Electronic Supplementary Material (ESI) for ChemComm.


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**Supporting information**

# Theoretical rationalization for the mechanism of *N*-heterocyclic carbene-halide reductive elimination at $Cu^{III}$, $Ag^{III}$ and $Au^{III}$

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## The supporting information includes:

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## COMPUTATIONAL DETAILS

Gaussian 09[S1] was used to fully optimize all the structures reported in this paper at the B3LYP level of density functional theory (DFT)[S1] in dichloromethane using the CPCM[S2] solvation model. The effective core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ)[S3] was chosen to describe Cu, Ag, Au and I. The 6-31G(d) basis set was used for other atoms[S4]. Polarization functions were also added for Cu ($\xi_f$ = 3.525) and I ($\xi_d$= 0.289)[S5]. This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for the structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC)[S6] calculations were used to confirm the connectivity between transition structures and minima. To further refine the energies obtained from the B3LYP/BS1 calculations, we carried out single-point energy calculations for all of the structures with a larger basis set (BS2) in dichloromethane using the CPCM solvation model at the M06[S7] levels. BS2 utilizes the quadrupole-ξ valence polarized def2-QZVP[S8] basis set on I, Au, Ag and Cu and the 6-311+G(2d,p) basis set on other atoms. An effective core potential including scalar relativistic effect was used for I, Au, and Ag atoms[S10]. All thermodynamic data were calculated at the standard state (298.15 K and 1 atm). To estimate the corresponding Gibbs free energies in dichloromethane, entropy corrections were calculated at the B3LYP/BS1 level and added to the single point potential energies[S11].

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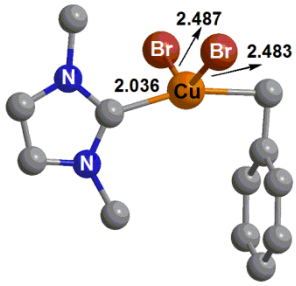
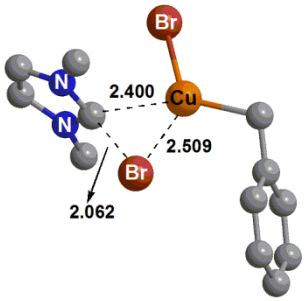



$Cu^{III}$_Bn_Br

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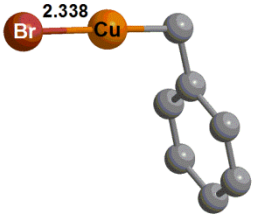


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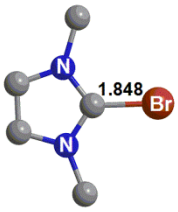
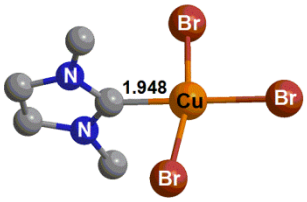



prod_Br

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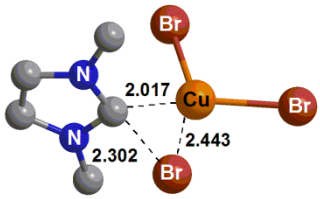


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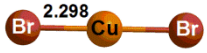


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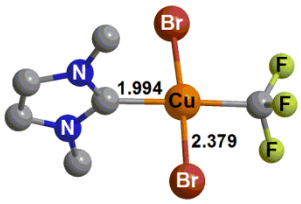


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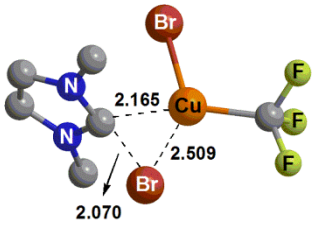


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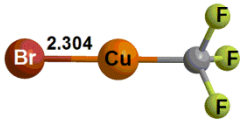


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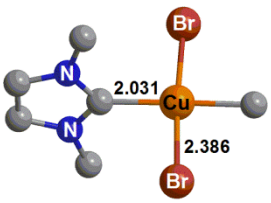


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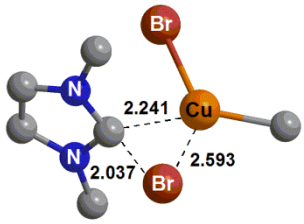


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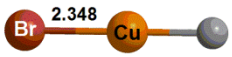


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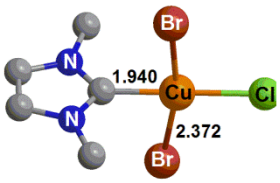


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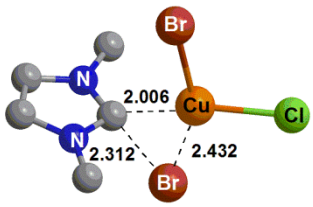


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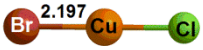


$Cu^{I}$_Cl

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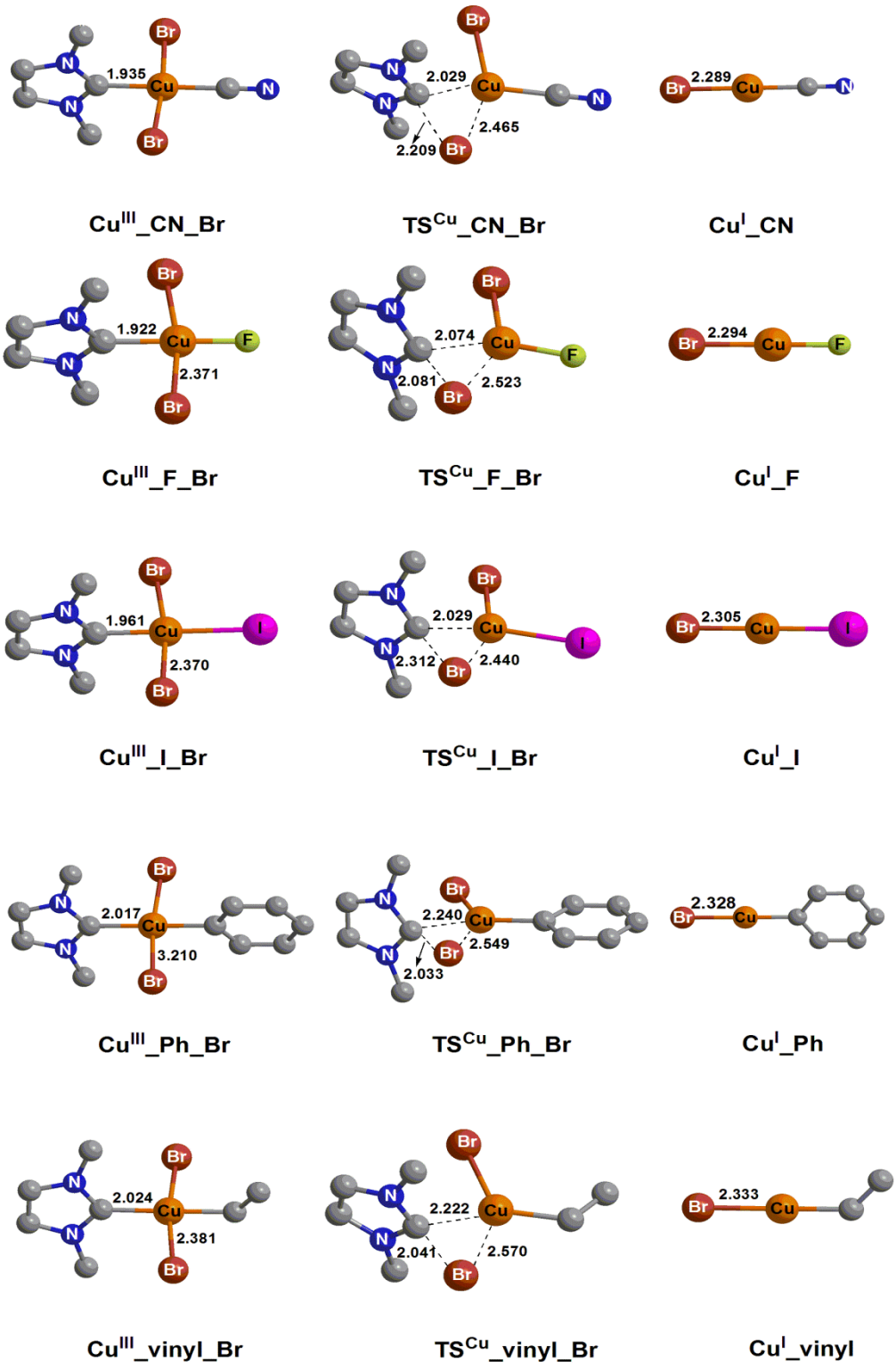


**Figure S1.** Optimized structures of intermediates, transition states and products for NHC-Br reductive elimination from trans-(NHC)Cu(Br)$_2$X complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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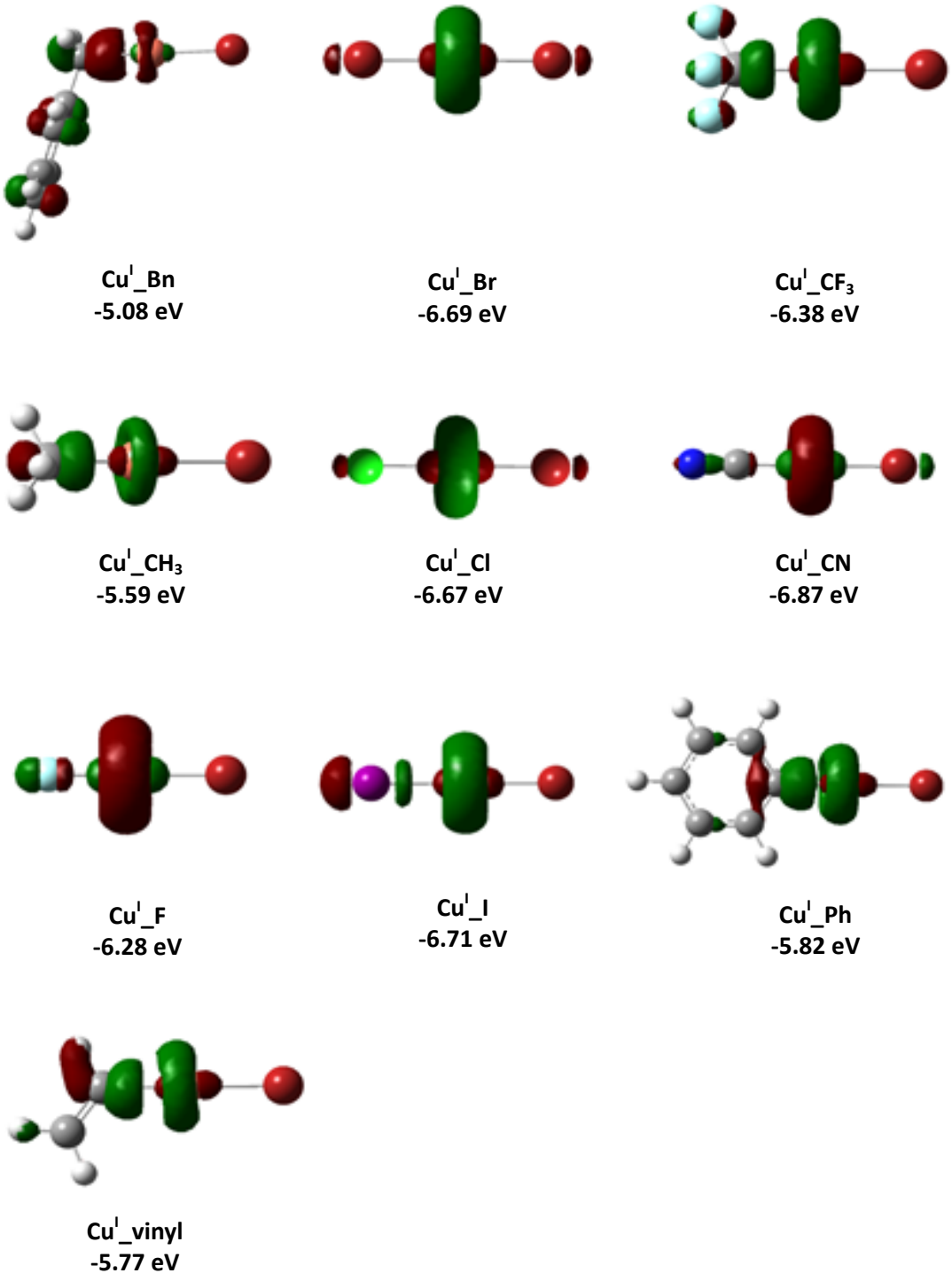
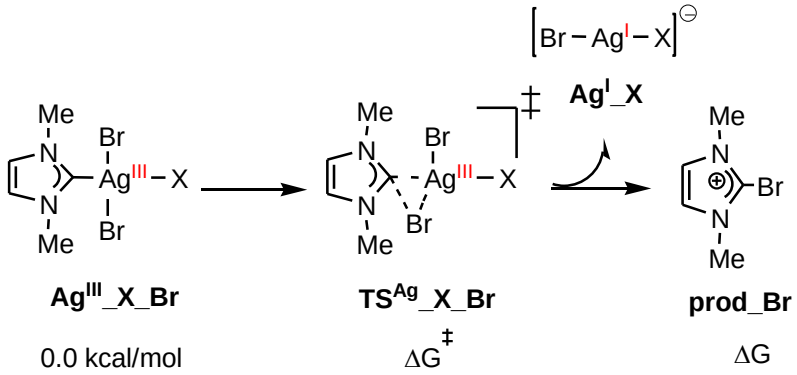



**Figure S2.** Spatial plots and energies (eV) of the s-$d_z^2$ hybrid orbital for **Cu$^{I}$_X** complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.




(S1)

**Table S1.** Calculated Gibbs activation energy ($\Delta G^{\ddagger}$), the reaction Gibbs energy ($\Delta G$), the HOMO energy of **$Ag^{I}$_X**.

| X | $\Delta G^{\ddagger}$ (kcal/mol) | $\Delta G$ (kcal/mol) | HOMO energy of **$Ag^{I}$_X** (eV) |
|---|---|---|---|
| Bn | 33 | 9 | -4.99 |
| $CH_3$ | 31.2 | 5.1 | -5.57 |
| vinyl | 29.8 | 2.1 | -5.74 |
| Ph | 26.7 | 1.6 | -5.78 |
| $CF_3$ | 18 | -10 | -6.39 |
| I | 12.3 | -21 | -6.69 |
| CN | 11.9 | -22.3 | -6.98 |
| F | 9.3 | -17.4 | -6.63 |
| Br | 8.3 | -23 | -6.88 |
| Cl | 7.6 | -22.7 | -6.89 |

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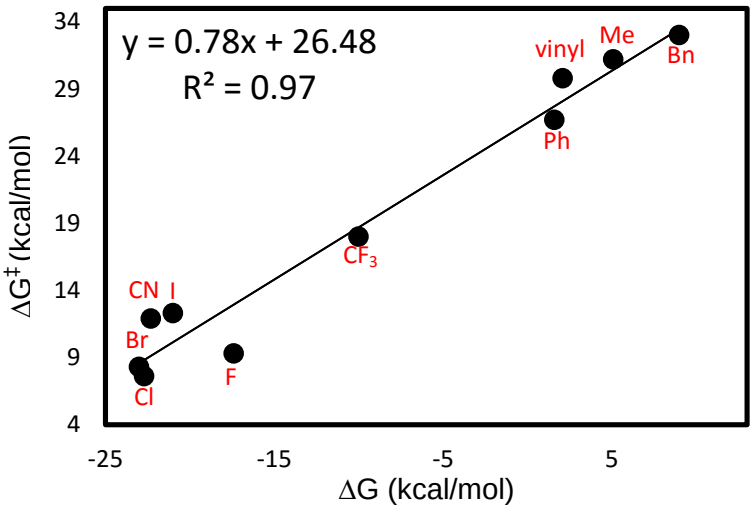



**Figure S3.** Plot of $\Delta G^{\ddagger}$ versus $\Delta G$ for reductive elimination of NHC-Br from trans-(NHC)Ag$(Br)_2$X complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

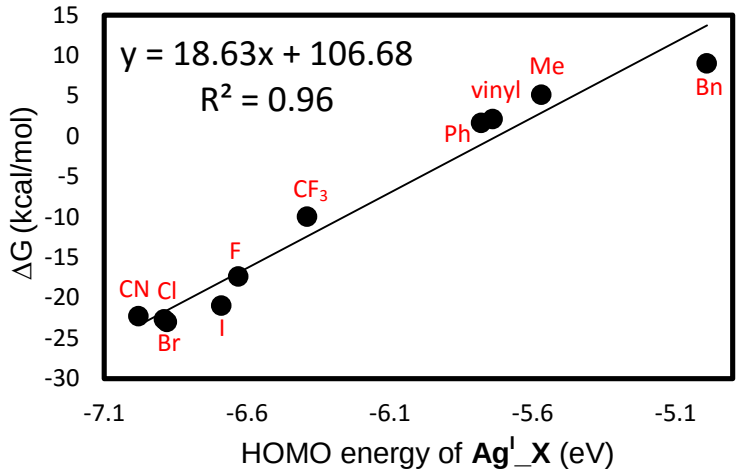
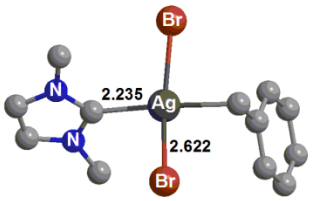



**Figure S4.** Plot of $\Delta G$ versus the HOMO energy of $Ag^{I}(Br)(X)$ complex where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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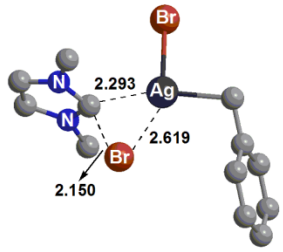


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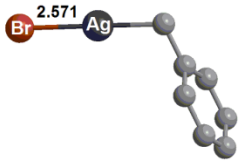


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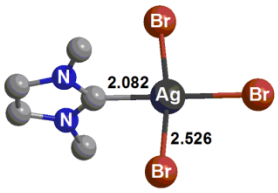


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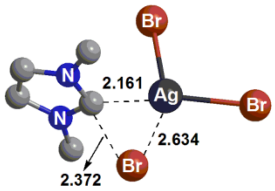


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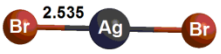


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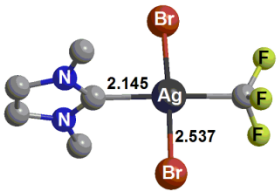


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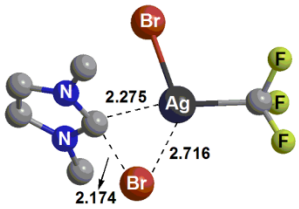


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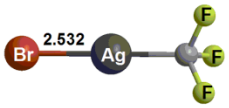


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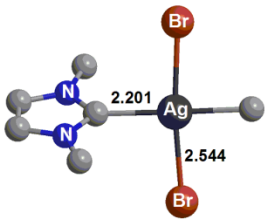
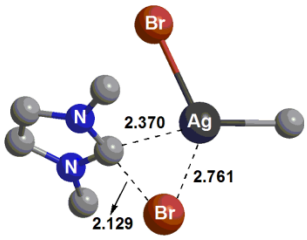



$Ag^{III}$_$CH_3$_Br

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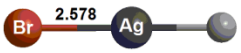


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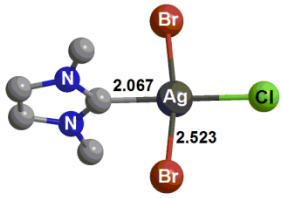


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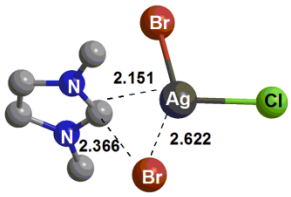
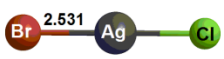



$TS^{Ag}$_Cl_Br




$Ag^{I}$_Cl

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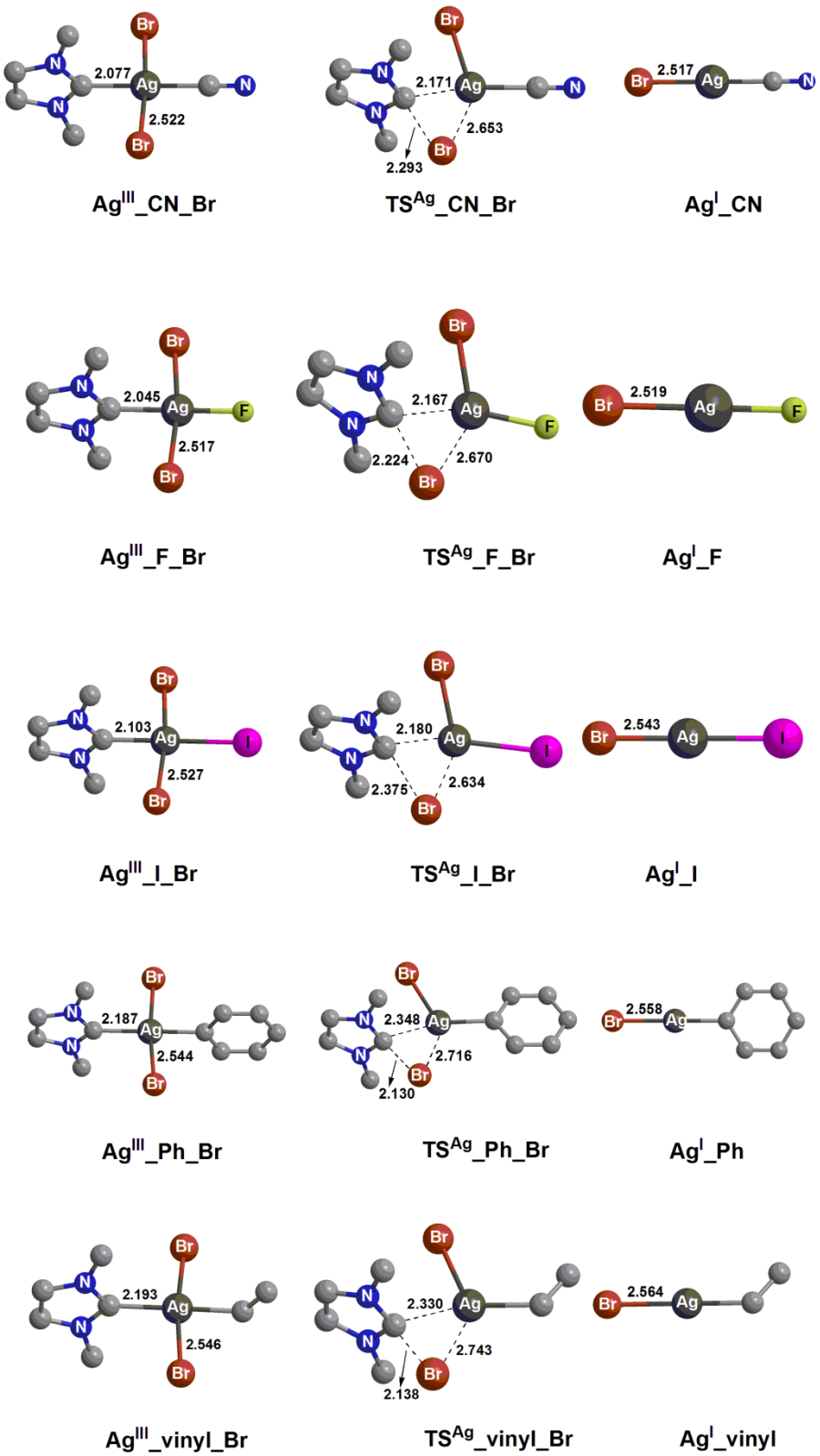


**Figure S5.** Optimized structures of intermediates, transition states and products for NHC-Br reductive elimination from trans-(NHC)Ag(Br)$_2$X complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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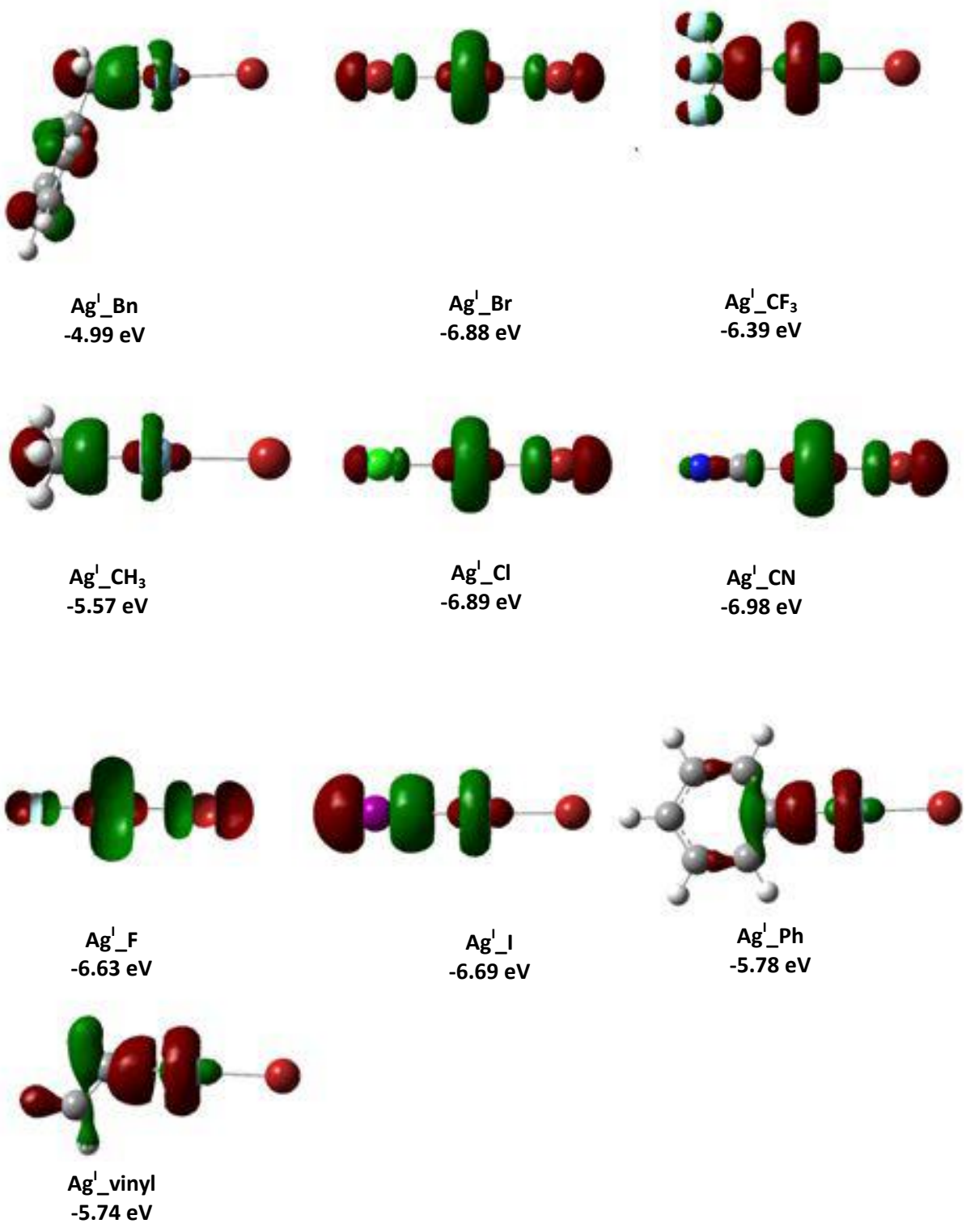


**Figure S6.** Spatial plots and energies (eV) of the s-$d_z^2$ hybrid orbital for **Ag$^{I}$_X** complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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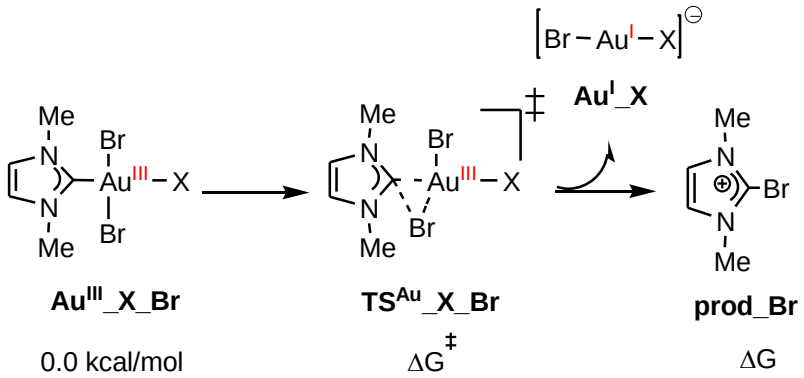


(S2)

**Table S2**. Calculated Gibbs activation energy ($\Delta G^{‡}$), the reaction Gibbs energy ($\Delta G$), the HOMO energy of **Au$^{I}$_X**.

| X | $\Delta G^{‡}$ (kcal/mol) | $\Delta G$ (kcal/mol) | HOMO energy of **Au$^{I}$_X** (eV) |
|---|---|---|---|
| Bn | 44.7 | 14.9 | -5.48 |
| Ph | 44.7 | 11.8 | -6.21 |
| vinyl | 44.2 | 11.2 | -6.16 |
| $CH_3$ | 43.8 | 13.8 | -6.08 |
| $CF_3$ | 39.1 | 4.5 | -6.64 |
| F | 31.9 | 7.7 | -6.80 |
| CN | 30.8 | -3.1 | -7.23 |
| I | 26.9 | 0.1 | -7.02 |
| Cl | 26.3 | 0 | -7.05 |
| Br | 26.3 | -0.4 | -7.06 |

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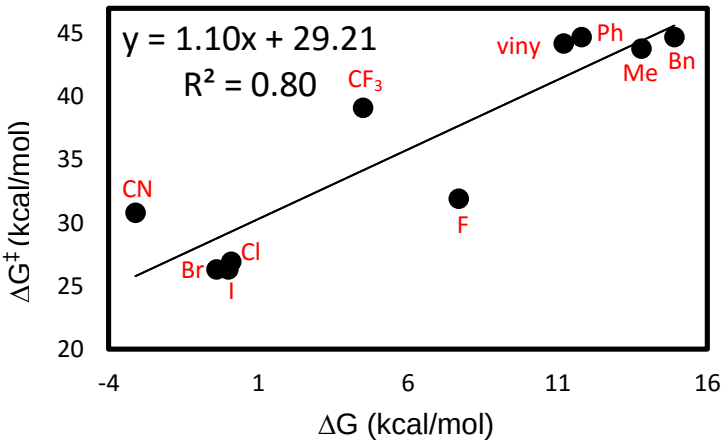



**Figure S7.** Plot of $\Delta G^{\ddagger}$ versus $\Delta G$ for reductive elimination of NHC-Br from trans-(NHC)Au$(Br)_2$X complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

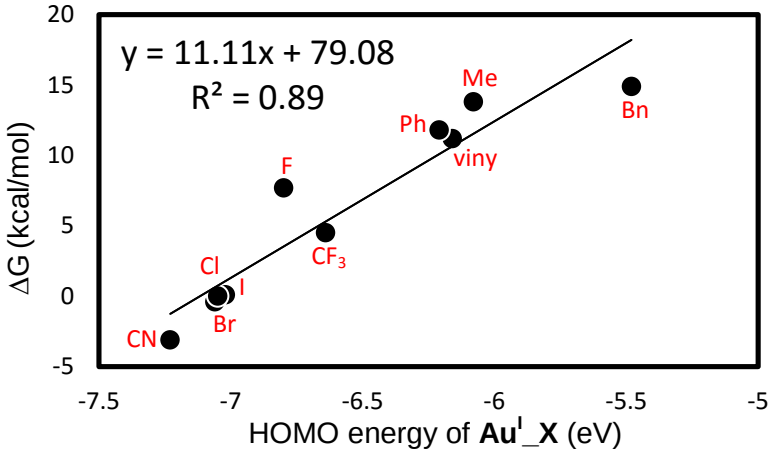
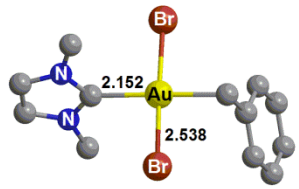
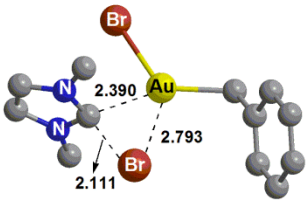


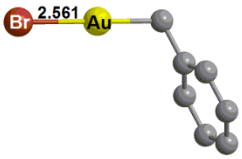

**Figure S8.** Plot of $\Delta G$ versus the HOMO energy of $Au^{I}(Br)(X)$ complex where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.



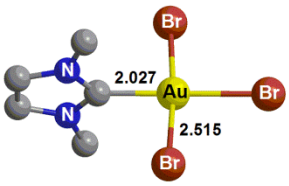

$Au^{III}$_Bn_Br



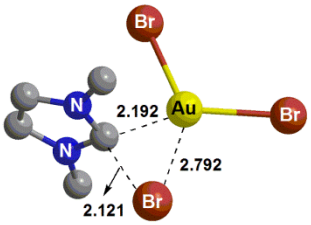

$TS^{Au}$_Bn_Br



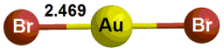

$Au^{I}$_Bn



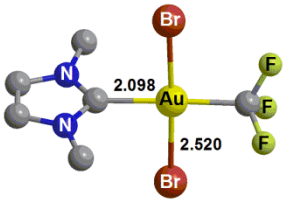

$Au^{III}$_Br_Br



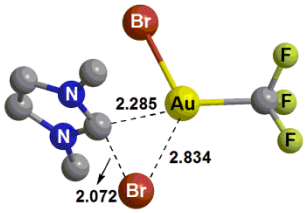

$TS^{Au}$_Br_Br



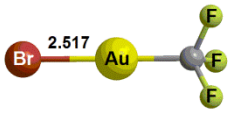

$Au^{I}$_Br



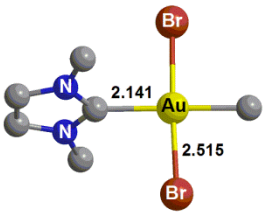

$Au^{III}$_$CF_3$_Br



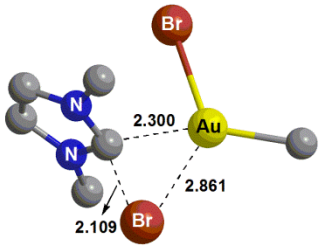

$TS^{Au}$_$CF_3$_Br



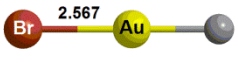

$Au^{I}$_$CF_3$



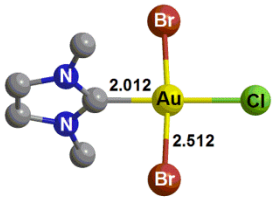

$Au^{III}$_$CH_3$_Br



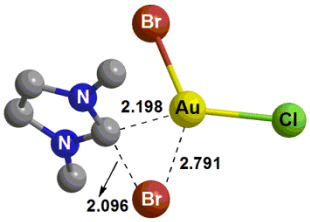

$TS^{Au}$_$CH_3$_Br



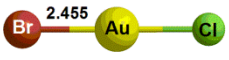

$Au^{I}$_$CH_3$




$Au^{III}$_Cl_Br




$TS^{Au}$_Cl_Br




$Au^{I}$_Cl

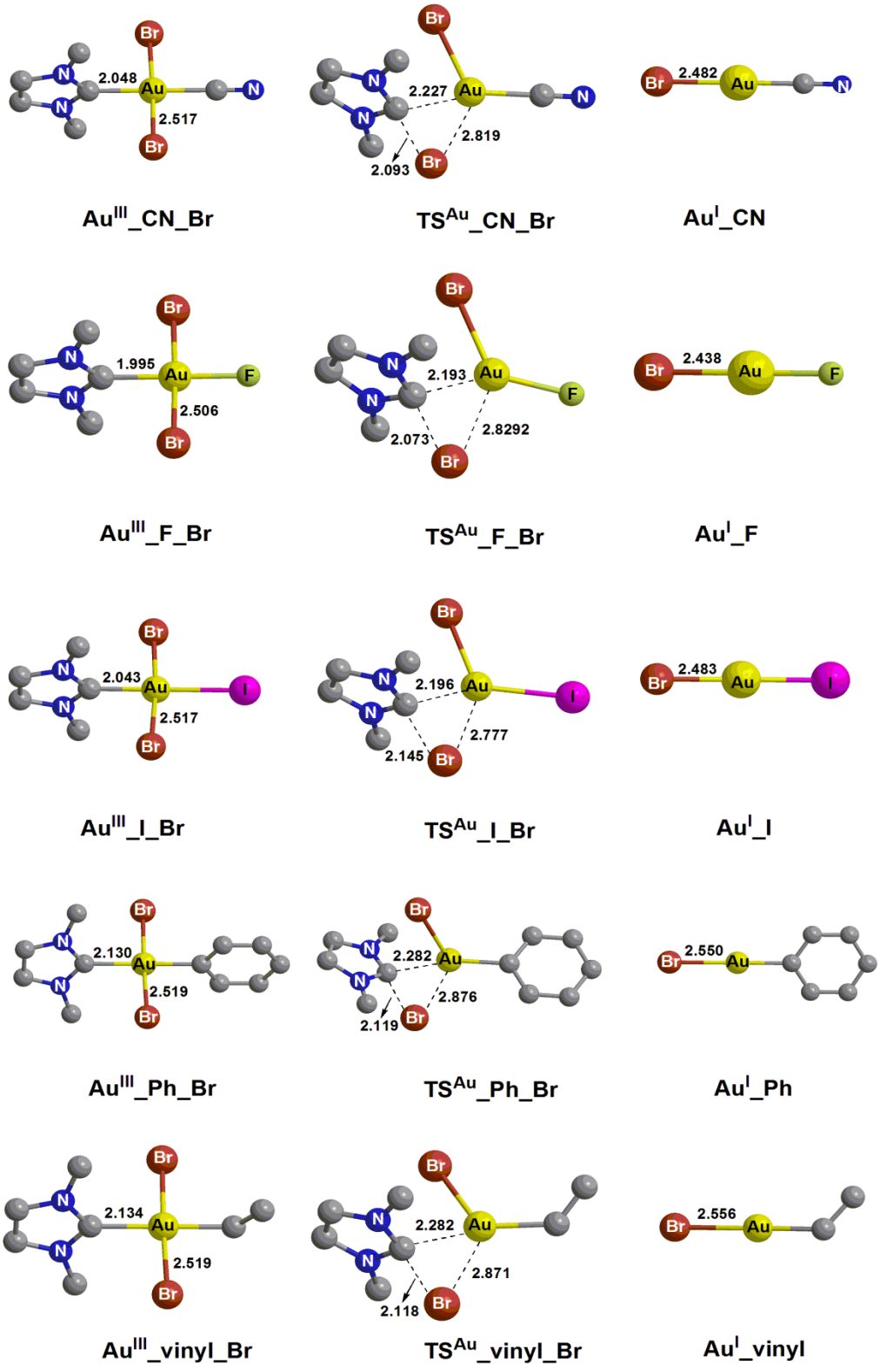



**Figure S9.** Optimized structures of intermediates, transition states and products for NHC-Br reductive elimination from trans-(NHC)Au(Br)$_2$X complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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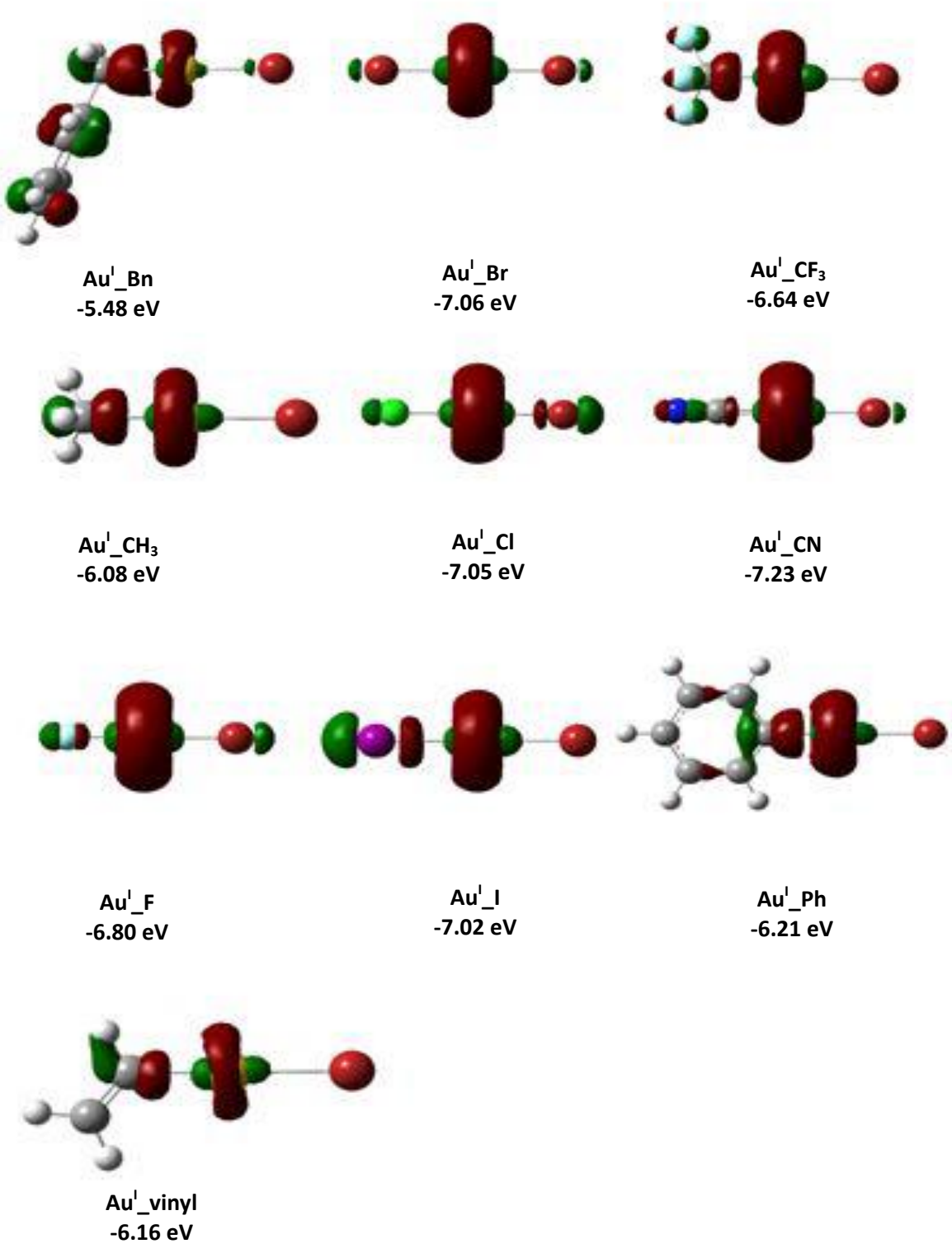


**Figure S10.** Spatial plots and energies (eV) of the s-$d_z^2$ hybrid orbital for **Au$^{I}$_X** complexes where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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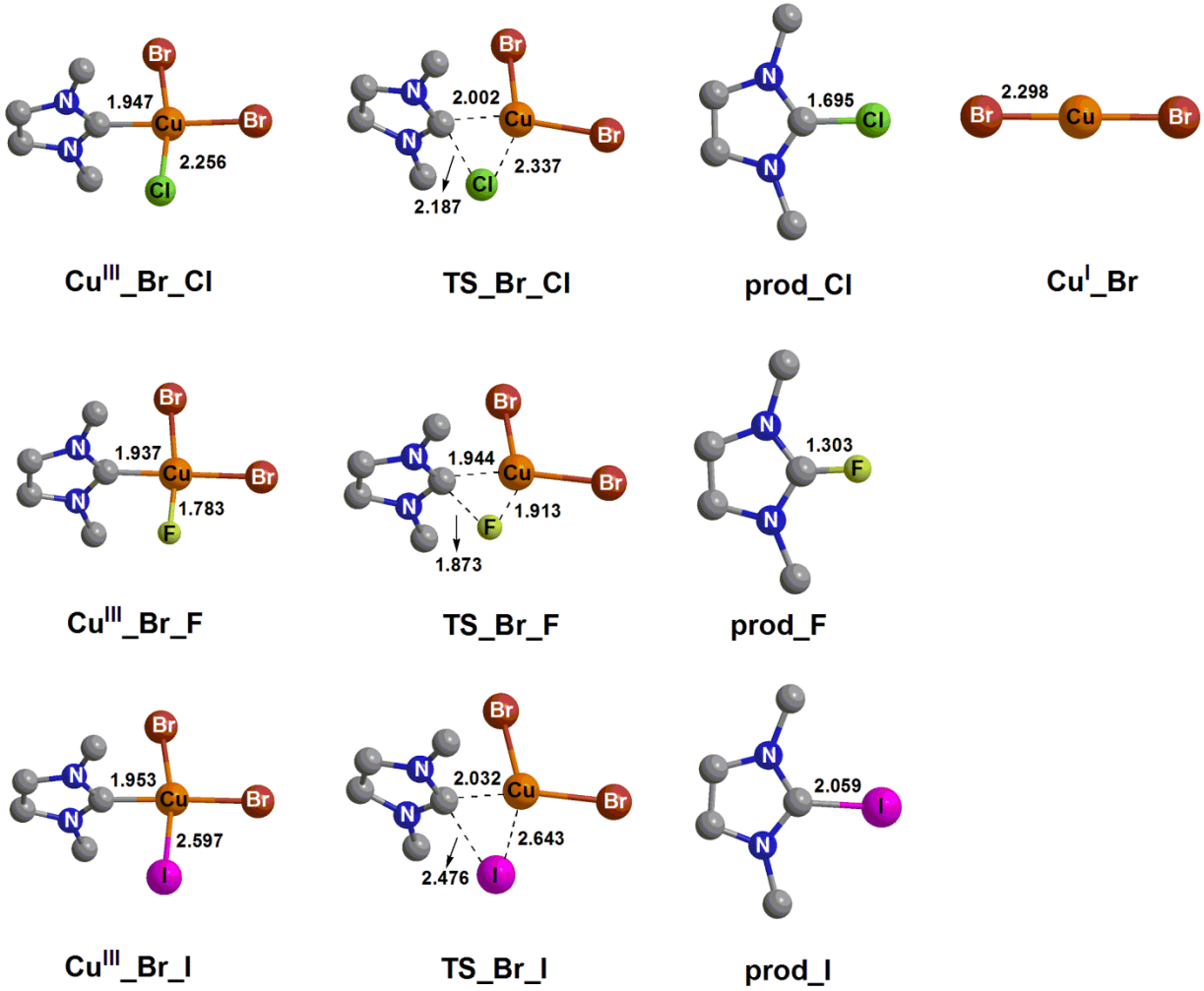


**Figure S11.** Optimized structures of intermediates, transition states and products in **$Cu^{III}$_Br_Y** [$D_e$(Cu-Y)] complexes where Y = F, Cl, Br and I.

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**Table S3**. Calculated Gibbs activation energy ($\Delta G^{‡}$), the reaction Gibbs energy ($\Delta G$), the HOMO energy of **$Cu^{I}$_X** in acetonitrile.

| X | $\Delta G^{‡}$ (kcal/mol) | $\Delta G$ (kcal/mol) | HOMO energy of **$Cu^{I}$_X** (eV) |
|---|---|---|---|
| Bn | 31.7 | 7.9 | -5.38 |
| $CH_3$ | 29.1 | 2.8 | -5.96 |
| vinyl | 27.3 | 0.1 | -5.76 |
| Ph | 24.3 | -0.3 | -6.15 |
| $CF_3$ | 13.7 | -12.3 | -6.71 |
| CN | 8.4 | -19.3 | -7.20 |
| I | 7.6 | -20.5 | -7.04 |
| F | 5.6 | -13.3 | -6.66 |
| Br | 5.2 | -21.9 | -7.05 |
| Cl | 4.5 | -22.2 | -7.02 |

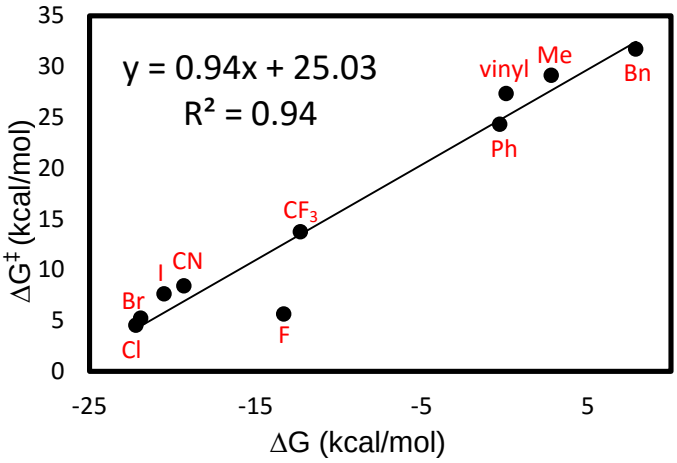


**Figure S12.** Plot of $\Delta G^{‡}$ versus $\Delta G$ for reductive elimination of NHC-Br from trans-(NHC)Cu$(Br)_2$X complexes in acetonitrile where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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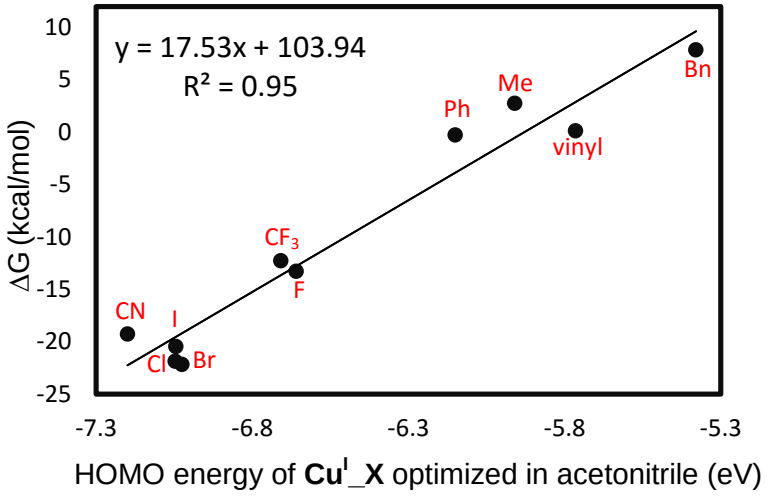


**Figure S13.** Plot of ΔG versus the HOMO energy of $Cu^{I}$(Br)(X) complex in acetonitrile where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl.

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**Table S4.** Total potential (E), enthalpy (H), Gibbs free energies (G) of all the structures optimized at the B3LYP/BS1 level of theory along with the total potential energies calculated by M06/BS2 for the structures optimized by B3LYP/BS1.

| species | E (B3LYP/BS1) (au) | H (B3LYP/BS1) (au) | G (B3LYP/BS1) (au) | E (M06/BS2// B3LYP/BS1) (au) |
|---|---|---|---|---|
| $Cu^{III}$_Bn_Br | -5914.844501 | -5914.573349 | -5914.647486 | -7364.157050 |
| $Cu^{III}$_Br_Br | -8215.314562 | -8215.165839 | -8215.228815 | -9667.385042 |
| $Cu^{III}$_$CF_3$_Br | -5981.482448 | -5981.318696 | -5981.387449 | -7430.955449 |
| $Cu^{III}$_$CH_3$_Br | -5683.778345 | -5683.594019 | -5683.657796 | -7133.213797 |
| $Cu^{III}$_Cl_Br | -6104.098427 | -6103.949584 | -6104.011204 | -7553.565440 |
| $Cu^{III}$_CN_Br | -5736.707460 | -5736.550872 | -5736.614299 | -7186.142660 |
| $Cu^{III}$_F_Br | -5743.716993 | -5743.567526 | -5743.627395 | -7193.194807 |
| $Cu^{III}$_I_Br | -5655.297075 | -5655.148476 | -5655.213636 | -5655.213636 |
| $Cu^{III}$_Ph_Br | -5875.509092 | -5875.267887 | -5875.339113 | -7324.847344 |
| $Cu^{III}$_vinyl_Br | -5721.851160 | -5721.661448 | -5721.726847 | -7171.269485 |
| $TS^{Cu}$_Bn_Br | -5914.783787 | -5914.515551 | -5914.589546 | -7364.103527 |
| $TS^{Cu}$_Br_Br | -8215.308024 | -8215.160722 | -8215.222762 | -9667.375495 |
| $TS^{Cu}$_$CF_3$_Br | -5981.451068 | -5981.290453 | -5981.356963 | -7430.929946 |
| $TS^{Cu}$_$CH_3$_Br | -5683.725016 | -5683.543267 | -5683.605556 | -7133.164389 |
| $TS^{Cu}$_Cl_Br | -6104.092770 | -6103.945350 | -6104.006740 | -7553.556735 |
| $TS^{Cu}$_CN_Br | -5736.694102 | -6103.945350 | -5736.599421 | -7186.127949 |
| $TS^{Cu}$_F_Br | -5743.702140 | -5743.554480 | -5743.613650 | -7193.183309 |
| $TS^{Cu}$_I_Br | -5655.289426 | -5655.142174 | -5655.205442 | -7391.127131 |
| $TS^{Cu}$_Ph_Br | -5875.462863 | -5875.223197 | -5875.294779 | -7324.805523 |
| $TS^{Cu}$_vinyl_Br | -5721.802844 | -5721.614483 | -5721.679702 | -7171.225912 |
| $Cu^{I}$_Bn | -3038.718776 | -3038.590917 | -3038.639621 | -4485.563628 |
| $Cu^{I}$_Br | -5339.253254 | -5339.245928 | -5339.280598 | -6788.843790 |
| $Cu^{I}$_$CF_3$ | -3105.394442 | -3105.373149 | -3105.414868 | -4552.396271 |
| $Cu^{I}$_$CH_3$ | -2807.665591 | -2807.624186 | -2807.659234 | -4254.630822 |
| $Cu^{I}$_Cl | -3228.037058 | -3228.029657 | -3228.063743 | -4675.023880 |
| $Cu^{I}$_CN | -2860.643001 | -2860.628675 | -2860.659640 | -4307.601026 |
| $Cu^{I}$_F | -2867.634297 | -2867.626947 | -2867.655022 | -4314.642540 |
| $Cu^{I}$_I | -2779.236999 | -2779.229721 | -2779.266131 | -4512.597050 |
| $Cu^{I}$_Ph | -2999.402904 | -2999.303637 | -2999.348743 | -4446.268080 |
| $Cu^{I}$_vinyl | -2845.744321 | -2845.696024 | -2845.734626 | -4292.690852 |
| $Au^{III}$_Bn_Br | -5854.152855 | -5853.881370 | -5853.957056 | -5859.394585 |
| $Au^{III}$_Br_Br | -8154.635279 | -8154.486315 | -8154.550830 | -8162.629268 |
| $Au^{III}$_$CF_3$_Br | -5920.809435 | -5920.645428 | -5920.716080 | -5926.205802 |
| $Au^{III}$_$CH_3$_Br | -5623.099695 | -5622.914669 | -5622.979094 | -5628.460221 |
| $Au^{III}$_Cl_Br | -6043.418660 | -6043.269488 | -6043.332184 | -6048.808332 |
| $Au^{III}$_CN_Br | -5676.036430 | -5675.879592 | -5675.944450 | -5681.391541 |
| $Au^{III}$_F_Br | -5683.032724 | -5682.883154 | -5682.944721 | -5688.432439 |

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|---|---|---|---|---|
| $Au^{III}$_I_Br | -5594.618981 | -5594.470146 | -5594.536299 | -5886.385696 |
| $Au^{III}$_Ph_Br | -5814.830738 | -5814.588912 | -5814.662645 | -5814.830738 |
| $Au^{III}$_vinyl_Br | -5661.172022 | -5660.981252 | -5661.048138 | -5666.515234 |
| $TS^{Au}$_Bn_Br | -5854.076337 | -5853.807504 | -5853.882488 | -5859.321429 |
| $TS^{Au}$_Br_Br | -8154.591445 | -8154.444379 | -8154.507800 | -8162.586537 |
| $TS^{Au}$_$CF_3$_Br | -5920.742868 | -5920.582169 | -5920.649239 | -5926.143795 |
| $TS^{Au}$_$CH_3$_Br | -5623.025074 | -5622.842742 | -5622.908004 | -5628.386968 |
| $TS^{Au}$_Cl_Br | -6043.373324 | -6043.226195 | -6043.288724 | -6048.764504 |
| $TS^{Au}$_CN_Br | -5675.982511 | -5675.827986 | -5675.891155 | -5681.341781 |
| $TS^{Au}$_F_Br | -5682.970675 | -5682.823441 | -5682.885184 | -5688.379109 |
| $TS^{Au}$_I_Br | -5594.577627 | -5594.430532 | -5594.494161 | -5886.343613 |
| $TS^{Au}$_Ph_Br | -5814.758513 | -5814.518791 | -5814.590626 | -5820.021804 |
| $TS^{Au}$_vinyl_Br | -5661.100752 | -5660.911904 | -5660.977006 | -5666.444607 |
| $Au^{I}$_Bn | -2978.038833 | -2977.909983 | -2977.959713 | -2980.801840 |
| $Au^{I}$_Br | -5278.546786 | -5278.539542 | -5278.575496 | -5284.064498 |
| $Au^{I}$_$CF_3$ | -3044.710850 | -3044.689256 | -3044.732654 | -3047.631192 |
| $Au^{I}$_$CH_3$ | -2746.989512 | -2746.946963 | -2746.983876 | -2749.870966 |
| $Au^{I}$_Cl | -3167.327800 | -3167.320481 | -3167.355823 | -3170.241550 |
| $Au^{I}$_CN | -2799.950791 | -2799.935849 | -2799.972033 | -2802.830979 |
| $Au^{I}$_F | -2806.922012 | -2806.914411 | -2806.948544 | -2809.853352 |
| $Au^{I}$_I | -2718.534570 | -2718.527839 | -2718.561910 | -3007.823179 |
| $Au^{I}$_Ph | -2938.724406 | -2938.624679 | -2938.670524 | -2941.507940 |
| $Au^{I}$_vinyl | -2785.066640 | -2785.017768 | -2785.057153 | -2787.930618 |
| $Ag^{III}$_Bn_Br | -5864.443193 | -5864.172296 | -5864.249496 | -5870.644567 |
| $Ag^{III}$_Br_Br | -8164.915113 | -8164.767344 | -8164.830155 | -8173.874194 |
| $Ag^{III}$_$CF_3$_Br | -5931.083401 | -5930.919597 | -5930.990834 | -5937.444365 |
| $Ag^{III}$_$CH_3$_Br | -5633.379487 | -5633.195185 | -5633.259710 | -5639.703878 |
| $Ag^{III}$_Cl_Br | -6053.697843 | -6053.549917 | -6053.611512 | -6060.052427 |
| $Ag^{III}$_CN_Br | -5686.304656 | -5686.148164 | -5686.213371 | -5692.628271 |
| $Ag^{III}$_F_Br | -5693.305346 | -5693.155918 | -5693.217300 | -5699.674945 |
| $Ag^{III}$_I_Br | -5604.900578 | -5604.751937 | -5604.818019 | -5897.631976 |
| $Ag^{III}$_Ph_Br | -5825.107466 | -5824.866338 | -5824.939255 | -5831.335233 |
| $Ag^{III}$_vinyl_Br | -5671.449504 | -5671.259703 | -5671.327005 | -5677.757543 |
| $TS^{Ag}$_Bn_Br | -5864.389724 | -5864.121327 | -5864.199739 | -5859.321429 |
| $TS^{Ag}$_Br_Br | -8164.903680 | -8164.756330 | -8164.819464 | -8162.586537 |
| $TS^{Ag}$_$CF_3$_Br | -5931.046370 | -5930.884876 | -5930.956022 | -5929.141379 |
| $TS^{Ag}$_$CH_3$_Br | -5633.323288 | -5633.141527 | -5633.205721 | -5628.386968 |
| $TS^{Ag}$_Cl_Br | -6053.687164 | -6053.539804 | -6053.601948 | -6048.764504 |
| $TS^{Ag}$_CN_Br | -5686.286426 | -5686.131707 | -5686.193924 | -5681.341781 |
| $TS^{Ag}$_F_Br | -5693.285474 | -5693.139062 | -5693.196745 | -5688.379109 |
| $TS^{Ag}$_I_Br | -5604.888759 | -5604.742518 | -5604.803676 | -5886.343616 |
| $TS^{Ag}$_Ph_Br | -5825.058030 | -5824.818669 | -5824.891752 | -5820.021804 |
| $TS^{Ag}$_vinyl_Br | -5671.398881 | -5671.211729 | -5671.274741 | -5666.444607 |
| $Ag^{I}$_Bn | -2795.352316 | -2795.304107 | -2795.343853 | -2980.801840 |
| $Ag^{I}$_Br | -5288.863794 | -5288.856571 | -5288.892885 | -5284.064498 |
| $Ag^{I}$_$CF_3$ | -3055.001525 | -3054.980401 | -3055.023463 | -3047.631192 |

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|---|---|---|---|---|
| $Ag^{I}$_$CH_3$ | -2757.275625 | -2757.234032 | -2757.270220 | -2749.870966 |
| $Ag^{I}$_Cl | -3177.646890 | -3177.639606 | -3177.674842 | -3170.241550 |
| $Ag^{I}$_CN | -2810.249159 | -2810.234571 | -2810.271433 | -2802.830979 |
| $Ag^{I}$_F | -2817.232320 | -2817.224801 | -2817.258520 | -2809.853352 |
| $Ag^{I}$_I | -2728.850537 | -2728.843344 | -2728.881218 | -3007.823179 |
| $Ag^{I}$_Ph | -2949.010422 | -2948.911264 | -2948.957531 | -2941.507940 |
| $Ag^{I}$_vinyl | -2795.352316 | -2795.304107 | -2795.343853 | -2799.187851 |
| Prod_Br | -2876.083017 | -2875.942447 | -2875.986790 | -2878.548536 |
| $Cu^{III}$_Br_Cl | -6104.094820 | -6103.945989 | -6104.008041 | -7553.561193 |
| $Cu^{III}$_Br_F | -5743.709865 | -5743.560444 | -5743.619872 | -7193.182730 |
| $Cu^{III}$_Br_I | -5655.300978 | -5655.152406 | -5655.217887 | -7391.145883 |
| $TS^{Cu}$_Br_Cl | -6104.084812 | -6103.937369 | -6103.998702 | -7553.546955 |
| $TS^{Cu}$_Br_F | -5743.696777 | -5743.548998 | -5743.608961 | -7193.160829 |
| $TS^{Cu}$_Br_I | -5655.300978 | -5655.152406 | -5655.217887 | -7391.142229 |
| prod_Cl | -764.880650 | -764.739731 | -764.782833 | -764.729914 |
| prod_F | -404.518969 | -404.376789 | -404.418988 | -404.373624 |
| prod_I | -316.065394 | -315.925124 | -315.970441 | -602.307772 |

`

**Table S5.** Total potential (E), enthalpy (H), Gibbs free energies (G) of all the structures for NHC-Br reductive elimination from trans-(NHC)Cu(Br)$_2$X complexes in acetonitrile where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl optimized at the B3LYP/BS1 level of theory along with the total potential energies calculated by M06/BS2 for the structures optimized by B3LYP/BS1.

| species | E (B3LYP/BS1) (au) | H (B3LYP/BS1) (au) | G (B3LYP/BS1) (au) | E (M06/BS2// B3LYP/BS1) (au) |
|---|---|---|---|---|
| $Cu^{III}$_Bn_Br | -5914.846999 | -5914.575859 | -5914.650245 | -7364.15921 |
| $Cu^{III}$_Br_Br | -8215.317255 | -8215.168536 | -8215.231572 | -9667.387436 |
| $Cu^{III}$_$CF_3$_Br | -5981.484228 | -5981.320508 | -5981.389269 | -7430.957342 |
| $Cu^{III}$_$CH_3$_Br | -5683.779808 | -5683.595497 | -5683.659369 | -7133.215183 |
| $Cu^{III}$_Cl_Br | -6104.101482 | -6103.952648 | -6104.014325 | -7553.568074 |
| $Cu^{III}$_CN_Br | -5736.710343 | -5736.553764 | -5736.617325 | -7186.145554 |
| $Cu^{III}$_F_Br | -5743.719798 | -5743.570359 | -5743.630382 | -7193.197825 |
| $Cu^{III}$_I_Br | -5655.299529 | -5655.150937 | -5655.216342 | -7391.141945 |
| $Cu^{III}$_Ph_Br | -5875.51106 | -5875.269853 | -5875.340946 | -7324.84921 |
| $Cu^{III}$_vinyl_Br | -5721.852909 | -5721.663226 | -5721.728873 | -7171.271154 |
| $TS^{Cu}$_Bn_Br | -5914.786608 | -5914.518356 | -5914.592102 | -7364.106371 |
| $TS^{Cu}$_Br_Br | -8215.311621 | -8215.164298 | -8215.226371 | -9667.378727 |
| $TS^{Cu}$_$CF_3$_Br | -5981.454771 | -5981.293135 | -5981.36174 | -7430.93363 |
| $TS^{Cu}$_$CH_3$_Br | -5683.728122 | -5683.546383 | -5683.609137 | -7133.167374 |
| $TS^{Cu}$_Cl_Br | -6104.096686 | -6103.949197 | -6104.010315 | -7553.560172 |
| $TS^{Cu}$_CN_Br | -5736.698193 | -5736.543398 | -5736.605556 | -7186.131795 |
| $TS^{Cu}$_F_Br | -5743.706395 | -5743.558725 | -5743.61841 | -7193.187549 |
| $TS^{Cu}$_I_Br | -5655.2929 | -5655.145626 | -5655.209394 | -7391.13014 |
| $TS^{Cu}$_Ph_Br | -5875.466182 | -5875.226496 | -5875.297853 | -7324.808742 |
| $TS^{Cu}$_vinyl_Br | -5721.806102 | -5721.618676 | -5721.680622 | -7171.229064 |
| $Cu^{I}$_Bn | -3038.725492 | -3038.597607 | -3038.646286 | -4485.570245 |
| $Cu^{I}$_Br | -5339.259953 | -5339.252627 | -5339.287326 | -6788.850343 |
| $Cu^{I}$_$CF_3$ | -3105.400891 | -3105.379613 | -3105.421344 | -4552.402597 |
| $Cu^{I}$_$CH_3$ | -2807.672691 | -2807.631296 | -2807.66635 | -4254.637797 |
| $Cu^{I}$_Cl | -3228.043959 | -3228.036559 | -3228.070672 | -4675.030646 |
| $Cu^{I}$_CN | -2860.64974 | -2860.635415 | -2860.66639 | -4307.607708 |
| $Cu^{I}$_F | -2867.641678 | -2867.634329 | -2867.662409 | -4314.649948 |
| $Cu^{I}$_I | -2779.243408 | -2779.236131 | -2779.272576 | -4512.603335 |
| $Cu^{I}$_Ph | -2999.409751 | -2999.310447 | -2999.355585 | -4446.274823 |
| $Cu^{I}$_vinyl | -2845.751303 | -2845.702986 | -2845.74161 | -4292.697718 |
| prod _Br | -2876.397974 | -2876.257420 | -2876.301919 | -2878.554953 |

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**Cartesian coordinates for all the calculated structures**

**$Cu^{III}$_Bn_Br**

| | | | |
|---|---|---|---|
| Cu | -0.12497400 | -0.49455700 | 0.07159900 |
| C | 1.52999500 | -1.77632200 | 0.36353100 |
| H | 1.39428200 | -2.13742500 | 1.37529400 |
| Br | -0.72838900 | -0.84178900 | 2.46943000 |
| Br | -0.67504700 | -1.79340000 | -1.98335800 |
| C | 2.36394600 | -0.63094300 | 0.14470800 |
| C | 2.77011200 | 0.19174800 | 1.23544000 |
| C | 2.83750000 | -0.31608600 | -1.16243500 |
| C | 3.65228800 | 1.24203300 | 1.03091400 |
| H | 2.38593900 | -0.02669900 | 2.22669700 |
| C | 3.71935900 | 0.73720600 | -1.35351900 |
| H | 2.50915100 | -0.92409000 | -1.99948400 |
| C | 4.13093600 | 1.51335500 | -0.25933200 |
| H | 3.97202000 | 1.85391800 | 1.86827700 |
| H | 4.09141900 | 0.96087700 | -2.34820500 |
| H | 4.82126600 | 2.33712200 | -0.41434000 |
| C | -1.23972700 | 1.17726600 | -0.26426000 |
| C | -3.06048500 | 2.50926700 | -0.45757900 |
| C | -1.96414100 | 3.29976700 | -0.58816200 |
| H | -4.11261900 | 2.74483300 | -0.49581000 |
| H | -1.86966900 | 4.36043000 | -0.76094300 |
| N | -0.86181800 | 2.46569100 | -0.47079500 |
| N | -2.59758000 | 1.21722900 | -0.26413300 |
| C | 0.51757300 | 2.93972900 | -0.52089600 |
| H | 1.17189400 | 2.10073000 | -0.75301000 |
| H | 0.61338000 | 3.69478000 | -1.30417100 |
| H | 0.80922800 | 3.37539200 | 0.43901200 |
| C | -3.46248900 | 0.05573200 | -0.05606700 |
| H | -4.48313000 | 0.32544800 | -0.33132900 |
| H | -3.11749800 | -0.76581000 | -0.68610500 |
| H | -3.43052600 | -0.25162000 | 0.99191200 |
| H | 1.43593500 | -2.51108400 | -0.42622400 |

**$Cu^{III}$_Br_Br**

| | | | |
|---|---|---|---|
| C | -1.50059900 | 0.00003300 | -0.00002900 |
| C | -3.61767100 | -0.00005600 | 0.67947600 |
| C | -3.61768900 | 0.00000300 | -0.67948200 |
| H | -4.42742400 | -0.00011600 | 1.39157500 |
| H | -4.42746000 | 0.00004800 | -1.39156000 |
| N | -2.28948000 | -0.00004600 | 1.08575900 |
| N | -2.28950900 | 0.00012600 | -1.08579700 |
| C | -1.81720100 | -0.00016000 | 2.47167100 |
| H | -2.68437400 | 0.00015000 | 3.13097800 |

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| | | | |
|---|---|---|---|
| H | -1.21877800 | -0.89551000 | 2.65376900 |
| H | -1.21820500 | 0.89481600 | 2.65371000 |
| C | -1.81726400 | 0.00023200 | -2.47172100 |
| H | -2.68445200 | 0.00039700 | -3.13100200 |
| H | -1.21846600 | 0.89535200 | -2.65370900 |
| H | -1.21865300 | -0.89497300 | -2.65390200 |
| Cu | 0.44734000 | -0.00000300 | -0.00005200 |
| Br | 0.19483500 | -2.36260100 | -0.00012000 |
| Br | 0.19488800 | 2.36260400 | 0.00003100 |
| Br | 2.82171800 | -0.00003000 | 0.00015900 |

**$Cu^{III}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.57017900 | -0.02354900 | 0.00211200 |
| C | -3.70464300 | -0.23239100 | -0.65825200 |
| C | -3.71100400 | 0.04482100 | 0.67146800 |
| H | -4.51270300 | -0.39910200 | -1.35293300 |
| H | -4.52530500 | 0.15824300 | 1.36962300 |
| N | -2.37369000 | -0.27397500 | -1.05184800 |
| N | -2.38404300 | 0.17448300 | 1.05931000 |
| C | -1.90891600 | -0.50779300 | -2.41917100 |
| H | -2.69360200 | -1.02350800 | -2.97358400 |
| H | -1.67813300 | 0.44103700 | -2.91045600 |
| H | -1.01764500 | -1.13696600 | -2.39009900 |
| C | -1.93131500 | 0.43673500 | 2.42550100 |
| H | -1.07099700 | 1.10733200 | 2.39383700 |
| H | -2.73970900 | 0.91720300 | 2.97752400 |
| H | -1.65551300 | -0.49779500 | 2.92104900 |
| Cu | 0.42207100 | 0.03496400 | -0.00108100 |
| Br | 0.27938400 | 2.38629700 | -0.17237200 |
| Br | 0.41994300 | -2.33929200 | 0.15857600 |
| C | 2.42370900 | 0.04044900 | 0.00496600 |
| F | 2.86359600 | -0.68796900 | -1.04729600 |
| F | 3.04827400 | 1.22902400 | -0.06700900 |
| F | 2.85427400 | -0.54980500 | 1.14400300 |

**$Cu^{III}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.21819300 | -0.01565800 | 0.00041600 |
| C | -3.36539200 | -0.27276300 | -0.64552100 |
| C | -3.37502700 | 0.16070300 | 0.64145600 |
| H | -4.17235800 | -0.50846800 | -1.32152100 |
| H | -4.19185500 | 0.36557900 | 1.31566600 |
| N | -2.03243400 | -0.37872600 | -1.01829300 |
| N | -2.04779500 | 0.31710600 | 1.01702400 |
| C | -1.57391900 | -0.77073900 | -2.34966700 |
| H | -2.30031600 | -1.45645200 | -2.78908200 |
| H | -1.46839600 | 0.10687300 | -2.99360800 |
| H | -0.61325000 | -1.27900300 | -2.25734800 |
| C | -1.60708300 | 0.72545200 | 2.34942500 |
| H | -2.35335700 | 1.39351000 | 2.78287500 |
| H | -1.48169500 | -0.14698400 | 2.99684800 |

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| | | | |
|---|---|---|---|
| H | -0.65964900 | 1.25829900 | 2.26004300 |
| Cu | 0.81203100 | 0.01953100 | 0.00310400 |
| Br | 0.86150000 | 2.38442400 | -0.25397500 |
| Br | 0.93152200 | -2.35157000 | 0.25021400 |
| C | 2.83454800 | 0.00901700 | 0.00839200 |
| H | 3.17130800 | 1.03580600 | -0.08089200 |
| H | 3.07893400 | -0.45665200 | 0.96123700 |
| H | 3.07795800 | -0.61355000 | -0.85071300 |

**$Cu^{III}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | 1.17540700 | -0.00163000 | -0.00000900 |
| C | 3.28967200 | -0.00345800 | 0.67959100 |
| C | 3.28975300 | -0.00322900 | -0.67935300 |
| H | 4.09920300 | -0.00441200 | 1.39188300 |
| H | 4.09936100 | -0.00394800 | -1.39155600 |
| N | 1.96169300 | -0.00244900 | 1.08680900 |
| N | 1.96181900 | -0.00220800 | -1.08672300 |
| C | 1.49022500 | -0.00145700 | 2.47329700 |
| H | 2.35827700 | -0.00631200 | 3.13130100 |
| H | 0.89621900 | 0.89659100 | 2.65636500 |
| H | 0.88779800 | -0.89421200 | 2.65460900 |
| C | 1.49048000 | -0.00083500 | -2.47325800 |
| H | 2.35858900 | -0.00578900 | -3.13118600 |
| H | 0.88784200 | -0.89340300 | -2.65479000 |
| H | 0.89671100 | 0.89739600 | -2.65619800 |
| Cu | -0.76417600 | 0.00073300 | 0.00001500 |
| Br | -0.49511900 | 2.35782700 | 0.00005900 |
| Br | -0.50095100 | -2.35699200 | -0.00016200 |
| Cl | -3.01989800 | 0.00352300 | 0.00003000 |

**$Cu^{III}$_CN_Br**

| | | | |
|---|---|---|---|
| C | 1.18214000 | 0.00037900 | 0.00003800 |
| C | 3.30589400 | 0.00105200 | 0.67966400 |
| C | 3.30596300 | 0.00066200 | -0.67936900 |
| H | 4.11613000 | 0.00145000 | 1.39119400 |
| H | 4.11626800 | 0.00065300 | -1.39082000 |
| N | 1.97807400 | 0.00087500 | 1.08350100 |
| N | 1.97818400 | 0.00026900 | -1.08333900 |
| C | 1.51054300 | 0.00100700 | 2.47142200 |
| H | 2.37975500 | 0.00248400 | 3.12821600 |
| H | 0.91148100 | 0.89514200 | 2.65713700 |
| H | 0.91372200 | -0.89442700 | 2.65812000 |
| C | 1.51078100 | -0.00038300 | -2.47130500 |
| H | 0.91187200 | 0.89372600 | -2.65763600 |
| H | 2.38005300 | 0.00054400 | -3.12802100 |
| H | 0.91383900 | -0.89584300 | -2.65749100 |
| Cu | -0.75206800 | -0.00017900 | 0.00002000 |
| Br | -0.63759400 | 2.36815200 | -0.00031800 |
| Br | -0.63611500 | -2.36844300 | 0.00029100 |
| C | -2.66677200 | -0.00077800 | -0.00024300 |

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| | | | |
|---|---|---|---|
| N | -3.83406700 | -0.00114500 | -0.00038900 |

**$Cu^{III}$_F_Br**

| | | | |
|---|---|---|---|
| C | 0.00387000 | 1.00239900 | 0.00012600 |
| C | 0.02143000 | 3.12157500 | 0.67963000 |
| C | 0.01628200 | 3.12157100 | -0.67956400 |
| H | 0.02945300 | 3.93163700 | 1.39132700 |
| H | 0.01914800 | 3.93152800 | -1.39141400 |
| N | 0.01335100 | 1.79350600 | 1.08497300 |
| N | 0.00506500 | 1.79343700 | -1.08478900 |
| C | 0.01803800 | 1.31304700 | 2.46776500 |
| H | 0.00991000 | 2.17478200 | 3.13426800 |
| H | -0.87135000 | 0.70395400 | 2.64421600 |
| H | 0.91805600 | 0.71970200 | 2.64449000 |
| C | -0.00185600 | 1.31296900 | -2.46754800 |
| H | -0.89552700 | 0.70864900 | -2.63833500 |
| H | -0.00937200 | 2.17470700 | -3.13401200 |
| H | 0.89387800 | 0.71484000 | -2.64991700 |
| Cu | -0.00538100 | -0.92055300 | 0.00041800 |
| Br | -2.36439700 | -0.68175200 | 0.00313100 |
| Br | 2.35614200 | -0.70609100 | -0.00378000 |
| F | -0.01385600 | -2.68080300 | 0.00068800 |

**$Cu^{III}$_I_Br**

| | | | |
|---|---|---|---|
| C | 1.83997400 | 0.00034800 | 0.00033800 |
| C | 3.96207100 | 0.00032100 | -0.67778700 |
| C | 3.96120300 | -0.00045400 | 0.68118500 |
| H | 4.77262100 | 0.00073300 | -1.38907100 |
| H | 4.77085100 | -0.00100600 | 1.39349900 |
| N | 2.63371600 | 0.00076400 | -1.08329900 |
| N | 2.63233800 | -0.00037400 | 1.08499300 |
| C | 2.16149800 | 0.00164600 | -2.46895600 |
| H | 3.02800700 | 0.00314000 | -3.12956700 |
| H | 1.56311200 | -0.89355200 | -2.65233800 |
| H | 1.56144600 | 0.89608600 | -2.65052300 |
| C | 2.15834000 | -0.00180000 | 2.47004100 |
| H | 3.02400500 | 0.00167100 | 3.13172800 |
| H | 1.55560300 | 0.89085800 | 2.65149700 |
| H | 1.56217000 | -0.89876900 | 2.65206100 |
| Cu | -0.12191900 | 0.00013400 | -0.00041100 |
| Br | 0.07337200 | -2.36230700 | -0.00142400 |
| Br | 0.07279300 | 2.36259300 | -0.00025700 |
| I | -2.73167700 | -0.00030500 | 0.00042800 |

**$Cu^{III}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | 1.99255700 | 0.00002200 | 0.00014200 |
| C | 4.14508000 | -0.25093000 | 0.63077500 |
| C | 4.14493800 | 0.25115200 | -0.63096700 |
| H | 4.95729600 | -0.50698500 | 1.29294900 |
| H | 4.95701900 | 0.50741300 | -1.29321700 |
| N | 2.81515100 | -0.40230000 | 0.99735700 |

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| | | | |
|---|---|---|---|
| N | 2.81493500 | 0.40235500 | -0.99734500 |
| C | 2.36720400 | -0.87292100 | 2.30655800 |
| H | 3.08695300 | -1.59798000 | 2.69097200 |
| H | 2.28384300 | -0.03719900 | 3.00709900 |
| H | 1.39742400 | -1.35875500 | 2.19301500 |
| C | 2.36670500 | 0.87325600 | -2.30638800 |
| H | 1.39695800 | 1.35903300 | -2.19249700 |
| H | 3.08634700 | 1.59846700 | -2.69078100 |
| H | 2.28323600 | 0.03767900 | -3.00707300 |
| Cu | -0.02467400 | -0.00003800 | 0.00001600 |
| Br | -0.16484200 | 2.35337500 | 0.33339000 |
| Br | -0.16452700 | -2.35336400 | -0.33352800 |
| C | -1.99651600 | -0.00015000 | 0.00002400 |
| C | -2.66605700 | 0.16262600 | -1.20608700 |
| C | -2.66594400 | -0.16291300 | 1.20615000 |
| C | -4.06814600 | 0.16176500 | -1.19818100 |
| H | -2.13048300 | 0.28881100 | -2.14244300 |
| C | -4.06804600 | -0.16194900 | 1.19838000 |
| H | -2.13032200 | -0.28928700 | 2.14245900 |
| C | -4.76707700 | -0.00006100 | 0.00015100 |
| H | -4.60515800 | 0.28794200 | -2.13496600 |
| H | -4.60494300 | -0.28816700 | 2.13522800 |
| H | -5.85351300 | -0.00001500 | 0.00019300 |

**$Cu^{III}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | 1.38477100 | 0.01031200 | 0.08505000 |
| C | 3.57914700 | 0.26465400 | -0.38211500 |
| C | 3.48681700 | -0.28736000 | 0.85529200 |
| H | 4.43788100 | 0.53891000 | -0.97475900 |
| H | 4.24825300 | -0.57728700 | 1.56234400 |
| N | 2.27968700 | 0.44376100 | -0.83458400 |
| N | 2.13348900 | -0.43941300 | 1.12053800 |
| C | 1.92976000 | 0.96804900 | -2.15362800 |
| H | 2.71085400 | 1.65669300 | -2.48054900 |
| H | 1.83784200 | 0.15374700 | -2.87797000 |
| H | 0.98480300 | 1.50731200 | -2.07913100 |
| C | 1.59209400 | -0.96006700 | 2.37427800 |
| H | 2.28064800 | -1.70412100 | 2.77897400 |
| H | 1.46111900 | -0.15345600 | 3.10120300 |
| H | 0.63151100 | -1.43582600 | 2.17323200 |
| Cu | -0.63541000 | 0.00471300 | -0.04808600 |
| Br | -0.76615700 | -2.32765600 | -0.50834200 |
| Br | -0.85595200 | 2.36668800 | 0.14611300 |
| C | -2.59698400 | -0.01739700 | -0.14514500 |
| H | -2.91269400 | 0.10957900 | -1.17775000 |
| C | -3.36518000 | -0.17074100 | 0.91759500 |
| H | -2.98202800 | -0.29212900 | 1.92829300 |
| H | -4.45226400 | -0.18138700 | 0.80896300 |

**$TS^{Cu}$_Bn_Br**

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| | | | |
|---|---|---|---|
| Cu | 0.09139500 | 0.85292600 | -0.34543500 |
| C | -1.67996300 | 1.70995900 | -0.92796800 |
| H | -1.64600400 | 2.73687800 | -0.55388900 |
| Br | 2.01091500 | 2.24072000 | 0.02615700 |
| Br | -0.54460700 | -1.56890500 | -0.18508500 |
| C | -2.80078000 | 0.92725700 | -0.40738700 |
| C | -3.42409000 | 1.24884200 | 0.82663000 |
| C | -3.28422000 | -0.22736300 | -1.07720800 |
| C | -4.46830900 | 0.48805700 | 1.33859000 |
| H | -3.07802400 | 2.12482200 | 1.37280600 |
| C | -4.34397500 | -0.98433500 | -0.56334600 |
| H | -2.85618000 | -0.49150800 | -2.04195600 |
| C | -4.94376400 | -0.63761400 | 0.64643000 |
| H | -4.92854800 | 0.77671400 | 2.28127800 |
| H | -4.69981100 | -1.84882900 | -1.11978200 |
| H | -5.76577100 | -1.22490400 | 1.04643300 |
| C | 1.43194700 | -1.07786500 | 0.14079700 |
| C | 3.57724300 | -1.64560200 | -0.06827100 |
| C | 3.31886100 | -1.47480100 | 1.25753100 |
| H | 4.49285100 | -1.88936600 | -0.58353500 |
| H | 3.96688400 | -1.53902900 | 2.11727600 |
| N | 1.97888900 | -1.15967200 | 1.37908200 |
| N | 2.39288400 | -1.43155600 | -0.74918200 |
| C | 1.30292100 | -0.81255900 | 2.62792600 |
| H | 1.21936900 | 0.27436200 | 2.71068800 |
| H | 0.30970600 | -1.26400100 | 2.64137400 |
| H | 1.89204400 | -1.20352200 | 3.45736000 |
| C | 2.23479200 | -1.47661700 | -2.20267000 |
| H | 3.05541200 | -2.06028800 | -2.61948800 |
| H | 1.28635800 | -1.95631300 | -2.44880500 |
| H | 2.25492000 | -0.46428400 | -2.61425700 |
| H | -1.60083600 | 1.69532100 | -2.02102100 |

**$TS^{Cu}$_Br_Br**

| | | | |
|---|---|---|---|
| C | 1.42675000 | -0.19894200 | 0.00001300 |
| C | 3.43632600 | 0.46474300 | -0.68121500 |
| C | 3.43630900 | 0.46481800 | 0.68122100 |
| H | 4.19813500 | 0.75067600 | -1.38882200 |
| H | 4.19809800 | 0.75082800 | 1.38881700 |
| N | 2.19189600 | 0.02403700 | -1.09242000 |
| N | 2.19186700 | 0.02415600 | 1.09244200 |
| C | 1.73603800 | -0.07189600 | -2.47942300 |
| H | 2.60856500 | -0.03953400 | -3.13118000 |
| H | 1.20962000 | -1.01741000 | -2.62099200 |
| H | 1.07115100 | 0.76552700 | -2.70629000 |
| C | 1.73598000 | -0.07163100 | 2.47944600 |
| H | 2.60849900 | -0.03926400 | 3.13121500 |
| H | 1.07113700 | 0.76584700 | 2.70623600 |
| H | 1.20950800 | -1.01710500 | 2.62108800 |

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| | | | |
|---|---|---|---|
| Cu | -0.57704400 | 0.03233300 | 0.00000200 |
| Br | 0.34429800 | -2.23073500 | 0.00011400 |
| Br | -0.34994300 | 2.40798800 | -0.00031800 |
| Br | -2.93021800 | -0.34060000 | 0.00018800 |

**$TS^{Cu}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.42503100 | -0.38052800 | 0.00171400 |
| C | 3.30354400 | 0.61275400 | -0.66452200 |
| C | 3.29836300 | 0.60102900 | 0.69951100 |
| H | 4.00995200 | 1.03475000 | -1.36173100 |
| H | 3.99964600 | 1.01079900 | 1.40907800 |
| N | 2.16433100 | -0.03616500 | -1.08882300 |
| N | 2.15587400 | -0.05505400 | 1.10381600 |
| C | 1.73742200 | -0.17034200 | -2.48134200 |
| H | 2.61790400 | -0.09876700 | -3.11933700 |
| H | 1.26455300 | -1.14330000 | -2.62247500 |
| H | 1.03194700 | 0.62745200 | -2.72871300 |
| C | 1.72080200 | -0.21652600 | 2.49103600 |
| H | 1.23875400 | -1.18814900 | 2.60774000 |
| H | 2.59874700 | -0.16746300 | 3.13470000 |
| H | 1.02126100 | 0.58144600 | 2.75405300 |
| Cu | -0.69874900 | 0.04258500 | 0.00131300 |
| Br | 0.43178300 | -2.19681600 | -0.01752300 |
| Br | -0.25053600 | 2.42178500 | -0.00126300 |
| C | -2.65695400 | -0.29016000 | 0.00445200 |
| F | -3.31510700 | 0.24796200 | -1.08744400 |
| F | -3.04637200 | -1.61861500 | 0.00740800 |
| F | -3.31333900 | 0.25237600 | 1.09515900 |

**$TS^{Cu}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | 0.81765600 | 0.65081700 | 0.01895100 |
| C | 0.58798200 | 2.82929700 | -0.38756000 |
| C | 0.73689700 | 2.67142200 | 0.95847200 |
| H | 0.40558800 | 3.71486300 | -0.97565800 |
| H | 0.71262000 | 3.39313700 | 1.75953100 |
| N | 0.68597500 | 1.58291200 | -0.96563500 |
| N | 0.92378200 | 1.32626600 | 1.19895500 |
| C | 0.46880200 | 1.28762500 | -2.37974100 |
| H | 0.62825300 | 2.20230800 | -2.95047100 |
| H | 1.17890100 | 0.52580500 | -2.70564200 |
| H | -0.55538100 | 0.93089000 | -2.51866600 |
| C | 1.08166900 | 0.72651200 | 2.52419100 |
| H | 1.51268000 | 1.47500400 | 3.18941200 |
| H | 0.11152200 | 0.40367900 | 2.91020600 |
| H | 1.75575600 | -0.12798500 | 2.45545300 |
| Cu | -0.54212200 | -1.12986900 | 0.07487000 |
| Br | 2.01838100 | -0.96210500 | -0.30448200 |
| Br | -2.45247400 | 0.38591600 | -0.02623200 |
| C | -0.89749000 | -3.08581200 | 0.23721700 |
| H | -0.13999100 | -3.57091100 | 0.87077900 |

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| | | | |
|---|---|---|---|
| H | -1.88700000 | -3.30007200 | 0.66230100 |
| H | -0.84956200 | -3.55733200 | -0.75589700 |

**$TS^{Cu}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | 1.12119300 | -0.12239100 | 0.00170700 |
| C | 2.83138400 | -1.36712800 | -0.67910100 |
| C | 2.83669600 | -1.35934800 | 0.68332100 |
| H | 3.46874900 | -1.87439200 | -1.38579700 |
| H | 3.47903500 | -1.85921100 | 1.39081800 |
| N | 1.77699300 | -0.57265200 | -1.09099100 |
| N | 1.78582400 | -0.55963300 | 1.09444200 |
| C | 1.36757700 | -0.34302800 | -2.47713100 |
| H | 2.17080700 | -0.67682200 | -3.13296900 |
| H | 0.45665100 | -0.90883000 | -2.68874600 |
| H | 1.19047400 | 0.72323700 | -2.62951600 |
| C | 1.38793400 | -0.31820900 | 2.48205100 |
| H | 2.22025000 | -0.58867900 | 3.13094400 |
| H | 1.15478300 | 0.74019200 | 2.61037300 |
| H | 0.51348300 | -0.92708800 | 2.72558600 |
| Cu | -0.84370000 | 0.28110700 | 0.00294600 |
| Br | -1.38599800 | -2.04083400 | 0.00110400 |
| Br | 0.70909100 | 2.15272000 | -0.01072600 |
| Cl | -2.86491900 | 1.31118100 | 0.00831800 |

**$TS^{Cu}$_CN_Br**

| | | | |
|---|---|---|---|
| C | -1.06042700 | -0.13748200 | 0.00002800 |
| C | -2.54099100 | -1.65293300 | -0.68179900 |
| C | -2.54093100 | -1.65296600 | 0.68191300 |
| H | -3.08510300 | -2.26062100 | -1.38729200 |
| H | -3.08497700 | -2.26069400 | 1.38742200 |
| N | -1.64699300 | -0.68603000 | -1.09435300 |
| N | -1.64690100 | -0.68607800 | 1.09443600 |
| C | -1.27877500 | -0.40640800 | -2.48253100 |
| H | -2.06578100 | -0.79035100 | -3.13081200 |
| H | -1.18645800 | 0.67212600 | -2.62135400 |
| H | -0.33032500 | -0.89704000 | -2.71687500 |
| C | -1.27849900 | -0.40658600 | 2.48259200 |
| H | -1.18597400 | 0.67192400 | 2.62145100 |
| H | -2.06551700 | -0.79041000 | 3.13093000 |
| H | -0.33011700 | -0.89740500 | 2.71682200 |
| Cu | 0.88972300 | 0.42463100 | -0.00000300 |
| Br | -0.94696400 | 2.06912800 | 0.00001300 |
| Br | 1.59250700 | -1.89009300 | -0.00008100 |
| C | 2.55406300 | 1.45064000 | 0.00001600 |
| N | 3.55269400 | 2.05873200 | 0.00003800 |

**$TS^{Cu}$_F_Br**

| | | | |
|---|---|---|---|
| C | -0.73600800 | 0.66219200 | 0.00001200 |
| C | -0.52350000 | 2.77179800 | 0.68214200 |
| C | -0.52353200 | 2.77183100 | -0.68202300 |
| H | -0.39650700 | 3.57919600 | 1.38587200 |

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| | | | |
|---|---|---|---|
| H | -0.39657600 | 3.57926500 | -1.38571900 |
| N | -0.70152900 | 1.46969800 | 1.09716000 |
| N | -0.70157800 | 1.46975100 | -1.09709700 |
| C | -0.65147100 | 1.00506300 | 2.48275300 |
| H | -0.88408200 | 1.84510400 | 3.13666600 |
| H | -1.39048400 | 0.21542300 | 2.62644800 |
| H | 0.34975400 | 0.62467000 | 2.70373400 |
| C | -0.65161900 | 1.00518900 | -2.48271800 |
| H | -1.39069400 | 0.21560700 | -2.62642200 |
| H | -0.88420600 | 1.84528200 | -3.13657200 |
| H | 0.34956800 | 0.62473900 | -2.70377000 |
| Cu | 0.42499600 | -1.05678300 | -0.00001300 |
| Br | -2.09438100 | -0.91479700 | -0.00000200 |
| Br | 2.48708200 | 0.16655900 | -0.00003600 |
| F | 0.76804000 | -2.84075800 | 0.00000300 |

**$TS^{Cu}$_I_Br**

| | | | |
|---|---|---|---|
| C | 1.74779800 | -0.24650100 | 0.00002800 |
| C | 3.79238800 | 0.29985500 | 0.68128200 |
| C | 3.79240800 | 0.29980300 | -0.68120800 |
| H | 4.56944900 | 0.54099300 | 1.38904100 |
| H | 4.56949000 | 0.54088700 | -1.38896200 |
| N | 2.52437100 | -0.06789500 | 1.09217600 |
| N | 2.52440300 | -0.06797700 | -1.09211100 |
| C | 2.06588200 | -0.14319900 | 2.47968500 |
| H | 2.93962000 | -0.14154300 | 3.13055000 |
| H | 1.43377400 | 0.71950600 | 2.70514600 |
| H | 1.50418100 | -1.06766100 | 2.62449400 |
| C | 2.06595700 | -0.14339100 | -2.47962800 |
| H | 2.93971400 | -0.14178500 | -3.13046600 |
| H | 1.50426000 | -1.06786400 | -2.62438100 |
| H | 1.43385400 | 0.71929600 | -2.70517600 |
| Cu | -0.25302100 | 0.08858800 | -0.00000400 |
| Br | 0.07112700 | 2.44400800 | -0.00011000 |
| Br | 0.54139000 | -2.21860400 | 0.00008100 |
| I | -2.85137500 | -0.18883600 | -0.00001000 |

**$TS^{Cu}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | -1.72413700 | -0.56583100 | 0.00668100 |
| C | -3.69855800 | 0.24095000 | -0.63145800 |
| C | -3.67799900 | 0.21758000 | 0.73195200 |
| H | -4.44899900 | 0.59885000 | -1.31837700 |
| H | -4.40722200 | 0.55115400 | 1.45311400 |
| N | -2.50468100 | -0.28743600 | -1.07289900 |
| N | -2.47120000 | -0.32483500 | 1.11873600 |
| C | -2.07927500 | -0.36908500 | -2.46910600 |
| H | -2.96512100 | -0.31236700 | -3.10105600 |
| H | -1.40581900 | 0.46147800 | -2.69682900 |
| H | -1.57045100 | -1.31917900 | -2.63945500 |
| C | -2.00933000 | -0.46329000 | 2.49924800 |

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| | | | |
|---|---|---|---|
| H | -1.33299900 | 0.35896200 | 2.74711600 |
| H | -2.87906700 | -0.43775800 | 3.15517900 |
| H | -1.49333900 | -1.41759900 | 2.61570000 |
| Cu | 0.38163600 | 0.19961600 | -0.00010500 |
| Br | -0.48834600 | 2.46818500 | -0.00697500 |
| Br | -0.50343800 | -2.19053400 | -0.04072000 |
| C | 2.35920700 | 0.02162500 | 0.00525700 |
| C | 3.00647800 | -1.22872900 | 0.00070200 |
| C | 3.19916700 | 1.15497300 | 0.01215700 |
| C | 4.40150400 | -1.35344800 | 0.00310900 |
| H | 2.41286700 | -2.14602500 | -0.00512900 |
| C | 4.59536200 | 1.05048400 | 0.01424700 |
| H | 2.75305100 | 2.14927600 | 0.01553100 |
| C | 5.20304200 | -0.20863600 | 0.00980000 |
| H | 4.86288200 | -2.33987700 | -0.00039900 |
| H | 5.21028100 | 1.94917800 | 0.01919700 |
| H | 6.28732600 | -0.29640800 | 0.01138800 |

**$TS^{Cu}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | 1.20043200 | -0.01970200 | 0.00115100 |
| C | 2.43049000 | -1.74507400 | 0.68855100 |
| C | 2.43331500 | -1.74743000 | -0.67512600 |
| H | 2.86734400 | -2.43318100 | 1.39467300 |
| H | 2.87317100 | -2.43793600 | -1.37702800 |
| N | 1.70653400 | -0.64711000 | 1.09994300 |
| N | 1.71098600 | -0.65097700 | -1.09331700 |
| C | 1.36940500 | -0.33165800 | 2.48712000 |
| H | 2.10985000 | -0.79963300 | 3.13568900 |
| H | 1.39198000 | 0.74981400 | 2.62944900 |
| H | 0.37315200 | -0.71819300 | 2.71865500 |
| C | 1.38033700 | -0.33963900 | -2.48295000 |
| H | 2.12085700 | -0.81382400 | -3.12688700 |
| H | 0.38312300 | -0.72250600 | -2.71640700 |
| H | 1.40849300 | 0.74113000 | -2.62973500 |
| Cu | -0.96671300 | 0.47069300 | -0.00097000 |
| Br | 1.08338700 | 2.01813000 | -0.00292300 |
| Br | -1.46192000 | -1.91138600 | -0.00246400 |
| C | -2.51543400 | 1.68852100 | 0.00090200 |
| H | -2.33194000 | 2.77435700 | 0.00079400 |
| C | -3.81137600 | 1.33237400 | 0.00270100 |
| H | -4.12037800 | 0.28480100 | 0.00289700 |
| H | -4.63798300 | 2.05126400 | 0.00411000 |

**$Cu^{I}$_Bn**

| | | | |
|---|---|---|---|
| Cu | 0.96198300 | 0.60658600 | -0.00001400 |
| Br | 2.96276400 | -0.60412000 | 0.00001700 |
| C | -0.73408500 | 1.60705500 | -0.00004300 |
| H | -0.73873100 | 2.25235900 | 0.88858900 |
| H | -0.73872300 | 2.25230300 | -0.88871600 |
| C | -1.90202500 | 0.68491500 | -0.00001900 |

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| | | | |
|---|---|---|---|
| C | -2.48216200 | 0.21835900 | -1.20118900 |
| C | -2.48217800 | 0.21844100 | 1.20117500 |
| C | -3.56348300 | -0.66280500 | -1.20290300 |
| H | -2.06853900 | 0.55932100 | -2.14929500 |
| C | -3.56349900 | -0.66272300 | 1.20293400 |
| H | -2.06856900 | 0.55946800 | 2.14926400 |
| C | -4.11583000 | -1.11599600 | 0.00002700 |
| H | -3.98071900 | -0.99578800 | -2.15140300 |
| H | -3.98074600 | -0.99564200 | 2.15145100 |
| H | -4.95864900 | -1.80230900 | 0.00004500 |

**$Cu^{I}$_Br**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | 0.00000000 |
| Br | 0.00000000 | 0.00000000 | 2.29773100 |
| Br | 0.00000000 | 0.00000000 | -2.29773100 |

**$Cu^{I}$_$CF_3$**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.01051500 |
| Br | 0.00000000 | 0.00000000 | 2.29371900 |
| C | 0.00000000 | 0.00000000 | -1.94343600 |
| F | 0.00000000 | 1.25835600 | -2.53017000 |
| F | 1.08976800 | -0.62917800 | -2.53017000 |
| F | -1.08976800 | -0.62917800 | -2.53017000 |

**$Cu^{I}$_$CH_3$**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.86925100 |
| Br | 0.00000000 | 0.00000000 | 1.47897300 |
| C | 0.00000000 | 0.00000000 | -2.81399600 |
| H | 0.00000000 | 1.02180000 | -3.22394100 |
| H | 0.88490500 | -0.51090000 | -3.22394100 |
| H | -0.88490500 | -0.51090000 | -3.22394100 |

**$Cu^{I}$_Cl**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.52847400 |
| Br | 0.00000000 | 0.00000000 | 1.76185000 |
| Cl | 0.00000000 | 0.00000000 | -2.72582400 |

**$Cu^{I}$_CN**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.61513600 | 0.00000000 |
| Br | -0.00155400 | -1.67417100 | 0.00000000 |
| C | 0.00312100 | 2.50451400 | 0.00000000 |
| N | 0.00509600 | 3.67570900 | 0.00000000 |

**$Cu^{I}$_F**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.88079600 | 0.00000000 |
| Br | -0.00066200 | -1.41405200 | 0.00000000 |
| F | 0.00257600 | 2.66097000 | 0.00000000 |

**$Cu^{I}$_I**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.44001100 |
| Br | 0.00000000 | 0.00000000 | -2.74460700 |
| I | 0.00000000 | 0.00000000 | 2.05323700 |

**$Cu^{I}$_Ph**

| | | | |
|---|---|---|---|
| Cu | -0.56998700 | -0.00002600 | -0.00001000 |
| Br | -2.89765900 | 0.00001300 | -0.00001200 |

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| | | | |
|---|---|---|---|
| C | 1.36365700 | -0.00002000 | 0.00000300 |
| C | 2.12165300 | 1.19529200 | 0.00001100 |
| C | 2.12169500 | -1.19530300 | 0.00000900 |
| C | 3.52186200 | 1.20437700 | 0.00002500 |
| H | 1.60768000 | 2.15659300 | 0.00000600 |
| C | 3.52190400 | -1.20433800 | 0.00002300 |
| H | 1.60775500 | -2.15662300 | 0.00000300 |
| C | 4.23125500 | 0.00003200 | 0.00003100 |
| H | 4.06038700 | 2.15106700 | 0.00003100 |
| H | 4.06046200 | -2.15100900 | 0.00002800 |
| H | 5.31924500 | 0.00005100 | 0.00004200 |

**$Cu^{I}$_vinyl**

| | | | |
|---|---|---|---|
| Cu | -0.55426000 | -0.17794400 | -0.00000200 |
| Br | 1.76290300 | 0.09720800 | 0.00000200 |
| C | -2.46127300 | -0.39147300 | -0.00000500 |
| H | -2.88746300 | -1.40611000 | 0.00001200 |
| C | -3.39422800 | 0.58141300 | -0.00000100 |
| H | -3.13549700 | 1.64251900 | 0.00000700 |
| H | -4.47212900 | 0.38203300 | 0.00000400 |

**$Ag^{III}$_Bn_Br**

| | | | |
|---|---|---|---|
| C | 2.21414489 | -0.11759520 | 0.19400420 |
| C | 3.97928855 | -0.64246410 | 1.46160157 |
| C | 4.14305164 | -1.24614368 | 0.25542816 |
| H | 4.57718481 | -0.68611975 | 2.35823095 |
| H | 4.91077207 | -1.91582385 | -0.09878049 |
| N | 2.81518819 | 0.09747546 | 1.40189930 |
| N | 3.07923004 | -0.87591138 | -0.54296759 |
| C | 2.16019182 | 0.72593055 | 2.54540772 |
| H | 2.92141680 | 0.99386710 | 3.27972446 |
| H | 1.64178829 | 1.62850204 | 2.21620539 |
| H | 1.44475100 | 0.02073630 | 2.98130340 |
| C | 2.75538835 | -1.46768513 | -1.83777698 |
| H | 2.27759730 | -0.71745757 | -2.47072554 |
| H | 3.68046197 | -1.80248586 | -2.30961435 |
| H | 2.07910896 | -2.31546088 | -1.68586960 |
| Br | 1.51600614 | 0.84880374 | -2.55759543 |
| Br | -0.98197543 | -0.77268433 | 1.42554372 |
| C | -1.78619134 | 0.13220352 | -1.17690938 |
| H | -2.20189625 | -0.85349924 | -1.15498315 |
| H | -1.75737224 | 0.48475516 | -2.18674867 |
| C | -2.73066778 | 1.05600376 | -0.38560932 |
| C | -3.72111077 | 0.50772682 | 0.42979702 |
| C | -2.59589434 | 2.44081675 | -0.48398041 |
| C | -4.57697574 | 1.34415563 | 1.14610941 |
| H | -3.82759972 | -0.58406611 | 0.50653810 |
| C | -3.45130576 | 3.27763198 | 0.23325066 |
| H | -1.81521062 | 2.87311118 | -1.12646393 |
| C | -4.44183854 | 2.72956155 | 1.04811274 |

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| | | | |
|---|---|---|---|
| H | -5.35808142 | 0.91207547 | 1.78835382 |
| H | -3.34454182 | 4.36945584 | 0.15581372 |
| H | -5.11673631 | 3.38885446 | 1.61303942 |
| Ag | 0.20321719 | 0.00443934 | -0.48551147 |

**$Ag^{III}$_Br_Br**

| | | | |
|---|---|---|---|
| C | -1.68168200 | 0.00618200 | -0.00015500 |
| C | -3.80174400 | 0.00966800 | 0.68072400 |
| C | -3.80256000 | 0.00939300 | -0.67849300 |
| H | -4.61201900 | 0.01277000 | 1.39229400 |
| H | -4.61368700 | 0.01143500 | -1.38911000 |
| N | -2.47583800 | 0.00781200 | -1.08442100 |
| N | -2.47443500 | 0.00774500 | 1.08511200 |
| C | -2.01490700 | 0.00203000 | 2.47716700 |
| H | -1.44004200 | -0.90622900 | 2.66970200 |
| H | -1.39474100 | 0.88152500 | 2.66157400 |
| H | -2.88892800 | 0.02760600 | 3.12707100 |
| C | -2.01829600 | -0.00510400 | -2.47704400 |
| H | -1.36697900 | 0.85260000 | -2.65586800 |
| H | -1.47696500 | -0.93220700 | -2.67742400 |
| H | -2.89146800 | 0.05786000 | -3.12561000 |
| Br | 0.20750400 | 2.51883800 | -0.00103700 |
| Br | 0.18905300 | -2.51739900 | 0.00092100 |
| Ag | 0.40008500 | -0.00031500 | -0.00024300 |
| Br | 2.93052500 | -0.00808200 | -0.00014800 |

**$Ag^{III}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.74747700 | -0.02719300 | 0.01754000 |
| C | -3.87987400 | -0.14306700 | -0.68045300 |
| C | -3.89361000 | -0.10679400 | 0.67774600 |
| H | -4.68376500 | -0.19432600 | -1.39768100 |
| H | -4.71233600 | -0.12057700 | 1.37973800 |
| N | -2.54848000 | -0.09134500 | -1.06698000 |
| N | -2.56996800 | -0.03283800 | 1.08796000 |
| C | -2.07557500 | -0.11863400 | -2.45220200 |
| H | -2.93729400 | -0.04969000 | -3.11633000 |
| H | -1.41230700 | 0.73034500 | -2.62953000 |
| H | -1.53968300 | -1.05105300 | -2.64500000 |
| C | -2.12808800 | 0.00210500 | 2.48315200 |
| H | -1.39734200 | 0.80205700 | 2.61516400 |
| H | -2.99264700 | 0.19708200 | 3.11817800 |
| H | -1.68091300 | -0.95557200 | 2.76071500 |
| Br | 0.26228400 | 2.55813900 | -0.05854700 |
| Br | 0.43682600 | -2.50150200 | -0.01881200 |
| Ag | 0.39814900 | 0.03465900 | 0.02714200 |
| C | 2.52128700 | 0.03395000 | 0.02960900 |
| F | 3.10031200 | 1.24260000 | 0.10536500 |
| F | 2.95978200 | -0.55162900 | -1.10387900 |
| F | 2.96474700 | -0.68457500 | 1.08155900 |

**$Ag^{III}$_$CH_3$_Br**

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| | | | |
|---|---|---|---|
| C | 1.42542900 | -0.25706000 | 0.00339600 |
| C | 3.48057600 | -0.98614400 | -0.58654300 |
| C | 3.60982600 | -0.29894600 | 0.57793600 |
| H | 4.21355700 | -1.48444700 | -1.20161100 |
| H | 4.47560900 | -0.09043900 | 1.18686800 |
| N | 2.13425900 | -0.95236200 | -0.91886800 |
| N | 2.33992600 | 0.14280900 | 0.91977200 |
| C | 1.56870300 | -1.54140800 | -2.13238000 |
| H | 2.23356700 | -2.33241600 | -2.48303700 |
| H | 0.59285000 | -1.96880300 | -1.89802200 |
| H | 1.46528600 | -0.78368500 | -2.91412700 |
| C | 2.03096800 | 0.88312100 | 2.14239800 |
| H | 1.80952300 | 0.19351800 | 2.96193300 |
| H | 2.89133100 | 1.49898200 | 2.41094600 |
| H | 1.17180200 | 1.52860900 | 1.95803200 |
| Br | -1.34398400 | -2.30953200 | 0.35298200 |
| Br | -0.41558100 | 2.63529500 | -0.35460300 |
| Ag | -0.74093000 | 0.13695400 | -0.00177200 |
| C | -2.85088000 | 0.48533700 | 0.00701600 |
| H | -3.23283400 | -0.19594200 | -0.74960400 |
| H | -3.14084900 | 0.21685900 | 1.02122600 |
| H | -2.97842300 | 1.53668800 | -0.22985800 |

**$Ag^{III}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | 1.37146500 | -0.00059400 | 0.00310200 |
| C | 3.48934200 | -0.00659500 | -0.67679500 |
| C | 3.48953300 | -0.01200400 | 0.68236300 |
| H | 4.29969200 | -0.00618500 | -1.38822100 |
| H | 4.30001100 | -0.01793500 | 1.39363300 |
| N | 2.16271100 | 0.00069000 | -1.08264500 |
| N | 2.16303400 | -0.00741100 | 1.08870900 |
| C | 1.70619700 | 0.00508500 | -2.47602100 |
| H | 2.58231900 | 0.03536000 | -3.12267500 |
| H | 1.13211700 | -0.90189200 | -2.67642000 |
| H | 1.08693700 | 0.88620600 | -2.65501000 |
| C | 1.70787600 | -0.01952200 | 2.48253300 |
| H | 1.15957900 | -0.94263400 | 2.68186400 |
| H | 2.58353200 | 0.03442100 | 3.12834800 |
| H | 1.06487600 | 0.84373200 | 2.66437100 |
| Br | -0.48613800 | -2.51250600 | -0.01170400 |
| Br | -0.47181600 | 2.51585600 | -0.00388500 |
| Ag | -0.69574600 | 0.00210900 | 0.00471900 |
| Cl | -3.10866600 | 0.00596500 | 0.00967300 |

**$Ag^{III}$_CN_Br**

| | | | |
|---|---|---|---|
| C | 1.36973600 | -0.00039900 | 0.00051400 |
| C | 3.49622400 | -0.00240600 | -0.68026300 |
| C | 3.49694700 | 0.00005400 | 0.67886700 |
| H | 4.30680900 | -0.00305100 | -1.39145200 |
| H | 4.30833500 | 0.00017300 | 1.38910800 |

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| | | | |
|---|---|---|---|
| N | 2.16920700 | -0.00315000 | -1.08265800 |
| N | 2.17029900 | 0.00175100 | 1.08267800 |
| C | 1.71338500 | 0.00140100 | -2.47598700 |
| H | 2.58810900 | -0.04331500 | -3.12403200 |
| H | 1.07976600 | -0.86901500 | -2.65757400 |
| H | 1.15393300 | 0.91724600 | -2.67813700 |
| C | 1.71569900 | -0.00291400 | 2.47626900 |
| H | 1.15782600 | -0.91952700 | 2.67915600 |
| H | 2.59089200 | 0.04344700 | 3.12357300 |
| H | 1.08090300 | 0.86661100 | 2.65791100 |
| Br | -0.60301300 | -2.51939100 | -0.00080700 |
| Br | -0.60055900 | 2.51962700 | -0.00025600 |
| Ag | -0.70687300 | 0.00014300 | 0.00065300 |
| C | -2.75996600 | 0.00170000 | 0.00083600 |
| N | -3.92674300 | 0.00252300 | 0.00091500 |

**$Ag^{III}$_F_Br**

| | | | |
|---|---|---|---|
| C | -0.03610800 | 1.20598400 | 0.00089300 |
| C | -0.11833000 | 3.32495900 | 0.68152100 |
| C | -0.11739500 | 3.32559900 | -0.67779700 |
| H | -0.14891500 | 4.13464100 | 1.39306900 |
| H | -0.14710300 | 4.13595600 | -1.38861000 |
| N | -0.06515800 | 2.00017300 | -1.08333300 |
| N | -0.06666700 | 1.99915800 | 1.08586400 |
| C | -0.05940500 | 1.53751600 | 2.47718400 |
| H | -0.03377800 | 2.41037400 | 3.12856900 |
| H | -0.96228000 | 0.95598600 | 2.67547200 |
| H | 0.82545400 | 0.92253500 | 2.65255400 |
| C | -0.05688700 | 1.53979700 | -2.47506200 |
| H | 0.82591700 | 0.92154400 | -2.64915300 |
| H | -0.96162900 | 0.96200000 | -2.67579300 |
| H | -0.02636100 | 2.41314300 | -3.12560300 |
| Br | 2.53319000 | -0.57629800 | -0.00238800 |
| Br | -2.48507500 | -0.73663700 | -0.00331100 |
| Ag | 0.02972200 | -0.83816800 | 0.00147600 |
| F | 0.08880700 | -2.78978000 | 0.00682800 |

**$Ag^{III}$_I_Br**

| | | | |
|---|---|---|---|
| C | 1.99812300 | 0.01091900 | 0.00057500 |
| C | 4.12218400 | 0.00520700 | -0.67714000 |
| C | 4.12098300 | 0.00525500 | 0.68207700 |
| H | 4.93353100 | 0.00492700 | -1.38755700 |
| H | 4.93106100 | 0.00518900 | 1.39394400 |
| N | 2.79317200 | 0.00936000 | 1.08497500 |
| N | 2.79508400 | 0.00939800 | -1.08241300 |
| C | 2.33782300 | -0.00357500 | -2.47480500 |
| H | 1.80756400 | -0.93605500 | -2.67978000 |
| H | 1.67637000 | 0.84689300 | -2.65045700 |
| H | 3.20982200 | 0.07271300 | -3.12365900 |
| C | 2.33333400 | -0.00183100 | 2.47653800 |

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| | | | |
|---|---|---|---|
| H | 1.67888800 | 0.85402100 | 2.65250100 |
| H | 1.79467200 | -0.93004300 | 2.67885200 |
| H | 3.20480200 | 0.06559000 | 3.12706300 |
| Br | 0.04536100 | 2.52623300 | -0.00124600 |
| Br | 0.07465700 | -2.51742000 | -0.00078000 |
| I | -2.85093100 | -0.01268500 | 0.00076000 |
| Ag | -0.10490300 | 0.00326500 | -0.00088600 |

**$Ag^{III}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | -2.14549200 | 0.04528100 | 0.00251400 |
| C | -4.29689700 | -0.01013800 | 0.68723600 |
| C | -4.30068000 | -0.01031400 | -0.67030600 |
| H | -5.10726900 | -0.02195900 | 1.39939300 |
| H | -5.11503000 | -0.02235100 | -1.37791500 |
| N | -2.97221500 | 0.02732200 | -1.07036600 |
| N | -2.96625700 | 0.02771100 | 1.07994400 |
| C | -2.52775000 | -0.00370900 | 2.47359700 |
| H | -2.57721200 | -1.02370900 | 2.86480800 |
| H | -1.50167300 | 0.35795300 | 2.53281600 |
| H | -3.17091400 | 0.64662900 | 3.07006400 |
| C | -2.54155700 | -0.00409500 | -2.46645200 |
| H | -1.51438600 | 0.35352100 | -2.53093200 |
| H | -2.59720900 | -1.02343100 | -2.85852500 |
| H | -3.18538800 | 0.64949500 | -3.05865400 |
| Br | 0.24583400 | 2.55534300 | -0.00457300 |
| Br | 0.12812600 | -2.52309600 | -0.00469000 |
| C | 2.13263700 | -0.02417900 | 0.00105000 |
| C | 2.79589500 | -0.04070200 | 1.22060900 |
| C | 2.80127500 | -0.04053300 | -1.21555300 |
| C | 4.19782600 | -0.07615400 | 1.21530300 |
| H | 2.25681900 | -0.02703400 | 2.16317200 |
| C | 4.20315800 | -0.07596000 | -1.20413600 |
| H | 2.26624900 | -0.02677000 | -2.16041100 |
| C | 4.89816700 | -0.09380600 | 0.00712500 |
| H | 4.73314300 | -0.08983700 | 2.16126500 |
| H | 4.74265600 | -0.08947800 | -2.14772200 |
| H | 5.98422900 | -0.12129800 | 0.00953400 |
| Ag | 0.04185500 | 0.01979200 | -0.00246100 |

**$Ag^{III}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | 1.56572100 | -0.14167600 | 0.08001700 |
| C | 3.66890000 | -0.28693100 | 0.89115300 |
| C | 3.75885000 | -0.18104100 | -0.45942300 |
| H | 4.43185800 | -0.38637200 | 1.64738800 |
| H | 4.61602000 | -0.17076400 | -1.11448900 |
| N | 2.45868400 | -0.09684000 | -0.93761400 |
| N | 2.31645100 | -0.26517500 | 1.20123900 |
| C | 1.78991600 | -0.31263500 | 2.56430700 |
| H | 1.76065100 | 0.69104400 | 2.99763000 |
| H | 0.78372500 | -0.73174600 | 2.54667900 |

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| | | | |
|---|---|---|---|
| H | 2.43091200 | -0.95254800 | 3.17365700 |
| C | 2.11863700 | 0.07049600 | -2.34926000 |
| H | 1.08576800 | -0.23895900 | -2.50684700 |
| H | 2.23490400 | 1.11615800 | -2.64745500 |
| H | 2.77556800 | -0.55634300 | -2.95581300 |
| Br | -1.00616000 | -2.47714300 | -0.22516400 |
| Br | -0.55291800 | 2.57414600 | -0.09932900 |
| Ag | -0.61644300 | 0.03261600 | -0.04478400 |
| C | -2.68859100 | 0.21580600 | -0.15789800 |
| H | -3.00266300 | 0.23456700 | -1.19823700 |
| C | -3.44822100 | 0.29330200 | 0.91836700 |
| H | -3.06120700 | 0.27087700 | 1.93456800 |
| H | -4.53217100 | 0.38624200 | 0.81610200 |

**$TS^{Ag}$_Bn_Br**

| | | | |
|---|---|---|---|
| C | -1.68489200 | -1.89769600 | 0.00801200 |
| C | -3.62180400 | -2.38607200 | 1.08522500 |
| C | -3.91633300 | -2.23433200 | -0.23191400 |
| H | -4.25190400 | -2.62047800 | 1.92979000 |
| H | -4.85381600 | -2.31056900 | -0.76159700 |
| N | -2.25270700 | -2.17606100 | 1.20837900 |
| N | -2.71772200 | -1.93658200 | -0.87097800 |
| C | -1.51955900 | -2.24287700 | 2.46857700 |
| H | -1.89748500 | -1.49122200 | 3.16747700 |
| H | -1.62621600 | -3.23512400 | 2.91605900 |
| H | -0.46778000 | -2.04927900 | 2.25989700 |
| C | -2.58807200 | -1.69117600 | -2.30378300 |
| H | -2.92766000 | -2.56379900 | -2.86886200 |
| H | -3.18311700 | -0.82080200 | -2.59461700 |
| H | -1.53737000 | -1.50263700 | -2.52235300 |
| Br | 0.81617100 | -1.39325500 | -0.48808300 |
| Br | -1.90631500 | 2.89134900 | 0.35637500 |
| C | 2.43498400 | 1.74389700 | -0.97702600 |
| H | 2.54152200 | 2.73324800 | -0.54039300 |
| H | 2.11245900 | 1.69467100 | -2.01452100 |
| C | 2.95921300 | 0.64176100 | -0.34506300 |
| C | 3.59670900 | 0.73734600 | 0.95519500 |
| C | 2.88137900 | -0.71366800 | -0.95427800 |
| C | 4.27825500 | -0.31373200 | 1.48510500 |
| H | 3.56306800 | 1.69354600 | 1.47096500 |
| C | 3.74853200 | -1.75387800 | -0.39881500 |
| H | 2.78751000 | -0.71516000 | -2.03802400 |
| C | 4.39039500 | -1.57221300 | 0.78203300 |
| H | 4.78197000 | -0.20239700 | 2.44161100 |
| H | 3.82421100 | -2.69252400 | -0.94026000 |
| H | 4.99990200 | -2.36315800 | 1.20903400 |
| Ag | 0.07084900 | 1.33822800 | -0.17672000 |

**$TS^{Ag}$_Br_Br**

| | | | |
|---|---|---|---|
| C | -1.60107400 | -0.09696700 | 0.00014600 |

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| | | | |
|---|---|---|---|
| C | -3.53451200 | 0.76277900 | 0.68147900 |
| C | -3.53467100 | 0.76339300 | -0.67994900 |
| H | -4.26469700 | 1.12055000 | 1.38989300 |
| H | -4.26501300 | 1.12181100 | -1.38787300 |
| N | -2.33591500 | 0.20536700 | 1.09219300 |
| N | -2.33617800 | 0.20633800 | -1.09145000 |
| C | -1.91771500 | 0.02198200 | 2.48362400 |
| H | -2.79159300 | 0.14641200 | 3.12210200 |
| H | -1.51452000 | -0.98481300 | 2.60601100 |
| H | -1.15892800 | 0.76330900 | 2.74494200 |
| C | -1.91824200 | 0.02433900 | -2.48314000 |
| H | -1.51510900 | -0.98234600 | -2.60662800 |
| H | -2.79223000 | 0.14946500 | -3.12133200 |
| H | -1.15947100 | 0.76591100 | -2.74381300 |
| Br | -0.75416500 | -2.31337000 | -0.00084500 |
| Br | 0.56467400 | 2.54066300 | -0.00006500 |
| Ag | 0.55936700 | -0.03016400 | 0.00005300 |
| Br | 3.07272600 | -0.58208300 | 0.00022600 |

**$TS^{Ag}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.06749200 | 0.58374000 | 0.01723000 |
| C | 1.40560900 | 2.73890600 | -0.45521600 |
| C | 1.55194600 | 2.58156000 | 0.89067600 |
| H | 1.44620300 | 3.62459400 | -1.06953000 |
| H | 1.74840700 | 3.30292100 | 1.66805400 |
| N | 1.14385800 | 1.49458000 | -0.99013600 |
| N | 1.37473000 | 1.24101700 | 1.16974000 |
| C | 0.82544200 | 1.22903700 | -2.39141000 |
| H | 1.22661800 | 2.04155300 | -2.99720600 |
| H | 1.28566400 | 0.28664100 | -2.69277400 |
| H | -0.25963600 | 1.17062000 | -2.51110500 |
| C | 1.41959600 | 0.65127500 | 2.50782600 |
| H | 1.86320300 | -0.34326800 | 2.44561500 |
| H | 2.03761300 | 1.28622600 | 3.14287400 |
| H | 0.41149100 | 0.58088100 | 2.92348200 |
| Br | 1.98478900 | -1.31328600 | -0.29106300 |
| Br | -2.36933900 | 1.12973200 | -0.01530500 |
| C | -1.85542200 | -2.80718700 | 0.16212900 |
| H | -2.54969400 | -2.78632200 | 1.00964200 |
| H | -2.42928200 | -2.93126500 | -0.76344300 |
| H | -1.17145500 | -3.65713900 | 0.27630200 |
| Ag | -0.72910600 | -0.96094100 | 0.07758200 |

**$TS^{Ag}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.06749200 | 0.58374000 | 0.01723000 |
| C | 1.40560900 | 2.73890600 | -0.45521600 |
| C | 1.55194600 | 2.58156000 | 0.89067600 |
| H | 1.44620300 | 3.62459400 | -1.06953000 |
| H | 1.74840700 | 3.30292100 | 1.66805400 |
| N | 1.14385800 | 1.49458000 | -0.99013600 |

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| | | | |
|---|---|---|---|
| N | 1.37473000 | 1.24101700 | 1.16974000 |
| C | 0.82544200 | 1.22903700 | -2.39141000 |
| H | 1.22661800 | 2.04155300 | -2.99720600 |
| H | 1.28566400 | 0.28664100 | -2.69277400 |
| H | -0.25963600 | 1.17062000 | -2.51110500 |
| C | 1.41959600 | 0.65127500 | 2.50782600 |
| H | 1.86320300 | -0.34326800 | 2.44561500 |
| H | 2.03761300 | 1.28622600 | 3.14287400 |
| H | 0.41149100 | 0.58088100 | 2.92348200 |
| Br | 1.98478900 | -1.31328600 | -0.29106300 |
| Br | -2.36933900 | 1.12973200 | -0.01530500 |
| C | -1.85542200 | -2.80718700 | 0.16212900 |
| H | -2.54969400 | -2.78632200 | 1.00964200 |
| H | -2.42928200 | -2.93126500 | -0.76344300 |
| H | -1.17145500 | -3.65713900 | 0.27630200 |
| Ag | -0.72910600 | -0.96094100 | 0.07758200 |

**$TS^{Ag}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | 1.26785700 | -0.30037100 | 0.00005900 |
| C | 2.79216100 | -1.76637100 | 0.68106500 |
| C | 2.79210800 | -1.76667200 | -0.68041100 |
| H | 3.35868300 | -2.34976700 | 1.38936300 |
| H | 3.35856400 | -2.35039100 | -1.38849600 |
| N | 1.85426400 | -0.83532900 | 1.09241400 |
| N | 1.85418300 | -0.83581200 | -1.09209900 |
| C | 1.51336200 | -0.53032900 | 2.48348500 |
| H | 2.29561100 | -0.93629800 | 3.12384700 |
| H | 1.46108200 | 0.55240900 | 2.61022600 |
| H | 0.55242600 | -0.98423100 | 2.73708800 |
| C | 1.51308500 | -0.53151100 | -2.48327000 |
| H | 1.46036500 | 0.55115600 | -2.61043100 |
| H | 2.29545700 | -0.93741600 | -3.12352100 |
| H | 0.55230800 | -0.98589200 | -2.73662800 |
| Br | 1.23646000 | 2.06544100 | -0.00037800 |
| Br | -1.68927300 | -2.01977500 | 0.00002300 |
| Cl | -2.84579100 | 1.70752700 | 0.00024500 |
| Ag | -0.77315300 | 0.38050400 | -0.00002100 |

**$TS^{Ag}$_CN_Br**

| | | | |
|---|---|---|---|
| C | -1.19277400 | -0.30721200 | 0.00008200 |
| C | -2.54458900 | -1.93965400 | -0.68067300 |
| C | -2.54471900 | -1.93922100 | 0.68162000 |
| H | -3.03878100 | -2.58708600 | -1.38742600 |
| H | -3.03904600 | -2.58620100 | 1.38869100 |
| N | -1.72369400 | -0.90706000 | -1.09241600 |
| N | -1.72391200 | -0.90636200 | 1.09286200 |
| C | -1.41481600 | -0.57628000 | -2.48418100 |
| H | -2.16264400 | -1.04627200 | -3.12214900 |
| H | -1.45284400 | 0.50688100 | -2.61237000 |
| H | -0.42001700 | -0.94859000 | -2.74078700 |

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| | | | |
|---|---|---|---|
| C | -1.41517800 | -0.57479700 | 2.48446900 |
| H | -1.45249800 | 0.50848200 | 2.61185400 |
| H | -2.16350100 | -1.04379200 | 3.12259400 |
| H | -0.42068900 | -0.94759200 | 2.74159200 |
| Br | -1.39270800 | 1.97744300 | -0.00051600 |
| Br | 1.79682200 | -1.90902000 | -0.00004900 |
| C | 2.58145700 | 1.68527500 | -0.00000300 |
| N | 3.55439200 | 2.33338500 | 0.00006300 |
| Ag | 0.81792000 | 0.51108400 | 0.00013400 |

**$TS^{Ag}$_F_Br**

| | | | |
|---|---|---|---|
| C | 0.90339400 | 0.69897500 | 0.00040300 |
| C | 1.20409900 | 2.79840200 | -0.67882300 |
| C | 1.20570900 | 2.79696900 | 0.68340100 |
| H | 1.28698400 | 3.60935400 | -1.38507100 |
| H | 1.29022600 | 3.60644400 | 1.39115300 |
| N | 1.04468100 | 1.48931800 | -1.09252600 |
| N | 1.04731300 | 1.48698800 | 1.09468900 |
| C | 0.91192800 | 1.04731800 | -2.48051300 |
| H | 1.43315200 | 1.75767300 | -3.12207600 |
| H | 1.36452100 | 0.06020100 | -2.58418200 |
| H | -0.14567600 | 1.00095100 | -2.75269800 |
| C | 0.91779500 | 1.04207700 | 2.48207200 |
| H | 1.36938300 | 0.05416000 | 2.58229700 |
| H | 1.44168800 | 1.75032200 | 3.12379400 |
| H | -0.13910800 | 0.99646100 | 2.75711400 |
| Br | 2.11773200 | -1.16446000 | -0.00342000 |
| Br | -2.56001300 | 0.70469200 | -0.00076300 |
| F | -1.38998600 | -2.75189400 | 0.00175800 |
| Ag | -0.54070200 | -0.91730300 | 0.00140100 |

**$TS^{Ag}$_I_Br**

| | | | |
|---|---|---|---|
| C | -1.90751100 | -0.18637300 | 0.00000700 |
| C | -3.91132800 | 0.49607700 | 0.68084800 |
| C | -3.91131900 | 0.49617400 | -0.68076300 |
| H | -4.67119700 | 0.78563100 | 1.38913200 |
| H | -4.67117200 | 0.78584200 | -1.38901700 |
| N | -2.66702900 | 0.05067800 | 1.09139400 |
| N | -2.66702000 | 0.05081900 | -1.09135500 |
| C | -2.23157400 | -0.08281500 | 2.48301400 |
| H | -3.11257700 | -0.04176200 | 3.12269100 |
| H | -1.73080300 | -1.04413400 | 2.61048800 |
| H | -1.54907600 | 0.73138300 | 2.73791300 |
| C | -2.23151000 | -0.08232700 | -2.48299000 |
| H | -1.72998400 | -1.04324900 | -2.61046600 |
| H | -3.11256900 | -0.04199500 | -3.12263700 |
| H | -1.54966600 | 0.73241100 | -2.73791700 |
| Br | -0.87559200 | -2.32551900 | -0.00012800 |
| Br | 0.09718900 | 2.61584400 | 0.00002900 |
| I | 3.01276600 | -0.33955700 | 0.00000600 |

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| | | | |
|---|---|---|---|
| Ag | 0.25941200 | 0.05140700 | 0.00004300 |

**$TS^{Ag}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | -1.87685700 | -0.49846200 | 0.00004700 |
| C | -3.83180600 | 0.33311700 | 0.68177300 |
| C | -3.83189700 | 0.33321800 | -0.68129000 |
| H | -4.56656900 | 0.68807800 | 1.38708800 |
| H | -4.56675200 | 0.68828800 | -1.38645500 |
| N | -2.63409300 | -0.21559600 | 1.09363300 |
| N | -2.63424200 | -0.21543700 | -1.09339300 |
| C | -2.20277300 | -0.35186900 | 2.48422900 |
| H | -3.08644700 | -0.33289900 | 3.12177500 |
| H | -1.68379400 | -1.30363100 | 2.60826800 |
| H | -1.53543600 | 0.47212700 | 2.74914800 |
| C | -2.20308400 | -0.35145700 | -2.48406300 |
| H | -1.68415000 | -1.30321200 | -2.60834600 |
| H | -3.08682900 | -0.33233400 | -3.12150600 |
| H | -1.53575200 | 0.47257200 | -2.74889000 |
| Br | -0.78655800 | -2.32815200 | -0.00016300 |
| Br | -0.36597600 | 2.65010200 | -0.00009100 |
| C | 2.52874400 | -0.06139600 | 0.00002700 |
| C | 3.11636900 | -1.33908200 | -0.00012700 |
| C | 3.39861500 | 1.04373900 | 0.00018900 |
| C | 4.50677200 | -1.51292100 | -0.00012000 |
| H | 2.48559300 | -2.23020800 | -0.00025600 |
| C | 4.79021500 | 0.88368000 | 0.00020000 |
| H | 2.98906800 | 2.05304200 | 0.00030500 |
| C | 5.34875400 | -0.39776100 | 0.00004500 |
| H | 4.93109000 | -2.51556500 | -0.00024300 |
| H | 5.43875900 | 1.75810800 | 0.00032800 |
| H | 6.42883800 | -0.52585800 | 0.00005200 |
| Ag | 0.38789600 | 0.12075800 | 0.00001000 |

**$TS^{Ag}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | -1.33167300 | 0.19709700 | 0.00155500 |
| C | -2.48262200 | 1.97964200 | 0.69308300 |
| C | -2.48141700 | 1.98788000 | -0.67006000 |
| H | -2.89071800 | 2.68238700 | 1.40221000 |
| H | -2.88851000 | 2.69909400 | -1.37123400 |
| N | -1.80106800 | 0.85031600 | 1.09913900 |
| N | -1.79919100 | 0.86364300 | -1.08871800 |
| C | -1.50546300 | 0.49804400 | 2.48723400 |
| H | -2.25381200 | 0.96401400 | 3.12852100 |
| H | -1.55231900 | -0.58608700 | 2.60004800 |
| H | -0.50837700 | 0.85644700 | 2.75578800 |
| C | -1.50014500 | 0.52814700 | -2.48022200 |
| H | -1.56228600 | -0.55335500 | -2.61027800 |
| H | -2.23732200 | 1.01525700 | -3.11869600 |
| H | -0.49619300 | 0.87599900 | -2.73676000 |
| Br | -1.51063800 | -1.93389400 | -0.01158600 |

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| | | | |
|---|---|---|---|
| Br | 1.64300500 | 1.96176700 | -0.00246400 |
| C | 2.58091300 | -1.84425400 | 0.00439100 |
| H | 2.39678500 | -2.92693900 | 0.00441900 |
| C | 3.86325800 | -1.45680400 | 0.00533300 |
| H | 4.15249400 | -0.40463600 | 0.00522200 |
| H | 4.70009600 | -2.16387200 | 0.00622500 |
| Ag | 0.86919200 | -0.56957700 | 0.00224400 |

**$Ag^{I}$_Bn**

| | | | |
|---|---|---|---|
| Br | -3.08827300 | -0.70521200 | 0.00066000 |
| Ag | -0.83142000 | 0.52718200 | -0.00028300 |
| C | 1.07324000 | 1.55318100 | -0.00235100 |
| H | 1.07602000 | 2.19142200 | -0.89277200 |
| H | 1.07636700 | 2.19431500 | 0.88598700 |
| C | 2.22306200 | 0.61453600 | -0.00105000 |
| C | 2.80008700 | 0.14687200 | 1.20136400 |
| C | 2.79953800 | 0.14287300 | -1.20216300 |
| C | 3.87435600 | -0.74246700 | 1.20402500 |
| H | 2.38854600 | 0.49182900 | 2.14884800 |
| C | 3.87380800 | -0.74647000 | -1.20235100 |
| H | 2.38757200 | 0.48468300 | -2.15060200 |
| C | 4.42263900 | -1.20196600 | 0.00147300 |
| H | 4.28936800 | -1.07714200 | 2.15282300 |
| H | 4.28839300 | -1.08429300 | -2.15021900 |
| H | 5.25964800 | -1.89527300 | 0.00243600 |

**$Ag^{I}$_Br**

| | | | |
|---|---|---|---|
| Br | 0.00000000 | 0.00000000 | 2.53516100 |
| Ag | 0.00000000 | 0.00000000 | 0.00000000 |
| Br | 0.00000000 | 0.00000000 | -2.53516100 |

**$Ag^{I}$_$CF_3$**

| | | | |
|---|---|---|---|
| Br | 0.00000000 | 0.00000000 | -2.51210000 |
| Ag | 0.00000000 | 0.00000000 | 0.02031900 |
| C | 0.00000000 | 0.00000000 | 2.15134300 |
| F | 0.00000000 | 1.25440200 | 2.74298100 |
| F | 1.08634400 | -0.62720100 | 2.74298100 |
| F | -1.08634400 | -0.62720100 | 2.74298100 |

**$Ag^{I}$_$CH_3$**

| | | | |
|---|---|---|---|
| Br | 0.00000000 | 0.00000000 | -1.81040400 |
| Ag | 0.00000000 | 0.00000000 | 0.76804800 |
| C | 0.00000000 | 0.00000000 | 2.89714200 |
| H | 1.02339300 | 0.00000000 | 3.29434200 |
| H | -0.51169700 | 0.88628400 | 3.29434200 |
| H | -0.51169700 | -0.88628400 | 3.29434200 |

**$Ag^{I}$_Cl**

| | | | |
|---|---|---|---|
| Br | 0.00000000 | 0.00000000 | -2.05590000 |
| Ag | 0.00000000 | 0.00000000 | 0.47489700 |
| Cl | 0.00000000 | 0.00000000 | 2.91978700 |

**$Ag^{I}$_CN**

| | | | |
|---|---|---|---|
| Br | 0.00000000 | 0.00000000 | -1.96105000 |

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| | | | |
|---|---|---|---|
| Ag | 0.00000000 | 0.00000000 | 0.55625900 |
| C | 0.00000000 | 0.00000000 | 2.63844900 |
| N | 0.00000000 | 0.00000000 | 3.80884200 |
| **$Ag^{I}$_F** | | | |
| Br | 0.00000000 | 0.00000000 | -1.75095400 |
| Ag | 0.00000000 | 0.00000000 | 0.76799000 |
| F | 0.00000000 | 0.00000000 | 2.79864900 |
| **$Ag^{I}$_I** | | | |
| Br | 0.00000000 | 0.00000000 | -2.95771400 |
| Ag | 0.00000000 | 0.00000000 | -0.41444300 |
| I | 0.00000000 | 0.00000000 | 2.32073200 |
| **$Ag^{I}$_Ph** | | | |
| Br | -3.03871800 | 0.00043600 | -0.00002200 |
| C | 1.63675700 | -0.00006600 | 0.00001100 |
| C | 2.38895500 | 1.19597000 | 0.00001600 |
| C | 2.38948800 | -1.19576700 | 0.00001600 |
| C | 3.78932100 | 1.20454200 | 0.00002600 |
| H | 1.87458700 | 2.15654300 | 0.00001300 |
| C | 3.78985800 | -1.20371600 | 0.00002600 |
| H | 1.87555000 | -2.15657000 | 0.00001300 |
| C | 4.49865400 | 0.00057200 | 0.00003100 |
| H | 4.32709100 | 2.15151500 | 0.00003000 |
| H | 4.32805100 | -2.15044800 | 0.00003000 |
| H | 5.58658000 | 0.00081400 | 0.00003900 |
| Ag | -0.48074300 | -0.00056000 | -0.00000300 |
| **$Ag^{I}$_vinyl** | | | |
| Br | -0.42158900 | -2.00238200 | 0.00000000 |
| Ag | 0.00000000 | 0.52636300 | 0.00000000 |
| C | 0.34141800 | 2.59992000 | 0.00000000 |
| H | -0.53093700 | 3.26559500 | 0.00000000 |
| C | 1.52437600 | 3.23907600 | 0.00000000 |
| H | 2.48063400 | 2.71313100 | 0.00000000 |
| H | 1.61117000 | 4.33158100 | 0.00000000 |
| **$Au^{III}$_Bn_Br** | | | |
| C | 2.05401000 | -0.10524800 | 0.59839300 |
| C | 4.25238600 | -0.04173300 | 1.09011200 |
| C | 3.60854600 | -0.57558000 | 2.16078500 |
| H | 5.29809400 | 0.16006500 | 0.91935300 |
| H | 3.98105000 | -0.92438900 | 3.11105800 |
| N | 3.27944900 | 0.24370000 | 0.14359300 |
| N | 2.26040300 | -0.60709500 | 1.83809100 |
| C | 3.55201500 | 0.79641900 | -1.18345100 |
| H | 4.49226000 | 1.34882200 | -1.14849800 |
| H | 3.62913800 | -0.00610300 | -1.92205100 |
| H | 2.74436600 | 1.47556300 | -1.45835600 |
| C | 1.20082900 | -1.10496200 | 2.71669700 |
| H | 0.64043700 | -1.88910400 | 2.20372100 |
| H | 1.65818700 | -1.51294300 | 3.61862400 |

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| | | | |
|---|---|---|---|
| H | 0.52555200 | -0.29054800 | 2.98946200 |
| Br | 0.15244200 | -2.44050300 | -0.86529400 |
| Br | 0.17472500 | 2.58361400 | -0.17299800 |
| Au | 0.16363600 | 0.05788700 | -0.41707500 |
| C | -1.75366800 | 0.19790400 | -1.36760900 |
| H | -1.75609900 | -0.62173900 | -2.08547200 |
| H | -1.73606300 | 1.16347000 | -1.87220800 |
| C | -2.82262400 | 0.08678000 | -0.34479200 |
| C | -3.35966300 | 1.23528500 | 0.27157200 |
| C | -3.34434200 | -1.16979000 | 0.02529800 |
| C | -4.38214700 | 1.13202400 | 1.21313100 |

**$Au^{III}$_Br_Br**

| | | | |
|---|---|---|---|
| C | -1.72132900 | -0.00044900 | 0.00003400 |
| C | -3.84382100 | 0.14213000 | -0.66464800 |
| C | -3.84385800 | -0.14334100 | 0.66450100 |
| H | -4.65603000 | 0.29140000 | -1.35799100 |
| H | -4.65609500 | -0.29256700 | 1.35782100 |
| N | -2.51847400 | 0.22757200 | -1.05999300 |
| N | -2.51853800 | -0.22861200 | 1.05998400 |
| C | -2.05852600 | 0.53074000 | -2.41905700 |
| H | -2.93286100 | 0.68513800 | -3.05055400 |
| H | -1.45055900 | 1.43727900 | -2.40266300 |
| H | -1.47109000 | -0.30478900 | -2.80482900 |
| C | -2.05882300 | -0.53085500 | 2.41931500 |
| H | -1.47310000 | 0.30572600 | 2.80541300 |
| H | -2.93322600 | -0.68691100 | 3.05030000 |
| H | -1.44909600 | -1.43622100 | 2.40335100 |
| Br | 0.19959000 | -2.50716600 | -0.17176000 |
| Au | 0.30573700 | 0.00005000 | 0.00011600 |
| Br | 2.83870700 | 0.00040700 | 0.00016000 |
| Br | 0.19844600 | 2.50718500 | 0.17129100 |

**$Au^{III}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.75982500 | -0.07289400 | 0.00558100 |
| C | 3.90398400 | 0.01221600 | 0.66125100 |
| C | 3.88746600 | -0.36671200 | -0.64391400 |
| H | 4.72368500 | 0.16794000 | 1.34446700 |
| H | 4.69034400 | -0.60366100 | -1.32379700 |
| N | 2.58321400 | 0.18876700 | 1.04262200 |
| N | 2.55676100 | -0.41490800 | -1.02870300 |
| C | 2.14174600 | 0.60609900 | 2.37564400 |
| H | 3.02205900 | 0.76971200 | 2.99715200 |
| H | 1.57016700 | 1.53303400 | 2.29667800 |
| H | 1.52081000 | -0.17319900 | 2.82278300 |
| C | 2.08048000 | -0.77779500 | -2.36558100 |
| H | 1.61475600 | 0.08684700 | -2.84391200 |
| H | 2.93224900 | -1.10733400 | -2.96054200 |
| H | 1.35554200 | -1.58998300 | -2.28443600 |
| Br | -0.13744700 | 2.52831600 | -0.23016000 |

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| | | | |
|---|---|---|---|
| Br | -0.42541000 | -2.47841200 | 0.21021300 |
| Au | -0.33576900 | 0.03140900 | 0.00146800 |
| C | -2.41935500 | 0.07274400 | 0.00594200 |
| F | -2.91172900 | -0.51817000 | 1.12683900 |
| F | -2.98795700 | 1.29784600 | -0.04944900 |
| F | -2.91237600 | -0.62081200 | -1.05485400 |

**$Au^{III}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.47971800 | -0.15502100 | 0.00260800 |
| C | -3.59297300 | -0.62083900 | -0.62440100 |
| C | -3.63966400 | -0.13173400 | 0.64233500 |
| H | -4.37696600 | -0.95707000 | -1.28446600 |
| H | -4.47143600 | 0.03499000 | 1.30840800 |
| N | -2.25744500 | -0.62983900 | -0.99733700 |
| N | -2.33225700 | 0.15059800 | 1.00758100 |
| C | -1.76104100 | -1.05618800 | -2.30648600 |
| H | -2.54571700 | -1.62093700 | -2.81116100 |
| H | -1.49272900 | -0.18657100 | -2.91178800 |
| H | -0.88649300 | -1.69399400 | -2.16993400 |
| C | -1.92579400 | 0.68043900 | 2.30990900 |
| H | -1.25862700 | 1.53131300 | 2.16167600 |
| H | -2.81686600 | 1.00655300 | 2.84734600 |
| H | -1.41463600 | -0.09207600 | 2.88970900 |
| Br | 0.42283600 | 2.55871400 | -0.27411900 |
| Br | 0.97085400 | -2.41077100 | 0.26955100 |
| Au | 0.64975200 | 0.06888400 | -0.00224900 |
| C | 2.74087800 | 0.26114000 | 0.00766700 |
| H | 3.08356100 | -0.02288600 | 1.00586800 |
| H | 3.14118900 | -0.42485700 | -0.74138000 |
| H | 3.00690300 | 1.29357900 | -0.21821800 |

**$Au^{III}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | -1.46788800 | -0.01531100 | 0.00181700 |
| C | -3.58718000 | -0.17895900 | -0.66356800 |
| C | -3.59043100 | 0.09689400 | 0.66746800 |
| H | -4.39724600 | -0.33626400 | -1.35760500 |
| H | -4.40418200 | 0.22879500 | 1.36249000 |
| N | -2.26142400 | -0.24215200 | -1.06119700 |
| N | -2.26647300 | 0.19307600 | 1.06448000 |
| C | -1.80172000 | -0.53614400 | -2.42241700 |
| H | -2.67622400 | -0.63025300 | -3.06546700 |
| H | -1.17058700 | 0.27858500 | -2.78211600 |
| H | -1.23832400 | -1.47140100 | -2.42327300 |
| C | -1.81108300 | 0.50583400 | 2.42346100 |
| H | -1.28361400 | 1.46159800 | 2.41922000 |
| H | -2.68475400 | 0.56930500 | 3.07140100 |
| H | -1.14921800 | -0.28477600 | 2.78109700 |
| Br | 0.40895800 | 2.50888200 | -0.17212700 |
| Br | 0.47183200 | -2.50053500 | 0.16404200 |
| Au | 0.54481100 | 0.00591900 | 0.00215400 |

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| | | | |
|---|---|---|---|
| Cl | 2.96361800 | 0.03143100 | 0.00255900 |

**$Au^{III}$_CN_Br**

| | | | |
|---|---|---|---|
| C | 1.46954800 | -0.00465800 | 0.00018700 |
| C | 3.59960800 | -0.16826800 | -0.66069500 |
| C | 3.60033400 | 0.14963300 | 0.66094800 |
| H | 4.41176800 | -0.33426800 | -1.35030100 |
| H | 4.41322200 | 0.31149400 | 1.35068100 |
| N | 2.27377000 | -0.26097100 | -1.05110400 |
| N | 2.27495700 | 0.24798500 | 1.05149700 |
| C | 1.81567400 | -0.58576800 | -2.40533200 |
| H | 2.68674900 | -0.81947200 | -3.01695300 |
| H | 1.15304700 | -1.45234500 | -2.36700200 |
| H | 1.28648400 | 0.26791300 | -2.83405300 |
| C | 1.81851600 | 0.57678100 | 2.40532200 |
| H | 1.27027400 | -0.26765100 | 2.82830200 |
| H | 2.69195000 | 0.78945300 | 3.02120400 |
| H | 1.17388300 | 1.45695700 | 2.36845800 |
| Br | -0.53837000 | -2.50804300 | 0.18705800 |
| Br | -0.52252600 | 2.51051500 | -0.18738500 |
| Au | -0.57869300 | 0.00158800 | 0.00010100 |
| C | -2.59572200 | 0.00746900 | -0.00006300 |
| N | -3.76115200 | 0.01082000 | -0.00026400 |

**$Au^{III}$_F_Br**

| | | | |
|---|---|---|---|
| C | -0.00397800 | 1.34268400 | -0.00012500 |
| C | -0.15398000 | 3.46695500 | 0.66495400 |
| C | 0.13344300 | 3.46823800 | -0.66352200 |
| H | -0.30582500 | 4.27852700 | 1.35846300 |
| H | 0.28004700 | 4.28121300 | -1.35649400 |
| N | -0.23596900 | 2.14134300 | 1.05917000 |
| N | 0.22348000 | 2.14342900 | -1.05877200 |
| C | -0.53439300 | 1.67976500 | 2.41850900 |
| H | -0.72118100 | 2.55221200 | 3.04402500 |
| H | -1.42150900 | 1.04396600 | 2.39944700 |
| H | 0.31561700 | 1.12004800 | 2.81407000 |
| C | 0.52475400 | 1.68508600 | -2.41850200 |
| H | -0.32221500 | 1.12142000 | -2.81499400 |
| H | 0.70696200 | 2.55936200 | -3.04285000 |
| H | 1.41531200 | 1.05412300 | -2.40004600 |
| Br | -2.49838500 | -0.61641200 | -0.17145800 |
| Br | 2.50188500 | -0.60246000 | 0.17223800 |
| Au | 0.00193500 | -0.65274500 | -0.00041300 |
| F | 0.00775100 | -2.62591900 | -0.00077200 |

**$Au^{III}$_I_Br**

| | | | |
|---|---|---|---|
| C | 1.97750400 | 0.00248900 | -0.00014700 |
| C | 4.10117700 | -0.14067200 | -0.66451400 |
| C | 4.10112400 | 0.14240400 | 0.66506400 |
| H | 4.91346100 | -0.28862500 | -1.35810000 |
| H | 4.91341100 | 0.28952400 | 1.35882100 |

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| | | | |
|---|---|---|---|
| N | 2.77551500 | -0.22394700 | -1.05998800 |
| N | 2.77541900 | 0.22822100 | 1.05994300 |
| C | 2.31614800 | -0.52345600 | -2.41984300 |
| H | 3.19058200 | -0.67302200 | -3.05242000 |
| H | 1.71069700 | -1.43173200 | -2.40697300 |
| H | 1.72637300 | 0.31179100 | -2.80257600 |
| C | 2.31594100 | 0.52484300 | 2.42041200 |
| H | 1.74895700 | -0.32215100 | 2.81188100 |
| H | 3.18969600 | 0.70091400 | 3.04709100 |
| H | 1.68833100 | 1.41781700 | 2.40487300 |
| Br | 0.04417600 | -2.50800800 | 0.16894900 |
| Br | 0.03712500 | 2.50925900 | -0.16996900 |
| Au | -0.06525900 | 0.00054700 | 0.00007500 |
| I | -2.80187700 | -0.00292600 | 0.00041000 |

**$Au^{III}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | 2.07894500 | 0.00001100 | 0.00001100 |
| C | 4.22570600 | -0.26108800 | 0.62724700 |
| C | 4.22572300 | 0.26106700 | -0.62718300 |
| H | 5.03789100 | -0.53038600 | 1.28382200 |
| H | 5.03792700 | 0.53035400 | -1.28374100 |
| N | 2.89754700 | -0.41621800 | 0.99299500 |
| N | 2.89757700 | 0.41622700 | -0.99295800 |
| C | 2.44318300 | -0.93282600 | 2.28500900 |
| H | 3.29673900 | -1.36708000 | 2.80646800 |
| H | 2.02195300 | -0.12495400 | 2.88848700 |
| H | 1.68781800 | -1.70307800 | 2.12112900 |
| C | 2.44326000 | 0.93286100 | -2.28497700 |
| H | 1.68780800 | 1.70303000 | -2.12110600 |
| H | 3.29681100 | 1.36722800 | -2.80635200 |
| H | 2.02214900 | 0.12498300 | -2.88853200 |
| Br | -0.09383900 | 2.49713500 | 0.33053800 |
| Br | -0.09381600 | -2.49713500 | -0.33056800 |
| Au | -0.05118900 | -0.00000100 | -0.00000600 |
| C | -2.10946900 | -0.00000300 | -0.00001000 |
| C | -2.81356800 | 0.17005300 | -1.19558500 |
| C | -2.81353800 | -0.17006300 | 1.19558600 |
| C | -4.21340300 | 0.17006100 | -1.19505300 |
| H | -2.28234000 | 0.30372900 | -2.13461300 |
| C | -4.21337200 | -0.17007200 | 1.19509100 |
| H | -2.28228600 | -0.30374100 | 2.13460000 |
| C | -4.91583200 | -0.00000600 | 0.00002800 |
| H | -4.75085500 | 0.30348400 | -2.13080100 |
| H | -4.75080000 | -0.30350000 | 2.13085200 |
| H | -6.00262100 | -0.00000600 | 0.00004100 |

**$Au^{III}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | -1.58065500 | -0.06827000 | 0.08385100 |
| C | -3.75071500 | -0.34411800 | -0.45136000 |
| C | -3.69857400 | 0.09940900 | 0.83166000 |

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| | | | |
|---|---|---|---|
| H | -4.58864900 | -0.60439000 | -1.07868500 |
| H | -4.48189900 | 0.30539400 | 1.54395600 |
| N | -2.43991100 | -0.44215100 | -0.89180400 |
| N | -2.35635600 | 0.25918700 | 1.14233200 |
| C | -2.03712600 | -0.88405000 | -2.22786600 |
| H | -2.91916400 | -1.24807800 | -2.75540100 |
| H | -1.60087400 | -0.05079800 | -2.78401600 |
| H | -1.30615900 | -1.68994300 | -2.13928200 |
| C | -1.86331500 | 0.77578500 | 2.41860900 |
| H | -1.82300000 | 1.86785000 | 2.39497400 |
| H | -2.53219800 | 0.44958300 | 3.21670000 |
| H | -0.86460900 | 0.38040800 | 2.60300600 |
| Br | 0.46501800 | 2.51788600 | -0.35565200 |
| Br | 0.71721600 | -2.48796000 | 0.15975400 |
| Au | 0.54692400 | 0.01595800 | -0.05843100 |
| C | 2.58767100 | 0.11324200 | -0.21727500 |
| H | 2.94086700 | 0.14165900 | -1.24864700 |
| C | 3.43346200 | 0.15412000 | 0.80819000 |
| H | 4.51020000 | 0.21803900 | 0.64443800 |
| H | 3.10972300 | 0.12627700 | 1.84688800 |

**$TS^{Au}$_Bn_Br**

| | | | |
|---|---|---|---|
| C | 1.40304000 | 1.23272900 | 0.15172300 |
| C | 3.25703600 | 1.70123300 | 1.30584900 |
| C | 3.56814200 | 1.75432100 | -0.01982200 |
| H | 3.87501100 | 1.82861700 | 2.18069000 |
| H | 4.50835300 | 1.93572700 | -0.51640700 |
| N | 1.91037600 | 1.41454200 | 1.40222300 |
| N | 2.40954800 | 1.49988300 | -0.72552000 |
| C | 1.18494900 | 1.19125000 | 2.65128500 |
| H | 1.66814900 | 1.76738100 | 3.44094900 |
| H | 0.15478800 | 1.52852000 | 2.53102700 |
| H | 1.19798500 | 0.12768000 | 2.90349000 |
| C | 2.31784300 | 1.37599500 | -2.17843400 |
| H | 1.34150100 | 1.73479100 | -2.50650000 |
| H | 3.10122900 | 1.98582700 | -2.62917100 |
| H | 2.44388600 | 0.32949200 | -2.46827900 |
| Br | -0.50557300 | 2.03633800 | -0.26179700 |
| Br | 2.24446500 | -2.08501400 | 0.17763100 |
| Au | 0.05156200 | -0.70027500 | -0.23462800 |
| C | -1.79864700 | -1.69676400 | -0.69832400 |
| H | -1.77101200 | -2.67980600 | -0.21999800 |
| H | -1.79232700 | -1.83241900 | -1.78504500 |
| C | -2.96723600 | -0.89135300 | -0.24630200 |
| C | -3.58471900 | -1.12890800 | 0.99953400 |
| C | -3.49701600 | 0.14726000 | -1.04095400 |
| C | -4.67712800 | -0.37464900 | 1.42577200 |
| H | -3.20045900 | -1.92502100 | 1.63476500 |
| C | -4.59472800 | 0.89985200 | -0.61786300 |

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| | | | |
|---|---|---|---|
| H | -3.04592600 | 0.35166400 | -2.00979200 |
| C | -5.19300200 | 0.64629500 | 0.61919800 |
| H | -5.13412700 | -0.58907900 | 2.38922700 |
| H | -4.98488200 | 1.68647700 | -1.25974700 |
| H | -6.04744400 | 1.23097900 | 0.94925900 |

**$TS^{Au}$_Br_Br**

| | | | |
|---|---|---|---|
| C | 1.60503300 | -0.34499500 | 0.00003500 |
| C | 3.43687600 | 0.73501900 | -0.68135100 |
| C | 3.43674400 | 0.73481900 | 0.68210300 |
| H | 4.12205500 | 1.18112200 | -1.38463400 |
| H | 4.12178300 | 1.18071400 | 1.38565700 |
| N | 2.32589300 | 0.03317200 | -1.09684400 |
| N | 2.32567600 | 0.03285500 | 1.09716500 |
| C | 1.92594800 | -0.16728600 | -2.48950500 |
| H | 2.81194500 | -0.07369100 | -3.11719600 |
| H | 1.50488800 | -1.16763100 | -2.60056900 |
| H | 1.18403300 | 0.58195300 | -2.77741900 |
| C | 1.92550000 | -0.16807900 | 2.48969100 |
| H | 1.50375300 | -1.16819600 | 2.60017100 |
| H | 2.81151100 | -0.07544300 | 3.11750500 |
| H | 1.18406600 | 0.58150100 | 2.77796200 |
| Br | 0.88255000 | -2.33940600 | -0.00033300 |
| Br | -0.19711100 | 2.60896500 | -0.00009000 |
| Au | -0.54941900 | 0.05723900 | 0.00005400 |
| Br | -3.03919800 | -0.57702400 | 0.00002700 |

**$TS^{Au}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.62814300 | -0.29879900 | 0.02466300 |
| C | -3.28327200 | 0.92640200 | 0.88891200 |
| C | -3.33814400 | 1.04703100 | -0.47237400 |
| H | -3.87471900 | 1.39613700 | 1.65891800 |
| H | -3.98481500 | 1.64241000 | -1.09753500 |
| N | -2.26032300 | 0.06113900 | 1.18644200 |
| N | -2.35053400 | 0.25392800 | -0.99898500 |
| C | -1.82854900 | -0.29393000 | 2.53877200 |
| H | -2.69179300 | -0.23319100 | 3.20169800 |
| H | -1.44167300 | -1.31347600 | 2.53435300 |
| H | -1.05008100 | 0.39560200 | 2.87457100 |
| C | -2.00537100 | 0.17182500 | -2.41716600 |
| H | -1.64795600 | -0.83388100 | -2.64194300 |
| H | -2.90094300 | 0.38153800 | -3.00207600 |
| H | -1.22629400 | 0.90376100 | -2.64617900 |
| Br | -1.10796500 | -2.29476500 | -0.17247000 |
| Br | 0.21150200 | 2.58224300 | -0.03441900 |
| Au | 0.64636500 | -0.07522100 | 0.00502700 |
| C | 2.70074200 | -0.46525600 | 0.03240700 |
| F | 3.03350100 | -1.79954100 | 0.02965000 |
| F | 3.33957200 | 0.04991600 | 1.13355600 |
| F | 3.37182700 | 0.06214600 | -1.04334500 |

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**$TS^{Au}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.13243900 | 0.63614000 | 0.00384500 |
| C | 1.50743100 | 2.74617600 | -0.63216700 |
| C | 1.52919700 | 2.71244400 | 0.73248000 |
| H | 1.60063500 | 3.57479100 | -1.31638400 |
| H | 1.64584100 | 3.50615100 | 1.45361000 |
| N | 1.30324600 | 1.45934300 | -1.07403800 |
| N | 1.33724700 | 1.40482000 | 1.11588800 |
| C | 1.11126500 | 1.06950600 | -2.46885800 |
| H | 1.63413000 | 1.78510500 | -3.10385700 |
| H | 1.52571900 | 0.07213200 | -2.62242300 |
| H | 0.04391400 | 1.06761700 | -2.70499000 |
| C | 1.20998500 | 0.94402900 | 2.49674100 |
| H | 1.62870500 | -0.05979500 | 2.57935700 |
| H | 1.76499700 | 1.62613900 | 3.14119300 |
| H | 0.15601200 | 0.92983800 | 2.78613400 |
| Br | 2.17639700 | -1.19549000 | -0.05523200 |
| Br | -2.16024800 | 1.40841700 | -0.00565700 |
| Au | -0.65770000 | -0.80869600 | 0.00725000 |
| C | -1.71743600 | -2.64197300 | 0.02784400 |
| H | -2.39948600 | -2.67689300 | 0.88454600 |
| H | -2.30512900 | -2.75050900 | -0.89054700 |
| H | -1.02303100 | -3.48711800 | 0.09946100 |

**$TS^{Au}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | -1.40554800 | 0.15271900 | 0.01146200 |
| C | -2.63069900 | 1.85111500 | 0.78674200 |
| C | -2.62472600 | 1.92874200 | -0.57473900 |
| H | -3.07046100 | 2.50043400 | 1.52703300 |
| H | -3.05816500 | 2.65863500 | -1.23976800 |
| N | -1.91298200 | 0.72996300 | 1.14227000 |
| N | -1.90457800 | 0.85468200 | -1.04967000 |
| C | -1.62983300 | 0.31315900 | 2.51569000 |
| H | -2.42504100 | 0.69047600 | 3.15855400 |
| H | -1.60900400 | -0.77636100 | 2.56251400 |
| H | -0.66622100 | 0.71746800 | 2.83632300 |
| C | -1.59303300 | 0.60547700 | -2.45661900 |
| H | -1.57284400 | -0.47057300 | -2.63450500 |
| H | -2.37259300 | 1.06124000 | -3.06709700 |
| H | -0.62122500 | 1.04129400 | -2.70268700 |
| Br | -1.52392200 | -1.93665900 | -0.10068400 |
| Br | 1.43457300 | 2.16503300 | -0.00816500 |
| Au | 0.74246100 | -0.31158100 | 0.00242200 |
| Cl | 2.69966600 | -1.82356200 | 0.04909300 |

**$TS^{Au}$_CN_Br**

| | | | |
|---|---|---|---|
| C | 1.34100700 | 0.16108400 | 0.00005500 |
| C | 2.51661100 | 1.93317100 | -0.68316300 |
| C | 2.51667400 | 1.93273600 | 0.68431600 |
| H | 2.93007100 | 2.64073100 | -1.38427700 |

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| | | | |
|---|---|---|---|
| H | 2.93020700 | 2.63983800 | 1.38585300 |
| N | 1.83235900 | 0.81822900 | -1.09811900 |
| N | 1.83244600 | 0.81753000 | 1.09861100 |
| C | 1.53637500 | 0.48445500 | -2.49076700 |
| H | 2.31369500 | 0.91725500 | -3.12057800 |
| H | 1.53374400 | -0.60012300 | -2.60696100 |
| H | 0.56014600 | 0.89104200 | -2.76729800 |
| C | 1.53681600 | 0.48276900 | 2.49109900 |
| H | 1.53347900 | -0.60190200 | 2.60635500 |
| H | 2.31471500 | 0.91447200 | 3.12094800 |
| H | 0.56098600 | 0.88978200 | 2.76841300 |
| Br | 1.57940100 | -1.91847200 | -0.00063000 |
| Br | -1.39689200 | 2.16829300 | -0.00008700 |
| C | -2.51152000 | -1.54597900 | 0.00018900 |
| N | -3.48740700 | -2.18825400 | 0.00023300 |
| Au | -0.80914500 | -0.42097200 | 0.00009100 |

**$TS^{Au}$_F_Br**

| | | | |
|---|---|---|---|
| C | -0.98471600 | 0.76598500 | 0.00027700 |
| C | -0.86399800 | 2.89188200 | 0.68662400 |
| C | -0.86170100 | 2.89446100 | -0.67751300 |
| H | -0.77299300 | 3.70365500 | 1.39089300 |
| H | -0.76809500 | 3.70884300 | -1.37841600 |
| N | -0.99191300 | 1.58546200 | 1.10017200 |
| N | -0.98831500 | 1.58964100 | -1.09647000 |
| C | -0.94259300 | 1.13692100 | 2.48991300 |
| H | -1.37528200 | 1.91426100 | 3.12038200 |
| H | -1.52447600 | 0.22003700 | 2.58970400 |
| H | 0.09438500 | 0.95069900 | 2.78222200 |
| C | -0.93286400 | 1.14643600 | -2.48764100 |
| H | -1.51360400 | 0.22950100 | -2.59348100 |
| H | -1.36344000 | 1.92589900 | -3.11695600 |
| H | 0.10552500 | 0.96220500 | -2.77619600 |
| Br | -2.39021800 | -0.75802300 | -0.00454400 |
| Br | 2.42031300 | 0.86651900 | -0.00045400 |
| Au | 0.50101100 | -0.84652800 | 0.00049300 |
| F | 0.87351000 | -2.86406500 | 0.00244200 |

**$TS^{Au}$_I_Br**

| | | | |
|---|---|---|---|
| C | -1.83315900 | -0.44104000 | 0.00004600 |
| C | -3.77555100 | 0.42170500 | 0.68211900 |
| C | -3.77580300 | 0.42199600 | -0.68095200 |
| H | -4.50649400 | 0.78472200 | 1.38706800 |
| H | -4.50698600 | 0.78533600 | -1.38548600 |
| N | -2.58746000 | -0.14334700 | 1.09627700 |
| N | -2.58788800 | -0.14293200 | -1.09578300 |
| C | -2.16571600 | -0.29702900 | 2.48845600 |
| H | -3.05424200 | -0.28023200 | 3.11912800 |
| H | -1.65407400 | -1.25378300 | 2.60415600 |
| H | -1.49541400 | 0.51983300 | 2.76797100 |

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| | | | |
|---|---|---|---|
| C | -2.16648100 | -0.29557400 | -2.48817900 |
| H | -1.65430600 | -1.25195500 | -2.60458600 |
| H | -3.05521200 | -0.27895500 | -3.11857400 |
| H | -1.49675900 | 0.52185500 | -2.76742000 |
| Br | -0.90825200 | -2.37620200 | -0.00036900 |
| Br | -0.29082900 | 2.63692300 | 0.00010800 |
| Au | 0.28690800 | 0.13007000 | -0.00014300 |
| I | 3.00477900 | -0.29818900 | 0.00010800 |

**$TS^{Au}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | 1.79306200 | -0.54977500 | 0.10126100 |
| C | 3.82289300 | 0.29762200 | -0.29977300 |
| C | 3.67269100 | 0.20188500 | 1.05418300 |
| H | 4.63340600 | 0.69581100 | -0.88966500 |
| H | 4.33013500 | 0.49626900 | 1.85704000 |
| N | 2.68173600 | -0.20494900 | -0.87897000 |
| N | 2.43752900 | -0.35556500 | 1.29320400 |
| C | 2.38441200 | -0.18746600 | -2.30884200 |
| H | 3.32530100 | -0.20609300 | -2.85944300 |
| H | 1.79416400 | -1.06921000 | -2.56255300 |
| H | 1.82291900 | 0.71888800 | -2.55121800 |
| C | 1.86493100 | -0.59004500 | 2.61816800 |
| H | 1.22124100 | -1.46936500 | 2.57650400 |
| H | 2.68012500 | -0.76699900 | 3.32035700 |
| H | 1.28221200 | 0.27838400 | 2.93551300 |
| Br | 0.86729900 | -2.44196400 | -0.13570200 |
| Br | 0.64238700 | 2.60411100 | -0.21911300 |
| Au | -0.37524400 | 0.14975800 | -0.02152500 |
| C | -2.44924000 | -0.02104000 | 0.01770900 |
| C | -3.15743700 | -0.62837000 | -1.03988200 |
| C | -3.20992400 | 0.43416100 | 1.11428200 |
| C | -4.54776700 | -0.77825200 | -1.00507200 |
| H | -2.61893800 | -0.99522300 | -1.91162100 |
| C | -4.60000000 | 0.28619800 | 1.15818400 |
| H | -2.71326700 | 0.91798000 | 1.95303500 |
| C | -5.27557700 | -0.32204000 | 0.09684700 |
| H | -5.06256900 | -1.25174900 | -1.83854500 |
| H | -5.15622500 | 0.64830900 | 2.02036900 |
| H | -6.35637100 | -0.43672400 | 0.12717500 |

**$TS^{Au}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | -1.38824900 | 0.09533400 | 0.11355100 |
| C | -2.60946700 | 1.58603800 | 1.24998200 |
| C | -2.71667400 | 1.88294000 | -0.07903900 |
| H | -3.01168700 | 2.08615600 | 2.11680000 |
| H | -3.22481400 | 2.69273500 | -0.57864300 |
| N | -1.82335900 | 0.46248000 | 1.35875100 |
| N | -1.99991100 | 0.93784200 | -0.77319200 |
| C | -1.41733300 | -0.15849100 | 2.61909400 |
| H | -2.20299500 | 0.01004500 | 3.35633700 |

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| | | | |
|---|---|---|---|
| H | -1.28715300 | -1.22973300 | 2.46213700 |
| H | -0.47844600 | 0.27922700 | 2.96704700 |
| C | -1.75916400 | 0.95211600 | -2.21362100 |
| H | -1.72651900 | -0.07441500 | -2.58184400 |
| H | -2.57637500 | 1.48868000 | -2.69597000 |
| H | -0.80743600 | 1.45158700 | -2.41481700 |
| Br | -1.54002200 | -1.96975600 | -0.33278000 |
| Br | 1.19684000 | 2.27138400 | -0.10327400 |
| Au | 0.83550700 | -0.37773200 | -0.08124800 |
| C | 2.55465400 | -1.52985000 | -0.14275300 |
| H | 2.63904000 | -2.25638400 | -0.95660300 |
| C | 3.57141900 | -1.49532000 | 0.73352900 |
| H | 3.59832500 | -0.80537000 | 1.57659600 |
| H | 4.43612000 | -2.15751500 | 0.64604300 |

**$Au^{I}$_Bn**

| | | | |
|---|---|---|---|
| Au | -0.66340200 | -0.41241800 | -0.00020600 |
| C | 1.15263500 | -1.43363000 | -0.00066400 |
| H | 1.16295900 | -2.08011400 | -0.88635600 |
| H | 1.16293000 | -2.08080500 | 0.88453300 |
| C | 2.34238500 | -0.52007300 | -0.00026800 |
| C | 2.92584800 | -0.07750800 | 1.20220400 |
| C | 2.92530900 | -0.07571600 | -1.20233500 |
| C | 4.03193700 | 0.77363900 | 1.20509600 |
| H | 2.49898900 | -0.40732500 | 2.14761400 |
| C | 4.03141700 | 0.77542700 | -1.20445600 |
| H | 2.49801900 | -0.40410500 | -2.14804700 |
| C | 4.59308200 | 1.20881000 | 0.00051400 |
| H | 4.45911800 | 1.09624200 | 2.15203100 |
| H | 4.45813200 | 1.09946300 | -2.15111000 |
| H | 5.45470800 | 1.87126800 | 0.00082800 |
| Br | -2.89433700 | 0.84516300 | 0.00046500 |

**$Au^{I}$_Br**

| | | | |
|---|---|---|---|
| Au | 0.00000000 | 0.00000000 | 0.00000000 |
| Br | 0.00000000 | 0.00000000 | 2.46901500 |
| Br | 0.00000000 | 0.00000000 | -2.46901500 |

**$Au^{I}$_$CF_3$**

| | | | |
|---|---|---|---|
| Au | 0.04189300 | -0.00003400 | 0.00006700 |
| Br | -2.47531600 | -0.00000100 | -0.00003000 |
| C | 2.06568000 | -0.00051100 | 0.00020800 |
| F | 2.62657900 | 1.25491200 | -0.05530300 |
| F | 2.62783800 | -0.57938600 | 1.11329900 |
| F | 2.62696200 | -0.67488000 | -1.05860400 |

**$Au^{I}$_$CH_3$**

| | | | |
|---|---|---|---|
| Au | 0.57024700 | -0.00002300 | -0.00017900 |
| C | 2.63050800 | 0.00015900 | 0.00074000 |
| H | 3.02022400 | 0.97981800 | -0.30305900 |
| H | 3.01888800 | -0.22643100 | 1.00159200 |
| H | 3.01999100 | -0.75342000 | -0.69514100 |

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| | | | |
|---|---|---|---|
| Br | -1.99690400 | 0.00002600 | 0.00018100 |
| **$Au^{I}$_Cl** | | | |
| Au | 0.00000000 | 0.00000000 | 0.34686700 |
| Br | 0.00000000 | 0.00000000 | -2.10799500 |
| Cl | 0.00000000 | 0.00000000 | 2.72807700 |
| **$Au^{I}$_CN** | | | |
| Au | 0.00000000 | 0.00000000 | 0.41793300 |
| Br | 0.00000000 | 0.00000000 | -2.06460200 |
| C | 0.00000000 | 0.00000000 | 2.38899100 |
| N | 0.00000000 | 0.00000000 | 3.55862800 |
| **$Au^{I}$_F** | | | |
| Au | 0.00000000 | 0.00000000 | 0.54777700 |
| Br | 0.00000000 | 0.00000000 | -1.89081600 |
| F | 0.00000000 | 0.00000000 | 2.54490700 |
| **$Au^{I}$_I** | | | |
| Au | 0.57250100 | 0.00000000 | -0.00002100 |
| Br | -1.90749900 | 0.00005022 | -0.00004599 |
| I | 3.24250100 | -0.00000405 | 0.00002932 |
| **$Au^{I}$_Ph** | | | |
| Br | 2.90713400 | 0.00004100 | -0.00003000 |
| C | -1.67160000 | -0.00001800 | 0.00002600 |
| C | -2.41257100 | -1.20078700 | 0.00002900 |
| C | -2.41250300 | 1.20079600 | 0.00002900 |
| C | -3.81160600 | -1.20459300 | 0.00003000 |
| H | -1.89101700 | -2.15538800 | 0.00002500 |
| C | -3.81153800 | 1.20468300 | 0.00003000 |
| H | -1.89089500 | 2.15536700 | 0.00002500 |
| C | -4.51929800 | 0.00006500 | 0.00003000 |
| H | -4.34909800 | -2.15088500 | 0.00002900 |
| H | -4.34897500 | 2.15100700 | 0.00003000 |
| H | -5.60678400 | 0.00009700 | 0.00003000 |
| Au | 0.35660500 | -0.00003200 | -0.00000200 |
| **$Au^{I}$_vinyl** | | | |
| Au | -0.39143900 | -0.10024100 | -0.00012700 |
| C | -2.39652100 | -0.29646100 | 0.00025400 |
| H | -2.78884200 | -1.31833700 | 0.00135700 |
| C | -3.30956200 | 0.68862400 | 0.00016300 |
| H | -4.38208000 | 0.47903400 | 0.00134000 |
| H | -3.04082600 | 1.74415500 | -0.00044300 |
| Br | 2.15348300 | 0.13317700 | 0.00015000 |
| **prod_Br** | | | |
| C | -2.30445400 | -0.68082700 | -0.00038500 |
| C | -0.20451800 | 0.00000000 | -0.00010600 |
| C | -2.30445400 | 0.68083100 | -0.00048600 |
| N | -0.98436000 | 1.09421400 | -0.00014100 |
| N | -0.98435900 | -1.09421200 | -0.00013500 |
| Br | 1.64424300 | -0.00000100 | 0.00022000 |
| H | -3.11699800 | -1.38923500 | -0.00057000 |

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| | | | |
|---|---|---|---|
| H | -3.11699700 | 1.38924100 | -0.00062700 |
| C | -0.51596600 | -2.48492800 | 0.00009300 |
| H | 0.08060600 | -2.67289700 | -0.89426800 |
| H | 0.08014000 | -2.67277700 | 0.89479100 |
| H | -1.39145000 | -3.13224800 | -0.00009100 |
| C | -0.51595900 | 2.48492700 | 0.00002200 |
| H | 0.08025300 | 2.67278600 | 0.89464800 |
| H | 0.08050900 | 2.67288000 | -0.89441200 |
| H | -1.39143900 | 3.13225300 | -0.00006900 |

**$Cu^{III}$_Br_Cl**

| | | | |
|---|---|---|---|
| C | -1.48618000 | -0.20093800 | 0.00092300 |
| C | -3.60180300 | -0.19941700 | 0.68302900 |
| C | -3.60341700 | -0.20157500 | -0.67615500 |
| H | -4.41088100 | -0.20421500 | 1.39591700 |
| H | -4.41416900 | -0.20889900 | -1.38711100 |
| N | -2.27308800 | -0.19680400 | 1.08754500 |
| N | -2.27566900 | -0.20009500 | -1.08382800 |
| C | -1.79700100 | -0.18914700 | 2.47254400 |
| H | -2.66236000 | -0.19711400 | 3.13433100 |
| H | -1.18823900 | -1.07713400 | 2.65567800 |
| H | -1.20734300 | 0.71280500 | 2.65071800 |
| C | -1.80271400 | -0.19968800 | -2.46991600 |
| H | -2.66958500 | -0.19416700 | -3.12975100 |
| H | -1.20010700 | 0.69342300 | -2.64915100 |
| H | -1.20758800 | -1.09659400 | -2.65458500 |
| Cu | 0.45930200 | -0.28241400 | -0.00084200 |
| Br | 0.25646300 | 2.07104200 | -0.00383100 |
| Br | 2.82937700 | -0.31758700 | 0.00177200 |
| Cl | 0.18965100 | -2.52271400 | -0.00047800 |

**$Cu^{III}$_Br_F**

| | | | |
|---|---|---|---|
| C | -1.51310800 | -0.22556700 | 0.10160600 |
| C | -3.64279000 | 0.11781800 | 0.64271100 |
| C | -3.61570900 | -0.72245900 | -0.42521000 |
| H | -4.46694500 | 0.52555800 | 1.20616100 |
| H | -4.41211400 | -1.18923600 | -0.98285300 |
| N | -2.32343400 | 0.41942200 | 0.95583900 |
| N | -2.28111900 | -0.92914200 | -0.74451500 |
| C | -1.89699600 | 1.25338700 | 2.08211400 |
| H | -2.64939500 | 2.02433000 | 2.25116400 |
| H | -1.78597700 | 0.64094300 | 2.98015300 |
| H | -0.94691700 | 1.72438000 | 1.83044100 |
| C | -1.77430700 | -1.80704800 | -1.80409100 |
| H | -2.59720900 | -2.42275500 | -2.16613900 |
| H | -1.37242500 | -1.21032000 | -2.62621600 |
| H | -0.99635700 | -2.44019500 | -1.37614600 |
| Cu | 0.41825300 | -0.36842500 | 0.15776100 |
| Br | 0.43794600 | 1.78663800 | -0.76629300 |
| Br | 2.78729700 | -0.55303500 | 0.27049600 |

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| | | | |
|---|---|---|---|
| F | 0.12264700 | -2.03035600 | 0.73324900 |

**$Cu^{III}$_Br_I**

| | | | |
|---|---|---|---|
| C | 1.52912200 | 0.00962700 | 0.00406400 |
| C | 3.64617200 | -0.18330500 | -0.66457500 |
| C | 3.63967000 | -0.17982500 | 0.69419100 |
| H | 4.45646800 | -0.25785500 | -1.37217300 |
| H | 4.44328100 | -0.25082000 | 1.40975800 |
| N | 2.32590100 | -0.06578900 | -1.07666100 |
| N | 2.31544700 | -0.05998700 | 1.09294000 |
| C | 1.87091600 | -0.00260800 | -2.46641000 |
| H | 2.73458400 | -0.13062300 | -3.11822500 |
| H | 1.15095800 | -0.80240300 | -2.65428800 |
| H | 1.40857200 | 0.96877100 | -2.65650200 |
| C | 1.84581900 | 0.00467500 | 2.47787500 |
| H | 2.70625200 | -0.09576400 | 3.13883700 |
| H | 1.35801100 | 0.96623700 | 2.65421900 |
| H | 1.14406700 | -0.81098500 | 2.66674600 |
| Cu | -0.39903200 | 0.32241900 | -0.00363100 |
| Br | 0.17977400 | 2.64943200 | -0.00967800 |
| Br | -2.74189300 | 0.62248600 | 0.00708800 |
| I | -0.48746600 | -2.27292100 | -0.00485400 |

**$TS^{Cu}$_Br_Cl**

| | | | |
|---|---|---|---|
| C | 1.43641100 | -0.47570700 | 0.00021400 |
| C | 3.48725900 | 0.03299100 | -0.68078500 |
| C | 3.48708300 | 0.03317600 | 0.68160200 |
| H | 4.26710900 | 0.26420900 | -1.38878000 |
| H | 4.26675100 | 0.26458100 | 1.38973500 |
| N | 2.21243700 | -0.31355000 | -1.09269200 |
| N | 2.21215400 | -0.31324800 | 1.09327600 |
| C | 1.74671500 | -0.38156800 | -2.47822600 |
| H | 2.61725100 | -0.37659200 | -3.13323800 |
| H | 1.18368100 | -1.30472000 | -2.62655700 |
| H | 1.11424900 | 0.48306100 | -2.69539900 |
| C | 1.74609000 | -0.38094400 | 2.47871100 |
| H | 2.61645600 | -0.37544900 | 3.13394500 |
| H | 1.11329700 | 0.48356300 | 2.69541700 |
| H | 1.18331000 | -1.30422300 | 2.62722200 |
| Cu | -0.54351900 | -0.17894300 | -0.00009200 |
| Cl | 0.31406900 | -2.35277700 | 0.00029300 |
| Br | -0.25353000 | 2.17503300 | -0.00025400 |
| Br | -2.89883300 | -0.50440400 | -0.00025500 |

**$TS^{Cu}$_Br_F**

| | | | |
|---|---|---|---|
| C | 1.45598800 | -0.42636900 | 0.05209400 |
| C | 3.55379400 | -0.40923800 | -0.65720000 |
| C | 3.56117100 | -0.14209900 | 0.67659000 |
| H | 4.35461800 | -0.44465100 | -1.37858700 |
| H | 4.36898700 | 0.10141700 | 1.34803700 |
| N | 2.23007700 | -0.61219600 | -1.02939100 |

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| | | | |
|---|---|---|---|
| N | 2.24156400 | -0.18086300 | 1.11267100 |
| C | 1.74155700 | -0.96663000 | -2.36295000 |
| H | 2.59859600 | -1.21621000 | -2.98722400 |
| H | 1.08361000 | -1.83347200 | -2.27891300 |
| H | 1.19989000 | -0.12435600 | -2.80004200 |
| C | 1.76785800 | 0.02785800 | 2.48162200 |
| H | 2.63144300 | 0.21229200 | 3.11948600 |
| H | 1.09850500 | 0.89102200 | 2.50891000 |
| H | 1.24103700 | -0.86587500 | 2.82297000 |
| Cu | -0.48102900 | -0.25715700 | 0.03722900 |
| F | 0.38521400 | -1.93885800 | 0.32179000 |
| Br | -0.39352300 | 2.06267900 | -0.26382700 |
| Br | -2.80297700 | -0.77018200 | 0.09084700 |

**$TS^{Cu}$_Br_I**

| | | | |
|---|---|---|---|
| C | -1.39650100 | 0.14408500 | 0.00000300 |
| C | -3.29114000 | 1.10071900 | 0.68138300 |
| C | -3.29112600 | 1.10079200 | -0.68131400 |
| H | -4.00667000 | 1.49001500 | 1.38811600 |
| H | -4.00663900 | 1.49016700 | -1.38802000 |
| N | -2.12557500 | 0.48559400 | 1.09140600 |
| N | -2.12555500 | 0.48570700 | -1.09137800 |
| C | -1.69293300 | 0.34593500 | 2.48255600 |
| H | -2.54928900 | 0.53633200 | 3.12858000 |
| H | -1.32872500 | -0.66895300 | 2.65233700 |
| H | -0.90082100 | 1.06870100 | 2.69417800 |
| C | -1.69285300 | 0.34625700 | -2.48252900 |
| H | -2.54925500 | 0.53642200 | -3.12856000 |
| H | -0.90095100 | 1.06927100 | -2.69409200 |
| H | -1.32833100 | -0.66851000 | -2.65235000 |
| Cu | 0.63449600 | 0.21201500 | 0.00001800 |
| I | -0.51341300 | -2.16897600 | -0.00010300 |
| Br | 0.60568300 | 2.61807200 | 0.00007800 |
| Br | 2.94650000 | -0.36298600 | 0.00003400 |

**prod_Cl**

| | | | |
|---|---|---|---|
| C | 0.68037000 | -1.83761400 | -0.00032200 |
| C | 0.00000000 | 0.25927200 | -0.00000100 |
| C | -0.68036800 | -1.83761500 | -0.00042100 |
| N | -1.09472900 | -0.51726200 | -0.00008700 |
| N | 1.09472900 | -0.51726000 | -0.00007700 |
| Cl | -0.00000100 | 1.95388200 | 0.00030900 |
| H | 1.38911600 | -2.64991500 | -0.00045900 |
| H | -1.38911300 | -2.64991600 | -0.00059800 |
| C | 2.48549600 | -0.04516700 | 0.00009900 |
| H | 2.67132700 | 0.55118000 | -0.89460700 |
| H | 2.67127200 | 0.55069800 | 0.89513900 |
| H | 3.13302200 | -0.92025300 | -0.00011600 |
| C | -2.48549500 | -0.04517000 | 0.00003700 |
| H | -2.67128200 | 0.55079200 | 0.89501000 |

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| | | | |
|---|---|---|---|
| H | -2.67131800 | 0.55108100 | -0.89473500 |
| H | -3.13302100 | -0.92025600 | -0.00009100 |

**prod_F**

| | | | |
|---|---|---|---|
| C | -0.67889500 | 1.53007200 | -0.00237900 |
| C | 0.00000500 | -0.55147600 | -0.00028300 |
| C | 0.67889700 | 1.53008600 | 0.00206900 |
| N | 1.09759700 | 0.20184500 | 0.00416200 |
| N | -1.09759700 | 0.20183500 | -0.00479900 |
| F | 0.00000600 | -1.85494800 | -0.00046100 |
| H | -1.38846300 | 2.34166300 | -0.00360300 |
| H | 1.38845700 | 2.34169000 | 0.00310300 |
| C | -2.48308700 | -0.28579400 | 0.00284300 |
| H | -3.01769400 | 0.15646400 | -0.83837000 |
| H | -2.47214500 | -1.37011300 | -0.09745400 |
| H | -2.95779800 | -0.00487600 | 0.94411900 |
| C | 2.48308200 | -0.28577700 | -0.00151900 |
| H | 2.47144300 | -1.37126500 | 0.08507600 |
| H | 2.96285400 | 0.00665700 | -0.93665900 |
| H | 3.01327300 | 0.14588200 | 0.84800800 |

**prod_I**

| | | | |
|---|---|---|---|
| C | 2.69347600 | -0.68078800 | -0.00005400 |
| C | 0.58490900 | 0.00000000 | -0.00009900 |
| C | 2.69347600 | 0.68078800 | -0.00018000 |
| N | 1.37493300 | 1.09206300 | 0.00002200 |
| N | 1.37493400 | -1.09206300 | 0.00002100 |
| I | -1.47398700 | 0.00000000 | -0.00002300 |
| H | 3.50677800 | -1.38857200 | -0.00002100 |
| H | 3.50677700 | 1.38857200 | -0.00025500 |
| C | 0.92403200 | -2.48904700 | 0.00014900 |
| H | 0.33083300 | -2.68558100 | 0.89496000 |
| H | 0.33094100 | -2.68576000 | -0.89469300 |
| H | 1.80779500 | -3.12528000 | 0.00027000 |
| C | 0.92403100 | 2.48904700 | 0.00018500 |
| H | 0.33077900 | 2.68571600 | -0.89455900 |
| H | 0.33099300 | 2.68562500 | 0.89509400 |
| H | 1.80779400 | 3.12528000 | 0.00011100 |

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**Cartesian coordinates for all the structures involved in NHC-Br reductive elimination from trans-(NHC)Cu(Br)$_2$X complexes in acetonitrile where X = Bn, Br, $CF_3$, $CH_3$, Cl, I, CN, F, Ph, and vinyl**

**$Cu^{III}$_Bn_Br**

| | | | |
|---|---|---|---|
| Cu | -0.12497400 | -0.49455700 | 0.07159900 |
| C | 1.52999500 | -1.77632200 | 0.36353100 |
| H | 1.39428200 | -2.13742500 | 1.37529400 |
| Br | -0.72838900 | -0.84178900 | 2.46943000 |
| Br | -0.67504700 | -1.79340000 | -1.98335800 |
| C | 2.36394600 | -0.63094300 | 0.14470800 |
| C | 2.77011200 | 0.19174800 | 1.23544000 |
| C | 2.83750000 | -0.31608600 | -1.16243500 |
| C | 3.65228800 | 1.24203300 | 1.03091400 |
| H | 2.38593900 | -0.02669900 | 2.22669700 |
| C | 3.71935900 | 0.73720600 | -1.35351900 |
| H | 2.50915100 | -0.92409000 | -1.99948400 |
| C | 4.13093600 | 1.51335500 | -0.25933200 |
| H | 3.97202000 | 1.85391800 | 1.86827700 |
| H | 4.09141900 | 0.96087700 | -2.34820500 |
| H | 4.82126600 | 2.33712200 | -0.41434000 |
| C | -1.23972700 | 1.17726600 | -0.26426000 |
| C | -3.06048500 | 2.50926700 | -0.45757900 |
| C | -1.96414100 | 3.29976700 | -0.58816200 |
| H | -4.11261900 | 2.74483300 | -0.49581000 |
| H | -1.86966900 | 4.36043000 | -0.76094300 |
| N | -0.86181800 | 2.46569100 | -0.47079500 |
| N | -2.59758000 | 1.21722900 | -0.26413300 |
| C | 0.51757300 | 2.93972900 | -0.52089600 |
| H | 1.17189400 | 2.10073000 | -0.75301000 |
| H | 0.61338000 | 3.69478000 | -1.30417100 |
| H | 0.80922800 | 3.37539200 | 0.43901200 |
| C | -3.46248900 | 0.05573200 | -0.05606700 |
| H | -4.48313000 | 0.32544800 | -0.33132900 |
| H | -3.11749800 | -0.76581000 | -0.68610500 |
| H | -3.43052600 | -0.25162000 | 0.99191200 |
| H | 1.43593500 | -2.51108400 | -0.42622400 |

**$Cu^{III}$_Br_Br**

| | | | |
|---|---|---|---|
| C | -1.50059900 | 0.00003300 | -0.00002900 |
| C | -3.61767100 | -0.00005600 | 0.67947600 |
| C | -3.61768900 | 0.00000300 | -0.67948200 |
| H | -4.42742400 | -0.00011600 | 1.39157500 |
| H | -4.42746000 | 0.00004800 | -1.39156000 |
| N | -2.28948000 | -0.00004600 | 1.08575900 |
| N | -2.28950900 | 0.00012600 | -1.08579700 |

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| | | | |
|---|---|---|---|
| C | -1.81720100 | -0.00016000 | 2.47167100 |
| H | -2.68437400 | 0.00015000 | 3.13097800 |
| H | -1.21877800 | -0.89551000 | 2.65376900 |
| H | -1.21820500 | 0.89481600 | 2.65371000 |
| C | -1.81726400 | 0.00023200 | -2.47172100 |
| H | -2.68445200 | 0.00039700 | -3.13100200 |
| H | -1.21846600 | 0.89535200 | -2.65370900 |
| H | -1.21865300 | -0.89497300 | -2.65390200 |
| Cu | 0.44734000 | -0.00000300 | -0.00005200 |
| Br | 0.19483500 | -2.36260100 | -0.00012000 |
| Br | 0.19488800 | 2.36260400 | 0.00003100 |
| Br | 2.82171800 | -0.00003000 | 0.00015900 |

**$Cu^{III}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.57017900 | -0.02354900 | 0.00211200 |
| C | -3.70464300 | -0.23239100 | -0.65825200 |
| C | -3.71100400 | 0.04482100 | 0.67146800 |
| H | -4.51270300 | -0.39910200 | -1.35293300 |
| H | -4.52530500 | 0.15824300 | 1.36962300 |
| N | -2.37369000 | -0.27397500 | -1.05184800 |
| N | -2.38404300 | 0.17448300 | 1.05931000 |
| C | -1.90891600 | -0.50779300 | -2.41917100 |
| H | -2.69360200 | -1.02350800 | -2.97358400 |
| H | -1.67813300 | 0.44103700 | -2.91045600 |
| H | -1.01764500 | -1.13696600 | -2.39009900 |
| C | -1.93131500 | 0.43673500 | 2.42550100 |
| H | -1.07099700 | 1.10733200 | 2.39383700 |
| H | -2.73970900 | 0.91720300 | 2.97752400 |
| H | -1.65551300 | -0.49779500 | 2.92104900 |
| Cu | 0.42207100 | 0.03496400 | -0.00108100 |
| Br | 0.27938400 | 2.38629700 | -0.17237200 |
| Br | 0.41994300 | -2.33929200 | 0.15857600 |
| C | 2.42370900 | 0.04044900 | 0.00496600 |
| F | 2.86359600 | -0.68796900 | -1.04729600 |
| F | 3.04827400 | 1.22902400 | -0.06700900 |
| F | 2.85427400 | -0.54980500 | 1.14400300 |

**$Cu^{III}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | -1.21819300 | -0.01565800 | 0.00041600 |
| C | -3.36539200 | -0.27276300 | -0.64552100 |
| C | -3.37502700 | 0.16070300 | 0.64145600 |
| H | -4.17235800 | -0.50846800 | -1.32152100 |
| H | -4.19185500 | 0.36557900 | 1.31566600 |
| N | -2.03243400 | -0.37872600 | -1.01829300 |
| N | -2.04779500 | 0.31710600 | 1.01702400 |
| C | -1.57391900 | -0.77073900 | -2.34966700 |
| H | -2.30031600 | -1.45645200 | -2.78908200 |
| H | -1.46839600 | 0.10687300 | -2.99360800 |
| H | -0.61325000 | -1.27900300 | -2.25734800 |
| C | -1.60708300 | 0.72545200 | 2.34942500 |

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| | | | |
|---|---|---|---|
| H | -2.35335700 | 1.39351000 | 2.78287500 |
| H | -1.48169500 | -0.14698400 | 2.99684800 |
| H | -0.65964900 | 1.25829900 | 2.26004300 |
| Cu | 0.81203100 | 0.01953100 | 0.00310400 |
| Br | 0.86150000 | 2.38442400 | -0.25397500 |
| Br | 0.93152200 | -2.35157000 | 0.25021400 |
| C | 2.83454800 | 0.00901700 | 0.00839200 |
| H | 3.17130800 | 1.03580600 | -0.08089200 |
| H | 3.07893400 | -0.45665200 | 0.96123700 |
| H | 3.07795800 | -0.61355000 | -0.85071300 |

**$Cu^{III}$_Cl_Br**

| | | | |
|---|---|---|---|
| C | 1.17540700 | -0.00163000 | -0.00000900 |
| C | 3.28967200 | -0.00345800 | 0.67959100 |
| C | 3.28975300 | -0.00322900 | -0.67935300 |
| H | 4.09920300 | -0.00441200 | 1.39188300 |
| H | 4.09936100 | -0.00394800 | -1.39155600 |
| N | 1.96169300 | -0.00244900 | 1.08680900 |
| N | 1.96181900 | -0.00220800 | -1.08672300 |
| C | 1.49022500 | -0.00145700 | 2.47329700 |
| H | 2.35827700 | -0.00631200 | 3.13130100 |
| H | 0.89621900 | 0.89659100 | 2.65636500 |
| H | 0.88779800 | -0.89421200 | 2.65460900 |
| C | 1.49048000 | -0.00083500 | -2.47325800 |
| H | 2.35858900 | -0.00578900 | -3.13118600 |
| H | 0.88784200 | -0.89340300 | -2.65479000 |
| H | 0.89671100 | 0.89739600 | -2.65619800 |
| Cu | -0.76417600 | 0.00073300 | 0.00001500 |
| Br | -0.49511900 | 2.35782700 | 0.00005900 |
| Br | -0.50095100 | -2.35699200 | -0.00016200 |
| Cl | -3.01989800 | 0.00352300 | 0.00003000 |

**$Cu^{III}$_CN_Br**

| | | | |
|---|---|---|---|
| C | 1.18214000 | 0.00037900 | 0.00003800 |
| C | 3.30589400 | 0.00105200 | 0.67966400 |
| C | 3.30596300 | 0.00066200 | -0.67936900 |
| H | 4.11613000 | 0.00145000 | 1.39119400 |
| H | 4.11626800 | 0.00065300 | -1.39082000 |
| N | 1.97807400 | 0.00087500 | 1.08350100 |
| N | 1.97818400 | 0.00026900 | -1.08333900 |
| C | 1.51054300 | 0.00100700 | 2.47142200 |
| H | 2.37975500 | 0.00248400 | 3.12821600 |
| H | 0.91148100 | 0.89514200 | 2.65713700 |
| H | 0.91372200 | -0.89442700 | 2.65812000 |
| C | 1.51078100 | -0.00038300 | -2.47130500 |
| H | 0.91187200 | 0.89372600 | -2.65763600 |
| H | 2.38005300 | 0.00054400 | -3.12802100 |
| H | 0.91383900 | -0.89584300 | -2.65749100 |
| Cu | -0.75206800 | -0.00017900 | 0.00002000 |
| Br | -0.63759400 | 2.36815200 | -0.00031800 |

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| | | | |
|---|---|---|---|
| Br | -0.63611500 | -2.36844300 | 0.00029100 |
| C | -2.66677200 | -0.00077800 | -0.00024300 |
| N | -3.83406700 | -0.00114500 | -0.00038900 |

**$Cu^{III}$_F_Br**

| | | | |
|---|---|---|---|
| C | 0.02092500 | 1.00516900 | 0.00000100 |
| C | 0.07676700 | 3.12268500 | 0.67947000 |
| C | 0.07552100 | 3.12260700 | -0.67980500 |
| H | 0.09905500 | 3.93228000 | 1.39137100 |
| H | 0.09634900 | 3.93213000 | -1.39183400 |
| N | 0.04184500 | 1.79508500 | 1.08518300 |
| N | 0.03975700 | 1.79497600 | -1.08530100 |
| C | 0.03232800 | 1.31694600 | 2.46900000 |
| H | 0.04138800 | 2.18010800 | 3.13344400 |
| H | -0.87067000 | 0.72797400 | 2.64443400 |
| H | 0.91874300 | 0.70472500 | 2.64956300 |
| C | 0.02629000 | 1.31670400 | -2.46903600 |
| H | -0.87979100 | 0.73217100 | -2.64347100 |
| H | 0.03909500 | 2.17970900 | -3.13362100 |
| H | 0.90947400 | 0.70008000 | -2.65039500 |
| Cu | -0.02181100 | -0.91810900 | 0.00005200 |
| Br | -2.37690700 | -0.64727200 | 0.00106200 |
| Br | 2.34326200 | -0.74623900 | -0.00097400 |
| F | -0.05619600 | -2.68068900 | -0.00011300 |

**$Cu^{III}$_I_Br**

| | | | |
|---|---|---|---|
| C | -1.84020200 | 0.00118500 | 0.00000000 |
| C | -3.96054800 | -0.00049300 | -0.67924300 |
| C | -3.96040400 | 0.00038800 | 0.67973300 |
| H | -4.77049900 | -0.00122100 | -1.39117500 |
| H | -4.77020900 | 0.00068300 | 1.39183400 |
| N | -2.63206200 | 0.00016100 | -1.08457000 |
| N | -2.63183200 | 0.00162100 | 1.08476700 |
| C | -2.16101000 | -0.00232300 | -2.47083000 |
| H | -3.02836000 | 0.00950400 | -3.12996900 |
| H | -1.55210300 | 0.88606600 | -2.65195300 |
| H | -1.57256200 | -0.90356600 | -2.65634500 |
| C | -2.16052000 | 0.00196100 | 2.47093100 |
| H | -1.55535900 | 0.89302500 | 2.65151300 |
| H | -3.02781000 | 0.01031000 | 3.13020300 |
| H | -1.56823800 | -0.89669000 | 2.65676700 |
| Cu | 0.12082200 | 0.00033400 | -0.00002100 |
| Br | -0.07514700 | 2.36254900 | -0.00082400 |
| Br | -0.07731600 | -2.36173700 | 0.00061900 |
| I | 2.73624200 | -0.00100000 | 0.00003700 |

**$Cu^{III}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | 1.99269600 | -0.00002100 | -0.00000800 |
| C | 4.14479900 | -0.24290400 | 0.63414500 |
| C | 4.14484300 | 0.24296400 | -0.63397400 |
| H | 4.95687200 | -0.49057100 | 1.29965500 |

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| | | | |
|---|---|---|---|
| H | 4.95696100 | 0.49066600 | -1.29941500 |
| N | 2.81485600 | -0.38949900 | 1.00266100 |
| N | 2.81492500 | 0.38946000 | -1.00262100 |
| C | 2.36814100 | -0.84333100 | 2.31837900 |
| H | 3.08113300 | -1.57340800 | 2.70570500 |
| H | 2.29864200 | -0.00055200 | 3.01184700 |
| H | 1.39188600 | -1.31816600 | 2.21474400 |
| C | 2.36829400 | 0.84324600 | -2.31838400 |
| H | 1.39200900 | 1.31803600 | -2.21483000 |
| H | 3.08128300 | 1.57335200 | -2.70566000 |
| H | 2.29889100 | 0.00045500 | -3.01184600 |
| Cu | -0.02397500 | -0.00000600 | -0.00002800 |
| Br | -0.16523100 | 2.35622300 | 0.32272500 |
| Br | -0.16527900 | -2.35623300 | -0.32276400 |
| C | -1.99642700 | 0.00002400 | 0.00000700 |
| C | -2.66593300 | 0.15521800 | -1.20726100 |
| C | -2.66591400 | -0.15516200 | 1.20728400 |
| C | -4.06820400 | 0.15434100 | -1.19938600 |
| H | -2.13034600 | 0.27567100 | -2.14444000 |
| C | -4.06818600 | -0.15427400 | 1.19943300 |
| H | -2.13031300 | -0.27561900 | 2.14445500 |
| C | -4.76718100 | 0.00003700 | 0.00003000 |
| H | -4.60518200 | 0.27460900 | -2.13695700 |
| H | -4.60514900 | -0.27453700 | 2.13701300 |
| H | -5.85360300 | 0.00004300 | 0.00003800 |

**$Cu^{III}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | 1.38408600 | 0.01129700 | 0.08570800 |
| C | 3.57759700 | 0.25225200 | -0.39113000 |
| C | 3.48677400 | -0.26970300 | 0.85940800 |
| H | 4.43554600 | 0.51152800 | -0.99159100 |
| H | 4.24906100 | -0.54314000 | 1.57206200 |
| N | 2.27755200 | 0.42175400 | -0.84572800 |
| N | 2.13371700 | -0.41398700 | 1.13069100 |
| C | 1.92638500 | 0.91474400 | -2.17652100 |
| H | 2.70336300 | 1.60109600 | -2.51753000 |
| H | 1.84086500 | 0.08425200 | -2.88294700 |
| H | 0.97769100 | 1.44910100 | -2.11559000 |
| C | 1.59515100 | -0.90140400 | 2.39911600 |
| H | 2.28113900 | -1.63965100 | 2.81824800 |
| H | 1.47308300 | -0.07682900 | 3.10707100 |
| H | 0.63041700 | -1.37554700 | 2.21516500 |
| Cu | -0.63556100 | 0.00402900 | -0.04708500 |
| Br | -0.76503000 | -2.33258700 | -0.49251400 |
| Br | -0.85567500 | 2.36877500 | 0.13038100 |
| C | -2.59754800 | -0.01927000 | -0.14604600 |
| H | -2.91242600 | 0.10425800 | -1.17943700 |
| C | -3.36649300 | -0.16892100 | 0.91680400 |
| H | -2.98379400 | -0.28749600 | 1.92809000 |

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| | | | |
|---|---|---|---|
| H | -4.45361500 | -0.17932700 | 0.80780400 |

**$TS^{Cu}$_Bn_Br**

| | | | |
|---|---|---|---|
| Cu | 0.09739600 | 0.83170300 | -0.33717400 |
| C | -1.66956200 | 1.70235500 | -0.91363500 |
| H | -1.63437100 | 2.72803500 | -0.53546700 |
| Br | 1.99664600 | 2.26429900 | 0.01372100 |
| Br | -0.53403600 | -1.58612400 | -0.18052800 |
| C | -2.80039000 | 0.92561300 | -0.40236400 |
| C | -3.42819000 | 1.24670500 | 0.82914200 |
| C | -3.29005600 | -0.22076600 | -1.08082400 |
| C | -4.48214100 | 0.49221500 | 1.33179700 |
| H | -3.07794100 | 2.11687500 | 1.38208900 |
| C | -4.35844600 | -0.97153100 | -0.57686000 |
| H | -2.85624700 | -0.48616700 | -2.04266000 |
| C | -4.96284000 | -0.62575400 | 0.63148900 |
| H | -4.94496000 | 0.78007500 | 2.27347600 |
| H | -4.71764500 | -1.83078500 | -1.13920600 |
| H | -5.79174000 | -1.20849800 | 1.02385900 |
| C | 1.43777800 | -1.06928900 | 0.14231600 |
| C | 3.58328600 | -1.63573500 | -0.06526000 |
| C | 3.32428900 | -1.46280300 | 1.26070300 |
| H | 4.49941000 | -1.87984900 | -0.57942800 |
| H | 3.97227500 | -1.52512600 | 2.12059800 |
| N | 1.98467800 | -1.14857200 | 1.38140200 |
| N | 2.39975500 | -1.42402100 | -0.74695600 |
| C | 1.30551800 | -0.81253900 | 2.63175300 |
| H | 1.20673000 | 0.27276100 | 2.71763100 |
| H | 0.31895300 | -1.27825700 | 2.64623500 |
| H | 1.90159500 | -1.19642800 | 3.45932000 |
| C | 2.23989800 | -1.48671700 | -2.19999000 |
| H | 3.06991000 | -2.06037800 | -2.61158000 |
| H | 1.29966100 | -1.98551400 | -2.43948800 |
| H | 2.24220000 | -0.47899900 | -2.62289300 |
| H | -1.58954600 | 1.69436400 | -2.00692800 |

**$TS^{Cu}$_Br_Br**

| | | | |
|---|---|---|---|
| C | 1.43683700 | -0.16562000 | 0.00001400 |
| C | 3.45061100 | 0.48063700 | -0.68137200 |
| C | 3.45060600 | 0.48071700 | 0.68133700 |
| H | 4.21463400 | 0.76021300 | -1.38909200 |
| H | 4.21462500 | 0.76037700 | 1.38902900 |
| N | 2.20228400 | 0.05111900 | -1.09231300 |
| N | 2.20227700 | 0.05124700 | 1.09232100 |
| C | 1.75064000 | -0.05255700 | -2.48058500 |
| H | 2.62530100 | -0.02126100 | -3.12927000 |
| H | 1.22725500 | -1.00015000 | -2.61900700 |
| H | 1.08498600 | 0.78211800 | -2.71437700 |
| C | 1.75061400 | -0.05224900 | 2.48059900 |
| H | 2.62526300 | -0.02082800 | 3.12929400 |

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| | | | |
|---|---|---|---|
| H | 1.08492700 | 0.78243800 | 2.71425700 |
| H | 1.22725800 | -0.99983900 | 2.61914900 |
| Cu | -0.56399600 | 0.02257700 | -0.00000800 |
| Br | 0.35615300 | -2.22900800 | 0.00011400 |
| Br | -0.39981000 | 2.40659800 | -0.00002000 |
| Br | -2.92251800 | -0.36501700 | -0.00008700 |

**$TS^{Cu}$_$CF_3$_Br**

| | | | |
|---|---|---|---|
| C | 1.43404300 | -0.33160800 | 0.00137400 |
| C | 3.29756000 | 0.70217500 | -0.64540800 |
| C | 3.29945600 | 0.65180000 | 0.71827500 |
| H | 3.99571000 | 1.15149400 | -1.33378900 |
| H | 4.00077400 | 1.04776800 | 1.43562900 |
| N | 2.16366000 | 0.05327500 | -1.08204900 |
| N | 2.16608200 | -0.02736700 | 1.10880200 |
| C | 1.73304000 | -0.04930400 | -2.47638600 |
| H | 2.60807600 | 0.06562300 | -3.11526300 |
| H | 1.28540700 | -1.02975100 | -2.64554900 |
| H | 1.00574000 | 0.73703000 | -2.69516200 |
| C | 1.75592700 | -0.25583100 | 2.49482000 |
| H | 1.27813400 | -1.23322200 | 2.57263100 |
| H | 2.64552900 | -0.23605600 | 3.12374200 |
| H | 1.06009500 | 0.52564200 | 2.81107000 |
| Cu | -0.68212900 | 0.01146400 | 0.00862300 |
| Br | 0.48894200 | -2.19364600 | -0.06173200 |
| Br | -0.35027300 | 2.41789400 | 0.01237100 |
| C | -2.63699800 | -0.34377000 | 0.01649300 |
| F | -3.30340200 | 0.19042800 | -1.07359900 |
| F | -3.01616600 | -1.67467800 | 0.01816400 |
| F | -3.29793000 | 0.19183100 | 1.10898800 |

**$TS^{Cu}$_$CH_3$_Br**

| | | | |
|---|---|---|---|
| C | 0.82148200 | 0.63930700 | 0.01678300 |
| C | 0.65049100 | 2.81740400 | -0.42052500 |
| C | 0.79418700 | 2.67408100 | 0.92824500 |
| H | 0.49417800 | 3.69959400 | -1.02107000 |
| H | 0.79040500 | 3.40754900 | 1.71891300 |
| N | 0.71409200 | 1.56104900 | -0.98060900 |
| N | 0.94394800 | 1.32836500 | 1.18742400 |
| C | 0.50371000 | 1.25396900 | -2.39348200 |
| H | 0.69099500 | 2.15755200 | -2.97311900 |
| H | 1.19855200 | 0.47159100 | -2.70291600 |
| H | -0.52695900 | 0.92033100 | -2.54052900 |
| C | 1.09592400 | 0.74397200 | 2.52054200 |
| H | 1.53879700 | 1.49506000 | 3.17469200 |
| H | 0.12228400 | 0.44049300 | 2.91319100 |
| H | 1.75780200 | -0.12072400 | 2.46176700 |
| Cu | -0.54877800 | -1.11017600 | 0.07473500 |
| Br | 2.00385800 | -1.00311900 | -0.28510400 |
| Br | -2.46316800 | 0.41481900 | -0.01855600 |

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| | | | |
|---|---|---|---|
| C | -0.96264600 | -3.05717900 | 0.22394800 |
| H | -0.21856100 | -3.56554800 | 0.85517400 |
| H | -1.95782600 | -3.25160700 | 0.64594800 |
| H | -0.92444000 | -3.52392400 | -0.77204000 |

**$TS^{Cu}$_Cl_Br (optimized in acetonitrile)**

| | | | |
|---|---|---|---|
| C | 1.12224000 | -0.14954300 | 0.00000000 |
| C | 2.85292300 | -1.36275300 | -0.68128000 |
| C | 2.85289600 | -1.36276600 | 0.68132700 |
| H | 3.50073600 | -1.85598200 | -1.38843400 |
| H | 3.50068400 | -1.85600700 | 1.38849600 |
| N | 1.78775600 | -0.58223900 | -1.09262900 |
| N | 1.78770800 | -0.58226600 | 1.09264900 |
| C | 1.38755500 | -0.34658700 | -2.48102800 |
| H | 2.22230200 | -0.61070000 | -3.12915100 |
| H | 0.51899100 | -0.96380700 | -2.72395200 |
| H | 1.14529800 | 0.70954200 | -2.61063500 |
| C | 1.38745200 | -0.34659900 | 2.48103000 |
| H | 2.22200900 | -0.61115600 | 3.12921500 |
| H | 1.14563500 | 0.70962100 | 2.61073200 |
| H | 0.51859800 | -0.96347600 | 2.72378600 |
| Cu | -0.82829600 | 0.28379200 | -0.00001300 |
| Br | -1.41421800 | -2.03097500 | -0.00000900 |
| Br | 0.70512200 | 2.15739500 | 0.00001200 |
| Cl | -2.85776200 | 1.31460600 | -0.00001300 |

**$TS^{Cu}$_CN_Br**

| | | | |
|---|---|---|---|
| C | -1.05708300 | -0.17450000 | 0.00004700 |
| C | -2.53598100 | -1.69021300 | -0.68169500 |
| C | -2.53583900 | -1.69006300 | 0.68242700 |
| H | -3.07976400 | -2.29818500 | -1.38716400 |
| H | -3.07949100 | -2.29786500 | 1.38814000 |
| N | -1.64153200 | -0.72391400 | -1.09402100 |
| N | -1.64129500 | -0.72368600 | 1.09436100 |
| C | -1.28390200 | -0.43507700 | -2.48358700 |
| H | -2.06272800 | -0.83946600 | -3.12899700 |
| H | -1.21965900 | 0.64539700 | -2.62288200 |
| H | -0.32447900 | -0.90185200 | -2.72105700 |
| C | -1.28336900 | -0.43453200 | 2.48379000 |
| H | -1.21991800 | 0.64599200 | 2.62305800 |
| H | -2.06161200 | -0.83957200 | 3.12949500 |
| H | -0.32348400 | -0.90054600 | 2.72089500 |
| Cu | 0.86789100 | 0.43892400 | -0.00009500 |
| Br | -0.97893300 | 2.05676000 | -0.00016900 |
| Br | 1.65375300 | -1.85388100 | -0.00009000 |
| C | 2.52190100 | 1.48624700 | 0.00009900 |
| N | 3.51557700 | 2.10264800 | 0.00020900 |

**$TS^{Cu}$_F_Br**

| | | | |
|---|---|---|---|
| C | -0.73984500 | 0.65056300 | 0.00004600 |
| C | -0.67140500 | 2.76888200 | 0.68241400 |

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| | | | |
|---|---|---|---|
| C | -0.67144100 | 2.76890900 | -0.68223800 |
| H | -0.60326800 | 3.58279400 | 1.38673700 |
| H | -0.60333900 | 3.58285000 | -1.38653100 |
| N | -0.75552200 | 1.45700600 | 1.09655400 |
| N | -0.75558100 | 1.45705100 | -1.09642700 |
| C | -0.69511900 | 0.99458600 | 2.48290300 |
| H | -0.90988900 | 1.83943900 | 3.13616200 |
| H | -1.44095100 | 0.21331400 | 2.63825000 |
| H | 0.30447100 | 0.60562900 | 2.69481600 |
| C | -0.69523500 | 0.99468400 | -2.48279500 |
| H | -1.44107600 | 0.21342100 | -2.63814300 |
| H | -0.91002700 | 1.83956200 | -3.13601500 |
| H | 0.30434600 | 0.60573200 | -2.69476100 |
| Cu | 0.44869100 | -1.02791100 | -0.00002200 |
| Br | -2.04760800 | -1.00628300 | 0.00005200 |
| Br | 2.49578700 | 0.23414300 | -0.00012200 |
| F | 0.89082300 | -2.79028700 | -0.00003200 |

**$TS^{Cu}$_I_Br**

| | | | |
|---|---|---|---|
| C | 1.75835200 | -0.21861800 | 0.00002400 |
| C | 3.80869400 | 0.30008900 | 0.68141000 |
| C | 3.80871300 | 0.30003600 | -0.68134200 |
| H | 4.58869800 | 0.53103000 | 1.38931800 |
| H | 4.58873900 | 0.53092200 | -1.38924500 |
| N | 2.53572400 | -0.05020400 | 1.09206000 |
| N | 2.53575600 | -0.05028800 | -1.09200300 |
| C | 2.08001600 | -0.12934300 | 2.48068400 |
| H | 2.95547100 | -0.13312400 | 3.12896000 |
| H | 1.45183500 | 0.73456900 | 2.71167300 |
| H | 1.51588800 | -1.05262500 | 2.62307100 |
| C | 2.08009200 | -0.12954000 | -2.48063600 |
| H | 2.95556900 | -0.13338000 | -3.12888200 |
| H | 1.51596300 | -1.05283100 | -2.62296400 |
| H | 1.45192400 | 0.73435600 | -2.71171800 |
| Cu | -0.24002400 | 0.08234300 | -0.00000500 |
| Br | 0.03456300 | 2.44691900 | -0.00008100 |
| Br | 0.54177900 | -2.21727100 | 0.00007600 |
| I | -2.84813100 | -0.20031800 | -0.00002100 |

**$TS^{Cu}$_Ph_Br**

| | | | |
|---|---|---|---|
| C | 1.72671000 | -0.54202300 | -0.00815600 |
| C | 3.70658900 | 0.25341900 | 0.62878200 |
| C | 3.68407400 | 0.23209700 | -0.73522500 |
| H | 4.46067700 | 0.60480600 | 1.31508300 |
| H | 4.41472900 | 0.56178100 | -1.45673500 |
| N | 2.51015500 | -0.26751600 | 1.07062100 |
| N | 2.47373500 | -0.30201700 | -1.12079000 |
| C | 2.09468800 | -0.36919200 | 2.46878800 |
| H | 1.61141900 | -1.33323300 | 2.63547700 |
| H | 2.98259600 | -0.29406600 | 3.09557400 |

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| | | | |
|---|---|---|---|
| H | 1.40215700 | 0.44197500 | 2.70787300 |
| C | 2.01605800 | -0.45081800 | -2.50194400 |
| H | 1.33288100 | 0.36356300 | -2.75625500 |
| H | 2.88711100 | -0.42008800 | -3.15564500 |
| H | 1.50960200 | -1.41061500 | -2.61501500 |
| Cu | -0.36927900 | 0.18455300 | 0.00126900 |
| Br | 0.44087300 | 2.48344000 | 0.01002000 |
| Br | 0.51810700 | -2.19074000 | 0.03986800 |
| C | -2.34932100 | 0.00849100 | -0.00444300 |
| C | -2.99190500 | -1.24460800 | -0.00026600 |
| C | -3.19456200 | 1.13801300 | -0.01182400 |
| C | -4.38652200 | -1.37516000 | -0.00348900 |
| H | -2.39442500 | -2.15924900 | 0.00587000 |
| C | -4.59051200 | 1.02794200 | -0.01478600 |
| H | -2.75265700 | 2.13427300 | -0.01500800 |
| C | -5.19308400 | -0.23373100 | -0.01068600 |
| H | -4.84363100 | -2.36353400 | -0.00025100 |
| H | -5.20920800 | 1.92406400 | -0.02018200 |
| H | -6.27696300 | -0.32605900 | -0.01295400 |

**$TS^{Cu}$_vinyl_Br**

| | | | |
|---|---|---|---|
| C | 1.19213900 | -0.05123000 | -0.00033700 |
| C | 2.41870900 | -1.78198500 | 0.68087400 |
| C | 2.41723800 | -1.78231300 | -0.68335300 |
| H | 2.85693700 | -2.47176800 | 1.38450000 |
| H | 2.85389900 | -2.47246800 | -1.38758700 |
| N | 1.69828600 | -0.68360000 | 1.09576300 |
| N | 1.69598600 | -0.68409300 | -1.09721400 |
| C | 1.38111100 | -0.36038500 | 2.48618600 |
| H | 2.11847700 | -0.84297500 | 3.12725500 |
| H | 1.42735900 | 0.72047700 | 2.62737100 |
| H | 0.38008400 | -0.72646100 | 2.72941500 |
| C | 1.37501000 | -0.36200800 | -2.48702300 |
| H | 2.11123300 | -0.84423700 | -3.12968100 |
| H | 0.37371300 | -0.72923300 | -2.72743300 |
| H | 1.41983200 | 0.71881600 | -2.62892800 |
| Cu | -0.94054200 | 0.48779600 | 0.00063200 |
| Br | 1.11659100 | 2.00200700 | -0.00056000 |
| Br | -1.52145700 | -1.88304800 | 0.00099200 |
| C | -2.47997400 | 1.72087800 | 0.00050700 |
| H | -2.27719200 | 2.80340500 | 0.00064000 |
| C | -3.78264700 | 1.38972600 | 0.00005300 |
| H | -4.11228500 | 0.34833300 | -0.00011700 |
| H | -4.59543500 | 2.12421200 | -0.00019200 |

**$Cu^{I}$_Bn**

| | | | |
|---|---|---|---|
| Cu | 0.96198300 | 0.60658600 | -0.00001400 |
| Br | 2.96276400 | -0.60412000 | 0.00001700 |
| C | -0.73408500 | 1.60705500 | -0.00004300 |
| H | -0.73873100 | 2.25235900 | 0.88858900 |

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| | | | |
|---|---|---|---|
| H | -0.73872300 | 2.25230300 | -0.88871600 |
| C | -1.90202500 | 0.68491500 | -0.00001900 |
| C | -2.48216200 | 0.21835900 | -1.20118900 |
| C | -2.48217800 | 0.21844100 | 1.20117500 |
| C | -3.56348300 | -0.66280500 | -1.20290300 |
| H | -2.06853900 | 0.55932100 | -2.14929500 |
| C | -3.56349900 | -0.66272300 | 1.20293400 |
| H | -2.06856900 | 0.55946800 | 2.14926400 |
| C | -4.11583000 | -1.11599600 | 0.00002700 |
| H | -3.98071900 | -0.99578800 | -2.15140300 |
| H | -3.98074600 | -0.99564200 | 2.15145100 |
| H | -4.95864900 | -1.80230900 | 0.00004500 |

**$Cu^{I}$_Br**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | 0.00000000 |
| Br | 0.00000000 | 0.00000000 | 2.29773100 |
| Br | 0.00000000 | 0.00000000 | -2.29773100 |

**$Cu^{I}$_$CF_3$**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.01051500 |
| Br | 0.00000000 | 0.00000000 | 2.29371900 |
| C | 0.00000000 | 0.00000000 | -1.94343600 |
| F | 0.00000000 | 1.25835600 | -2.53017000 |
| F | 1.08976800 | -0.62917800 | -2.53017000 |
| F | -1.08976800 | -0.62917800 | -2.53017000 |

**$Cu^{I}$_$CH_3$**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.86925100 |
| Br | 0.00000000 | 0.00000000 | 1.47897300 |
| C | 0.00000000 | 0.00000000 | -2.81399600 |
| H | 0.00000000 | 1.02180000 | -3.22394100 |
| H | 0.88490500 | -0.51090000 | -3.22394100 |
| H | -0.88490500 | -0.51090000 | -3.22394100 |

**$Cu^{I}$_Cl**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.52847400 |
| Br | 0.00000000 | 0.00000000 | 1.76185000 |
| Cl | 0.00000000 | 0.00000000 | -2.72582400 |

**$Cu^{I}$_CN**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.61513600 | 0.00000000 |
| Br | -0.00155400 | -1.67417100 | 0.00000000 |
| C | 0.00312100 | 2.50451400 | 0.00000000 |
| N | 0.00509700 | 3.67570900 | 0.00000000 |

**$Cu^{I}$_F**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.88079600 | 0.00000000 |
| Br | -0.00066200 | -1.41405200 | 0.00000000 |
| F | 0.00257600 | 2.66097000 | 0.00000000 |

**$Cu^{I}$_I**

| | | | |
|---|---|---|---|
| Cu | 0.00000000 | 0.00000000 | -0.44001100 |
| Br | 0.00000000 | 0.00000000 | -2.74460700 |
| I | 0.00000000 | 0.00000000 | 2.05323700 |

**$Cu^{I}$_Ph**

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| | | | |
|---|---|---|---|
| Cu | -0.56998700 | -0.00002600 | -0.00001000 |
| Br | -2.89765900 | 0.00001300 | -0.00001200 |
| C | 1.36365700 | -0.00002000 | 0.00000300 |
| C | 2.12165300 | 1.19529200 | 0.00001100 |
| C | 2.12169500 | -1.19530300 | 0.00000900 |
| C | 3.52186200 | 1.20437700 | 0.00002500 |
| H | 1.60768000 | 2.15659300 | 0.00000600 |
| C | 3.52190400 | -1.20433800 | 0.00002300 |
| H | 1.60775500 | -2.15662300 | 0.00000300 |
| C | 4.23125500 | 0.00003200 | 0.00003100 |
| H | 4.06038700 | 2.15106700 | 0.00003100 |
| H | 4.06046200 | -2.15100900 | 0.00002800 |
| H | 5.31924500 | 0.00005100 | 0.00004200 |

**$Cu^{I}$_vinyl**

| | | | |
|---|---|---|---|
| Cu | -0.55426000 | -0.17794400 | -0.00000200 |
| Br | 1.76290300 | 0.09720800 | 0.00000200 |
| C | -2.46127300 | -0.39147300 | -0.00000500 |
| H | -2.88746300 | -1.40611000 | 0.00001200 |
| C | -3.39422800 | 0.58141300 | 0.00000000 |
| H | -3.13549700 | 1.64251900 | 0.00000700 |
| H | -4.47212900 | 0.38203300 | 0.00000400 |

**prod_Br**

| | | | |
|---|---|---|---|
| C | 2.30423700 | 0.68081600 | -0.00038500 |
| C | 0.20602700 | 0.00000000 | -0.00011100 |
| C | 2.30423700 | -0.68081900 | -0.00048900 |
| N | 0.98400200 | -1.09362400 | -0.00013900 |
| N | 0.98400100 | 1.09362200 | -0.00013300 |
| Br | -1.63945500 | 0.00000100 | 0.00021500 |
| H | 3.11636900 | 1.38956300 | -0.00056100 |
| H | 3.11636900 | -1.38956600 | -0.00063200 |
| C | 0.50759000 | 2.48103000 | 0.00010200 |
| H | -0.09080700 | 2.66361600 | -0.89408400 |
| H | -0.09034700 | 2.66349000 | 0.89462200 |
| H | 1.37821000 | 3.13441900 | -0.00007600 |
| C | 0.50758600 | -2.48102900 | 0.00003300 |
| H | -0.09045600 | -2.66349800 | 0.89448200 |
| H | -0.09070800 | -2.66360100 | -0.89422600 |
| H | 1.37820200 | -3.13442200 | -0.00005100 |

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**Note about G09 input files**

The input files used for this study are available via the University of York data repository. They can be accessed at www.york.ac.uk/