

## Supplementary Information

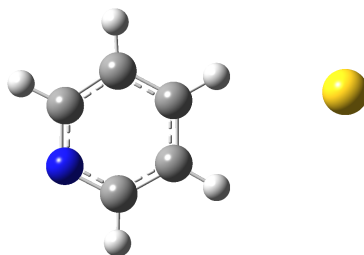
# Experimental and Theoretical Study on Activation of the C-H Bond in Pyridine by $[M_m]^-$ (M=Cu, Ag, Au, m=1-3)

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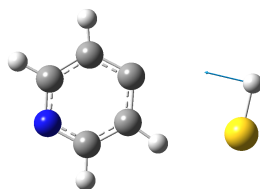
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The Cartesian coordinates and energies of all reaction complex, transition state, intermediate and product have been listed here. The imaginary frequency of each transition state with a picture of the associated displacement vectors have also been inserted here.



C	2.01365200	0.49327000	0.00137800
C	3.10964800	1.35287200	0.00041700
C	4.39276800	0.80708000	-0.00071900
C	3.57686200	-1.32340400	-0.00007900
C	2.25761200	-0.87784400	0.00128300
H	0.98270700	0.84488700	0.00199700
H	2.97596500	2.42954500	0.00042700
H	5.26615300	1.45622000	-0.00145000
H	3.79732200	-2.38846000	-0.00036000
H	1.42052400	-1.56792100	0.00192900
N	4.64126800	-0.50767300	-0.00104200
Au	-1.75993400	0.00085600	-0.00011300



C	1.99911600	0.98402200	0.00022900
C	3.35831400	1.34892500	0.00001400
C	4.37461200	0.38904200	-0.00017500

C	2.86527300	-1.30394100	0.00008600
C	1.80412100	-0.39578100	0.00026700
H	-1.61419100	1.54620400	0.00022500
H	3.66239200	2.39847700	-0.00003900
H	5.42440900	0.69391700	-0.00038300
H	2.67745700	-2.38098500	0.00014200
H	0.78480000	-0.82783100	0.00038600
N	4.15416900	-0.93406800	-0.00013600
Au	-1.60028700	-0.01297400	-0.00002400

Freq = -329.34

Zero-point correction= 0.078963 (Hartree/Particle)

Thermal correction to Energy= 0.086432

Thermal correction to Enthalpy= 0.087376

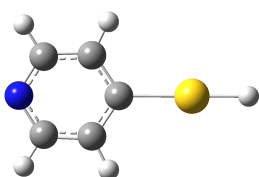
Thermal correction to Gibbs Free Energy= 0.042338

Sum of electronic and zero-point Energies= -383.698893

Sum of electronic and thermal Energies= -383.691424

Sum of electronic and thermal Enthalpies= -383.690480

Sum of electronic and thermal Free Energies= -383.735518



C	-0.90002900	-0.00002500	0.00309700
C	-1.67937800	1.17615000	0.00099300
C	-3.07192500	1.13262900	-0.00020800
C	-3.07196000	-1.13260500	-0.00020800
C	-1.67941400	-1.17617100	0.00099300
H	2.85114900	0.00001900	-0.00212100
H	-1.19683300	2.15040400	0.00049700
H	-3.64917300	2.05807500	-0.00183700
H	-3.64923600	-2.05803500	-0.00183900
H	-1.19690200	-2.15044200	0.00049900
N	-3.79008700	0.00002200	-0.00145800
Au	1.21250400	-0.00000100	-0.00016500

Zero-point correction= 0.083830 (Hartree/Particle)

Thermal correction to Energy= 0.090158

Thermal correction to Enthalpy= 0.091102

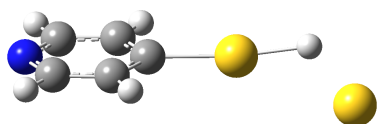
Thermal correction to Gibbs Free Energy= 0.050979

Sum of electronic and zero-point Energies= -383.801399

Sum of electronic and thermal Energies= -383.795072

Sum of electronic and thermal Enthalpies= -383.794128

Sum of electronic and thermal Free Energies= -383.834250



C	2.48294000	0.00003200	-0.03022500
C	3.23279700	1.18073100	-0.18596600
C	4.59680300	1.13395700	-0.46641000
C	4.59702700	-1.13302900	-0.46752400
C	3.23303300	-1.18035600	-0.18713100
H	-1.17854300	-0.00116700	0.98937200
H	2.75702600	2.15153300	-0.08770800
H	5.16177800	2.05830300	-0.58361800
H	5.16219300	-2.05714600	-0.58561200
H	2.75746400	-2.15134900	-0.08978700
N	5.29661300	0.00060500	-0.61029700
Au	-2.48861000	0.00022800	-0.24933700
Au	0.45580300	-0.00038500	0.40950100

Zero-point correction= 0.084111 (Hartree/Particle)

Thermal correction to Energy= 0.092864

Thermal correction to Enthalpy= 0.093808

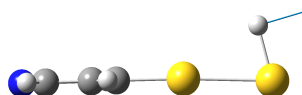
Thermal correction to Gibbs Free Energy= 0.043280

Sum of electronic and zero-point Energies= -519.284220

Sum of electronic and thermal Energies= -519.275467

Sum of electronic and thermal Enthalpies= -519.274523

Sum of electronic and thermal Free Energies= -519.325051



C	-2.38464400	0.00000400	0.00392900
C	-3.14339700	-1.18395100	-0.01331100
C	-4.53512200	-1.13356700	-0.04325100
C	-4.53511000	1.13360000	-0.04324500
C	-3.14338400	1.18396700	-0.01330600
H	1.92306500	-0.00002600	1.59573700
H	-2.65563000	-2.15238100	-0.00338100
H	-5.11124100	-2.05798000	-0.05553500
H	-5.11121900	2.05801800	-0.05552100
H	-2.65560700	2.15239200	-0.00336900
N	-5.24886600	0.00002000	-0.05849800
Au	2.34110700	0.00000900	-0.04106300
Au	-0.35626400	-0.00001500	0.03583100

Freq = -443.27

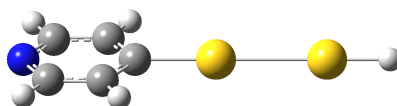
Zero-point correction= 0.081513 (Hartree/Particle)

Thermal correction to Energy= 0.090511

Thermal correction to Enthalpy= 0.091455

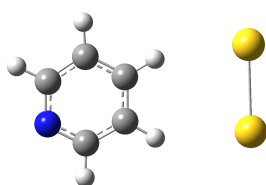
Thermal correction to Gibbs Free Energy= 0.041245

Sum of electronic and zero-point Energies=	-519.263426
Sum of electronic and thermal Energies=	-519.254428
Sum of electronic and thermal Enthalpies=	-519.253484
Sum of electronic and thermal Free Energies=	-519.303694



C	2.48991300	0.00002200	-0.00000500
C	3.24318400	-1.18431200	0.00002700
C	4.63621900	-1.13422100	0.00008900
C	4.63594600	1.13477800	0.00008800
C	3.24289900	1.18453500	0.00002700
H	-4.04037400	-0.00096500	0.00046500
H	2.75328500	-2.15235800	0.00000500
H	5.21376700	-2.05788700	0.00011500
H	5.21327400	2.05858100	0.00011500
H	2.75276700	2.15246300	0.00000700
N	5.34813200	0.00036400	0.00012100
Au	-2.42477900	0.00014500	0.00003800
Au	0.41441700	-0.00023600	-0.00007500
Zero-point correction=			0.081965 (Hartree/Particle)
Thermal correction to Energy=			0.091957
Thermal correction to Enthalpy=			0.092901

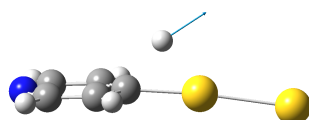
Thermal correction to Gibbs Free Energy=	0.039215
Sum of electronic and zero-point Energies=	-519.282833
Sum of electronic and thermal Energies=	-519.272841
Sum of electronic and thermal Enthalpies=	-519.271897
Sum of electronic and thermal Free Energies=	-519.325583



C	-2.78272000	-0.69044000	0.00184700
C	-3.95799000	-1.43833700	0.00116900
C	-5.18025700	-0.76783800	-0.00050400
C	-4.15588700	1.27094900	-0.00070900
C	-2.88536900	0.69888300	0.00099200
H	-1.80221100	-1.15989200	0.00258700
H	-3.93193200	-2.52274300	0.00189800
H	-6.11349900	-1.32717900	-0.00103000
H	-4.26816500	2.35232600	-0.00151000
H	-1.98741600	1.31044500	0.00158200
N	-5.29569800	0.56486200	-0.00153200
Au	0.99771700	1.38578500	0.00008200
Au	1.14084600	-1.34839700	-0.00020300

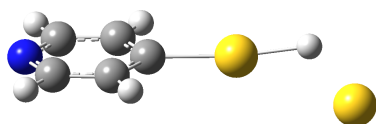


Zero-point correction=	0.089074 (Hartree/Particle)
Thermal correction to Energy=	0.098257
Thermal correction to Enthalpy=	0.099201
Thermal correction to Gibbs Free Energy=	0.045775
Sum of electronic and zero-point Energies=	-519.297841
Sum of electronic and thermal Energies=	-519.288658
Sum of electronic and thermal Enthalpies=	-519.287713
Sum of electronic and thermal Free Energies=	-519.341140



C	-2.38474400	0.00002800	0.05581900
C	-3.14748800	-1.19329300	-0.01642600
C	-4.52592600	-1.13557700	-0.14414300
C	-4.52581100	1.13586200	-0.14405300
C	-3.14736700	1.19343100	-0.01632200
H	-1.45847400	-0.00011700	1.49134000
H	-2.65960600	-2.16100800	0.02748000
H	-5.09619700	-2.06162100	-0.21151200
H	-5.09598700	2.06196900	-0.21134900
H	-2.65939100	2.16109500	0.02768100
N	-5.24703400	0.00018200	-0.20813300

Au	2.33200300	0.00007400	-0.06975800
Au	-0.30558600	-0.00012800	0.09411300
Freq = -1032.83			
Zero-point correction=			0.080738 (Hartree/Particle)
Thermal correction to Energy=			0.089289
Thermal correction to Enthalpy=			0.090233
Thermal correction to Gibbs Free Energy=			0.041651
Sum of electronic and zero-point Energies=			-519.236873
Sum of electronic and thermal Energies=			-519.228322
Sum of electronic and thermal Enthalpies=			-519.227377
Sum of electronic and thermal Free Energies=			-519.275959



C	2.48294000	0.00003200	-0.03022500
C	3.23279700	1.18073100	-0.18596600
C	4.59680300	1.13395700	-0.46641000
C	4.59702700	-1.13302900	-0.46752400
C	3.23303300	-1.18035600	-0.18713100
H	-1.17854300	-0.00116700	0.98937200
H	2.75702600	2.15153300	-0.08770800
H	5.16177800	2.05830300	-0.58361800

H	5.16219300	-2.05714600	-0.58561200
H	2.75746400	-2.15134900	-0.08978700
N	5.29661300	0.00060500	-0.61029700
Au	-2.48861000	0.00022800	-0.24933700
Au	0.45580300	-0.00038500	0.40950100

Zero-point correction= 0.084111 (Hartree/Particle)

Thermal correction to Energy= 0.092864

Thermal correction to Enthalpy= 0.093808

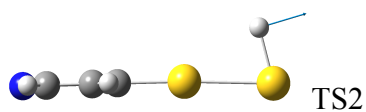
Thermal correction to Gibbs Free Energy= 0.043280

Sum of electronic and zero-point Energies= -519.284220

Sum of electronic and thermal Energies= -519.275467

Sum of electronic and thermal Enthalpies= -519.274523

Sum of electronic and thermal Free Energies= -519.325051

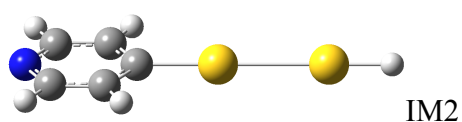


C	-2.38464400	0.00000400	0.00392900
C	-3.14339700	-1.18395100	-0.01331100
C	-4.53512200	-1.13356700	-0.04325100
C	-4.53511000	1.13360000	-0.04324500
C	-3.14338400	1.18396700	-0.01330600

H	1.92306500	-0.00002600	1.59573700
H	-2.65563000	-2.15238100	-0.00338100
H	-5.11124100	-2.05798000	-0.05553500
H	-5.11121900	2.05801800	-0.05552100
H	-2.65560700	2.15239200	-0.00336900
N	-5.24886600	0.00002000	-0.05849800
Au	2.34110700	0.00000900	-0.04106300
Au	-0.35626400	-0.00001500	0.03583100

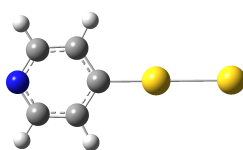
Freq = -443.27

Zero-point correction=	0.081513 (Hartree/Particle)
Thermal correction to Energy=	0.090511
Thermal correction to Enthalpy=	0.091455
Thermal correction to Gibbs Free Energy=	0.041245
Sum of electronic and zero-point Energies=	-519.263426
Sum of electronic and thermal Energies=	-519.254428
Sum of electronic and thermal Enthalpies=	-519.253484
Sum of electronic and thermal Free Energies=	-519.303694



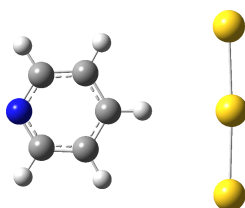
C	2.48991300	0.00002200	-0.00000500
C	3.24318400	-1.18431200	0.00002700
C	4.63621900	-1.13422100	0.00008900

C	4.63594600	1.13477800	0.00008800
C	3.24289900	1.18453500	0.00002700
H	-4.04037400	-0.00096500	0.00046500
H	2.75328500	-2.15235800	0.00000500
H	5.21376700	-2.05788700	0.00011500
H	5.21327400	2.05858100	0.00011500
H	2.75276700	2.15246300	0.00000700
N	5.34813200	0.00036400	0.00012100
Au	-2.42477900	0.00014500	0.00003800
Au	0.41441700	-0.00023600	-0.00007500
Zero-point correction=			0.081965 (Hartree/Particle)
Thermal correction to Energy=			0.091957
Thermal correction to Enthalpy=			0.092901
Thermal correction to Gibbs Free Energy=			0.039215
Sum of electronic and zero-point Energies=			-519.282833
Sum of electronic and thermal Energies=			-519.272841
Sum of electronic and thermal Enthalpies=			-519.271897
Sum of electronic and thermal Free Energies=			-519.325583

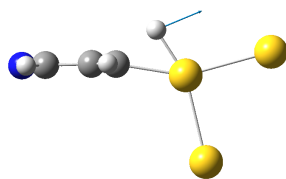


C	2.37942800	0.00000000	-0.00000600
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C	3.14266600	-1.18207200	0.00000800
C	4.53502400	-1.13327200	0.00003300
C	4.53502400	1.13327400	0.00003400
C	3.14266500	1.18207200	0.00000800
H	2.65564300	-2.15164400	-0.00000200
H	5.11217100	-2.05795200	0.00004300
H	5.11217000	2.05795400	0.00004300
H	2.65564200	2.15164400	-0.00000200
N	5.24955100	0.00000100	0.00004600
Au	-2.34086700	0.00000000	0.00001800
Au	0.33211600	-0.00000100	-0.00002900
Zero-point correction=			0.077921 (Hartree/Particle)
Thermal correction to Energy=			0.086113
Thermal correction to Enthalpy=			0.087057
Thermal correction to Gibbs Free Energy=			0.039658
Sum of electronic and zero-point Energies=			-518.728086
Sum of electronic and thermal Energies=			-518.719893
Sum of electronic and thermal Enthalpies=			-518.718949
Sum of electronic and thermal Free Energies=			-518.766348



C	0.00197800	3.05976300	0.00020800
C	-1.19231800	3.77525300	0.00043800
C	-1.13628300	5.16708200	0.00025100
C	1.14338600	5.16539200	-0.00037200
C	1.19734900	3.77349800	-0.00021300
H	0.00123500	1.97397800	0.00030600
H	-2.14413300	3.25670400	0.00074200
H	-2.05304600	5.75281600	0.00042900
H	2.06101100	5.74977300	-0.00069500
H	2.14837900	3.25351300	-0.00040400
N	0.00406100	5.86825800	-0.00014800
Au	2.64745200	-0.76410100	0.00001000
Au	-0.00056100	-0.83838700	0.00003100
Au	-2.64849300	-0.76093600	-0.00005600
Zero-point correction=			0.089580 (Hartree/Particle)
Thermal correction to Energy=			0.101319
Thermal correction to Enthalpy=			0.102263
Thermal correction to Gibbs Free Energy=			0.038742
Sum of electronic and zero-point Energies=			-654.822568
Sum of electronic and thermal Energies=			-654.810830
Sum of electronic and thermal Enthalpies=			-654.809885
Sum of electronic and thermal Free Energies=			-654.873407



C	-2.44522400	-0.91639300	-0.00007500
C	-3.18253100	-0.94789100	-1.19168000
C	-4.57234000	-0.96285000	-1.13603500
C	-4.57178600	-0.96316500	1.13692800
C	-3.18194700	-0.94824800	1.19188500
H	-1.19336600	-1.90237100	-0.00053400
H	-2.68219500	-0.94635500	-2.15287800
H	-5.14994200	-0.96897000	-2.05827200
H	-5.14892800	-0.96954700	2.05945200
H	-2.68114200	-0.94705300	2.15284200
N	-5.28159500	-0.97092700	0.00062200
Au	0.16415300	2.13537700	0.00009800
Au	-0.35893800	-0.50017800	-0.00041100
Au	2.23971800	-1.11669100	0.00017200

Freq = -890.49

Zero-point correction= 0.084098 (Hartree/Particle)

Thermal correction to Energy= 0.094904

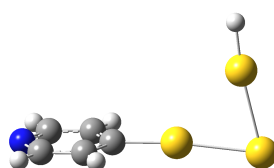
Thermal correction to Enthalpy= 0.095848

Thermal correction to Gibbs Free Energy= 0.039249

Sum of electronic and zero-point Energies= -654.756574

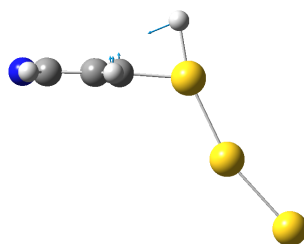


Sum of electronic and thermal Energies= -654.745767  
Sum of electronic and thermal Enthalpies= -654.744823  
Sum of electronic and thermal Free Energies= -654.801422



C	2.95102200	0.00433700	-0.00078000
C	3.68998500	0.18758200	-1.18169000
C	5.05374600	0.46818500	-1.12693100
C	5.05674200	0.41525300	1.14020700
C	3.69310900	0.13222600	1.18547700
H	-1.79506100	3.06053300	0.01321800
H	3.21027300	0.11341700	-2.15146700
H	5.61688700	0.60834500	-2.04862000
H	5.62236900	0.51196200	2.06595000
H	3.21602200	0.01277000	2.15202200
N	5.75316300	0.58486000	0.00906800
Au	-1.61466300	-1.26903800	-0.00167900
Au	0.95543800	-0.41968600	-0.00637700
Au	-1.60419600	1.49066700	0.00562200

Zero-point correction=	0.084837 (Hartree/Particle)
Thermal correction to Energy=	0.096212
Thermal correction to Enthalpy=	0.097156
Thermal correction to Gibbs Free Energy=	0.038466
Sum of electronic and zero-point Energies=	-654.822283
Sum of electronic and thermal Energies=	-654.810908
Sum of electronic and thermal Enthalpies=	-654.809964
Sum of electronic and thermal Free Energies=	-654.868654

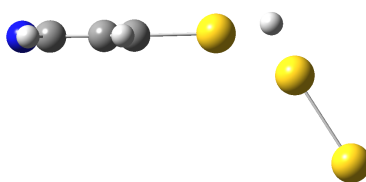


C	3.31998900	0.23241100	-0.00001100
C	3.86390100	0.69490300	1.19766300
C	4.91790700	1.60382100	1.13548600
C	4.91784600	1.60392500	-1.13547000
C	3.86383700	0.69501300	-1.19767300
H	3.02959800	-2.04430700	-0.00010700
H	3.48105500	0.37340600	2.15702200
H	5.35066800	1.98092600	2.05946100
H	5.35055700	1.98111400	-2.05943300
H	3.48093800	0.37360400	-2.15704100

N	5.45612900	2.06371600	0.00001500
Au	1.72103800	-0.97668300	-0.00002600
Au	-0.67469100	0.04589200	0.00004000
Au	-3.37782300	0.34735800	-0.00001500

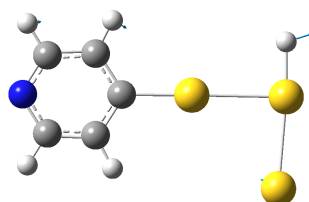
Freq = -523.87

Zero-point correction=	0.083722 (Hartree/Particle)
Thermal correction to Energy=	0.095107
Thermal correction to Enthalpy=	0.096051
Thermal correction to Gibbs Free Energy=	0.038150
Sum of electronic and zero-point Energies=	-654.745346
Sum of electronic and thermal Energies=	-654.733961
Sum of electronic and thermal Enthalpies=	-654.733017
Sum of electronic and thermal Free Energies=	-654.790918



C	-3.75818200	0.26130500	0.06024000
C	-4.32627200	1.15819600	-0.86185700
C	-5.63728500	1.60499000	-0.70813000
C	-5.91543800	0.38301300	1.18203000
C	-4.61578400	-0.11452500	1.10914200

H	-0.35378300	-1.39846800	-0.38013600
H	-3.75085900	1.51760700	-1.70851100
H	-6.06471300	2.29966600	-1.42996500
H	-6.56972300	0.08184500	1.99912800
H	-4.27925100	-0.80174700	1.87839500
N	-6.44425800	1.23469700	0.29429600
Au	-1.83224000	-0.44191500	-0.11611100
Au	1.04694800	-0.48162500	-0.12031100
Au	3.46435400	0.54253200	0.14645400
Zero-point correction=			0.085681 (Hartree/Particle)
Thermal correction to Energy=			0.096649
Thermal correction to Enthalpy=			0.097593
Thermal correction to Gibbs Free Energy=			0.040259
Sum of electronic and zero-point Energies=			-654.829292
Sum of electronic and thermal Energies=			-654.818323
Sum of electronic and thermal Enthalpies=			-654.817379
Sum of electronic and thermal Free Energies=			-654.874713

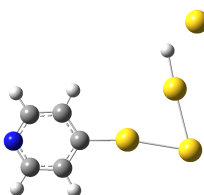


C	4.18119100	-0.70221000	0.00028700
C	3.09691700	0.19006000	0.00003400

C	3.44147700	1.55133700	-0.00014300
C	4.78088800	1.93616700	-0.00001900
C	5.48857100	-0.21910500	0.00036800
H	4.01759700	-1.77373500	0.00043900
H	-0.93958100	-2.75301400	-0.00001600
H	2.67326500	2.31587000	-0.00034100
H	5.04111000	2.99346300	-0.00012500
H	6.32465700	-0.91694700	0.00056300
Au	1.16851900	-0.43017800	-0.00016600
Au	-2.05794700	1.36510000	0.00004000
Au	-1.43621500	-1.23826800	0.00006100
N	5.81064700	1.08017600	0.00020900

Freq = -28.15

Zero-point correction=	0.085084 (Hartree/Particle)
Thermal correction to Energy=	0.095405
Thermal correction to Enthalpy=	0.096349
Thermal correction to Gibbs Free Energy=	0.040921
Sum of electronic and zero-point Energies=	-654.809312
Sum of electronic and thermal Energies=	-654.798992
Sum of electronic and thermal Enthalpies=	-654.798048
Sum of electronic and thermal Free Energies=	-654.853475



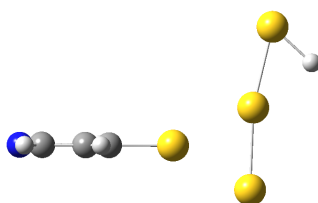
C	3.40082200	1.42210100	-0.00202600
C	4.77994900	1.15748200	-0.00526100
C	5.69867500	2.20569000	-0.00287900
C	4.04729600	3.76125700	0.00539500
C	3.05474900	2.78282800	0.00360900
H	-1.99610600	1.26541900	0.03201400
H	5.15013500	0.13822200	-0.00952600
H	6.76660600	1.99214700	-0.00530900
H	3.77097200	4.81435200	0.00951800
H	2.01495900	3.08938600	0.00651600
N	5.36084400	3.50070100	0.00229000
Au	0.49914500	-2.35379800	-0.00237800
Au	1.99728100	-0.06144900	-0.00474300
Au	-0.99604100	-0.07759700	0.01328900
Au	-3.76774400	1.17916500	-0.00670300

Zero-point correction= 0.084782 (Hartree/Particle)

Thermal correction to Energy= 0.098615

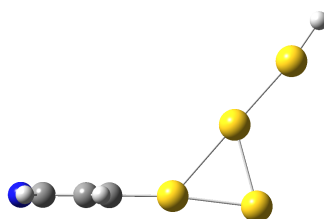
Thermal correction to Enthalpy= 0.099559

Thermal correction to Gibbs Free Energy=	0.030840
Sum of electronic and zero-point Energies=	-790.297940
Sum of electronic and thermal Energies=	-790.284107
Sum of electronic and thermal Enthalpies=	-790.283163
Sum of electronic and thermal Free Energies=	-790.351883



C	3.89134100	-1.77594100	-1.17569800
C	3.33234900	-1.25127100	0.00172000
C	4.02727000	-1.57275600	1.17978400
C	5.18209200	-2.35096600	1.13007200
C	5.05150500	-2.54609400	-1.12601300
H	3.42885600	-1.58986200	-2.13893100
H	-3.53990300	0.12090600	0.00001300
H	3.67647300	-1.21998200	2.14353300
H	5.71439500	-2.59311200	2.04892000
H	5.47738900	-2.94736600	-2.04460500
N	5.70918300	-2.84349400	0.00193800
Au	1.63000800	-0.11010400	0.00060400
Au	0.36412400	2.43787900	-0.01478400
Au	-1.18358100	0.28608300	0.00239800

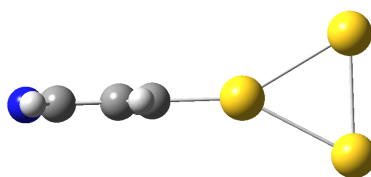
Au	-3.13496700	-1.53644000	0.01074800
Freq = -809.87			
Zero-point correction=			0.082195 (Hartree/Particle)
Thermal correction to Energy=			0.096049
Thermal correction to Enthalpy=			0.096993
Thermal correction to Gibbs Free Energy=			0.028811
Sum of electronic and zero-point Energies=			-790.266970
Sum of electronic and thermal Energies=			-790.253117
Sum of electronic and thermal Enthalpies=			-790.252172
Sum of electronic and thermal Free Energies=			-790.320355



C	4.18891400	-1.51948200	-1.16490400
C	3.67780800	-0.93857900	0.00611800
C	4.37813400	-1.24692800	1.18273100
C	5.49950100	-2.07335200	1.13685600
C	5.31789600	-2.33486300	-1.10957800
H	3.71525200	-1.34472600	-2.12431900
H	-5.10413000	-1.56229600	0.03572700

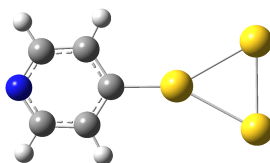


H	4.05935400	-0.84922000	2.13960400
H	6.03873700	-2.30801100	2.05318500
H	5.70917500	-2.78277200	-2.02154900
N	5.98328900	-2.62172100	0.01586100
Au	2.04037600	0.27602100	-0.00259000
Au	0.04042900	2.13214800	-0.01863600
Au	-0.92903200	-0.42485500	-0.00677500
Au	-3.61601200	-1.02283000	0.02166000
Zero-point correction=			0.084712 (Hartree/Particle)
Thermal correction to Energy=			0.098848
Thermal correction to Enthalpy=			0.099792
Thermal correction to Gibbs Free Energy=			0.029830
Sum of electronic and zero-point Energies=			-790.298578
Sum of electronic and thermal Energies=			-790.284443
Sum of electronic and thermal Enthalpies=			-790.283499
Sum of electronic and thermal Free Energies=			-790.353460



C	3.68684600	-0.00157800	-1.18384400
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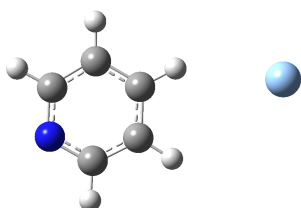
C	5.07910800	-0.00134800	-1.13383900
C	5.07908100	0.00167700	1.13389400
C	3.68681700	0.00157800	1.18386400
C	2.92846600	-0.00008800	0.00000100
H	5.65573700	0.00298700	2.05797200
H	3.19916500	0.00282200	2.15253900
H	3.19921800	-0.00293500	-2.15253000
H	5.65578700	-0.00252300	-2.05790400
N	5.79223100	0.00024800	0.00003600
Au	-1.58985700	-1.38088900	0.00031300
Au	0.88804900	-0.00030500	-0.00002400
Au	-1.58955100	1.38115000	-0.00029900
Zero-point correction=			0.078279 (Hartree/Particle)
Thermal correction to Energy=			0.089041
Thermal correction to Enthalpy=			0.089985
Thermal correction to Gibbs Free Energy=			0.031980
Sum of electronic and zero-point Energies=			-654.209902
Sum of electronic and thermal Energies=			-654.199140
Sum of electronic and thermal Enthalpies=			-654.198196
Sum of electronic and thermal Free Energies=			-654.256201



C	0.00011500	3.69163800	1.18387600
C	0.00008400	5.08434200	1.13393800
C	0.00008400	5.08434200	-1.13393800
C	0.00011500	3.69163800	-1.18387600
C	0.00015500	2.93436500	0.00000000
H	0.00008200	5.66100700	-2.05791100
H	0.00012600	3.20310200	-2.15190900
H	0.00012600	3.20310200	2.15190900
N	0.00011500	5.79692500	0.00000000
H	0.00008200	5.66100700	2.05791100
Au	-0.00022600	0.89002500	0.00000000
Au	0.00008400	-1.59200400	1.38160600
Au	0.00008400	-1.59200400	-1.38160600
Zero-point correction=			0.078315 (Hartree/Particle)
Thermal correction to Energy=			0.089077
Thermal correction to Enthalpy=			0.090021
Thermal correction to Gibbs Free Energy=			0.031876
Sum of electronic and zero-point Energies=			-654.209651
Sum of electronic and thermal Energies=			-654.198889

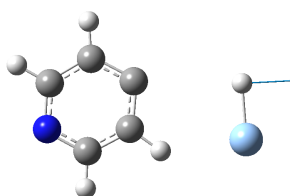
Sum of electronic and thermal Enthalpies= -654.197944

Sum of electronic and thermal Free Energies= -654.256089



C	1.43280000	0.45589800	0.00014300
C	2.50311200	1.34648400	0.00003600
C	3.80107100	0.83773500	-0.00005600
C	3.04633900	-1.31513900	-0.00002500
C	1.71504400	-0.90694800	0.00011800
H	0.39437400	0.78535500	0.00023200
H	2.33726700	2.41877800	0.00003000
H	4.65565000	1.51131400	-0.00016900
H	3.29645600	-2.37370100	-0.00001500
H	0.90074200	-1.62420600	0.00019500
N	4.08669600	-0.46967700	-0.00010100
Ag	-2.45067100	0.00131900	-0.00001800
Zero-point correction=			0.088328 (Hartree/Particle)
Thermal correction to Energy=			0.095126
Thermal correction to Enthalpy=			0.096070

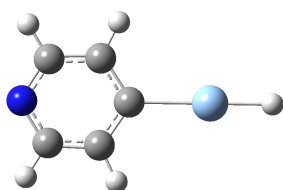
Thermal correction to Gibbs Free Energy=	0.052861
Sum of electronic and zero-point Energies=	-394.079873
Sum of electronic and thermal Energies=	-394.073076
Sum of electronic and thermal Enthalpies=	-394.072131
Sum of electronic and thermal Free Energies=	-394.115341



C	-1.39086100	0.96647000	0.00015800
C	-2.74533300	1.34765400	0.00000600
C	-3.77381700	0.40092700	-0.00011600
C	-2.28595300	-1.31026700	0.00005500
C	-1.21312400	-0.41635800	0.00017300
H	1.70778600	1.56270500	0.00012800
H	-3.03584100	2.40115900	-0.00002000
H	-4.81974700	0.71913200	-0.00024000
H	-2.11161000	-2.38988100	0.00007600
H	-0.20140200	-0.86201400	0.00027000
N	-3.57054100	-0.92525400	-0.00009100
Ag	2.16827900	-0.01882700	-0.00002600

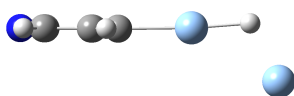
Freq = -357.73

Zero-point correction=	0.077690 (Hartree/Particle)
Thermal correction to Energy=	0.085215
Thermal correction to Enthalpy=	0.086159
Thermal correction to Gibbs Free Energy=	0.041402
Sum of electronic and zero-point Energies=	-393.986817
Sum of electronic and thermal Energies=	-393.979292
Sum of electronic and thermal Enthalpies=	-393.978348
Sum of electronic and thermal Free Energies=	-394.023104



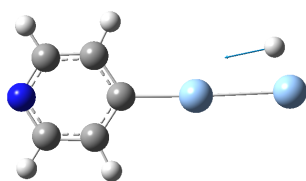
C	-0.50232400	0.00000300	-0.00012300
C	-1.28528500	1.17402800	-0.00004900
C	-2.67906800	1.13253000	-0.00001900
C	-2.67906400	-1.13253200	-0.00001900
C	-1.28528000	-1.17402500	-0.00004900
H	3.36911600	-0.00000200	0.00045500
H	-0.80885000	2.15263600	0.00005700
H	-3.25691100	2.05801500	0.00013200
H	-3.25690400	-2.05801900	0.00013200

H	-0.80884200	-2.15263200	0.00005700
N	-3.39684300	-0.00000300	0.00009900
Ag	1.68354100	0.00000000	0.00000100
Zero-point correction=			0.081759 (Hartree/Particle)
Thermal correction to Energy=			0.088448
Thermal correction to Enthalpy=			0.089392
Thermal correction to Gibbs Free Energy=			0.049153
Sum of electronic and zero-point Energies=			-394.076360
Sum of electronic and thermal Energies=			-394.069672
Sum of electronic and thermal Enthalpies=			-394.068727
Sum of electronic and thermal Free Energies=			-394.108966



C	-2.02806300	-0.00017800	0.06715700
C	-2.78417900	-1.17641600	-0.10640900
C	-4.14324200	-1.13205400	-0.41518100
C	-4.14261100	1.13425800	-0.41190100
C	-2.78351700	1.17695600	-0.10302900
H	1.72777000	-0.00265000	1.10280600

H	-2.31843500	-2.15359800	-0.00296200
H	-4.70702200	-2.05619100	-0.54512600
H	-4.70585900	2.05907500	-0.53922500
H	-2.31722300	2.15360200	0.00321900
N	-4.84037400	0.00152700	-0.57117200
Ag	2.93825800	0.00088700	-0.37348000
Ag	0.07223200	-0.00144700	0.58189900
Zero-point correction=			0.082578 (Hartree/Particle)
Thermal correction to Energy=			0.090713
Thermal correction to Enthalpy=			0.091657
Thermal correction to Gibbs Free Energy=			0.044635
Sum of electronic and zero-point Energies=			-539.865347
Sum of electronic and thermal Energies=			-539.857212
Sum of electronic and thermal Enthalpies=			-539.856268
Sum of electronic and thermal Free Energies=			-539.903290



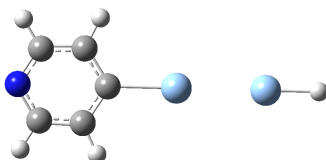
C	2.01545000	-0.00576200	0.00160200
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C	2.76212600	1.18650900	-0.02912400
C	4.15672400	1.16691200	-0.02013200
C	4.19795700	-1.09859300	0.04995500
C	2.80510900	-1.16941600	0.04156100
H	-2.42970400	1.30411500	1.09752900
H	2.26516100	2.15254000	-0.05989300
H	4.71764800	2.10139200	-0.04525400
H	4.79266200	-2.01173000	0.08276500
H	2.34298100	-2.15291200	0.06586800
N	4.89138400	0.04729600	0.01921200
Ag	-2.86416600	0.00175200	-0.00460200
Ag	-0.14759200	-0.04861100	-0.02813600

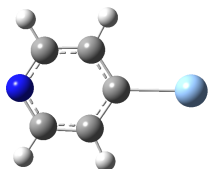
Freq = -404.67

Zero-point correction=	0.079982 (Hartree/Particle)
Thermal correction to Energy=	0.089223
Thermal correction to Enthalpy=	0.090167
Thermal correction to Gibbs Free Energy=	0.040290
Sum of electronic and zero-point Energies=	-539.840643
Sum of electronic and thermal Energies=	-539.831402
Sum of electronic and thermal Enthalpies=	-539.830457
Sum of electronic and thermal Free Energies=	-539.880335



C	-2.10250800	-0.00077400	0.00125200
C	-2.86707600	1.17885000	-0.00011400
C	-4.26148700	1.13461500	-0.00268800
C	-4.26302400	-1.13311200	-0.00258100
C	-2.86877600	-1.17920900	-0.00008500
H	4.65068700	0.00058700	-0.00550300
H	-2.38627500	2.15395900	0.00073000
H	-4.83941800	2.05902900	-0.00334600
H	-4.84202100	-2.05690500	-0.00398600
H	-2.38920700	-2.15500700	0.00082000
N	-4.97556900	0.00120400	-0.00394100
Ag	2.94532200	0.00027200	-0.00202800
Ag	0.09324100	-0.00053400	0.00339300
Zero-point correction=			0.080709 (Hartree/Particle)
Thermal correction to Energy=			0.090529
Thermal correction to Enthalpy=			0.091473
Thermal correction to Gibbs Free Energy=			0.040035
Sum of electronic and zero-point Energies=			-539.856259
Sum of electronic and thermal Energies=			-539.846439
Sum of electronic and thermal Enthalpies=			-539.845495

Sum of electronic and thermal Free Energies= -539.896933



C	0.00000000	0.00000000	-0.49637900
C	0.00000000	1.17674200	-1.26668900
C	0.00000000	1.13372500	-2.66068000
C	0.00000000	-1.13372500	-2.66068000
C	0.00000000	-1.17674200	-1.26668900
H	0.00000000	2.15356500	-0.78574300
H	0.00000000	2.05890900	-3.23928300
H	0.00000000	-2.05890900	-3.23928300
H	0.00000000	-2.15356500	-0.78574300
N	0.00000000	0.00000000	-3.37673400
Ag	0.00000000	0.00000000	1.74029600

Zero-point correction= 0.075787 (Hartree/Particle)

Thermal correction to Energy= 0.082083

Thermal correction to Enthalpy= 0.083027

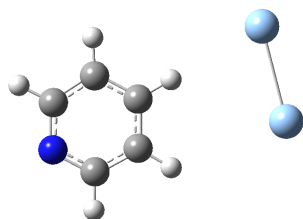
Thermal correction to Gibbs Free Energy= 0.043167

Sum of electronic and zero-point Energies= -393.459333

Sum of electronic and thermal Energies= -393.453038

Sum of electronic and thermal Enthalpies= -393.452093

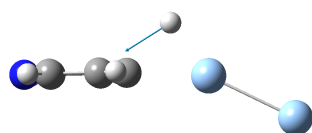
Sum of electronic and thermal Free Energies= -393.491953



C	2.28261400	-0.37881100	0.00193200
C	3.27748100	-1.35323400	-0.00926500
C	4.61168400	-0.95063500	-0.00985100
C	4.03390900	1.25647000	0.01025700
C	2.67289500	0.95816700	0.01196600
H	1.22855500	-0.64479300	0.00218100
H	3.02197700	-2.40707900	-0.01730800
H	5.40891500	-1.69055100	-0.01855900
H	4.36832700	2.29111500	0.01777900
H	1.92708800	1.74561600	0.02034300
N	5.00121900	0.32971200	-0.00042300
Ag	-1.56916600	1.40179300	-0.00355100
Ag	-1.66987500	-1.37613400	0.00287700

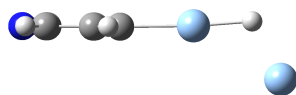
Zero-point correction= 0.088583 (Hartree/Particle)

Thermal correction to Energy=	0.097965
Thermal correction to Enthalpy=	0.098909
Thermal correction to Gibbs Free Energy=	0.044546
Sum of electronic and zero-point Energies=	-539.885401
Sum of electronic and thermal Energies=	-539.876018
Sum of electronic and thermal Enthalpies=	-539.875074
Sum of electronic and thermal Free Energies=	-539.929437



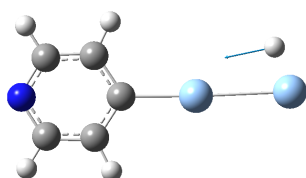
C	2.02908200	-0.00015000	0.09713600
C	2.76834900	1.18848200	-0.04222000
C	4.13012400	1.13661000	-0.31996500
C	4.13065700	-1.13544000	-0.32129400
C	2.76891400	-1.18827000	-0.04358400
H	1.07057600	-0.00142000	1.66963600
H	2.29013300	2.15871900	0.06491300
H	4.69479100	2.06103500	-0.44337300
H	4.69575500	-2.05945500	-0.44578900
H	2.29115800	-2.15885400	0.06246300
N	4.83296300	0.00083500	-0.46302600
Ag	-2.82536700	0.00045800	-0.29019800

Ag	-0.23497200	-0.00074000	0.42026000
Freq = -713.13			
Zero-point correction=			0.079581 (Hartree/Particle)
Thermal correction to Energy=			0.088605
Thermal correction to Enthalpy=			0.089550
Thermal correction to Gibbs Free Energy=			0.040116
Sum of electronic and zero-point Energies=			-539.816879
Sum of electronic and thermal Energies=			-539.807855
Sum of electronic and thermal Enthalpies=			-539.806911
Sum of electronic and thermal Free Energies=			-539.856344



C	-2.02806300	-0.00017800	0.06715700
C	-2.78417900	-1.17641600	-0.10640900
C	-4.14324200	-1.13205400	-0.41518100
C	-4.14261100	1.13425800	-0.41190100
C	-2.78351700	1.17695600	-0.10302900
H	1.72777000	-0.00265000	1.10280600
H	-2.31843500	-2.15359800	-0.00296200
H	-4.70702200	-2.05619100	-0.54512600

H	-4.70585900	2.05907500	-0.53922500
H	-2.31722300	2.15360200	0.00321900
N	-4.84037400	0.00152700	-0.57117200
Ag	2.93825800	0.00088700	-0.37348000
Ag	0.07223200	-0.00144700	0.58189900
Zero-point correction=			0.082578 (Hartree/Particle)
Thermal correction to Energy=			0.090713
Thermal correction to Enthalpy=			0.091657
Thermal correction to Gibbs Free Energy=			0.044635
Sum of electronic and zero-point Energies=			-539.865347
Sum of electronic and thermal Energies=			-539.857212
Sum of electronic and thermal Enthalpies=			-539.856268
Sum of electronic and thermal Free Energies=			-539.903290



C	2.01545000	-0.00576200	0.00160200
C	2.76212600	1.18650900	-0.02912400
C	4.15672400	1.16691200	-0.02013200

C	4.19795700	-1.09859300	0.04995500
C	2.80510900	-1.16941600	0.04156100
H	-2.42970400	1.30411500	1.09752900
H	2.26516100	2.15254000	-0.05989300
H	4.71764800	2.10139200	-0.04525400
H	4.79266200	-2.01173000	0.08276500
H	2.34298100	-2.15291200	0.06586800
N	4.89138400	0.04729600	0.01921200
Ag	-2.86416600	0.00175200	-0.00460200
Ag	-0.14759200	-0.04861100	-0.02813600

Freq = -404.67

Zero-point correction= 0.079982 (Hartree/Particle)

Thermal correction to Energy= 0.089223

Thermal correction to Enthalpy= 0.090167

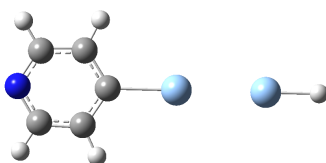
Thermal correction to Gibbs Free Energy= 0.040290

Sum of electronic and zero-point Energies= -539.840643

Sum of electronic and thermal Energies= -539.831402

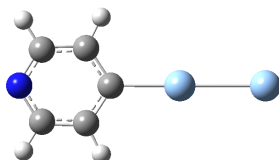
Sum of electronic and thermal Enthalpies= -539.830457

Sum of electronic and thermal Free Energies= -539.880335



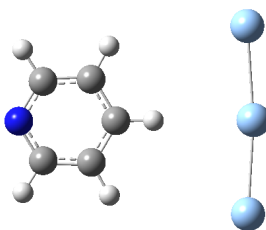


C	-2.10250800	-0.00077400	0.00125200
C	-2.86707600	1.17885000	-0.00011400
C	-4.26148700	1.13461500	-0.00268800
C	-4.26302400	-1.13311200	-0.00258100
C	-2.86877600	-1.17920900	-0.00008500
H	4.65068700	0.00058700	-0.00550300
H	-2.38627500	2.15395900	0.00073000
H	-4.83941800	2.05902900	-0.00334600
H	-4.84202100	-2.05690500	-0.00398600
H	-2.38920700	-2.15500700	0.00082000
N	-4.97556900	0.00120400	-0.00394100
Ag	2.94532200	0.00027200	-0.00202800
Ag	0.09324100	-0.00053400	0.00339300
Zero-point correction=			0.080709 (Hartree/Particle)
Thermal correction to Energy=			0.090529
Thermal correction to Enthalpy=			0.091473
Thermal correction to Gibbs Free Energy=			0.040035
Sum of electronic and zero-point Energies=			-539.856259
Sum of electronic and thermal Energies=			-539.846439
Sum of electronic and thermal Enthalpies=			-539.845495
Sum of electronic and thermal Free Energies=			-539.896933



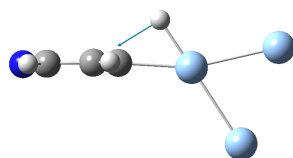
C	2.00556100	0.00000000	-0.00001600
C	2.77845200	-1.17698000	-0.00000100
C	4.17239000	-1.13310200	0.00002600
C	4.17238800	1.13310300	0.00002600
C	2.77845100	1.17698000	-0.00000100
H	2.29990200	-2.15366000	-0.00001100
H	4.75063500	-2.05804200	0.00003700
H	4.75063300	2.05804500	0.00003700
H	2.29990000	2.15366000	-0.00001100
N	4.88759300	0.00000100	0.00004100
Ag	-2.88108000	0.00000100	0.00002300
Ag	-0.17759400	-0.00000100	-0.00003400
Zero-point correction=			0.076820 (Hartree/Particle)
Thermal correction to Energy=			0.085324
Thermal correction to Enthalpy=			0.086268
Thermal correction to Gibbs Free Energy=			0.038761
Sum of electronic and zero-point Energies=			-539.300747

Sum of electronic and thermal Energies= -539.292243  
Sum of electronic and thermal Enthalpies= -539.291299  
Sum of electronic and thermal Free Energies= -539.338806



C	2.66023200	-0.00634600	-0.00014100
C	3.37098700	-1.20312100	0.00022800
C	4.76296500	-1.15105300	0.00057000
C	4.76799700	1.12910100	-0.00025000
C	3.37625700	1.18727800	-0.00070000
H	1.57466900	-0.00377800	-0.00077100
H	2.84841500	-2.15296000	0.00049600
H	5.34604500	-2.06944100	0.00100700
H	5.35512400	2.04490500	-0.00046800
H	2.85775500	2.13935300	-0.00125700
N	5.46708800	-0.01252200	0.00035700

Ag	-1.14104200	2.71189900	-0.00057300
Ag	-1.31616500	0.00305400	0.00130200
Ag	-1.15730800	-2.70656100	-0.00072300
Zero-point correction=			0.089545 (Hartree/Particle)
Thermal correction to Energy=			0.101284
Thermal correction to Enthalpy=			0.102229
Thermal correction to Gibbs Free Energy=			0.040303
Sum of electronic and zero-point Energies=			-685.705517
Sum of electronic and thermal Energies=			-685.693778
Sum of electronic and thermal Enthalpies=			-685.692834
Sum of electronic and thermal Free Energies=			-685.754760

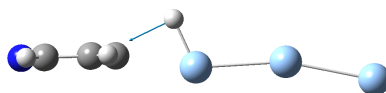


C	2.46096700	-0.25754000	-0.00032700
C	3.20601100	-0.18253700	1.18866800
C	4.58390000	-0.00035500	1.13650300
C	4.58496700	0.00146500	-1.13475600
C	3.20711800	-0.18059600	-1.18850500
H	1.35665600	-1.66233400	-0.00140100
H	2.72041300	-0.25881300	2.15684100
H	5.15507200	0.07829200	2.06099600

H	5.15700600	0.08160400	-2.05858500
H	2.72243500	-0.25522400	-2.15726300
N	5.29338600	0.09576700	0.00128000
Ag	-1.45839400	1.72051100	0.00044300
Ag	0.26635400	-0.36684300	-0.00117300
Ag	-2.26377000	-1.24593300	0.00032500

Freq = -891.75

Zero-point correction=	0.081952 (Hartree/Particle)
Thermal correction to Energy=	0.092962
Thermal correction to Enthalpy=	0.093906
Thermal correction to Gibbs Free Energy=	0.038616
Sum of electronic and zero-point Energies=	-685.621347
Sum of electronic and thermal Energies=	-685.610338
Sum of electronic and thermal Enthalpies=	-685.609393
Sum of electronic and thermal Free Energies=	-685.664683



C	3.07098300	0.14831000	-0.00007600
C	3.70605000	-0.22296600	-1.19491200
C	4.90527300	-0.92360000	-1.13430000
C	4.90549200	-0.92281000	1.13453700

C	3.70628700	-0.22212200	1.19489500
H	2.72843700	2.07559900	-0.00070900
H	3.28349700	0.02439100	-2.16128500
H	5.39458300	-1.22176400	-2.06050800
H	5.39497900	-1.22033400	2.06085800
H	3.28394000	0.02594000	2.16117600
N	5.52602800	-1.28247100	0.00018400
Ag	1.16992100	1.05283600	-0.00020100
Ag	-1.13396700	-0.35206900	0.00018800
Ag	-3.87706300	-0.22943500	-0.00002300

Freq = -907.35

Zero-point correction= 0.080968 (Hartree/Particle)

Thermal correction to Energy= 0.092760

Thermal correction to Enthalpy= 0.093704

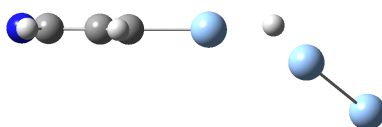
Thermal correction to Gibbs Free Energy= 0.034868

Sum of electronic and zero-point Energies= -685.606673

Sum of electronic and thermal Energies= -685.594880

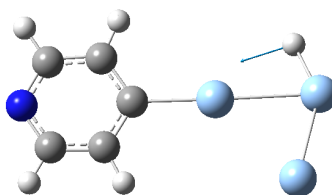
Sum of electronic and thermal Enthalpies= -685.593936

Sum of electronic and thermal Free Energies= -685.652772



C	3.36565900	0.10961900	0.01173400
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C	4.44144400	-0.55991300	0.62629900
C	5.70732000	0.01905700	0.70944300
C	5.00098200	1.88780500	-0.36197500
C	3.70764600	1.38143000	-0.48690000
H	-0.13235400	-1.58340000	-0.34882400
H	4.30671000	-1.55074900	1.05316100
H	6.52575100	-0.51749700	1.18962700
H	5.24367600	2.87506700	-0.75483800
H	2.96424900	2.00028200	-0.98270800
N	6.00966200	1.23124500	0.22645900
Ag	-3.94338700	0.69684800	0.17186000
Ag	1.39338200	-0.74014100	-0.16414500
Ag	-1.58433500	-0.52841800	-0.10842200
Zero-point correction=			0.083910 (Hartree/Particle)
Thermal correction to Energy=			0.095183
Thermal correction to Enthalpy=			0.096127
Thermal correction to Gibbs Free Energy=			0.038555
Sum of electronic and zero-point Energies=			-685.701526
Sum of electronic and thermal Energies=			-685.690254
Sum of electronic and thermal Enthalpies=			-685.689310
Sum of electronic and thermal Free Energies=			-685.746881



Freq = -262.62

C	3.66176600	-0.99221300	0.34808800
C	2.66838200	-0.06364800	-0.01242400
C	3.17056000	1.20549200	-0.35293700
C	4.53924300	1.47173900	-0.32341000
C	5.01152300	-0.63996900	0.35303200
H	3.39714400	-2.00737900	0.63108600
H	-1.09721800	-2.58000700	-0.18171100
H	2.49813700	2.00728600	-0.64513600
H	4.91040500	2.46077800	-0.59197900
H	5.76736000	-1.37254800	0.63650900
Ag	0.56253400	-0.52768100	-0.04119300
Ag	-2.07154700	1.52271200	0.11290400
Ag	-2.06722900	-1.17407500	-0.07355900
N	5.47124300	0.57407600	0.02342500

Zero-point correction= 0.081564 (Hartree/Particle)

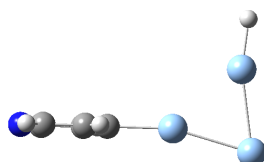
Thermal correction to Energy= 0.092826

Thermal correction to Enthalpy= 0.093771

Thermal correction to Gibbs Free Energy= 0.036758



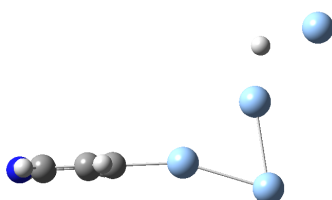
Sum of electronic and zero-point Energies=	-685.676680
Sum of electronic and thermal Energies=	-685.665418
Sum of electronic and thermal Enthalpies=	-685.664474
Sum of electronic and thermal Free Energies=	-685.721486



C	-2.63074300	-0.05882300	-0.00000200
C	-3.39399900	0.02231100	1.17879100
C	-4.78044500	0.16786300	1.13373800
C	-4.78046200	0.16802400	-1.13367900
C	-3.39401600	0.02248000	-1.17877200
H	2.30023100	3.11383700	0.00021600
H	-2.91732400	-0.02570300	2.15448800
H	-5.35538700	0.22926100	2.05780000
H	-5.35541700	0.22955500	-2.05772300
H	-2.91735500	-0.02539400	-2.15448300
N	-5.48998600	0.24119700	0.00004000
Ag	2.07040100	-1.30710400	-0.00008400
Ag	-0.47396800	-0.31198900	-0.00003000
Ag	1.94725100	1.46715500	0.00009200

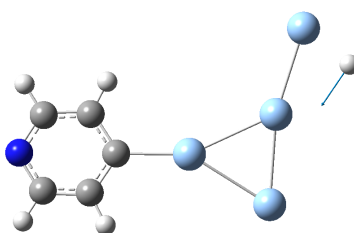
Zero-point correction= 0.082312 (Hartree/Particle)

Thermal correction to Energy=	0.094099
Thermal correction to Enthalpy=	0.095044
Thermal correction to Gibbs Free Energy=	0.037453
Sum of electronic and zero-point Energies=	-685.681311
Sum of electronic and thermal Energies=	-685.669523
Sum of electronic and thermal Enthalpies=	-685.668579
Sum of electronic and thermal Free Energies=	-685.726170



C	4.11008700	-1.13054500	-1.15824500
C	3.51136600	-0.59752900	-0.00272100
C	4.28983400	-0.73722300	1.16025300
C	5.53974700	-1.35519900	1.12209800
C	5.36727100	-1.73264300	-1.10732500
H	3.60411000	-1.08547700	-2.11903400
H	-2.27541200	-1.67641900	0.14814600
H	3.93267700	-0.36670900	2.11762300
H	6.12960600	-1.45543400	2.03308300
H	5.81675700	-2.13999400	-2.01276000
N	6.09467400	-1.85493100	0.01046800

Ag	1.56893400	0.36896700	-0.01401900
Ag	-0.36135500	2.34106000	-0.05899800
Ag	-1.28715000	-0.22984600	0.06306200
Ag	-4.10724300	-1.35193900	0.00304700
Zero-point correction=			0.083026 (Hartree/Particle)
Thermal correction to Energy=			0.097093
Thermal correction to Enthalpy=			0.098037
Thermal correction to Gibbs Free Energy=			0.030378
Sum of electronic and zero-point Energies=			-831.475356
Sum of electronic and thermal Energies=			-831.461289
Sum of electronic and thermal Enthalpies=			-831.460345
Sum of electronic and thermal Free Energies=			-831.528004



C	3.45111700	-2.07541000	-0.31484200
C	3.24131200	-0.72280700	0.00943000
C	4.41952600	-0.02606600	0.33373000
C	5.66191400	-0.66016400	0.32042800
C	4.73042700	-2.63117300	-0.30335700
H	2.61648800	-2.71847700	-0.58141300

H	-4.17132000	-0.23571400	0.03731300
H	4.38696500	1.02670200	0.60295200
H	6.56430300	-0.10370500	0.57433900
H	4.87394400	-3.68128400	-0.55764000
N	5.84126300	-1.95001500	0.00770000
Ag	1.27689100	0.20879500	0.00050900
Ag	-0.24501200	2.58207100	-0.06314000
Ag	-1.55999300	0.20133400	0.00856400
Ag	-3.39071700	-1.79951200	0.04551900

Freq = -450.80

Zero-point correction= 0.081133 (Hartree/Particle)

Thermal correction to Energy= 0.095119

Thermal correction to Enthalpy= 0.096063

Thermal correction to Gibbs Free Energy= 0.028810

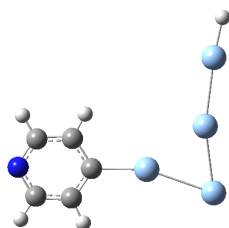
Sum of electronic and zero-point Energies= -831.458575

Sum of electronic and thermal Energies= -831.444590

Sum of electronic and thermal Enthalpies= -831.443645

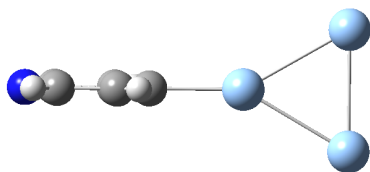
Sum of electronic and thermal Free Energies= -831.510899

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C	3.11959000	-2.18607800	-0.17382800
C	3.16334300	-0.79182900	0.00036100
C	4.45823200	-0.27355400	0.17522000
C	5.57467600	-1.10998700	0.16858900
C	4.28828400	-2.94772800	-0.16659400
H	2.17359800	-2.70046500	-0.31687700
H	-4.57229200	-3.06141800	0.01477500
H	4.61849900	0.79158700	0.31988100
H	6.57229700	-0.69294800	0.30544200
H	4.23830200	-4.02760500	-0.30240100
N	5.51499800	-2.43686800	0.00078500
Ag	1.38569200	0.44447100	-0.00478800
Ag	-0.23796000	2.70139100	-0.03361100
Ag	-1.51097500	0.24562400	0.01807700
Ag	-3.36569600	-1.88927300	0.01928300
Zero-point correction=			0.082254 (Hartree/Particle)
Thermal correction to Energy=			0.096772
Thermal correction to Enthalpy=			0.097716
Thermal correction to Gibbs Free Energy=			0.029050
Sum of electronic and zero-point Energies=			-831.475447
Sum of electronic and thermal Energies=			-831.460928
Sum of electronic and thermal Enthalpies=			-831.459984

Sum of electronic and thermal Free Energies= -831.528650



C	-3.37823700	-0.00023900	1.17850400
C	-4.77218200	0.00014100	1.13368700
C	-4.77224700	0.00016500	-1.13339900
C	-3.37830400	-0.00021000	-1.17829500
C	-2.60917700	-0.00041300	0.00008300
H	-5.35038200	0.00035800	-2.05763100
H	-2.89949200	-0.00036700	-2.15421100
H	-2.89937000	-0.00042200	2.15439300
H	-5.35026500	0.00030600	2.05795200
N	-5.48633900	0.00039000	0.00016400
Ag	2.00862800	1.40893200	-0.00003400
Ag	2.00875000	-1.40877700	-0.00009400
Ag	-0.43514800	-0.00014000	0.00001900

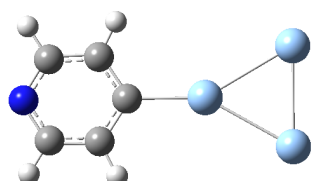
Zero-point correction= 0.077412 (Hartree/Particle)

Thermal correction to Energy= 0.088337

Thermal correction to Enthalpy= 0.089281

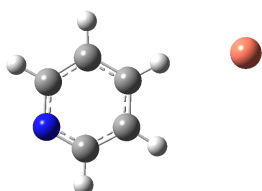
Thermal correction to Gibbs Free Energy= 0.032409

Sum of electronic and zero-point Energies=	-685.095457
Sum of electronic and thermal Energies=	-685.084532
Sum of electronic and thermal Enthalpies=	-685.083588
Sum of electronic and thermal Free Energies=	-685.140460



C	-3.37726800	1.17863700	-0.00013500
C	-4.77140600	1.13367900	0.00026200
C	-4.77140600	-1.13367900	0.00026100
C	-3.37726800	-1.17863700	-0.00013600
C	-2.60897100	0.00000000	-0.00031700
H	-5.34957300	-2.05786800	0.00042500
H	-2.89733700	-2.15384600	-0.00032700
H	-2.89733700	2.15384600	-0.00032500
N	-5.48523600	0.00000000	0.00049300
H	-5.34957300	2.05786800	0.00042700
Ag	-0.43453300	0.00000000	-0.00028500
Ag	2.00799400	1.40961500	0.00010700
Ag	2.00799400	-1.40961500	0.00010800
Zero-point correction=			0.077408 (Hartree/Particle)

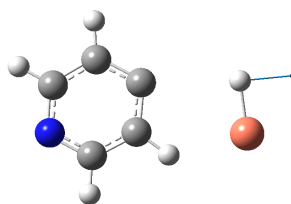
Thermal correction to Energy=	0.088343
Thermal correction to Enthalpy=	0.089288
Thermal correction to Gibbs Free Energy=	0.032264
Sum of electronic and zero-point Energies=	-685.095524
Sum of electronic and thermal Energies=	-685.084589
Sum of electronic and thermal Enthalpies=	-685.083645
Sum of electronic and thermal Free Energies=	-685.140668



C	-1.23624800	-0.00009200	0.14160800
C	-2.00388000	-1.17627900	0.00113100
C	-3.37458100	-1.13308400	-0.24753400
C	-3.37441100	1.13328200	-0.24742300
C	-2.00370400	1.17624700	0.00132600
H	2.20110500	0.00039100	1.03902200
H	-1.53486000	-2.15404600	0.08580500
H	-3.94306900	-2.05764100	-0.35100600
H	-3.94277400	2.05791100	-0.35060900
H	-1.53456700	2.15393400	0.08620300
N	-4.07931400	0.00016300	-0.37396600
Cu	3.07897600	0.00007900	-0.39403200

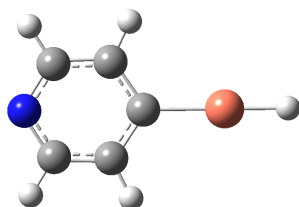


Cu	0.68882700	-0.00015300	0.53933200
Zero-point correction=			0.087978 (Hartree/Particle)
Thermal correction to Energy=			0.094800
Thermal correction to Enthalpy=			0.095744
Thermal correction to Gibbs Free Energy=			0.052970
Sum of electronic and zero-point Energies=			-444.436107
Sum of electronic and thermal Energies=			-444.429285
Sum of electronic and thermal Enthalpies=			-444.428341
Sum of electronic and thermal Free Energies=			-444.471115



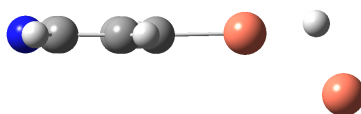
C	-0.63611600	0.90006700	0.24063900
C	-1.95034500	1.35721300	0.03165200
C	-3.01396400	0.46998100	-0.15595500
C	-1.64271400	-1.32289700	0.06471700
C	-0.53836100	-0.48937100	0.24829400
H	2.05570700	1.40142700	0.05554100
H	-2.17976400	2.42543000	0.00609000
H	-4.02538800	0.84625100	-0.33062200
H	-1.53079800	-2.41050300	0.08280200

H	0.43862000	-0.99237100	0.39855600
N	-2.88657400	-0.86581200	-0.14261100
Cu	2.48747000	-0.02412100	-0.06173000
Freq = -430.25			
Zero-point correction=			0.078287 (Hartree/Particle)
Thermal correction to Energy=			0.085561
Thermal correction to Enthalpy=			0.086505
Thermal correction to Gibbs Free Energy=			0.043905
Sum of electronic and zero-point Energies=			-444.362276
Sum of electronic and thermal Energies=			-444.355002
Sum of electronic and thermal Enthalpies=			-444.354058
Sum of electronic and thermal Free Energies=			-444.396658



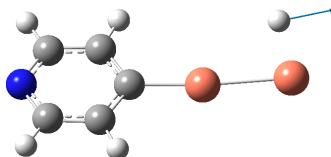
C	0.01308300	-0.00145100	-0.00028100
C	-0.77366800	1.17320300	0.00001500
C	-2.16685000	1.13324200	0.00003000
C	-2.16900800	-1.13183800	0.00009700
C	-0.77582000	-1.17448000	-0.00003900
H	3.54750700	0.00108600	0.00048700
H	-0.29687800	2.15209900	-0.00002900

H	-2.74394200	2.05929700	0.00011900
H	-2.74773800	-2.05688600	0.00017700
H	-0.30096000	-2.15433300	-0.00011600
N	-2.88674200	0.00132300	0.00000800
Cu	1.99940600	-0.00008900	0.00001300
Zero-point correction=			0.081817 (Hartree/Particle)
Thermal correction to Energy=			0.088435
Thermal correction to Enthalpy=			0.089380
Thermal correction to Gibbs Free Energy=			0.050012
Sum of electronic and zero-point Energies=			-444.463086
Sum of electronic and thermal Energies=			-444.456468
Sum of electronic and thermal Enthalpies=			-444.455524
Sum of electronic and thermal Free Energies=			-444.494891



C	-1.23624800	-0.00009200	0.14160800
C	-2.00388000	-1.17627900	0.00113100
C	-3.37458100	-1.13308400	-0.24753400
C	-3.37441100	1.13328200	-0.24742300
C	-2.00370400	1.17624700	0.00132600
H	2.20110500	0.00039100	1.03902200

H	-1.53486000	-2.15404600	0.08580500
H	-3.94306900	-2.05764100	-0.35100600
H	-3.94277400	2.05791100	-0.35060900
H	-1.53456700	2.15393400	0.08620300
N	-4.07931400	0.00016300	-0.37396600
Cu	3.07897600	0.00007900	-0.39403200
Cu	0.68882700	-0.00015300	0.53933200
Zero-point correction=			0.083546 (Hartree/Particle)
Thermal correction to Energy=			0.092281
Thermal correction to Enthalpy=			0.093225
Thermal correction to Gibbs Free Energy=			0.045557
Sum of electronic and zero-point Energies=			-640.624627
Sum of electronic and thermal Energies=			-640.615892
Sum of electronic and thermal Enthalpies=			-640.614948
Sum of electronic and thermal Free Energies=			-640.662616



C	-1.24938000	-0.02422000	-0.01203100
C	-2.06282500	-1.17513300	0.02735200
C	-3.45369800	-1.08458400	0.04510500

C	-3.37929300	1.18034500	-0.01029600
C	-1.98534500	1.17867700	-0.02843100
H	2.80003700	1.35234300	0.77127200
H	-1.61553100	-2.16618400	0.04165400
H	-4.06167000	-1.98926700	0.07580300
H	-3.92649200	2.12337100	-0.02474400
H	-1.47461500	2.13811500	-0.05543000
N	-4.13170000	0.07158600	0.02638400
Cu	3.08325500	0.00981900	0.00337300
Cu	0.70927700	-0.09292200	-0.04211200

Freq = -416.91

Zero-point correction= 0.080789 (Hartree/Particle)

Thermal correction to Energy= 0.089705

Thermal correction to Enthalpy= 0.090649

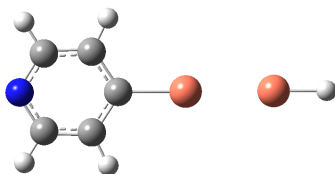
Thermal correction to Gibbs Free Energy= 0.043059

Sum of electronic and zero-point Energies= -640.601073

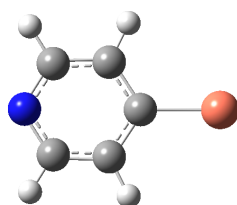
Sum of electronic and thermal Energies= -640.592157

Sum of electronic and thermal Enthalpies= -640.591213

Sum of electronic and thermal Free Energies= -640.638803

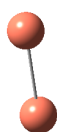
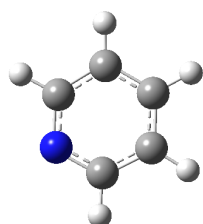


C	-1.33763400	-0.00014300	0.00030500
C	-2.10875400	1.17862200	0.00003300
C	-3.50237700	1.13418900	-0.00041800
C	-3.50281600	-1.13363800	-0.00041900
C	-2.10921000	-1.17860900	0.00003200
H	4.75986700	0.00034300	-0.00135800
H	-1.62851100	2.15434700	0.00019200
H	-4.08071600	2.05837100	-0.00060900
H	-4.08151200	-2.05759700	-0.00061100
H	-1.62934800	-2.15452000	0.00019100
N	-4.21681900	0.00041300	-0.00064800
Cu	0.63668100	-0.00046700	0.00083000
Cu	3.20961900	0.00024700	-0.00050100
Zero-point correction=			0.080705 (Hartree/Particle)
Thermal correction to Energy=			0.090617
Thermal correction to Enthalpy=			0.091561
Thermal correction to Gibbs Free Energy=			0.040730
Sum of electronic and zero-point Energies=			-640.611965
Sum of electronic and thermal Energies=			-640.602053
Sum of electronic and thermal Enthalpies=			-640.601109
Sum of electronic and thermal Free Energies=			-640.651939



C	0.00000000	0.00000000	0.05582500
C	0.00000000	1.17710700	-0.71758500
C	0.00000000	1.13350200	-2.11069600
C	0.00000000	-1.13350200	-2.11069600
C	0.00000000	-1.17710700	-0.71758500
H	0.00000000	2.15381500	-0.23636300
H	0.00000000	2.05870800	-2.69024200
H	0.00000000	-2.05870800	-2.69024200
H	0.00000000	-2.15381500	-0.23636300
N	0.00000000	0.00000000	-2.82726800
Cu	0.00000000	0.00000000	2.04305200
Zero-point correction=			0.076009 (Hartree/Particle)
Thermal correction to Energy=			0.082162
Thermal correction to Enthalpy=			0.083107
Thermal correction to Gibbs Free Energy=			0.044409
Sum of electronic and zero-point Energies=			-443.837450

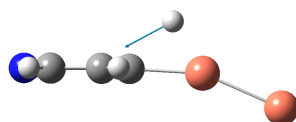
Sum of electronic and thermal Energies= -443.831297  
Sum of electronic and thermal Enthalpies= -443.830353  
Sum of electronic and thermal Free Energies= -443.869050



C	1.61247200	0.52261300	0.20177100
C	2.75563000	1.28307700	0.43558800
C	4.00379200	0.69968300	0.22455800
C	3.06395100	-1.27708600	-0.42097500
C	1.77247800	-0.78750500	-0.24121300
H	0.61185000	0.92306500	0.34910400
H	2.68274700	2.31089100	0.77446800
H	4.91359900	1.26962500	0.40111200
H	3.22031700	-2.29809300	-0.76031800
H	0.90009300	-1.40471000	-0.43239500
N	4.17391800	-0.55967300	-0.19466500
Cu	-2.05677800	1.18719200	-0.22269700
Cu	-2.10860000	-1.17090700	0.21691500



Zero-point correction=	0.088785 (Hartree/Particle)
Thermal correction to Energy=	0.097963
Thermal correction to Enthalpy=	0.098907
Thermal correction to Gibbs Free Energy=	0.047062
Sum of electronic and zero-point Energies=	-640.611557
Sum of electronic and thermal Energies=	-640.602378
Sum of electronic and thermal Enthalpies=	-640.601434
Sum of electronic and thermal Free Energies=	-640.653279

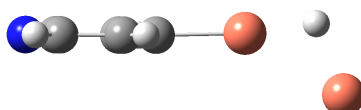


C	1.21416600	-0.00021900	0.13210300
C	1.97570600	1.18861100	0.02673200
C	3.34598500	1.13576500	-0.18579700
C	3.34647100	-1.13515600	-0.18626900
C	1.97621900	-1.18867600	0.02625100
H	0.25132300	-0.00086100	1.58898900
H	1.49613100	2.16090600	0.10877200
H	3.91380900	2.06149200	-0.28407000
H	3.91469400	-2.06059800	-0.28492500
H	1.49706600	-2.16121000	0.10792900
N	4.06036300	0.00048100	-0.29549200

Cu	-3.04487900	0.00029500	-0.26210000
Cu	-0.77053000	-0.00046800	0.32946700

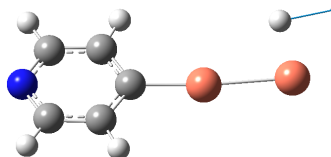
Freq = -841.69

Zero-point correction=	0.080498 (Hartree/Particle)
Thermal correction to Energy=	0.089116
Thermal correction to Enthalpy=	0.090060
Thermal correction to Gibbs Free Energy=	0.043150
Sum of electronic and zero-point Energies=	-640.572689
Sum of electronic and thermal Energies=	-640.564070
Sum of electronic and thermal Enthalpies=	-640.563126
Sum of electronic and thermal Free Energies=	-640.610037



C	-1.23624800	-0.00009200	0.14160800
C	-2.00388000	-1.17627900	0.00113100
C	-3.37458100	-1.13308400	-0.24753400
C	-3.37441100	1.13328200	-0.24742300
C	-2.00370400	1.17624700	0.00132600
H	2.20110500	0.00039100	1.03902200
H	-1.53486000	-2.15404600	0.08580500

H	-3.94306900	-2.05764100	-0.35100600
H	-3.94277400	2.05791100	-0.35060900
H	-1.53456700	2.15393400	0.08620300
N	-4.07931400	0.00016300	-0.37396600
Cu	3.07897600	0.00007900	-0.39403200
Cu	0.68882700	-0.00015300	0.53933200
Zero-point correction=			0.083546 (Hartree/Particle)
Thermal correction to Energy=			0.092281
Thermal correction to Enthalpy=			0.093225
Thermal correction to Gibbs Free Energy=			0.045557
Sum of electronic and zero-point Energies=			-640.624627
Sum of electronic and thermal Energies=			-640.615892
Sum of electronic and thermal Enthalpies=			-640.614948
Sum of electronic and thermal Free Energies=			-640.662616



C	-1.24938000	-0.02422000	-0.01203100
C	-2.06282500	-1.17513300	0.02735200
C	-3.45369800	-1.08458400	0.04510500

C	-3.37929300	1.18034500	-0.01029600
C	-1.98534500	1.17867700	-0.02843100
H	2.80003700	1.35234300	0.77127200
H	-1.61553100	-2.16618400	0.04165400
H	-4.06167000	-1.98926700	0.07580300
H	-3.92649200	2.12337100	-0.02474400
H	-1.47461500	2.13811500	-0.05543000
N	-4.13170000	0.07158600	0.02638400
Cu	3.08325500	0.00981900	0.00337300
Cu	0.70927700	-0.09292200	-0.04211200

Freq = -416.91

Zero-point correction= 0.080789 (Hartree/Particle)

Thermal correction to Energy= 0.089705

Thermal correction to Enthalpy= 0.090649

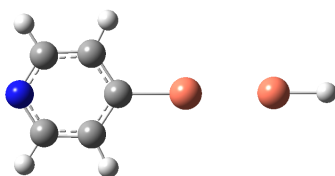
Thermal correction to Gibbs Free Energy= 0.043059

Sum of electronic and zero-point Energies= -640.601073

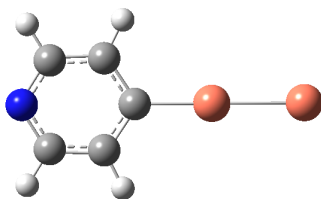
Sum of electronic and thermal Energies= -640.592157

Sum of electronic and thermal Enthalpies= -640.591213

Sum of electronic and thermal Free Energies= -640.638803



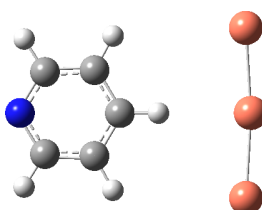
C	-1.33763400	-0.00014300	0.00030500
C	-2.10875400	1.17862200	0.00003300
C	-3.50237700	1.13418900	-0.00041800
C	-3.50281600	-1.13363800	-0.00041900
C	-2.10921000	-1.17860900	0.00003200
H	4.75986700	0.00034300	-0.00135800
H	-1.62851100	2.15434700	0.00019200
H	-4.08071600	2.05837100	-0.00060900
H	-4.08151200	-2.05759700	-0.00061100
H	-1.62934800	-2.15452000	0.00019100
N	-4.21681900	0.00041300	-0.00064800
Cu	0.63668100	-0.00046700	0.00083000
Cu	3.20961900	0.00024700	-0.00050100
Zero-point correction=			0.080705 (Hartree/Particle)
Thermal correction to Energy=			0.090617
Thermal correction to Enthalpy=			0.091561
Thermal correction to Gibbs Free Energy=			0.040730
Sum of electronic and zero-point Energies=			-640.611965
Sum of electronic and thermal Energies=			-640.602053
Sum of electronic and thermal Enthalpies=			-640.601109
Sum of electronic and thermal Free Energies=			-640.651939



C	1.22816500	0.00000000	-0.00001700
C	2.00785600	-1.17618100	-0.00000500
C	3.40106700	-1.13319800	0.00001600
C	3.40106600	1.13319900	0.00001700
C	2.00785500	1.17618100	-0.00000500
H	1.52991900	-2.15365000	-0.00001200
H	3.97896100	-2.05820300	0.00002500
H	3.97896000	2.05820500	0.00002500
H	1.52991800	2.15365000	-0.00001200
N	4.11788200	0.00000100	0.00002700
Cu	-3.11889000	0.00000000	0.00002300
Cu	-0.74728200	-0.00000100	-0.00003200
Zero-point correction=			0.076928 (Hartree/Particle)
Thermal correction to Energy=			0.085235
Thermal correction to Enthalpy=			0.086179
Thermal correction to Gibbs Free Energy=			0.040446
Sum of electronic and zero-point Energies=			-640.047358
Sum of electronic and thermal Energies=			-640.039050

Sum of electronic and thermal Enthalpies= -640.038106

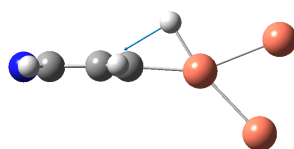
Sum of electronic and thermal Free Energies= -640.083840



C	-1.95890200	-0.00281800	0.18522400
C	-2.66949700	-1.19680900	0.10079800
C	-4.05316600	-1.14192600	-0.05424100
C	-4.05091500	1.14005300	-0.05578600
C	-2.66714900	1.19245600	0.09921400
H	-0.87867800	-0.00377000	0.30348600
H	-2.15167000	-2.14798100	0.15248000
H	-4.63520000	-2.05827400	-0.12141000
H	-4.63115000	2.05744700	-0.12420400
H	-2.14735600	2.14262800	0.14960500
N	-4.74905300	-0.00030700	-0.13165100
Cu	1.56817400	-2.36494900	0.00523700
Cu	1.69904700	0.00085200	-0.04865300
Cu	1.56330300	2.36638500	0.00584200

Zero-point correction= 0.089148 (Hartree/Particle)

Thermal correction to Energy=	0.100671
Thermal correction to Enthalpy=	0.101615
Thermal correction to Gibbs Free Energy=	0.042651
Sum of electronic and zero-point Energies=	-836.810278
Sum of electronic and thermal Energies=	-836.798755
Sum of electronic and thermal Enthalpies=	-836.797811
Sum of electronic and thermal Free Energies=	-836.856775



C	1.73669000	-0.12872600	-0.00000900
C	2.50111600	-0.08589400	1.18821400
C	3.88278900	0.03561200	1.13503100
C	3.88283100	0.03568900	-1.13495600
C	2.50116000	-0.08580900	-1.18820000
H	0.67378800	-1.40651700	-0.00010800
H	2.01591400	-0.13936900	2.15870400
H	4.45606500	0.09000700	2.06031600
H	4.45614200	0.09014900	-2.06021700
H	2.01599500	-0.13920500	-2.15871300
N	4.60036800	0.10034900	0.00005200



Cu	-1.99510300	1.40863100	0.00004200
Cu	-0.23743700	-0.15662300	-0.00008700
Cu	-2.34842500	-1.17693000	0.00001600

Freq = -947.04

Zero-point correction= 0.082869 (Hartree/Particle)

Thermal correction to Energy= 0.093396

Thermal correction to Enthalpy= 0.094341

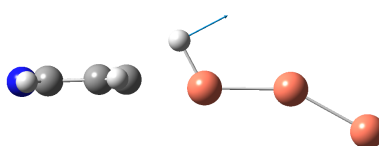
Thermal correction to Gibbs Free Energy= 0.042242

Sum of electronic and zero-point Energies= -836.755284

Sum of electronic and thermal Energies= -836.744756

Sum of electronic and thermal Enthalpies= -836.743812

Sum of electronic and thermal Free Energies= -836.795910



C	-3.28119600	1.18493300	-0.01759800
C	-2.54091900	-0.00022300	0.08092000
C	-3.28188800	-1.18490200	-0.01813900
C	-4.65558000	-1.13814300	-0.25000000
C	-4.65491000	1.13908400	-0.24950500
H	-2.79491800	2.15483400	0.08106700

H	-1.25549200	-0.00041200	1.33683500
H	-2.79618600	-2.15513800	0.08007400
H	-5.23145500	-2.05843100	-0.34688200
H	-5.23023800	2.05975500	-0.34600100
Cu	-0.39821500	-0.00060100	0.14519000
Cu	1.93310200	-0.00004500	0.43684900
Cu	4.16389300	0.00030000	-0.42683300
N	-5.35276700	0.00070300	-0.36859200

Freq =-1068.21

Zero-point correction= 0.082006 (Hartree/Particle)

Thermal correction to Energy= 0.093276

Thermal correction to Enthalpy= 0.094220

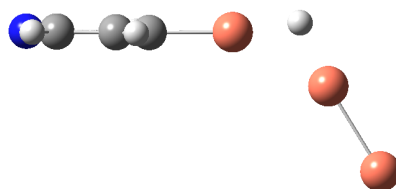
Thermal correction to Gibbs Free Energy= 0.038872

Sum of electronic and zero-point Energies= -836.729100

Sum of electronic and thermal Energies= -836.717830

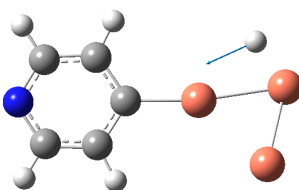
Sum of electronic and thermal Enthalpies= -836.716886

Sum of electronic and thermal Free Energies= -836.772234



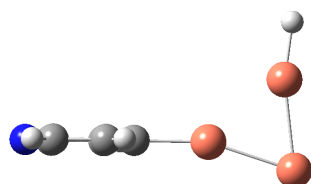
C	-2.37747000	-0.12938700	-0.00001800
C	-3.10292900	0.15284900	-1.17673200

C	-4.40136000	0.65792600	-1.13326700
C	-4.40148400	0.65707600	1.13359700
C	-3.10305500	0.15197200	1.17682600
H	0.82814000	-1.66227900	-0.00068700
H	-2.65808400	-0.01885400	-2.15431900
H	-4.94003500	0.86828400	-2.05739800
H	-4.94026400	0.86673500	2.05782500
H	-2.65832200	-0.02047400	2.15433300
N	-5.06802600	0.91589800	0.00022500
Cu	3.87739900	0.86722400	0.00024600
Cu	-0.55890400	-0.86799600	-0.00023900
Cu	1.99745500	-0.52982500	-0.00013600
Zero-point correction=			0.084605 (Hartree/Particle)
Thermal correction to Energy=			0.094689
Thermal correction to Enthalpy=			0.095633
Thermal correction to Gibbs Free Energy=			0.044173
Sum of electronic and zero-point Energies=			-836.832041
Sum of electronic and thermal Energies=			-836.821957
Sum of electronic and thermal Enthalpies=			-836.821013
Sum of electronic and thermal Free Energies=			-836.872473



C	2.73273900	-1.15449400	0.29148300
C	1.82880000	-0.11774000	-0.01955500
C	2.46433600	1.10696500	-0.30970100
C	3.85236400	1.23274500	-0.28302100
C	4.11070000	-0.94241500	0.30042600
H	2.36759000	-2.15019900	0.53080600
H	-1.48035100	-2.25339900	-0.29149500
H	1.87610400	1.98599000	-0.56142500
H	4.32093000	2.18988400	-0.51393000
H	4.78965600	-1.75972700	0.54548200
N	4.69186400	0.23185900	0.01771800
Cu	-0.12088100	-0.35487600	-0.04902600
Cu	-2.39579800	-0.99901600	-0.12841600
Cu	-2.12644600	1.34058400	0.18739800
Zero-point correction=			0.082338 (Hartree/Particle)
Thermal correction to Energy=			0.093116
Thermal correction to Enthalpy=			0.094061
Thermal correction to Gibbs Free Energy=			0.040695
Sum of electronic and zero-point Energies=			-836.812828

Sum of electronic and thermal Energies= -836.802050  
 Sum of electronic and thermal Enthalpies= -836.801106  
 Sum of electronic and thermal Free Energies= -836.854471

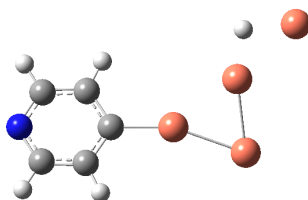


C	-1.85631300	-0.07381300	-0.00000700
C	-2.62817600	-0.01132400	1.17773000
C	-4.01735900	0.09616400	1.13367000
C	-4.01744400	0.09535500	-1.13364100
C	-2.62826500	-0.01215600	-1.17773200
H	2.53983000	2.77002100	-0.00124700
H	-2.15100000	-0.04522700	2.15443100
H	-4.59374400	0.14228800	2.05790900
H	-4.59389500	0.14085400	-2.05787000
H	-2.15115400	-0.04673000	-2.15444100
N	-4.73005200	0.14914500	0.00002200
Cu	2.31894200	-1.16413500	0.00022000
Cu	0.10548100	-0.25427200	-0.00000200
Cu	2.22887600	1.26080100	-0.00018500

Zero-point correction= 0.082800 (Hartree/Particle)

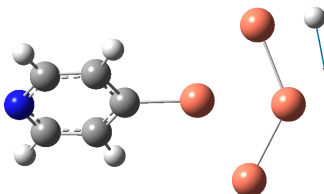
Thermal correction to Energy= 0.094201

Thermal correction to Enthalpy=	0.095145
Thermal correction to Gibbs Free Energy=	0.040316
Sum of electronic and zero-point Energies=	-836.821442
Sum of electronic and thermal Energies=	-836.810042
Sum of electronic and thermal Enthalpies=	-836.809097
Sum of electronic and thermal Free Energies=	-836.863927



C	2.68543700	-0.15931900	0.00444300
C	3.77359100	0.60428000	0.47217400
C	5.07294100	0.09853400	0.46806000
C	4.37977300	-1.87108900	-0.41652200
C	3.05344300	-1.44280500	-0.44612500
H	-2.31456500	-1.68272000	0.27248000
H	3.62179400	1.61315000	0.84933700
H	5.90006700	0.70720000	0.83398500
H	4.64241400	-2.86782300	-0.77081100
H	2.30360600	-2.13031900	-0.82952200
N	5.39905500	-1.12525200	0.03166000

Cu	0.82915000	0.50470600	-0.02531300
Cu	-1.03631100	2.03053000	-0.19487100
Cu	-1.58984100	-0.26327000	0.09801300
Cu	-3.91809500	-1.27680600	0.08530000
Zero-point correction=			0.084388 (Hartree/Particle)
Thermal correction to Energy=			0.097847
Thermal correction to Enthalpy=			0.098791
Thermal correction to Gibbs Free Energy=			0.035684
Sum of electronic and zero-point Energies=			-1032.981116
Sum of electronic and thermal Energies=			-1032.967657
Sum of electronic and thermal Enthalpies=			-1032.966713
Sum of electronic and thermal Free Energies=			-1033.029820



C	-2.88411600	-0.92235200	-0.82417400
C	-2.11809400	-0.07397100	-0.00005900
C	-2.90031600	0.74701800	0.83721900
C	-4.29299700	0.68809800	0.82023600
C	-4.27748000	-0.91190800	-0.78580000
H	-2.39755900	-1.60815600	-1.51416300

H	3.16348300	-2.18666800	0.24902100
H	-2.42853100	1.44852200	1.52148700
H	-4.87733000	1.33076600	1.47937600
H	-4.84925800	-1.57428600	-1.43640600
Cu	1.19944900	2.17374200	-0.20894700
Cu	-0.13259300	-0.05656600	-0.00701000
Cu	2.35114900	0.14846700	0.00254800
Cu	1.58994400	-2.04843700	0.18777700
N	-5.00047500	-0.12435000	0.02278200

Freq = -458.89

Zero-point correction= 0.082262 (Hartree/Particle)

Thermal correction to Energy= 0.095528

Thermal correction to Enthalpy= 0.096472

Thermal correction to Gibbs Free Energy= 0.035553

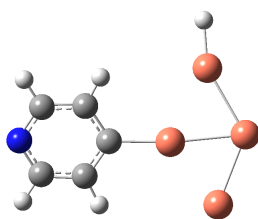
Sum of electronic and zero-point Energies= -1032.971340

Sum of electronic and thermal Energies= -1032.958074

Sum of electronic and thermal Enthalpies= -1032.957130

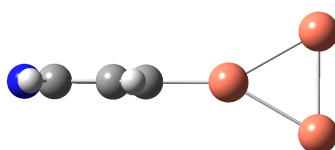
Sum of electronic and thermal Free Energies= -1033.018049





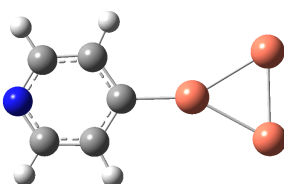
C	-2.02272900	-0.09026600	0.00132000
C	-2.76582000	1.04573000	0.37649100
C	-4.15999300	1.03013700	0.37079500
C	-4.20956700	-1.11893100	-0.35276200
C	-2.81725300	-1.19176600	-0.37194000
H	1.07605800	3.74393000	-0.15133500
H	-2.26355100	1.96069600	0.67708900
H	-4.71825200	1.91833300	0.66580100
H	-4.80772700	-1.98238400	-0.64431700
H	-2.35785900	-2.12689200	-0.68162100
N	-4.89809800	-0.02981200	0.01342400
Cu	1.46079900	-2.16989500	0.11509700
Cu	-0.05315200	-0.14709600	-0.00387000
Cu	2.36088300	0.06192900	-0.00214100
Cu	1.16975400	2.20835800	-0.11263900
Zero-point correction=			0.083356 (Hartree/Particle)
Thermal correction to Energy=			0.097152
Thermal correction to Enthalpy=			0.098097
Thermal correction to Gibbs Free Energy=			0.035364

Sum of electronic and zero-point Energies=	-1032.982959
Sum of electronic and thermal Energies=	-1032.969164
Sum of electronic and thermal Enthalpies=	-1032.968219
Sum of electronic and thermal Free Energies=	-1033.030952



C	2.59898100	-0.00011800	1.17749300
C	3.99206700	0.00012900	1.13368500
C	3.99214000	0.00011000	-1.13340000
C	2.59905700	-0.00013600	-1.17729800
C	1.82289800	-0.00026000	0.00007200
H	4.57010200	0.00021400	-2.05788900
H	2.12115300	-0.00022200	-2.15431500
H	2.12101300	-0.00018900	2.15447800
H	4.56996900	0.00024500	2.05821100
N	4.70771800	0.00025400	0.00016600
Cu	-2.27913000	-1.21725600	-0.00008900
Cu	-0.14487700	-0.00061400	0.00000200
Cu	-2.27830700	1.21786400	-0.00008400
Zero-point correction=			0.077826 (Hartree/Particle)

Thermal correction to Energy=	0.088336
Thermal correction to Enthalpy=	0.089280
Thermal correction to Gibbs Free Energy=	0.035668
Sum of electronic and zero-point Energies=	-836.216635
Sum of electronic and thermal Energies=	-836.206124
Sum of electronic and thermal Enthalpies=	-836.205180
Sum of electronic and thermal Free Energies=	-836.258793



C	2.59791200	-1.17771600	-0.00486700
C	3.99142900	-1.13364300	-0.00460400
C	3.99117400	1.13382500	0.00485800
C	2.59764800	1.17758900	0.00493300
C	1.82277800	-0.00015100	-0.00002500
H	4.56937800	2.05814300	0.00877600
H	2.11751900	2.15314600	0.00895800
H	2.11800200	-2.15338200	-0.00895600
N	4.70621100	0.00017100	0.00017600
H	4.56983900	-2.05783200	-0.00843900
Cu	-0.14729800	-0.00028100	-0.00012400

Cu	-2.27696100	-1.21858600	0.00318700
Cu	-2.27656400	1.21884300	-0.00317800
Zero-point correction=			0.077839 (Hartree/Particle)
Thermal correction to Energy=			0.088378
Thermal correction to Enthalpy=			0.089322
Thermal correction to Gibbs Free Energy=			0.034640
Sum of electronic and zero-point Energies=			-836.216523
Sum of electronic and thermal Energies=			-836.205984
Sum of electronic and thermal Enthalpies=			-836.205040
Sum of electronic and thermal Free Energies=			-836.259723