Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Bond Tuning with Heterocyclic Carbenes

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Supplementary Information

PMe3

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P     0.141496   3.165298   0.000000
C     1.923862   3.780736   0.000000
C    -0.542305   4.173343   1.417570
C    -0.542305   4.173343  -1.417570
H    -0.312674   5.245676  -1.323727
H    -0.124677   3.798177  -2.362832
H    -1.633353   4.042771  -1.459278
H    -0.312674   5.245676   1.323727
H    -1.633353   4.042771   1.459278
H    -0.124677   3.798177   2.362832
H     2.126818   4.391144   0.890828
H     2.616642   2.928385   0.000000
H     2.126818   4.391144  -0.890828
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-2.366309082727810 hartree
-1484.88       kcal/mol
-6212.74         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000004
 Gradient (Max):   0.000867
 Gradient (RMS):   0.000229
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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Phosphorus (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
-----------------------------------------------------
C     2.905719  -1.864768   1.230687
C     2.215500  -1.894951   0.000000
C     2.905719  -1.864768  -1.230687
C     4.300218  -1.737874  -1.201764
C     5.014409  -1.660289   0.000000
C     4.300218  -1.737874   1.201764
N     0.787165  -2.064713   0.000000
C    -0.182998  -1.103447   0.000000
N    -1.382361  -1.742870   0.000000
C    -1.263070  -3.222303   0.000000
C     0.251795  -3.445569   0.000000
C    -2.719100  -1.197745   0.000000
C    -3.390704  -1.030540   1.230122
C    -4.741822  -0.659964   1.200474
C    -5.437707  -0.478908   0.000000
C    -4.741822  -0.659964  -1.200474
C    -3.390704  -1.030540  -1.230122
Ru    0.202201   0.953507   0.000000
Cl    0.054602   1.053124   2.424574
C     2.024649   0.966457   0.000000
P     0.328067   3.361661   0.000000
Cl    0.054602   1.053124  -2.424574
C     2.169172  -1.921531  -2.543229
C     6.518892  -1.521613   0.000000
C     2.169172  -1.921531   2.543229
C    -2.698483  -1.261261  -2.548515
C    -6.914523  -0.158406   0.000000
C    -2.698483  -1.261261   2.548515
C     1.214891   4.108822  -1.434364
C     1.214891   4.108822   1.434364
C    -1.306865   4.253527   0.000000
H     0.602107  -3.989807   0.889194
H     0.602107  -3.989807  -0.889194
H    -1.756860  -3.640217   0.889359
H    -1.756860  -3.640217  -0.889359
H     4.839922  -1.687547  -2.151175
H     4.839922  -1.687547   2.151175
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H    -5.267577  -0.530662  -2.150214
H    -5.267577  -0.530662   2.150214
H     2.604886   1.001881   0.940010
H     2.604886   1.001881  -0.940010
H    -3.398806  -1.110928   3.379642
H    -2.305164  -2.286657   2.625966
H    -1.845663  -0.576256   2.676847
H    -3.398806  -1.110928  -3.379642
H    -1.845663  -0.576256  -2.676847
H    -2.305164  -2.286657  -2.625966
H    -7.202496   0.415981   0.890178
H    -7.202496   0.415981  -0.890178
H    -7.512858  -1.083697   0.000000
H     6.870054  -0.982010   0.889497
H     7.007408  -2.508601   0.000000
H     6.870054  -0.982010  -0.889497
H     2.876062  -1.914060   3.382230
H     1.487197  -1.062172   2.651921
H     1.558187  -2.832893   2.628256
H     2.876062  -1.914060  -3.382230
H     1.558187  -2.832893  -2.628256
H     1.487197  -1.062172  -2.651921
H     1.182817   5.206706   1.385991
H     0.756060   3.744905   2.363174
H     2.261408   3.770806   1.417320
H     1.182817   5.206706  -1.385991
H     2.261408   3.770806  -1.417320
H     0.756060   3.744905  -2.363174
H    -1.383802   4.885717  -0.895106
H    -2.138243   3.537376   0.000000
H    -1.383802   4.885717   0.895106
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-14.333719507293688 hartree
-8994.55       kcal/mol
-37633.18        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000022
 Gradient (Max):   0.000586
 Gradient (RMS):   0.000175
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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.758905  -1.819702   1.231400
C     2.076396  -1.936767   0.000000
C     2.758905  -1.819702  -1.231400
C     4.122046  -1.500177  -1.201119
C     4.817961  -1.322992   0.000000
C     4.122046  -1.500177   1.201119
N     0.674008  -2.276678   0.000000
C    -0.355058  -1.378511   0.000000
N    -1.529180  -2.074055   0.000000
C    -1.321711  -3.537683   0.000000
C     0.211832  -3.678367   0.000000
C    -2.861613  -1.541004   0.000000
C    -3.523318  -1.338530  -1.231821
C    -4.858910  -0.921161  -1.202877
C    -5.545761  -0.712811   0.000000
C    -4.858910  -0.921161   1.202877
C    -3.523318  -1.338530   1.231821
C    -2.804499  -1.527060  -2.542748
C    -2.804499  -1.527060   2.542748
C    -6.998272  -0.299439   0.000000
Ru   -0.011220   0.533942   0.000000
Cl    0.191578   0.965973   2.309155
C     2.061159  -2.026215  -2.550795
C     6.291574  -0.990783   0.000000
C     2.061159  -2.026215   2.550795
Cl    0.191578   0.965973  -2.309155
C    -1.775187   1.020461   0.000000
H    -1.785269  -3.989817  -0.889385
H    -1.785269  -3.989817   0.889385
H     0.584887  -4.206508  -0.889983
H     0.584887  -4.206508   0.889983
H    -5.375246  -0.750948   2.151121
H    -5.375246  -0.750948  -2.151121
H     4.652381  -1.387767   2.150155
H     4.652381  -1.387767  -2.150155
H    -2.316445   1.229865  -0.938806
H    -2.316445   1.229865   0.938806
H     2.790352  -2.036441  -3.370207
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H     1.510706  -2.977988  -2.577375
H     1.341251  -1.215861  -2.742313
H     2.790352  -2.036441   3.370207
H     1.341251  -1.215861   2.742313
H     1.510706  -2.977988   2.577375
H     6.570029  -0.410969  -0.889557
H     6.570029  -0.410969   0.889557
H     6.901662  -1.907812   0.000000
H    -7.246821   0.293223  -0.889903
H    -7.655342  -1.183471   0.000000
H    -7.246821   0.293223   0.889903
H    -3.484348  -1.349466  -3.384823
H    -1.953063  -0.833483  -2.630835
H    -2.400908  -2.545365  -2.644756
H    -3.484348  -1.349466   3.384823
H    -2.400908  -2.545365   2.644756
H    -1.953063  -0.833483   2.630835
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.920455778456372 hartree
-7480.20       kcal/mol
-31297.15        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000037
 Gradient (Max):   0.000868
 Gradient (RMS):   0.000134
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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.989091   1.219560  -1.231054
C     2.298782   1.299638   0.000000
C     2.989091   1.219560   1.231054
C     4.360452   0.933694   1.199836
C     5.061292   0.770204   0.000000
C     4.360452   0.933694  -1.199836
N     0.886018   1.612432   0.000000
C    -0.142234   0.727927   0.000000
N    -1.305546   1.420011   0.000000
C    -1.093011   2.889862   0.000000
C     0.435471   3.023809   0.000000
C    -2.664775   0.932851   0.000000
C    -3.335912   0.766468   1.229966
C    -4.673118   0.349927   1.199923
C    -5.356913   0.125606   0.000000
C    -4.673118   0.349927  -1.199923
C    -3.335912   0.766468  -1.229966
C    -2.657177   1.030352   2.548953
C    -2.657177   1.030352  -2.548953
C    -6.805697  -0.302878   0.000000
Ru    0.252390  -1.322228   0.000000
Cl    0.103635  -1.207228  -2.447201
C     2.305104   1.467313   2.550026
C     6.544692   0.484335   0.000000
C     2.305104   1.467313  -2.550026
Cl    0.103635  -1.207228   2.447201
C    -1.451528  -1.966182   0.000000
H    -1.559584   3.334628   0.889700
H    -1.559584   3.334628  -0.889700
H     0.817364   3.542637   0.890396
H     0.817364   3.542637  -0.890396
H    -5.192672   0.199917  -2.149865
H    -5.192672   0.199917   2.149865
H     4.894656   0.847431  -2.149539
H     4.894656   0.847431   2.149539
H    -1.969905  -2.179260   0.947925
H    -1.969905  -2.179260  -0.947925
H     3.022311   1.370400   3.374387
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H	1.883167	2.483305	2.596366
H	1.484993	0.752908	2.716637
H	3.022311	1.370400	-3.374387
H	1.484993	0.752908	-2.716637
H	1.883167	2.483305	-2.596366
H	6.842617	-0.085434	0.889752
H	6.842617	-0.085434	-0.889752
H	7.124465	1.420837	0.000000
H	-7.046990	-0.899152	0.889685
H	-7.474175	0.572583	0.000000
H	-7.046990	-0.899152	-0.889685
H	-3.344250	0.827222	3.379671
H	-1.762251	0.400995	2.671103
H	-2.336823	2.080589	2.634877
H	-3.344250	0.827222	-3.379671
H	-2.336823	2.080589	-2.634877
H	-1.762251	0.400995	-2.671103
C	1.565783	-3.021958	-0.693491
C	1.565783	-3.021958	0.693491
H	2.365249	-2.538809	-1.256052
H	0.932328	-3.693969	-1.269819
H	0.932328	-3.693969	1.269819
H	2.365249	-2.538809	1.256052

Net Charge: 0.00

Total Bonding Energy:
-13.101889242752160 hartree
-8221.56 kcal/mol
-34399.01 kJ/mol

Summary Geometry Optimization:

Energy Change :	0.000240
Gradient (Max):	0.000584
Gradient (RMS):	0.000106

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ADF - Version 2008.01
GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Nitrogen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.135716   1.204660   0.000000
C    -0.090964  -0.809889   0.000000
Cl    0.148254   1.317726  -2.411494
Cl    0.148254   1.317726   2.411494
C     1.642095   2.488507   0.000000
C    -1.048377   2.790690   0.000000
H    -1.599309   2.962277  -0.929883
H    -1.599309   2.962277   0.929883
C     0.389100   3.460931   0.000000
H     0.454686   4.045057   0.925144
H     0.454686   4.045057  -0.925144
H     2.217365   2.533661  -0.929883
H     2.217365   2.533661   0.929883
N     0.918021  -1.711746   0.000000
N    -1.275676  -1.463901   0.000000
C     0.422682  -3.109573   0.000000
C    -1.104685  -2.936981   0.000000
H    -1.581611  -3.371244   0.890036
H    -1.581611  -3.371244  -0.890036
H     0.790757  -3.639240   0.890062
H     0.790757  -3.639240  -0.890062
C    -2.600253  -0.886258   0.000000
C    -3.253686  -0.665987   1.230802
C    -4.557800  -0.155585   1.200765
C    -5.222927   0.116496   0.000000
C    -4.557800  -0.155585  -1.200765
C    -3.253686  -0.665987  -1.230802
C    -2.588911  -0.963678   2.549506
H    -5.069493   0.022568   2.150037
C    -6.617350   0.696832   0.000000
H    -5.069493   0.022568  -2.150037
C    -2.588911  -0.963678  -2.549506
C     2.338108  -1.444530   0.000000
C     3.024155  -1.375772  -1.230845
C     4.409099  -1.168050  -1.200799
C     5.118029  -1.050443   0.000000
C     4.409099  -1.168050   1.200799
C     3.024155  -1.375772   1.230845
C     2.309726  -1.518529  -2.549468
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H     4.947634  -1.108188  -2.150053
C     6.606508  -0.794287   0.000000
H     4.947634  -1.108188   2.150053
C     2.309726  -1.518529   2.549468
H    -7.181021   0.387788  -0.890108
H    -7.181021   0.387788   0.890108
H    -6.581715   1.797559   0.000000
H    -3.292909  -0.807254   3.376181
H    -2.235195  -2.004163   2.603604
H    -1.715214  -0.311542   2.707063
H    -2.235195  -2.004163  -2.603604
H    -3.292909  -0.807254  -3.376181
H    -1.715214  -0.311542  -2.707063
H     7.087487  -1.220779  -0.890119
H     6.816190   0.286865   0.000000
H     7.087487  -1.220779   0.890119
H     3.030757  -1.522142  -3.376242
H     1.733897  -2.454566  -2.603571
H     1.602439  -0.688823  -2.706912
H     1.733897  -2.454566   2.603571
H     3.030757  -1.522142   3.376242
H     1.602439  -0.688823   2.706912
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.121245793775138 hartree
-8233.71       kcal/mol
-34449.83        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000069
 Gradient (Max):   0.000808
 Gradient (RMS):   0.000147
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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.493767  -1.934148   1.234728
C     2.798374  -2.004947   0.000000
C     3.493767  -1.934148  -1.234728
C     4.887283  -1.802918  -1.203518
C     5.599710  -1.735975   0.000000
C     4.887283  -1.802918   1.203518
P     0.996518  -2.178441   0.000000
C    -0.195538  -0.936037   0.000000
P    -1.711897  -1.743530   0.000000
C    -1.395150  -3.593710   0.000000
C     0.140944  -3.845770   0.000000
C    -3.421009  -1.148909   0.000000
C    -4.100638  -0.984513   1.234599
C    -5.471692  -0.701108   1.203345
C    -6.176653  -0.575520   0.000000
C    -5.471692  -0.701108  -1.203345
C    -4.100638  -0.984513  -1.234599
Ru    0.328127   1.064752   0.000000
Cl    0.158864   1.096741   2.424377
C     2.151630   1.088507   0.000000
P     0.379664   3.448333   0.000000
Cl    0.158864   1.096741  -2.424377
C     2.771561  -1.959064  -2.558072
C     7.104238  -1.610733   0.000000
C     2.771561  -1.959064   2.558072
C    -3.390264  -1.108880  -2.559845
C    -7.668422  -0.342750   0.000000
C    -3.390264  -1.108880   2.559845
C     1.217558   4.236620  -1.440190
C     1.217558   4.236620   1.440190
C    -1.308089   4.235106   0.000000
H     0.440347  -4.418275   0.887638
H     0.440347  -4.418275  -0.887638
H    -1.862050  -4.041090   0.887183
H    -1.862050  -4.041090  -0.887183
H     5.429942  -1.738019  -2.149989
H     5.429942  -1.738019   2.149989
H    -6.004658  -0.580984  -2.149944
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```
H    -6.004658  -0.580984   2.149944
H     2.729875   1.104558   0.941960
H     2.729875   1.104558  -0.941960
H    -4.064055  -0.845608   3.385657
H    -3.036099  -2.137156   2.727415
H    -2.503047  -0.460114   2.602535
H    -4.064055  -0.845608  -3.385657
H    -2.503047  -0.460114  -2.602535
H    -3.036099  -2.137156  -2.727415
H    -7.990061   0.211948   0.890855
H    -7.990061   0.211948  -0.890855
H    -8.207876  -1.303412   0.000000
H     7.461769  -1.077479   0.890458
H     7.578315  -2.604844   0.000000
H     7.461769  -1.077479  -0.890458
H     3.483752  -1.883121   3.390126
H     2.050837  -1.129544   2.631390
H     2.197537  -2.888714   2.683019
H     3.483752  -1.883121  -3.390126
H     2.197537  -2.888714  -2.683019
H     2.050837  -1.129544  -2.631390
H     1.110778   5.330437   1.407864
H     0.783712   3.826553   2.362330
H     2.284252   3.969701   1.417128
H     1.110778   5.330437  -1.407864
H     2.284252   3.969701  -1.417128
H     0.783712   3.826553  -2.362330
H    -1.425623   4.860223  -0.895745
H    -2.092941   3.467940   0.000000
H    -1.425623   4.860223   0.895745
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-14.005896061651290 hartree
-8788.83       kcal/mol
-36772.47        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000026
 Gradient (Max):   0.000497
 Gradient (RMS):   0.000143
 -----------------------------------------------------
```

I-2 a-P

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	3.306436	-1.836573	1.236520
C	2.637982	-2.044323	0.000000
C	3.306436	-1.836573	-1.236520
C	4.643060	-1.422969	-1.203420
C	5.325888	-1.209778	0.000000
C	4.643060	-1.422969	1.203420
P	0.895248	-2.529669	0.000000
C	0.223367	-4.280179	0.000000
C	-1.339182	-4.236502	0.000000
P	-1.894472	-2.449883	0.000000
C	-0.474381	-1.463413	0.000000
Ru	-0.264122	0.466889	0.000000
Cl	-0.010330	0.825667	2.312146
C	2.613268	-2.004543	-2.564100
C	6.772000	-0.777708	0.000000
C	2.613268	-2.004543	2.564100
C	-3.610042	-1.876144	0.000000
C	-4.277030	-1.656334	-1.235164
C	-5.611549	-1.236055	-1.203492
C	-6.296491	-1.026892	0.000000
C	-5.611549	-1.236055	1.203492
C	-4.277030	-1.656334	1.235164
C	-3.583652	-1.839231	-2.562074
C	-3.583652	-1.839231	2.562074
C	-7.745248	-0.604292	0.000000
Cl	-0.010330	0.825667	-2.312146
C	-2.036903	0.896976	0.000000
H	-1.732270	-4.748289	-0.887608
H	-1.732270	-4.748289	0.887608
H	0.587967	-4.811927	-0.888025
H	0.587967	-4.811927	0.888025
H	-6.128924	-1.058441	2.149449
H	-6.128924	-1.058441	-2.149449
H	5.161573	-1.250596	2.149700
H	5.161573	-1.250596	-2.149700
H	-2.589739	1.060715	-0.941701
H	-2.589739	1.060715	0.941701
H	3.333200	-1.927512	-3.389040

```
H     2.104239  -2.975755  -2.634590
H     1.843122  -1.228410  -2.699049
H     3.333200  -1.927512   3.389040
H     1.843122  -1.228410   2.699049
H     2.104239  -2.975755   2.634590
H     7.011596  -0.182377  -0.890446
H     7.011596  -0.182377   0.890446
H     7.439698  -1.653662   0.000000
H    -7.990567  -0.011667  -0.890630
H    -8.405413  -1.485984   0.000000
H    -7.990567  -0.011667   0.890630
H    -4.257436  -1.582464  -3.389580
H    -2.685313  -1.209221  -2.630975
H    -3.252409  -2.878559  -2.700421
H    -4.257436  -1.582464   3.389580
H    -3.252409  -2.878559   2.700421
H    -2.685313  -1.209221   2.630975
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.586883948603111 hartree
-7270.88       kcal/mol
-30421.36        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------
 Energy Change :   0.000010
 Gradient (Max):   0.000431
 Gradient (RMS):   0.000101
 -----------------------------------------------
```

I-3 a-P

ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	3.657532	1.270993	-1.236801
C	2.972529	1.409284	0.000000
C	3.657532	1.270993	1.236801
C	5.028736	0.990940	1.203771
C	5.730005	0.849555	0.000000
C	5.028736	0.990940	-1.203771
P	1.198363	1.760499	0.000000
C	-0.098714	0.637933	0.000000
P	-1.559262	1.523651	0.000000
C	-1.109664	3.343465	0.000000
C	0.445033	3.478244	0.000000
C	-3.262594	0.920476	0.000000
C	-3.920977	0.691449	1.236094
C	-5.246243	0.242207	1.203706
C	-5.924809	0.015391	0.000000
C	-5.246243	0.242207	-1.203706
C	-3.920977	0.691449	-1.236094
C	-3.228169	0.894889	2.559721
C	-3.228169	0.894889	-2.559721
C	-7.362920	-0.443629	0.000000
Ru	0.189226	-1.412104	0.000000
Cl	0.079105	-1.172425	-2.441191
C	2.950204	1.397901	2.562022
C	7.214302	0.574569	0.000000
C	2.950204	1.397901	-2.562022
Cl	0.079105	-1.172425	2.441191
C	-1.508457	-2.066939	0.000000
H	-1.537665	3.828101	0.886930
H	-1.537665	3.828101	-0.886930
H	0.785057	4.027469	0.887273
H	0.785057	4.027469	-0.887273
H	-5.759607	0.054917	-2.150020
H	-5.759607	0.054917	2.150020
H	5.562381	0.872948	-2.150001
H	5.562381	0.872948	2.150001
H	-2.028455	-2.270368	0.949528
H	-2.028455	-2.270368	-0.949528
H	3.653598	1.249646	3.391558

```
H     2.494281   2.392361   2.676524
H     2.136159   0.661010   2.651832
H     3.653598   1.249646  -3.391558
H     2.136159   0.661010  -2.651832
H     2.494281   2.392361  -2.676524
H     7.517255   0.008962   0.890514
H     7.517255   0.008962  -0.890514
H     7.783766   1.517356   0.000000
H    -7.592718  -1.042740   0.890537
H    -8.046075   0.420370   0.000000
H    -7.592718  -1.042740  -0.890537
H    -3.890537   0.617987   3.390061
H    -2.307405   0.294048   2.623713
H    -2.934142   1.946087   2.698048
H    -3.890537   0.617987  -3.390061
H    -2.934142   1.946087  -2.698048
H    -2.307405   0.294048  -2.623713
C     1.430433  -3.128887  -0.697055
C     1.430433  -3.128887   0.697055
H     2.250992  -2.680966  -1.258437
H     0.785026  -3.790315  -1.272564
H     0.785026  -3.790315   1.272564
H     2.250992  -2.680966   1.258437
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-12.774973853023074 hartree
-8016.42       kcal/mol
-33540.69        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000034
 Gradient (Max):   0.000865
 Gradient (RMS):   0.000157
 -------------------------------------------------
```

I-4 a-P

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Phosphorus (TZP, 2p frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.140174   1.240636   0.000000
C    -0.083290  -0.736737   0.000000
Cl    0.144612   1.277536  -2.413096
Cl    0.144612   1.277536   2.413096
C     1.649435   2.519868   0.000000
C    -1.044902   2.824871   0.000000
H    -1.595513   3.002144  -0.929859
H    -1.595513   3.002144   0.929859
C     0.395227   3.493052   0.000000
H     0.461435   4.078032   0.924917
H     0.461435   4.078032  -0.924917
H     2.225760   2.569443  -0.929859
H     2.225760   2.569443   0.929859
P     1.187428  -1.892900   0.000000
P    -1.579679  -1.580600   0.000000
C     0.380023  -3.586065   0.000000
C    -1.169995  -3.411100   0.000000
H    -1.608825  -3.882945   0.888205
H    -1.608825  -3.882945  -0.888205
H     0.702640  -4.143924   0.888239
H     0.702640  -4.143924  -0.888239
C    -3.236943  -0.859801   0.000000
C    -3.870271  -0.568237   1.236420
C    -5.145421   0.008173   1.203741
C    -5.796659   0.303614   0.000000
C    -5.145421   0.008173  -1.203741
C    -3.870271  -0.568237  -1.236420
C    -3.200377  -0.829801   2.561273
H    -5.640846   0.238846   2.150037
C    -7.154566   0.962681   0.000000
H    -5.640846   0.238846  -2.150037
C    -3.200377  -0.829801  -2.561273
C     2.963631  -1.559294   0.000000
C     3.645912  -1.415676  -1.236403
C     5.017327  -1.137271  -1.203737
C     5.718149  -0.994900   0.000000
C     5.017327  -1.137271   1.203737
C     3.645912  -1.415676   1.236403
```

C	2.934474	-1.521296	-2.561197
H	5.551515	-1.021856	-2.150041
C	7.188981	-0.655910	0.000000
H	5.551515	-1.021856	2.150041
C	2.934474	-1.521296	2.561197
H	-7.734579	0.689589	-0.890941
H	-7.734579	0.689589	0.890941
H	-7.049855	2.059119	0.000000
H	-3.870388	-0.571079	3.391305
H	-2.915146	-1.886374	2.666786
H	-2.276154	-0.238083	2.657588
H	-2.915146	-1.886374	-2.666786
H	-3.870388	-0.571079	-3.391305
H	-2.276154	-0.238083	-2.657588
H	7.693354	-1.051665	-0.890947
H	7.331855	0.436197	0.000000
H	7.693354	-1.051665	0.890947
H	3.645233	-1.418319	-3.391272
H	2.420912	-2.487702	-2.666737
H	2.165370	-0.738465	-2.657368
H	2.420912	-2.487702	2.666737
H	3.645233	-1.418319	3.391272
H	2.165370	-0.738465	2.657368

Net Charge: 0.00

Total Bonding Energy:
-12.793086786173239 hartree
-8027.78 kcal/mol
-33588.24 kJ/mol

Summary Geometry Optimization:

Energy Change :	0.000049
Gradient (Max):	0.000758
Gradient (RMS):	0.000132

I-1 b-N

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Phosphorus (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.877670  -1.912270   1.234395
C     2.200056  -1.927123   0.000000
C     2.877670  -1.912270  -1.234395
C     4.275390  -1.830293  -1.202878
C     4.990349  -1.778382   0.000000
C     4.275390  -1.830293   1.202878
N     0.757875  -2.039382   0.000000
C    -0.191904  -1.023037   0.000000
N    -1.360339  -1.725693   0.000000
N    -1.190330  -3.109992   0.000000
C     0.104549  -3.252096   0.000000
C    -2.726713  -1.247107   0.000000
C    -3.388256  -1.102866   1.233338
C    -4.747724  -0.766926   1.202229
C    -5.445948  -0.604325   0.000000
C    -4.747724  -0.766926  -1.202229
C    -3.388256  -1.102866  -1.233338
Ru    0.222047   1.022379   0.000000
Cl    0.071261   1.099424   2.422846
C     2.043919   1.003483   0.000000
P     0.345303   3.420312   0.000000
Cl    0.071261   1.099424  -2.422846
C     2.134366  -1.952133  -2.543594
C     6.498664  -1.696492   0.000000
C     2.134366  -1.952133   2.543594
C    -2.683456  -1.340544  -2.542907
C    -6.931138  -0.326383   0.000000
C    -2.683456  -1.340544   2.542907
C     1.222540   4.170314  -1.436901
C     1.222540   4.170314   1.436901
C    -1.302667   4.284652   0.000000
H     4.816781  -1.799209  -2.151708
H     4.816781  -1.799209   2.151708
H    -5.278254  -0.655167  -2.151215
H    -5.278254  -0.655167   2.151215
H     2.624236   1.023340   0.940725
H     2.624236   1.023340  -0.940725
```

```
H    -3.379082  -1.209904   3.380814
H    -2.281255  -2.363632   2.588689
H    -1.840340  -0.644687   2.676063
H    -3.379082  -1.209904  -3.380814
H    -1.840340  -0.644687  -2.676063
H    -2.281255  -2.363632  -2.588689
H    -7.235730   0.238927   0.890387
H    -7.235730   0.238927  -0.890387
H    -7.500811  -1.269515   0.000000
H     6.870247  -1.171502   0.889725
H     6.947363  -2.702134   0.000000
H     6.870247  -1.171502  -0.889725
H     2.838476  -1.971394   3.384123
H     1.480817  -1.070628   2.654938
H     1.492703  -2.842699   2.618401
H     2.838476  -1.971394  -3.384123
H     1.492703  -2.842699  -2.618401
H     1.480817  -1.070628  -2.654938
H     1.178131   5.267904   1.393872
H     0.766023   3.796443   2.362942
H     2.272645   3.843868   1.419088
H     1.178131   5.267904  -1.393872
H     2.272645   3.843868  -1.419088
H     0.766023   3.796443  -2.362942
H    -1.390209   4.914901  -0.895413
H    -2.122072   3.554641   0.000000
H    -1.390209   4.914901   0.895413
H     0.621468  -4.205224   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.891626037439346 hartree
-8717.13       kcal/mol
-36472.46        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000002
 Gradient (Max):   0.000549
 Gradient (RMS):   0.000174
 -------------------------------------------------
```

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.749746	-1.886999	1.234999
C	2.078379	-1.978070	0.000000
C	2.749746	-1.886999	-1.234999
C	4.124599	-1.625642	-1.202974
C	4.825678	-1.480122	0.000000
C	4.124599	-1.625642	1.202974
N	0.656240	-2.229996	0.000000
C	-0.332270	-1.282233	0.000000
N	-1.493770	-2.042719	0.000000
C	-1.125619	-3.374924	0.000000
N	0.168884	-3.532145	0.000000
C	-2.858322	-1.573140	0.000000
C	-3.513407	-1.393123	-1.235323
C	-4.862702	-1.022260	-1.203710
C	-5.555032	-0.837262	0.000000
C	-4.862702	-1.022260	1.203710
C	-3.513407	-1.393123	1.235323
C	-2.787991	-1.569268	-2.544336
C	-2.787991	-1.569268	2.544336
C	-7.021363	-0.477371	0.000000
Ru	-0.022122	0.634781	0.000000
Cl	0.187247	1.029187	2.312397
C	2.030657	-2.071828	-2.545060
C	6.312817	-1.216614	0.000000
C	2.030657	-2.071828	2.545060
Cl	0.187247	1.029187	-2.312397
C	-1.798613	1.069763	0.000000
H	-5.385979	-0.874766	2.151565
H	-5.385979	-0.874766	-2.151565
H	4.660426	-1.538322	2.151291
H	4.660426	-1.538322	-2.151291
H	-2.347892	1.253069	-0.939818
H	-2.347892	1.253069	0.939818
H	2.749775	-2.119389	-3.371581
H	1.441396	-2.999635	-2.545683
H	1.344364	-1.232192	-2.736647
H	2.749775	-2.119389	3.371581
H	1.344364	-1.232192	2.736647

```
H     1.441396  -2.999635   2.545683
H     6.618564  -0.651235  -0.889820
H     6.618564  -0.651235   0.889820
H     6.877445  -2.162249   0.000000
H    -7.291686   0.105142  -0.890072
H    -7.644078  -1.385825   0.000000
H    -7.291686   0.105142   0.890072
H    -3.472970  -1.416996  -3.386655
H    -1.957996  -0.850726  -2.638373
H    -2.354039  -2.575669  -2.636804
H    -3.472970  -1.416996   3.386655
H    -2.354039  -2.575669   2.636804
H    -1.957996  -0.850726   2.638373
H    -1.846434  -4.184921   0.000000
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.474004255294323 hartree
-7200.05       kcal/mol
-30124.99        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000036
 Gradient (Max):   0.000621
 Gradient (RMS):   0.000141
 -----------------------------------------------------
```

I-3 b-N

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.981231	1.311687	-1.234713
C	2.303775	1.352473	0.000000
C	2.981231	1.311687	1.234713
C	4.366679	1.108918	1.201845
C	5.073955	0.989343	0.000000
C	4.366679	1.108918	-1.201845
N	0.869174	1.566515	0.000000
C	-0.111796	0.624754	0.000000
N	-1.267374	1.381644	0.000000
C	-0.903844	2.712144	0.000000
N	0.390957	2.869213	0.000000
C	-2.656065	0.957290	0.000000
C	-3.319747	0.818067	1.234074
C	-4.674541	0.463987	1.201567
C	-5.367167	0.275635	0.000000
C	-4.674541	0.463987	-1.201567
C	-3.319747	0.818067	-1.234074
C	-2.621463	1.054017	2.547753
C	-2.621463	1.054017	-2.547753
C	-6.836358	-0.074747	0.000000
Ru	0.243586	-1.425943	0.000000
Cl	0.117020	-1.273816	-2.443798
C	2.269849	1.525455	2.543809
C	6.572647	0.800522	0.000000
C	2.269849	1.525455	-2.543809
Cl	0.117020	-1.273816	2.443798
C	-1.481149	-2.010821	0.000000
H	-5.201263	0.339224	-2.150796
H	-5.201263	0.339224	2.150796
H	4.906654	1.059888	-2.150644
H	4.906654	1.059888	2.150644
H	-2.008033	-2.203283	0.948008
H	-2.008033	-2.203283	-0.948008
H	2.986764	1.509419	3.373582
H	1.757727	2.499055	2.551540
H	1.513826	0.745301	2.721279
H	2.986764	1.509419	-3.373582
H	1.513826	0.745301	-2.721279

```
H     1.757727   2.499055  -2.551540
H     6.907523   0.252180   0.890025
H     6.907523   0.252180  -0.890025
H     7.088248   1.773793   0.000000
H    -7.109583  -0.656339   0.889912
H    -7.455016   0.836457   0.000000
H    -7.109583  -0.656339  -0.889912
H    -3.313838   0.891358   3.382424
H    -1.758785   0.379796   2.669525
H    -2.243541   2.085476   2.621604
H    -3.313838   0.891358  -3.382424
H    -2.243541   2.085476  -2.621604
H    -1.758785   0.379796  -2.669525
C     1.474152  -3.179279  -0.693853
C     1.474152  -3.179279   0.693853
H     2.294758  -2.733475  -1.256793
H     0.812466  -3.824026  -1.269573
H     0.812466  -3.824026   1.269573
H     2.294758  -2.733475   1.256793
H    -1.625227   3.521343   0.000000
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-12.658267987538832 hartree
-7943.18       kcal/mol
-33234.28        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000025
 Gradient (Max):   0.000214
 Gradient (RMS):   0.000041
 -----------------------------------------------------
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I-4 b-N

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Nitrogen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.143406   1.307426   0.000000
C    -0.089530  -0.706911   0.000000
Cl    0.157284   1.388894  -2.408391
Cl    0.157284   1.388894   2.408391
C     1.656659   2.579831   0.000000
C    -1.038282   2.893083   0.000000
H    -1.588310   3.065286  -0.930170
H    -1.588310   3.065286   0.930170
C     0.403349   3.554059   0.000000
H     0.471500   4.136258   0.925763
H     0.471500   4.136258  -0.925763
H     2.231384   2.624609  -0.930272
H     2.231384   2.624609   0.930272
N     0.896359  -1.669159   0.000000
N    -1.240785  -1.425845   0.000000
C     0.276030  -2.902977   0.000000
N    -1.023242  -2.801658   0.000000
C    -2.599896  -0.928962   0.000000
C    -3.248711  -0.742337   1.234453
C    -4.574932  -0.294389   1.202618
C    -5.250732  -0.056173   0.000000
C    -4.574932  -0.294389  -1.202618
C    -3.248711  -0.742337  -1.234453
C    -2.563809  -1.031003   2.543790
H    -5.096547  -0.144672   2.151098
C    -6.673790   0.449500   0.000000
H    -5.096547  -0.144672  -2.151098
C    -2.563809  -1.031003  -2.543790
C     2.337333  -1.478514   0.000000
C     3.012432  -1.440281  -1.234670
C     4.406690  -1.310075  -1.202024
C     5.119864  -1.234727   0.000000
C     4.406690  -1.310075   1.202024
C     3.012432  -1.440281   1.234670
C     2.282847  -1.541095  -2.548730
H     4.947828  -1.278492  -2.150777
C     6.620479  -1.065418   0.000000
H     4.947828  -1.278492   2.150777
```

C	2.282847	-1.541095	2.548730
H	-7.219759	0.110338	-0.890096
H	-7.219759	0.110338	0.890096
H	-6.696715	1.550534	0.000000
H	-3.265630	-0.907305	3.377388
H	-2.178975	-2.060854	2.568899
H	-1.712031	-0.350998	2.703902
H	-2.178975	-2.060854	-2.568899
H	-3.265630	-0.907305	-3.377388
H	-1.712031	-0.350998	-2.703902
H	7.075534	-1.519058	-0.890135
H	6.891563	0.001887	0.000000
H	7.075534	-1.519058	0.890135
H	2.997579	-1.572462	-3.379762
H	1.662395	-2.448172	-2.601537
H	1.614158	-0.677504	-2.696597
H	1.662395	-2.448172	2.601537
H	2.997579	-1.572462	3.379762
H	1.614158	-0.677504	2.696597
H	0.826120	-3.837501	0.000000

Net Charge: 0.00

Total Bonding Energy:
-12.675473759726462 hartree
-7953.98 kcal/mol
-33279.45 kJ/mol

Summary Geometry Optimization:

Energy Change :	0.000017
Gradient (Max):	0.000980
Gradient (RMS):	0.000176

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.427552  -1.997079   1.238170
C     2.740021  -2.048332   0.000000
C     3.427552  -1.997079  -1.238170
C     4.823717  -1.915623  -1.204914
C     5.537370  -1.876985   0.000000
C     4.823717  -1.915623   1.204914
P     0.939950  -2.173649   0.000000
C    -0.209684  -0.872519   0.000000
P    -1.660295  -1.778598   0.000000
N    -1.342586  -3.409242   0.000000
C    -0.023693  -3.632338   0.000000
C    -3.383326  -1.269414   0.000000
C    -4.051948  -1.107167   1.237920
C    -5.417287  -0.804289   1.205089
C    -6.117645  -0.663551   0.000000
C    -5.417287  -0.804289  -1.205089
C    -4.051948  -1.107167  -1.237920
Ru    0.341567   1.135976   0.000000
Cl    0.174750   1.139548   2.425360
C     2.165058   1.158667   0.000000
P     0.377884   3.505991   0.000000
Cl    0.174750   1.139548  -2.425360
C     2.695885  -1.995529  -2.556527
C     7.045348  -1.812340   0.000000
C     2.695885  -1.995529   2.556527
C    -3.334098  -1.260178  -2.555557
C    -7.603923  -0.400059   0.000000
C    -3.334098  -1.260178   2.555557
C     1.204268   4.302720  -1.441954
C     1.204268   4.302720   1.441954
C    -1.320412   4.270384   0.000000
H     5.368122  -1.870162  -2.151285
H     5.368122  -1.870162   2.151285
H    -5.949437  -0.680460  -2.151353
H    -5.949437  -0.680460   2.151353
H     2.743373   1.171149   0.942246
H     2.743373   1.171149  -0.942246
```

```
H    -4.009407  -1.046376   3.393200
H    -2.953068  -2.284958   2.677781
H    -2.468637  -0.583048   2.623290
H    -4.009407  -1.046376  -3.393200
H    -2.468637  -0.583048  -2.623290
H    -2.953068  -2.284958  -2.677781
H    -7.913568   0.161017   0.891001
H    -7.913568   0.161017  -0.891001
H    -8.161799  -1.349929   0.000000
H     7.424508  -1.294849   0.890668
H     7.476805  -2.825670   0.000000
H     7.424508  -1.294849  -0.890668
H     3.403605  -1.946926   3.393334
H     2.010705  -1.134838   2.629106
H     2.085133  -2.902140   2.676552
H     3.403605  -1.946926  -3.393334
H     2.085133  -2.902140  -2.676552
H     2.010705  -1.134838  -2.629106
H     1.086223   5.395363   1.410211
H     0.771624   3.887875   2.362515
H     2.273596   4.046607   1.421878
H     1.086223   5.395363  -1.410211
H     2.273596   4.046607  -1.421878
H     0.771624   3.887875  -2.362515
H    -1.445771   4.893877  -0.895823
H    -2.096101   3.493741   0.000000
H    -1.445771   4.893877   0.895823
H     0.373498  -4.648455   0.000000
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.595528044941993 hartree
-8531.32       kcal/mol
-35695.05        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------
 Energy Change :   0.000005
 Gradient (Max):   0.000765
 Gradient (RMS):   0.000180
 -----------------------------------------------
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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.364040  -1.961578   1.239978
C     2.690141  -2.105061   0.000000
C     3.364040  -1.961578  -1.239978
C     4.732900  -1.678902  -1.205290
C     5.431777  -1.533539   0.000000
C     4.732900  -1.678902   1.205290
P     0.917433  -2.375270   0.000000
C    -0.329568  -1.178855   0.000000
P    -1.752806  -2.184672   0.000000
C    -1.108647  -3.815122   0.000000
N     0.224778  -3.883774   0.000000
C    -3.458302  -1.599641   0.000000
C    -4.112973  -1.374986  -1.238570
C    -5.444554  -0.949271  -1.204948
C    -6.128139  -0.738933   0.000000
C    -5.444554  -0.949271   1.204948
C    -4.112973  -1.374986   1.238570
C    -3.411181  -1.562086  -2.560467
C    -3.411181  -1.562086   2.560467
C    -7.575564  -0.313673   0.000000
Ru   -0.065789   0.757891   0.000000
Cl    0.206533   1.055206   2.320752
C     2.645022  -2.072010  -2.559601
C     6.912730  -1.245362   0.000000
C     2.645022  -2.072010   2.559601
Cl    0.206533   1.055206  -2.320752
C    -1.825080   1.237056   0.000000
H    -5.961030  -0.769604   2.150872
H    -5.961030  -0.769604  -2.150872
H     5.266362  -1.559189   2.151154
H     5.266362  -1.559189  -2.151154
H    -2.374583   1.413277  -0.941902
H    -2.374583   1.413277   0.941902
H     3.359439  -2.068456  -3.391950
H     2.051393  -2.995056  -2.617105
H     1.952625  -1.225324  -2.696718
H     3.359439  -2.068456   3.391950
```

```
H     1.952625  -1.225324   2.696718
H     2.051393  -2.995056   2.617105
H     7.209929  -0.677219  -0.890679
H     7.209929  -0.677219   0.890679
H     7.489096  -2.183805   0.000000
H    -7.820139   0.278728  -0.890840
H    -8.235734  -1.195324   0.000000
H    -7.820139   0.278728   0.890840
H    -4.085308  -1.329098  -3.393662
H    -2.527710  -0.910296  -2.638084
H    -3.057574  -2.595839  -2.684067
H    -4.085308  -1.329098   3.393662
H    -3.057574  -2.595839   2.684067
H    -2.527710  -0.910296   2.638084
H    -1.715252  -4.721348   0.000000
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.171796803072688 hartree
-7010.41       kcal/mol
-29331.55        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000591
 Gradient (RMS):   0.000089
 -------------------------------------------------
```

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.606814   1.409653  -1.240048
C     2.927055   1.509259   0.000000
C     3.606814   1.409653   1.240048
C     4.990361   1.209224   1.205600
C     5.696924   1.107762   0.000000
C     4.990361   1.209224  -1.205600
P     1.146721   1.721934   0.000000
C    -0.068605   0.523896   0.000000
P    -1.490287   1.505761   0.000000
C    -0.875343   3.141216   0.000000
N     0.462479   3.228726   0.000000
C    -3.210155   0.970917   0.000000
C    -3.868415   0.770799   1.239345
C    -5.211836   0.383079   1.205106
C    -5.899879   0.190070   0.000000
C    -5.211836   0.383079  -1.205106
C    -3.868415   0.770799  -1.239345
C    -3.159307   0.946872   2.558195
C    -3.159307   0.946872  -2.558195
C    -7.358252  -0.197728   0.000000
Ru    0.174592  -1.538758   0.000000
Cl    0.083232  -1.271790  -2.438065
C     2.878965   1.504736   2.556485
C     7.194057   0.918812   0.000000
C     2.878965   1.504736  -2.556485
Cl    0.083232  -1.271790   2.438065
C    -1.538918  -2.150074   0.000000
H    -5.732992   0.219142  -2.151333
H    -5.732992   0.219142   2.151333
H     5.530426   1.125088  -2.151583
H     5.530426   1.125088   2.151583
H    -2.065713  -2.339510   0.949107
H    -2.065713  -2.339510  -0.949107
H     3.578532   1.404007   3.395240
H     2.366125   2.472809   2.653914
H     2.112073   0.717975   2.647626
H     3.578532   1.404007  -3.395240
```

```
H     2.112073   0.717975  -2.647626
H     2.366125   2.472809  -2.653914
H     7.529500   0.372514   0.890782
H     7.529500   0.372514  -0.890782
H     7.705807   1.894037   0.000000
H    -7.617481  -0.784166   0.890741
H    -7.996591   0.699838   0.000000
H    -7.617481  -0.784166  -0.890741
H    -3.825963   0.697778   3.392851
H    -2.265877   0.304170   2.620875
H    -2.820023   1.984733   2.692505
H    -3.825963   0.697778  -3.392851
H    -2.820023   1.984733  -2.692505
H    -2.265877   0.304170  -2.620875
C     1.348723  -3.291849  -0.697939
C     1.348723  -3.291849   0.697939
H     2.186420  -2.875674  -1.258722
H     0.685315  -3.935144  -1.273425
H     0.685315  -3.935144   1.273425
H     2.186420  -2.875674   1.258722
H    -1.491856   4.040883   0.000000
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-12.363810599171426 hartree
-7758.41       kcal/mol
-32461.18        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000006
 Gradient (Max):   0.000900
 Gradient (RMS):   0.000156
 -------------------------------------------------
```

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.166228   1.392891   0.000000
C    -0.082326  -0.595462   0.000000
Cl    0.167367   1.402813  -2.411520
Cl    0.167367   1.402813   2.411520
C     1.689168   2.651976   0.000000
C    -1.006528   2.984028   0.000000
H    -1.555417   3.168815  -0.929543
H    -1.555417   3.168815   0.929543
C     0.441202   3.634843   0.000000
H     0.513640   4.218995   0.924852
H     0.513640   4.218995  -0.924852
H     2.266510   2.699984  -0.929540
H     2.266510   2.699984   0.929540
P     1.131871  -1.833484   0.000000
P    -1.515161  -1.530024   0.000000
C     0.196868  -3.316024   0.000000
N    -1.127355  -3.142066   0.000000
C    -3.210420  -0.950464   0.000000
C    -3.852920  -0.708807   1.239843
C    -5.168051  -0.234895   1.205593
C    -5.839282   0.007480   0.000000
C    -5.168051  -0.234895  -1.205593
C    -3.852920  -0.708807  -1.239843
C    -3.153696  -0.930960   2.556528
H    -5.682257  -0.049013   2.151468
C    -7.247061   0.551068   0.000000
H    -5.682257  -0.049013  -2.151468
C    -3.153696  -0.930960  -2.556528
C     2.918140  -1.596853   0.000000
C     3.600519  -1.507695  -1.239636
C     4.990298  -1.353705  -1.205097
C     5.700611  -1.277046   0.000000
C     4.990298  -1.353705   1.205097
C     3.600519  -1.507695   1.239636
C     2.872633  -1.548642  -2.559238
H     5.532809  -1.288876  -2.151292
C     7.196757  -1.079431   0.000000
```

```
H      5.532809  -1.288876   2.151292
C      2.872633  -1.548642   2.559238
H     -7.801728   0.229791  -0.890880
H     -7.801728   0.229791   0.890880
H     -7.234349   1.652368   0.000000
H     -3.830622  -0.726655   3.395074
H     -2.796603  -1.966857   2.648416
H     -2.274921  -0.272513   2.652772
H     -2.796603  -1.966857  -2.648416
H     -3.830622  -0.726655  -3.395074
H     -2.274921  -0.272513  -2.652772
H      7.660431  -1.522156  -0.890859
H      7.443582  -0.006094   0.000000
H      7.660431  -1.522156   0.890859
H      3.580567  -1.480892  -3.394318
H      2.296546  -2.478379  -2.673006
H      2.157336  -0.713762  -2.642046
H      2.296546  -2.478379   2.673006
H      3.580567  -1.480892   3.394318
H      2.157336  -0.713762   2.642046
H      0.633016  -4.315728   0.000000
-------------------------------------------------
Net Charge:          0.00

Total  Bonding  Energy:
-12.380099615753727 hartree
-7768.63       kcal/mol
-32503.95        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000017
 Gradient (Max):   0.000889
 Gradient (RMS):   0.000145
 -------------------------------------------------
```

I-1 c-N

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Phosphorus (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.930063  -1.845839   1.234073
C     2.247890  -1.880597   0.000000
C     2.930063  -1.845839  -1.234073
C     4.319871  -1.687706  -1.203195
C     5.030716  -1.594551   0.000000
C     4.319871  -1.687706   1.203195
N     0.819002  -2.086023   0.000000
C    -0.173024  -1.093103   0.000000
N    -1.389440  -1.764107   0.000000
C    -1.231736  -3.166504   0.000000
C     0.279243  -3.382671   0.000000
C    -2.721346  -1.186433   0.000000
C    -3.379901  -1.011845   1.232454
C    -4.715219  -0.591421   1.201344
C    -5.401865  -0.382505   0.000000
C    -4.715219  -0.591421  -1.201344
C    -3.379901  -1.011845  -1.232454
Ru    0.162610   0.881935   0.000000
Cl    0.024027   1.090166   2.394181
C     1.992122   0.848273   0.000000
P     0.327499   3.361203   0.000000
Cl    0.024027   1.090166  -2.394181
C     2.193073  -1.957106  -2.541566
C     6.532183  -1.434357   0.000000
C     2.193073  -1.957106   2.541566
C    -2.706818  -1.314602  -2.545719
C    -6.867343  -0.015937   0.000000
C    -2.706818  -1.314602   2.545719
C     1.228960   4.092034  -1.431494
C     1.228960   4.092034   1.431494
C    -1.301491   4.255818   0.000000
H     4.860143  -1.636108  -2.151697
H     4.860143  -1.636108   2.151697
H    -5.239573  -0.455378  -2.150418
H    -5.239573  -0.455378   2.150418
H     2.568388   0.890914   0.939835
```

```
H     2.568388   0.890914  -0.939835
H    -3.394887  -1.125601   3.378548
H    -2.403717  -2.371532   2.596105
H    -1.808749  -0.696271   2.691920
H    -3.394887  -1.125601  -3.378548
H    -1.808749  -0.696271  -2.691920
H    -2.403717  -2.371532  -2.596105
H    -7.138238   0.565888   0.890577
H    -7.138238   0.565888  -0.890577
H    -7.490744  -0.924319   0.000000
H     6.876852  -0.891901   0.890060
H     7.030058  -2.416472   0.000000
H     6.876852  -0.891901  -0.890060
H     2.894386  -1.911491   3.383252
H     1.459435  -1.143666   2.658523
H     1.648573  -2.910815   2.606555
H     2.894386  -1.911491  -3.383252
H     1.648573  -2.910815  -2.606555
H     1.459435  -1.143666  -2.658523
H     1.227256   5.189317   1.364688
H     0.756360   3.758466   2.363887
H     2.265966   3.726070   1.423249
H     1.227256   5.189317  -1.364688
H     2.265966   3.726070  -1.423249
H     0.756360   3.758466  -2.363887
H    -1.375618   4.887644  -0.895337
H    -2.134400   3.541718   0.000000
H    -1.375618   4.887644   0.895337
O    -2.105367  -4.009460   0.000000
O     0.880354  -4.439379   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-14.284492980790812 hartree
-8963.66       kcal/mol
-37503.93        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000013
 Gradient (Max):   0.000536
 Gradient (RMS):   0.000173
 -------------------------------------------------
```

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.749392  -1.813187   1.234351
C     2.083462  -1.947446   0.000000
C     2.749392  -1.813187  -1.234351
C     4.099068  -1.444795  -1.202418
C     4.786822  -1.243116   0.000000
C     4.099068  -1.444795   1.202418
N     0.681216  -2.320230   0.000000
C    -0.354577  -1.391349   0.000000
N    -1.549805  -2.106322   0.000000
C    -1.322209  -3.497641   0.000000
C     0.204774  -3.642481   0.000000
C    -2.874582  -1.535891   0.000000
C    -3.529332  -1.336260  -1.235686
C    -4.850609  -0.881098  -1.204295
C    -5.528839  -0.650340   0.000000
C    -4.850609  -0.881098   1.204295
C    -3.529332  -1.336260   1.235686
C    -2.829913  -1.594792  -2.543600
C    -2.829913  -1.594792   2.543600
C    -6.969770  -0.202151   0.000000
Ru   -0.012418   0.472494   0.000000
Cl    0.240068   1.044022   2.238783
C     2.057522  -2.077810  -2.546220
C     6.249183  -0.866709   0.000000
C     2.057522  -2.077810   2.546220
Cl    0.240068   1.044022  -2.238783
C    -1.799972   0.924172   0.000000
H    -5.366990  -0.709703   2.151698
H    -5.366990  -0.709703  -2.151698
H     4.627574  -1.321802   2.150701
H     4.627574  -1.321802  -2.150701
H    -2.338169   1.136236  -0.937607
H    -2.338169   1.136236   0.937607
H     2.778839  -2.036902  -3.370869
H     1.589751  -3.072879  -2.554005
H     1.277344  -1.328232  -2.742933
H     2.778839  -2.036902   3.370869
```

```
H     1.277344  -1.328232   2.742933
H     1.589751  -3.072879   2.554005
H     6.511239  -0.280159  -0.889939
H     6.511239  -0.280159   0.889939
H     6.883039  -1.767292   0.000000
H    -7.205474   0.394371  -0.890534
H    -7.643318  -1.073534   0.000000
H    -7.205474   0.394371   0.890534
H    -3.497510  -1.380069  -3.386039
H    -1.930504  -0.968755  -2.649241
H    -2.513021  -2.645140  -2.621275
H    -3.497510  -1.380069   3.386039
H    -2.513021  -2.645140   2.621275
H    -1.930504  -0.968755   2.649241
O     0.859674  -4.665556   0.000000
O    -2.158598  -4.378270   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.877340321106610 hartree
-7453.14       kcal/mol
-31183.95        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000014
 Gradient (Max):   0.000607
 Gradient (RMS):   0.000084
 -------------------------------------------------
```

I-3 c-N

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     2.974909   1.167249  -1.234732
C     2.299408   1.262886   0.000000
C     2.974909   1.167249   1.234732
C     4.333303   0.828681   1.201736
C     5.025641   0.639275   0.000000
C     4.333303   0.828681  -1.201736
N     0.890095   1.623943   0.000000
C    -0.158605   0.715407   0.000000
N    -1.340002   1.440362   0.000000
C    -1.091100   2.832604   0.000000
C     0.437449   2.955789   0.000000
C    -2.694581   0.923329   0.000000
C    -3.352338   0.747741   1.233809
C    -4.676507   0.295656   1.201892
C    -5.352597   0.055052   0.000000
C    -4.676507   0.295656  -1.201892
C    -3.352338   0.747741  -1.233809
C    -2.681118   1.057143   2.545799
C    -2.681118   1.057143  -2.545799
C    -6.792903  -0.398537   0.000000
Ru    0.245401  -1.220436   0.000000
Cl    0.105372  -1.269312  -2.440578
C     2.298098   1.472828   2.544273
C     6.500310   0.313806   0.000000
C     2.298098   1.472828  -2.544273
Cl    0.105372  -1.269312   2.440578
C    -1.503845  -1.766411   0.000000
H    -5.195827   0.140634  -2.150669
H    -5.195827   0.140634   2.150669
H     4.867910   0.735612  -2.150130
H     4.867910   0.735612   2.150130
H    -2.025616  -1.967409   0.946733
H    -2.025616  -1.967409  -0.946733
H     3.013566   1.385030   3.370613
H     1.905970   2.501013   2.546853
H     1.462827   0.784246   2.738883
H     3.013566   1.385030  -3.370613
```

```
H     1.462827   0.784246  -2.738883
H     1.905970   2.501013  -2.546853
H     6.784484  -0.261839   0.890270
H     6.784484  -0.261839  -0.890270
H     7.100654   1.237090   0.000000
H    -7.025036  -0.997296   0.890205
H    -7.472415   0.468134   0.000000
H    -7.025036  -0.997296  -0.890205
H    -3.359851   0.845642   3.380628
H    -1.767256   0.459676   2.683739
H    -2.403653   2.120817   2.601372
H    -3.359851   0.845642  -3.380628
H    -2.403653   2.120817  -2.601372
H    -1.767256   0.459676  -2.683739
C     1.767986  -2.908234  -0.684633
C     1.767986  -2.908234   0.684633
H     2.501906  -2.338460  -1.254771
H     1.148845  -3.595704  -1.258909
H     1.148845  -3.595704   1.258909
H     2.501906  -2.338460   1.254771
O    -1.907665   3.727290   0.000000
O     1.106799   3.966891   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.044584276714888 hartree
-8185.60       kcal/mol
-34248.55        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000008
 Gradient (Max):   0.000617
 Gradient (RMS):   0.000111
 -------------------------------------------------
```

I-4 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Nitrogen (TZP, 1s frozen)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.128435   1.141874   0.000000
C    -0.092028  -0.814096   0.000000
Cl    0.147854   1.307412  -2.395393
Cl    0.147854   1.307412   2.395393
C     1.635090   2.443064   0.000000
C    -1.051280   2.745136   0.000000
H    -1.602915   2.901648  -0.930040
H    -1.602915   2.901648   0.930040
C     0.384541   3.416103   0.000000
H     0.449735   3.997470   0.926157
H     0.449735   3.997470  -0.926157
H     2.207692   2.472675  -0.930058
H     2.207692   2.472675   0.930058
N     0.931808  -1.737894   0.000000
N    -1.295599  -1.487481   0.000000
C     0.428965  -3.058225   0.000000
C    -1.098771  -2.886428   0.000000
C    -2.613856  -0.872738   0.000000
C    -3.251195  -0.642643   1.233814
C    -4.532995  -0.080531   1.201689
C    -5.184550   0.220178   0.000000
C    -4.532995  -0.080531  -1.201689
C    -3.251195  -0.642643  -1.233814
C    -2.611378  -1.011489   2.546417
H    -5.042127   0.106486   2.150204
C    -6.557235   0.849367   0.000000
H    -5.042127   0.106486  -2.150204
C    -2.611378  -1.011489  -2.546417
C     2.353767  -1.432408   0.000000
C     3.026313  -1.351018  -1.233841
C     4.401188  -1.089025  -1.201742
C     5.103341  -0.941167   0.000000
C     4.401188  -1.089025   1.201742
C     3.026313  -1.351018   1.233841
C     2.320359  -1.569333  -2.546224
H     4.939245  -1.020647  -2.150250
C     6.581817  -0.634193   0.000000
```

```
H     4.939245  -1.020647   2.150250
C     2.320359  -1.569333   2.546224
H    -7.130826   0.559672  -0.890048
H    -7.130826   0.559672   0.890048
H    -6.482957   1.948168   0.000000
H    -3.301118  -0.810359   3.374777
H    -2.354990  -2.081006   2.575202
H    -1.690665  -0.434222   2.719536
H    -2.354990  -2.081006  -2.575202
H    -3.301118  -0.810359  -3.374777
H    -1.690665  -0.434222  -2.719536
H     7.076198  -1.044676  -0.890053
H     6.754808   0.453446   0.000000
H     7.076198  -1.044676   0.890053
H     3.037646  -1.528575  -3.374591
H     1.831512  -2.554567  -2.573721
H     1.551794  -0.801262  -2.720395
H     1.831512  -2.554567   2.573721
H     3.037646  -1.528575   3.374591
H     1.551794  -0.801262   2.720395
O     1.064157  -4.088989   0.000000
O    -1.947156  -3.750219   0.000000
-----------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.067752415844680 hartree
-8200.14       kcal/mol
-34309.38        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000009
 Gradient (Max):   0.000850
 Gradient (RMS):   0.000101
 -------------------------------------------------
```

I-1 c-P

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.536195  -1.879693   1.237988
C     2.847759  -1.956405   0.000000
C     3.536195  -1.879693  -1.237988
C     4.924847  -1.715749  -1.204920
C     5.635009  -1.631977   0.000000
C     4.924847  -1.715749   1.204920
P     1.057188  -2.215409   0.000000
C    -0.172804  -0.963656   0.000000
P    -1.722364  -1.769361   0.000000
C    -1.366871  -3.549478   0.000000
C     0.208557  -3.802325   0.000000
C    -3.399390  -1.091719   0.000000
C    -4.067965  -0.910872   1.237646
C    -5.420192  -0.553952   1.204371
C    -6.115268  -0.384255   0.000000
C    -5.420192  -0.553952  -1.204371
C    -4.067965  -0.910872  -1.237646
Ru    0.283929   0.985904   0.000000
Cl    0.117568   1.131464   2.401763
C     2.111561   1.019607   0.000000
P     0.341230   3.440582   0.000000
Cl    0.117568   1.131464  -2.401763
C     2.813653  -1.954468  -2.559045
C     7.136439  -1.481600   0.000000
C     2.813653  -1.954468   2.559045
C    -3.371133  -1.105208  -2.560830
C    -7.590810  -0.067574   0.000000
C    -3.371133  -1.105208   2.560830
C     1.189336   4.218387  -1.437878
C     1.189336   4.218387   1.437878
C    -1.343455   4.226732   0.000000
H     5.467054  -1.647553  -2.151332
H     5.467054  -1.647553   2.151332
H    -5.948330  -0.415232  -2.151055
H    -5.948330  -0.415232   2.151055
H     2.684484   1.054041   0.942641
H     2.684484   1.054041  -0.942641
```

```
H    -4.038420  -0.842352   3.391200
H    -3.062976  -2.153215   2.691534
H    -2.461976  -0.489934   2.633682
H    -4.038420  -0.842352  -3.391200
H    -2.461976  -0.489934  -2.633682
H    -3.062976  -2.153215  -2.691534
H    -7.880580   0.503789   0.891261
H    -7.880580   0.503789  -0.891261
H    -8.181880  -0.997220   0.000000
H     7.486012  -0.944199   0.891007
H     7.623351  -2.469443   0.000000
H     7.486012  -0.944199  -0.891007
H     3.519359  -1.854695   3.393216
H     2.055719  -1.160630   2.646839
H     2.288264  -2.914311   2.667273
H     3.519359  -1.854695  -3.393216
H     2.288264  -2.914311  -2.667273
H     2.055719  -1.160630  -2.646839
H     1.106082   5.313408   1.386127
H     0.741552   3.835909   2.364346
H     2.250239   3.929059   1.424069
H     1.106082   5.313408  -1.386127
H     2.250239   3.929059  -1.424069
H     0.741552   3.835909  -2.364346
H    -1.458277   4.852270  -0.895718
H    -2.130014   3.461633   0.000000
H    -1.458277   4.852270   0.895718
O    -2.156273  -4.477473   0.000000
O     0.666442  -4.934144   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-13.943220162698934 hartree
-8749.50       kcal/mol
-36607.92        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000025
 Gradient (Max):   0.000768
 Gradient (RMS):   0.000182
 -------------------------------------------------
```

I-2 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.397505  -1.789525   1.239507
C     2.728578  -1.968552   0.000000
C     3.397505  -1.789525  -1.239507
C     4.741060  -1.403472  -1.204771
C     5.427067  -1.203114   0.000000
C     4.741060  -1.403472   1.204771
P     0.985851  -2.453457   0.000000
C    -0.364431  -1.314557   0.000000
P    -1.859590  -2.231121   0.000000
C    -1.372609  -3.973433   0.000000
C     0.216668  -4.095671   0.000000
C    -3.510369  -1.486194   0.000000
C    -4.157791  -1.233790  -1.238565
C    -5.457985  -0.720449  -1.205010
C    -6.124816  -0.461305   0.000000
C    -5.457985  -0.720449   1.205010
C    -4.157791  -1.233790   1.238565
C    -3.487769  -1.500552  -2.562626
C    -3.487769  -1.500552   2.562626
C    -7.541586   0.056057   0.000000
Ru   -0.048239   0.564790   0.000000
Cl    0.273831   1.091945   2.239333
C     2.705232  -1.981536  -2.564355
C     6.883341  -0.809061   0.000000
C     2.705232  -1.981536   2.564355
Cl    0.273831   1.091945  -2.239333
C    -1.806499   1.084924   0.000000
H    -5.965906  -0.517007   2.150653
H    -5.965906  -0.517007  -2.150653
H     5.266327  -1.252290   2.150716
H     5.266327  -1.252290  -2.150716
H    -2.346746   1.282141  -0.940537
H    -2.346746   1.282141   0.940537
H     3.426501  -1.921395  -3.388622
H     2.200894  -2.956424  -2.615217
```

```
H     1.939614  -1.206267  -2.722157
H     3.426501  -1.921395   3.388622
H     1.939614  -1.206267   2.722157
H     2.200894  -2.956424   2.615217
H     7.139394  -0.221358  -0.890806
H     7.139394  -0.221358   0.890806
H     7.525214  -1.704037   0.000000
H    -7.748440   0.662222  -0.891107
H    -8.255764  -0.782459   0.000000
H    -7.748440   0.662222   0.891107
H    -4.141605  -1.207821  -3.393235
H    -2.542118  -0.947184  -2.654878
H    -3.246765  -2.567473  -2.674811
H    -4.141605  -1.207821   3.393235
H    -3.246765  -2.567473   2.674811
H    -2.542118  -0.947184   2.654878
O     0.768668  -5.181558   0.000000
O    -2.082741  -4.963139   0.000000
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-11.532421514980435 hartree
-7236.70       kcal/mol
-30278.37        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000016
 Gradient (Max):   0.000467
 Gradient (RMS):   0.000127
 -----------------------------------------------------
```

I-3 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Ruthenium (TZP, 3d frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     3.651312   1.158169  -1.240508
C     2.974158   1.295686   0.000000
C     3.651312   1.158169   1.240508
C     5.015600   0.850880   1.205145
C     5.712851   0.694040   0.000000
C     5.015600   0.850880  -1.205145
P     1.222756   1.742404   0.000000
C    -0.125317   0.629828   0.000000
P    -1.620439   1.512172   0.000000
C    -1.136502   3.256211   0.000000
C     0.472193   3.386913   0.000000
C    -3.299203   0.849818   0.000000
C    -3.950170   0.625095   1.239855
C    -5.268322   0.158534   1.205159
C    -5.942481  -0.078402   0.000000
C    -5.268322   0.158534  -1.205159
C    -3.950170   0.625095  -1.239855
C    -3.268085   0.870234   2.561224
C    -3.268085   0.870234  -2.561224
C    -7.375674  -0.550012   0.000000
Ru    0.203623  -1.345180   0.000000
Cl    0.059207  -1.198700  -2.446929
C     2.951268   1.336120   2.563077
C     7.192725   0.400336   0.000000
C     2.951268   1.336120  -2.563077
Cl    0.059207  -1.198700   2.446929
C    -1.486002  -2.036891   0.000000
H    -5.782588  -0.026439  -2.151263
H    -5.782588  -0.026439   2.151263
H     5.549766   0.734555  -2.151193
H     5.549766   0.734555   2.151193
H    -1.988917  -2.264563   0.950799
H    -1.988917  -2.264563  -0.950799
H     3.647092   1.165357   3.393827
H     2.548984   2.355247   2.660553
H     2.104100   0.640026   2.669307
H     3.647092   1.165357  -3.393827
```

```
H     2.104100   0.640026  -2.669307
H     2.548984   2.355247  -2.660553
H     7.489814  -0.167351   0.891071
H     7.489814  -0.167351  -0.891071
H     7.770578   1.338023   0.000000
H    -7.601239  -1.149827   0.891020
H    -8.063659   0.310120   0.000000
H    -7.601239  -1.149827  -0.891020
H    -3.922909   0.583092   3.393162
H    -2.329635   0.299685   2.642190
H    -3.014532   1.934017   2.681537
H    -3.922909   0.583092  -3.393162
H    -3.014532   1.934017  -2.681537
H    -2.329635   0.299685  -2.642190
C     1.635335  -2.974319  -0.692183
C     1.635335  -2.974319   0.692183
H     2.401149  -2.443593  -1.258252
H     1.026806  -3.670172  -1.268015
H     1.026806  -3.670172   1.268015
H     2.401149  -2.443593   1.258252
O    -1.833691   4.251380   0.000000
O     1.007117   4.478741   0.000000
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-12.705033708299283 hartree
-7972.53       kcal/mol
-33357.06        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000009
 Gradient (Max):   0.000995
 Gradient (RMS):   0.000152
 -------------------------------------------------
```

I-4 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Ruthenium (TZP, 3d frozen)
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)
Phosphorus (TZP, 2p frozen)
Oxygen (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
Ru    0.135864   1.204361   0.000000
C    -0.081769  -0.725216   0.000000
Cl    0.147537   1.309024  -2.401521
Cl    0.147537   1.309024   2.401521
C     1.641899   2.511202   0.000000
C    -1.041303   2.813792   0.000000
H    -1.594451   2.973938  -0.929201
H    -1.594451   2.973938   0.929201
C     0.393270   3.486965   0.000000
H     0.459054   4.070804   0.925189
H     0.459054   4.070804  -0.925189
H     2.216803   2.544145  -0.929203
H     2.216803   2.544145   0.929203
P     1.231015  -1.876658   0.000000
P    -1.618152  -1.555071   0.000000
C     0.413446  -3.490885   0.000000
C    -1.180951  -3.310950   0.000000
C    -3.245240  -0.769772   0.000000
C    -3.876240  -0.492604   1.239933
C    -5.152526   0.078691   1.205016
C    -5.804037   0.371997   0.000000
C    -5.152526   0.078691  -1.205016
C    -3.876240  -0.492604  -1.239933
C    -3.214544  -0.784519   2.562019
H    -5.654214   0.295831   2.150942
C    -7.170089   1.013170   0.000000
H    -5.654214   0.295831  -2.150942
C    -3.214544  -0.784519  -2.562019
C     2.992234  -1.473848   0.000000
C     3.669188  -1.344657  -1.239929
C     5.040718  -1.072314  -1.205023
C     5.741039  -0.930863   0.000000
C     5.040718  -1.072314   1.205023
C     3.669188  -1.344657   1.239929
C     2.959277  -1.482740  -2.562008
H     5.578354  -0.973222  -2.150917
C     7.215351  -0.609113   0.000000
```

```
H     5.578354  -0.973222   2.150917
C     2.959277  -1.482740   2.562008
H    -7.745945   0.731302  -0.890773
H    -7.745945   0.731302   0.890773
H    -7.080909   2.110948   0.000000
H    -3.877406  -0.514471   3.393264
H    -2.965588  -1.851373   2.655420
H    -2.275442  -0.219316   2.670228
H    -2.965588  -1.851373  -2.655420
H    -3.877406  -0.514471  -3.393264
H    -2.275442  -0.219316  -2.670228
H     7.714203  -1.011838  -0.890784
H     7.372243   0.481072   0.000000
H     7.714203  -1.011838   0.890784
H     3.665674  -1.367272  -3.393241
H     2.479380  -2.467606  -2.654963
H     2.169375  -0.722947  -2.670674
H     2.479380  -2.467606   2.654963
H     3.665674  -1.367272   3.393241
H     2.169375  -0.722947   2.670674
O     0.913462  -4.599339   0.000000
O    -1.915382  -4.280116   0.000000
-----------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-12.729821157344087 hartree
-7988.08       kcal/mol
-33422.14        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000013
 Gradient (Max):   0.000926
 Gradient (RMS):   0.000128
 -----------------------------------------------------
```

II-1 a-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(2V)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N     0.000000   2.877548  -1.080364
C     0.000000   2.023686   0.002493
N     0.000000   2.893736   1.070949
C     0.000000   4.221604   0.666269
C     0.000000   4.211891  -0.696494
Pd    0.000000   0.000000   0.009109
C     0.000000  -2.023686   0.002493
N     0.000000  -2.893736   1.070949
C     0.000000  -4.221604   0.666269
C     0.000000  -4.211891  -0.696494
N     0.000000  -2.877548  -1.080364
C     0.000000  -2.444633   2.458171
C     0.000000  -2.409728  -2.459327
C     0.000000   2.444633   2.458171
C     0.000000   2.409728  -2.459327
H     0.000000  -5.050367   1.364073
H     0.000000  -5.030832  -1.405611
H     0.000000  -1.312585  -2.408073
H    -0.897737  -2.760756  -2.986827
H     0.897737  -2.760756  -2.986827
H     0.000000   5.050367   1.364073
H     0.000000   5.030832  -1.405611
H     0.897737   2.760756  -2.986827
H    -0.897737   2.760756  -2.986827
H     0.000000   1.312585  -2.408073
H     0.000000  -3.320933   3.117042
H     0.889697  -1.833659   2.651197
H    -0.889697  -1.833659   2.651197
H     0.000000   3.320933   3.117042
H    -0.889697   1.833659   2.651197
H     0.889697   1.833659   2.651197
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-6.614480067622109 hartree
-4150.65       kcal/mol
-17366.31        kJ/mol
Summary Geometry Optimization:
```

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---------------------------------------------------
Energy Change :   0.000048
Gradient (Max):   0.000718
Gradient (RMS):   0.000214
---------------------------------------------------
```

II-2 a-N

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N    -1.089831   2.830260   0.000000
C    -0.004511   1.981382   0.000000
N     1.072278   2.839917   0.000000
C     0.666414   4.168569   0.000000
C    -0.695724   4.163015   0.000000
Pd    0.012701   0.043999   0.000000
C     2.458810   2.387400   0.000000
C    -2.472786   2.372227   0.000000
H     1.367168   4.994708   0.000000
H    -1.402365   4.984016   0.000000
H    -2.995470   2.729241  -0.897805
H    -2.995470   2.729241   0.897805
H    -2.437092   1.275054   0.000000
H     3.117004   3.263934   0.000000
H     2.651575   1.776911   0.889951
H     2.651575   1.776911  -0.889951
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.314788326706880 hartree
-2080.06       kcal/mol
-8702.98         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000691
 Gradient (RMS):   0.000206
 ------------------------------------------------
```

II-RHC a-N

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     0.002289  -2.016208   0.000000
N     1.059911  -2.892653   0.000000
C     0.665562  -4.228227   0.000000
C    -0.696952  -4.218169   0.000000
N    -1.068276  -2.874936   0.000000
C     2.447944  -2.442969   0.000000
C    -2.448118  -2.408525   0.000000
H     1.362486  -5.059044   0.000000
H    -1.406030  -5.038529   0.000000
H    -2.420948  -1.315376   0.000000
H    -2.978269  -2.762024   0.895097
H    -2.978269  -2.762024  -0.895097
H     3.112637  -3.313930   0.000000
H     2.647296  -1.836762  -0.891315
H     2.647296  -1.836762   0.891315
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.226217395740234 hartree
-2024.48       kcal/mol
-8470.43         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000010
 Gradient (Max):   0.000607
 Gradient (RMS):   0.000183
 ------------------------------------------------
```

II-3 a-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -3.966813   1.368176   0.000000
N    -2.580691   1.468141   0.000000
C    -1.981242   0.237553   0.000000
N    -3.047240  -0.629897   0.000000
C    -4.262871   0.039541   0.000000
C    -1.868753   2.744501   0.000000
Pd    0.025352  -0.431426   0.000000
C    -2.889563  -2.081617   0.000000
H    -5.216995  -0.473153   0.000000
H    -4.614679   2.236226   0.000000
H    -0.794390   2.541047   0.000000
H    -2.133536   3.320336   0.895987
H    -2.133536   3.320336  -0.895987
H    -3.878311  -2.551681   0.000000
H    -2.340963  -2.402829  -0.894278
H    -2.340963  -2.402829   0.894278
C     1.230886   1.167854   0.000000
C     1.787096  -1.419543   0.000000
C     2.358219  -1.871574  -1.205701
C     3.419097  -2.786309  -1.207984
C     3.952356  -3.248830   0.000000
C     3.419097  -2.786309   1.207984
C     2.358219  -1.871574   1.205701
H     1.973013  -1.511127  -2.162901
H     3.838435  -3.129211  -2.156794
H     4.787279  -3.952387   0.000000
H     3.838435  -3.129211   2.156794
H     1.973013  -1.511127   2.162901
C     1.610164   1.771448   1.209633
C     2.310382   2.985406   1.206558
C     2.660084   3.600865   0.000000
C     2.310382   2.985406  -1.206558
C     1.610164   1.771448  -1.209633
H     1.356224   1.305459   2.162803
H     2.590688   3.444281   2.157330
H     3.212093   4.542406   0.000000
H     2.590688   3.444281  -2.157330
H     1.356224   1.305459  -2.162803
------------------------------------------------
```

```
Net Charge:         0.00

Total  Bonding  Energy:
-8.525816044111375 hartree
-5350.03       kcal/mol
-22384.53        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000087
 Gradient (Max):   0.000847
 Gradient (RMS):   0.000138
 -------------------------------------------------
```

II-1 a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(2V)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P     0.000000   3.122681  -1.311206
C     0.000000   2.005394  -0.010333
P     0.000000   3.096394   1.312788
C     0.000000   4.733393   0.715793
C     0.000000   4.747768  -0.682353
Pd    0.000000   0.000000  -0.011752
C     0.000000  -2.005394  -0.010333
P     0.000000  -3.096394   1.312788
C     0.000000  -4.733393   0.715793
C     0.000000  -4.747768  -0.682353
P     0.000000  -3.122681  -1.311206
C     0.000000  -2.698184   3.096926
C     0.000000  -2.709034  -3.091862
C     0.000000   2.698184   3.096926
C     0.000000   2.709034  -3.091862
H     0.000000  -5.633025   1.329610
H     0.000000  -5.659473  -1.277779
H     0.000000  -1.611433  -3.120798
H    -0.901025  -3.090301  -3.588351
H     0.901025  -3.090301  -3.588351
H     0.000000   5.633025   1.329610
H     0.000000   5.659473  -1.277779
H     0.901025   3.090301  -3.588351
H    -0.901025   3.090301  -3.588351
H     0.000000   1.611433  -3.120798
H     0.000000  -3.647547   3.648886
H     0.896552  -2.121694   3.353456
H    -0.896552  -2.121694   3.353456
H     0.000000   3.647547   3.648886
H    -0.896552   2.121694   3.353456
H     0.896552   2.121694   3.353456
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-5.992438382543274 hartree
-3760.31       kcal/mol
-15733.14        kJ/mol
Summary Geometry Optimization:
```

```
---------------------------------------------------
Energy Change :   0.000002
Gradient (Max):   0.000250
Gradient (RMS):   0.000071
---------------------------------------------------
```

II-2 a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P    -1.326503   3.081156   0.000000
C    -0.012518   1.976055   0.000000
P     1.324129   3.053263   0.000000
C     0.714579   4.685518   0.000000
C    -0.682345   4.700288   0.000000
Pd   -0.009181   0.050385   0.000000
C     3.107476   2.654199   0.000000
C    -3.109304   2.677270   0.000000
H     1.327594   5.585801   0.000000
H    -1.276147   5.613137   0.000000
H    -3.600799   3.064437  -0.901228
H    -3.600799   3.064437   0.901228
H    -3.151432   1.580277   0.000000
H     3.657232   3.605074   0.000000
H     3.364084   2.078087   0.896782
H     3.364084   2.078087  -0.896782
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.003299715994420 hartree
-1884.60       kcal/mol
-7885.16         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000002
 Gradient (Max):   0.000437
 Gradient (RMS):   0.000129
 ------------------------------------------------
```

II-RHC a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.008642  -1.987160   0.000000
P     1.279675  -3.095711   0.000000
C     0.715508  -4.748746   0.000000
C    -0.685487  -4.761588   0.000000
P    -1.276546  -3.117840   0.000000
C     3.063764  -2.695996   0.000000
C    -3.059384  -2.710731   0.000000
H     1.331527  -5.646944   0.000000
H    -1.285519  -5.670556   0.000000
H    -3.118178  -1.615424   0.000000
H    -3.554333  -3.099898   0.898220
H    -3.554333  -3.099898  -0.898220
H     3.615971  -3.644099   0.000000
H     3.328074  -2.122015  -0.896184
H     3.328074  -2.122015   0.896184
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-2.923578633905685 hartree
-1834.57       kcal/mol
-7675.85         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000003
 Gradient (Max):   0.000567
 Gradient (RMS):   0.000186
 ------------------------------------------------
```

II-3 a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -4.214503   1.624574   0.000000
P    -2.478627   1.618454   0.000000
C    -1.920374  -0.006190   0.000000
P    -3.426868  -0.828708   0.000000
C    -4.724519   0.325017   0.000000
C    -1.510194   3.159786   0.000000
Pd    0.094876  -0.687215   0.000000
C    -3.729561  -2.629849   0.000000
H    -5.785695   0.084141   0.000000
H    -4.831983   2.521215   0.000000
H    -0.449109   2.876854   0.000000
H    -1.734053   3.741591   0.901899
H    -1.734053   3.741591  -0.901899
H    -4.819708  -2.761533   0.000000
H    -3.309900  -3.097317  -0.898346
H    -3.309900  -3.097317   0.898346
C     1.162790   0.992343   0.000000
C     1.969027  -1.473273   0.000000
C     2.635433  -1.774225  -1.204183
C     3.901001  -2.374665  -1.207130
C     4.542586  -2.671348   0.000000
C     3.901001  -2.374665   1.207130
C     2.635433  -1.774225   1.204183
H     2.172222  -1.525167  -2.162357
H     4.398282  -2.588335  -2.156207
H     5.542325  -3.110752   0.000000
H     4.398282  -2.588335   2.156207
H     2.172222  -1.525167   2.162357
C     1.482250   1.628513   1.210097
C     2.053908   2.907639   1.207412
C     2.334224   3.557484   0.000000
C     2.053908   2.907639  -1.207412
C     1.482250   1.628513  -1.210097
H     1.272903   1.137588   2.161291
H     2.282459   3.393895   2.158154
H     2.779687   4.553538   0.000000
H     2.282459   3.393895  -2.158154
H     1.272903   1.137588  -2.161291
------------------------------------------------
```

```
Net Charge:         0.00

Total  Bonding  Energy:
-8.214283295446222 hartree
-5154.54       kcal/mol
-21566.60        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000029
 Gradient (Max):   0.000792
 Gradient (RMS):   0.000310
 -------------------------------------------------
```

II-1 b-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
---------------------------------------------------
N    -1.054114   2.892534   0.000000
C    -0.009353   2.016978   0.000000
N     1.066754   2.890422   0.000000
C     0.607502   4.183487   0.000000
N    -0.701844   4.229118   0.000000
Pd    0.004972  -0.000649   0.000000
C     0.010875  -2.018434   0.000000
N     1.049017  -2.900255   0.000000
N     0.685697  -4.234721   0.000000
C    -0.623781  -4.179559   0.000000
N    -1.073051  -2.882546   0.000000
C     2.462370  -2.551171   0.000000
C    -2.464475  -2.444110   0.000000
C     2.462533   2.467218   0.000000
C    -2.462125   2.534543   0.000000
H    -1.267762  -5.052060   0.000000
H    -2.435712  -1.346913   0.000000
H    -2.982348  -2.804879   0.898346
H    -2.982348  -2.804879  -0.898346
H     1.247670   5.059185   0.000000
H    -2.950908   2.937022  -0.896195
H    -2.950908   2.937022   0.896195
H    -2.502502   1.439807   0.000000
H     3.032606  -3.484754   0.000000
H     2.698785  -1.959771  -0.892125
H     2.698785  -1.959771   0.892125
H     3.104466   3.356180   0.000000
H     2.663845   1.860684   0.890272
H     2.663845   1.860684  -0.890272
---------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-6.273526794579221 hartree
-3936.70       kcal/mol
-16471.14        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000005
```

```
Gradient (Max):   0.000284
Gradient (RMS):   0.000075
--------------------------------------------------
```

II-2 b-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
-------------------------------------------------
N    -1.090299   2.828275   0.000000
C    -0.004751   1.965059   0.000000
N     1.043206   2.837287   0.000000
N     0.679721   4.170879   0.000000
C    -0.629817   4.122296   0.000000
Pd    0.008683   0.032433   0.000000
C     2.453976   2.478446   0.000000
C    -2.485528   2.402029   0.000000
H    -1.268767   4.998887   0.000000
H    -2.998608   2.769138  -0.898318
H    -2.998608   2.769138   0.898318
H    -2.472303   1.304965   0.000000
H     3.028303   3.409559   0.000000
H     2.687455   1.885635   0.891984
H     2.687455   1.885635  -0.891984
-------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.143012542827536 hartree
-1972.27       kcal/mol
-8251.98         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000026
 Gradient (Max):   0.000640
 Gradient (RMS):   0.000178
 -------------------------------------------------
```

II-RHC b-N

```
============================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     0.009521  -1.987077   0.000000
N     1.064778  -2.878471   0.000000
C     0.598757  -4.175950   0.000000
N    -0.709548  -4.207165   0.000000
N    -1.031535  -2.850304   0.000000
C     2.466406  -2.474064   0.000000
C    -2.437138  -2.480001   0.000000
H     1.229304  -5.059307   0.000000
H    -2.486162  -1.388278   0.000000
H    -2.931289  -2.880290   0.894002
H    -2.931289  -2.880290  -0.894002
H     3.101237  -3.367390   0.000000
H     2.683048  -1.875284  -0.891760
H     2.683048  -1.875284   0.891760
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.057478925498728 hartree
-1918.60       kcal/mol
-8027.41         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000014
 Gradient (Max):   0.000284
 Gradient (RMS):   0.000095
 ------------------------------------------------
```

II-3 b-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N    -3.962810   1.365984   0.000000
N    -2.579691   1.430687   0.000000
C    -1.955917   0.229018   0.000000
N    -3.029208  -0.641826   0.000000
C    -4.197993   0.078989   0.000000
C    -1.952949   2.746070   0.000000
Pd    0.046661  -0.426515   0.000000
C    -2.902638  -2.097043   0.000000
H    -5.188031  -0.363748   0.000000
H    -0.868271   2.605301   0.000000
H    -2.265583   3.297024   0.894676
H    -2.265583   3.297024  -0.894676
H    -3.901969  -2.544870   0.000000
H    -2.359881  -2.426465  -0.894243
H    -2.359881  -2.426465   0.894243
C     1.230143   1.192496   0.000000
C     1.804014  -1.417337   0.000000
C     2.360210  -1.884350  -1.206622
C     3.390820  -2.833118  -1.208279
C     3.908022  -3.312597   0.000000
C     3.390820  -2.833118   1.208279
C     2.360210  -1.884350   1.206622
H     1.985700  -1.512284  -2.163476
H     3.797787  -3.190763  -2.156852
H     4.718536  -4.044090   0.000000
H     3.797787  -3.190763   2.156852
H     1.985700  -1.512284   2.163476
C     1.601069   1.798334   1.210163
C     2.291729   3.018105   1.206649
C     2.637157   3.635234   0.000000
C     2.291729   3.018105  -1.206649
C     1.601069   1.798334  -1.210163
H     1.351691   1.330058   2.163284
H     2.567978   3.479545   2.157216
H     3.181661   4.581083   0.000000
H     2.567978   3.479545  -2.157216
H     1.351691   1.330058  -2.163284
------------------------------------------------
Net Charge:         0.00
```

```
Total  Bonding  Energy:
-8.353628801063669 hartree
-5241.98       kcal/mol
-21932.45        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000034
 Gradient (Max):   0.000530
 Gradient (RMS):   0.000108
 -------------------------------------------------
```

II-1 b-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P    -1.281977   3.160361   0.000000
C    -0.028538   2.002096   0.000000
P     1.300540   3.110287   0.000000
C     0.615296   4.723141   0.000000
N    -0.729448   4.726942   0.000000
Pd   -0.013744  -0.000199   0.000000
C     0.006647  -2.002827   0.000000
P     1.285993  -3.133264   0.000000
N     0.766170  -4.712437   0.000000
C    -0.578379  -4.737396   0.000000
P    -1.298186  -3.139122   0.000000
C     3.089693  -2.892125   0.000000
C    -3.081502  -2.720214   0.000000
C     3.084024   2.702437   0.000000
C    -3.084967   2.914999   0.000000
H    -1.113684  -5.688297   0.000000
H    -3.111286  -1.622855   0.000000
H    -3.574506  -3.103827   0.901592
H    -3.574506  -3.103827  -0.901592
H     1.171339   5.662341   0.000000
H    -3.532259   3.354722  -0.899746
H    -3.532259   3.354722   0.899746
H    -3.236736   1.828941   0.000000
H     3.531015  -3.897216   0.000000
H     3.401260  -2.345163  -0.897372
H     3.401260  -2.345163   0.897372
H     3.642669   3.648393   0.000000
H     3.332536   2.123992   0.897614
H     3.332536   2.123992  -0.897614
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-5.682806752315281 hartree
-3566.02       kcal/mol
-14920.21        kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
```

```
Energy Change :   0.000007
Gradient (Max):   0.000814
Gradient (RMS):   0.000231
--------------------------------------------------
```

II-2 b-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P    -1.331884   2.912982   0.000000
C    -0.010138   1.792299   0.000000
P     1.276259   2.917774   0.000000
N     0.738152   4.489462   0.000000
C    -0.605313   4.508432   0.000000
Pd    0.005574  -0.128931   0.000000
C     3.078975   2.672582   0.000000
C    -3.116586   2.498317   0.000000
H    -1.145011   5.456826   0.000000
H    -3.606869   2.885766  -0.901499
H    -3.606869   2.885766   0.901499
H    -3.157640   1.401343   0.000000
H     3.523559   3.676389   0.000000
H     3.388342   2.124411   0.897333
H     3.388342   2.124411  -0.897333
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-2.847746967621680 hartree
-1786.99       kcal/mol
-7476.76         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000008
 Gradient (Max):   0.000872
 Gradient (RMS):   0.000305
 -------------------------------------------------
```

II-RHC b-P

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================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
---------------------------------------------------
C     0.008615  -1.676430   0.000000
P     1.278085  -2.831226   0.000000
C     0.583726  -4.445197   0.000000
N    -0.763181  -4.416559   0.000000
P    -1.238198  -2.817393   0.000000
C     3.070768  -2.459597   0.000000
C    -3.031502  -2.507279   0.000000
H     1.119569  -5.395494   0.000000
H    -3.159448  -1.418176   0.000000
H    -3.495101  -2.934087   0.897207
H    -3.495101  -2.934087  -0.897207
H     3.610957  -3.415079   0.000000
H     3.339042  -1.888632  -0.896932
H     3.339042  -1.888632   0.896932
---------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-2.769255060592511 hartree
-1737.73       kcal/mol
-7270.68         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000001
 Gradient (Max):   0.000822
 Gradient (RMS):   0.000207
 -------------------------------------------------
```

II-3 b-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N    -4.236342   1.594584   0.000000
P    -2.580106   1.657777   0.000000
C    -1.864266   0.114228   0.000000
P    -3.313875  -0.822461   0.000000
C    -4.644271   0.315244   0.000000
C    -1.778083   3.281679   0.000000
Pd    0.151005  -0.497366   0.000000
C    -3.407775  -2.648839   0.000000
H    -5.705799   0.065662   0.000000
H    -0.694673   3.088460   0.000000
H    -2.062139   3.838327   0.900666
H    -2.062139   3.838327  -0.900666
H    -4.470633  -2.923899   0.000000
H    -2.925245  -3.051011  -0.898853
H    -2.925245  -3.051011   0.898853
C     1.265687   1.160794   0.000000
C     1.932129  -1.442695   0.000000
C     2.507651  -1.885271  -1.206575
C     3.578258  -2.788721  -1.207956
C     4.116566  -3.244825   0.000000
C     3.578258  -2.788721   1.207956
C     2.507651  -1.885271   1.206575
H     2.116003  -1.531157  -2.163261
H     3.998980  -3.129559  -2.156760
H     4.958082  -3.940434   0.000000
H     3.998980  -3.129559   2.156760
H     2.116003  -1.531157   2.163261
C     1.606908   1.787189   1.209798
C     2.240432   3.037780   1.206654
C     2.557220   3.670772   0.000000
C     2.240432   3.037780  -1.206654
C     1.606908   1.787189  -1.209798
H     1.380560   1.307115   2.162682
H     2.496818   3.510679   2.157195
H     3.060254   4.639349   0.000000
H     2.496818   3.510679  -2.157195
H     1.380560   1.307115  -2.162682
------------------------------------------------
```

```
Net Charge:         0.00

Total  Bonding  Energy:
-8.060670507207643 hartree
-5058.15       kcal/mol
-21163.29        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000693
 Gradient (RMS):   0.000192
 -------------------------------------------------
```

II-1 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(2V)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N     0.000000   2.846757  -1.108583
C     0.000000   2.015572  -0.004062
N     0.000000   2.845247   1.103199
C     0.000000   4.203344   0.771896
C     0.000000   4.202683  -0.774454
Pd    0.000000   0.000000  -0.005005
C     0.000000  -2.015572  -0.004062
N     0.000000  -2.845247   1.103199
C     0.000000  -4.203344   0.771896
C     0.000000  -4.202683  -0.774454
N     0.000000  -2.846757  -1.108583
C     0.000000  -2.367881   2.483538
C     0.000000  -2.377331  -2.490270
C     0.000000   2.367881   2.483538
C     0.000000   2.377331  -2.490270
O     0.000000  -5.155715   1.525014
O     0.000000  -5.151025  -1.532519
H     0.000000  -1.282134  -2.449255
H    -0.893237  -2.744272  -3.010045
H     0.893237  -2.744272  -3.010045
O     0.000000   5.155715   1.525014
O     0.000000   5.151025  -1.532519
H     0.893237   2.744272  -3.010045
H    -0.893237   2.744272  -3.010045
H     0.000000   1.282134  -2.449255
H     0.000000  -3.249607   3.133005
H     0.893761  -1.761531   2.667228
H    -0.893761  -1.761531   2.667228
H     0.000000   3.249607   3.133005
H    -0.893761   1.761531   2.667228
H     0.893761   1.761531   2.667228
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-7.058702129904379 hartree
-4429.40       kcal/mol
-18532.62        kJ/mol
```

```
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000010
 Gradient (Max):   0.000482
 Gradient (RMS):   0.000157
 -------------------------------------------------
```

II-2 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Nitrogen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
N    -1.117653   2.786828   0.000000
C    -0.004475   1.960314   0.000000
N     1.102333   2.796232   0.000000
C     0.759478   4.151421   0.000000
C    -0.784622   4.142699   0.000000
Pd    0.012789   0.044614   0.000000
C     2.484605   2.329378   0.000000
C    -2.498999   2.319439   0.000000
O     1.508629   5.107986   0.000000
O    -1.548032   5.088038   0.000000
H    -3.017828   2.688604  -0.893066
H    -3.017828   2.688604   0.893066
H    -2.464359   1.223547   0.000000
H     3.126448   3.216815   0.000000
H     2.673570   1.723570   0.893441
H     2.673570   1.723570  -0.893441
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.541006267304258 hartree
-2222.02       kcal/mol
-9296.91         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000361
 Gradient (RMS):   0.000112
 ------------------------------------------------
```

II-RHC c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     0.000867  -2.010990   0.000000
N     1.093832  -2.855547   0.000000
C     0.764641  -4.214196   0.000000
C    -0.790842  -4.201351   0.000000
N    -1.101002  -2.837314   0.000000
C     2.472955  -2.371100   0.000000
C    -2.473267  -2.338557   0.000000
O     1.503971  -5.176278   0.000000
O    -1.550413  -5.146712   0.000000
H    -2.422272  -1.246196   0.000000
H    -3.004865  -2.694104   0.891764
H    -3.004865  -2.694104  -0.891764
H     3.135318  -3.243646   0.000000
H     2.656297  -1.763921  -0.893762
H     2.656297  -1.763921   0.893762
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.442734902354398 hartree
-2160.35       kcal/mol
-9038.90         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000011
 Gradient (Max):   0.000933
 Gradient (RMS):   0.000357
 -------------------------------------------------
```

II-3 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)

---------------------------------------------------
C    -3.921072   1.447755   0.000000
N    -2.520194   1.488999   0.000000
C    -1.947789   0.237628   0.000000
N    -2.998402  -0.669715   0.000000
C    -4.254475  -0.060462   0.000000
C    -1.801676   2.763437   0.000000
Pd    0.004250  -0.432375   0.000000
C    -2.818093  -2.119074   0.000000
O    -5.343580  -0.596260   0.000000
O    -4.683151   2.390941   0.000000
H    -0.729259   2.555304   0.000000
H    -2.080018   3.337483   0.891518
H    -2.080018   3.337483  -0.891518
H    -3.814393  -2.573512   0.000000
H    -2.270928  -2.433647  -0.897286
H    -2.270928  -2.433647   0.897286
C     1.250817   1.156249   0.000000
C     1.784817  -1.406034   0.000000
C     2.351508  -1.851298  -1.208035
C     3.414879  -2.762596  -1.208661
C     3.949303  -3.220909   0.000000
C     3.414879  -2.762596   1.208661
C     2.351508  -1.851298   1.208035
H     1.965664  -1.491108  -2.164672
H     3.834817  -3.104548  -2.156960
H     4.787897  -3.919659   0.000000
H     3.834817  -3.104548   2.156960
H     1.965664  -1.491108   2.164672
C     1.626182   1.751981   1.211565
C     2.322640   2.968320   1.207231
C     2.668856   3.583298   0.000000
C     2.322640   2.968320  -1.207231
C     1.626182   1.751981  -1.211565
H     1.372862   1.285429   2.164325
H     2.599964   3.428790   2.157514
H     3.215498   4.527571   0.000000
H     2.599964   3.428790  -2.157514
```

```
H     1.372862   1.285429  -2.164325
-----------------------------------------------------
Net Charge:          0.00

Total  Bonding  Energy:
-8.741303213076737 hartree
-5485.25       kcal/mol
-22950.29        kJ/mol
Summary Geometry Optimization:
 -----------------------------------------------------
 Energy Change :   0.000048
 Gradient (Max):   0.000509
 Gradient (RMS):   0.000144
 -----------------------------------------------------
```

II-1 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(2V)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P     0.000000   3.035726  -1.399363
C     0.000000   2.004183  -0.018562
P     0.000000   3.008273   1.385072
C     0.000000   4.724609   0.829263
C     0.000000   4.743449  -0.799477
Pd    0.000000   0.000000  -0.023490
C     0.000000  -2.004183  -0.018562
P     0.000000  -3.008273   1.385072
C     0.000000  -4.724609   0.829263
C     0.000000  -4.743449  -0.799477
P     0.000000  -3.035726  -1.399363
C     0.000000  -2.512547   3.150291
C     0.000000  -2.508376  -3.158520
C     0.000000   2.512547   3.150291
C     0.000000   2.508376  -3.158520
O     0.000000  -5.763420   1.462573
O     0.000000  -5.794211  -1.410390
H     0.000000  -1.410541  -3.122929
H    -0.901785  -2.868730  -3.667366
H     0.901785  -2.868730  -3.667366
O     0.000000   5.763420   1.462573
O     0.000000   5.794211  -1.410390
H     0.901785   2.868730  -3.667366
H    -0.901785   2.868730  -3.667366
H     0.000000   1.410541  -3.122929
H     0.000000  -3.453571   3.717494
H     0.902625  -1.936914   3.386729
H    -0.902625  -1.936914   3.386729
H     0.000000   3.453571   3.717494
H    -0.902625   1.936914   3.386729
H     0.902625   1.936914   3.386729
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-6.373064666008656 hartree
-3999.16       kcal/mol
-16732.48        kJ/mol
```

```
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000014
 Gradient (Max):   0.000922
 Gradient (RMS):   0.000255
 ------------------------------------------------
```

II-2 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Phosphorus (TZP, 2p frozen)
Carbon (TZP, 1s frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
P    -1.415188   2.792555   0.000000
C    -0.012872   1.778280   0.000000
P     1.390238   2.795844   0.000000
C     0.801618   4.502675   0.000000
C    -0.819295   4.503057   0.000000
Pd    0.011148  -0.127690   0.000000
C     3.161319   2.318449   0.000000
C    -3.171564   2.251591   0.000000
O     1.429957   5.545384   0.000000
O    -1.448096   5.544183   0.000000
H    -3.682453   2.609116  -0.901874
H    -3.682453   2.609116   0.901874
H    -3.130959   1.153218   0.000000
H     3.719083   3.265279   0.000000
H     3.402680   1.743970   0.902286
H     3.402680   1.743970  -0.902286
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.198216339998325 hartree
-2006.91       kcal/mol
-8396.92         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000011
 Gradient (Max):   0.000890
 Gradient (RMS):   0.000329
 -------------------------------------------------
```

II-RHC c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.007052  -1.721361   0.000000
P     1.357537  -2.733707   0.000000
C     0.817573  -4.461754   0.000000
C    -0.838252  -4.458732   0.000000
P    -1.376187  -2.720894   0.000000
C     3.119621  -2.224256   0.000000
C    -3.119742  -2.145832   0.000000
O     1.426240  -5.512012   0.000000
O    -1.452775  -5.503585   0.000000
H    -3.065578  -1.048525   0.000000
H    -3.642301  -2.491618   0.899782
H    -3.642301  -2.491618  -0.899782
H     3.704169  -3.153987   0.000000
H     3.352467  -1.644188  -0.901183
H     3.352467  -1.644188   0.901183
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.104293127367899 hartree
-1947.97       kcal/mol
-8150.32         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000029
 Gradient (Max):   0.000606
 Gradient (RMS):   0.000224
 -------------------------------------------------
```

II-4 c-P

```
================================================================
```

ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Palladium (TZP, 3d frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	-4.324752	1.549459	0.000000
P	-2.522978	1.731303	0.000000
C	-1.851267	0.148246	0.000000
P	-3.168341	-0.977329	0.000000
C	-4.702729	-0.031210	0.000000
C	-1.613875	3.318983	0.000000
Pd	0.131846	-0.430302	0.000000
C	-3.041496	-2.807223	0.000000
O	-5.861795	-0.399018	0.000000
O	-5.197886	2.394682	0.000000
H	-0.544298	3.059071	0.000000
H	-1.862812	3.890982	0.901191
H	-1.862812	3.890982	-0.901191
H	-4.077351	-3.172726	0.000000
H	-2.528904	-3.161967	-0.902327
H	-2.528904	-3.161967	0.902327
C	1.355204	1.169118	0.000000
C	1.912221	-1.400351	0.000000
C	2.470400	-1.853496	-1.208677
C	3.517795	-2.783337	-1.208473
C	4.043402	-3.251649	0.000000
C	3.517795	-2.783337	1.208473
C	2.470400	-1.853496	1.208677
H	2.087947	-1.489079	-2.164902
H	3.930391	-3.133913	-2.156813
H	4.867199	-3.967744	0.000000
H	3.930391	-3.133913	2.156813
H	2.087947	-1.489079	2.164902
C	1.726440	1.769924	1.211344
C	2.419714	2.988328	1.207191
C	2.765630	3.604010	0.000000
C	2.419714	2.988328	-1.207191
C	1.726440	1.769924	-1.211344
H	1.476692	1.301488	2.163991
H	2.697972	3.448630	2.157380
H	3.313909	4.547461	0.000000
H	2.697972	3.448630	-2.157380
H	1.476692	1.301488	-2.163991

Net Charge: 0.00

```
Total  Bonding  Energy:
-8.399170254173640 hartree
-5270.56       kcal/mol
-22052.02        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000006
 Gradient (Max):   0.000859
 Gradient (RMS):   0.000153
 -------------------------------------------------
```

tBuB(OH)$_2$

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  NOSYM

Basis:
Boron (TZP, 1s frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)
Carbon (TZP, 1s frozen)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
B    -1.459040   0.122980  -0.000185
O    -2.595019   0.920652  -0.000538
H    -2.342699   1.860687  -0.002608
O    -1.632242  -1.251097   0.004476
H    -2.582802  -1.461784   0.006928
O    -0.229923   0.730653  -0.002884
C     1.067326   0.038955  -0.001058
C     2.100527   1.168997   0.002107
C     1.194571  -0.810500   1.267469
C     1.200063  -0.808657  -1.270248
H     2.194807  -1.266157   1.316384
H     1.059005  -0.182689   2.159886
H     0.446113  -1.612398   1.281314
H     3.119036   0.754904   0.004447
H     1.981686   1.800540  -0.889654
H     1.977259   1.799333   0.894131
H     2.200793  -1.263601  -1.315504
H     0.452209  -1.610977  -1.288263
H     1.067894  -0.179607  -2.162275
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.892401490240226 hartree
-2442.52       kcal/mol
-10219.50        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000004
 Gradient (Max):   0.000377
 Gradient (RMS):   0.000122
 -------------------------------------------------
```

tBuO$^-$

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Oxygen (TZP, 1s frozen)
Carbon (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
O    -0.066473   0.322533   0.000000
C     0.170882  -1.003009   0.000000
C     1.712617  -1.324046   0.000000
C    -0.444363  -1.709781   1.265206
C    -0.444363  -1.709781  -1.265206
H    -0.273747  -2.806504   1.316236
H    -0.015649  -1.243112   2.168026
H    -1.530938  -1.520466   1.276288
H     1.963724  -2.406371   0.000000
H     2.166053  -0.856114  -0.889959
H     2.166053  -0.856114   0.889959
H    -0.273747  -2.806504  -1.316236
H    -1.530938  -1.520466  -1.276288
H    -0.015649  -1.243112  -2.168026
------------------------------------------------
Net Charge:         -1.00

Total  Bonding  Energy:
-2.758648747246755 hartree
-1731.08       kcal/mol
-7242.83         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000041
 Gradient (Max):   0.000746
 Gradient (RMS):   0.000290
 -------------------------------------------------
```

Cl^-

```
================================================================
ADF - Version 2008.01

SINGLE POINT
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  ATOM

Basis:
Chlorine (TZP, 2p frozen)

Molecular Geometry   (x,y,z in Angstrom)
-------------------------------------------------
Cl    0.000000   0.000000   0.000000
-------------------------------------------------
Net Charge:         -1.00

Total  Bonding  Energy:
-0.143555263768652 hartree
-90.08         kcal/mol
-376.90          kJ/mol
```

PhCl

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Chlorine (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.014854   0.744916   0.000000
C    -1.234680   0.066538   0.000000
C    -1.293603  -1.328166   0.000000
C    -0.099386  -2.054758   0.000000
C     1.132696  -1.393833   0.000000
C     1.170515   0.003615   0.000000
Cl   -2.735945   0.992430   0.000000
H    -2.259671  -1.831919   0.000000
H     2.060690  -1.966465   0.000000
H     0.002145   1.834295   0.000000
H    -0.137926  -3.144667   0.000000
H     2.127043   0.527466   0.000000
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-2.683947485122870 hartree
-1684.20       kcal/mol
-7046.70         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000003
 Gradient (Max):   0.000408
 Gradient (RMS):   0.000132
 ------------------------------------------------
```

$PhB(OH)_2$

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  NOSYM

Basis:
Carbon (TZP, 1s frozen)
Boron (TZP, 1s frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C     1.701435  -0.538144  -0.023142
C     2.467673  -0.417628   1.153750
C     1.775269  -0.284302   2.372701
C     0.379728  -0.270659   2.422269
C    -0.358041  -0.390142   1.239897
C     0.305712  -0.527504   0.016159
B     4.032878  -0.435550   1.075449
O     4.631812  -0.568539  -0.157791
H     2.324749  -0.187492   3.314849
H     2.217473  -0.641622  -0.978483
O     4.867889  -0.328258   2.173173
H     4.373017  -0.239281   3.004837
H     5.602367  -0.567233  -0.073232
H    -0.133835  -0.167480   3.379354
H    -1.448947  -0.377149   1.273277
H    -0.267236  -0.626597  -0.907329
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.701694708141589 hartree
-2322.85       kcal/mol
-9718.80         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000025
 Gradient (Max):   0.000483
 Gradient (RMS):   0.000159
 -------------------------------------------------
```

OH^-

```
============================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(LIN)

Basis:
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
-------------------------------------------------
O     0.000000   0.000000   4.876022
H     0.000000   0.000000   5.854627
-------------------------------------------------
Net Charge:         -1.00

Total  Bonding  Energy:
-0.340711528447369 hartree
-213.80        kcal/mol
-894.54          kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000008
 Gradient (RMS):   0.000005
 -------------------------------------------------
```

III-1 a-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.261790   0.163494   0.000000
N     1.109439   0.158274   0.000000
C     1.934266   1.363242   0.000000
Au   -1.486094   1.729052   0.000000
O    -2.640836   3.362053   0.000000
H    -3.565479   3.050848   0.000000
N    -0.600936  -1.164915   0.000000
C    -1.980058  -1.647582   0.000000
C     0.528953  -1.970970   0.000000
C     1.606346  -1.138683   0.000000
H     0.473231  -3.052199   0.000000
H     2.666599  -1.358326   0.000000
H     1.260190   2.226200   0.000000
H     2.565780   1.390880  -0.897300
H     2.565780   1.390880   0.897300
H    -1.969645  -2.742417   0.000000
H    -2.503949  -1.284039   0.891568
H    -2.503949  -1.284039  -0.891568
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.726347700469631 hartree
-2338.32       kcal/mol
-9783.52         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000035
 Gradient (Max):   0.000926
 Gradient (RMS):   0.000239
 ------------------------------------------------
```

III-2 a-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.251580   0.154647   0.000000
N     1.103068   0.187447   0.000000
C     1.947434   1.388867   0.000000
Au   -1.474663   1.707456   0.000000
N    -0.620981  -1.149783   0.000000
C    -2.003681  -1.648902   0.000000
C     0.513563  -1.944824   0.000000
C     1.591222  -1.110013   0.000000
H     0.457748  -3.026617   0.000000
H     2.653010  -1.325472   0.000000
H     1.300134   2.270265   0.000000
H     2.575097   1.394773  -0.898020
H     2.575097   1.394773   0.898020
H    -1.973824  -2.741652   0.000000
H    -2.524706  -1.300724   0.898155
H    -2.524706  -1.300724  -0.898155
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-3.087656251810198 hartree
-1937.53       kcal/mol
-8106.64         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000015
 Gradient (Max):   0.000678
 Gradient (RMS):   0.000146
 ------------------------------------------------
```

III-1 a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.315428   0.220883   0.000000
P     1.404056   0.173327   0.000000
C     2.504705   1.626926   0.000000
Au   -1.533078   1.793185   0.000000
O    -2.676628   3.443229   0.000000
H    -3.604003   3.138145   0.000000
P    -0.693013  -1.457293   0.000000
C    -2.355792  -2.206268   0.000000
C     0.797679  -2.348031   0.000000
C     1.900344  -1.491236   0.000000
H     0.874465  -3.433330   0.000000
H     2.933050  -1.833772   0.000000
H     1.836237   2.497895   0.000000
H     3.128646   1.644792  -0.901598
H     3.128646   1.644792   0.901598
H    -2.224648  -3.296011   0.000000
H    -2.905846  -1.900334   0.897543
H    -2.905846  -1.900334  -0.897543
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.409843048673616 hartree
-2139.71       kcal/mol
-8952.54         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000049
 Gradient (Max):   0.000950
 Gradient (RMS):   0.000268
 ------------------------------------------------
```

III-2 a-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Gold (TZP, 4f frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.296343   0.209111   0.000000
P     1.420819   0.216183   0.000000
C     2.518509   1.665609   0.000000
Au   -1.516130   1.760479   0.000000
P    -0.731001  -1.452605   0.000000
C    -2.399606  -2.172530   0.000000
C     0.768380  -2.303964   0.000000
C     1.872272  -1.447835   0.000000
H     0.850304  -3.389490   0.000000
H     2.903372  -1.797005   0.000000
H     1.873343   2.553155   0.000000
H     3.140928   1.662217  -0.902980
H     3.140928   1.662217   0.902980
H    -2.270019  -3.262941   0.000000
H    -2.941212  -1.866604   0.902900
H    -2.941212  -1.866604  -0.902900
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-2.782478671408388 hartree
-1746.03       kcal/mol
-7305.40         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000010
 Gradient (Max):   0.000941
 Gradient (RMS):   0.000241
 ------------------------------------------------
```

III-1 b-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.241801   0.236854   0.000000
N     1.129689   0.158239   0.000000
C     1.640518   1.439439   0.000000
N     0.518689   2.202978   0.000000
N    -0.654521   1.479840   0.000000
Au    3.536440   2.011730   0.000000
O     5.473042   2.487215   0.000000
C     1.928441  -1.066858   0.000000
C     0.468782   3.660021   0.000000
H     5.534007   3.460670   0.000000
H    -0.901068  -0.623800   0.000000
H     2.982327  -0.771425   0.000000
H     1.713451  -1.659086  -0.897988
H     1.713451  -1.659086   0.897988
H    -0.585115   3.950434   0.000000
H     0.969735   4.049793   0.893597
H     0.969735   4.049793  -0.893597
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.552280085721362 hartree
-2229.09       kcal/mol
-9326.51         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000011
 Gradient (Max):   0.000668
 Gradient (RMS):   0.000194
 ------------------------------------------------
```

III-2 b-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.210626   0.245461   0.000000
N     1.161647   0.153350   0.000000
C     1.636214   1.430385   0.000000
N     0.549913   2.220748   0.000000
N    -0.610199   1.495000   0.000000
Au    3.524868   2.008949   0.000000
C     1.944024  -1.092892   0.000000
C     0.491248   3.686243   0.000000
H    -0.876723  -0.611076   0.000000
H     3.006431  -0.835461   0.000000
H     1.706751  -1.672560  -0.898646
H     1.706751  -1.672560   0.898646
H    -0.566858   3.959308   0.000000
H     0.978992   4.075514   0.900028
H     0.978992   4.075514  -0.900028
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-2.902811363493535 hartree
-1821.54       kcal/mol
-7621.33         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000006
 Gradient (Max):   0.000757
 Gradient (RMS):   0.000222
 ------------------------------------------------
```

III-1 b-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.676507   0.131333   0.000000
P     1.056082  -0.108370   0.000000
C     1.742235   1.486623   0.000000
P     0.294373   2.396596   0.000000
N    -1.041582   1.423122   0.000000
Au    3.648169   2.038333   0.000000
O     5.601360   2.483987   0.000000
C     2.020353  -1.661731   0.000000
C     0.041297   4.193703   0.000000
H     5.664826   3.457974   0.000000
H    -1.428805  -0.657993   0.000000
H     3.073563  -1.351270   0.000000
H     1.808918  -2.247779  -0.902112
H     1.808918  -2.247779   0.902112
H    -1.045543   4.346621   0.000000
H     0.484221   4.638766   0.898410
H     0.484221   4.638766  -0.898410
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.252605216034704 hartree
-2041.04       kcal/mol
-8539.71         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000001
 Gradient (Max):   0.000907
 Gradient (RMS):   0.000244
 ------------------------------------------------
```

III-2 b-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.617474   0.149273   0.000000
P     1.097154  -0.135783   0.000000
C     1.738772   1.476412   0.000000
P     0.331552   2.438188   0.000000
N    -0.964250   1.446199   0.000000
Au    3.631197   2.032214   0.000000
C     2.050778  -1.690947   0.000000
C     0.105624   4.230961   0.000000
H    -1.381068  -0.629217   0.000000
H     3.113356  -1.417334   0.000000
H     1.815874  -2.266679  -0.903547
H     1.815874  -2.266679   0.903547
H    -0.982245   4.386084   0.000000
H     0.547832   4.668062   0.903265
H     0.547832   4.668062  -0.903265
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-2.617747279535898 hartree
-1642.66       kcal/mol
-6872.89         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000002
 Gradient (Max):   0.000947
 Gradient (RMS):   0.000238
 ------------------------------------------------
```

III-1 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.204788   0.062416   0.000000
N     1.193883   0.131565   0.000000
C     1.652173   1.431257   0.000000
N     0.547444   2.257127   0.000000
C    -0.654870   1.537629   0.000000
Au    3.521305   2.009629   0.000000
O     5.436799   2.502636   0.000000
C     2.035386  -1.063601   0.000000
C     0.599010   3.717950   0.000000
H     5.503629   3.477306   0.000000
O    -0.887881  -0.940545   0.000000
H     3.081092  -0.740932   0.000000
H     1.823518  -1.663625  -0.892787
H     1.823518  -1.663625   0.892787
H    -0.435971   4.074784   0.000000
H     1.119978   4.075940   0.895096
H     1.119978   4.075940  -0.895096
O    -1.783215   1.984226   0.000000
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.944830409433814 hartree
-2475.42       kcal/mol
-10357.15        kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000002
 Gradient (Max):   0.000382
 Gradient (RMS):   0.000104
 -------------------------------------------------
```

III-2 c-N

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.211681   0.054192   0.000000
N     1.226861   0.131091   0.000000
C     1.620115   1.418699   0.000000
N     0.573368   2.270221   0.000000
C    -0.663113   1.537079   0.000000
Au    3.510082   2.009201   0.000000
C     2.063456  -1.075417   0.000000
C     0.622843   3.739763   0.000000
O    -0.861930  -0.950535   0.000000
H     3.113617  -0.767005   0.000000
H     1.842174  -1.667252  -0.894967
H     1.842174  -1.667252   0.894967
H    -0.413144   4.092136   0.000000
H     1.133232   4.095318   0.901521
H     1.133232   4.095318  -0.901521
O    -1.766885   2.000954   0.000000
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-3.271449864683599 hartree
-2052.87       kcal/mol
-8589.19         kJ/mol
Summary Geometry Optimization:
 -------------------------------------------------
 Energy Change :   0.000003
 Gradient (Max):   0.000899
 Gradient (RMS):   0.000187
 -------------------------------------------------
```

III-1 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.602090  -0.090408   0.000000
P     1.204338  -0.169616   0.000000
C     1.769767   1.472421   0.000000
P     0.384195   2.522556   0.000000
C    -1.071355   1.459604   0.000000
Au    3.645303   2.043866   0.000000
O     5.573343   2.524633   0.000000
C     2.281912  -1.653577   0.000000
C     0.393171   4.354148   0.000000
H     5.639482   3.499708   0.000000
O    -1.419374  -0.989687   0.000000
H     3.311084  -1.267692   0.000000
H     2.106696  -2.251153  -0.902075
H     2.106696  -2.251153   0.902075
H    -0.664351   4.651851   0.000000
H     0.885158   4.734577   0.902977
H     0.885158   4.734577  -0.902977
O    -2.251537   1.753770   0.000000
------------------------------------------------
Net Charge:         0.00

Total  Bonding  Energy:
-3.598139259771075 hartree
-2257.87       kcal/mol
-9446.91         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000011
 Gradient (Max):   0.000809
 Gradient (RMS):   0.000224
 ------------------------------------------------
```

III-2 c-P

```
================================================================
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional:  VWN  Becke88 Perdew86
Relativistic Corrections:  scalar(ZORA,SAPA)
General Accuracy:     5.00
Symmetry:  C(S)

Basis:
Carbon (TZP, 1s frozen)
Phosphorus (TZP, 2p frozen)
Gold (TZP, 4f frozen)
Oxygen (TZP, 1s frozen)
Hydrogen (TZP)

Final Geometry   (x,y,z in Angstrom)
------------------------------------------------
C    -0.587087  -0.091690   0.000000
P     1.253856  -0.200744   0.000000
C     1.737292   1.454816   0.000000
P     0.413319   2.566970   0.000000
C    -1.056373   1.469270   0.000000
Au    3.625250   2.041072   0.000000
C     2.347539  -1.670827   0.000000
C     0.474409   4.395683   0.000000
O    -1.382768  -0.989870   0.000000
H     3.376437  -1.283794   0.000000
H     2.166133  -2.262492  -0.905367
H     2.166133  -2.262492   0.905367
H    -0.576813   4.718367   0.000000
H     0.971944   4.755105   0.908891
H     0.971944   4.755105  -0.908891
O    -2.218065   1.775852   0.000000
------------------------------------------------
Net Charge:         1.00

Total  Bonding  Energy:
-2.940254796847603 hartree
-1845.04       kcal/mol
-7719.64         kJ/mol
Summary Geometry Optimization:
 ------------------------------------------------
 Energy Change :   0.000000
 Gradient (Max):   0.000714
 Gradient (RMS):   0.000199
 ------------------------------------------------
```