G3(MP2) Ring Strain in Bicyclic Phosphorus Heterocycles and Their Hydrocarbon Analogues

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Computational Details.

All geometry optimizations were performed with the Gaussian 98 suite of programs, using the B3LYP exchange-correlation potentials and 6-31G(*) basis-set (see mss). All structures were confirmed to have only positive force constants. The global minimum was subjected to a G3(MP2) evaluation of the energy. All values in kcal/mol.

2-Aza-1-Phosphabicyclo[1.1.0]butane (1A)

H	-2.141	-0.245	0.275
N	1.041	-0.612	-0.440
C	-0.029	-0.812	0.506
P	0.103	0.948	0.074
H	1.939	-0.626	0.069
H	0.042	-1.297	1.473
C	-1.203	-0.362	-0.265
H	-1.281	-0.728	-1.288

E(QCISD/6-31G*)=-297271.32

G3(MP2) Enthalpy=-297439.30

2-Aza-1-Phosphabicyclo[2.1.0]pentane (1B)

H	-1.623	1.261	0.779
C	-1.279	0.641	-0.061
N	-1.070	-0.790	0.282
C	0.139	0.955	-0.504
P	0.614	-0.854	-0.265
H	0.800	0.880	1.625
H	2.136	1.028	0.386
H	-2.006	0.723	-0.874
H	0.376	1.592	-1.351
C	1.113	0.718	0.594
H	-1.242	-1.031	1.259

E(QCISD/6-31G*)=-321869.43

G3(MP2) Enthalpy=-322071.00

2-Aza-1-Phosphabicyclo[3.1.0]hexane (1C)

H	-0.581	0.711	1.787
C	-0.417	1.037	-0.419
P	-0.997	-0.714	-0.331
N	0.627	-1.268	-0.030
C	1.538	-0.199	0.390
C	1.099	1.046	-0.382
H	-0.894	1.717	-1.121
H	1.492	1.954	0.092
C	-1.143	0.721	0.856
H	1.485	1.002	-1.405
H	0.681	-2.095	0.561
H	1.487	-0.004	1.471
H	2.572	-0.474	0.157
H	-2.146	1.130	0.962

E(QCISD/6-31G*)=-371061.78

G3(MP2) Enthalpy=-371326.33

2-Aza-1-Phosphabicyclo[4.1.0]heptane (1D)

H	0.850	2.478	0.081
C	0.768	1.477	-0.362
C	1.524	-0.918	-0.121
P	-1.226	-0.708	-0.361
N	0.221	-1.444	0.289
C	-0.691	1.072	-0.392
C	1.687	0.508	0.379
H	1.678	-0.935	-1.214
H	-2.437	1.095	0.986
C	-1.437	0.690	0.846
H	-0.870	0.562	1.764
H	1.484	0.521	1.455
H	1.121	1.560	-1.398
H	2.293	-1.559	0.325
H	2.726	0.831	0.242
H	0.171	-2.451	0.149
H	-1.278	1.657	-1.100

E(QCISD/6-31G*)=-371061.78

G3(MP2) Enthalpy=-371326.33

2-Aza-1-Phosphabicyclo[5.1.0]octane (1E)

H	0.667	1.476	-1.644
C	0.493	1.639	-0.573
H	0.535	2.726	-0.419
C	-0.921	1.201	-0.228
H	2.539	1.631	-0.012
P	-1.589	-0.508	-0.309
H	-0.482	0.395	1.798
H	-2.166	1.039	1.634
H	-1.659	1.904	-0.619
C	-1.296	0.635	1.121
N	-0.206	-1.542	-0.424
C	1.002	-1.477	0.397
H	1.478	1.150861	0.290
H	-0.545	-2.498	-0.497
H	0.783	-1.317	1.465
H	1.481	-2.460	0.323
C	1.996	-0.429	-0.088
C	1.651	1.027	0.214
H	2.131	-0.563	-1.167
H	2.962	-0.649	0.387

E(QCISD/6-31G*)=-395644.61

G3(MP2) Enthalpy=-395942.49

**2-Aza-1-Phosphabicyclo[5.1.0]octane (1E)
second conformer**

H	0.792	1.496	-1.532
C	0.376	1.602	-0.521
H	0.223	2.680	-0.371
C	-1.013	0.978	-0.492
H	2.129	1.912	0.675
P	-1.438	-0.821	-0.262
H	-1.199	0.715	1.702
H	-2.784	1.044	0.853
H	-1.647	1.395	-1.276
C	-1.755	0.702	0.769
N	0.052	-1.380	0.460
C	1.247	-1.271	-0.387
H	0.904	0.942	1.465
H	-0.068	-2.321	0.825
H	1.793	-2.222	-0.386
H	0.967	-1.078	-1.432
C	2.159	-0.151	0.108
C	1.399	1.112	0.505
H	2.889	0.082	-0.679
H	2.730	-0.502	0.976

E(QCISD/6-31G*)= -395644.94
G3(MP2) Enthalpy= -395941.11

Bicyclo[2.1.0]pentane

H	-0.609	1.459	1.278
C	0.246	0.988	0.779
C	0.246	0.988	-0.779
C	0.246	-0.538	0.763
C	0.246	-0.538	-0.763
H	-1.870	-0.463	0.000
H	-1.081	-2.112	0.000
H	1.166	1.413	1.187
H	0.794	-1.181	1.444
C	-0.943	-1.035	0.000
H	1.166	1.413	-1.187
H	-0.609	1.459	-1.278
H	0.794	-1.181	-1.444

E(QCISD/6-31G*)=-122142.55
G3(MP2) Enthalpy=-122300.84

Bicyclo[3.1.0]hexane

C	-0.916	-1.292	0.000
C	0.292	-0.809	0.754
C	0.292	-0.809	-0.754
C	0.292	0.633	-1.220
C	-0.197	1.432	0.000
C	0.292	0.633	1.220
H	0.874	-1.540	1.309
H	-1.820	-0.689	0.000
H	0.874	-1.540	-1.309
H	1.317	0.925	-1.479
H	-0.332	0.803	-2.105
H	-1.289	1.488	0.000
H	0.171	2.462	0.000
H	-0.332	0.803	2.105
H	1.317	0.925	1.479
H	-1.103	-2.361	0.000

E(QCISD/6-31G*)=-146754.68
G3(MP2) Enthalpy=-146943.73

Bicyclo[4.1.0]heptane

H	-0.469	2.408	-0.614
C	-0.346	1.514	0.007
C	-1.317	-0.760	0.478
C	1.032	-0.675	-0.470
C	-0.215	-1.508	-0.272
C	0.966	0.831	-0.353
C	-1.560	0.600	-0.166
H	-1.045	-0.625	1.533
H	1.224	-0.065	1.662
H	-0.607	-1.788	-1.259
H	1.603	1.383	-1.040
H	-1.758	0.453	-1.236
H	-0.308	1.866	1.046
H	-2.234	-1.361	0.470
H	1.710	-1.059	-1.231
H	0.036	-2.444	0.243
C	1.693	0.015	0.685
H	-2.449	1.081	0.259
H	2.777	0.051	0.717

E(QCISD/6-31G*)=-171342.72
G3(MP2) Enthalpy=-171563.25

Bicyclo[5.1.0]octane

H	1.414	1.126	1.349
C	0.326	1.264	1.305
C	0.326	1.264	-1.305
C	0.326	-1.201	-0.752
C	-0.361	-0.090	-1.510
C	-0.361	-0.090	1.510
C	-0.051	1.969	0.000
H	0.066	1.933	-2.135
H	1.249	-1.544	-1.216
H	-0.373	-0.347	-2.577
H	-1.413	-0.015	1.207
H	0.411	2.965	0.000
H	0.066	1.933	2.135
H	1.414	1.126	-1.349
H	1.249	-1.544	1.216
H	-1.413	-0.015	-1.207
C	0.326	-1.201	0.752
H	-1.137	2.140	0.000
C	-0.453	-2.247	0.000
H	-1.536	-2.154	0.000
H	-0.373	-0.347	2.577
H	-0.095	-3.272	0.000

E(QCISD/6-31G*)=-195929.75

G3(MP2) Enthalpy=-196182.78

2-Aza-1-Phosphabicyclo[1.1.0]butene (2A)

C	0.403	-1.017	0.518
N	-0.065	1.141	0.393
C	-0.371	-0.033	1.132
P	0.031	-0.097	-0.916
H	-0.849	1.806	0.342
H	0.656	-2.041	0.749

E(QCISD/6-31G*)=-296487.32

G3(MP2) Enthalpy=-296651.58

2-Aza-1-Phosphabicyclo[2.1.0]pentene (2B)

C	0.049	0.878	-0.540
C	1.011	1.066	0.368
P	0.801	-0.709	-0.192
H	1.022	1.579	1.328
C	-1.363	0.472	-0.181
H	-2.009	0.192	-1.021
H	-1.873	1.196	0.462
N	-0.848	-0.748	0.548
H	-1.397	-1.597	0.387

E(QCISD/6-31G*)=-321069.07

G3(MP2) Enthalpy=-321267.84

Bicyclo[5.1.0]octane, second conformer

H	0.271	1.839	2.124
C	-0.030	1.188	1.293
C	-0.030	1.188	-1.293
C	-0.030	-1.361	-0.752
C	0.452	-0.222	-1.625
C	0.452	-0.222	1.625
C	0.520	1.786	0.000
H	-1.126	1.216	-1.275
H	0.218	-2.330	-1.183
H	1.551	-0.223	-1.631
H	0.146	-0.448	2.655
H	1.615	1.697	0.000
H	-1.126	1.216	1.275
H	0.271	1.839	-2.124
H	0.218	-2.330	1.183
H	0.146	-0.448	-2.655
C	-0.030	-1.361	0.752
H	0.300	2.861	0.000
C	-1.335	-1.336	0.000
H	-1.900	-0.411	0.000
H	1.551	-0.223	1.631
H	-1.956	-2.227	0.000

E(QCISD/6-31G*)=-195928.12

G3(MP2) Enthalpy=-196180.93

2-Aza-1-Phosphabicyclo[2.1.0]pentene (2B-flat)

H	-1.955	-0.727	0.885
C	-1.382	-0.419	0.000
N	-0.084	-1.149	0.000
C	-1.186	1.044	0.000
P	1.211	-0.137	0.000
C	0.187	1.284	0.000
H	0.636	2.274	0.000
H	-1.955	-0.728	-0.885
H	-0.014	-2.164	0.000

E(QCISD/6-31G*)=-321091.51

G3(MP2) Enthalpy=-321291.55

2-Aza-1-Phosphabicyclo[3.1.0]hexene (2C)

H	1.511	0.800	-1.499
N	0.365	-1.297	0.141
P	-1.131	-0.522	-0.344
C	-0.237	1.034	-0.285
C	1.234	0.934	-0.450
C	1.489	-0.373	0.360
H	0.339	-2.078	0.792
H	2.424	-0.838	0.029
C	-1.148	1.048	0.676
H	1.595	-0.100	1.420
H	-1.285	1.504	1.653
H	1.803	1.767	-0.026

E(QCISD/6-31G*)=-345689.19

G3(MP2) Enthalpy=-345920.29

2-Aza-1-Phosphabicyclo[4.1.0]hexene (2D)

C	1.378	-1.082	0.678
P	1.361	0.409	-0.402
C	-1.217	1.167	-0.069
C	-1.038	-1.386	-0.399
C	-1.751	-0.220	0.318
C	0.403	-1.106	-0.204
N	0.158	1.409	0.404
H	-1.866	1.921	0.389
H	-1.336	-2.347	0.032
H	-2.824	-0.255	0.095
H	1.707	-1.513	1.615
H	0.383	2.402	0.351
H	-1.627	-0.345	1.399
H	-1.314	1.282	-1.163
H	-1.294	-1.389	-1.465

E(QCISD/6-31G*)=-370288.86

G3(MP2) Enthalpy=-370551.33

2-Aza-1-Phosphabicyclo[5.1.0]octene (2E)

H	-0.335	1.162	1.539
C	-0.377	1.587	0.523
H	-1.416	1.099	-1.296
N	0.881	1.434	-0.206
H	-0.532	2.665	0.642
P	1.657	-0.096	-0.438
H	-3.022	-0.610	-0.232
H	1.534	2.197	-0.040
H	-2.044	-0.526	1.229
C	1.179	-1.190	0.959
C	0.305	-1.209	-0.035
H	-2.456	1.646	0.012
H	1.305	-1.530	1.981
C	-1.088	-1.532	-0.417
H	-1.390	-2.505	-0.014
H	-1.178	-1.576	-1.508
C	-2.005	-0.430	0.137
C	-1.596	1.005	-0.218

E(QCISD/6-31G*)=-394881.30

G3(MP2) Enthalpy=-395176.69

Bicyclo[1.1.0]butene

H	1.3453	-0.4029	1.1479
C	1.0914	-0.0877	0.1417
C	-0.1578	-0.8891	-0.3553
C	-0.0206	0.8569	0.0049
H	1.9572	0.0080	-0.5130
H	-2.1703	-0.0383	0.3082
C	-1.0989	-0.0739	0.1852
H	-0.0166	1.5966	-0.8019

E(QCISD/6-31G*)=-96756.96

G3(MP2) Enthalpy=-96881.69

Bicyclo[2.1.0]pentene

H	1.414	-1.455	0.720
C	1.062	-0.756	-0.046
C	0.855	0.784	0.328
C	-0.403	-0.734	-0.362
C	-0.518	0.763	-0.374
H	-2.024	-0.392	1.185
H	-0.770	1.366	-1.241
H	1.694	-0.835	-0.935
H	0.799	0.920	1.416
C	-1.449	-0.234	0.277
H	1.608	1.462	-0.086

E(QCISD/6-31G*)=-121330.94

G3(MP2) Enthalpy=-121487.95

Bicyclo[3.1.0]hexene

C	1.578	-0.346	0.489
C	0.921	0.626	-0.444
C	0.619	-0.835	-0.269
C	-0.820	-1.168	-0.268
C	-1.338	0.156	0.387
C	-0.378	1.316	-0.006
H	1.436	0.998	-1.329
H	2.112	-0.450	1.426
H	-0.779	1.880	-0.855
H	-1.207	-1.283	-1.286
H	-1.096	-2.050	0.318
H	-1.320	0.012	1.471
H	-2.372	0.367	0.096
H	-0.259	2.023	0.824

E(QCISD/6-31G*)=-145957.63

G3(MP2) Enthalpy=-146144.98

Bicyclo[4.1.0]heptene

C	1.890	-0.367	0.412
C	0.833	-0.825	-0.207
C	0.061	1.517	0.172
C	-1.465	-0.544	0.377
C	-1.314	0.899	-0.135
C	-0.460	-1.528	-0.265
C	1.133	0.625	-0.437
H	0.199	1.585	1.260
H	-1.310	-0.555	1.463
H	-1.463	0.907	-1.223
H	-0.742	-1.716	-1.308
H	1.541	0.940	-1.401
H	-0.452	-2.487	0.263
H	0.111	2.538	-0.222
H	-2.487	-0.897	0.195
H	-2.115	1.513	0.296
H	2.643	-0.494	1.177

E(QCISD/6-31G*)=-170558.31

G3(MP2) Enthalpy=-170777.20

Bicyclo[5.1.0]octene

H	1.213	1.128	-1.272
C	1.322	1.084	-0.180
C	-1.260	1.243	-0.299
C	-0.425	-1.212	-0.085
C	-1.503	-0.246	-0.486
C	1.822	-0.307	0.231
C	0.015	1.562	0.484
H	-2.121	1.718	0.193
H	2.866	-0.426	-0.083
H	-2.131	-0.495	-1.347
H	1.175	-1.555	-1.419
H	0.065	2.650	0.609
H	2.115	1.798	0.073
H	-1.181	1.709	-1.291
C	1.003	-1.476	-0.339
C	-1.487	-1.205	0.677
H	1.811	-0.376	1.326
H	-0.054	1.145	1.497
H	1.320	-2.419	0.119
H	-1.996	-1.542	1.569

E(QCISD/6-31G*)=-195149.86

G3(MP2) Enthalpy=-195400.54

Cyclopropane

H	0.000	1.456	0.910
C	0.000	0.867	0.000
C	0.751	-0.433	0.000
C	-0.751	-0.433	0.000
H	0.000	1.456	-0.910
H	1.261	-0.728	0.910
H	1.261	-0.728	-0.910
H	-1.261	-0.728	0.910
H	-1.261	-0.728	-0.910

E(QCISD/6-31G*)=-73730.11

G3(MP2) Enthalpy=-73828.41

Cyclobutane

H	1.986	0.000	0.451
C	1.071	0.000	-0.147
C	0.000	1.071	0.147
C	0.000	-1.071	0.147
C	-1.071	0.000	-0.147
H	-1.986	0.000	0.451
H	-1.344	0.000	-1.207
H	1.344	0.000	-1.207
H	0.000	-1.986	-0.451
H	0.000	-1.344	1.207
H	0.000	1.986	-0.451
H	0.000	1.344	1.207

E(QCISD/6-31G*)=-98319.95

G3(MP2) Enthalpy=-98449.02

Cyclopentane

H	1.911	1.218	0.144
C	1.063	0.656	-0.259
C	0.976	-0.778	0.260
C	-0.438	-1.201	-0.147
C	-1.296	0.077	0.002
C	-0.293	1.246	0.143
H	1.162	0.644	-1.351
H	1.072	-0.778	1.353
H	1.753	-1.437	-0.139
H	-0.428	-1.527	-1.193
H	-0.821	-2.038	0.445
H	-1.950	0.016	0.877
H	-1.948	0.213	-0.866
H	-0.246	1.577	1.186
H	-0.573	2.117	-0.456

E(QCISD/6-31G*)=-122926.76

G3(MP2) Enthalpy=-123088.15

Cyclohexane-chair

H	-2.489	0.000	-0.131
C	-1.455	0.000	0.233
C	0.727	-1.260	0.233
C	0.727	1.260	0.233
C	1.455	0.000	-0.233
C	-0.727	1.260	-0.233
C	-0.727	-1.260	-0.233
H	0.754	-1.306	1.330
H	0.754	1.306	1.330
H	1.508	0.000	-1.330
H	-0.754	1.306	-1.330
H	-0.754	-1.306	-1.330
H	-1.508	0.000	1.330
H	1.245	-2.156	-0.131
H	1.245	2.156	-0.131
H	2.489	0.000	0.131
H	-1.245	2.156	0.131
H	-1.245	-2.156	0.131

E(QCISD/6-31G*)=-147520.39

G3(MP2) Enthalpy=-147713.04

Cyclohexane-boat

H	-2.173	0.269	0.835
C	-1.516	0.000	0.000
C	0.653	1.211	0.395
C	0.653	-1.211	-0.395
C	1.516	0.000	0.000
C	-0.653	-1.211	0.395
C	-0.653	1.211	-0.395
H	1.209	2.141	0.235
H	-1.209	-2.141	0.235
H	2.173	-0.269	0.835
H	-0.418	-1.174	1.465
H	-1.210	2.141	-0.235
H	-2.172	-0.269	-0.835
H	0.418	1.174	1.465
H	1.210	-2.141	-0.235
H	2.172	0.269	-0.835
H	0.418	-1.174	-1.465
H	-0.418	1.174	-1.465

E(QCISD/6-31G*)=-147513.90

G3(MP2) Enthalpy=-147706.78

Cycloheptane

H	-1.186	2.319	-0.522
C	-0.874	1.290	-0.302
C	0.147	-0.749	-1.535
C	0.000	-1.298	0.956
C	0.874	-1.290	-0.302
C	0.000	1.298	0.956
C	-0.147	0.749	-1.535
H	-0.797	-1.300	-1.640
H	0.314	-2.113	1.619
H	1.799	-0.725	-0.125
H	-0.314	2.113	1.619
H	0.797	1.300	-1.640
H	-1.799	0.725	-0.125
H	0.735	-0.982	-2.432
H	0.875	0.011	2.430
H	1.186	-2.319	-0.522
C	0.000	0.000	1.769
H	-0.735	0.982	-2.432
H	-0.875	-0.011	2.430
H	-1.026	-1.543	0.654
H	1.026	1.543	0.654

E(QCISD/6-31G*)=-172100.85

G3(MP2) Enthalpy=-172325.85

Cyclopropene

H	-0.913	1.456	0.000
C	0.000	0.858	0.000
C	0.000	-0.499	0.651
C	0.000	-0.499	-0.651
H	0.913	1.456	0.000
H	0.000	-1.038	-1.584
H	0.000	-1.038	1.584

E(QCISD/6-31G*)=-72947.08

G3(MP2) Enthalpy=-73043.58

Aza-phosphacyclobutane

H	-1.422	-0.176	1.294
C	-1.275	-0.131	0.203
N	-0.255	-1.078	-0.283
C	-0.451	1.116	-0.158
H	-2.248	-0.242	-0.291
H	-0.538	1.977	0.506
H	-0.607	1.421	-1.194
P	1.074	0.037	-0.010
H	1.087	0.126	1.427
H	-0.242	-2.015	0.119

E(QCISD/6-31G*)=-298032.93

G3(MP2) Enthalpy=-298207.60

Aza-phosphacyclopentane

H	-0.029	1.858	1.005
C	-0.040	1.361	0.031
P	1.294	0.028	-0.044
N	0.156	-1.283	-0.163
C	-1.153	-0.820	0.310
C	-1.362	0.611	-0.195
H	0.125	2.124	-0.733
H	-2.203	1.106	0.302
H	1.500	-0.047	1.358
H	-1.588	0.573	-1.267
H	0.105	-1.627	-1.120
H	-1.137	-0.831	1.406
H	-1.939	-1.507	-0.020

E(QCISD/6-31G*)=-322638.46

G3(MP2) Enthalpy=-322844.58

Aza-phosphacyclohexane

H	0.961	1.260	1.355
C	1.013	1.247	0.259
C	0.926	-1.290	0.228
P	-1.505	-0.023	0.090
N	-0.412	-1.273	-0.358
C	-0.398	1.399	-0.309
C	1.696	-0.044	-0.192
H	1.449	-2.184	-0.129
H	1.790	-0.049	-1.284
H	-0.361	1.483	-1.401
H	-0.869	2.314	0.068
H	2.709	-0.091	0.225
H	1.627	2.107	-0.036
H	0.893	-1.343	1.331
H	-1.307	0.068	1.510
H	-0.852	-2.188	-0.393

E(QCISD/6-31G*)=-371061.78

G3(MP2) Enthalpy=-371326.33

Aza-phosphacycloheptane

H	-0.376	1.277	-1.464
C	-0.569	1.546	-0.416
C	-1.777	-0.752	-0.120
N	0.649	-1.336	-0.338
C	-0.575	-1.522	0.428
C	0.702	1.384	0.426
C	-1.772	0.758	0.112
H	-2.691	-1.163	0.329
P	1.754	-0.052	-0.125
H	-0.813	-2.594	0.445
H	0.425	1.309	1.483
H	-2.681	1.167	-0.346
H	-0.846	2.607	-0.424
H	-1.847	-0.958	-1.197
H	1.330	2.278	0.331
H	-0.372	-1.232	1.466
H	2.261	-0.382	1.161
H	-1.864	0.954	1.189
H	0.556	-1.615	-1.309

E(QCISD/6-31G*)=-371811.17

G3(MP2) Enthalpy=-372082.32

NH₂-C(PH₂)=CH₂

N	1.119	-1.177	0.090
C	0.487	0.076	-0.001
C	1.151	1.245	-0.001
P	-1.344	-0.075	-0.088
H	2.238	1.275	-0.026
H	0.633	2.193	0.050
H	0.738	-1.872	-0.546
H	2.128	-1.119	-0.023
H	-1.593	-0.345	1.279
H	-1.639	1.305	-0.027

E(QCISD/6-31G*)=-298029.09

G3(MP2) Enthalpy=-298207.52

Me₂-C=CH₂

H	0.000	0.924	2.028
C	0.000	0.000	1.459
C	0.000	0.000	0.120
H	0.000	-0.924	2.028
C	0.000	1.273	-0.679
C	0.000	-1.273	-0.679
H	0.880	1.324	-1.330
H	0.000	2.153	-0.032
H	-0.880	1.324	-1.330
H	-0.880	-1.324	-1.330
H	0.000	-2.153	-0.032
H	0.880	-1.324	-1.330

E(QCISD/6-31G*)=-98327.77

G3(MP2) Enthalpy=-98460.19

NH₂-CH(PH₂)-CH₃

H	-0.493	0.087	-1.493
C	-0.436	0.059	-0.399
P	1.390	-0.168	0.002
C	-1.206	-1.161	0.092
N	-1.101	1.264	0.094
H	-0.807	-2.086	-0.332
H	-2.257	-1.063	-0.188
H	-1.152	-1.238	1.184
H	-1.036	1.289	1.112
H	-0.610	2.094	-0.238
H	1.801	1.158	-0.289
H	1.266	0.045	1.400

E(QCISD/6-31G*)=-298782.72

G3(MP2) Enthalpy=-298963.01

NH₂-PH-CH₃

H	-2.200	0.254	-0.373
N	-1.300	0.582	-0.044
H	-1.409	1.130	0.804
P	-0.066	-0.619	-0.085
C	1.416	0.471	-0.014
H	0.015	-1.071	1.266
H	2.310	-0.136	0.152
H	1.353	1.219	0.781
H	1.523	0.988	-0.969

E(QCISD/6-31G*)=-274207.16

G3(MP2) Enthalpy=-274345.08

PH₂-C(CH₃)=CH₂

H	1.518	-0.914	1.037
P	1.373	0.045	0.000
H	1.518	-0.914	-1.037
C	-0.463	0.122	0.000
C	-1.036	1.336	0.000
C	-1.274	-1.143	0.000
H	-2.346	-0.926	0.000
H	-1.045	-1.753	0.880
H	-1.045	-1.753	-0.880
H	-0.447	2.248	0.000
H	-2.117	1.452	0.000

E(QCISD/6-31G*)=-287979.85

G3(MP2) Enthalpy=-288140.22

Ethane

H	0.000	1.019	1.157
C	0.000	0.000	0.762
H	0.882	-0.509	1.157
C	0.000	0.000	-0.762
H	-0.882	-0.509	1.157
H	0.882	0.509	-1.157
H	-0.882	0.509	-1.157
H	0.000	-1.019	-1.157

E(QCISD/6-31G*)=-49908.68

G3(MP2) Enthalpy=-49979.06

Ethene

H	0.923	0.000	-1.238
C	0.000	0.000	-0.667
C	0.000	0.000	0.667
H	-0.923	0.000	-1.238
H	0.923	0.000	1.238
H	-0.923	0.000	1.238

E(QCISD/6-31G*)=-49147.87

G3(MP2) Enthalpy=-49216.