.7838427942\C,0,0
.,1.1084879087,0.7838427942\C,0,1.1084879087,0.,0.7838427942\C,0,0.,-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.108488	0.783843
2	6	0	1.108488	0.000000	0.783843
3	6	0	0.000000	-1.108488	0.783843
4	6	0	-1.108488	0.000000	0.783843
5	6	0	0.000000	1.108488	-0.783843
6	6	0	1.108488	0.000000	-0.783843
7	6	0	0.000000	-1.108488	-0.783843
8	6	0	-1.108488	0.000000	-0.783843
9	1	0	0.000000	1.995440	1.411221
10	1	0	1.995440	0.000000	1.411221
11	1	0	0.000000	-1.995440	1.411221
12	1	0	-1.995440	0.000000	1.411221

13	1	0	0.000000	1.995440	-1.411221
14	1	0	1.995440	0.000000	-1.411221
15	1	0	0.000000	-1.995440	-1.411221
16	1	0	-1.995440	0.000000	-1.411221

[3.4.4.4]Fenestrane

Species name: 3444fenestrane
Full file name: 3444fenestrane_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.149771 E(Thermal)= 0.156759
W1BD (0 K)= -310.500397 W1BD Energy= -310.493409
W1BD Enthalpy= -310.492465 W1BD Free Energy= -310.530228
1\1\GINC-NODE36\Mixed\W1BD\W1BD\C8H10\RABLENP\23-Dec-2019\0\\#n W1BD f
opt=(calcfc,tight)\\[3.4.4.4]Fenestrane\\0,1\C,0,0.,0.,-0.1116063709\C
,0,-0.5035044209,0.6031660247,-1.3328695163\C,0,0.5310633553,1.0396633

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.112183
2	6	0	0.000000	0.785701	-1.333447
3	6	0	1.073939	0.457804	0.751191
4	6	0	-1.073939	-0.457804	0.751191
5	6	0	0.000000	-0.785701	-1.333447
6	6	0	1.147784	1.553060	-0.416911
7	6	0	0.000000	0.000000	1.901156
8	6	0	-1.147784	-1.553060	-0.416911
9	1	0	-0.827789	1.374681	-1.700946
10	1	0	1.978708	-0.139258	0.812830
11	1	0	-1.978708	0.139258	0.812830
12	1	0	0.827789	-1.374681	-1.700946
13	1	0	0.726049	2.526092	-0.180735
14	1	0	2.148944	1.666994	-0.831663
15	1	0	-0.456698	0.762469	2.528596
16	1	0	0.456698	-0.762469	2.528596
17	1	0	-2.148944	-1.666994	-0.831663
18	1	0	-0.726049	-2.526092	-0.180735

[2.2.2]Propellane

Species name: 222propellane
Full file name: 222propellane_w1bd.log
Method: W1BD calculation

Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.175188 E(Thermal)= 0.182335
W1BD (0 K)= -311.862873 W1BD Energy= -311.855725
W1BD Enthalpy= -311.854781 W1BD Free Energy= -311.892620
1\1\GINC-NODE44\Mixed\W1BD\W1BD\C8H12\RABLENP\26-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\[2.2.2]Propellane\\0,1\C,0,0.,0.0000000014,0.76787
40185\C,0,0.,0.0000000014,-0.7678740185\C,0,0.,1.550832652,0.786268588

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.767874
2	6	0	0.000000	0.000000	-0.767874
3	6	0	0.000000	1.550833	0.786269
4	6	0	0.000000	1.550833	-0.786269
5	6	0	1.343060	-0.775416	0.786269
6	6	0	1.343060	-0.775416	-0.786269
7	6	0	-1.343060	-0.775416	0.786269
8	6	0	-1.343060	-0.775416	-0.786269
9	1	0	0.881809	2.001533	1.242576
10	1	0	-0.881809	2.001533	1.242576
11	1	0	0.881809	2.001533	-1.242576
12	1	0	-0.881809	2.001533	-1.242576
13	1	0	1.292474	-1.764435	1.242576
14	1	0	2.174282	-0.237098	1.242576
15	1	0	1.292474	-1.764435	-1.242576
16	1	0	2.174282	-0.237098	-1.242576
17	1	0	-2.174282	-0.237098	1.242576
18	1	0	-1.292474	-1.764435	1.242576
19	1	0	-2.174282	-0.237098	-1.242576
20	1	0	-1.292474	-1.764435	-1.242576

[2.2.2]Bicyclooctene

Species name: bce
Full file name: bce_w1bd.log
Method: W1BD calculation
Point group: C2V
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.179413 E(Thermal)= 0.185810
W1BD (0 K)= -311.958578 W1BD Energy= -311.952180
W1BD Enthalpy= -311.951236 W1BD Free Energy= -311.987925
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C8H12\RABLENP\22-Oct-2018\0\\#n W1BD f
opt=(calcfc,tight)\\[2.2.2]Bicyclooctene\\0,1\C,0,-1.2868270331,0.,0.0
871146881\C,0,1.2868270331,0.,0.0871146881\C,0,-0.6660301349,0.,1.4602

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.286827	0.089860
2	6	0	0.000000	-1.286827	0.089860
3	6	0	0.000000	0.666030	1.462971
4	6	0	0.000000	-0.666030	1.462971
5	6	0	-1.251205	0.775451	-0.670056
6	6	0	-1.251205	-0.775451	-0.670056
7	6	0	1.251205	0.775451	-0.670056
8	6	0	1.251205	-0.775451	-0.670056
9	1	0	0.000000	2.375578	0.131940
10	1	0	0.000000	-2.375578	0.131940
11	1	0	0.000000	1.269384	2.361612
12	1	0	0.000000	-1.269384	2.361612
13	1	0	-1.235651	1.164915	-1.690227
14	1	0	-2.152334	1.162796	-0.194704
15	1	0	-1.235651	-1.164915	-1.690227
16	1	0	-2.152334	-1.162796	-0.194704
17	1	0	2.152334	1.162796	-0.194704
18	1	0	1.235651	1.164915	-1.690227
19	1	0	2.152334	-1.162796	-0.194704
20	1	0	1.235651	-1.164915	-1.690227

[2.2.2]Bicyclooctane

Species name: bco
Full file name: bco_w1bd.log
Method: W1BD calculation
Point group: D3H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.202486 E(Thermal)= 0.209520
W1BD (0 K)= -313.166170 W1BD Energy= -313.159135
W1BD Enthalpy= -313.158191 W1BD Free Energy= -313.196063
1\1\GINC-NODE39\Mixed\W1BD\W1BD\C8H14\RABLENP\30-Sep-2018\0\\#n W1BD f
opt=(calcfc,tight)\\[2.2.2]Bicyclooctane\\0,1\C,0,0.,-0.0000000007,1.2
951617677\C,0,0.,-0.0000000007,-1.2951617677\C,0,0.,1.4474362164,0.777

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.295162
2	6	0	0.000000	0.000000	-1.295162
3	6	0	0.000000	1.447436	0.777466
4	6	0	0.000000	1.447436	-0.777466
5	6	0	1.253517	-0.723718	0.777466

6	6	0	1.253517	-0.723718	-0.777466
7	6	0	-1.253517	-0.723718	0.777466
8	6	0	-1.253517	-0.723718	-0.777466
9	1	0	0.000000	0.000000	2.387203
10	1	0	0.000000	0.000000	-2.387203
11	1	0	0.874937	1.974752	1.163155
12	1	0	-0.874937	1.974752	1.163155
13	1	0	0.874937	1.974752	-1.163155
14	1	0	-0.874937	1.974752	-1.163155
15	1	0	1.272717	-1.745094	1.163155
16	1	0	2.147654	-0.229658	1.163155
17	1	0	1.272717	-1.745094	-1.163155
18	1	0	2.147654	-0.229658	-1.163155
19	1	0	-2.147654	-0.229658	1.163155
20	1	0	-1.272717	-1.745094	1.163155
21	1	0	-2.147654	-0.229658	-1.163155
22	1	0	-1.272717	-1.745094	-1.163155

Equatorial cis-1,3-dimethylcyclohexane

Species name: eq_cis13dmcyclohex
Full file name: eq_cis13dmcyclohex_w1bd.log
Method: W1BD calculation
Point group: CS
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.221818 E(Thermal)= 0.230537
W1BD (0 K)= -314.363359 W1BD Energy= -314.354640
W1BD Enthalpy= -314.353696 W1BD Free Energy= -314.395799
1\1\GINC-NODE34\Mixed\W1BD\W1BD\C8H16\RABLENP\12-Feb-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Equatorial cis-1,3-dimethylcyclohexane\\0,1\C,0,-1
.0630894036,-0.0755379838,0.\H,0,-2.0656543207,0.3624480471,0.\H,0,-1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.458880	-0.963911	0.000000
2	1	0	-1.333327	-1.621414	0.000000
3	1	0	0.419541	-1.621563	0.000000
4	6	0	-0.446630	-0.119484	1.281428
5	6	0	-0.446630	-0.119484	-1.281428
6	6	0	0.740341	0.853070	1.266224
7	6	0	0.740341	0.853070	-1.266224
8	6	0	0.765116	1.712507	0.000000
9	6	0	-0.446630	-0.995355	2.533963
10	6	0	-0.446630	-0.995355	-2.533963
11	1	0	-1.364692	0.481262	1.289905
12	1	0	-1.364692	0.481262	-1.289905
13	1	0	0.710612	1.489925	2.154264
14	1	0	1.670062	0.275605	1.330613

15	1	0	0.710612	1.489925	-2.154264
16	1	0	1.670062	0.275605	-1.330613
17	1	0	-0.103610	2.379324	0.000000
18	1	0	1.647249	2.357006	0.000000
19	1	0	0.450640	-1.617974	2.574506
20	1	0	-0.470757	-0.389953	3.442154
21	1	0	-1.311983	-1.660716	2.553248
22	1	0	0.450640	-1.617974	-2.574506
23	1	0	-0.470757	-0.389953	-3.442154
24	1	0	-1.311983	-1.660716	-2.553248

Equatorial trans-1,4-dimethylcyclohexane

Species name: eq_trans14dmcyclohex
Full file name: eq_trans14dmcyclohex_w1bd.log
Method: W1BD calculation
Point group: C2H
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.221637 E(Thermal)= 0.230382
W1BD (0 K)= -314.363519 W1BD Energy= -314.354774
W1BD Enthalpy= -314.353830 W1BD Free Energy= -314.395340
1\1\GINC-NODE33\Mixed\W1BD\W1BD\C8H16\RABLENP\06-Feb-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Equatorial trans-1,4-dimethylcyclohexane\\0,1\C,0,
-0.3358249359,1.4635043347,0.\C,0,0.0420468418,2.9443771127,0.\C,0,0.1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.226858	1.484304	0.000000
2	6	0	0.259314	2.933237	0.000000
3	6	0	0.226858	0.731287	1.257212
4	6	0	0.226858	0.731287	-1.257212
5	6	0	-0.226858	-0.731287	1.257212
6	6	0	-0.226858	-0.731287	-1.257212
7	6	0	0.226858	-1.484304	0.000000
8	6	0	-0.259314	-2.933237	0.000000
9	1	0	-1.324063	1.496422	0.000000
10	1	0	1.351382	2.978659	0.000000
11	1	0	-0.093816	3.471199	-0.881978
12	1	0	-0.093816	3.471199	0.881978
13	1	0	-0.147490	1.239694	2.149652
14	1	0	1.320810	0.771146	1.316213
15	1	0	-0.147490	1.239694	-2.149652
16	1	0	1.320810	0.771146	-1.316213
17	1	0	-1.320810	-0.771146	1.316213
18	1	0	0.147490	-1.239694	2.149652
19	1	0	-1.320810	-0.771146	-1.316213
20	1	0	0.147490	-1.239694	-2.149652
21	1	0	1.324063	-1.496422	0.000000

22	1	0	-1.351382	-2.978659	0.000000
23	1	0	0.093816	-3.471199	-0.881978
24	1	0	0.093816	-3.471199	0.881978

[4.4.4.4]Fenestrane

Species name: 4444fenestrane
Full file name: 4444fenestrane_w1bd.log
Method: W1BD calculation
Point group: D2D
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.179715 E(Thermal)= 0.187328
W1BD (0 K)= -349.869759 W1BD Energy= -349.862147
W1BD Enthalpy= -349.861202 W1BD Free Energy= -349.900005
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C9H12\RABLENP\31-Jan-2020\0\\#n W1BD f
opt=(calcfc,tight)\\[4.4.4.4]Fenestrane\\0,1\C,0,0.,0.,0.\C,0,1.353111
1593,0.,-0.6233093261\C,0,0.,1.3531111593,0.6233093261\C,0,-1.35311115

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	1.353111	0.623309
3	6	0	1.353111	0.000000	-0.623309
4	6	0	0.000000	-1.353111	0.623309
5	6	0	-1.353111	0.000000	-0.623309
6	6	0	1.474609	1.474609	0.000000
7	6	0	1.474609	-1.474609	0.000000
8	6	0	-1.474609	-1.474609	0.000000
9	6	0	-1.474609	1.474609	0.000000
10	1	0	0.000000	1.458281	1.705949
11	1	0	1.458281	0.000000	-1.705949
12	1	0	0.000000	-1.458281	1.705949
13	1	0	-1.458281	0.000000	-1.705949
14	1	0	2.216173	1.636094	0.782436
15	1	0	1.636094	2.216173	-0.782436
16	1	0	2.216173	-1.636094	0.782436
17	1	0	1.636094	-2.216173	-0.782436
18	1	0	-2.216173	-1.636094	0.782436
19	1	0	-1.636094	-2.216173	-0.782436
20	1	0	-2.216173	1.636094	0.782436
21	1	0	-1.636094	2.216173	-0.782436

Equatorial cis-1,3,5-trimethylcyclohexane

Species name: eq_cis135tmcyclohex

Full file name: eq_cis135tmcyclohex_w1bd.log
Method: W1BD calculation
Point group: C3V
NImag: 0

Temperature=   298.150000 Pressure=   1.000000
E(ZPE)=   0.248925 E(Thermal)=   0.259167
W1BD (0 K)=   -353.662185 W1BD Energy=   -353.651943
W1BD Enthalpy=   -353.650998 W1BD Free Energy=   -353.695391
1\1\GINC-NODE32\Mixed\W1BD\W1BD\C9H18\RABLENP\12-Mar-2020\0\\#n W1BD f
opt=(calcfc,tight)\\Equatorial cis-1,3,5-trimethylcyclohexane\\0,1\C,0
,1.2786080639,-0.7382047093,0.3321552426\C,0,0.0000000005,-1.453551027

                        Standard orientation:

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

     1   6   0   1.278608   0.738205   -0.333600
     2   6   0   0.000000   1.453551   0.119483
     3   6   0   -1.278608   0.738205   -0.333600
     4   6   0   -1.258812   -0.726776   0.119483
     5   6   0   0.000000   -1.476409   -0.333600
     6   6   0   1.258812   -0.726776   0.119483
     7   6   0   2.533998   1.463004   0.152038
     8   6   0   -2.533998   1.463004   0.152038
     9   6   0   0.000000   -2.926009   0.152038
    10   1   0   1.290543   0.745096   -1.430515
    11   1   0   0.000000   2.482283   -0.252506
    12   1   0   0.000000   1.522246   1.214684
    13   1   0   -1.290543   0.745096   -1.430515
    14   1   0   -2.149720   -1.241141   -0.252506
    15   1   0   -1.318304   -0.761123   1.214684
    16   1   0   0.000000   -1.490191   -1.430515
    17   1   0   2.149720   -1.241141   -0.252506
    18   1   0   1.318304   -0.761123   1.214684
    19   1   0   2.573878   1.486029   1.244008
    20   1   0   3.440564   0.968006   -0.201599
    21   1   0   2.558600   2.495613   -0.201599
    22   1   0   -2.573878   1.486029   1.244008
    23   1   0   -2.558600   2.495613   -0.201599
    24   1   0   -3.440564   0.968006   -0.201599
    25   1   0   0.000000   -2.972059   1.244008
    26   1   0   -0.881964   -3.463619   -0.201599
    27   1   0   0.881964   -3.463619   -0.201599

[4.4.4.5]Fenestrane

Species name: 4445fenestrane
Full file name: 4445fenestrane_w1bd.log
Method: W1BD calculation
Point group: C2
NImag: 0

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.210661 E(Thermal)= 0.218704
W1BD (0 K)= -389.259942 W1BD Energy= -389.251899
W1BD Enthalpy= -389.250955 W1BD Free Energy= -389.291508
1\1\GINC-NODE33\Mixed\W1BD\W1BD\C10H14\RABLENP\12-Mar-2020\0\\#n W1BD
fopt=(calcfc,tight)\\[4.4.4.5]Fenestrane\\0,1\C,0,0.,0.,0.1395872872\C
,0,0.,0.,2.2835317643\C,0,0.5799410775,1.1311444115,-0.6661636825\C,0,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.139470
2	6	0	0.000000	0.000000	2.283415
3	6	0	0.592592	1.124568	-0.666281
4	6	0	-0.592592	-1.124568	-0.666281
5	6	0	0.000000	0.786566	-2.057022
6	6	0	0.000000	-0.786566	-2.057022
7	6	0	0.002577	2.104417	0.428721
8	6	0	-0.002577	-2.104417	0.428721
9	6	0	-0.675875	0.890296	1.173688
10	6	0	0.675875	-0.890296	1.173688
11	1	0	0.726567	0.501350	2.924709
12	1	0	-0.726567	-0.501350	2.924709
13	1	0	1.682268	1.148714	-0.724510
14	1	0	-1.682268	-1.148714	-0.724510
15	1	0	0.560673	1.204275	-2.893891
16	1	0	-1.030362	1.142537	-2.143095
17	1	0	1.030362	-1.142537	-2.143095
18	1	0	-0.560673	-1.204275	-2.893891
19	1	0	0.776220	2.634171	0.985084
20	1	0	-0.720307	2.837331	0.069834
21	1	0	-0.776220	-2.634171	0.985084
22	1	0	0.720307	-2.837331	0.069834
23	1	0	-1.760351	0.961304	1.238579
24	1	0	1.760351	-0.961304	1.238579