P-heterocyclic carbenes as potential ligands for the design of new metathesis catalysts

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Supplementary Material

p1

Atom Coordinates (x,y,z) in Angstrom

Ru	0.262769	-0.015109	0.134448
Cl	0.281856	2.323020	-0.123579
Cl	0.329197	-2.078008	-0.986830
C	-1.705067	0.009047	0.095013
C	0.333899	-0.375181	1.930734
P	2.724645	-0.004247	-0.062946
H	-0.574668	-0.420695	2.572129
H	1.291160	-0.555853	2.468893
C	3.620928	-1.557684	0.390212
C	3.614419	1.307739	0.890239
C	3.262452	0.302416	-1.805078
P	-2.743601	-1.394426	0.448792
C	-4.399154	-0.643110	0.329839
C	-4.395366	0.565169	-0.297170
P	-2.763168	1.383896	-0.358570
H	-2.502084	-1.756181	1.817451
H	-5.316608	1.095109	-0.594478
H	-2.538355	1.724916	-1.730610
H	-5.317039	-1.207588	0.565576
H	4.702640	1.315059	0.672828
H	3.167158	2.287481	0.628388
H	3.460940	1.142286	1.976046
H	4.367903	0.327591	-1.898154
H	2.853150	-0.501822	-2.448876
H	2.839800	1.270734	-2.140929
H	4.710338	-1.483326	0.192642
H	3.460812	-1.777066	1.465613
H	3.184307	-2.389800	-0.197125

Energy E(RB-P86) -2314.67909472 a.u.
-6077189.96 kJ/mol
-1452483.12 kcal/mol
SCF Convergence: 0.9828D-08
Maximum Force: 0.000013
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.192425 a.u.
Lowest Frequency 33.0752 cm-1

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p2

Atom Coordinates (x,y,z) in Angstrom

Ru	1.079293	0.062239	0.111911
Cl	1.305496	1.964889	1.363239
Cl	1.664996	-0.663015	-1.984892
C	-0.755590	-0.158021	0.014730
C	1.429914	-1.339275	1.214067
H	0.672964	-2.090068	1.537019
H	2.473863	-1.483871	1.579808
P	-1.815616	-1.006695	1.259267
C	-3.403948	-0.629126	0.421224
C	-3.341571	-0.098017	-0.824680
P	-1.719635	0.559566	-1.376753
H	-1.775947	-0.013588	2.301950
H	-4.243325	0.074793	-1.437729
H	-1.302743	-0.357434	-2.408018
H	-4.356142	-0.946640	0.881216

Energy E(RB-P86) -1853.71724796 a.u.
-4866934.63 kJ/mol

```
                    -1163225.18 kcal/mol
SCF Convergence: 0.8784D-08
  Maximum Force: 0.000014
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.081604 a.u.
Lowest Frequency    44.7695 cm-1
```

p3

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru  -0.888370  -0.053004   0.107674
 Cl  -0.722169  -2.343277  -0.420233
 Cl  -0.967960   2.196391  -0.564453
 C    1.050803   0.023926   0.049786
 C   -0.876300  -0.038711   1.946073
 H    0.058862  -0.071145   2.545731
 H   -1.816843  -0.017825   2.534057
 C   -3.333712   0.269300   0.395264
 C   -3.109625  -0.352601  -0.806409
 H   -3.387562   1.365309   0.480147
 H   -3.621207  -0.322749   1.279794
 H   -3.217053  -1.441741  -0.919313
 H   -2.985912   0.234107  -1.733230
 P    2.036333   1.417267   0.559644
 C    3.710627   0.750317   0.318945
 C    3.739023  -0.364161  -0.462853
 P    2.143722  -1.239724  -0.597076
 H    1.814533   1.612223   1.963846
 H    4.671481  -0.811445  -0.847338
 H    1.909018  -1.428038  -1.995669
 H    4.609448   1.318992   0.610616
------------------------------------
Energy E(RB-P86)  -1932.24785639 a.u.
                    -5073116.75 kJ/mol
                    -1212503.89 kcal/mol
SCF Convergence: 0.3457D-08
  Maximum Force: 0.000043
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.134396 a.u.
Lowest Frequency    36.6639 cm-1
```

p4

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru   0.246261  -0.879225   0.089229
 C    2.041397  -1.024373   0.387730
 C   -0.039451   1.025907   0.043130
 Cl  -0.184967  -0.875568   2.468338
 Cl   0.876818  -0.605605  -2.279987
 H    2.397795  -1.351200   1.387310
 H    2.777987  -0.841491  -0.420914
 C   -0.933829  -2.838669   0.385090
 C   -0.642683  -2.756296  -0.967727
 H   -0.312425  -3.433037   1.073778
 H    0.222163  -3.276684  -1.407073
 H   -1.366764  -2.347556  -1.690723
 H   -1.904413  -2.508385   0.789725
 P   -1.723359   1.494397   0.486313
 P    0.937540   2.386448  -0.565845
 C   -1.573950   3.258064   0.004723
 C   -0.432061   3.602366  -0.646487
 H   -1.601691   1.400202   1.921709
```

```
 H    1.156656   1.850311  -1.892148
 H   -0.268497   4.611852  -1.061762
 H   -2.426994   3.947182   0.126273
-----------------------------------
Energy E(RB-P86)  -1932.23581914 a.u.
                    -5073085.14 kJ/mol
                    -1212496.33 kcal/mol
SCF Convergence: 0.8122D-08
  Maximum Force: 0.000009
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.133590 a.u.
Lowest Frequency    42.2770 cm-1
```

(p4-p5)≠

```
Atom Coordinates (x,y,z) in Angstrom
-----------------------------------
 Ru   0.062726   0.859355   0.037894
 Cl  -0.339578   1.059494  -2.290841
 Cl   0.041512   0.675046   2.416232
 P    0.538659  -2.125035  -1.392289
 P   -0.771471  -2.086043   1.187318
 C   -0.006142  -1.076616  -0.058527
 C    0.132208  -3.758602  -0.701384
 C   -0.718378  -3.708104   0.363228
 C   -0.984303   2.889032   0.380765
 C    0.293382   3.319219   0.050126
 C    1.853743   1.234526  -0.145325
 H    1.969725  -2.045769  -1.474902
 H   -2.151655  -1.743995   1.365977
 H    0.407441  -4.692493  -1.219853
 H   -1.189636  -4.600017   0.809660
 H   -1.758944   2.834139  -0.402987
 H   -1.308677   2.858924   1.432876
 H    0.553208   3.559924  -0.992714
 H    1.003984   3.619811   0.837048
 H    2.263468   1.714403  -1.062533
 H    2.587374   0.965706   0.649715
-----------------------------------
Energy E(RB-P86)  -1932.23570939 a.u.
                    -5073084.86 kJ/mol
                    -1212496.26 kcal/mol
SCF Convergence: 0.3844D-08
  Maximum Force: 0.000013
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.133549 a.u.
Lowest Frequency  -251.4749 cm-1
```

p5

```
Atom Coordinates (x,y,z) in Angstrom
-----------------------------------
 Ru   0.838036   0.026789   0.035087
 Cl   0.693343   2.346081   0.542070
 Cl   0.885959  -2.295357  -0.475823
 C   -1.078734  -0.034767  -0.044630
 C    2.259871  -0.338377   1.385028
 C    3.132201   0.100325   0.131348
 C    2.341777   0.487789  -1.191395
 H    2.287133   0.389346   2.217202
 H    2.409336  -1.393042   1.679925
 H    3.700145   1.000830   0.433342
 H    3.777516  -0.762845  -0.119917
 H    2.484721  -0.233492  -2.017325
```

```
 H    2.447577   1.550965  -1.474321
 P   -2.068550  -1.467765   0.295195
 C   -3.723594  -0.726575   0.156085
 C   -3.735923   0.486875  -0.470299
 P   -2.125958   1.332785  -0.470930
 H   -1.908978  -1.890195   1.655969
 H   -4.660234   1.002457  -0.781263
 H   -1.878971   1.768918  -1.814162
 H   -4.635929  -1.300882   0.389714
-------------------------------------
Energy E(RB-P86)  -1932.26109596 a.u.
                    -5073151.51 kJ/mol
                    -1212512.19 kcal/mol
SCF Convergence: 0.3435D-08
  Maximum Force: 0.000030
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.137527 a.u.
Lowest Frequency    40.9728 cm-1
```

(p1-p6)≠

```
Atom Coordinates (x,y,z) in Angstrom
-------------------------------------
 Ru   0.175196  -0.014263  -0.216258
 Cl   0.027750  -2.306063  -0.650681
 Cl   0.470128   0.337035   2.196149
 C   -1.767370   0.050268  -0.106920
 C    0.255256   0.626907  -1.954328
 P    2.687808  -0.398802  -0.099996
 H    1.207341   0.840211  -2.488426
 H   -0.651907   0.921868  -2.531307
 C    3.903215   0.837170   0.565084
 C    3.473840  -0.888310  -1.708055
 C    3.045512  -1.855775   0.979664
 P   -2.824683   1.505462  -0.284527
 C   -4.463514   0.720604  -0.082046
 C   -4.417130  -0.541604   0.419170
 P   -2.800660  -1.378940   0.256444
 H   -2.690409   1.801418  -1.689455
 H   -5.318502  -1.096059   0.733482
 H   -2.433947  -1.814828   1.570816
 C    1.301220   2.866351   0.046329
 C   -0.002998   3.208838   0.134283
 H   -0.554152   3.620943  -0.727525
 H   -0.554885   3.109812   1.082043
 H    1.840433   2.497987   0.929339
 H    1.870516   2.993328  -0.889550
 H   -5.395346   1.302901  -0.182704
 H    4.913428   0.383570   0.638478
 H    3.959292   1.729821  -0.088058
 H    3.574030   1.150513   1.575983
 H    4.127611  -2.100110   0.986100
 H    2.701440  -1.611058   2.004135
 H    2.457551  -2.719898   0.613741
 H    4.530439  -1.197561  -1.569387
 H    2.897477  -1.731944  -2.138320
 H    3.441866  -0.042358  -2.424895
-------------------------------------
Energy E(RB-P86)  -2393.17829753 a.u.
                    -6283289.62 kJ/mol
                    -1501742.12 kcal/mol
SCF Convergence: 0.9861D-08
  Maximum Force: 0.000004
```

```
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.243270 a.u.
Lowest Frequency  -122.8563 cm-1
```

p6

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru  -0.375582  -0.253590  -0.314471
 Cl   1.899638  -1.131612   0.000404
 Cl   0.202298   2.270780  -0.200146
 C   -0.306982  -0.102491   1.705885
 C   -0.872136  -2.026692  -0.561365
 P    0.525543   0.098791  -2.576343
 H   -0.135390  -2.863130  -0.562196
 H   -1.918846  -2.358531  -0.778233
 C   -0.441354   1.127906  -3.768117
 C    0.810623  -1.476246  -3.500676
 C    2.170699   0.920205  -2.600957
 P   -0.562725  -1.459808   2.832926
 C    0.023584  -0.705684   4.388769
 C    0.184019   0.641295   4.302920
 P    0.291936   1.295503   2.596678
 H    0.416453  -2.418835   2.414791
 H    0.415067   1.280997   5.171995
 C   -2.493801   0.263059   0.154374
 C   -2.267248   0.434058  -1.225824
 H   -2.130064   1.453460  -1.619026
 H   -2.650605  -0.318992  -1.937050
 H   -3.020985  -0.625351   0.540053
 H   -2.513888   1.146415   0.812289
 H   -0.569881   2.423857   2.493365
 H    0.070729  -1.275560   5.331707
 H    1.311676  -1.288081  -4.472560
 H    1.451589  -2.124503  -2.870517
 H   -0.156889  -1.987879  -3.675383
 H    2.514599   1.038815  -3.649026
 H    2.064741   1.902720  -2.101623
 H    2.878387   0.302542  -2.016896
 H    0.120128   1.233025  -4.719049
 H   -1.427613   0.670531  -3.977546
 H   -0.592231   2.130821  -3.321694
------------------------------------
Energy E(RB-P86)  -2393.21457227 a.u.
                    -6283384.86 kJ/mol
                    -1501764.88 kcal/mol
SCF Convergence: 0.6185D-08
  Maximum Force: 0.000010
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.246681 a.u.
Lowest Frequency    37.8911 cm-1
```

(p6-p7)≠

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru  -0.343684  -0.211305  -0.274759
 Cl   1.952491  -1.044946  -0.032039
 Cl   0.614167   2.193037  -0.139059
 C   -0.355476  -0.047057   1.708630
 C   -0.752141  -2.020006  -0.592301
 P    0.433110   0.001960  -2.642989
 H    0.072274  -2.766492  -0.611330
 H   -1.743284  -2.452172  -0.858661
```

C	-0.649349	0.866920	-3.873810
C	0.758819	-1.622033	-3.466702
C	2.038260	0.879824	-2.827468
P	-0.774521	-1.392439	2.817271
C	-0.220170	-0.674734	4.405353
C	0.053865	0.653669	4.330736
P	0.324980	1.297119	2.635991
H	0.193964	-2.387524	2.455221
H	0.286201	1.273394	5.214273
C	-2.589261	-0.106816	-0.127433
C	-2.135017	1.029779	-0.807128
H	-1.994084	1.992516	-0.293739
H	-2.255802	1.099580	-1.898089
H	-3.051302	-0.938037	-0.684847
H	-2.871418	-0.054771	0.935997
H	-0.462084	2.478057	2.501381
H	-0.269389	-1.243354	5.349182
H	1.203428	-1.481038	-4.473501
H	1.464407	-2.187858	-2.826227
H	-0.185187	-2.195873	-3.557178
H	2.329961	0.914726	-3.897252
H	1.937554	1.896837	-2.402389
H	2.790879	0.331339	-2.228727
H	-0.159357	0.881078	-4.869275
H	-1.626774	0.351643	-3.965639
H	-0.821784	1.910933	-3.544491

Energy E(RB-P86) -2393.20668424 a.u.
-6283364.15 kJ/mol
-1501759.93 kcal/mol
SCF Convergence: 0.9381D-08
Maximum Force: 0.000002
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.246561 a.u.
Lowest Frequency -83.0336 cm-1

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p7

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.268851	-0.208666	-0.263234
Cl	2.004092	-1.103827	-0.263458
Cl	0.838360	2.105113	-0.015566
C	-0.255292	-0.218138	1.717823
C	-0.739775	-2.009352	-0.592916
P	0.185289	0.280645	-2.664726
H	0.075891	-2.764096	-0.632331
H	-1.743871	-2.429056	-0.824648
C	-0.856620	1.587099	-3.460678
C	-0.011287	-1.163792	-3.805952
C	1.897723	0.853618	-3.004154
P	-0.733422	-1.629162	2.713115
C	-0.200468	-1.046113	4.363982
C	0.118702	0.274101	4.393593
P	0.456754	1.029838	2.757851
H	0.223870	-2.617649	2.299885
H	0.348343	0.818398	5.326172
H	-0.299900	2.238124	2.691716
C	-2.486584	-0.061722	-0.453561
C	-1.991574	1.230403	-0.231545
H	-2.027600	1.684301	0.770653
H	-1.878867	1.954572	-1.050107
H	-2.793757	-0.374273	-1.466191

H	-2.945036	-0.638444	0.367134
H	-0.292176	-1.677824	5.263517
H	2.040311	1.024504	-4.091015
H	2.066958	1.782928	-2.426376
H	2.596698	0.084470	-2.622294
H	0.242931	-0.896620	-4.852516
H	0.664937	-1.970800	-3.459493
H	-1.054624	-1.535992	-3.765366
H	-0.571548	1.715124	-4.525211
H	-1.931891	1.322380	-3.406427
H	-0.691167	2.542956	-2.924554

Energy E(RB-P86) -2393.20924264 a.u.
-6283370.87 kJ/mol
-1501761.54 kcal/mol
SCF Convergence: 0.5204D-08
Maximum Force: 0.000076
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.246396 a.u.
Lowest Frequency 30.6393 cm-1

(p7-p8)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.181531	-0.106637	-0.215085
Cl	1.953903	-1.411195	-0.566931
Cl	1.092122	2.002002	0.034411
C	-0.216360	-0.221924	1.745996
C	-0.435881	-1.994170	-0.490700
P	0.093841	0.331650	-2.683501
H	-0.068507	-2.770671	0.211861
H	-0.925951	-2.448610	-1.382199
C	-0.973928	1.651158	-3.432898
C	-0.193707	-1.100093	-3.827415
C	1.784479	0.892814	-3.159131
P	-0.983516	-1.513388	2.743056
C	-0.501760	-0.967186	4.417683
C	-0.010980	0.298626	4.455627
P	0.534580	0.981213	2.844139
H	-0.195421	-2.683829	2.471213
H	0.215352	0.825650	5.399121
H	-0.134564	2.235868	2.710555
C	-2.365193	-0.175442	-0.473956
C	-1.950834	1.156670	-0.200798
H	-2.100839	1.580561	0.805358
H	-1.892245	1.909406	-1.000091
H	-2.642169	-0.480799	-1.498541
H	-2.844344	-0.775099	0.318935
H	-0.745317	-1.561116	5.314862
H	1.839694	1.117820	-4.244045
H	2.026997	1.790238	-2.556615
H	2.505093	0.096991	-2.889252
H	-0.002589	-0.822179	-4.884305
H	0.491651	-1.922531	-3.539484
H	-1.238383	-1.462602	-3.737171
H	-0.745851	1.776573	-4.511545
H	-2.048082	1.398637	-3.323578
H	-0.778176	2.609181	-2.910394

Energy E(RB-P86) -2393.19711043 a.u.
-6283339.01 kJ/mol
-1501753.92 kcal/mol

SCF Convergence: 0.9122D-08
  Maximum Force: 0.000017
<S**2>:   0.0000
Charge: 0.0000
ZPE-correction: 0.245733 a.u.
Lowest Frequency -224.6514 cm-1

p8

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.174601	-0.125342	-0.300225
Cl	2.219981	-0.360185	-0.078651
Cl	0.219105	2.323123	0.275964
C	-0.349797	-0.398306	1.662231
C	-0.711315	-2.000092	-0.695574
P	0.413838	0.406141	-2.638712
H	-0.778975	-2.761503	0.111082
H	-0.509787	-2.474720	-1.675598
C	-0.905009	1.083266	-3.760503
C	1.084627	-1.007759	-3.632792
C	1.739832	1.675739	-2.790491
P	-0.195693	-1.935168	2.567029
C	-0.180172	-1.319042	4.282347
C	-0.533928	-0.008525	4.389239
P	-0.417072	0.925765	2.825319
H	1.123655	-2.406722	2.261768
H	-0.682906	0.499840	5.357349
H	-1.583676	1.736657	2.700135
C	-2.093727	-1.119855	-0.714274
C	-2.090471	0.447203	-0.543026
H	-2.633582	0.795883	0.354536
H	-2.382885	0.999755	-1.452745
H	-2.504728	-1.318301	-1.722886
H	-2.705912	-1.543646	0.104625
H	-0.044582	-1.995085	5.142859
H	-0.504042	1.283831	-4.775458
H	-1.749580	0.369430	-3.851727
H	-1.288977	2.032906	-3.335826
H	1.965793	1.894648	-3.854324
H	1.408772	2.587854	-2.255967
H	2.637108	1.289339	-2.269375
H	1.446697	-0.673628	-4.626985
H	1.923869	-1.454983	-3.063360
H	0.305393	-1.783310	-3.779980

Energy E(RB-P86) -2393.20180939 a.u.
                    -6283351.35 kJ/mol
                    -1501756.87 kcal/mol
SCF Convergence: 0.3313D-08
  Maximum Force: 0.000062
<S**2>:   0.0000
Charge: 0.0000
ZPE-correction: 0.247303 a.u.
Lowest Frequency   27.6406 cm-1

(p1-p9)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	0.349037	0.269132	0.001239
Cl	-0.149006	0.281237	2.303477
Cl	-0.430461	0.360896	-2.218108
C	0.289955	-1.703663	0.022050
C	2.180766	0.250747	-0.132285
P	0.428859	2.734092	0.009796

H	2.777090	-0.688427	-0.112423
H	2.795392	1.173312	-0.229663
C	1.228152	3.536375	-1.453299
C	1.307867	3.478862	1.456075
C	-1.230004	3.549019	0.066169
P	0.729451	-2.730520	-1.362894
C	0.641229	-4.390855	-0.617311
C	-0.023339	-4.406748	0.570821
P	-0.168135	-2.775845	1.379334
H	2.095870	-2.449368	-1.698171
H	-0.304816	-5.336389	1.094651
H	-1.551346	-2.603314	1.698646
H	0.927605	-5.299716	-1.172771
H	1.269429	4.587844	1.443007
H	0.835256	3.092009	2.380896
H	2.367165	3.151195	1.455336
H	-1.146572	4.654137	0.123025
H	-1.792731	3.268083	-0.846124
H	-1.784948	3.170884	0.947803
H	1.198198	4.643482	-1.387885
H	2.284258	3.207330	-1.530953
H	0.698420	3.196453	-2.365418
C	-3.486789	-0.710840	0.003038
C	-3.690616	0.607499	-0.149233
H	-3.844085	-1.251794	0.895703
H	-2.943139	-1.295347	-0.757675
H	-4.222198	1.206231	0.609527
H	-3.321456	1.137012	-1.043002

Energy E(RB-P86) -2393.20189660 a.u.
-6283351.58 kJ/mol
-1501756.93 kcal/mol
SCF Convergence: 0.3010D-08
Maximum Force: 0.000263
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.242642 a.u.
Lowest Frequency -33.9565 cm-1

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p9

Atom Coordinates (x,y,z) in Angstrom

Ru	0.264443	-0.004019	-0.020225
Cl	0.213508	2.412399	-0.014084
Cl	0.186956	-2.372719	-0.558517
C	-1.722887	0.005220	0.207252
C	0.385581	-0.284059	1.831600
P	2.727842	0.001017	0.104927
H	-0.505865	-0.362165	2.493409
H	1.323221	-0.422643	2.415208
C	3.446642	-1.564047	0.786045
C	3.372380	1.307646	1.248041
C	3.804341	0.275399	-1.380511
P	-2.710218	-1.465205	0.386709
C	-4.325508	-0.745773	0.838755
C	-4.403778	0.595283	0.623968
P	-2.780632	1.413872	0.466847
H	-2.238790	-2.229099	1.498473
H	-5.338580	1.175330	0.707846
H	-2.838459	2.250634	-0.689323
H	-5.195153	-1.378706	1.083668
H	4.479492	1.283993	1.313649
H	3.028991	2.292098	0.871993

```
 H    2.944037   1.170173   2.260618
 H    4.875361   0.254439  -1.091401
 H    3.620450  -0.513753  -2.135561
 H    3.574204   1.259767  -1.833827
 H    4.547552  -1.491324   0.901546
 H    2.990493  -1.787935   1.770875
 H    3.187815  -2.398187   0.104070
 C   -0.608828   0.219395  -2.330969
 C    0.765121   0.227624  -2.412287
 H   -1.172708   1.163428  -2.304908
 H   -1.177707  -0.712717  -2.469199
 H    1.308184   1.182443  -2.475568
 H    1.310790  -0.698882  -2.646054
------------------------------------
Energy E(RB-P86)  -2393.20571671 a.u.
                    -6283361.61 kJ/mol
                    -1501759.32 kcal/mol
SCF Convergence: 0.5662D-08
  Maximum Force: 0.000094
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.245683 a.u.
Lowest Frequency    27.1114 cm-1
```

p'1

Atom Coordinates (x,y,z) in Angstrom

Ru	0.347848	0.190286	0.200580
Cl	0.356835	2.494361	-0.284524
Cl	0.385058	-2.021218	-0.630361
C	-1.643570	0.194566	0.194548
C	0.449340	0.045066	2.024710
P	2.783670	0.193899	-0.018527
H	-0.448396	0.125421	2.673969
H	1.407715	-0.108339	2.571859
C	3.686394	-1.293146	0.612688
C	3.669958	1.606439	0.781761
C	3.325820	0.298539	-1.784142
P	-2.701084	-1.127052	0.683337
C	-4.357030	-0.437140	0.469659
C	-4.345077	0.706202	-0.271424
P	-2.703213	1.490285	-0.448195
C	-2.459955	-1.894077	2.326564
H	-5.254370	1.199054	-0.654133
C	-2.467415	1.785288	-2.254380
H	-5.269432	-0.988686	0.751047
H	4.760115	1.588610	0.575563
H	3.224881	2.549069	0.405502
H	3.503770	1.566175	1.877680
H	4.431482	0.317312	-1.879329
H	2.920856	-0.576503	-2.331213
H	2.899315	1.219198	-2.231053
H	4.774762	-1.242833	0.402675
H	3.532311	-1.377978	1.707884
H	3.247048	-2.191520	0.134900
C	-3.332972	-1.610582	3.403433
C	-3.153732	-2.254240	4.639741
C	-2.103990	-3.173664	4.814893
C	-1.413007	-2.830241	2.500691
C	-1.233942	-3.454797	3.745576
H	-4.144358	-0.876496	3.278811
H	-3.836526	-2.027648	5.474242
H	-1.966050	-3.674522	5.786329
H	-0.742663	-3.056514	1.654958
H	-0.412619	-4.177312	3.876655
C	-2.126444	0.733363	-3.134147
C	-1.966641	0.992872	-4.505766
C	-2.152115	2.293693	-5.008435
C	-2.641035	3.091576	-2.759409
C	-2.491114	3.341386	-4.134393
H	-1.977338	-0.285336	-2.742575
H	-1.694951	0.170023	-5.186329
H	-2.026265	2.492165	-6.084823
H	-2.882046	3.917777	-2.071486
H	-2.629276	4.363258	-4.522342

Energy E(RB-P86) -2776.45403795 a.u.
-7289580.08 kJ/mol
-1742251.29 kcal/mol
SCF Convergence: 0.3588D-08
Maximum Force: 0.000048
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.353608 a.u.
Lowest Frequency 22.1385 cm-1

p'2

Atom Coordinates (x,y,z) in Angstrom

Ru	1.250772	-0.083426	0.259479
Cl	1.584487	2.016892	1.106396
Cl	2.171028	-1.268897	-1.467335
C	-0.579369	-0.140852	-0.032287
C	1.299766	-1.238593	1.659787
H	0.427714	-1.856477	1.977591
H	2.249226	-1.381289	2.226874
P	-1.863793	-0.732579	1.158796
C	-3.289234	-0.120953	0.180480
C	-3.050908	0.328146	-1.074914
P	-1.303381	0.567728	-1.586080
C	-1.798520	0.406695	2.619896
H	-3.859338	0.633244	-1.762211
C	-1.051054	-0.735111	-2.886296
H	-4.307055	-0.214813	0.598474
C	-1.555944	-2.047013	-2.748002
C	-1.364442	-2.985097	-3.774446
C	-0.669125	-2.622878	-4.943550
C	-0.355868	-0.375402	-4.060178
C	-0.165536	-1.318990	-5.085100
H	-2.100771	-2.334786	-1.834398
H	-1.758020	-4.007790	-3.660057
H	-0.519820	-3.362154	-5.746557
H	0.039493	0.647211	-4.169340
H	0.380881	-1.032031	-5.997529
C	-1.884857	1.810791	2.485686
C	-1.853563	2.628637	3.626458
C	-1.735908	2.055843	4.906387
C	-1.680355	-0.163330	3.906187
C	-1.649009	0.660151	5.045679
H	-1.975157	2.263588	1.485912
H	-1.914012	3.722776	3.514122
H	-1.710089	2.701617	5.798490
H	-1.619398	-1.258487	4.016059
H	-1.559648	0.207398	6.046026

Energy E(RB-P86) -2315.48692478 a.u.
-6079310.92 kJ/mol
-1452990.04 kcal/mol
SCF Convergence: 0.5612D-08
Maximum Force: 0.000038
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.242152 a.u.
Lowest Frequency 15.1168 cm-1

p'3

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.001618	-1.489285	-0.107935
C	1.750332	-1.634592	-0.652249
C	0.096449	0.464573	-0.212172
Cl	-1.146314	-1.489760	-2.167202
Cl	0.085424	-1.333782	2.247762
H	2.288699	-2.604880	-0.677013
H	2.330148	-0.758936	-1.009519
C	-1.106248	-3.582927	0.165602
C	0.230321	-3.884108	0.286250
H	-1.718120	-3.364233	1.057610
H	-1.643405	-3.734847	-0.782906

H	0.789441	-4.280812	-0.576999
H	0.730490	-3.908372	1.266703
P	-0.936782	1.496666	-1.254388
P	1.071029	1.538827	0.795226
C	-0.436679	3.148282	-0.665032
C	0.671078	3.167204	0.129495
C	-2.738639	1.341804	-0.887166
C	2.874099	1.245562	0.899839
H	1.164462	4.084889	0.490143
H	-0.942990	4.056072	-1.033342
C	-3.214324	1.350109	0.443297
C	-4.592575	1.242448	0.693153
C	-5.499858	1.133333	-0.376783
C	-3.649038	1.222924	-1.958157
C	-5.027415	1.125269	-1.700694
H	-2.504620	1.428457	1.282228
H	-4.958822	1.241348	1.732204
H	-6.579808	1.048053	-0.176426
H	-3.275615	1.191697	-2.993726
H	-5.734469	1.032054	-2.540284
C	3.788563	2.050300	0.179578
C	5.170207	1.835831	0.318819
C	5.648203	0.819446	1.165361
C	3.357049	0.232361	1.761717
C	4.739898	0.017699	1.880266
H	3.419321	2.834378	-0.499759
H	5.877124	2.464375	-0.245937
H	6.732241	0.654065	1.269935
H	2.640032	-0.382849	2.330305
H	5.109976	-0.777205	2.547096

Energy E(RB-P86) -2394.02418075 a.u.
-6285510.49 kJ/mol
-1502272.92 kcal/mol
SCF Convergence: 0.1410D-08
Maximum Force: 0.000062
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.295401 a.u.
Lowest Frequency 17.8163 cm-1

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p'4

Atom Coordinates (x,y,z) in Angstrom

Ru	0.150623	-1.200378	0.112578
C	0.485351	-1.841490	-1.562772
C	-0.100521	0.745199	-0.136448
Cl	2.531980	-0.613679	0.218424
Cl	-2.238052	-1.378228	-0.247496
H	1.498527	-1.792778	-2.011784
H	-0.342438	-2.295931	-2.147848
C	0.982910	-2.691906	1.612091
C	-0.389215	-2.907574	1.489393
H	1.716246	-3.309890	1.071615
H	-0.792952	-3.708764	0.850548
H	-1.103076	-2.477507	2.211683
H	1.395854	-2.080354	2.430735
P	-1.527669	1.590777	0.489922
P	1.017291	1.940928	-0.788880
C	-1.007899	3.310628	0.274107
C	0.075187	3.461350	-0.546999
C	-1.912940	1.311903	2.270575
C	1.516355	1.773227	-2.542532

H	0.449520	4.435996	-0.901306
H	-1.612116	4.148163	0.660320
C	0.824154	2.477959	-3.557084
C	1.246732	2.376118	-4.892123
C	2.351728	1.572152	-5.226638
C	2.630268	0.971511	-2.879323
C	3.036645	0.868803	-4.220558
H	-0.052711	3.093124	-3.302437
H	0.701167	2.923298	-5.677412
H	2.677668	1.493410	-6.275990
H	3.160147	0.425978	-2.081792
H	3.902611	0.238293	-4.477649
C	-1.215509	2.031740	3.269269
C	-1.539698	1.844276	4.623065
C	-2.555387	0.942337	4.989046
C	-2.934258	0.408452	2.639348
C	-3.247427	0.224940	3.997701
H	-0.412698	2.730320	2.986273
H	-0.989786	2.403341	5.396849
H	-2.806565	0.798282	6.051975
H	-3.457129	-0.165516	1.858548
H	-4.042980	-0.482490	4.280816

Energy E(RB-P86) -2394.01740625 a.u.
-6285492.70 kJ/mol
-1502268.67 kcal/mol
SCF Convergence: 0.3687D-08
Maximum Force: 0.000492
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.295545 a.u.
Lowest Frequency 15.3118 cm-1

(p'4-p'5)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.086833	1.462350	0.300016
C	1.522519	1.995951	0.979161
C	0.075203	-0.469238	-0.014096
Cl	0.927560	1.751488	-1.896627
Cl	-1.124612	0.928665	2.394902
H	2.388250	2.257984	0.334976
H	1.648339	2.064886	2.083610
C	-1.339189	3.210870	-0.455008
C	-1.003714	3.658082	0.811192
H	-0.865852	3.608017	-1.365402
H	-0.198492	4.398356	0.944639
H	-1.609689	3.411466	1.695283
H	-2.262993	2.617185	-0.602413
P	-1.128316	-1.658561	0.530737
P	1.306984	-1.320175	-0.947769
C	-0.510708	-3.150214	-0.286873
C	0.761073	-3.031463	-0.775374
C	-2.865454	-1.374934	-0.014654
C	3.047300	-1.136537	-0.409065
H	1.345753	-3.872083	-1.184292
H	-1.072893	-4.098311	-0.255802
C	3.632136	-2.065829	0.484072
C	4.981135	-1.929146	0.849886
C	5.750516	-0.868937	0.336280
C	3.822548	-0.074337	-0.928048
C	5.168591	0.057600	-0.546439
H	3.028676	-2.887715	0.899855

H	5.431547	-2.653370	1.547238
H	6.808118	-0.765693	0.626968
H	3.353885	0.648027	-1.616338
H	5.768098	0.889098	-0.949824
C	-3.291788	-1.800564	-1.295272
C	-4.625622	-1.605995	-1.690176
C	-5.538926	-0.985919	-0.818066
C	-3.785122	-0.756359	0.860807
C	-5.115679	-0.559373	0.452875
H	-2.576357	-2.272816	-1.986596
H	-4.950366	-1.935783	-2.689911
H	-6.583923	-0.834056	-1.132045
H	-3.443493	-0.410056	1.848516
H	-5.827027	-0.072055	1.138434

Energy E(RB-P86) -2394.01382978 a.u.
-6285483.31 kJ/mol
-1502266.42 kcal/mol
SCF Convergence: 0.9667D-08
Maximum Force: 0.000008
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.294721 a.u.
Lowest Frequency -64.8023 cm-1

P'5

Atom Coordinates (x,y,z) in Angstrom

Ru	1.369332	0.043663	0.057783
Cl	1.262464	2.318110	0.763960
Cl	1.467421	-2.230970	-0.648779
C	-0.548946	-0.017452	-0.023280
C	2.792996	-0.398411	1.379509
C	3.663298	0.116674	0.155268
C	2.869060	0.579285	-1.139506
H	2.829536	0.273796	2.256666
H	2.932962	-1.472080	1.600809
H	4.227089	1.000138	0.510861
H	4.309671	-0.728598	-0.148901
H	3.022335	-0.086577	-2.008838
H	2.958792	1.660337	-1.350676
P	-1.544978	-1.405648	0.438111
C	-3.202751	-0.682187	0.222668
C	-3.209608	0.477494	-0.493345
P	-1.589049	1.305641	-0.570593
C	-1.305859	-1.943894	2.178098
H	-4.123489	0.975261	-0.857951
C	-1.239186	1.862688	-2.285729
H	-4.110480	-1.238131	0.510494
C	-0.513449	1.059513	-3.194611
C	-0.261684	1.532514	-4.493467
C	-0.734055	2.795151	-4.894400
C	-1.698301	3.137880	-2.684316
C	-1.454158	3.595525	-3.989810
H	-0.145346	0.069416	-2.881882
H	0.306629	0.904403	-5.197809
H	-0.534932	3.159730	-5.914622
H	-2.237057	3.780718	-1.969157
H	-1.816580	4.589446	-4.296565
C	-0.712319	-1.098358	3.142789
C	-0.541142	-1.557836	4.459497
C	-0.963686	-2.849271	4.822523
C	-1.714221	-3.246999	2.539935

```
 C    -1.552148  -3.691667   3.862571
 H    -0.383374  -0.085851   2.859565
 H    -0.075676  -0.896535   5.207576
 H    -0.828308  -3.203157   5.856863
 H    -2.148434  -3.921068   1.783603
 H    -1.874642  -4.707632   4.140311
------------------------------------
Energy E(RB-P86)  -2394.03942409 a.u.
                    -6285550.51 kJ/mol
                    -1502282.48 kcal/mol
SCF Convergence: 0.6583D-08
  Maximum Force: 0.000008
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.298228 a.u.
Lowest Frequency    22.0790 cm-1
```

pn1

Atom Coordinates (x,y,z) in Angstrom

Ru	0.792630	-0.014170	0.100610
Cl	0.819240	2.319920	-0.117550
Cl	0.862600	-2.061980	-1.034770
C	-1.146250	0.025510	0.073360
C	0.866310	-0.392160	1.895010
P	3.283110	-0.025060	-0.125380
H	-0.033800	-0.439210	2.546120
H	1.832190	-0.580870	2.412750
C	4.292670	-1.533780	0.280700
C	4.343100	1.235580	0.739250
C	3.941060	0.251120	-1.843290
P	-2.214500	-1.373540	0.396670
N	-3.822300	-0.673630	0.329590
C	-3.815000	0.487280	-0.241960
P	-2.204130	1.406690	-0.359070
H	-2.041850	-1.696880	1.785360
H	-4.775410	0.995040	-0.473220
H	-2.024920	1.774240	-1.731020
H	5.033400	0.226310	-1.823350
H	3.570870	-0.535090	-2.505900
H	3.605430	1.224380	-2.209810
H	5.394310	1.049260	0.505870
H	4.066880	2.237330	0.401030
H	4.190830	1.160700	1.818800
H	5.351050	-1.319990	0.112400
H	4.137810	-1.804640	1.328010
H	3.982210	-2.363030	-0.359760

Energy E(RB-P86) -2330.71005694 a.u.
-6119279.25 kJ/mol
-1462542.70 kcal/mol
SCF Convergence: 0.4184D-08
Maximum Force: 0.000004
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.181138 a.u.
Lowest Frequency 32.8626 cm-1

---

pn2

Atom Coordinates (x,y,z) in Angstrom

Ru	1.073204	0.052289	0.117916
Cl	1.359354	1.981429	1.311745
Cl	1.670785	-0.722150	-1.954772
C	-0.759742	-0.128686	0.014940
C	1.389469	-1.331311	1.252752
H	0.619531	-2.064478	1.586380
H	2.427935	-1.488175	1.628728
P	-1.872921	-1.011820	1.205540
N	-3.407671	-0.653006	0.433623
C	-3.344101	-0.110018	-0.730254
P	-1.733258	0.617435	-1.356962
H	-1.915544	-0.027104	2.255635
H	-4.279309	0.066049	-1.304635
H	-1.353303	-0.287852	-2.411602

Energy E(RB-P86) -1869.75384020 a.u.
-4909038.71 kJ/mol
-1173288.30 kcal/mol
SCF Convergence: 0.4009D-08

```
  Maximum Force: 0.000033
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.070167 a.u.
Lowest Frequency    45.5897 cm-1
```

pn3

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru  -0.888737  -0.042321   0.054760
 Cl  -0.714570  -2.338515  -0.441335
 Cl  -0.893939   2.194172  -0.662687
 C    1.043207   0.002469   0.107609
 C   -0.979934  -0.005751   1.890890
 H   -0.085604  -0.048168   2.548506
 H   -1.956075   0.039549   2.415737
 C   -3.352387   0.347055   0.192780
 C   -3.076216  -0.350449  -0.954202
 H   -3.377376   1.447124   0.212336
 H   -3.706131  -0.183848   1.092073
 H   -3.207919  -1.441130  -1.011933
 H   -2.878764   0.176408  -1.904216
 P    2.042177   1.388687   0.638476
 N    3.673719   0.755492   0.556710
 C    3.734289  -0.322139  -0.158438
 P    2.167364  -1.273915  -0.447735
 H    1.809716   1.549764   2.045883
 H    4.721537  -0.762700  -0.412733
 H    2.056760  -1.498175  -1.856625
------------------------------------
Energy E(RB-P86)  -1948.28391608 a.u.
                    -5115219.42 kJ/mol
                    -1222566.67 kcal/mol
SCF Convergence: 0.6801D-08
  Maximum Force: 0.000011
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.123004 a.u.
Lowest Frequency    34.6405 cm-1
```

pn4

no local minimum located

(pn4-pn5)≠

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru  -0.871789  -0.036414   0.087019
 Cl  -0.775948  -2.414154  -0.019336
 Cl  -0.822328   2.355976  -0.068494
 C   -1.268980   0.087360   1.878784
 C    1.060780  -0.006777  -0.073905
 P    2.142325   1.336416   0.361185
 N    3.727735   0.681588   0.011446
 C    3.665251  -0.369354  -0.744576
 P    2.052130  -1.280718  -0.809778
 C   -2.869949  -0.294459  -0.937026
 C   -3.310429   0.203281   0.286935
 H    2.166337   1.486864   1.786602
 H    4.592541  -0.810160  -1.166709
 H    1.724625  -1.503348  -2.186904
 H   -2.982861  -1.360377  -1.188996
 H   -2.685507   0.409897  -1.769934
 H   -3.754221  -0.477420   1.031439
 H   -3.424672   1.285447   0.454710
 H   -1.697560  -0.780731   2.426195
```

```
 H   -1.080270   1.014178   2.465381
-------------------------------------
Energy E(RB-P86)  -1948.27358042 a.u.
                    -5115192.29 kJ/mol
                    -1222560.18 kcal/mol
SCF Convergence: 0.7596D-08
  Maximum Force: 0.000116
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.122628 a.u.
Lowest Frequency  -160.0297 cm-1
```

pn5

```
Atom Coordinates (x,y,z) in Angstrom
-------------------------------------
 Ru   0.832432   0.018588   0.006844
 Cl   0.735344   2.337645   0.542117
 Cl   0.840742  -2.295048  -0.523663
 C   -1.076120   0.008110  -0.068579
 C    2.195208  -0.385748   1.403759
 C    3.126399   0.054038   0.191689
 C    2.396701   0.492851  -1.146558
 H    2.202916   0.330845   2.245689
 H    2.312660  -1.447140   1.689339
 H    3.698847   0.936133   0.536673
 H    3.763710  -0.817517  -0.051417
 H    2.542534  -0.212466  -1.985612
 H    2.532497   1.559317  -1.399452
 P   -2.082323  -1.413428   0.324606
 N   -3.694483  -0.743955   0.250056
 C   -3.730367   0.395460  -0.367345
 P   -2.147825   1.352450  -0.504121
 H   -1.943918  -1.744164   1.712819
 H   -4.705227   0.863354  -0.618582
 H   -1.981810   1.723685  -1.879743
-------------------------------------
Energy E(RB-P86)  -1948.29651406 a.u.
                    -5115252.50 kJ/mol
                    -1222574.57 kcal/mol
SCF Convergence: 0.5556D-08
  Maximum Force: 0.000001
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.126021 a.u.
Lowest Frequency    31.0913 cm-1
```

p1a

Atom Coordinates (x,y,z) in Angstrom

Ru	0.797979	-0.007529	0.110198
Cl	0.810343	2.329074	-0.112961
Cl	0.883626	-2.066820	-1.007021
C	-1.148632	0.008283	0.061308
C	0.859155	-0.379640	1.905319
P	3.280420	0.004149	-0.102140
H	-0.049858	-0.441105	2.543562
H	1.820115	-0.550875	2.438648
H	4.068625	-1.149590	0.220077
H	4.086735	0.984013	0.565547
H	3.797594	0.215681	-1.419539
P	-2.177687	-1.412247	0.376672
C	-3.831934	-0.659687	0.266292
C	-3.829156	0.562805	-0.332489
P	-2.203688	1.395279	-0.369371
H	-1.939201	-1.805146	1.736760
H	-4.751038	1.095599	-0.622289
H	-1.974937	1.759262	-1.734518
H	-4.748867	-1.233178	0.482715

Energy E(RB-P86) -2196.80218908 a.u.
-5767704.15 kJ/mol
-1378514.24 kcal/mol
SCF Convergence: 0.5353D-08
Maximum Force: 0.000057
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.107940 a.u.
Lowest Frequency 36.2488 cm-1

n1

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.019067	0.054732	0.086260
Cl	-0.101700	1.609667	-1.705074
Cl	-0.036737	-2.226410	0.741755
C	-2.057504	-0.004056	0.048126
C	-0.023969	1.040477	1.631623
P	2.373002	0.044201	0.006468
N	-2.887277	-0.941621	0.596119
C	-4.222879	-0.681614	0.323449
C	-4.242527	0.479235	-0.416476
N	-2.917906	0.868205	-0.557448
H	-2.475708	-1.767670	1.051338
H	-5.040383	-1.320838	0.671568
H	-5.080413	1.044740	-0.836308
H	-2.533377	1.639075	-1.120349
H	-0.961798	1.352623	2.145504
H	0.903829	1.384027	2.145855
C	3.239966	-0.751650	1.435488
C	3.198705	1.695673	-0.127366
C	3.053018	-0.874956	-1.450713
H	4.301773	1.608213	-0.211157
H	2.789516	2.215547	-1.016664
H	2.948173	2.303618	0.765666
H	4.162865	-0.865710	-1.465681
H	2.693352	-1.922964	-1.411531
H	2.667693	-0.407665	-2.379361
H	4.341790	-0.764297	1.304106
H	2.990326	-0.203340	2.366568
H	2.857149	-1.786691	1.538931

Energy E(RB-P86) -1741.62940240 a.u.
-4572648.00 kJ/mol
-1092889.00 kcal/mol
SCF Convergence: 0.1758D-08
Maximum Force: 0.000003
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.209104 a.u.
Lowest Frequency 33.8932 cm-1

n2

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.882461	0.001311	0.103986
Cl	-1.033295	-2.221561	-0.584624
Cl	-1.027080	2.223363	-0.588237
C	1.029948	-0.001448	0.032713
C	-0.987982	0.003005	1.913428
N	1.877797	1.078390	0.000522
C	3.206331	0.683023	-0.076941
C	3.204326	-0.691897	-0.078979
N	1.874664	-1.083631	-0.002754
H	1.493395	2.028554	-0.056101
H	4.035689	1.395891	-0.114005
H	4.031617	-1.407056	-0.118079
H	1.487384	-2.032529	-0.061592
H	-0.153878	0.002294	2.647900
H	-2.022491	0.005121	2.339446

Energy E(RB-P86) -1280.65209275 a.u.
-3362352.07 kJ/mol

-803621.35 kcal/mol
SCF Convergence: 0.5750D-08
Maximum Force: 0.000008
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.097904 a.u.
Lowest Frequency 40.4154 cm-1

n3

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.652642	-0.014337	0.051505
Cl	-0.390470	-2.259497	-0.719116
Cl	-0.472131	2.306069	-0.483865
C	1.385860	0.023966	0.014941
C	-0.608661	-0.107287	1.872977
N	2.207455	1.110418	0.079859
C	3.546346	0.750171	0.048560
C	3.571016	-0.624026	-0.022149
N	2.245935	-1.033286	-0.030476
H	1.785437	2.051187	0.039814
H	4.360238	1.481169	0.081153
H	4.410604	-1.324913	-0.063197
H	1.857749	-1.979457	-0.167680
H	0.324462	-0.121728	2.478268
H	-1.552013	-0.154663	2.466096
C	-2.852202	-0.747180	0.059837
C	-2.876953	0.634626	0.130860
H	-2.958498	-1.379158	0.956628
H	-2.982230	-1.271822	-0.899800
H	-3.027318	1.249867	-0.770212
H	-3.004129	1.167105	1.087523

Energy E(RB-P86) -1359.20070800 a.u.
-3568581.46 kJ/mol
-852911.36 kcal/mol
SCF Convergence: 0.3260D-08
Maximum Force: 0.000022
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.151153 a.u.
Lowest Frequency 62.5836 cm-1

n4

Atom Coordinates (x,y,z) in Angstrom

Ru	0.020196	0.021623	0.688782
C	1.401949	-1.124305	0.941422
C	-0.059144	-0.028503	-1.390370
Cl	1.586596	1.862827	0.292335
Cl	-1.539209	-1.858108	0.501449
N	-0.800785	-0.854646	-2.170297
N	0.581362	0.789961	-2.262552
C	-0.631347	-0.569631	-3.511720
C	0.256539	0.486889	-3.570973
H	2.451449	-0.754005	0.975439
H	1.222410	-2.216783	1.059795
H	-1.376724	-1.574739	-1.686954
H	1.215769	1.510589	-1.859825
C	-0.100573	1.146872	2.602102
C	-1.000734	0.074028	2.662831
H	0.885798	1.105409	3.089892
H	-0.759858	-0.856050	3.200924
H	-2.072885	0.219419	2.447860

```
 H   -0.443433   2.161540   2.337930
 H   -1.144566  -1.118901  -4.307456
 H    0.663656   1.032572  -4.428163
-----------------------------------
Energy E(RB-P86)  -1359.19594677 a.u.
                    -3568568.96 kJ/mol
                     -852908.37 kcal/mol
SCF Convergence: 0.7353D-08
  Maximum Force: 0.000014
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.150801 a.u.
Lowest Frequency    61.9211 cm-1
```

(n4-n5)≠

```
Atom Coordinates (x,y,z) in Angstrom
-----------------------------------
 Ru  -0.607375  -0.045856   0.040779
 Cl  -0.388722  -2.308436  -0.764290
 Cl  -0.529068   2.310410   0.644156
 C    1.423085   0.105943  -0.179740
 C   -1.006972  -0.491423   1.772031
 N    2.202445   1.199626   0.027128
 C    3.532563   0.927087  -0.221231
 C    3.590190  -0.401258  -0.601600
 N    2.290451  -0.867062  -0.567230
 H    1.725843   2.070531   0.336202
 H    4.326117   1.674073  -0.118003
 H    4.442812  -1.025422  -0.887557
 H    1.899533  -1.799561  -0.797139
 C   -2.891956  -0.538060   0.262423
 C   -2.585834   0.437609  -0.706454
 H   -1.047685  -1.556774   2.100145
 H   -1.215346   0.285110   2.544155
 H   -2.940906  -1.607511   0.003390
 H   -3.390534  -0.229723   1.197057
 H   -2.831975   1.500061  -0.546625
 H   -2.457661   0.105982  -1.755474
-----------------------------------
Energy E(RB-P86)  -1359.18788454 a.u.
                    -3568547.79 kJ/mol
                     -852903.31 kcal/mol
SCF Convergence: 0.6074D-08
  Maximum Force: 0.000035
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.150211 a.u.
Lowest Frequency  -138.1378 cm-1
```

n5

```
Atom Coordinates (x,y,z) in Angstrom
-----------------------------------
 Ru   0.566103   0.003254   0.036307
 Cl   0.371183   2.410639   0.167640
 Cl   0.546399  -2.393869  -0.106142
 C   -1.453975  -0.041582  -0.094687
 C    1.896377   0.023444   1.485756
 N   -2.249609  -1.139263  -0.208377
 C   -3.580948  -0.788805  -0.274964
 C   -3.620963   0.593760  -0.201586
 N   -2.312906   1.012373  -0.091652
 H   -1.788783  -2.068845  -0.230130
 H   -4.389274  -1.521425  -0.368137
 H   -4.471211   1.283107  -0.219156
```

H	-1.897742	1.962556	-0.011578
C	2.808552	0.053023	0.181726
C	2.073529	0.191784	-1.218215
H	1.958939	0.948451	2.092042
H	1.995283	-0.920863	2.055706
H	3.431758	0.962644	0.286082
H	3.395728	-0.883732	0.158785
H	2.254470	-0.675624	-1.881950
H	2.205590	1.183931	-1.692611

Energy E(RB-P86) -1359.20613832 a.u.
-3568595.72 kJ/mol
-852914.76 kcal/mol
SCF Convergence: 0.5953D-08
Maximum Force: 0.000443
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.153191 a.u.
Lowest Frequency 59.5189 cm-1

(n1-n6)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	0.032309	-0.033101	0.294297
Cl	2.353817	0.127433	0.806861
Cl	-0.921194	0.076831	-2.086251
C	0.004181	2.029572	0.196931
C	-0.221719	-0.425339	2.068236
P	0.511036	-2.280593	-0.333631
N	-0.369580	2.776465	-0.876874
C	-0.146787	4.128383	-0.674362
C	0.387050	4.244751	0.589038
N	0.466039	2.951679	1.092095
H	-0.724505	2.266907	-1.711525
H	-0.377505	4.890183	-1.425528
H	0.706910	5.125132	1.154997
H	0.894495	2.669399	1.975918
H	-1.258131	-0.402693	2.485310
H	0.569147	-0.733099	2.797222
C	1.344479	-3.319617	0.945586
C	1.684611	-2.318342	-1.753107
C	-0.900381	-3.328161	-0.905306
C	-3.246977	0.679793	0.652686
C	-3.445527	-0.648847	0.567486
H	-3.374877	-1.169240	-0.400852
H	-3.686990	-1.260617	1.453646
H	-3.318610	1.220506	1.611690
H	-3.013676	1.273850	-0.244306
H	-0.549061	-4.321503	-1.254226
H	-1.623986	-3.462757	-0.076649
H	-1.403861	-2.793638	-1.735361
H	1.914530	-3.360638	-2.056647
H	1.224223	-1.761996	-2.593039
H	2.609771	-1.793761	-1.442882
H	1.672264	-4.293084	0.526547
H	2.221347	-2.755252	1.321301
H	0.647973	-3.495048	1.789765

Energy E(RB-P86) -1820.12771554 a.u.
-4778745.32 kJ/mol
-1142147.43 kcal/mol
SCF Convergence: 0.3548D-08
Maximum Force: 0.000011

<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.259151 a.u.
Lowest Frequency -101.5477 cm-1

n6

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.265498	-0.035529	0.378554
Cl	2.181625	0.210685	0.313420
Cl	-0.675025	0.202199	-2.192960
C	-0.121764	2.035311	0.315005
C	-0.087995	-0.308607	2.201356
P	0.364717	-2.296207	-0.306163
N	-0.160480	2.767237	-0.822356
C	0.109461	4.105059	-0.582497
C	0.314488	4.223236	0.771488
N	0.156436	2.941371	1.293757
H	-0.322613	2.241520	-1.713937
H	0.135465	4.856007	-1.378018
H	0.552608	5.091810	1.392859
H	0.304657	2.665582	2.265132
H	-0.951515	-0.465070	2.898870
H	0.903818	-0.363731	2.711303
C	1.267842	-3.206449	1.023709
C	1.521332	-2.344601	-1.735660
C	-0.945563	-3.494401	-0.823264
C	-2.374440	0.529086	0.623688
C	-2.301220	-0.865491	0.416028
H	-2.551815	-1.264771	-0.579048
H	-2.447584	-1.557179	1.264882
H	-2.562689	0.934423	1.633125
H	-2.673493	1.184765	-0.210329
H	-0.482151	-4.458176	-1.118904
H	-1.663481	-3.673146	0.000860
H	-1.491812	-3.074610	-1.691094
H	1.788877	-3.395328	-1.971047
H	1.021969	-1.856611	-2.594999
H	2.418809	-1.753862	-1.471353
H	1.650235	-4.181488	0.658023
H	2.114199	-2.568488	1.347530
H	0.590968	-3.373390	1.885491

Energy E(RB-P86) -1820.17031514 a.u.
-4778857.16 kJ/mol
-1142174.16 kcal/mol
SCF Convergence: 0.6188D-08
Maximum Force: 0.000036
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.262820 a.u.
Lowest Frequency 28.9240 cm-1

(n6-n7)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.246319	0.040011	0.315902
Cl	2.207808	0.118252	0.327621
Cl	-0.066915	-0.051079	-2.289910
C	-0.126387	2.077596	0.007762
C	-0.072995	-0.045918	2.180953
P	0.144310	-2.373311	0.125164
N	0.033538	2.681974	-1.195254
C	0.234045	4.047013	-1.068619

C	0.184303	4.324194	0.276472
N	-0.045577	3.103414	0.907507
H	0.065993	2.055886	-2.033096
H	0.393060	4.704776	-1.928626
H	0.290207	5.265544	0.824238
H	-0.080977	2.947944	1.915491
H	-0.879499	-0.056732	2.951223
H	0.949072	-0.132626	2.614604
C	0.915367	-3.098548	1.641892
C	1.337354	-2.847720	-1.192154
C	-1.285751	-3.511849	-0.184828
C	-2.368198	0.413690	0.905884
C	-2.368732	-0.238858	-0.334085
H	-2.487236	0.320545	-1.273913
H	-2.627587	-1.305431	-0.401700
H	-2.623161	-0.141365	1.824781
H	-2.552875	1.499438	0.963213
H	-0.941585	-4.566601	-0.207276
H	-2.051414	-3.400385	0.609424
H	-1.746283	-3.266137	-1.162504
H	1.533426	-3.939337	-1.157903
H	0.928634	-2.544310	-2.174605
H	2.266821	-2.271359	-1.016409
H	1.186363	-4.163455	1.488465
H	1.828713	-2.510677	1.862606
H	0.216751	-3.013829	2.498314

Energy E(RB-P86) -1820.15758862 a.u.
-4778823.75 kJ/mol
-1142166.18 kcal/mol
SCF Convergence: 0.3713D-08
Maximum Force: 0.000002
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.262865 a.u.
Lowest Frequency -79.6424 cm-1

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n7

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.242397	-0.308879	0.042192
Cl	2.157619	-0.790224	0.173278
Cl	0.483246	2.196143	-0.133176
C	-0.112115	-0.000948	2.079965
C	-0.414958	-2.180296	0.052728
P	0.023624	-0.099144	-2.361178
N	0.290411	1.162494	2.650716
C	0.411471	1.052979	4.026389
C	0.055988	-0.235159	4.346464
N	-0.266680	-0.851268	3.138536
H	0.525175	1.950332	2.005574
H	0.735851	1.883363	4.661095
H	0.006882	-0.752528	5.309368
H	-0.524665	-1.830966	3.017679
H	0.516393	-2.788345	0.091645
H	-1.343285	-2.792284	-0.018263
C	-0.150322	-1.685509	-3.302123
C	1.669115	0.523939	-2.893249
C	-1.157523	1.029994	-3.227927
C	-2.163296	0.832132	0.097916
C	-2.455493	-0.530588	-0.057213
H	-2.761375	-0.932813	-1.038577
H	-2.804652	-1.125141	0.803848

H	-2.253098	1.319234	1.081857
H	-2.197512	1.529445	-0.751381
H	-0.938567	1.067335	-4.314891
H	-2.202207	0.688584	-3.081681
H	-1.043941	2.043454	-2.794021
H	-0.002679	-1.536030	-4.391769
H	0.610645	-2.396954	-2.923532
H	-1.154725	-2.119681	-3.124278
H	1.747365	0.527947	-3.999923
H	1.793143	1.544502	-2.481882
H	2.444347	-0.120090	-2.433841

Energy E(RB-P86) -1820.15946687 a.u.
-4778828.68 kJ/mol
-1142167.36 kcal/mol
SCF Convergence: 0.6728D-08
Maximum Force: 0.000003
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.262980 a.u.
Lowest Frequency 40.2238 cm-1

(n7-n8)≠

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.279750	-0.011749	0.007333
Cl	2.011810	-1.568435	0.368098
Cl	0.945238	2.050481	-0.121507
C	-0.227320	0.245792	2.034231
C	-0.421007	-1.923738	0.210144
P	0.005547	-0.068651	-2.380804
N	-0.875284	1.122900	2.862089
C	-0.377671	1.079560	4.162065
C	0.611052	0.124966	4.155793
N	0.667064	-0.369764	2.861361
H	-1.559880	1.793971	2.511309
H	-0.756974	1.716764	4.966910
H	1.264873	-0.230091	4.958530
H	1.371932	-1.001276	2.426886
H	-0.380151	-2.654289	-0.624284
C	-0.727595	-1.474048	-3.354928
C	1.777279	-0.109524	-2.896814
C	-0.644542	1.411071	-3.285464
C	-2.284709	0.449605	-0.088782
C	-2.200943	-1.034948	0.026979
H	-2.521910	-1.613104	-0.858768
H	-2.585235	-1.458377	0.973700
H	-2.665606	0.855841	-1.044616
H	-0.380612	1.383506	-4.362927
H	-1.747279	1.467844	-3.183630
H	-0.202130	2.308792	-2.809146
H	1.884510	-0.105700	-4.001315
H	2.270550	0.780251	-2.458000
H	2.255329	-1.008053	-2.459332
H	-0.501051	-1.377043	-4.436725
H	-0.312067	-2.437011	-2.994111
H	-1.829416	-1.497142	-3.226407
H	-0.488263	-2.431840	1.195608
H	-2.730395	0.974523	0.780183

Energy E(RB-P86) -1820.14338194 a.u.
-4778786.45 kJ/mol
-1142157.26 kcal/mol

```
SCF Convergence: 0.2780D-08
  Maximum Force: 0.000022
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.262463 a.u.
Lowest Frequency  -281.6267 cm-1
```

n8

```
/home/heiko/PHC/PMe3
Atom Coordinates (x,y,z) in Angstrom
-------------------------------------
 Ru  -0.281532  -0.037039   0.013722
 Cl   2.135841  -1.054701   0.234366
 Cl   0.881425   2.043535  -0.076459
 C   -0.220222   0.180193   2.056810
 C   -0.709894  -1.992595   0.184619
 P    0.012304  -0.089058  -2.377533
 N   -1.012771   0.836787   2.960700
 C   -0.454349   0.835352   4.236989
 C    0.726991   0.139349   4.128368
 N    0.830992  -0.251314   2.804623
 H   -1.859124   1.337970   2.687917
 H   -0.929962   1.318731   5.096057
 H    1.484382  -0.099574   4.881661
 H    1.619917  -0.703607   2.280047
 H   -0.533382  -2.473024   1.164678
 H   -0.486029  -2.672047  -0.656869
 C   -0.293435  -1.689468  -3.272579
 C    1.717156   0.339026  -2.933297
 C   -1.035915   1.102320  -3.337649
 C   -2.230404   0.347042  -0.049698
 C   -2.111439  -1.279481   0.072541
 H   -2.615612  -1.678359  -0.828487
 H   -2.658981  -1.523790   1.003739
 H   -2.781270   0.752924   0.825737
 H   -2.752147   0.634866  -0.984028
 H   -0.755878   1.123463  -4.411152
 H   -2.107411   0.828697  -3.254645
 H   -0.896764   2.110825  -2.898852
 H    1.797999   0.312336  -4.039425
 H    1.957452   1.348626  -2.546480
 H    2.422610  -0.374811  -2.464002
 H   -0.133570  -1.576280  -4.364729
 H    0.409227  -2.455708  -2.887043
 H   -1.330620  -2.044536  -3.103200
-------------------------------------
Energy E(RB-P86)  -1820.15303657 a.u.
                    -4778811.80 kJ/mol
                    -1142163.32 kcal/mol
SCF Convergence: 0.2344D-08
  Maximum Force: 0.000018
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.263903 a.u.
Lowest Frequency    19.4876 cm-1
```

(n1-n9)≠

```
Atom Coordinates (x,y,z) in Angstrom
-------------------------------------
 Ru   0.053419  -0.121396  -0.190951
 C   -1.975522  -0.063136  -0.042382
 C    0.033807   0.877084   1.370059
 Cl  -0.017883  -2.391532   0.604955
 Cl  -0.085376   1.564557  -1.904805
```

```
 P    2.475377   0.035488  -0.005523
 N   -2.790697  -0.913675   0.645255
 C   -4.117163  -0.500357   0.613473
 C   -4.136659   0.666147  -0.116213
 N   -2.821154   0.907318  -0.493728
 H   -2.384727  -1.765351   1.059270
 H   -4.927053  -1.051983   1.101103
 H   -4.966899   1.326065  -0.386778
 H   -2.441966   1.659664  -1.086830
 H   -0.899830   1.201119   1.885296
 H    0.936670   1.253233   1.903484
 C    3.109073  -0.658375   1.593818
 C    3.068883   1.792523   0.016866
 C    3.697333  -0.710690  -1.191335
 H    4.165351   1.856316   0.173834
 H    2.794887   2.258999  -0.950674
 H    2.552136   2.358831   0.816897
 H    4.739549  -0.486237  -0.882008
 H    3.561920  -1.814054  -1.224899
 H    3.531386  -0.297457  -2.210469
 H    4.204508  -0.517355   1.699184
 H    2.595228  -0.176788   2.449272
 H    2.860632  -1.738358   1.620898
 C    0.656566  -1.720278  -2.721700
 C   -0.683315  -1.581803  -2.554626
 H   -1.238658  -0.803725  -3.101207
 H   -1.255192  -2.330132  -1.984807
 H    1.190423  -2.594997  -2.312065
 H    1.204106  -1.058988  -3.413763
-------------------------------------
Energy E(RB-P86)  -1820.15027128 a.u.
                   -4778804.54 kJ/mol
                   -1142161.59 kcal/mol
SCF Convergence: 0.2468D-08
  Maximum Force: 0.005006
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.260308 a.u.
Lowest Frequency  -102.0138 cm-1
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n9

```
Atom Coordinates (x,y,z) in Angstrom
-------------------------------------
 Ru  -0.016279   0.018223   0.044735
 Cl  -0.190183   2.178480  -1.091960
 Cl  -0.051151  -2.312076   0.790132
 C   -2.052932   0.030326   0.224445
 C   -0.063858   0.745075   1.777622
 P    2.404269   0.130741   0.135800
 N   -2.849741  -0.937716   0.754286
 C   -4.184827  -0.550318   0.776987
 C   -4.224055   0.718249   0.245462
 N   -2.910999   1.043424  -0.075760
 H   -2.415784  -1.825643   1.052212
 H   -4.985349  -1.189453   1.162413
 H   -5.065370   1.398040   0.078261
 H   -2.530969   1.899864  -0.508887
 H   -1.004833   0.951011   2.336596
 H    0.818086   1.029973   2.387782
 C    3.146529   0.809284   1.701188
 C    3.251833   1.204200  -1.116326
 C    3.333765  -1.468294   0.003260
 H    4.332054   1.312891  -0.887885
```

```
 H    3.141110   0.764626  -2.126729
 H    2.759218   2.196993  -1.122662
 H    4.413005  -1.325248   0.216919
 H    2.894127  -2.193347   0.716954
 H    3.222006  -1.886185  -1.016187
 H    4.252705   0.809594   1.622580
 H    2.802088   1.848751   1.873834
 H    2.851941   0.187376   2.570316
 C    0.591332  -0.866222  -2.113220
 C   -0.790728  -0.874862  -2.030380
 H   -1.381155  -0.060832  -2.477611
 H   -1.326833  -1.794788  -1.751812
 H    1.158093  -1.789448  -1.918282
 H    1.103607  -0.050562  -2.645982
-------------------------------------
Energy E(RB-P86)  -1820.16221738 a.u.
                    -4778835.90 kJ/mol
                    -1142169.08 kcal/mol
SCF Convergence: 0.2568D-08
  Maximum Force: 0.000005
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.262130 a.u.
Lowest Frequency    36.3578 cm-1
```

n1a

Atom Coordinates (x,y,z) in Angstrom

Ru	0.537190	0.002397	0.069551
Cl	0.453746	2.276717	-0.582227
Cl	0.463996	-2.272209	-0.582557
C	-1.492223	-0.002144	0.062067
C	0.567817	0.002312	1.902894
P	2.917685	0.007077	-0.018110
N	-2.331621	-1.078125	0.043549
C	-3.663819	-0.695681	-0.010687
C	-3.666950	0.681446	-0.011103
N	-2.336512	1.069981	0.042875
H	-1.928536	-2.023257	-0.029662
H	-4.490469	-1.412447	-0.039534
H	-4.496855	1.394426	-0.040377
H	-1.937669	2.016890	-0.030758
H	-0.358629	0.000392	2.519613
H	1.512052	0.004162	2.495070
H	3.640973	0.007560	1.226488
H	3.627365	1.089658	-0.636135
H	3.630692	-1.072895	-0.636888

Energy E(RB-P86) -1623.75409594 a.u.
-4263166.38 kJ/mol
-1018921.12 kcal/mol
SCF Convergence: 0.4068D-08
Maximum Force: 0.000055
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.124994 a.u.
Lowest Frequency 59.2601 cm-1

C2H4

Atom Coordinates (x,y,z) in Angstrom

C	-0.671063	0.000028	-0.000001
C	0.671063	-0.000028	0.000002
H	1.251676	0.938111	0.000008
H	1.251600	-0.938213	-0.000007
H	-1.251675	-0.938111	-0.000011
H	-1.251601	0.938213	0.000004

Energy E(RB-P86) -78.52443283 a.u.
-206165.90 kJ/mol
-49274.83 kcal/mol
SCF Convergence: 0.1784D-10
Maximum Force: 0.000061
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.049270 a.u.
Lowest Frequency 795.3789 cm-1

PMe3

Atom Coordinates (x,y,z) in Angstrom

P	-0.316989	-0.348204	0.384496
C	1.552056	-0.421766	0.448067
C	-0.547451	1.507071	0.470081
C	-0.563548	-0.600498	-1.453248
H	1.888258	-1.456865	0.230656
H	2.036747	0.270394	-0.274848
H	1.897094	-0.167413	1.471745
H	-1.616500	1.754552	0.303777
H	-0.277251	1.864272	1.485557
H	0.067322	2.055641	-0.276649
H	-1.630950	-0.434468	-1.707826
H	0.061950	0.078568	-2.073105
H	-0.318164	-1.650461	-1.716145

Energy E(RB-P86) -460.93013297 a.u.
-1210172.06 kJ/mol
-289238.04 kcal/mol
SCF Convergence: 0.6669D-09
Maximum Force: 0.000148
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.108612 a.u.
Lowest Frequency 172.3156 cm-1

PH3

Atom Coordinates (x,y,z) in Angstrom

P	-0.096104	-0.001591	0.092380
H	0.176312	-1.102744	-0.797402
H	1.302647	0.171275	0.396136
H	-0.037394	0.955322	-0.984433

Energy E(RB-P86) -343.06911365 a.u.
-900727.96 kJ/mol
-215279.13 kcal/mol
SCF Convergence: 0.1931D-08
Maximum Force: 0.000043
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.023044 a.u.
Lowest Frequency 985.6905 cm-1

PH

Atom Coordinates (x,y,z) in Angstrom

C	-0.969148	-1.086492	-0.119894
P	0.756448	-1.138502	-0.123319
C	1.394989	0.566103	-0.051521
C	0.385442	1.431464	0.271779
P	-1.227284	0.609710	0.065261
H	1.369442	-1.888429	-1.171464
H	0.521418	2.506422	0.473413
H	-2.157736	1.008861	1.071012
H	2.461723	0.838572	-0.104279

Energy E(RB-P86) -799.07453048 a.u.
-2097970.18 kJ/mol
-501426.86 kcal/mol
SCF Convergence: 0.5518D-08
Maximum Force: 0.000198
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.053243 a.u.
Lowest Frequency 211.1099 cm-1

PPh

Atom Coordinates (x,y,z) in Angstrom

C	-0.532948	-0.598044	-0.065740
P	1.171096	-0.622048	-0.246886
C	1.810748	1.058724	-0.073268
C	0.821931	1.888452	0.403033
P	-0.779280	1.058405	0.297536
C	1.932601	-1.649203	-1.533956
H	0.980908	2.942455	0.680263
C	-2.026134	1.544143	1.522499
H	2.862348	1.360835	-0.199473
C	-2.919975	0.568824	2.022486
C	-3.929850	0.943881	2.922887
C	-4.056573	2.283148	3.334616
C	-2.163188	2.892792	1.925765
C	-3.169802	3.254367	2.835380
H	-2.804615	-0.478864	1.703039
H	-4.619671	0.178555	3.313054
H	-4.847198	2.571000	4.045435
H	-1.484261	3.665409	1.530391
H	-3.264744	4.305266	3.152056
C	1.130972	-2.571072	-2.246484
C	1.719696	-3.416295	-3.200565
C	3.101589	-3.349923	-3.455839
C	3.324057	-1.593128	-1.780851
C	3.900103	-2.435354	-2.745337
H	0.048301	-2.606645	-2.047590
H	1.089046	-4.128549	-3.756250
H	3.557437	-4.011503	-4.209315
H	3.962626	-0.891554	-1.220287
H	4.983222	-2.379641	-2.938822

Energy E(RB-P86) -1260.85681030 a.u.
-3310379.56 kJ/mol
-791199.63 kcal/mol
SCF Convergence: 0.4957D-08
Maximum Force: 0.000006
<S**2>: 0.0000
Charge: 0.0000

ZPE-correction: 0.214445 a.u.
Lowest Frequency 21.3342 cm-1

PNH

Atom Coordinates (x,y,z) in Angstrom

C	-0.823551	-1.183711	-0.040983
P	0.839809	-0.982554	0.404406
N	1.350088	0.699490	0.120344
C	0.300970	1.435427	-0.059134
P	-1.236513	0.439795	-0.390067
H	1.740984	-1.766348	-0.379359
H	0.369490	2.535186	-0.168206
H	-2.475039	0.965827	0.090763

Energy E(RB-P86) -815.11325586 a.u.
-2140079.85 kJ/mol
-511491.31 kcal/mol
SCF Convergence: 0.3079D-08
Maximum Force: 0.000046
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.041916 a.u.
Lowest Frequency 227.4164 cm-1

IH

Atom Coordinates (x,y,z) in Angstrom

C	0.809912	-1.001231	0.000000
N	1.074003	0.348960	0.000000
C	-0.058739	1.163815	0.000000
C	-1.125870	0.300602	0.000000
N	-0.565619	-0.977391	0.000000
H	2.030668	0.704158	0.000000
H	-0.024494	2.258740	0.000000
H	-2.203812	0.495740	0.000000
H	-1.112867	-1.838735	0.000000

Energy E(RB-P86) -226.01754042 a.u.
-593409.05 kJ/mol
-141828.15 kcal/mol
SCF Convergence: 0.4843D-08
Maximum Force: 0.000188
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.069391 a.u.
Lowest Frequency 583.4301 cm-1

RuCl2CH2PMe3

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.807648	-0.024633	0.158182
Cl	-1.094183	2.249001	-0.185522
Cl	-1.111450	-2.042656	-0.939510
C	-0.822514	-0.338760	1.947735
P	1.388545	0.002152	-0.043503
H	-1.838069	-0.416171	2.411017
H	0.030182	-0.465596	2.651610
C	2.235850	-1.566897	0.428709
C	2.247257	1.309599	0.934297
C	1.927941	0.305605	-1.781977
H	3.342512	1.281259	0.757368
H	1.836131	2.294507	0.638030
H	2.043622	1.159227	2.012831
H	3.035524	0.313634	-1.854933

```
 H    1.517155  -0.493023  -2.431064
 H    1.524811   1.281184  -2.119006
 H    3.331387  -1.488757   0.269408
 H    2.032967  -1.791115   1.494489
 H    1.816671  -2.388724  -0.184250
-----------------------------------
Energy E(RB-P86)  -1515.53274016 a.u.
                   -3979031.21 kJ/mol
                    -951011.19 kcal/mol
SCF Convergence: 0.1941D-08
  Maximum Force: 0.000015
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.137357 a.u.
Lowest Frequency    40.4386 cm-1
```

RuCl2CH2PH3

```
Atom Coordinates (x,y,z) in Angstrom
-----------------------------------
 Ru  -0.295225  -0.026689   0.110561
 P    1.877085  -0.081736  -0.080135
 C   -0.272530  -0.708056   1.795231
 Cl  -0.723635  -1.744899  -1.360540
 Cl  -0.480340   2.263203   0.257754
 H    2.444754  -0.886055  -1.121479
 H    2.568769   1.154687  -0.295729
 H    2.607175  -0.583519   1.050479
 H    0.596720  -1.013767   2.419624
 H   -1.281037  -0.833819   2.260433
-----------------------------------
Energy E(RB-P86)  -1397.64724561 a.u.
                   -3669522.84 kJ/mol
                    -877036.92 kcal/mol
SCF Convergence: 0.4752D-09
  Maximum Force: 0.000040
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.053561 a.u.
Lowest Frequency    98.1421 cm-1
```

n3-ii

Ru	0.017234	0.034447	0.653607
C	1.215409	-1.333966	0.795492
C	0.044671	-0.165992	-1.375430
Cl	-2.130142	-0.998110	0.491849
Cl	1.318150	1.994615	0.242738
N	-0.737240	-0.969660	-2.151501
N	0.882113	0.435119	-2.268243
C	-0.420358	-0.857838	-3.497037
C	0.617716	0.042649	-3.571858
H	1.581629	-1.672437	1.793127
H	1.636964	-1.891238	-0.070000
H	-1.518284	-1.476428	-1.706576
H	1.526399	1.164854	-1.925933
C	0.512079	0.701734	2.818376
C	-0.531542	-0.203931	2.893768
H	0.327671	1.787486	2.831788
H	1.557789	0.402467	2.996730
H	-0.365272	-1.266337	3.135741
H	-1.576821	0.134786	2.969427
H	-0.943105	-1.416115	-4.279913
H	1.176648	0.422554	-4.432732

Energy E(RB-P86) -1359.20070799 a.u.
-3568581.46 kJ/mol
-852911.36 kcal/mol
SCF Convergence: 0.7350D-08
Maximum Force: 0.000038
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.151151 a.u.
Lowest Frequency 62.6975 cm-1

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n3-ia

no local minimum

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n3-ai

Atom Coordinates (x,y,z) in Angstrom

Ru	0.020196	0.021623	0.688782
C	1.401949	-1.124305	0.941422
C	-0.059144	-0.028503	-1.390370
Cl	1.586596	1.862827	0.292335
Cl	-1.539209	-1.858108	0.501449
N	-0.800785	-0.854646	-2.170297
N	0.581362	0.789961	-2.262552
C	-0.631347	-0.569631	-3.511720
C	0.256539	0.486889	-3.570973
H	2.451449	-0.754005	0.975439
H	1.222410	-2.216783	1.059795
H	-1.376724	-1.574739	-1.686954
H	1.215769	1.510589	-1.859825
C	-0.100573	1.146872	2.602102
C	-1.000734	0.074028	2.662831
H	0.885798	1.105409	3.089892
H	-0.759858	-0.856050	3.200924
H	-2.072885	0.219419	2.447860
H	-0.443433	2.161540	2.337930
H	-1.144566	-1.118901	-4.307456
H	0.663656	1.032572	-4.428163

Energy E(RB-P86) -1359.19594677 a.u.
-3568568.96 kJ/mol

-852908.37 kcal/mol
SCF Convergence: 0.7353D-08
Maximum Force: 0.000014
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.150801 a.u.
Lowest Frequency 61.9211 cm-1

n3-aa

no local minimum

p3ii/p3ia

Atom Coordinates (x,y,z) in Angstrom

Ru	0.121432	-0.888798	0.002882
C	1.959241	-0.846814	-0.027493
C	0.032131	1.050718	-0.046097
Cl	-0.460122	-0.881283	-2.280538
Cl	-0.499086	-0.829721	2.267724
H	2.563493	-1.774669	0.041159
H	2.541794	0.093514	-0.134834
C	0.458286	-3.299925	0.479048
C	-0.759924	-3.136971	-0.129828
H	0.566939	-3.280916	1.574139
H	1.334976	-3.611904	-0.112142
H	-0.893780	-3.318577	-1.206654
H	-1.676349	-2.989929	0.467794
P	-0.659416	2.048163	-1.363932
P	0.554627	2.133321	1.267548
C	-0.533310	3.699478	-0.597635
C	0.272271	3.756537	0.498654
H	-2.057666	1.781010	-1.505653
H	1.965628	1.945800	1.448493
H	0.561081	4.694958	1.000867
H	-0.942895	4.594498	-1.096279

Energy E(RB-P86) -1932.24785654 a.u.
-5073116.75 kJ/mol
-1212503.89 kcal/mol
SCF Convergence: 0.4564D-08
Maximum Force: 0.000061
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.134405 a.u.
Lowest Frequency 36.6993 cm-1

p3-ai

Atom Coordinates (x,y,z) in Angstrom

Ru	0.246261	-0.879225	0.089229
C	2.041397	-1.024373	0.387730
C	-0.039451	1.025907	0.043130
Cl	-0.184967	-0.875568	2.468338
Cl	0.876818	-0.605605	-2.279987
H	2.397795	-1.351200	1.387310
H	2.777987	-0.841491	-0.420914
C	-0.933829	-2.838669	0.385090
C	-0.642683	-2.756296	-0.967727
H	-0.312425	-3.433037	1.073778
H	0.222163	-3.276684	-1.407073
H	-1.366764	-2.347556	-1.690723
H	-1.904413	-2.508385	0.789725
P	-1.723359	1.494397	0.486313
P	0.937540	2.386448	-0.565845
C	-1.573950	3.258064	0.004723

```
 C   -0.432061   3.602366  -0.646487
 H   -1.601691   1.400202   1.921709
 H    1.156656   1.850311  -1.892148
 H   -0.268497   4.611852  -1.061762
 H   -2.426994   3.947182   0.126273
-------------------------------------
Energy E(RB-P86)  -1932.23581914 a.u.
                    -5073085.14 kJ/mol
                    -1212496.33 kcal/mol
SCF Convergence: 0.8122D-08
  Maximum Force: 0.000009
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.133590 a.u.
Lowest Frequency    42.2770 cm-1
```

p3-aa

no local minimum

n3-ii

Atom Coordinates (x,y,z) in Angstrom

Ru	0.018821	0.030292	0.627944
C	1.212928	-1.327625	0.780183
C	0.047839	-0.170581	-1.399638
Cl	-2.135101	-1.012414	0.513476
Cl	1.325928	2.004870	0.264422
N	-0.731025	-0.966537	-2.168002
N	0.875658	0.432950	-2.283405
C	-0.415981	-0.852353	-3.509226
C	0.611519	0.042557	-3.583024
H	1.573362	-1.658880	1.771108
H	1.638968	-1.887325	-0.069526
H	-1.498797	-1.484472	-1.738952
H	1.524978	1.149276	-1.956180
C	0.495683	0.708585	2.897393
C	-0.530015	-0.184020	2.971095
H	0.313860	1.784845	2.871500
H	1.537667	0.409683	3.034110
H	-0.364149	-1.245314	3.170828
H	-1.570443	0.145090	3.006940
H	-0.935388	-1.404922	-4.286876
H	1.163501	0.423135	-4.437617

Energy E(RB+HF-LYP) -1359.03615499 a.u.
-3568149.42 kJ/mol
-852808.10 kcal/mol
SCF Convergence: 0.1911D-08
Maximum Force: 0.000025
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.155733 a.u.
Lowest Frequency 59.9390 cm-1

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n3-ia

Atom Coordinates (x,y,z) in Angstrom

Ru	0.015799	0.030053	-0.588344
C	0.720695	1.712951	-0.667895
C	0.055795	0.151129	1.420464
Cl	-2.337575	0.383953	-0.517245
Cl	1.918304	-1.398323	-0.494521
N	-0.916569	0.605248	2.245873
N	1.053736	-0.219890	2.256724
C	-0.548081	0.505106	3.574142
C	0.711427	-0.022333	3.581091
H	0.940326	2.225339	-1.618641
H	0.965193	2.308783	0.228275
H	-1.815359	0.892681	1.858466
H	1.892783	-0.660160	1.878974
C	-0.401289	-0.993888	-2.782096
C	0.112388	0.228877	-3.065226
H	0.243046	-1.874715	-2.720635
H	-1.481544	-1.152323	-2.729681
H	-0.540603	1.085651	-3.248973
H	1.182692	0.363788	-3.239850
H	1.374670	-0.265776	4.406143
H	-1.194551	0.810129	4.392008

Energy E(RB+HF-LYP) -1359.03531168 a.u.
-3568147.21 kJ/mol
-852807.57 kcal/mol

SCF Convergence: 0.4752D-08
  Maximum Force: 0.000033
<S**2>:   0.0000
Charge: 0.0000
ZPE-correction: 0.155297 a.u.
Lowest Frequency   24.8790 cm-1

n3-ai

Atom Coordinates (x,y,z) in Angstrom

Ru	0.013002	0.023290	0.674800
C	1.389093	-1.126699	0.890822
C	-0.043218	-0.035144	-1.411138
Cl	1.560761	1.897918	0.319223
Cl	-1.587656	-1.833348	0.508524
N	-0.770220	-0.859610	-2.190629
N	0.605820	0.771758	-2.273456
C	-0.582514	-0.583670	-3.527734
C	0.299264	0.461761	-3.580804
H	2.432635	-0.768827	0.919028
H	1.214900	-2.211551	0.993829
H	-1.357964	-1.569982	-1.738666
H	1.227694	1.495613	-1.894537
C	-0.077820	1.105026	2.677957
C	-0.966326	0.050712	2.731905
H	0.924371	1.039374	3.106057
H	-0.708806	-0.898851	3.205204
H	-2.030938	0.194993	2.528461
H	-0.411943	2.116243	2.430043
H	-1.081112	-1.133773	-4.320782
H	0.716204	0.997380	-4.428987

Energy E(RB+HF-LYP) -1359.03143496 a.u.
                    -3568137.03 kJ/mol
                     -852805.14 kcal/mol
SCF Convergence: 0.3271D-08
  Maximum Force: 0.000042
<S**2>:   0.0000
Charge: 0.0000
ZPE-correction: 0.155636 a.u.
Lowest Frequency   62.9814 cm-1

n3-aa

no local minimum

p3-ii

Atom Coordinates (x,y,z) in Angstrom

Ru	0.058256	-0.869109	0.018421
C	1.818082	-0.908703	-0.436081
C	0.000451	1.075988	-0.068226
Cl	-1.150103	-0.899476	-2.018480
Cl	-0.057614	-0.730244	2.373420
H	2.333633	-1.879811	-0.527585
H	2.440684	-0.026220	-0.651505
C	0.331604	-3.387123	0.764075
C	-0.171021	-3.420540	-0.487632
H	-0.315592	-3.412552	1.642193
H	1.405999	-3.413255	0.962344
H	0.468556	-3.478489	-1.371599
H	-1.245768	-3.483474	-0.672031
P	-0.712843	2.097389	-1.348843
P	0.719663	2.131236	1.159864
C	-0.378710	3.742346	-0.643566
C	0.505408	3.753278	0.375811

```
 H   -2.119013   1.933438  -1.358473
 H    2.103516   1.827692   1.245459
 H    0.905590   4.666880   0.825583
 H   -0.746867   4.650949  -1.130490
------------------------------------
Energy E(RB+HF-LYP)  -1932.04021151 a.u.
                     -5072571.58 kJ/mol
                     -1212373.59 kcal/mol
SCF Convergence: 0.3740D-08
  Maximum Force: 0.000030
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.138247 a.u.
Lowest Frequency    36.7930 cm-1
```

p3-ia

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru   0.072442  -0.835962  -0.005895
 C    1.867567  -0.943600  -0.298686
 C    0.095706   1.087556  -0.056002
 Cl  -0.890014  -0.907977  -2.154501
 Cl  -0.176135  -0.839743   2.330646
 H    2.371638  -1.922671  -0.330531
 H    2.526275  -0.076492  -0.467791
 C   -1.040358  -3.265833   0.159843
 C    0.282396  -3.516826   0.205988
 H   -1.613077  -3.093262   1.074999
 H   -1.589857  -3.284746  -0.784021
 H    0.839943  -3.754979  -0.704478
 H    0.823007  -3.554085   1.155113
 P   -0.742924   2.125054  -1.251441
 P    0.916833   2.128007   1.134772
 C   -0.374736   3.757281  -0.531793
 C    0.598834   3.759644   0.402355
 H   -2.140781   1.925392  -1.117306
 H    2.306757   1.845133   1.027940
 H    1.024274   4.671943   0.831422
 H   -0.796164   4.672075  -0.960635
------------------------------------
Energy E(RB+HF-LYP)  -1932.04159883 a.u.
                     -5072575.22 kJ/mol
                     -1212374.46 kcal/mol
SCF Convergence: 0.2851D-08
  Maximum Force: 0.000014
<S**2>:   0.0000
Charge:   0.0000
ZPE-correction:        0.137703 a.u.
Lowest Frequency    33.0572 cm-1
```

p3-ai

```
Atom Coordinates (x,y,z) in Angstrom
------------------------------------
 Ru   0.209713  -0.840692   0.080439
 C    2.004646  -0.923609   0.331211
 C   -0.038389   1.049648   0.040730
 Cl  -0.243293  -0.908109   2.451630
 Cl   0.652112  -0.667667  -2.325618
 H    2.416391  -1.204222   1.315041
 H    2.714119  -0.730401  -0.488876
 C   -0.786869  -3.104402   0.440016
 C   -0.504373  -3.056214  -0.886371
 H   -0.084331  -3.520024   1.165520
 H    0.439582  -3.427146  -1.290956
```

H	-1.246751	-2.740687	-1.622983
H	-1.772931	-2.839453	0.829414
P	-1.731976	1.608178	0.365902
P	1.057413	2.383070	-0.428667
C	-1.430374	3.374975	-0.019514
C	-0.230427	3.679387	-0.547207
H	-1.701617	1.505979	1.790589
H	1.312665	1.954598	-1.767256
H	0.020658	4.687981	-0.891916
H	-2.241933	4.104578	0.068179

Energy E(RB+HF-LYP) -1932.02953479 a.u.
-5072543.54 kJ/mol
-1212366.89 kcal/mol
SCF Convergence: 0.3362D-08
Maximum Force: 0.000018
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.137569 a.u.
Lowest Frequency 34.1441 cm-1

p3-aa

Atom Coordinates (x,y,z) in Angstrom

Ru	-0.786420	0.001918	0.065462
Cl	-0.775878	-2.172769	1.079859
Cl	-1.084725	2.041204	-1.157348
C	1.093381	0.093299	-0.007112
C	-1.187975	0.781930	1.667690
H	-1.431134	1.855648	1.734755
H	-1.228548	0.189975	2.597256
C	-3.368961	-0.121577	0.168288
C	-2.864527	-0.671044	-0.974723
H	-3.690268	0.922733	0.192789
H	-3.570628	-0.740693	1.045919
H	-2.679029	-1.746981	-1.033639
H	-2.806724	-0.079198	-1.891687
P	2.275504	0.438010	1.308073
C	3.775115	0.016308	0.339043
C	3.608732	-0.143977	-0.985033
P	1.885570	-0.301366	-1.604583
H	2.032434	-0.736702	2.084330
H	4.448511	-0.293137	-1.672034
H	1.642131	0.962080	-2.228494
H	4.765269	0.039207	0.806513

Energy E(RB+HF-LYP) -1932.03817581 a.u.
-5072566.23 kJ/mol
-1212372.31 kcal/mol
SCF Convergence: 0.2858D-08
Maximum Force: 0.000016
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.137877 a.u.
Lowest Frequency 32.0773 cm-1

[Ru]SIH-ii

Atom Coordinates (x,y,z) in Angstrom

N	1.062844	0.185483	-2.148520
C	0.725999	0.061532	-3.568900
C	-0.508423	-0.870346	-3.516336
N	-0.886870	-0.770026	-2.108981
C	0.048926	-0.194242	-1.349096

H	-1.706267	-1.186877	-1.670584
Ru	0.017547	0.028577	0.668415
Cl	1.286580	2.019397	0.299602
H	1.711052	0.882989	-1.787178
C	1.214368	-1.330217	0.812859
Cl	-2.160628	-0.958195	0.616799
C	-0.507418	-0.155299	3.045648
C	0.544071	0.702014	2.958562
H	0.475735	1.048077	-3.999048
H	1.555086	-0.365626	-4.152137
H	-0.248605	-1.911382	-3.780145
H	-1.319774	-0.542936	-4.183651
H	1.570965	-1.662573	1.804586
H	1.646142	-1.884285	-0.037376
H	1.578133	0.368522	3.073278
H	-0.374116	-1.222995	3.235549
H	0.397773	1.783244	2.925722
H	-1.536323	0.207197	3.088020

Energy E(RB+HF-LYP) -1360.23703630 a.u.
-3571302.34 kJ/mol
-853561.66 kcal/mol
SCF Convergence: 0.2596D-08
Maximum Force: 0.000002
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.178500 a.u.
Lowest Frequency 46.4860 cm-1

[Ru]SIH-ia

Atom Coordinates (x,y,z) in Angstrom

C	-0.639476	0.454508	3.589630
N	-1.006497	0.325314	2.180968
C	0.048467	0.170902	1.373342
N	1.156877	0.110607	2.133486
C	0.846326	0.018136	3.562568
Ru	0.005839	0.036394	-0.626491
Cl	-2.355987	0.315581	-0.601299
H	1.999405	-0.279403	1.716240
H	-1.927703	0.490578	1.780212
C	0.693054	1.726274	-0.703677
Cl	1.906994	-1.383442	-0.545366
H	1.490885	0.673459	4.166855
H	0.974578	-1.017883	3.924042
H	-1.259278	-0.185021	4.235901
H	-0.754519	1.498696	3.931624
H	0.885056	2.239298	-1.660366
H	0.956295	2.321716	0.187279
C	0.190095	0.190852	-3.145341
C	-0.405480	-0.993388	-2.873885
H	-0.404731	1.082606	-3.359730
H	-1.493750	-1.087923	-2.858023
H	0.185194	-1.906403	-2.760826
H	1.273982	0.267430	-3.261281

Energy E(RB+HF-LYP) -1360.23618972 a.u.
-3571300.12 kJ/mol
-853561.13 kcal/mol
SCF Convergence: 0.4333D-08
Maximum Force: 0.000002
<S**2>: 0.0000
Charge: 0.0000

ZPE-correction: 0.177947 a.u.
Lowest Frequency 36.3534 cm-1

[Ru]SIH-ai

Atom Coordinates (x,y,z) in Angstrom

N	0.807458	0.575892	-2.200881
C	0.403611	0.466119	-3.603356
C	-0.672346	-0.648224	-3.532363
N	-0.940715	-0.707844	-2.094856
C	-0.030474	-0.051973	-1.376782
H	-1.567259	-1.358190	-1.612980
Ru	0.009621	0.032544	0.724655
Cl	1.614546	1.857903	0.382365
H	1.455170	1.261035	-1.803673
C	1.350667	-1.167102	0.891023
Cl	-1.661370	-1.762231	0.611985
C	-0.947563	0.102221	2.799256
C	-0.013187	1.113516	2.740922
H	-0.015011	1.422258	-3.964771
H	1.250564	0.198854	-4.252668
H	-0.287267	-1.617298	-3.896387
H	-1.578325	-0.404686	-4.106949
H	1.139309	-2.243664	1.012163
H	2.408012	-0.850879	0.876287
H	-0.299969	2.140054	2.497730
H	-0.728729	-0.861986	3.262155
H	0.990794	0.997561	3.153765
H	-2.006042	0.294921	2.604515

Energy E(RB+HF-LYP) -1360.22928723 a.u.
-3571281.99 kJ/mol
-853556.80 kcal/mol
SCF Convergence: 0.3587D-08
Maximum Force: 0.000006
<S**2>: 0.0000
Charge: 0.0000
ZPE-correction: 0.178278 a.u.
Lowest Frequency 51.1371 cm-1