**Supplementary Material**

# A reduced electrophilicity for simple Lewis acids A involved in non-covalent interactions with Lewis bases B

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Index

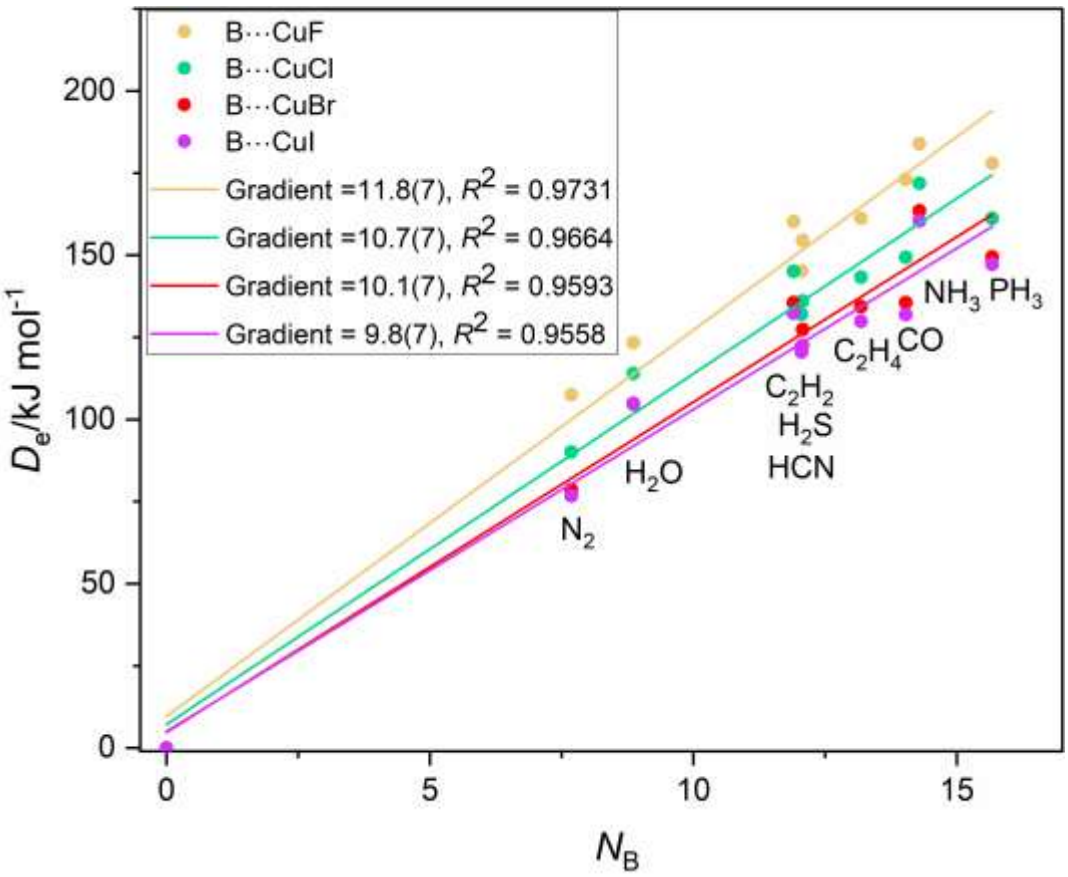


Figure S1. Dissociation energy $D_e$ plotted against the nucleophilicity of the Lewis base B for the four series of coinage-metal-bonded complexes B···CuX (X = F, Cl, Br, I). The straight lines are linear regression fits to the points (solid dots) for each series, with the origin taken as a point. The inset gives the gradient of each fitted line in kJ mol$^{-1}$ and the quality of the fit as measured by $R^2$.

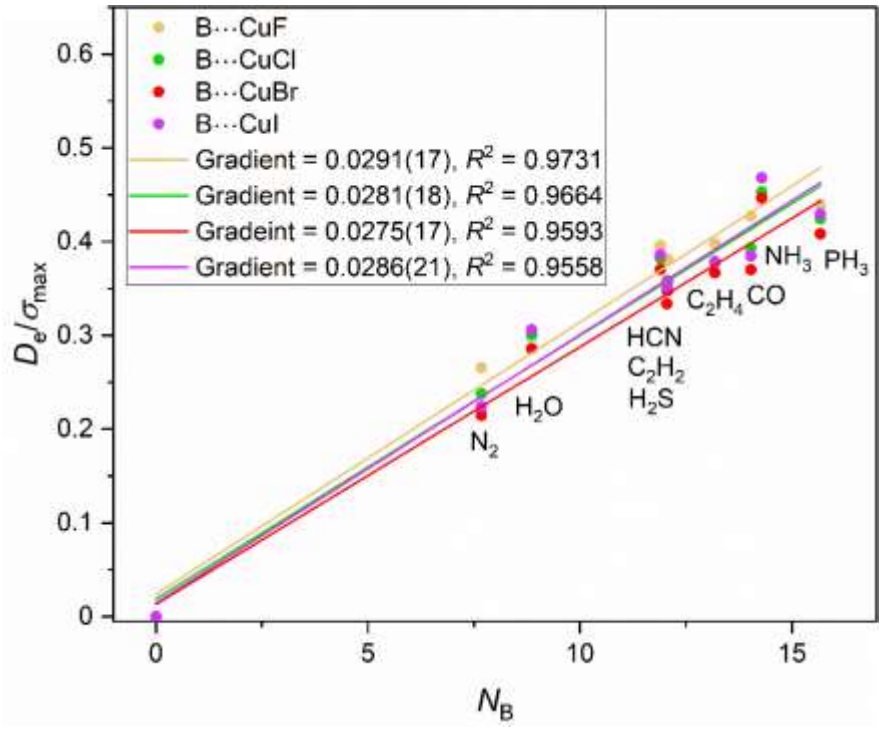


Figure S2. $D_e/\sigma_{max}$ plotted against the nucleophilicity $N_B$ of the Lewis base B for the four series of coinage-metal-bonded -bonded complexes- B···CuX (X = F, Cl, Br, I). The straight lines are linear regression fits to the points (solid dots) for each series, (origin as a point). The inset gives the gradient of each fit and the quality of the fit, as measured by $R^2$

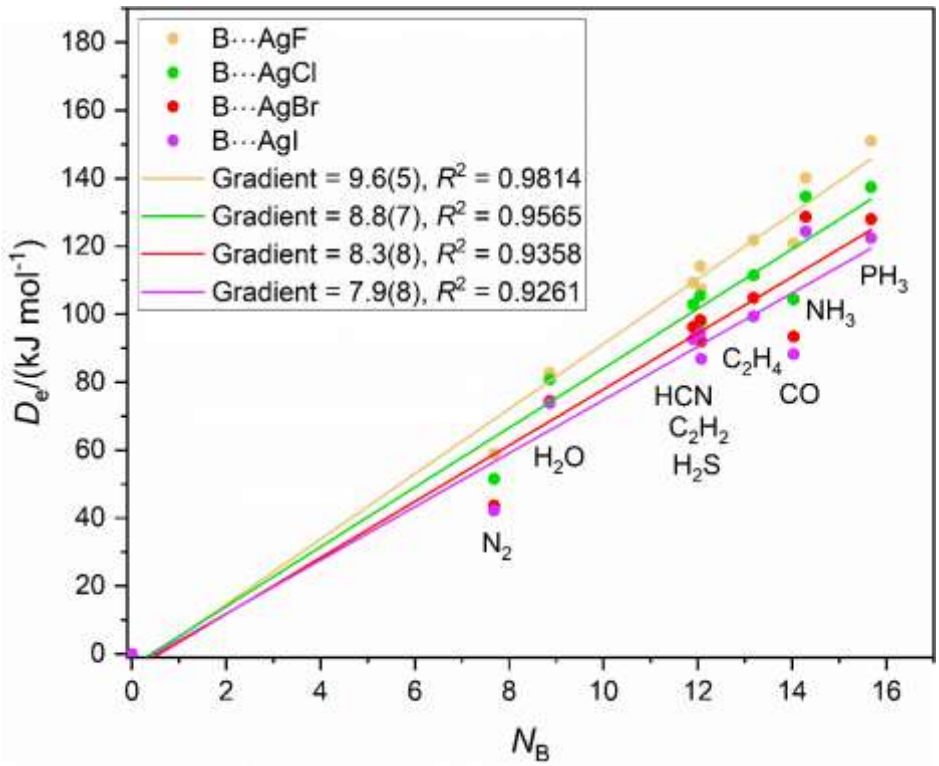


Figure S3. Dissociation energy $D_e$ plotted against the nucleophilicity of the Lewis base B for the four series of coinage-metal-bonded complexes B···AgX (X = F, Cl, Br, I). The straight lines are linear regression fits to the points (solid dots) for each series, with the origin taken as a point. The inset gives the gradient of each fitted line in kJ mol$^{-1}$ and the quality of the fit as measured by $R^2$

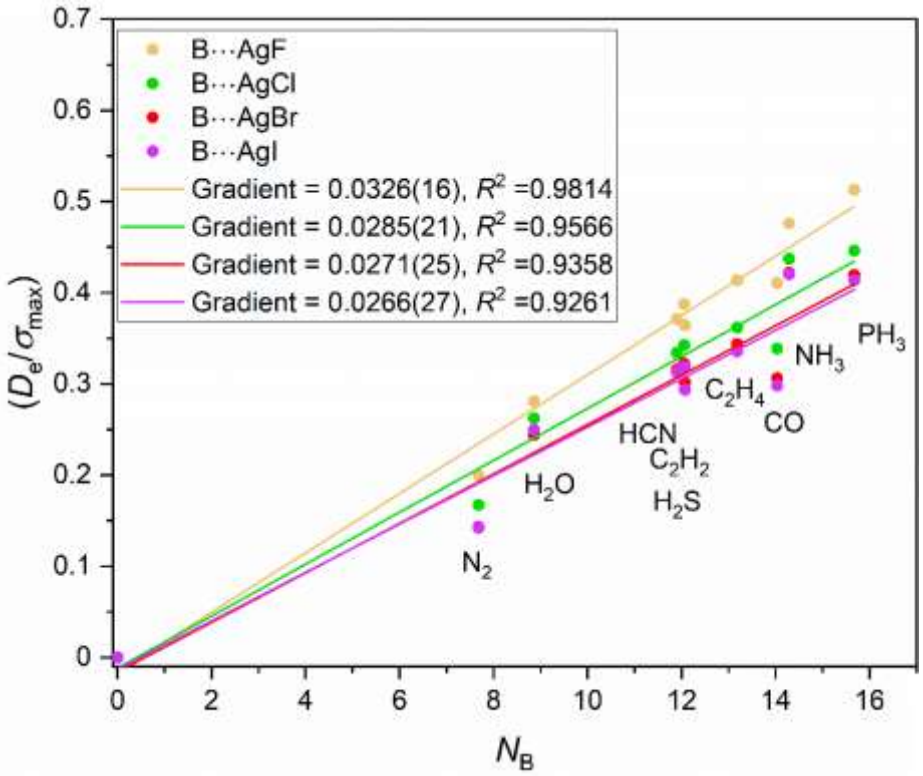


Figure S4. $D_e/\sigma_{max}$ plotted against the nucleophilicity $N_B$ of the Lewis base B for the four series of coinage-metal-bonded -bonded complexes- B···AgX (X = F, Cl, Br, I). The straight lines are linear regression fits to the points (solid dots) for each series, (origin as a point). The inset gives the gradient of each fit and the quality of the fit, as measured by $R^2$

Cartesian Coordinates (Å) of the calculated complexes

## Complexes B···IF.

| | |
|---|---|
| FI | CCSD(T)-F12C/USERDEF ENERGY=-394.56734930<br>F 0.0000000000 0.0000000000 -1.6592880148<br>I 0.0000000000 0.0000000000 0.2484041057 |
| FI:CO | CCSD(T)-F12C/USERDEF ENERGY=-507.76449772<br>F 0.0000000000 0.0000000000 -2.2398084787<br>I 0.0000000000 0.0000000000 -0.3072618601<br>C 0.0000000000 0.0000000000 2.2676637652<br>O 0.0000000000 0.0000000000 3.3944437854 |
| FI:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-473.04113832<br>F 0.0000000000 0.0000000000 -2.1724490968<br>I 0.0000000000 0.0000000000 -0.2283475498<br>C 0.0000000000 0.6735257200 2.5006689845<br>C 0.0000000000 -0.6735257200 2.5006689845<br>H -0.9241437091 1.2352446494 2.5250833968<br>H 0.9241437091 1.2352446494 2.5250833968<br>H 0.9241437091 -1.2352446494 2.5250833968<br>H -0.9241437091 -1.2352446494 2.5250833968 |
| FI:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-471.78555091<br>F 0.0000000000 0.0000000000 -2.1531579163<br>I 0.0000000000 0.0000000000 -0.2245632941<br>C 0.0000000000 0.6047562977 2.6629166915<br>C 0.0000000000 -0.6047562977 2.6629166915<br>H 0.0000000000 1.6690106802 2.6967238697<br>H 0.0000000000 -1.6690106802 2.6967238697 |
| FI:N2 | CCSD(T)-F12C/USERDEF ENERGY=-503.97647441<br>F 0.0000000000 0.0000000000 -2.2660363659<br>I 0.0000000000 0.0000000000 -0.3535611928<br>N 0.0000000000 0.0000000000 2.5893048698<br>N 0.0000000000 0.0000000000 3.6876837637 |
| FI:NCH | CCSD(T)-F12C/USERDEF ENERGY=-487.88177762<br>F 0.0000000000 0.0000000000 -2.2219929240<br>I 0.0000000000 0.0000000000 -0.2909821704<br>N 0.0000000000 0.0000000000 2.3339873752<br>C 0.0000000000 0.0000000000 3.4852217937<br>H 0.0000000000 0.0000000000 4.5529156745 |
| FI:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-451.08676465<br>F -0.0000000000 0.0000000000 -1.9970754149<br>I -0.0000000000 0.0000000000 -0.0387945876<br>N 0.0000000000 0.0000000000 2.4530195286<br>H 0.9460699354 0.0000000000 2.8129245718<br>H -0.4730349677 0.8193205978 2.8129245718<br>H -0.4730349677 -0.8193205978 2.8129245718 |
| FI:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-470.94155852<br>F 2.0870802761 0.0356997936 0.0000000000<br>I 0.1598563806 -0.0065557808 0.0000000000<br>O -2.4648911009 -0.0605866747 0.0000000000 |

| | | | | |
|---|---|---|---|---|
| | H | -2.8400124628 | 0.3836338960 | 0.7640582388 |
| | H | -2.8400124628 | 0.3836338960 | -0.7640582388 |
| FI:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-737.29227299 | | | |
| | F | -0.0000000000 | 0.0000000000 | -2.2915598743 |
| | I | -0.0000000000 | 0.0000000000 | -0.3125733158 |
| | P | 0.0000000000 | 0.0000000000 | 2.3872982868 |
| | H | 1.2310659779 | 0.0000000000 | 3.0622244320 |
| | H | -0.6155329889 | 1.0661344106 | 3.0622244320 |
| | H | -0.6155329889 | -1.0661344106 | 3.0622244320 |
| FI:SH2 | CCSD(T)-F12C/USERDEF ENERGY=-793.53204558 | | | |
| | F | 2.4133457948 | 0.0366058959 | 0.0000000000 |
| | I | 0.4733123053 | -0.0168880417 | 0.0000000000 |
| | S | -2.4637396173 | -0.0883435469 | 0.0000000000 |
| | H | -2.6465195514 | 0.8178781164 | 0.9676357742 |
| | H | -2.6465195514 | 0.8178781164 | -0.9676357742 |

**NOTE**: For the B···XY complexes in which XY =ICl, BrCl , $Br_2$, FCl, and $Cl_2$, the distances *r*(Z···X), where Z is the acceptor atom/centre in B, calculated at the CCSD(T)(F12c)/cc-pVDZ-F12 level, are available from the Supplementary Information associated with ref. 11. The exceptions are $N_2$···$Br_2$ and HCN···$Br_2$ which were first calculated here and the optimised cartesian coordinates are given immediately below. Likewise, the distances *r*(Z···H) calculated at the same level of theory for the B···HX (X = F,Cl,Br and I) complexes are also available from the Supplementary Information associated with ref.11 (*Phys.Chem.Chem. Phys. 2014, 16, 25199*).

**Complexes B···$Br_2$**

| | | | | |
|---|---|---|---|---|
| $Br_2$ | Br | 0.0000000000 | 0.0000000000 | -1.7411647138 |
| | Br | 0.0000000000 | 0.0000000000 | 0.5485213421 |
| $N_2$:$Br_2$ | Br | 0.0000000000 | 0.0000000000 | -1.8737123607 |
| | Br | 0.0000000000 | 0.0000000000 | 0.4177972883 |
| | N | 0.0000000000 | 0.0000000000 | 3.6033613056 |
| | N | 0.0000000000 | 0.0000000000 | 4.7021951741 |
| HCN:$Br_2$ | Br | 0.0000000000 | 0.0000000000 | -1.8220020900 |
| | Br | 0.0000000000 | 0.0000000000 | 0.4768246140 |
| | N | 0.0000000000 | 0.0000000000 | 3.3815708986 |
| | C | 0.0000000000 | 0.0000000000 | 4.5353028097 |
| | H | 0.0000000000 | 0.0000000000 | 5.6024067851 |

**Complexes B···IBr.**

| | | | | |
|---|---|---|---|---|
| BrI | CCSD(T)-F12C/USERDEF ENERGY=-710.54731815 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.5206560192 |
| | I | 0.0000000000 | 0.0000000000 | 0.9574572757 |
| BrI:CO | CCSD(T)-F12C/USERDEF ENERGY=-823.73850507 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -2.0902977687 |

| | | | | |
|---|---|---|---|---|
| | I | 0.0000000000 | 0.0000000000 | 0.3962705642 |
| | C | 0.0000000000 | 0.0000000000 | 3.5229305914 |
| | O | 0.0000000000 | 0.0000000000 | 4.6514468739 |
| BrI:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-789.01436503 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -2.0150690341 |
| | I | 0.0000000000 | 0.0000000000 | 0.4891457805 |
| | C | 0.0000000000 | 0.6697014627 | 3.5255471045 |
| | C | 0.0000000000 | -0.6697014627 | 3.5255471045 |
| | H | -0.9239993721 | 1.2330964360 | 3.5334798272 |
| | H | 0.9239993721 | 1.2330964360 | 3.5334798272 |
| | H | 0.9239993721 | -1.2330964360 | 3.5334798272 |
| | H | -0.9239993721 | -1.2330964360 | 3.5334798272 |
| BrI:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-787.76080821 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.9912760336 |
| | I | 0.0000000000 | 0.0000000000 | 0.5016134459 |
| | C | 0.0000000000 | 0.6037071544 | 3.6649061915 |
| | C | 0.0000000000 | -0.6037071544 | 3.6649061915 |
| | H | 0.0000000000 | 1.6679174804 | 3.6783383203 |
| | H | 0.0000000000 | -1.6679174804 | 3.6783383203 |
| BrI:N2 | CCSD(T)-F12C/USERDEF ENERGY=-819.95434564 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -2.0926480988 |
| | I | 0.0000000000 | 0.0000000000 | 0.3883941460 |
| | N | 0.0000000000 | 0.0000000000 | 3.6601002704 |
| | N | 0.0000000000 | 0.0000000000 | 4.7588448937 |
| BrI:NCH | CCSD(T)-F12C/USERDEF ENERGY=-803.85541405 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -2.0482884274 |
| | I | 0.0000000000 | 0.0000000000 | 0.4456963102 |
| | N | 0.0000000000 | 0.0000000000 | 3.3678360207 |
| | C | 0.0000000000 | 0.0000000000 | 4.5208761865 |
| | H | 0.0000000000 | 0.0000000000 | 5.5882863202 |
| BrI:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-767.05618640 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -1.8344444642 |
| | I | -0.0000000000 | 0.0000000000 | 0.6975593877 |
| | N | 0.0000000000 | 0.0000000000 | 3.3445428398 |
| | H | 0.9450071383 | 0.0000000000 | 3.7070292368 |
| | H | -0.4725035691 | 0.8184001885 | 3.7070292368 |
| | H | -0.4725035691 | -0.8184001885 | 3.7070292368 |
| BrI:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-786.91571734 | | | |
| | Br | 1.9292623053 | 0.0202390804 | 0.0000000000 |
| | I | -0.5645183244 | -0.0308666016 | 0.0000000000 |
| | O | -3.4029647414 | -0.0440767780 | 0.0000000000 |
| | H | -3.7875729875 | 0.3952534561 | 0.7615233517 |
| | H | -3.7875729875 | 0.3952534561 | -0.7615233517 |
| BrI:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-1053.26132039 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -2.1255130962 |
| | I | -0.0000000000 | 0.0000000000 | 0.4084728278 |
| | P | 0.0000000000 | 0.0000000000 | 3.4078868957 |
| | H | 1.2167900744 | 0.0000000000 | 4.1154963018 |
| | H | -0.6083950372 | 1.0537711155 | 4.1154963018 |

| | |
|---|---|
| | H -0.6083950372 -1.0537711155 4.1154963018 |
| BrI:SH2 | CCSD(T)-F12C/USERDEF ENERGY=-1109.50572102<br>Br -2.2691417303 -0.0163583814 0.0000000000<br>I 0.2350505394 0.0378065893 0.0000000000<br>S 3.4265101621 0.0597960974 0.0000000000<br>H 3.5291726128 -0.8597213443 0.9663855401<br>H 3.5291726128 -0.8597213443 -0.9663855401 |

## Complexes B···$I_2$.

| | |
|---|---|
| I2 | CCSD(T)-F12C/USERDEF ENERGY=-710.54731815<br>Br 0.0000000000 0.0000000000 -1.5206560192<br>I 0.0000000000 0.0000000000 0.9574572757 |
| I2:CO | CCSD(T)-F12C/USERDEF ENERGY=-702.87650791<br>I 0.0000000000 0.0000000000 -1.8682289848<br>I 0.0000000000 0.0000000000 0.8164085113<br>C 0.0000000000 0.0000000000 4.1204622463<br>O 0.0000000000 0.0000000000 5.2496234779 |
| I2:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-668.15161731<br>I 0.0000000000 0.0000000000 -1.7994996629<br>I 0.0000000000 0.0000000000 0.8979187686<br>C 0.0000000000 0.6686685488 4.0778094783<br>C 0.0000000000 -0.6686685488 4.0778094783<br>H -0.9238690364 1.2324550893 4.0821737244<br>H 0.9238690364 1.2324550893 4.0821737244<br>H 0.9238690364 -1.2324550893 4.0821737244<br>H -0.9238690364 -1.2324550893 4.0821737244 |
| I2:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-666.89854828<br>I 0.0000000000 0.0000000000 -1.7759640708<br>I 0.0000000000 0.0000000000 0.9136900854<br>C 0.0000000000 0.6034066803 4.2019819611<br>C 0.0000000000 -0.6034066803 4.2019819611<br>H 0.0000000000 1.6674229917 4.2101783660<br>H 0.0000000000 -1.6674229917 4.2101783660 |
| I2:N2 | CCSD(T)-F12C/USERDEF ENERGY=-699.09296945<br>I 0.0000000000 0.0000000000 -1.8655283438<br>I 0.0000000000 0.0000000000 0.8153197837<br>N 0.0000000000 0.0000000000 4.2082020458<br>N 0.0000000000 0.0000000000 5.3070397607 |
| I2:NCH | CCSD(T)-F12C/USERDEF ENERGY=-682.99264099<br>I 0.0000000000 0.0000000000 -1.8258143976<br>I 0.0000000000 0.0000000000 0.8650552227<br>N 0.0000000000 0.0000000000 3.9159423240<br>C 0.0000000000 0.0000000000 5.0695644712<br>H 0.0000000000 0.0000000000 6.1368327237 |
| I2:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-646.19135407<br>I -0.0000000000 0.0000000000 -1.6242121953<br>I -0.0000000000 0.0000000000 1.0989754337<br>N 0.0000000000 0.0000000000 3.8487550990 |

| | |
|---|---|
| | H 0.9434243007 0.0000000000 4.2155363993<br>H -0.4717121503 0.8170294109 4.2155363993<br>H -0.4717121503 -0.8170294109 4.2155363993 |
| I2:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-666.05293493<br>I 1.7625009975 0.0152292108 0.0000000000<br>I -0.9279130861 -0.0341217957 0.0000000000<br>O -3.8717144407 -0.0379726092 0.0000000000<br>H -4.2718141403 0.3884248820 0.7604254184<br>H -4.2718141403 0.3884248820 -0.7604254184 |
| I2:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-932.39728274<br>I -0.0000000000 0.0000000000 -1.9049931516<br>I -0.0000000000 0.0000000000 0.8061579417<br>P 0.0000000000 0.0000000000 4.0368973954<br>H 1.2069679771 0.0000000000 4.7655716204<br>H -0.6034839886 1.0452649297 4.7655716204<br>H -0.6034839886 -1.0452649297 4.7655716204 |
| I2:SH2 | CCSD(T)-F12C/USERDEF ENERGY=-988.64281809<br>I -2.0999056870 -0.0084896598 0.0000000000<br>I 0.5975077805 0.0495051050 0.0000000000<br>S 3.9322044407 0.0430221214 0.0000000000<br>H 3.9912843889 -0.8808054064 0.9655261812<br>H 3.9912843889 -0.8808054064 -0.9655261812 |

## Complexes B···ICN.

| | |
|---|---|
| NCI | CCSD(T)-F12C/USERDEF ENERGY=-387.53255620<br>I 0.0000000000 0.0000000000 -0.4466839221<br>C 0.0000000000 0.0000000000 1.5532815718<br>N 0.0000000000 0.0000000000 2.7151389585 |
| NCI:CO | CCSD(T)-F12C/USERDEF ENERGY=-500.72343266<br>C 0.0000000000 0.0000000000 -2.2371277654<br>I 0.0000000000 0.0000000000 -0.2309711639<br>N 0.0000000000 0.0000000000 -3.3990726660<br>C 0.0000000000 0.0000000000 3.0609211311<br>O 0.0000000000 0.0000000000 4.1893256587 |
| NCI:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-465.99790411<br>C 0.0000000000 0.0000000000 -2.1432982092<br>I 0.0000000000 0.0000000000 -0.1309401993<br>N 0.0000000000 0.0000000000 -3.3053741955<br>C 0.0000000000 0.6680923630 3.1592996992<br>C 0.0000000000 -0.6680923630 3.1592996992<br>H -0.9238288052 1.2322975781 3.1660764860<br>H 0.9238288052 1.2322975781 3.1660764860<br>H 0.9238288052 -1.2322975781 3.1660764860<br>H -0.9238288052 -1.2322975781 3.1660764860 |
| NCI:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-464.74542992<br>C 0.0000000000 0.0000000000 -2.1093499396<br>I 0.0000000000 0.0000000000 -0.1001679915<br>N 0.0000000000 0.0000000000 -3.2713966469 |

| | | | | |
|---|---|---|---|---|
| | C | 0.0000000000 | 0.6033217901 | 3.2198704013 |
| | C | 0.0000000000 | -0.6033217901 | 3.2198704013 |
| | H | 0.0000000000 | 1.6675400029 | 3.2348184367 |
| | H | 0.0000000000 | -1.6675400029 | 3.2348184367 |
| NCI:N2 | CCSD(T)-F12C/USERDEF ENERGY=-496.93971001 | | | |
| | C | 0.0000000000 | 0.0000000000 | -2.2232781124 |
| | I | 0.0000000000 | 0.0000000000 | -0.2203815775 |
| | N | 0.0000000000 | 0.0000000000 | -3.3851874934 |
| | N | 0.0000000000 | 0.0000000000 | 3.0948658699 |
| | N | 0.0000000000 | 0.0000000000 | 4.1935540515 |
| NCI:NCH | CCSD(T)-F12C/USERDEF ENERGY=-480.84148152 | | | |
| | C | 0.0000000000 | 0.0000000000 | -2.1732935414 |
| | I | 0.0000000000 | 0.0000000000 | -0.1621006548 |
| | N | 0.0000000000 | 0.0000000000 | -3.3354842504 |
| | N | 0.0000000000 | 0.0000000000 | 2.8604018537 |
| | C | 0.0000000000 | 0.0000000000 | 4.0136309425 |
| | H | 0.0000000000 | 0.0000000000 | 5.0811482038 |
| NCI:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-444.03866349 | | | |
| | C | -0.0000000000 | 0.0000000000 | -1.9162686383 |
| | I | -0.0000000000 | 0.0000000000 | 0.1129399412 |
| | N | 0.0000000000 | 0.0000000000 | -3.0786273070 |
| | N | 0.0000000000 | 0.0000000000 | 2.9745946792 |
| | H | 0.9391486398 | 0.0000000000 | 3.3536281958 |
| | H | -0.4695743199 | 0.8133265800 | 3.3536281958 |
| | H | -0.4695743199 | -0.8133265800 | 3.3536281958 |
| NCI:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-463.90157031 | | | |
| | N | 3.1224305886 | 0.0135778980 | 0.0000000000 |
| | C | 1.9602852565 | 0.0067782045 | 0.0000000000 |
| | I | -0.0509230366 | -0.0042936282 | 0.0000000000 |
| | O | -2.9688351347 | -0.0435841141 | 0.0000000000 |
| | H | -3.4983733152 | 0.2008915291 | 0.7611368763 |
| | H | -3.4983733152 | 0.2008915291 | -0.7611368763 |
| NCI:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-730.24346765 | | | |
| | C | -0.0000000000 | 0.0000000000 | -2.2857497073 |
| | I | -0.0000000000 | 0.0000000000 | -0.2695289997 |
| | N | 0.0000000000 | 0.0000000000 | -3.4479006079 |
| | P | 0.0000000000 | 0.0000000000 | 3.1685669679 |
| | H | 1.2024668671 | 0.0000000000 | 3.9056894558 |
| | H | -0.6012334336 | 1.0413668541 | 3.9056894558 |
| | H | -0.6012334336 | -1.0413668541 | 3.9056894558 |
| NCI:SH2 | CCSD(T)-F12C/USERDEF ENERGY=-786.48949054 | | | |
| | N | 3.5171199314 | 0.0587952855 | 0.0000000000 |
| | C | 2.3553657230 | 0.0296826542 | 0.0000000000 |
| | I | 0.3426069682 | -0.0200289698 | 0.0000000000 |
| | S | -3.0776919404 | -0.0663047341 | 0.0000000000 |
| | H | -3.2470306361 | 0.8428820470 | 0.9662460072 |
| | H | -3.2470306361 | 0.8428820470 | -0.9662460072 |

## Complexes B···ICCH.

| | |
|---|---|
| HCCI | CCSD(T)-F12C/USERDEF ENERGY=-371.43971537 |
| | I 0.0000000000 0.0000000000 -0.4394124120 |
| | C 0.0000000000 0.0000000000 1.5562121190 |
| | C 0.0000000000 0.0000000000 2.7652090011 |
| | H 0.0000000000 0.0000000000 3.8288180204 |
| HCCI:CO | CCSD(T)-F12C/USERDEF ENERGY=-484.62965738 |
| | C 0.0000000000 0.0000000000 -2.2547215533 |
| | I 0.0000000000 0.0000000000 -0.2551098542 |
| | C 0.0000000000 0.0000000000 -3.4642032059 |
| | H 0.0000000000 0.0000000000 -4.5277424711 |
| | C 0.0000000000 0.0000000000 3.1260538125 |
| | O 0.0000000000 0.0000000000 4.2552523085 |
| HCCI:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-449.90355575 |
| | C 0.0000000000 0.0000000000 -2.1601431503 |
| | I 0.0000000000 0.0000000000 -0.1565215098 |
| | C 0.0000000000 0.0000000000 -3.3698882243 |
| | H 0.0000000000 0.0000000000 -4.4334368103 |
| | C 0.0000000000 0.6676202741 3.2345571490 |
| | C 0.0000000000 -0.6676202741 3.2345571490 |
| | H -0.9236966757 1.2318649055 3.2374789453 |
| | H 0.9236966757 1.2318649055 3.2374789453 |
| | H 0.9236966757 -1.2318649055 3.2374789453 |
| | H -0.9236966757 -1.2318649055 3.2374789453 |
| HCCI:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-448.65120935 |
| | C 0.0000000000 0.0000000000 -2.1253852292 |
| | I 0.0000000000 0.0000000000 -0.1238585074 |
| | C 0.0000000000 0.0000000000 -3.3350371516 |
| | H 0.0000000000 0.0000000000 -4.3985725886 |
| | C 0.0000000000 0.6031257152 3.2922440165 |
| | C 0.0000000000 -0.6031257152 3.2922440165 |
| | H 0.0000000000 1.6670027478 3.2991339442 |
| | H 0.0000000000 -1.6670027478 3.2991339442 |
| HCCI:NCH | CCSD(T)-F12C/USERDEF ENERGY=-464.74570721 |
| | C 0.0000000000 0.0000000000 -2.1923118825 |
| | I 0.0000000000 0.0000000000 -0.1886474922 |
| | C 0.0000000000 0.0000000000 -3.4024512067 |
| | H 0.0000000000 0.0000000000 -4.4658270078 |
| | N 0.0000000000 0.0000000000 2.9432642559 |
| | C 0.0000000000 0.0000000000 4.0970548295 |
| | H 0.0000000000 0.0000000000 5.1642216610 |
| HCCI:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-427.94170012 |
| | C -0.0000000000 0.0000000000 -1.9241218956 |
| | I -0.0000000000 0.0000000000 0.0905738969 |
| | C 0.0000000000 0.0000000000 -3.1348953389 |
| | H 0.0000000000 0.0000000000 -4.1983173116 |
| | N 0.0000000000 0.0000000000 3.0741414596 |
| | H 0.9387668170 0.0000000000 3.4534509843 |
| | H -0.4693834085 0.8129959117 3.4534509843 |

| | |
|---|---|
| | H -0.4693834085 -0.8129959117 3.4534509843 |
| HCCI:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-447.80596968<br>H 4.2440291607 0.0334818391 0.0000000000<br>C 3.1808438277 0.0144979968 0.0000000000<br>C 1.9709357309 -0.0073883601 0.0000000000<br>I -0.0328657301 -0.0454716383 0.0000000000<br>O -3.0495133419 -0.1047113358 0.0000000000<br>H -3.5318823377 0.2255704498 0.7600023674<br>H -3.5318823377 0.2255704498 -0.7600023674 |
| HCCI:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-714.14867959<br>C -0.0000000000 0.0000000000 -2.3085101998<br>I -0.0000000000 0.0000000000 -0.3030478568<br>C 0.0000000000 0.0000000000 -3.5184123289<br>H 0.0000000000 0.0000000000 -4.5818835543<br>P 0.0000000000 0.0000000000 3.2592242722<br>H 1.1979726035 0.0000000000 4.0059954936<br>H -0.5989863018 1.0374747077 4.0059954936<br>H -0.5989863018 -1.0374747077 4.0059954936 |
| HCCI:SH2 | CCSD(T)-F12C/USERDEF ENERGY=-770.39488746<br>H -4.6312476187 -0.1091001344 0.0000000000<br>C -3.5680925623 -0.0761153352 0.0000000000<br>C -2.3587987351 -0.0394652923 0.0000000000<br>I -0.3561922893 0.0243868427 0.0000000000<br>S 3.1784854928 0.0574772079 0.0000000000<br>H 3.2699907613 -0.8635664194 0.9653739949<br>H 3.2699907613 -0.8635664194 -0.9653739949 |

## Complexes B···BrF.

| | |
|---|---|
| HCCI | CCSD(T)-F12C/USERDEF ENERGY=-515.41062412<br>Br 0.0000000000 0.0000000000 -0.3376893193<br>F 0.0000000000 0.0000000000 1.4202629228 |
| FBr:CO | CCSD(T)-F12C/USERDEF ENERGY=-628.60550772<br>F 0.0000000000 0.0000000000 -2.2143721024<br>Br 0.0000000000 0.0000000000 -0.4368891507<br>C 0.0000000000 0.0000000000 2.1045215441<br>O 0.0000000000 0.0000000000 3.2314534310 |
| FBr:C2H4 | CCSD(T)-F12C/USERDEF ENERGY=-593.88206026<br>F 0.0000000000 0.0000000000 -2.1026992379<br>Br 0.0000000000 0.0000000000 -0.3050797228<br>C 0.0000000000 0.6723914512 2.2904079824<br>C 0.0000000000 -0.6723914512 2.2904079824<br>H -0.9241458667 1.2342671474 2.3078846775<br>H 0.9241458667 1.2342671474 2.3078846775<br>H 0.9241458667 -1.2342671474 2.3078846775<br>H -0.9241458667 -1.2342671474 2.3078846775 |
| FBr:C2H2 | CCSD(T)-F12C/USERDEF ENERGY=-592.62710450<br>F 0.0000000000 0.0000000000 -2.0855380337 |

| | | | | |
|---|---|---|---|---|
| | Br | 0.0000000000 | 0.0000000000 | -0.3067683959 |
| | C | 0.0000000000 | 0.6043132109 | 2.4613263465 |
| | C | 0.0000000000 | -0.6043132109 | 2.4613263465 |
| | H | 0.0000000000 | 1.6685118171 | 2.4842413459 |
| | H | 0.0000000000 | -1.6685118171 | 2.4842413459 |
| FBr:N2 | CCSD(T)-F12C/USERDEF ENERGY=-624.81905587 | | | |
| | F | 0.0000000000 | 0.0000000000 | -2.2460928460 |
| | Br | 0.0000000000 | 0.0000000000 | -0.4842278466 |
| | N | 0.0000000000 | 0.0000000000 | 2.3552448112 |
| | N | 0.0000000000 | 0.0000000000 | 3.4536836958 |
| FBr:NCH | CCSD(T)-F12C/USERDEF ENERGY=-608.72231796 | | | |
| | F | 0.0000000000 | 0.0000000000 | -2.1831223339 |
| | Br | 0.0000000000 | 0.0000000000 | -0.4052269572 |
| | N | 0.0000000000 | 0.0000000000 | 2.1381451107 |
| | C | 0.0000000000 | 0.0000000000 | 3.2898842308 |
| | H | 0.0000000000 | 0.0000000000 | 4.3573388007 |
| FBr:NH3 | CCSD(T)-F12C/USERDEF ENERGY=-571.92713909 | | | |
| | F | 0.0000000000 | 0.0000000000 | -1.8721680477 |
| | Br | 0.0000000000 | 0.0000000000 | -0.0537797602 |
| | N | 0.0000000000 | 0.0000000000 | 2.2780588271 |
| | H | 0.9479801286 | 0.0000000000 | 2.6315503032 |
| | H | -0.4739900643 | 0.8209748737 | 2.6315503032 |
| | H | -0.4739900643 | -0.8209748737 | 2.6315503032 |
| FBr:OH2 | CCSD(T)-F12C/USERDEF ENERGY=-591.78259009 | | | |
| | F | 1.9762270301 | 0.0386786547 | 0.0000000000 |
| | Br | 0.1998814921 | -0.0206014753 | 0.0000000000 |
| | O | -2.3150957069 | -0.0767148088 | 0.0000000000 |
| | H | -2.6510994877 | 0.3993172047 | 0.7629610535 |
| | H | -2.6510994877 | 0.3993172047 | -0.7629610535 |
| FBr:PH3 | CCSD(T)-F12C/USERDEF ENERGY=-858.13480678 | | | |
| | F | 0.0000000000 | 0.0000000000 | -2.2441556854 |
| | Br | 0.0000000000 | 0.0000000000 | -0.3698040132 |
| | P | 0.0000000000 | 0.0000000000 | 2.0645548026 |
| | H | 1.2380306590 | 0.0000000000 | 2.7240936997 |
| | H | -0.6190153295 | 1.0721660013 | 2.7240936997 |
| | H | -0.6190153295 | -1.0721660013 | 2.7240936997 |

## Complexes B···HCN

| | | | | |
|---|---|---|---|---|
| NCH:N2 | N | 0.0000000000 | 0.0000000000 | -1.3722450524 |
| | C | 0.0000000000 | 0.0000000000 | -0.2169612492 |
| | H | 0.0000000000 | 0.0000000000 | 0.8511397654 |
| | N | 0.0000000000 | 0.0000000000 | 3.3414037302 |
| | N | 0.0000000000 | 0.0000000000 | 4.4400774247 |
| NCH:CO | N | 0.0000000000 | 0.0000000000 | -1.4028896314 |
| | C | 0.0000000000 | 0.0000000000 | -0.2475131425 |
| | H | 0.0000000000 | 0.0000000000 | 0.8217196563 |
| | C | 0.0000000000 | 0.0000000000 | 3.3717401885 |
| | O | 0.0000000000 | 0.0000000000 | 4.5003575480 |

| | | | | |
|---|---|---|---|---|
| NCH:PH3 | N | 0.0000000000 | 0.0000000000 | 1.3483995452 |
| | C | 0.0000000000 | 0.0000000000 | 0.1928062724 |
| | H | -0.0000000000 | 0.0000000000 | -0.8788016271 |
| | P | -0.0000000000 | 0.0000000000 | -3.6987838636 |
| | H | 1.1976536451 | 0.0000000000 | -4.4452654095 |
| | H | -0.5988268226 | -1.0371984816 | -4.4452654095 |
| | H | -0.5988268226 | 1.0371984816 | -4.4452654095 |
| NCH:C2H2 | C | 0.0000000000 | 0.6029721237 | -0.0102526191 |
| | C | 0.0000000000 | -0.6029721237 | -0.0102526191 |
| | H | 0.0000000000 | 1.6669662198 | -0.0202295286 |
| | H | 0.0000000000 | -1.6669662198 | -0.0202295286 |
| | H | 0.0000000000 | 0.0000000000 | 2.5524634145 |
| | C | 0.0000000000 | 0.0000000000 | 3.6231863839 |
| | N | 0.0000000000 | 0.0000000000 | 4.7787185815 |
| NCH:C2H4 | C | -0.0097590785 | 0.6673412265 | 0.0000000000 |
| | C | -0.0097590785 | -0.6673412265 | 0.0000000000 |
| | H | -0.0152691214 | 1.2317382976 | 0.9236043120 |
| | H | -0.0152691214 | 1.2317382976 | -0.9236043120 |
| | H | -0.0152691214 | -1.2317382976 | 0.9236043120 |
| | H | -0.0152691214 | -1.2317382976 | -0.9236043120 |
| | H | 2.6040046632 | 0.0000000000 | 0.0000000000 |
| | C | 3.6748282148 | 0.0000000000 | 0.0000000000 |
| | N | 4.8303720756 | 0.0000000000 | 0.0000000000 |
| NCH:NCH | N | 0.0000000000 | 0.0000000000 | -3.6841007575 |
| | C | 0.0000000000 | 0.0000000000 | -2.5284058081 |
| | H | 0.0000000000 | 0.0000000000 | -1.4555059138 |
| | N | 0.0000000000 | 0.0000000000 | 0.7625672393 |
| | C | 0.0000000000 | 0.0000000000 | 1.9160545306 |
| | H | 0.0000000000 | 0.0000000000 | 2.9833567472 |
| NCH:OH2 | N | 0.0000000000 | 0.0593680336 | 1.1546691136 |
| | C | 0.0000000000 | -0.0053534964 | 0.0007467906 |
| | H | 0.0000000000 | -0.0651614667 | -1.0719959108 |
| | O | 0.0000000000 | -0.1677950296 | -3.1245573680 |
| | H | 0.7604499900 | -0.1976439196 | -3.7068559209 |
| | H | -0.7604499900 | -0.1976439196 | -3.7068559209 |
| NCH:NH3 | N | 0.0000000000 | 0.0000000000 | 1.2754701741 |
| | C | -0.0000000000 | 0.0000000000 | 0.1191970414 |
| | H | -0.0000000000 | 0.0000000000 | -0.9623684769 |
| | N | -0.0000000000 | 0.0000000000 | -3.0810425497 |
| | H | 0.9364180618 | 0.0000000000 | -3.4668343540 |
| | H | -0.4682090309 | -0.8109618300 | -3.4668343540 |
| | H | -0.4682090309 | 0.8109618300 | -3.4668343540 |

## Complexes B···HCCH

| | | | | |
|---|---|---|---|---|
| HCCH:N2 | H | 0.0000000000 | 0.0000000000 | -4.1001357383 |
| | C | 0.0000000000 | 0.0000000000 | -3.0370556549 |
| | C | 0.0000000000 | 0.0000000000 | -1.8314597384 |
| | H | 0.0000000000 | 0.0000000000 | -0.7675774582 |

| | | | | |
|---|---|---|---|---|
| | N | 0.0000000000 | 0.0000000000 | 1.8503734208 |
| | N | 0.0000000000 | 0.0000000000 | 2.9492236801 |
| HCCH:CO | H | 0.0000000000 | 0.0000000000 | -4.1314927618 |
| | C | 0.0000000000 | 0.0000000000 | -3.0684392910 |
| | C | 0.0000000000 | 0.0000000000 | -1.8626815198 |
| | H | 0.0000000000 | 0.0000000000 | -0.7980917383 |
| | C | 0.0000000000 | 0.0000000000 | 1.8972585391 |
| | O | 0.0000000000 | 0.0000000000 | 3.026815283 |
| HCCH:PH3 | H | 0.0000000000 | 0.0000000000 | 2.5377316899 |
| | C | 0.0000000000 | 0.0000000000 | 1.4747249882 |
| | C | -0.0000000000 | 0.0000000000 | 0.2687318890 |
| | H | -0.0000000000 | 0.0000000000 | -0.7970820876 |
| | P | -0.0000000000 | 0.0000000000 | -3.7833724674 |
| | H | 1.1938674440 | 0.0000000000 | -4.5383033045 |
| | H | -0.5969337221 | -1.0339195353 | -4.5383033046 |
| | H | -0.5969337221 | 1.0339195353 | -4.5383033046 |
| HCCH:C2H2 | C | 0.0000000000 | 0.6028196059 | -0.0814353801 |
| | C | 0.0000000000 | -0.6028196059 | -0.0814353801 |
| | H | 0.0000000000 | 1.6664459751 | -0.0834574427 |
| | H | 0.0000000000 | -1.6664459751 | -0.0834574427 |
| | H | 0.0000000000 | 0.0000000000 | 2.6131912649 |
| | C | 0.0000000000 | 0.0000000000 | 3.6786717942 |
| | C | 0.0000000000 | 0.0000000000 | 4.8846396633 |
| | H | 0.0000000000 | 0.0000000000 | 5.9476870077 |
| HCCH:C2H4 | C | -0.0746736864 | 0.6670034778 | 0.0000000000 |
| | C | -0.0746736864 | -0.6670034778 | 0.0000000000 |
| | H | -0.0763450489 | 1.2313079659 | 0.9235089741 |
| | H | -0.0763450489 | 1.2313079659 | -0.9235089741 |
| | H | -0.0763450489 | -1.2313079659 | 0.9235089741 |
| | H | -0.0763450489 | -1.2313079659 | -0.9235089741 |
| | H | 2.6829766937 | 0.0000000000 | 0.0000000000 |
| | C | 3.7484734915 | 0.0000000000 | 0.0000000000 |
| | C | 4.9543995594 | 0.0000000000 | 0.0000000000 |
| | H | 6.0174881350 | 0.0000000000 | 0.0000000000 |
| HCCH:NCH | H | 0.0000000000 | 0.0000000000 | -4.0302052661 |
| | C | 0.0000000000 | 0.0000000000 | -2.9673069916 |
| | C | 0.0000000000 | 0.0000000000 | -1.7608886068 |
| | H | 0.0000000000 | 0.0000000000 | -0.6938001963 |
| | N | 0.0000000000 | 0.0000000000 | 1.6813499701 |
| | C | 0.0000000000 | 0.0000000000 | 2.8355593437 |
| | H | 0.0000000000 | 0.0000000000 | 3.9025380766 |
| HCCH:OH2 | H | 0.0000000000 | 0.1169579480 | 2.3157978973 |
| | C | 0.0000000000 | 0.0623900842 | 1.2542441023 |
| | C | 0.0000000000 | -0.0020545882 | 0.0494063768 |
| | H | 0.0000000000 | -0.0579863605 | -1.0170990623 |
| | O | 0.0000000000 | -0.1725279659 | -3.2133971328 |
| | H | 0.7595615643 | -0.2035044580 | -3.7969006988 |
| | H | -0.7595615643 | -0.2035044580 | -3.7969006988 |
| HCCH:NH3 | H | -0.0000000000 | 0.0000000000 | 2.4473510704 |

| | | | | |
|---|---|---|---|---|
| | C | 0.0000000000 | 0.0000000000 | 1.3844181679 |
| | C | 0.0000000000 | 0.0000000000 | 0.1772227712 |
| | H | 0.0000000000 | 0.0000000000 | -0.8946385983 |
| | N | -0.0000000000 | 0.0000000000 | -3.1818533675 |
| | H | 0.9368904155 | 0.0000000000 | -3.5655823056 |
| | H | -0.4684452077 | -0.8113709003 | -3.5655823056 |
| | H | -0.4684452077 | 0.8113709003 | -3.5655823056 |

## Complexes B···HCP

| | | | | |
|---|---|---|---|---|
| PCH:N2 | P | 0.0000000000 | 0.0000000000 | -4.2524717379 |
| | C | 0.0000000000 | 0.0000000000 | -2.7091182432 |
| | H | 0.0000000000 | 0.0000000000 | -1.6368264192 |
| | N | 0.0000000000 | 0.0000000000 | 0.9962814555 |
| | N | 0.0000000000 | 0.0000000000 | 2.0951746548 |
| PCH:CO | P | 0.0000000000 | 0.0000000000 | -4.2954597411 |
| | C | 0.0000000000 | 0.0000000000 | -2.7519071413 |
| | H | 0.0000000000 | 0.0000000000 | -1.6790304204 |
| | C | 0.0000000000 | 0.0000000000 | 1.0449134214 |
| | O | 0.0000000000 | 0.0000000000 | 2.1745235915 |
| PCH:PH3 | P | 0.0000000000 | 0.0000000000 | 1.8373116342 |
| | C | -0.0000000000 | 0.0000000000 | 0.2933428581 |
| | H | -0.0000000000 | 0.0000000000 | -0.7807509096 |
| | P | 0.0000000000 | 0.0000000000 | -3.7667848159 |
| | H | 1.1937768035 | 0.0000000000 | -4.5219512927 |
| | H | -0.5968884017 | -1.0338410382 | -4.5219512927 |
| | H | -0.5968884017 | 1.0338410382 | -4.5219512927 |
| PCH:C2H2 | C | 0.0000000000 | 0.6028278283 | -0.0452922559 |
| | C | 0.0000000000 | -0.6028278283 | -0.0452922559 |
| | H | 0.0000000000 | 1.6664252871 | -0.0482134648 |
| | H | 0.0000000000 | -1.6664252871 | -0.0482134648 |
| | H | 0.0000000000 | 0.0000000000 | 2.6554452569 |
| | C | 0.0000000000 | 0.0000000000 | 3.7291722268 |
| | P | 0.0000000000 | 0.0000000000 | 5.2730617073 |
| PCH:C2H4 | C | -0.0291432711 | 0.6669824814 | 0.0000000000 |
| | C | -0.0291432711 | -0.6669824814 | 0.0000000000 |
| | H | -0.0306694984 | 1.2313060189 | 0.9234969618 |
| | H | -0.0306694984 | 1.2313060189 | -0.9234969618 |
| | H | -0.0306694984 | -1.2313060189 | 0.9234969618 |
| | H | -0.0306694984 | -1.2313060189 | -0.9234969618 |
| | H | 2.7345969219 | 0.0000000000 | 0.0000000000 |
| | C | 3.8083968347 | 0.0000000000 | 0.0000000000 |
| | P | 5.3522927362 | 0.0000000000 | 0.0000000000 |
| PCH:NCH | P | 0.0000000000 | 0.0000000000 | -4.1467634618 |
| | C | 0.0000000000 | 0.0000000000 | -2.6022035951 |
| | H | 0.0000000000 | 0.0000000000 | -1.5272852262 |
| | N | 0.0000000000 | 0.0000000000 | 0.8598714976 |
| | C | 0.0000000000 | 0.0000000000 | 2.0141419716 |
| | H | 0.0000000000 | 0.0000000000 | 3.0811361228 |
| PCH:OH2 | P | 0.0000000000 | 0.0547876112 | 1.7830442347 |

| | | | | |
|---|---|---|---|---|
| | C | 0.0000000000 | -0.0131912975 | 0.2398400601 |
| | H | 0.0000000000 | -0.0622438235 | -0.8347543193 |
| | O | 0.0000000000 | -0.1641404460 | -3.0463481932 |
| | H | 0.7593875560 | -0.1947209213 | -3.6302349337 |
| | H | -0.7593875560 | -0.1947209213 | -3.6302349337 |
| PCH:NH3 | P | -0.0000000000 | 0.0000000000 | 1.8818291410 |
| | C | -0.0000000000 | 0.0000000000 | 0.3362532999 |
| | H | 0.0000000000 | 0.0000000000 | -0.7432301415 |
| | N | -0.0000000000 | 0.0000000000 | -3.0402858093 |
| | H | 0.9368521161 | 0.0000000000 | -3.4242452572 |
| | H | -0.4684260581 | -0.8113377321 | -3.4242452572 |
| | H | -0.4684260581 | 0.8113377321 | -3.4242452572 |
| PCH:SH2 | P | 0.0000000000 | 0.0452430699 | 1.9531502342 |
| | C | 0.0000000000 | 0.1034398719 | 0.4102514178 |
| | H | 0.0000000000 | 0.1428735827 | -0.6633866383 |
| | S | 0.0000000000 | 0.0008847225 | -3.5293709848 |
| | H | 0.9648907882 | -0.9176180775 | -3.6401259166 |
| | H | -0.9648907882 | -0.9176180775 | -3.6401259166 |

## Complexes B···CuBr.

| | | | | |
|---|---|---|---|---|
| BrCu | CCSD(T)/AVTZ ENERGY=-4212.16859941 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -0.9791284158 |
| | Cu | 0.0000000000 | 0.0000000000 | 1.2311754782 |
| BrCu:CO | CCSD(T)/AVTZ ENERGY=-4325.38500938 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.5818762108 |
| | Cu | 0.0000000000 | 0.0000000000 | 0.6238188127 |
| | C | 0.0000000000 | 0.0000000000 | 2.4497759553 |
| | O | 0.0000000000 | 0.0000000000 | 3.5834335962 |
| BrCu:C2H4 | CCSD(T)/AVTZ ENERGY=-4290.66518670 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.5041060890 |
| | Cu | 0.0000000000 | 0.0000000000 | 0.7126982332 |
| | C | 0.0000000000 | 0.6850734324 | 2.6575428865 |
| | C | 0.0000000000 | -0.6850734324 | 2.6575428865 |
| | H | -0.9250185030 | 1.2457841569 | 2.7420966988 |
| | H | 0.9250185030 | 1.2457841569 | 2.7420966988 |
| | H | 0.9250185030 | -1.2457841569 | 2.7420966988 |
| | H | -0.9250185030 | -1.2457841569 | 2.7420966988 |
| BrCu:C2H2 | CCSD(T)/AVTZ ENERGY=-4289.41015098 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.4700330612 |
| | Cu | 0.0000000000 | 0.0000000000 | 0.7464387300 |
| | C | 0.0000000000 | 0.6159176017 | 2.6733673126 |
| | C | 0.0000000000 | -0.6159176017 | 2.6733673126 |
| | H | 0.0000000000 | 1.6652159419 | 2.8814694347 |
| | H | 0.0000000000 | -1.6652159419 | 2.8814694347 |
| BrCu:N2 | CCSD(T)/AVTZ ENERGY=-4321.58212839 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.5699983008 |

| | | | | |
|---|---|---|---|---|
| | Cu | 0.0000000000 | 0.0000000000 | 0.6299786780 |
| | N | 0.0000000000 | 0.0000000000 | 2.4967946765 |
| | N | 0.0000000000 | 0.0000000000 | 3.6014668091 |
| BrCu:NCH | CCSD(T)/AVTZ ENERGY=-4305.50315828 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.5627648365 |
| | Cu | 0.0000000000 | 0.0000000000 | 0.6456587914 |
| | N | 0.0000000000 | 0.0000000000 | 2.5064370537 |
| | C | 0.0000000000 | 0.0000000000 | 3.6606357660 |
| | H | 0.0000000000 | 0.0000000000 | 4.7297655298 |
| BrCu:NH3 | CCSD(T)/AVTZ ENERGY=-4268.71203133 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -1.3226376751 |
| | Cu | -0.0000000000 | 0.0000000000 | 0.8868720224 |
| | N | 0.0000000000 | 0.0000000000 | 2.8288326505 |
| | H | 0.9426687608 | 0.0000000000 | 3.2092720369 |
| | H | -0.4713343804 | 0.8163750942 | 3.2092720369 |
| | H | -0.4713343804 | -0.8163750942 | 3.2092720369 |
| BrCu:OH2 | CCSD(T)/AVTZ ENERGY=-4288.55235807 | | | |
| | Cu | 0.0000000000 | 0.0159412252 | -0.8668533109 |
| | Br | 0.0000000000 | -0.0069250451 | 1.3356393335 |
| | O | 0.0000000000 | 0.0189508743 | -2.8192081150 |
| | H | 0.7704167639 | -0.3784277391 | -3.2403845954 |
| | H | -0.7704167639 | -0.3784277391 | -3.2403845954 |
| BrCu:PH3 | CCSD(T)/AVTZ ENERGY=-4554.92133055 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -1.6491378038 |
| | Cu | -0.0000000000 | 0.0000000000 | 0.5708473286 |
| | P | 0.0000000000 | 0.0000000000 | 2.7484465065 |
| | H | 1.2326453019 | 0.0000000000 | 3.4287491530 |
| | H | -0.6163226509 | 1.0675021453 | 3.4287491530 |
| | H | -0.6163226509 | -1.0675021453 | 3.4287491530 |
| BrCu:SH2 | CCSD(T)/AVTZ ENERGY=-4611.15594868 | | | |
| | Cu | 0.0000000000 | 0.0108611295 | -0.5715423659 |
| | Br | 0.0000000000 | -0.0055307095 | 1.6433539316 |
| | S | 0.0000000000 | 0.0455346736 | -2.7726659457 |
| | H | 0.9755899011 | -0.8473208483 | -3.0258007167 |
| | H | -0.9755899011 | -0.8473208483 | -3.0258007167 |

## Complexes B···AgBr.

| | | | | |
|---|---|---|---|---|
| BrAg | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2719.16426877 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.3864975177 |
| | Ag | 0.0000000000 | 0.0000000000 | 1.0270561449 |
| BrAg:CO | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2832.36371533 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.8505728385 |
| | Ag | 0.0000000000 | 0.0000000000 | 0.5354952640 |
| | C | 0.0000000000 | 0.0000000000 | 2.5710431875 |
| | O | 0.0000000000 | 0.0000000000 | 3.7016676956 |
| BrAg:C2H4 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2797.64853785 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.7979634531 |
| | Ag | 0.0000000000 | 0.0000000000 | 0.6031326335 |
| | C | 0.0000000000 | 0.6813326807 | 2.7923355997 |

| | | | | |
|---|---|---|---|---|
| | C | 0.0000000000 | -0.6813326807 | 2.7923355997 |
| | H | -0.9257331566 | 1.2419805603 | 2.8593354884 |
| | H | 0.9257331566 | 1.2419805603 | 2.8593354884 |
| | H | 0.9257331566 | -1.2419805603 | 2.8593354884 |
| | H | -0.9257331566 | -1.2419805603 | 2.8593354884 |
| BrAg:C2H2 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2796.39140181 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.7732052050 |
| | Ag | 0.0000000000 | 0.0000000000 | 0.6262950368 |
| | C | 0.0000000000 | 0.6118759370 | 2.8363802621 |
| | C | 0.0000000000 | -0.6118759370 | 2.8363802621 |
| | H | 0.0000000000 | 1.6713083212 | 2.9730657341 |
| | H | 0.0000000000 | -1.6713083212 | 2.9730657341 |
| BrAg:N2 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2828.56344616 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.8571704359 |
| | Ag | 0.0000000000 | 0.0000000000 | 0.5315923377 |
| | N | 0.0000000000 | 0.0000000000 | 2.6990027314 |
| | N | 0.0000000000 | 0.0000000000 | 3.8017032098 |
| BrAg:NCH | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2812.48269116 | | | |
| | Br | 0.0000000000 | 0.0000000000 | -1.8443445676 |
| | Ag | 0.0000000000 | 0.0000000000 | 0.5489622258 |
| | N | 0.0000000000 | 0.0000000000 | 2.6662740475 |
| | C | 0.0000000000 | 0.0000000000 | 3.8199172940 |
| | H | 0.0000000000 | 0.0000000000 | 4.8893920745 |
| BrAg:NH3 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2775.69328225 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -1.6465262742 |
| | Ag | -0.0000000000 | 0.0000000000 | 0.7489120597 |
| | N | 0.0000000000 | 0.0000000000 | 2.9147778540 |
| | H | 0.9428031512 | 0.0000000000 | 3.2918032831 |
| | H | -0.4714015756 | 0.8164914797 | 3.2918032831 |
| | H | -0.4714015756 | -0.8164914797 | 3.2918032831 |
| BrAg:OH2 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-2795.53536915 | | | |
| | Ag | 0.0000000000 | 0.0137192602 | -0.7311711113 |
| | Br | 0.0000000000 | -0.0098233504 | 1.6635776900 |
| | O | 0.0000000000 | 0.0059606770 | -2.9530700350 |
| | H | 0.7676072738 | -0.3920442558 | -3.3777066869 |
| | H | -0.7676072738 | -0.3920442558 | -3.3777066869 |
| BrAg:PH3 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-3061.90811305 | | | |
| | Br | -0.0000000000 | 0.0000000000 | -1.9073815111 |
| | Ag | -0.0000000000 | 0.0000000000 | 0.4979218927 |
| | P | 0.0000000000 | 0.0000000000 | 2.8425866373 |
| | H | 1.2319861812 | 0.0000000000 | 3.5226560022 |
| | H | -0.6159930906 | 1.0669313301 | 3.5226560022 |
| | H | -0.6159930906 | -1.0669313301 | 3.5226560022 |
| BrAg:SH2 | CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-3118.14194803 | | | |
| | Ag | 0.0000000000 | 0.0118418645 | -0.4919975500 |
| | Br | 0.0000000000 | -0.0089924756 | 1.9099206755 |
| | S | 0.0000000000 | 0.0369962624 | -2.9083790115 |
| | H | 0.9739820787 | -0.8655902197 | -3.1235889148 |
| | H | -0.9739820787 | -0.8655902197 | -3.1235889148 |

## Complexes B···AuBr.

| | |
|---|---|
| BrAu | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2707.86345084<br>Br 0.0000000000 0.0000000000 -1.6694614349<br>Au 0.0000000000 0.0000000000 0.6772555054 |
| BrAu:CO | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2821.09823672<br>Br 0.0000000000 0.0000000000 -1.9748259165<br>Au 0.0000000000 0.0000000000 0.3830081780<br>C 0.0000000000 0.0000000000 2.2917188974<br>O 0.0000000000 0.0000000000 3.4270581431 |
| BrAu:C2H4 | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2786.37555718<br>Br 0.0000000000 0.0000000000 -1.9420728619<br>Au 0.0000000000 0.0000000000 0.4305638059<br>C 0.0000000000 0.6933485633 2.4900276961<br>C 0.0000000000 -0.6933485633 2.4900276961<br>H -0.9229722175 1.2471999826 2.6185335373<br>H 0.9229722175 1.2471999826 2.6185335373<br>H 0.9229722175 -1.2471999826 2.6185335373<br>H -0.9229722175 -1.2471999826 2.6185335373 |
| BrAu:C2H2 | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2785.11579837<br>Br 0.0000000000 0.0000000000 -1.9216226022<br>Au 0.0000000000 0.0000000000 0.4456776837<br>C 0.0000000000 0.6206224493 2.5042103026<br>C 0.0000000000 -0.6206224493 2.5042103026<br>H 0.0000000000 1.6540848244 2.7807305103<br>H 0.0000000000 -1.6540848244 2.7807305103 |
| BrAu:N2 | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2817.27971921<br>Br 0.0000000000 0.0000000000 -1.9625320053<br>Au 0.0000000000 0.0000000000 0.3776700766<br>N 0.0000000000 0.0000000000 2.3899610432<br>N 0.0000000000 0.0000000000 3.4947801309 |
| BrAu:NCH | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2801.20109575<br>Br 0.0000000000 0.0000000000 -1.9625180333<br>Au 0.0000000000 0.0000000000 0.3864863684<br>N 0.0000000000 0.0000000000 2.3903364679<br>C 0.0000000000 0.0000000000 3.5432996145<br>H 0.0000000000 0.0000000000 4.6122548699 |
| BrAu:NH3 | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2764.41393691<br>Br -0.0000000000 0.0000000000 -1.8408881319<br>Au -0.0000000000 0.0000000000 0.5157767448<br>N 0.0000000000 0.0000000000 2.6066397219<br>H 0.9471305363 0.0000000000 2.9741070909<br>H -0.4735652682 0.8202391052 2.9741070909<br>H -0.4735652682 -0.8202391052 2.9741070909 |
| BrAu:OH2 | CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-2784.24592346<br>Au 0.0000000000 0.0049717947 -0.5001942354<br>Br 0.0000000000 -0.0067273264 1.8396926514<br>O 0.0000000000 0.0275534736 -2.6519400876 |

| | | | | |
|---|---|---|---|---|
| | H | 0.7704806011 | -0.4378116538 | -3.0001009586 |
| | H | -0.7704806011 | -0.4378116538 | -3.0001009586 |
| BrAu:PH3 | Br | -0.0000000000 | 0.0000000000 | -2.0225216899 |
| | Au | -0.0000000000 | 0.0000000000 | 0.3621017613 |
| | P | 0.0000000000 | 0.0000000000 | 2.5967855460 |
| | H | 1.2402237858 | 0.0000000000 | 3.2586080775 |
| | H | -0.6201118929 | 1.0740653049 | 3.2586080775 |
| | H | -0.6201118929 | -1.0740653049 | 3.2586080775 |
| BrAu:SH2 | Au | 0.0000000000 | 0.0016589841 | -0.3545937355 |
| | Br | 0.0000000000 | -0.0032971575 | 2.0138928375 |
| | S | 0.0000000000 | 0.0505538692 | -2.6559098679 |
| | H | 0.9746269039 | -0.8353995607 | -2.9399249530 |
| | H | -0.9746269039 | -0.8353995607 | -2.9399249530 |

## Complexes B···CuI.

| | |
|---|---|
| ICu | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-1934.34695594<br>Cu 0.0000000000 0.0000000000 -1.5868187324<br>I 0.0000000000 0.0000000000 0.7945759847 |
| ICu:CO | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2047.55920007<br>I 0.0000000000 0.0000000000 -1.3185247697<br>Cu 0.0000000000 0.0000000000 1.0669025646<br>C 0.0000000000 0.0000000000 2.9059252858<br>O 0.0000000000 0.0000000000 4.0393673720 |
| ICu:C2H4 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2012.84014658<br>I 0.0000000000 0.0000000000 -1.2573353450<br>Cu 0.0000000000 0.0000000000 1.1378437219<br>C 0.0000000000 0.6843506778 3.0989563763<br>C 0.0000000000 -0.6843506778 3.0989563763<br>H -0.9252346922 1.2453745008 3.1782888026<br>H 0.9252346922 1.2453745008 3.1782888026<br>H 0.9252346922 -1.2453745008 3.1782888026<br>H -0.9252346922 -1.2453745008 3.1782888026 |
| ICu:C2H2 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2011.58504562<br>I 0.0000000000 0.0000000000 -1.2266759883<br>Cu 0.0000000000 0.0000000000 1.1681307274<br>C 0.0000000000 0.6152168040 3.1127706032<br>C 0.0000000000 -0.6152168040 3.1127706032<br>H 0.0000000000 1.6669912952 3.3071394751<br>H 0.0000000000 -1.6669912952 3.3071394751 |
| ICu:N2 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2043.75731062<br>I 0.0000000000 0.0000000000 -1.3087758973<br>Cu 0.0000000000 0.0000000000 1.0683419341<br>N 0.0000000000 0.0000000000 2.9532977929<br>N 0.0000000000 0.0000000000 4.0577663561 |
| ICu:NCH | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2027.67827436<br>I 0.0000000000 0.0000000000 -1.3004943286<br>Cu 0.0000000000 0.0000000000 1.0851175169<br>N 0.0000000000 0.0000000000 2.9594457774<br>C 0.0000000000 0.0000000000 4.1136298571<br>H 0.0000000000 0.0000000000 5.1828460590 |
| ICu:NH3 | I -0.0000000000 0.0000000000 -1.0925476437<br>Cu -0.0000000000 0.0000000000 1.2936156791<br>N 0.0000000000 0.0000000000 3.2468574276<br>H 0.9426728110 0.0000000000 3.6273111070<br>H -0.4713364055 0.8163786018 3.6273111070<br>H -0.4713364055 -0.8163786018 3.6273111070 |
| ICu:OH2 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2010.72832177<br>I 2.0862992464 0.0169157243 0.0000000000<br>Cu -0.2905270795 -0.0386843833 0.0000000000<br>O -2.2564350913 -0.0520917210 0.0000000000<br>H -2.6838769117 0.3389375008 0.7701737714<br>H -2.6838769117 0.3389375008 -0.7701737714 |
| ICu:PH3 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2277.09631571 |

| | |
|---|---|
| | I -0.0000000000 0.0000000000 -1.3833495081<br>Cu -0.0000000000 0.0000000000 1.0148278046<br>P 0.0000000000 0.0000000000 3.2063142897<br>H 1.2323913585 0.0000000000 3.8873562908<br>H -0.6161956793 1.0672822239 3.8873562908<br>H -0.6161956793 -1.0672822239 3.8873562908 |
| ICu:SH2 | CCSD(T)/AVTZ,I=AVTZ-PP ENERGY=-2333.33141805<br>I 2.4193846659 0.0103885070 0.0000000000<br>Cu 0.0282953421 -0.0383867815 0.0000000000<br>S -2.1894075167 -0.0945102993 0.0000000000<br>H -2.4430487739 0.7980554554 0.9755334219<br>H -2.4430487739 0.7980554554 -0.9755334219 |

## Complexes B···AgI.

| | |
|---|---|
| IAg | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-441.34642131<br>I 0.0000000000 0.0000000000 -1.1802783951<br>Ag 0.0000000000 0.0000000000 1.3885807109 |
| IAg:CO | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-554.54243863<br>I 0.0000000000 0.0000000000 -1.6073211588<br>Ag 0.0000000000 0.0000000000 0.9434510621<br>C 0.0000000000 0.0000000000 3.0032311797<br>O 0.0000000000 0.0000000000 4.1337523301 |
| IAg:C2H4 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-519.82791373<br>I 0.0000000000 0.0000000000 -1.5623438247<br>Ag 0.0000000000 0.0000000000 1.0003217928<br>C 0.0000000000 0.6806279024 3.2123450960<br>C 0.0000000000 -0.6806279024 3.2123450960<br>H -0.9258650110 1.2417979558 3.2740051247<br>H 0.9258650110 1.2417979558 3.2740051247<br>H 0.9258650110 -1.2417979558 3.2740051247<br>H -0.9258650110 -1.2417979558 3.2740051247 |
| IAg:C2H2 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-518.57103898<br>I 0.0000000000 0.0000000000 -1.5387023758<br>Ag 0.0000000000 0.0000000000 1.0213062922<br>C 0.0000000000 0.6112870867 3.2587761341<br>C 0.0000000000 -0.6112870867 3.2587761341<br>H 0.0000000000 1.6722151762 3.3835589434<br>H 0.0000000000 -1.6722151762 3.3835589434 |
| IAg:N2 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-550.74368289<br>I 0.0000000000 0.0000000000 -1.6114931617<br>Ag 0.0000000000 0.0000000000 0.9373815370<br>N 0.0000000000 0.0000000000 3.1395161949<br>N 0.0000000000 0.0000000000 4.2422029233 |
| IAg:NCH | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-534.66254434<br>I 0.0000000000 0.0000000000 -1.5983164891<br>Ag 0.0000000000 0.0000000000 0.9556685390<br>N 0.0000000000 0.0000000000 3.0951676759<br>C 0.0000000000 0.0000000000 4.2490138527 |

| | |
|---|---|
| | H 0.0000000000 0.0000000000 5.3185286874 |
| IAg:NH3 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-497.87310080<br>I -0.0000000000 0.0000000000 -1.4195657930<br>Ag -0.0000000000 0.0000000000 1.1356763536<br>N 0.0000000000 0.0000000000 3.3179727095<br>H 0.9428048303 0.0000000000 3.6951116117<br>H -0.4714024151 0.8164929338 3.6951116117<br>H -0.4714024151 -0.8164929338 3.6951116117 |
| IAg:OH2 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-517.71610640<br>Ag 0.0000000000 0.0169200939 -1.1183894635<br>I 0.0000000000 -0.0072896315 1.4340346710<br>O 0.0000000000 -0.0053830031 -3.3578171454<br>H 0.7674478872 -0.4037550164 -3.7824798973<br>H -0.7674478872 -0.4037550164 -3.7824798973 |
| IAg:PH3 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-784.08705700<br>I -0.0000000000 0.0000000000 -1.6624918403<br>Ag -0.0000000000 0.0000000000 0.9057550066<br>P 0.0000000000 0.0000000000 3.2713277806<br>H 1.2317451485 0.0000000000 3.9525197382<br>H -0.6158725743 1.0667225896 3.9525197382<br>H -0.6158725743 -1.0667225896 3.9525197382 |
| IAg:SH2 | CCSD(T)/AVTZ,AG=AVTZ-PP,I=AVTZ-PP ENERGY=-840.32170084<br>Ag 0.0000000000 0.0152355996 -0.8988214182<br>I 0.0000000000 -0.0068816039 1.6636927521<br>S 0.0000000000 0.0309510603 -3.3386315214<br>H 0.9739172326 -0.8742658261 -3.5422838144<br>H -0.9739172326 -0.8742658261 -3.5422838144 |

## Complexes B···AuI.

| | |
|---|---|
| IAu | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-430.05063662<br>I 0.0000000000 0.0000000000 -1.5225753616<br>Au 0.0000000000 0.0000000000 0.9809944092 |
| IAu:CO | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-543.27629118<br>I 0.0000000000 0.0000000000 -1.8207294732<br>Au 0.0000000000 0.0000000000 0.7064122588<br>C 0.0000000000 0.0000000000 2.6332947552<br>O 0.0000000000 0.0000000000 3.7684131027 |
| IAu:C2H4 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-508.55515309<br>I 0.0000000000 0.0000000000 -1.7895270861<br>Au 0.0000000000 0.0000000000 0.7476093388<br>C 0.0000000000 0.6921330558 2.8288813416<br>C 0.0000000000 -0.6921330558 2.8288813416<br>H -0.9236229311 1.2466795693 2.9493988375<br>H 0.9236229311 1.2466795693 2.9493988375<br>H 0.9236229311 -1.2466795693 2.9493988375<br>H -0.9236229311 -1.2466795693 2.9493988375 |
| IAu:C2H2 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-507.29554811<br>I 0.0000000000 0.0000000000 -1.7697480811 |

| | |
|---|---|
| | Au 0.0000000000 0.0000000000 0.7616280478<br>C 0.0000000000 0.6195416337 2.8440345486<br>C 0.0000000000 -0.6195416337 2.8440345486<br>H 0.0000000000 1.6572001904 3.1033490743<br>H 0.0000000000 -1.6572001904 3.1033490743 |
| IAu:N2 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-539.46029395<br>I 0.0000000000 0.0000000000 -1.8085189872<br>Au 0.0000000000 0.0000000000 0.6961141733<br>N 0.0000000000 0.0000000000 2.7461324363<br>N 0.0000000000 0.0000000000 3.8506857408 |
| IAu:NCH | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-523.38112761<br>I 0.0000000000 0.0000000000 -1.8061415634<br>Au 0.0000000000 0.0000000000 0.7063512009<br>N 0.0000000000 0.0000000000 2.7377838410<br>C 0.0000000000 0.0000000000 3.8910084575<br>H 0.0000000000 0.0000000000 4.9599919109 |
| IAu:NH3 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-486.59422339<br>I -0.0000000000 0.0000000000 -1.6898363093<br>Au -0.0000000000 0.0000000000 0.8287338947<br>N 0.0000000000 0.0000000000 2.9421227360<br>H 0.9470068148 0.0000000000 3.3094256868<br>H -0.4735034074 0.8201319592 3.3094256868<br>H -0.4735034074 -0.8201319592 3.3094256868 |
| IAu:OH2 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-506.42811781<br>Au 0.0000000000 0.0062954810 -0.8109525685<br>I 0.0000000000 -0.0050818197 1.6891815229<br>O 0.0000000000 0.0192128775 -2.9938980145<br>H 0.7698678860 -0.4476868674 -3.3410698399<br>H -0.7698678860 -0.4476868674 -3.3410698399 |
| IAu:PH3 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-772.81970815<br>I -0.0000000000 0.0000000000 -1.8652784417<br>Au -0.0000000000 0.0000000000 0.6846115098<br>P 0.0000000000 0.0000000000 2.9372862291<br>H 1.2394467345 0.0000000000 3.6012643313<br>H -0.6197233672 1.0733923587 3.6012643313<br>H -0.6197233672 -1.0733923587 3.6012643313 |
| IAu:SH2 | CCSD(T)/AVTZ,AU=AVTZ-PP,I=AVTZ-PP ENERGY=-829.04422952<br>Au 0.0000000000 0.0025459784 -0.6741565548<br>I 0.0000000000 -0.0026398490 1.8566099921<br>S 0.0000000000 0.0477273655 -3.0015518021<br>H 0.9746767937 -0.8416179053 -3.2729258972<br>H -0.9746767937 -0.8416179053 -3.2729258972 |