Supporting Material

Synthesis, Structure, and Condensed-Phase Reactivity of $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Ph}_3](BF_4)$ (L^{Ph} = bis(diphenylphosphino)amine) with CS_2.

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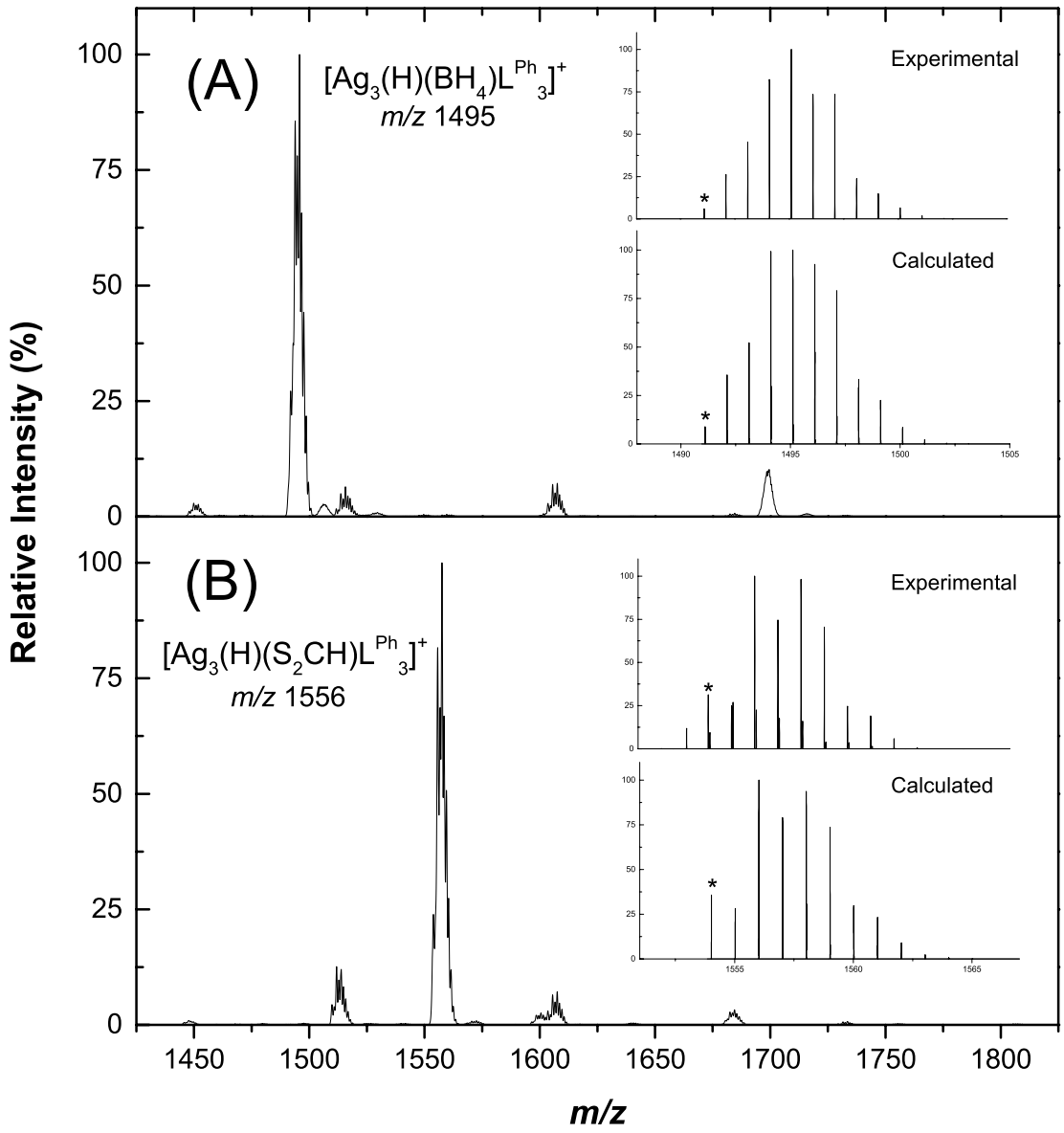


Figure S1: Mass Spectra from the Lumos mass spectrometer for ESI-MS of a 50 μM acetonitrile solution of: (A) the preparation of $[Ag_3(H)(BH_4)L^{Ph}_3]^+$ from stoichiometric equivalents of $AgBF_4$, bis(diphenylphosphino)amine L^{Ph} and $NaBH_4$; (B) the subsequent addition of CS_2 to give $[Ag_3(H)(S_2CH)L^{Ph}_3]^+$. Spectra were recorded 15 min after the addition of $NaBH_4$ and CS_2 respectively. The *m/z* values shown are of the most intense isotope peak for each cluster. Insets are the Ultra-High Resolution Accurate MS: top is experimental, bottom is theoretical isotope pattern. The * designates monoisotopic masses at 500,000 resolution: $[Ag_3(H)(BH_4)L^{Ph}_3]^+$ (*m/z* 1491.1075 (exp)/*m/z* 1491.1116 (calc)) and $[Ag_3(H)(S_2CH)L^{Ph}_3]^+$ (*m/z* 1554.0243 (exp)/*m/z* 1554.0193 (calc)).

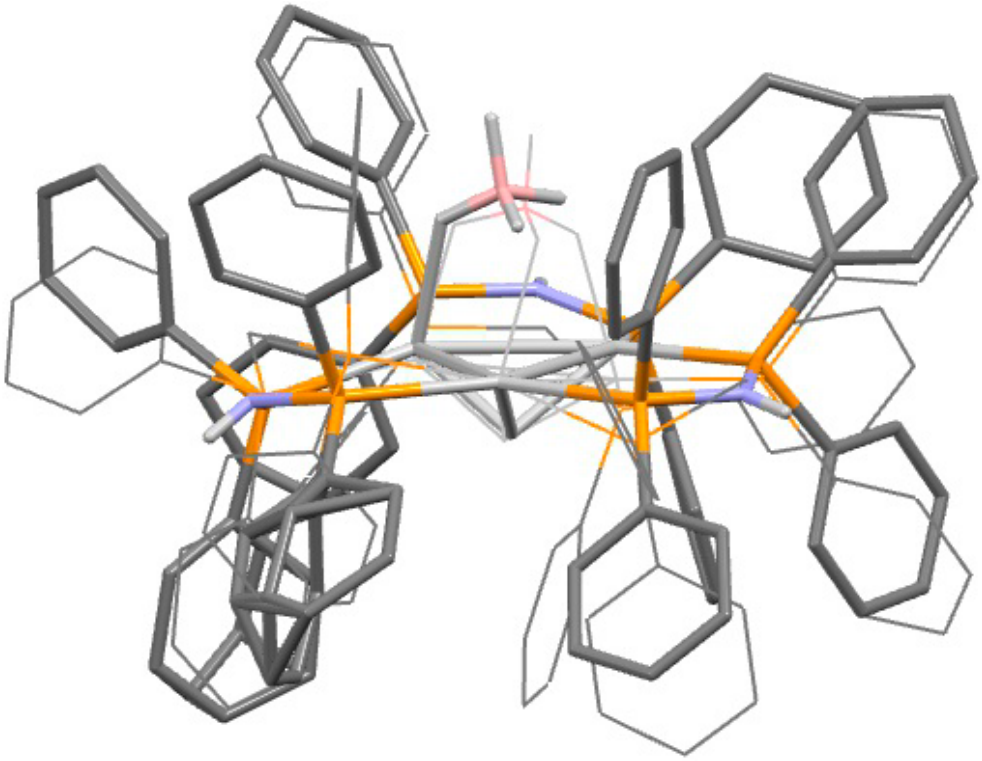


Figure S2: Overlayed perspective of the cations **3b.BF$_4$**, as a capped sticks model, on [Ag$_3$(μ_3-H)(μ_3-BH$_4$)L$_3$](BF$_4$) (L = (Ph$_2$P)$_2$CH$_2$ = dppm), **3c.BF$_4$**, as a wireframe model.

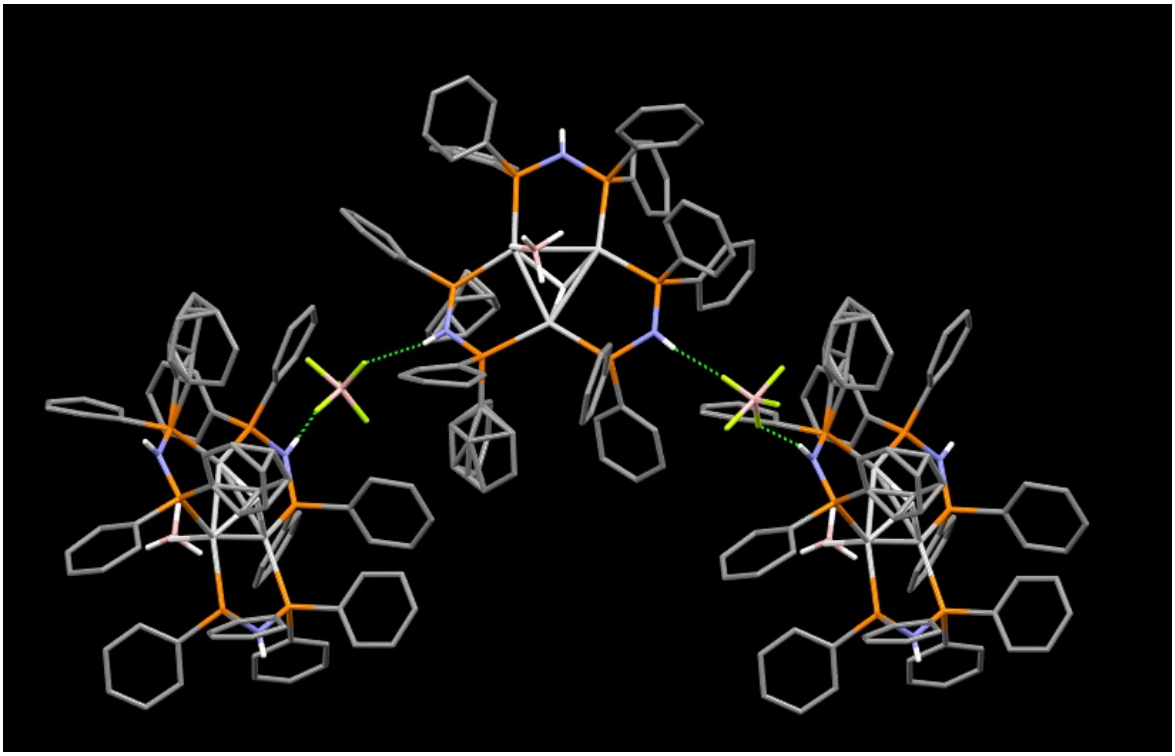


Figure S3: H bonding network between the cations **3b** and the BF_4^- counter ions.

Table S1: Crystal data and structure refinement for cluster **3bBF$_4$.**

Identification code	jmwhm1
Empirical formula	$C_{72}H_{68}Ag_3B_2F_4N_3P_6$
Formula weight	1582.34
Temperature/K	130.01(10)
Crystal system	Monoclinic
Space group	P 21/n
a/Å	18.3179(4)
b/Å	22.8489(4)
c/Å	21.3193(6)
β/°	114.712(3)
Volume/Å^3	8105.9(4)
Z	4
ρ_{calc}g/cm^3	1.455
μ/mm^{-1}	7.254
F(000)	3192
Crystal size/mm^3	0.35 × 0.05 × 0.03
Radiation	CuKα (λ = 1.54184)
□ range for data collection/°	3.87 to 77.03
Index ranges	-11<=h<=23, -28<=k<=28, -26<=l<=26
Reflections collected	60697
Independent reflections	16930 [R(int) = 0.0793]
Data / restraints / parameters	16930 / 1178 / 876
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1749
R indices (all data)	R1 = 0.0945, wR2 = 0.1979

Table S2: Bond distances of X-ray crystallography for cluster **3b.BF$_4$.**

C(1)-C(6)	1.377(12)
C(1)-C(2)	1.387(11)
C(1)-P(1)	1.819(8)
C(2)-C(3)	1.378(12)
C(3)-C(4)	1.359(14)
C(4)-C(5)	1.370(15)
C(5)-C(6)	1.384(13)
C(7)-C(8)	1.3900
C(7)-C(12)	1.3900
C(7)-P(1)	1.825(5)
C(8)-C(9)	1.3900
C(9)-C(10)	1.3900
C(10)-C(11)	1.3900
C(11)-C(12)	1.3900
C(13)-C(18)	1.385(12)
C(13)-C(14)	1.402(12)
C(13)-P(2)	1.816(8)
C(14)-C(15)	1.390(13)

C(15)-C(16)	1.371(17)
C(16)-C(17)	1.377(17)
C(17)-C(18)	1.413(12)
C(19)-C(20)	1.385(12)
C(19)-C(24)	1.390(12)
C(19)-P(2)	1.816(8)
C(20)-C(21)	1.390(12)
C(21)-C(22)	1.382(16)
C(22)-C(23)	1.364(18)
C(23)-C(24)	1.385(15)
C(25)-C(30)	1.383(13)
C(25)-C(26)	1.390(14)
C(25)-P(3)	1.828(9)
C(26)-C(27)	1.376(16)
C(27)-C(28)	1.33(2)
C(28)-C(29)	1.35(2)
C(29)-C(30)	1.384(15)
C(31)-C(36)	1.390(12)
C(31)-C(32)	1.389(12)
C(31)-P(3)	1.817(8)
C(32)-C(33)	1.383(11)
C(33)-C(34)	1.369(14)
C(34)-C(35)	1.394(16)
C(35)-C(36)	1.385(13)
C(37)-C(38)	1.3900
C(37)-C(42)	1.3900
C(37)-P(4)	1.808(5)
C(38)-C(39)	1.3900
C(39)-C(40)	1.3900
C(40)-C(41)	1.3900
C(41)-C(42)	1.3900
C(43)-C(48)	1.341(13)
C(43)-C(44)	1.391(11)
C(43)-P(4)	1.814(7)
C(44)-C(45)	1.379(12)
C(45)-C(46)	1.347(16)
C(46)-C(47)	1.338(18)
C(47)-C(48)	1.430(15)
C(49)-C(50)	1.3900
C(49)-C(54)	1.3900
C(49)-P(5)	1.804(5)

C(50)-C(51)	1.3900
C(51)-C(52)	1.3900
C(52)-C(53)	1.3900
C(53)-C(54)	1.3900
C(55)-C(56)	1.3900
C(55)-C(60)	1.3900
C(55)-P(5)	1.863(8)
C(56)-C(57)	1.3900
C(57)-C(58)	1.3900
C(58)-C(59)	1.3900
C(59)-C(60)	1.3900
C(55A)-C(56A)	1.3900
C(55A)-C(60A)	1.3900
C(55A)-P(5)	1.741(12)
C(56A)-C(57A)	1.3900
C(57A)-C(58A)	1.3900
C(58A)-C(59A)	1.3900
C(59A)-C(60A)	1.3900
C(61)-C(62)	1.341(15)
C(61)-C(66)	1.397(16)
C(61)-P(6)	1.835(10)
C(62)-C(63)	1.459(19)
C(63)-C(64)	1.34(2)
C(64)-C(65)	1.360(19)
C(65)-C(66)	1.399(15)
C(67)-C(68)	1.333(13)
C(67)-C(72)	1.357(19)
C(67)-C(72A)	1.55(4)
C(67)-P(6)	1.822(10)
C(68)-C(69)	1.386(16)
C(69)-C(70A)	1.28(5)
C(69)-C(70)	1.36(2)
C(70)-C(71)	1.39(2)
C(71)-C(72)	1.38(2)
C(70A)-C(71A)	1.42(5)
C(71A)-C(72A)	1.38(4)
B(1)-H(1B)	1.054(9)
B(1)-H(1D)	1.053(9)
B(1)-H(1A)	1.052(9)
B(1)-H(1C)	1.053(9)
B(2)-F(1)	1.255(15)

B(2)-F(2)	1.314(16)
B(2)-F(3)	1.343(18)
B(2)-F(4)	1.39(3)
B(2)-F(4A)	1.51(3)
N(1)-P(1)	1.686(7)
N(1)-P(2)	1.693(7)
N(1)-H(1F)	0.82(2)
N(2)-P(6)	1.671(7)
N(2)-P(5)	1.686(7)
N(2)-H(2A)	0.81(2)
N(3)-P(3)	1.672(6)
N(3)-P(4)	1.697(7)
N(3)-H(3A)	0.81(2)
F(3)-F(4)	1.73(3)
P(1)-Ag(1)	2.4514(18)
P(2)-Ag(2)	2.4578(18)
P(3)-Ag(2)	2.4361(19)
P(4)-Ag(3)	2.4633(18)
P(5)-Ag(3)	2.4774(19)
P(6)-Ag(1)	2.445(2)
Ag(1)-Ag(2)	2.8466(7)
Ag(1)-Ag(3)	2.9214(7)
Ag(1)-H(1B)	2.14(5)
Ag(1)-H(1E)	2.08(9)
Ag(2)-Ag(3)	2.9355(7)
Ag(2)-H(1E)	2.03(9)
Ag(3)-H(1E)	1.88(9)

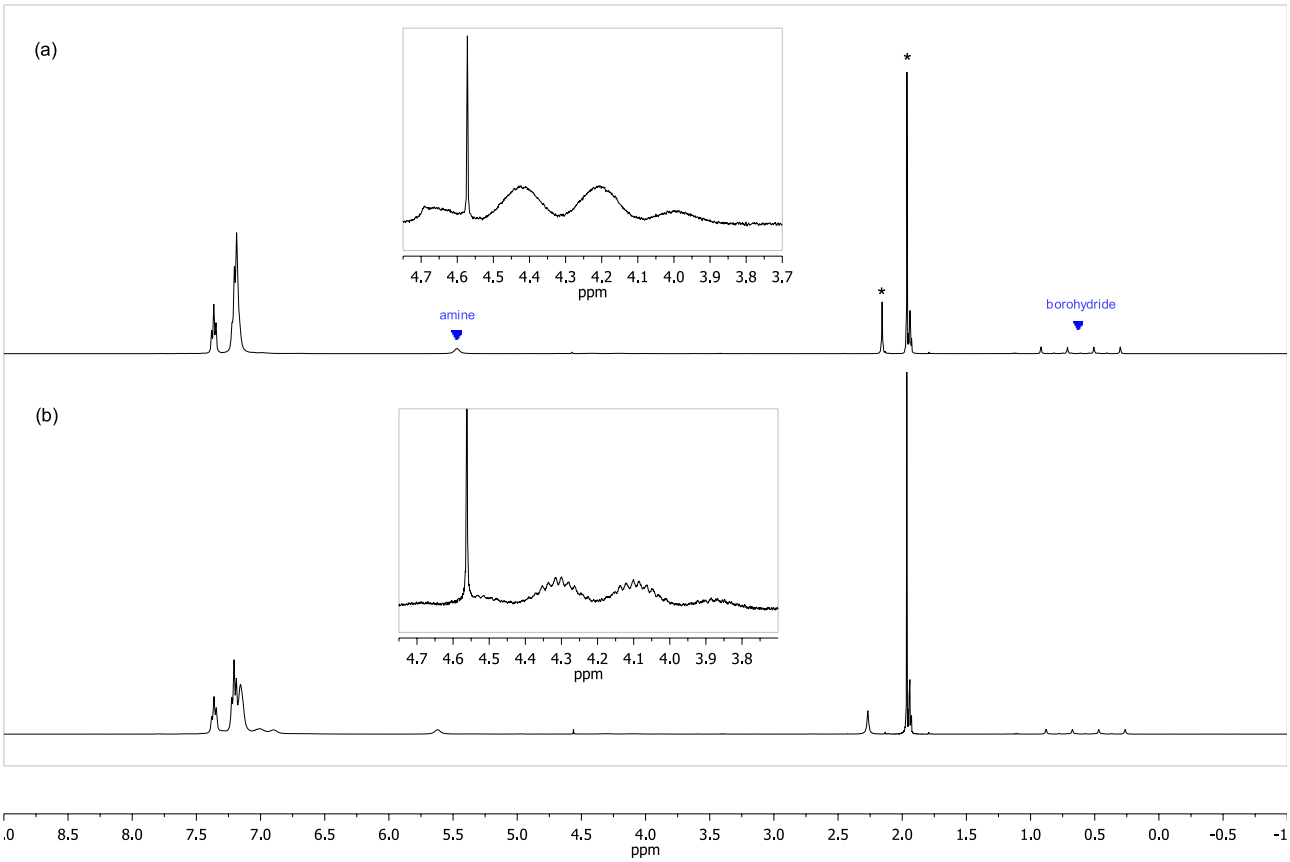


Figure S4: ^{1}H NMR spectra of cluster **3b.BF$_4$** at different temperatures: (a) RT; (b) 0 °C. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer.

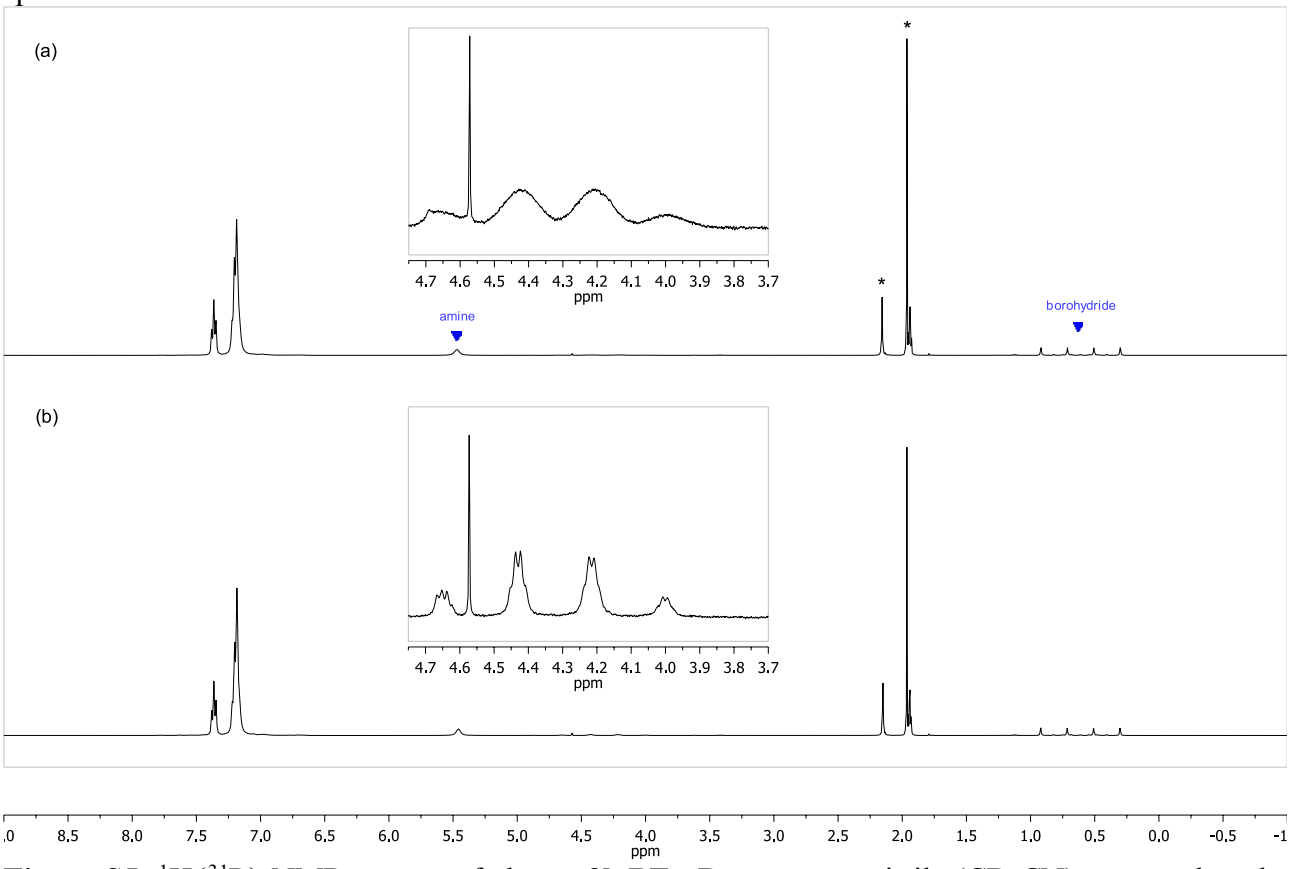


Figure S5: $^{1}H\{^{31}P\}$ NMR spectra of cluster **3b.BF$_4$**. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer.

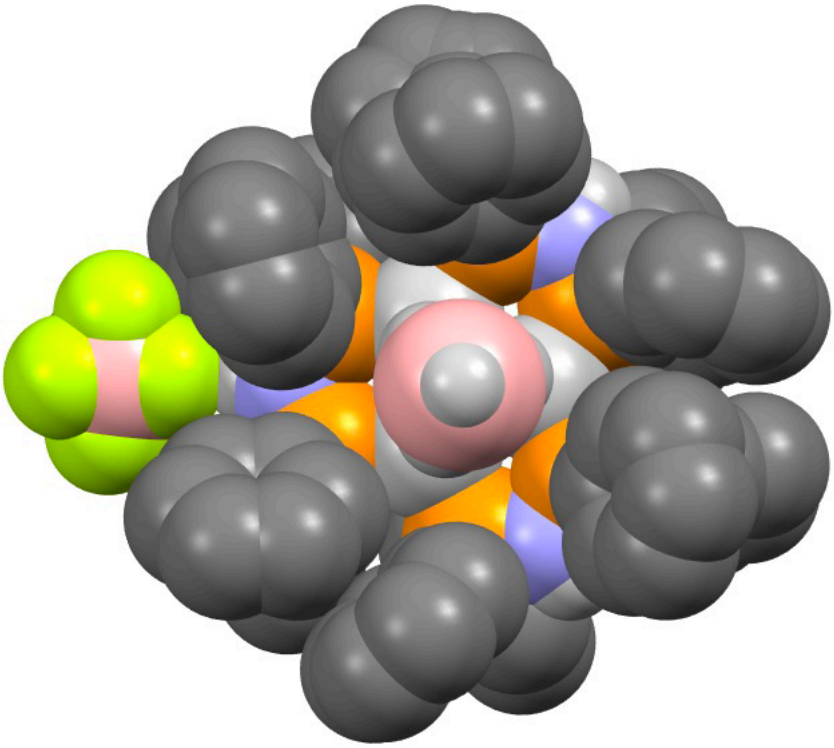


Figure S6: Space filling model of $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Ph}_3](BF_4)$.

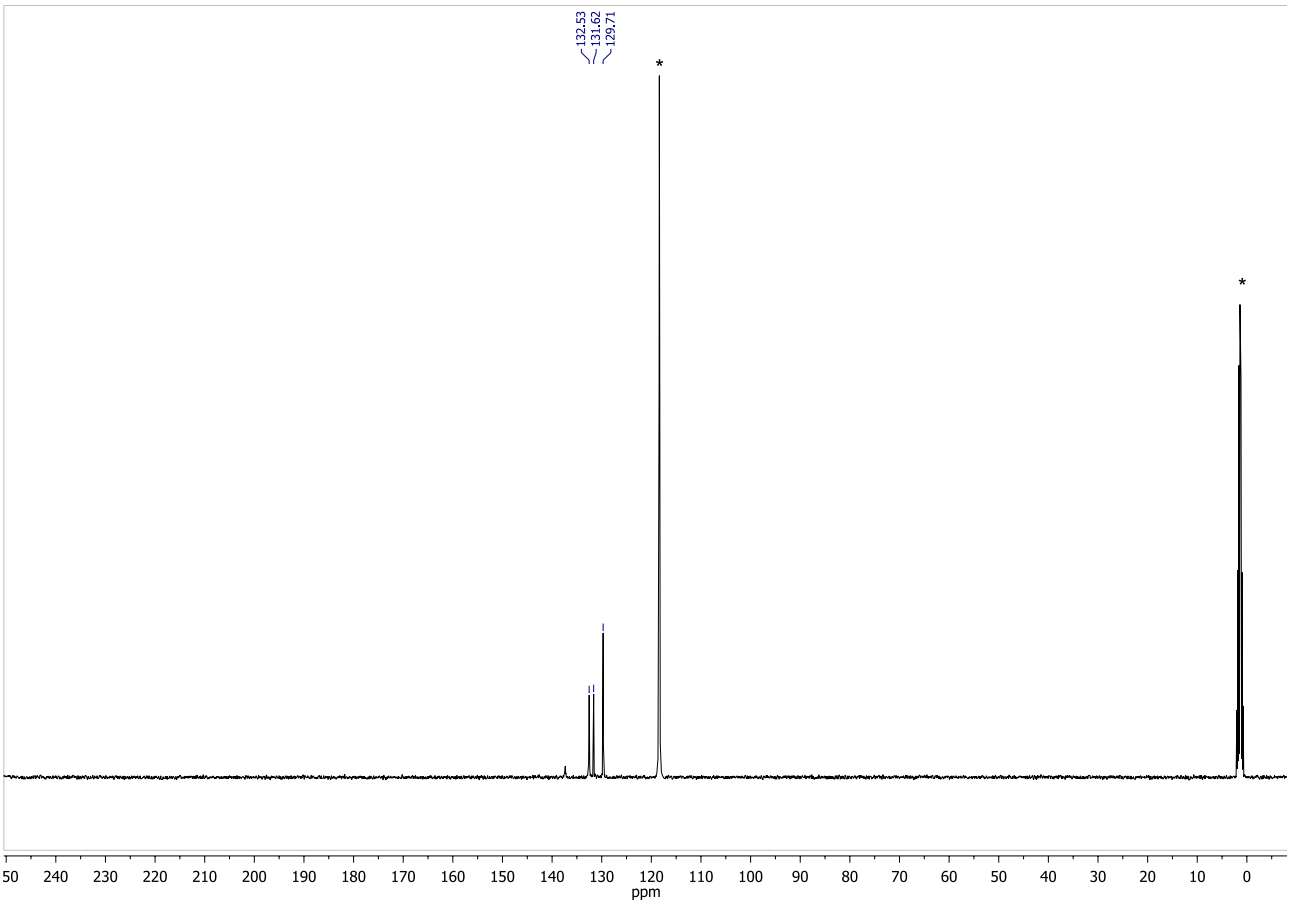


Figure S7: $^{13}C\{^1H\}$ NMR spectra of cluster **3b.BF$_4$**. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer. An * denotes a solvent impurity.

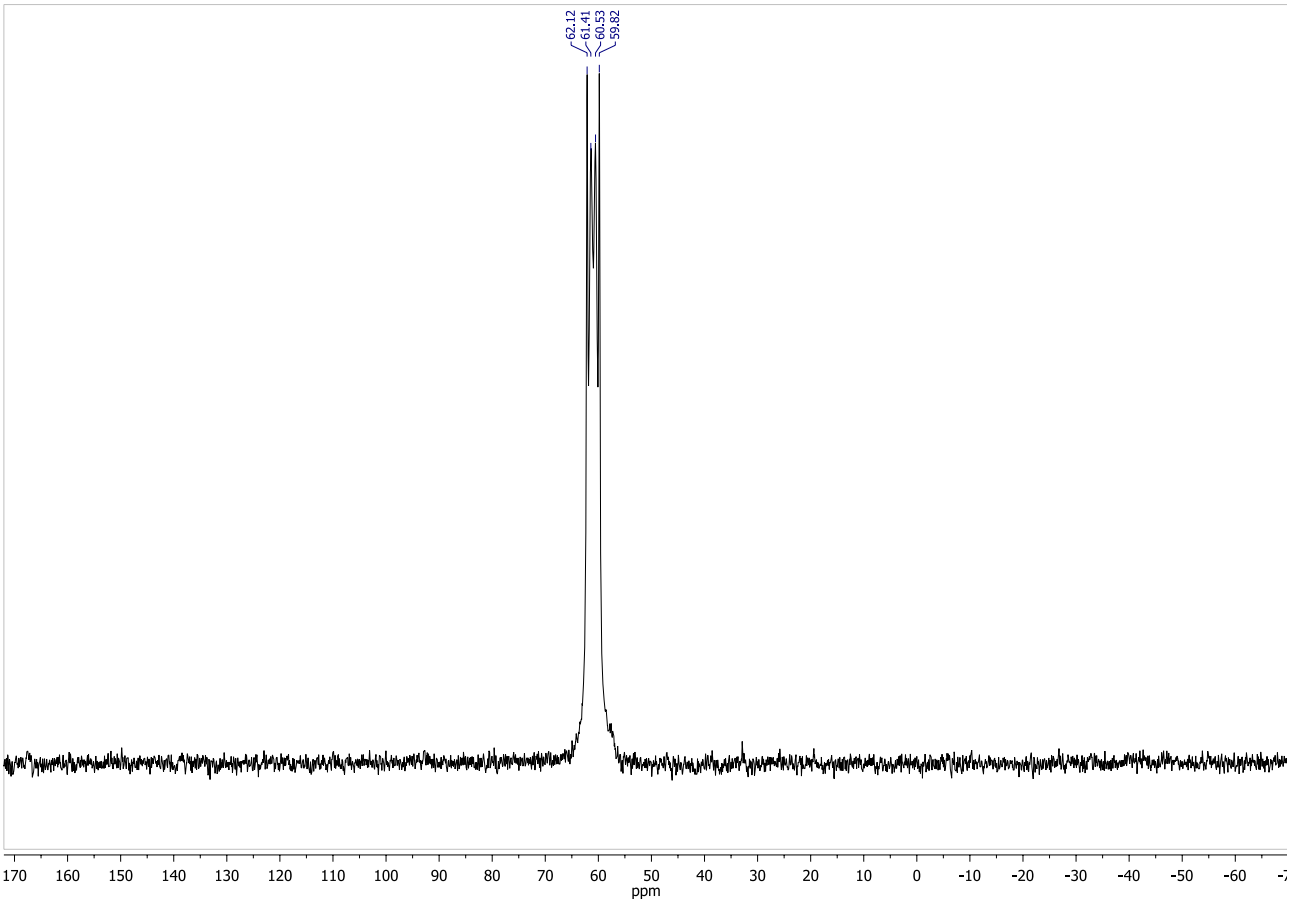


Figure S8: $^{31}P\{^{1}H\}$ NMR spectra of cluster **3b.BF$_4$**. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer.

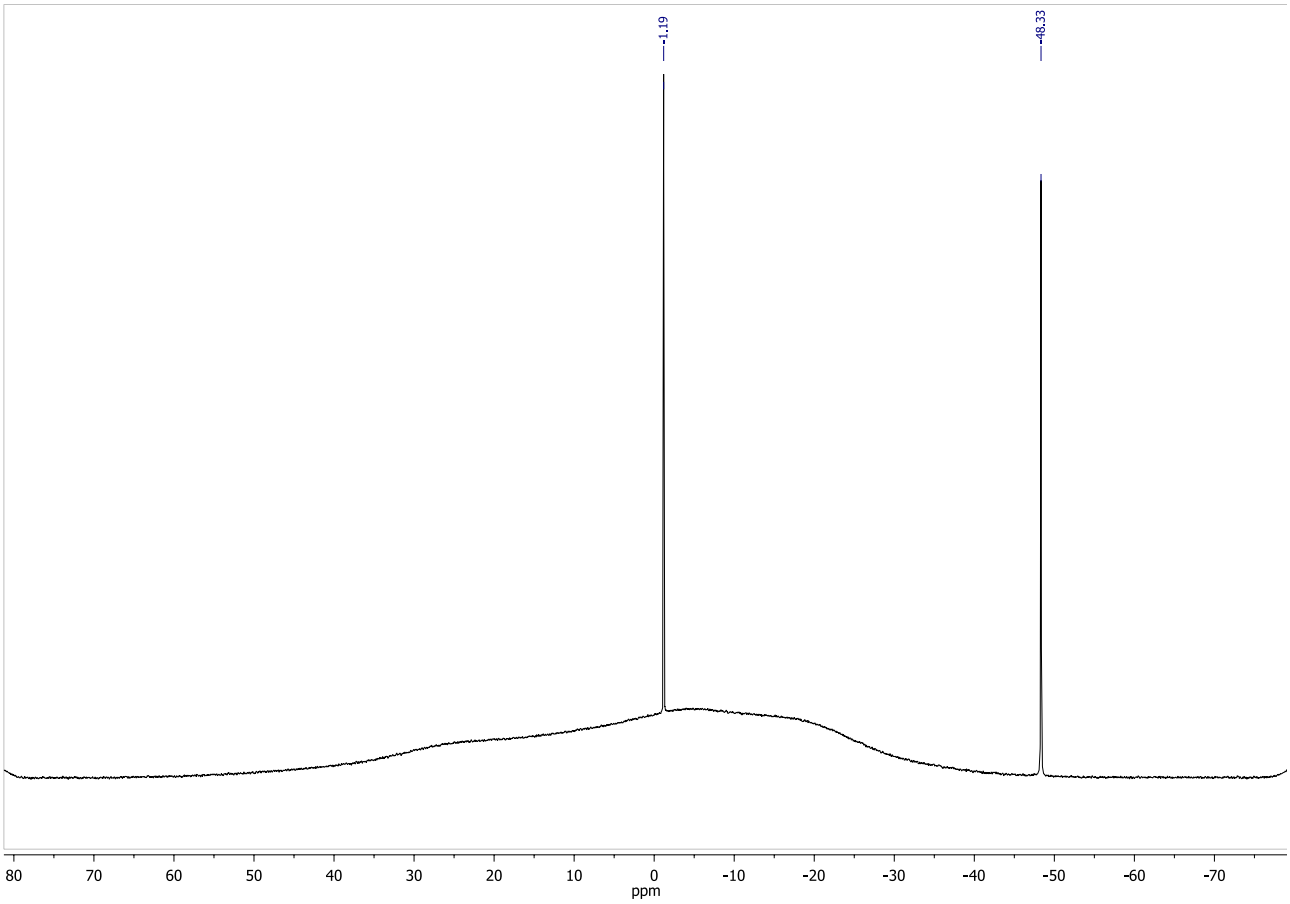


Figure S9: $^{11}B\{^{1}H\}$ NMR spectra of cluster **3b.BF$_4$**. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer.

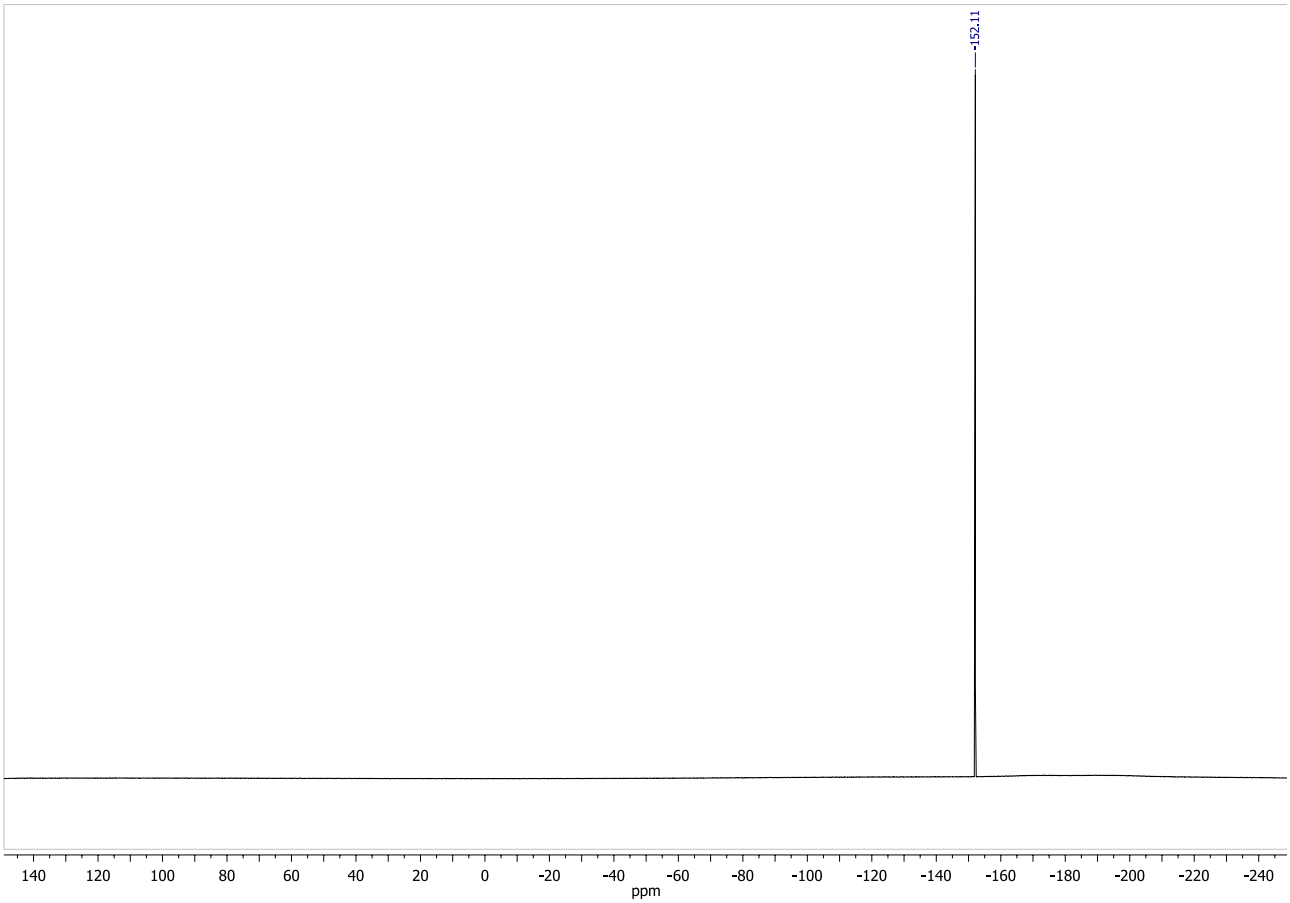


Figure S10: $^{19}F\{^{1}H\}$ NMR spectra of cluster **3b.BF$_4$**. Deuteroacetonitrile (CD_3CN) was used as the solvent for the measurement in a 400 MHz NMR spectrometer.

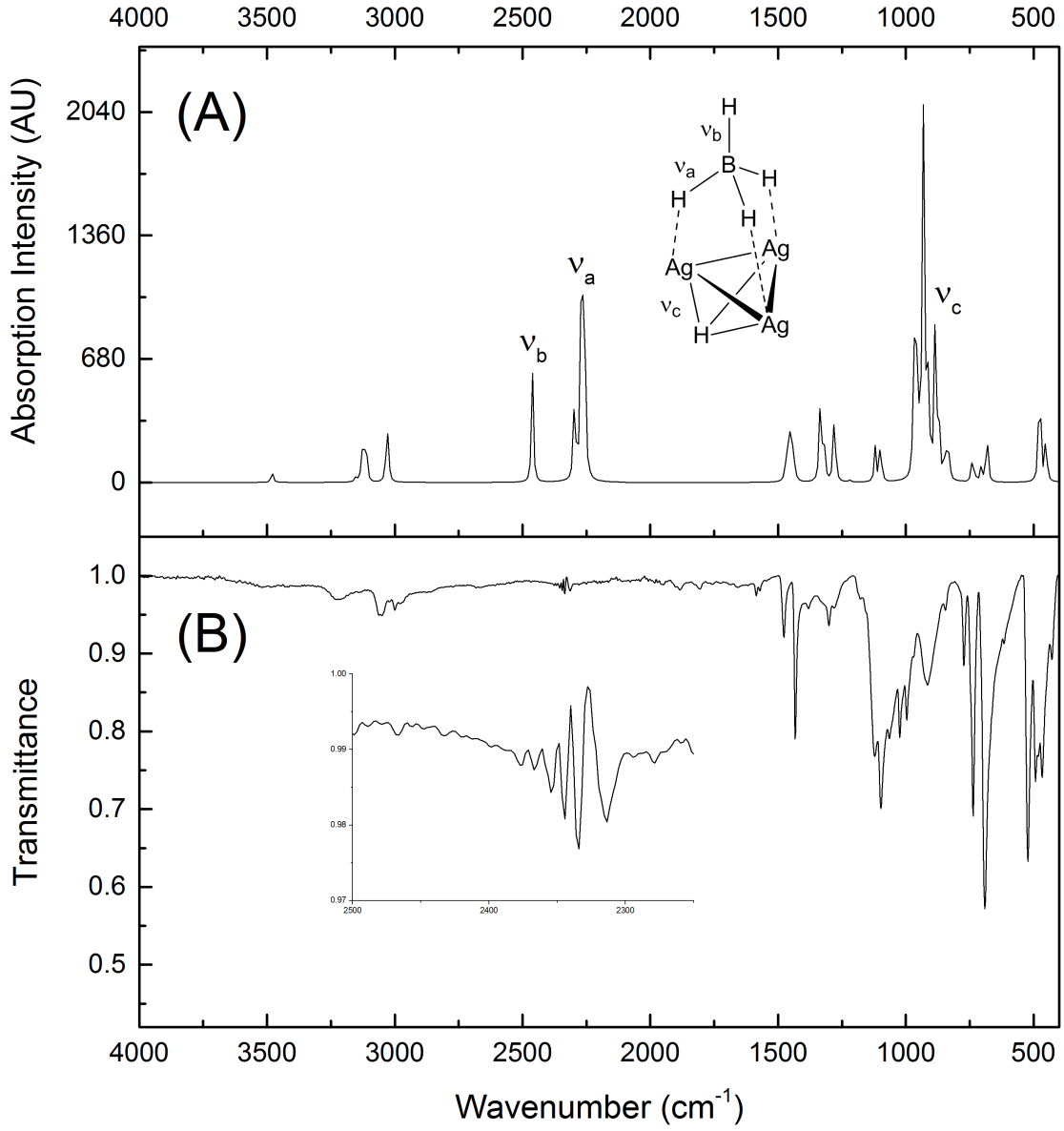


Figure S11: (A) DFT calculated IR spectrum of cluster $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Me}{}_3]^+$, **3d**, at the level of M06/6-31+G(d)/SDD. No scaling factors have been used. Simulated IR spectrum was plotted using GaussView with a resolution of 4 cm^{-1}. Inset illustrates the core structure of **3d** with L^{Me} atoms removed for clarity; (B) ATR-FTIR spectrum of cluster **3b.BF$_4$**. Spectrum was collected from isolated crystals and an average of 32 scans. Inset highlights the expanded region, 2500 – 2250 cm^{-1}, of the associated B-H stretching vibrations.

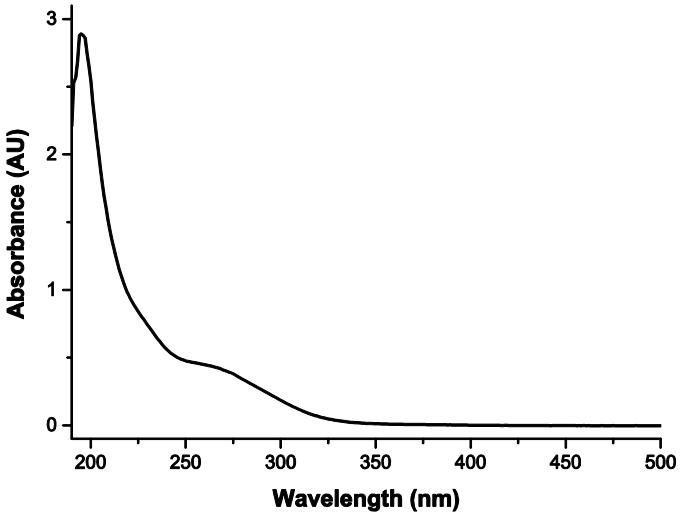


Figure S12: UV/Vis absorption spectra of cluster **3b.BF$_4$** dissolved in acetonitrile (CH_3CN) at a concentration of 100 µM.

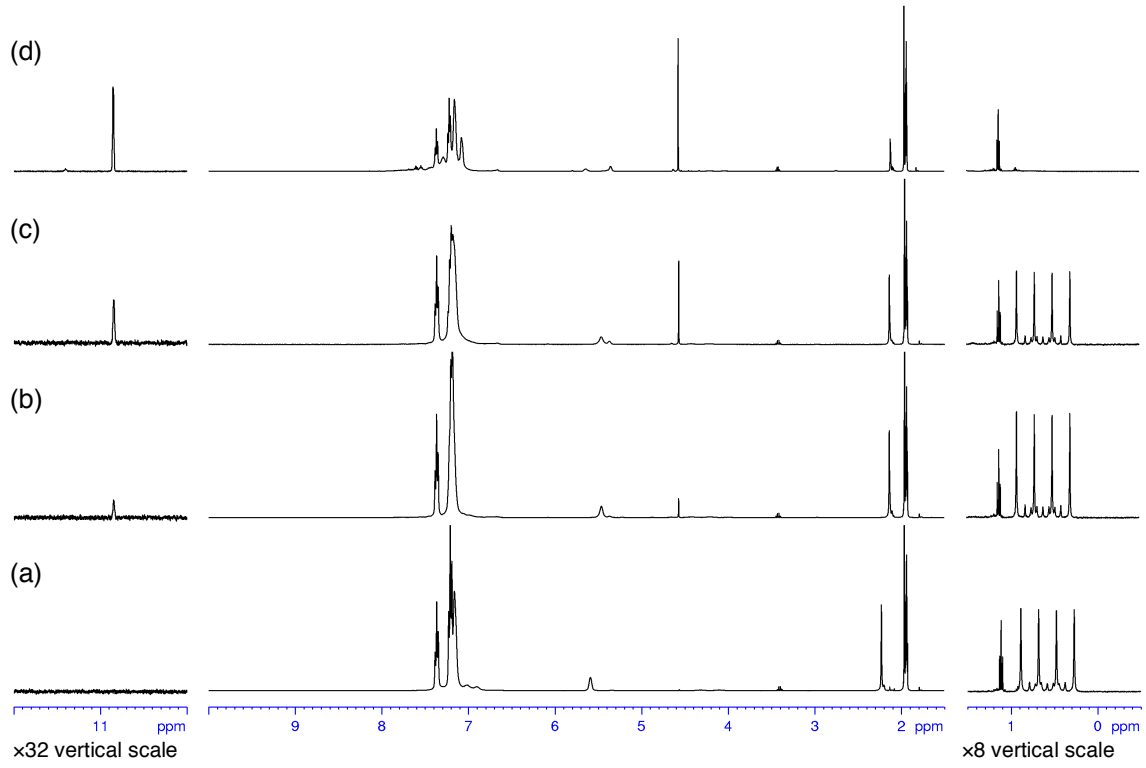


Figure S13: ^{1}H NMR spectra *in situ* reaction of $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Ph}_3](BF_4)$ with CS_2 (400 MHz, CD_3CN). (a) 0°C, 0 mins; (b) 25°C, 70 mins; (c) 25°C, 105 mins; (d) 25°C, 235 mins (500 MHz).

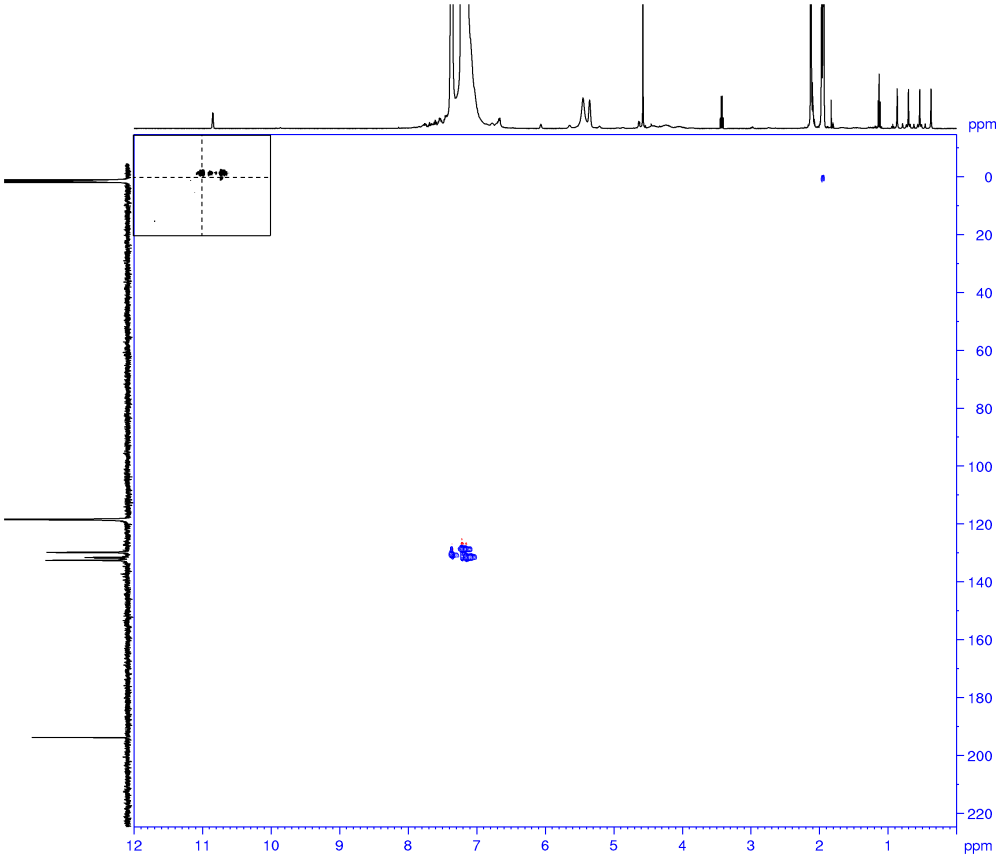


Figure S14: ^{1}H-^{13}C HSQC NMR spectrum of the *in situ* reaction of $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Ph}_3](BF_4)$ with CS_2 (500 MHz, CD_3CN, 25°C). The inset (×32 vertical intensity) shows the correlation between the dithioformate hydrogen (10.87 ppm) and carbon. Note that this peak is a foldback from *ca.* δ_C 240.7 ppm; ^{13}C spectral width collected was 224.64 to -14.68 ppm.

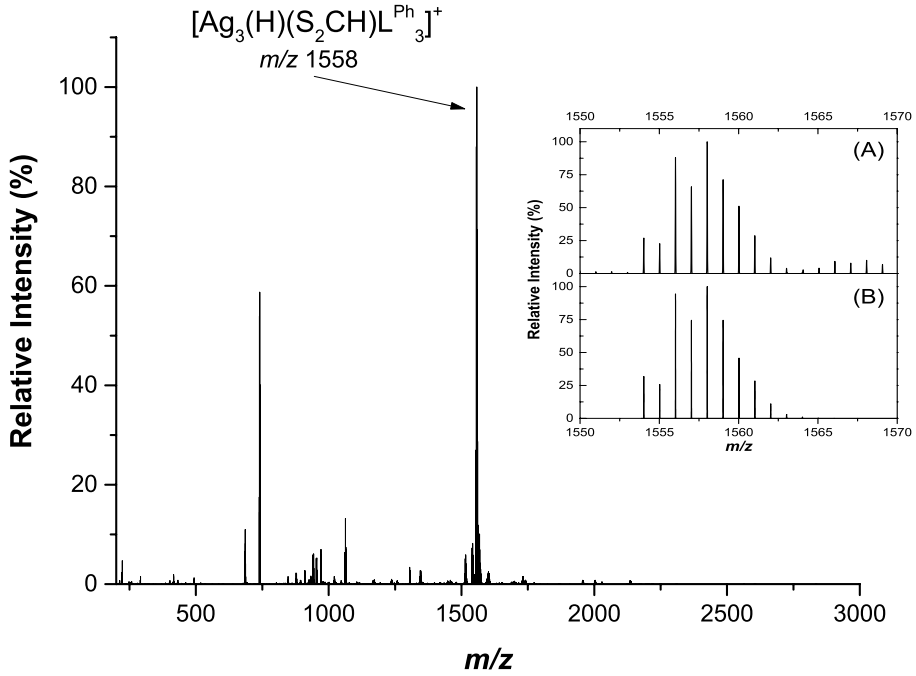


Figure S15: Positive mode ESI-MS of an aliquot taken from the in situ NMR experiments measured on a Q-Exactive Orbitrap. Labeled is the main product cluster formed $[Ag_3(H)(S_2CH)L^{Ph}_3]^+$ at *m/z* 1558 (most abundant isotope shown). Insets show the isotopic pattern of this same ion; (A) experimental and (B) simulated - set at 140,000 resolution.

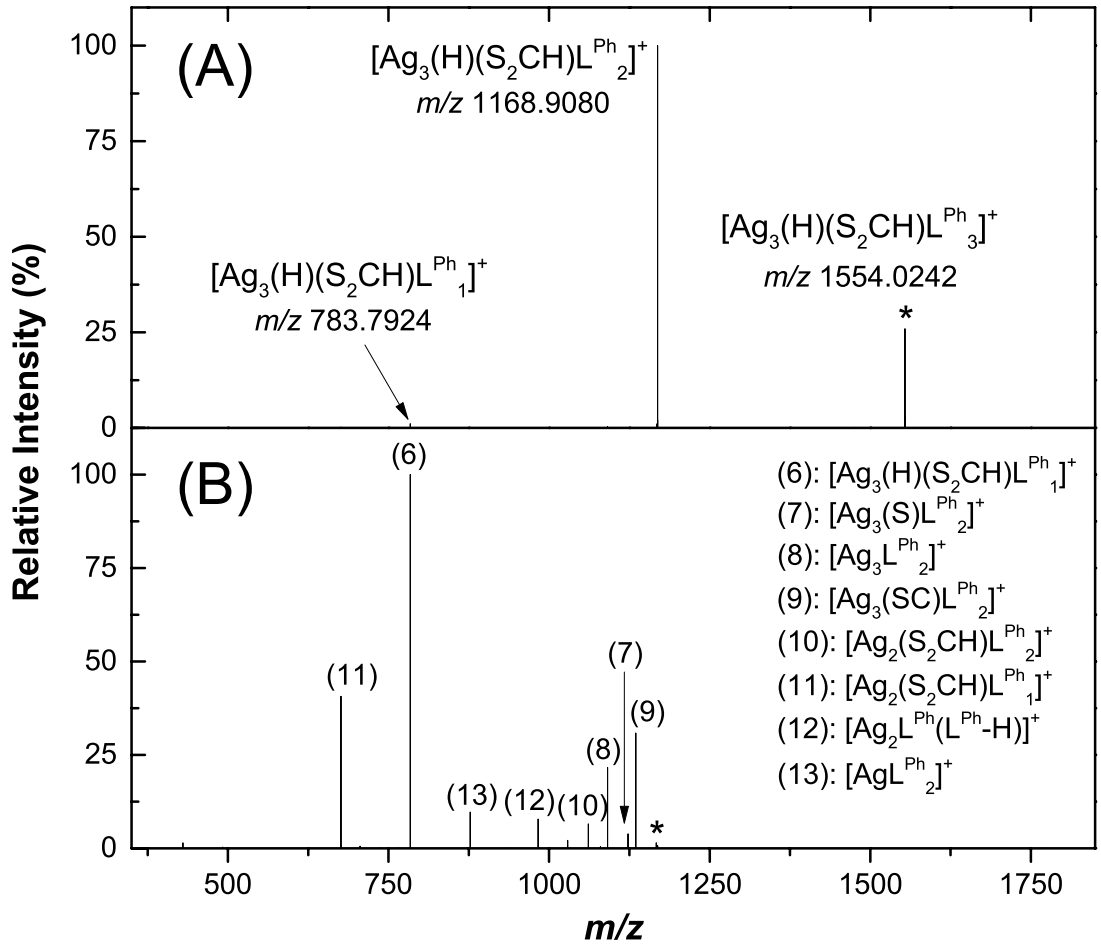


Figure S16: Single isotope multistage mass spectrometry low energy CID experiments carried out on the Lumos mass spectrometer. Mass spectra obtained using a Q value of 0.25 and an activation time of 30 ms with the given normalised collision energies (NCE) for the following species: (A) MS/MS on $[Ag_3(H)(S_2CH)L^{Ph}{}_3]^+$ (NCE = 15%); (B) MS^3 on $[Ag_3(H)(S_2CH)L^{Ph}{}_2]^+$ (NCE = 15%). A * designates the mass selected precursor ion.

Table S3: Comparison of experimentally determined accurate masses of product ions versus calculated mass for the product ions observed from the fragmentation chemistry of $[Ag_3(H)(S_2CH)L^{Ph}{}_2]^+$. Monoisotopic masses at 500,000 resolution.

Product ion	Experimental (m/z)	Calculated (m/z)
$\mathbf{[Ag_3(X)(S_2CX)L^{Ph}{}_1]^+}$	783.7925	783.7894
$\mathbf{[Ag_2(S_2CX)L^{Ph}{}_1]^+}$	675.8790	675.8765
$\mathbf{[Ag_3L^{Ph}{}_2]^+}$	1090.9481	1090.9446
$\mathbf{[Ag_3,L^{Ph}{}_2,C,S]^+}$	1134.9202	1134.9166
$\mathbf{[Ag_2L^{Ph}{}_1(L^{Ph}\text{-}H)]^+}$	983.0350	983.0317
$\mathbf{[AgL^{Ph}{}_2]^+}$	877.1376	877.1344
$\mathbf{[Ag_3(S)L^{Ph}{}_2]^+}$	1122.9201	1122.9166
$\mathbf{[Ag_3(S_2CX)L^{Ph}{}_2]^+}$	1060.9949	1060.9914

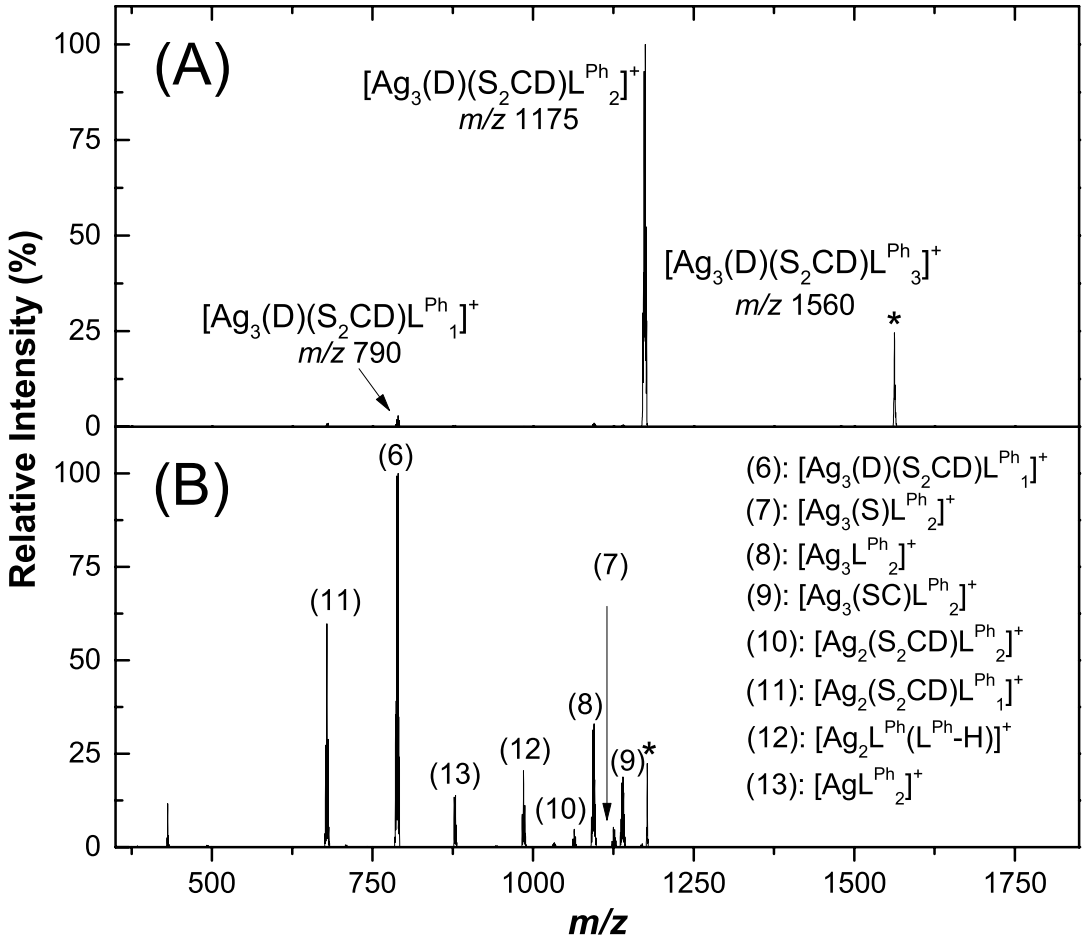


Figure S17: LTQ multistage mass spectrometry low energy CID experiments. Mass spectra obtained using a Q value of 0.25 and an activation time of 30 ms with the given normalised collision energies (NCE) for the following species: (A) MS/MS on $[Ag_3(D)(S_2CD)L^{Ph}_3]^+$ (NCE = 15%); (B) MS^3 on $[Ag_3(D)(S_2CD)L^{Ph}_2]^+$ (NCE = 15%). A * designates the mass selected precursor ion.

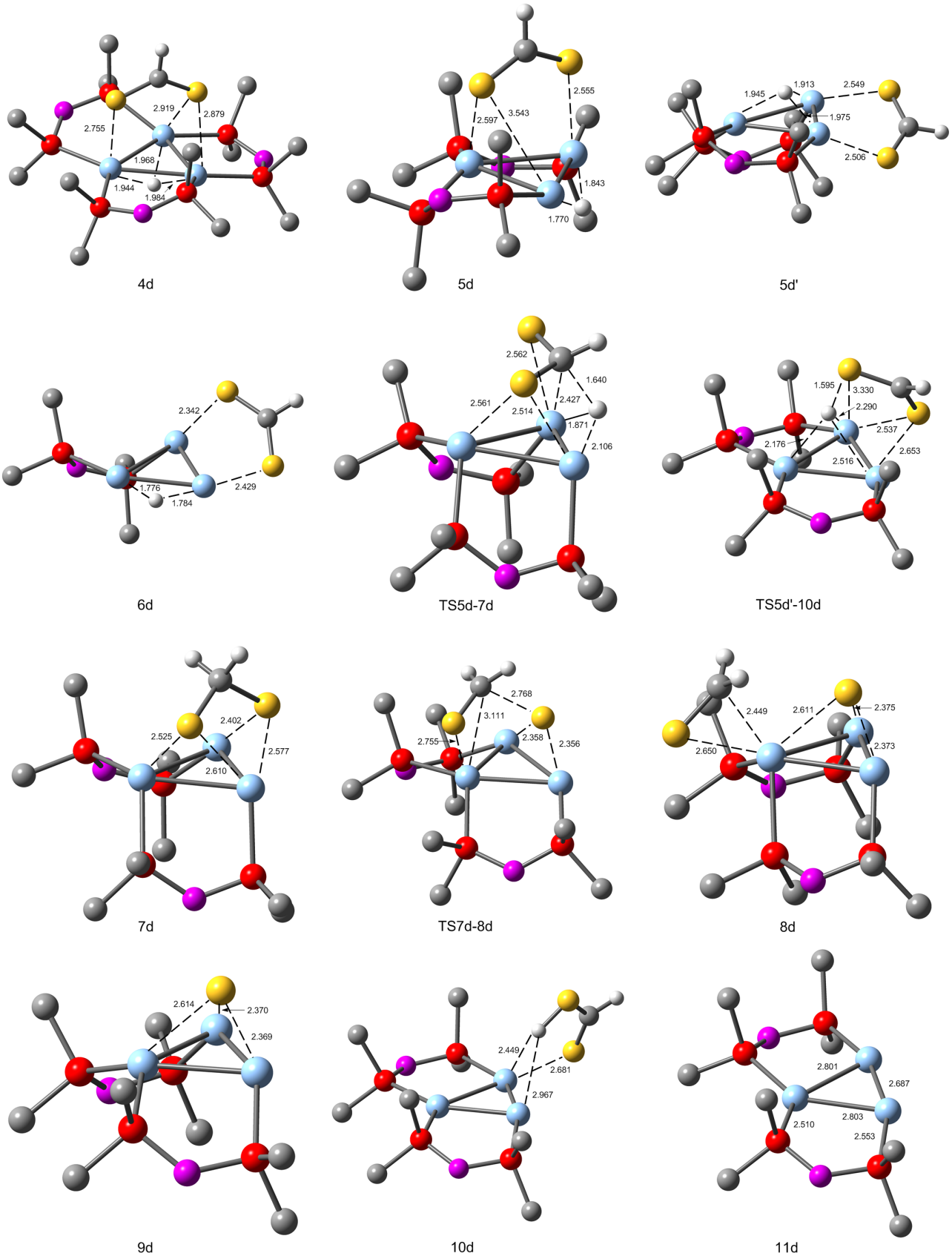


Figure S18. Full structural details of key bond distances associated with the ligand transformation reaction associated with the reactions shown in Figure 6.

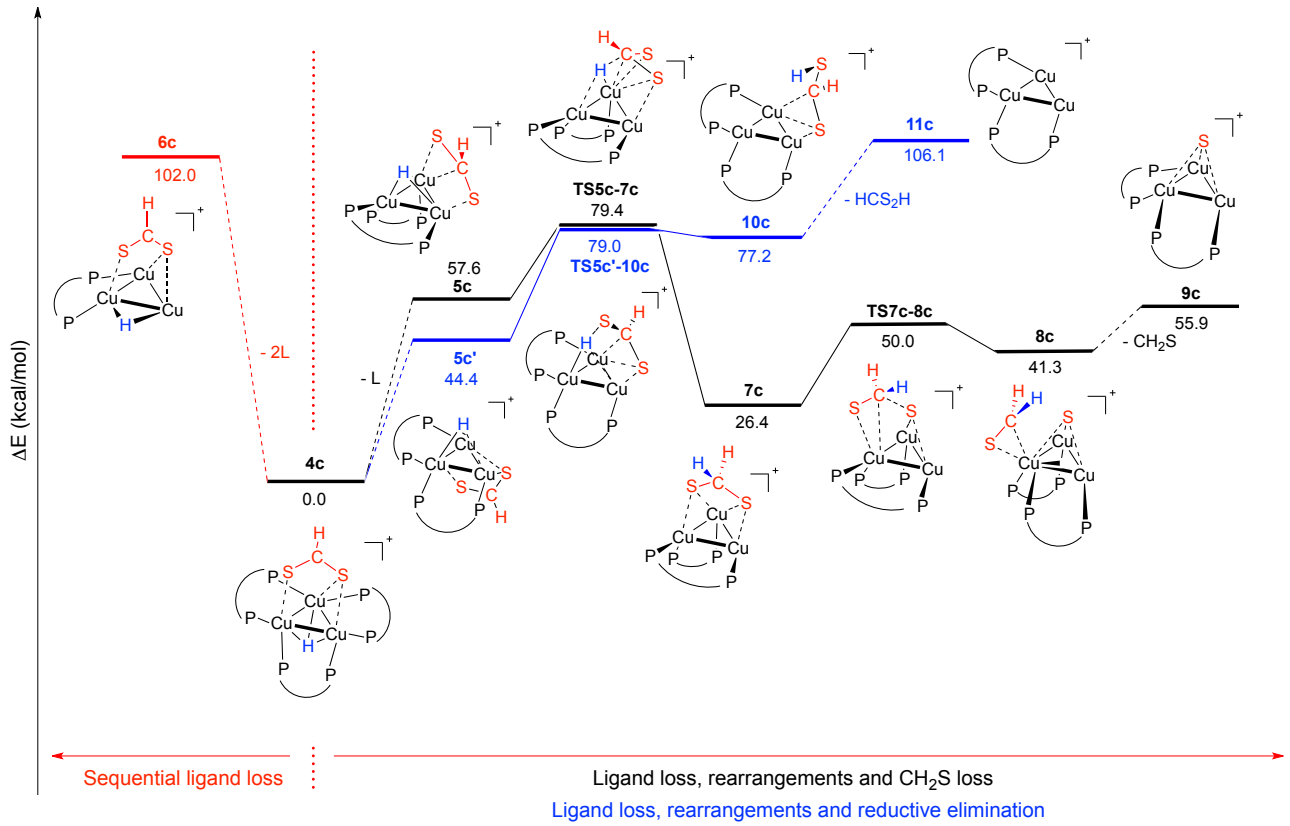
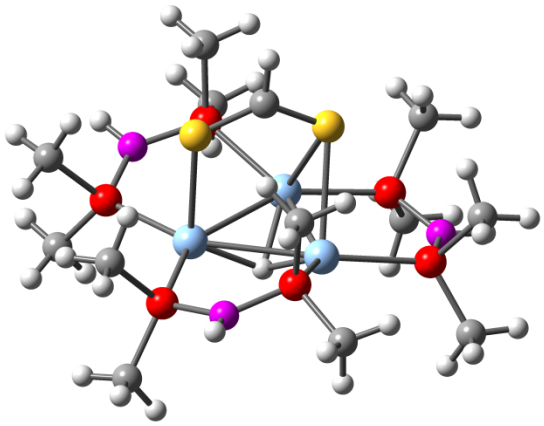


Figure S19. DFT energy surface showing competition between sequential ligand losses, versus ligand loss followed by either CH_2S loss or reductive elimination of HCS_2H from $[Cu_3(H)(S_2CH)L^{Me}_3]^+$, **4c**. Reactant, intermediates and transition states exhibit a wide range of configurations for weak interactions of organic fragments with the Cu_3 core. In view of the complexity of these interactions, bond orders within these fragments are not assigned. Energies (E), in kcal/mol, were calculated at the M06/def2-TZVP//M06/6-31+G(d)/SDD level of theory and are relative to **4c**.

Cartesian coordinates of DFT calculated structures associated with Figure 6

E(B1) = energy of optimized structure for basis set 1 (M06/6-31+G(d))
E(ZPE) = zero-point energy of optimized structure for basis set 1 (M06/6-31+G(d))
E(B2) = single point energy at basis set 2 (M06/def2-TZVP)

$[Ag_3(\mu_3\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_3]^+$ (4d)



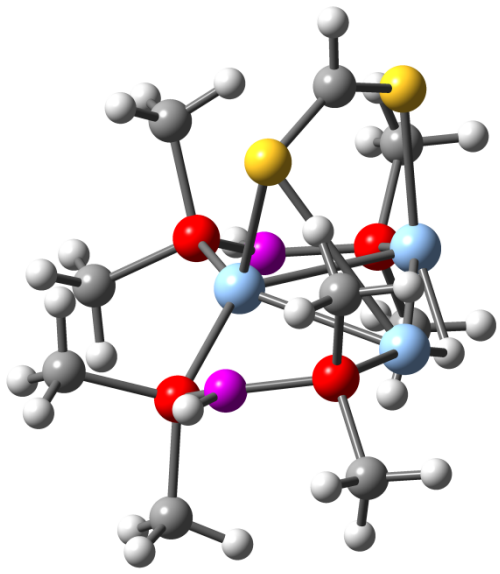
C13H41Ag3N3P6S2(1+)
E(B1) = -3968.629350 Hartrees
E(ZPE) = 0.533350 Hartrees

E(B2) = -3969.267538 Hartrees

Ag	1.625884	0.213336	-0.733484
Ag	-0.749817	-1.521521	-0.455726
Ag	-1.100980	1.330315	-0.412485
P	3.154693	-1.822430	-0.919402
P	0.767411	-3.373926	0.209453
P	2.636410	2.545709	-0.931362
P	-3.228434	-1.931251	-0.692130
P	-3.611572	1.109027	-0.640477
P	-0.055411	3.506192	0.164816
S	1.841202	0.236814	2.013322
S	-1.205907	-0.127443	2.068052
N	2.365561	-3.262035	-0.399216
N	-4.161643	-0.502135	-0.885532
N	1.508033	3.769727	-0.490544
H	1.897883	4.705283	-0.351070
C	-4.513803	1.648425	0.864024
C	4.599629	-1.736188	0.209653
C	0.118049	3.840256	1.958526
C	0.261126	-5.039936	-0.363002
C	-3.895478	-3.005736	-2.017141
C	0.337996	0.027199	2.732068
C	3.371786	3.256504	-2.453355
C	4.006097	2.809787	0.262380
C	-0.937588	5.012641	-0.391114
C	3.967493	-2.375497	-2.467685
C	0.970253	-3.668618	2.006007
C	-3.950222	-2.726599	0.796239
C	-4.526594	2.023647	-1.937099
H	0.358743	-0.013753	3.828864
H	-5.176141	-0.629612	-0.920052
H	2.968987	-4.071189	-0.234510
H	-0.134339	0.007226	-1.531471
H	5.274570	-0.934451	-0.118657
H	4.259898	-1.506677	1.227918
H	5.163809	-2.679940	0.219638
H	4.543716	-3.297594	-2.307403
H	3.212825	-2.554836	-3.241232
H	4.651289	-1.594121	-2.823710
H	0.981088	-5.814115	-0.061400
H	-0.714112	-5.284369	0.080522
H	0.159959	-5.049108	-1.454166
H	1.446819	-2.792970	2.464778
H	-0.016259	-3.806163	2.470213
H	1.584941	-4.559064	2.198853
H	-3.498830	-3.719717	0.932589
H	-3.719695	-2.124286	1.684443
H	-5.039857	-2.844454	0.710068
H	-3.466487	-4.011512	-1.914302
H	-4.990005	-3.087283	-1.956377
H	-3.617833	-2.608376	-2.999404
H	-4.153011	1.745709	-2.928585
H	-5.605696	1.820264	-1.888142

H -4.369979 3.101405 -1.795385
H -4.304016 2.710631 1.053875
H -5.600269 1.518301 0.756974
H -4.165134 1.074174 1.731932
H 0.542760 4.837366 2.141290
H -0.867205 3.775076 2.440925
H 0.768706 3.078803 2.408596
H -1.071424 4.990690 -1.478507
H -1.928041 5.042266 0.083256
H -0.395365 5.927765 -0.112843
H 4.344074 3.856057 0.268556
H 3.673463 2.530951 1.270474
H 4.858385 2.171318 -0.006693
H 4.229232 2.646873 -2.766219
H 2.632217 3.256844 -3.261316
H 3.719780 4.285464 -2.284510

$[Ag_3(\mu_2\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (5d)

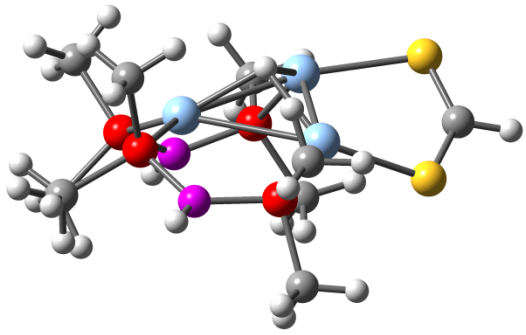


C9H28Ag3N2P4S2(1+)
E(B1) = -3071.237009 Hartrees
E(ZPE) = 0.365242 Hartrees
E(B2) = -3071.72793 Hartrees

Ag 2.156926 0.387158 0.117955
Ag -0.098742 -1.431077 0.712408
Ag -0.680404 1.311221 0.109367
P 3.332035 -1.801328 -0.069285
P 0.870453 -3.586628 -0.212097
P 2.415210 2.632304 -1.015234
P -0.127997 3.686608 0.291894
S 1.888983 1.261167 2.548285
S 0.500621 -1.415775 3.195653

N	2.511218	-3.212432	-0.588039
N	1.487393	3.861854	-0.246281
H	1.842841	4.817155	-0.326553
C	4.107226	-2.230095	1.531716
C	-0.130999	4.480243	1.932536
C	0.337224	-4.476769	-1.718067
C	1.288053	0.024722	3.528902
C	2.163925	2.919209	-2.807573
C	4.103867	3.283003	-0.750372
C	-1.071450	4.874644	-0.728902
C	4.773701	-1.802980	-1.195248
C	1.010050	-4.959323	0.994458
H	1.443224	0.204335	4.600096
H	3.114354	-4.007254	-0.816039
H	-1.068135	-0.336599	-0.409056
H	4.749154	-1.402817	1.864225
H	3.324078	-2.373081	2.287622
H	4.710285	-3.145178	1.451321
H	5.325697	-2.751863	-1.135459
H	4.448201	-1.639991	-2.228482
H	5.455066	-0.991981	-0.907820
H	1.023222	-5.303509	-1.950025
H	-0.667127	-4.890956	-1.565237
H	0.303700	-3.786676	-2.567702
H	1.449203	-4.586957	1.928571
H	0.013284	-5.358119	1.222791
H	1.630985	-5.777836	0.604060
H	0.271337	5.500594	1.868335
H	-1.156393	4.529671	2.319595
H	0.480878	3.890458	2.625359
H	-1.049885	4.566889	-1.781071
H	-2.117430	4.903395	-0.398789
H	-0.651196	5.886129	-0.640878
H	4.201615	4.314257	-1.118581
H	4.345917	3.254937	0.319115
H	4.825004	2.655834	-1.289471
H	2.826828	2.267812	-3.391798
H	1.127456	2.676939	-3.075677
H	2.368757	3.966201	-3.069953

$[Ag_3(\mu_3\text{-}H)(\mu_1,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (5d')

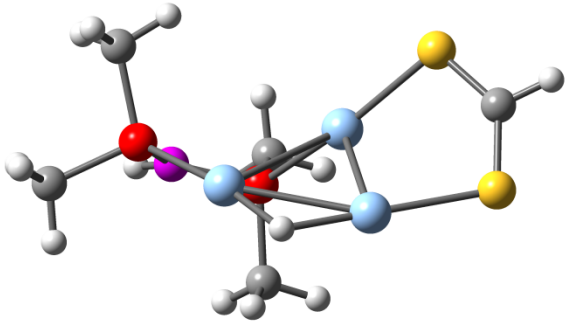


C9H28Ag3N2P4S2(1+)
E(B1) = -3071.232516 Hartrees

E(ZPE) = 0.364511 Hartrees
E(B2) = -3071.723029 Hartrees

Ag	2.695095	0.346016	0.226101
Ag	1.136925	-1.207605	2.199082
Ag	0.140234	1.339957	1.421824
P	3.401525	-1.813094	-0.845578
P	1.245670	-3.230556	0.751002
P	3.091534	2.668567	-0.701786
P	0.256758	3.453014	0.110418
S	-0.726646	-1.660929	3.877851
S	-2.102530	0.382759	2.000219
N	2.228854	-3.047035	-0.652811
N	1.650786	3.581759	-0.891834
H	1.757455	4.469069	-1.390341
C	4.964942	-2.523936	-0.203644
C	0.293922	4.975360	1.129456
C	-0.417542	-3.555163	0.069564
C	-1.992078	-0.785711	3.220055
C	3.878985	2.917592	-2.333520
C	4.159389	3.685981	0.387694
C	-1.095175	3.829922	-1.057979
C	3.679394	-1.861818	-2.652205
C	1.718653	-4.872926	1.403735
H	-2.968190	-1.010551	3.667382
H	2.318759	-3.858747	-1.267644
H	1.863792	0.547802	1.973078
H	5.804431	-1.846810	-0.409209
H	4.888686	-2.652809	0.883784
H	5.173622	-3.499043	-0.665067
H	3.974431	-2.866163	-2.987173
H	2.770639	-1.558008	-3.183631
H	4.485694	-1.163654	-2.910544
H	-0.414025	-4.393907	-0.639992
H	-1.098547	-3.789830	0.898829
H	-0.790344	-2.653562	-0.431276
H	2.759808	-4.860959	1.747244
H	1.076391	-5.115886	2.260382
H	1.597350	-5.657035	0.643267
H	0.355298	5.874084	0.499827
H	-0.619767	5.034758	1.734818
H	1.153198	4.953294	1.810427
H	-1.178251	3.037430	-1.809297
H	-2.041763	3.884206	-0.505273
H	-0.928556	4.791801	-1.562869
H	4.248032	4.713997	0.009672
H	3.729720	3.709760	1.397464
H	5.163056	3.246136	0.456723
H	4.886202	2.482333	-2.318364
H	3.294518	2.421848	-3.116609
H	3.972392	3.985410	-2.577080

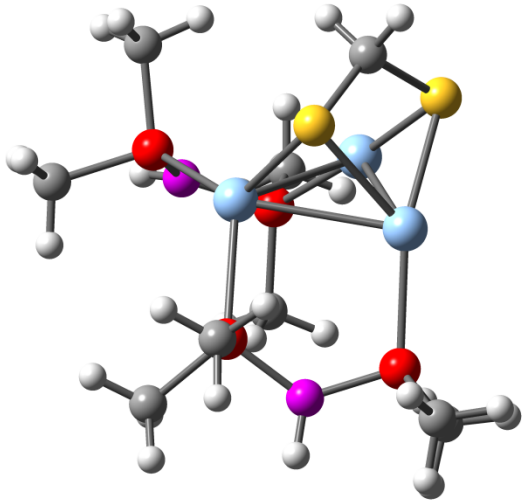
$[Ag_3(\mu_2\text{-}H)(\mu_1,\mu_1\text{-}S_2CH)(L^{Me})]^+$ (6d)



C5H15Ag3NP2S2(1+)
E(B1) = -2173.845438 Hartrees
E(ZPE) = 0.196414 Hartrees
E(B2) = -2174.18814 Hartrees

Ag	1.444670	-0.588321	-1.372034
Ag	0.789391	-1.322538	1.580078
Ag	-0.921685	0.396831	-0.181499
P	3.328956	-2.117038	-1.166591
P	1.358379	-3.517435	0.677710
S	0.445652	0.436057	3.225576
S	-2.279592	0.776181	1.796042
N	2.763928	-3.484037	-0.304740
C	4.823428	-1.558432	-0.285171
C	0.069857	-4.342595	-0.315355
C	-1.157270	0.916896	3.036083
C	3.989565	-2.838526	-2.703588
C	1.785885	-4.773497	1.925811
H	-1.551007	1.433411	3.920283
H	3.291996	-4.353442	-0.396286
H	0.001756	0.389517	-1.708501
H	5.292840	-0.730622	-0.831768
H	4.553280	-1.201917	0.716079
H	5.547695	-2.378477	-0.191828
H	4.743183	-3.606400	-2.480751
H	3.182578	-3.283613	-3.295598
H	4.467699	-2.052271	-3.300331
H	0.423245	-5.316946	-0.678132
H	-0.827802	-4.494597	0.298178
H	-0.204257	-3.717419	-1.174099
H	2.620802	-4.429637	2.545690
H	0.919812	-4.948838	2.575355
H	2.053431	-5.724922	1.445417

$[Ag_3(\mu_2,\mu_2\text{-}S_2CH_2)(L^{Me})_2]^+$ (7d)

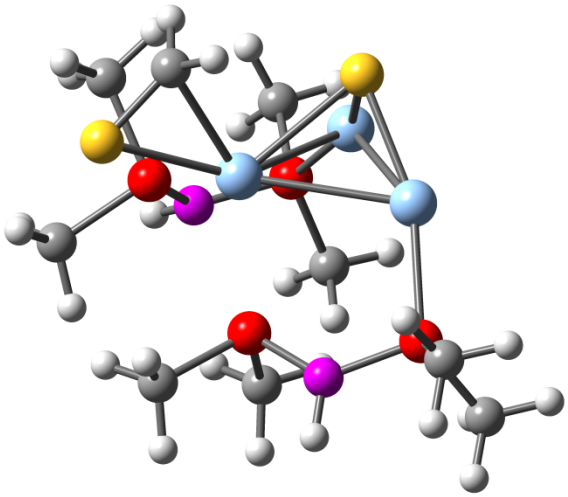


C9H28Ag3N2P4S2(1+)
E(B1) = -3071.267230 Hartrees
E(ZPE) = 0.370947 Hartrees
E(B2) = -3071.756824 Hartrees

Ag	2.807739	0.343633	0.980390
Ag	0.380341	-1.454993	1.588149
Ag	0.277913	1.582047	2.121392
P	3.683645	-1.874609	0.248658
P	0.845650	-2.639144	-0.474487
P	2.563306	2.344441	-0.606638
P	-0.337524	2.883270	0.173647
S	2.574071	1.261391	3.321010
S	0.005587	-0.418640	3.721979
N	2.537497	-2.832962	-0.609390
N	0.946870	2.831928	-0.972903
H	0.861744	3.492265	-1.750201
C	4.316622	-2.978656	1.561469
C	-0.640976	4.671479	0.414483
C	0.318676	-1.874802	-2.048081
C	1.744945	-0.086056	4.253080
C	3.276169	2.335389	-2.293538
C	3.354599	3.830631	0.120052
C	-1.778138	2.387765	-0.834741
C	5.080170	-1.828262	-0.930406
C	0.223950	-4.347067	-0.623826
H	2.333894	-1.009128	4.215699
H	2.884286	-3.614425	-1.167918
H	1.680854	0.231893	5.300790
H	5.109325	-2.465970	2.122237
H	3.502626	-3.210170	2.260182
H	4.715721	-3.915078	1.148214
H	5.388915	-2.838943	-1.232625
H	4.798585	-1.253072	-1.820626
H	5.937778	-1.336586	-0.454341
H	0.646032	-2.477141	-2.906201
H	-0.774556	-1.779404	-2.073690
H	0.758280	-0.871732	-2.123963
H	0.539634	-4.941976	0.240154

H -0.872244 -4.336051 -0.655274
H 0.591278 -4.818178 -1.546307
H -0.813208 5.175470 -0.547187
H -1.524804 4.817287 1.048168
H 0.218734 5.132269 0.915488
H -1.686682 1.329671 -1.106193
H -2.697696 2.517608 -0.250539
H -1.851646 2.991333 -1.750176
H 3.203614 4.716681 -0.512643
H 2.933185 4.019126 1.116508
H 4.432240 3.657714 0.243072
H 4.353669 2.139633 -2.223510
H 2.817201 1.542971 -2.896292
H 3.137646 3.300964 -2.800935

$[Ag_3(\mu_3\text{-}S)(\kappa^2\text{-}SCH_2)(L^{Me})_2]^+$ (8d)

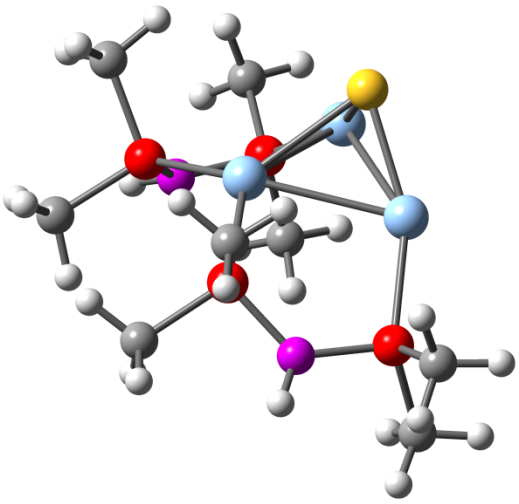


C9H28Ag3N2P4S2(1+)
E(B1) = -3071.238282 Hartrees
E(ZPE) = 0.369038 Hartrees
E(B2) = -3071.729557 Hartrees

Ag 2.016099 0.434954 1.750827
Ag 0.001643 -1.615365 0.967006
Ag -0.726728 1.556185 1.580006
P 3.372156 -1.572205 0.467795
P 0.972771 -2.932878 -0.807356
P 2.184930 2.209886 -0.139935
P -0.534281 3.536291 0.217888
S 4.237289 0.908609 3.116567
S -0.184636 -0.309902 2.942101
N 2.628888 -2.498302 -0.806547
N 1.115388 3.563488 -0.245027
H 1.398188 4.313034 -0.881118
C 3.857123 -2.831259 1.715931
C -0.788145 5.180965 0.964256
C 0.487273 -2.779170 -2.560781
C 2.965912 0.329143 4.005338
C 2.008830 1.401067 -1.782849
C 3.801705 3.046797 -0.307182
C -1.460424 3.674328 -1.353192

C	4.999639	-1.245911	-0.315242
C	0.969527	-4.744874	-0.561032
H	2.836956	-0.736559	4.219628
H	3.251124	-3.122264	-1.327167
H	2.286993	0.995592	4.544790
H	4.542307	-2.374517	2.443739
H	2.968971	-3.182339	2.259190
H	4.359081	-3.689184	1.246767
H	5.515616	-2.179473	-0.582848
H	4.882988	-0.636697	-1.219860
H	5.629512	-0.699908	0.399026
H	1.153592	-3.375153	-3.199488
H	-0.540900	-3.137503	-2.695152
H	0.538243	-1.730441	-2.873739
H	1.358571	-4.983397	0.436080
H	-0.053460	-5.134369	-0.634018
H	1.588950	-5.244904	-1.318748
H	-0.468793	5.973540	0.273571
H	-1.851135	5.323403	1.194501
H	-0.214110	5.261119	1.893485
H	-1.296937	2.778272	-1.963525
H	-2.534757	3.760555	-1.147630
H	-1.140757	4.559710	-1.920038
H	3.851958	3.671835	-1.210095
H	3.993764	3.664474	0.577433
H	4.589551	2.283958	-0.367067
H	2.714116	0.563076	-1.876255
H	0.991441	0.993946	-1.869015
H	2.181484	2.109163	-2.605431

$[Ag_3(\mu_3\text{-}S)(L^{Me})_2]^+$ (9d)

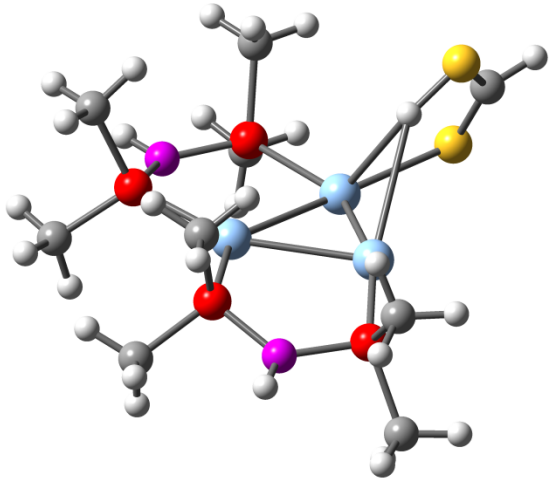


C8H26Ag3N2P4S(1+)
E(B1) = -2633.850227 Hartrees
E(ZPE) = 0.342004 Hartrees
E(B2) = -2634.298311 Hartrees

Ag	-0.000192	0.722948	-0.699838
Ag	-1.700812	-1.657287	-0.805294
Ag	1.695528	-1.660239	-0.813873

P	-2.229142	1.668801	0.121634
P	-3.440905	-1.080656	0.762889
P	2.228540	1.661567	0.129317
P	3.440839	-1.091763	0.751021
S	-0.006163	-1.253194	-2.411442
N	-3.228777	0.600261	1.044845
N	3.227611	0.586798	1.045886
H	3.986292	1.039723	1.561682
C	-3.300010	2.220913	-1.259550
C	5.167675	-1.231572	0.166463
C	-3.535716	-1.769470	2.450787
C	2.251387	3.118674	1.238345
C	-2.253317	3.133474	1.220608
C	-5.169640	-1.226390	0.185463
C	3.300453	2.223553	-1.247101
C	3.542136	-1.792045	2.433783
H	2.577739	-1.683940	2.941150
H	3.792639	-2.858539	2.377396
H	4.317182	-1.279541	3.020247
H	4.277411	2.567529	-0.880053
H	3.446521	1.397453	-1.955597
H	2.813137	3.044508	-1.789930
H	-3.279447	3.450522	1.456144
H	-1.720354	2.914253	2.152782
H	-1.747762	3.966818	0.716458
H	-2.812528	3.038384	-1.807458
H	-3.444975	1.389947	-1.962577
H	-4.277460	2.566872	-0.895711
H	-3.987104	1.056563	1.558141
H	5.866899	-0.783177	0.886069
H	5.432141	-2.288242	0.034394
H	5.273319	-0.727581	-0.801741
H	-4.309236	-1.253659	3.036352
H	-3.785391	-2.836568	2.402626
H	-2.569690	-1.656943	2.954070
H	1.746687	3.955451	0.739020
H	1.716928	2.893065	2.168124
H	3.277191	3.433991	1.477628
H	-5.279160	-0.730579	-0.786503
H	-5.433835	-2.284318	0.063284
H	-5.866618	-0.772509	0.903816

$[Ag_3(\mu_{2,}\mu_1\text{-}HS_2CH)(L^{Me})_2]^+$ (10d)

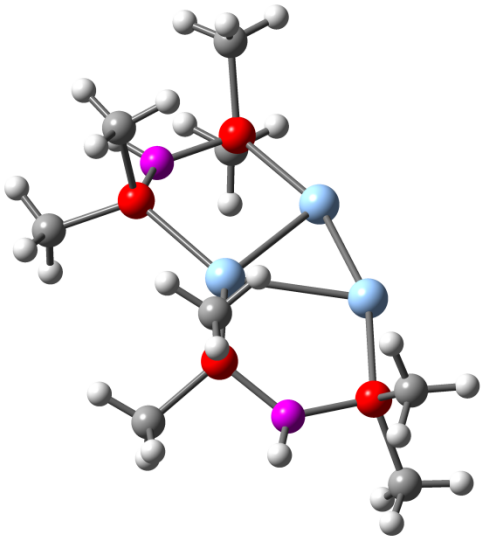


C9H28Ag3N2P4S2(1+)
E(B1) = -3071.195625 Hartrees
E(ZPE) = 0.366253 Hartrees
E(B2) = -3071.690743 Hartrees

Ag	1.940997	0.270621	-0.464981
Ag	-0.094573	-1.156678	0.867521
Ag	-0.125781	1.558105	0.870156
P	3.238747	-1.785757	-1.090109
P	1.025383	-3.394166	0.283502
P	2.689636	2.659958	-0.972874
P	0.149951	3.994707	0.146963
S	-0.350665	-0.629425	4.428669
S	-1.985116	-2.251903	2.421252
N	2.372899	-3.232331	-0.781876
N	1.490098	3.898895	-0.934341
H	1.794471	4.793809	-1.327370
C	4.789583	-1.984373	-0.127473
C	0.629168	5.348066	1.292475
C	0.222169	-4.893542	-0.393824
C	-1.603669	-1.688926	3.920386
C	3.532883	3.098736	-2.538736
C	3.938662	3.194589	0.264379
C	-1.089801	4.842669	-0.899159
C	3.838416	-2.075756	-2.795600
C	1.756619	-4.061773	1.832462
H	-2.219721	-2.003674	4.770286
H	2.874636	-4.097035	-1.000449
H	0.093428	-0.316153	3.160053
H	5.485228	-1.166130	-0.356841
H	4.562221	-1.952608	0.945513
H	5.281516	-2.939675	-0.358722
H	4.350377	-3.045238	-2.876922
H	2.998371	-2.057024	-3.498091
H	4.546676	-1.285182	-3.074447
H	0.928053	-5.733390	-0.466020
H	-0.597458	-5.187136	0.275062
H	-0.196187	-4.687388	-1.384787
H	2.354979	-3.281231	2.321372
H	0.951194	-4.352444	2.521483

H 2.393186 -4.937594 1.642896
H 0.924012 6.249805 0.736645
H -0.215266 5.602586 1.945528
H 1.466617 5.028844 1.924347
H -1.401713 4.182299 -1.715436
H -1.971717 5.095949 -0.297836
H -0.679409 5.769748 -1.324059
H 4.214833 4.248958 0.121806
H 3.530238 3.064481 1.275256
H 4.842366 2.575035 0.181980
H 4.425671 2.471219 -2.653858
H 2.868550 2.918956 -3.390953
H 3.849566 4.152014 -2.543656

$[Ag_3(L^{Me})_2]^+$ (11d)

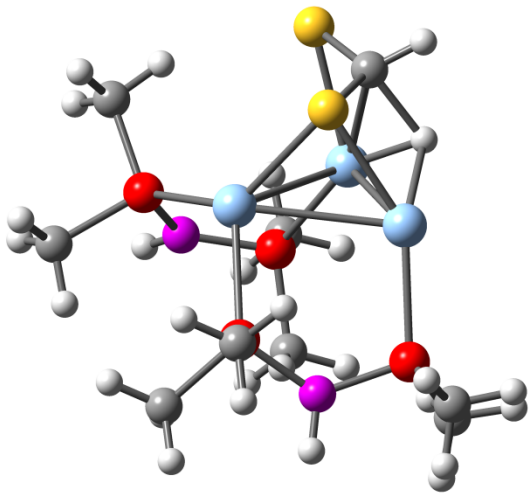


C8H26Ag3N2P4(1+)
E(B1) = -2235.633205 Hartrees
E(ZPE) = 0.339586 Hartrees
E(B2) = -2236.052144 Hartrees

Ag 2.054921 0.400087 -0.594946
Ag 0.302311 -1.105366 0.988527
Ag -0.023447 1.559506 0.886094
P 3.248119 -1.780702 -0.958732
P 1.076892 -3.473549 0.435699
P 2.690298 2.767822 -1.133484
P 0.168871 3.997248 0.151229
N 2.329437 -3.217465 -0.723721
N 1.454993 3.958182 -0.999366
H 1.707182 4.867766 -1.395122
C 4.644351 -1.920299 0.225275
C 0.674889 5.334761 1.301837
C 0.013927 -4.669318 -0.452714
C 3.399839 3.237495 -2.753118
C 4.000975 3.327475 0.023518
C -1.141547 4.834007 -0.814157
C 4.069716 -2.188137 -2.542157

C	1.873219	-4.561479	1.681194
H	2.793877	-4.069229	-1.050374
H	5.389840	-1.139155	0.022877
H	4.273067	-1.778369	1.248656
H	5.129995	-2.903721	0.153432
H	4.589027	-3.155761	-2.483419
H	3.334833	-2.223360	-3.353638
H	4.810819	-1.413331	-2.773943
H	0.600406	-5.524071	-0.818611
H	-0.762769	-5.044910	0.224941
H	-0.472002	-4.177889	-1.302357
H	2.644271	-4.005412	2.227653
H	1.126988	-4.911717	2.405628
H	2.333905	-5.438002	1.203731
H	0.909454	6.259927	0.756241
H	-0.135294	5.544403	2.011691
H	1.557397	5.023502	1.873732
H	-1.481230	4.181110	-1.625269
H	-1.995927	5.055611	-0.162701
H	-0.775496	5.778258	-1.241632
H	4.239506	4.389477	-0.129275
H	3.660282	3.182156	1.057179
H	4.913032	2.732667	-0.121761
H	4.298223	2.637916	-2.944145
H	2.675724	3.045495	-3.552319
H	3.683196	4.299971	-2.771247

$[Ag_3(\mu_2\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (TS5d-7d)



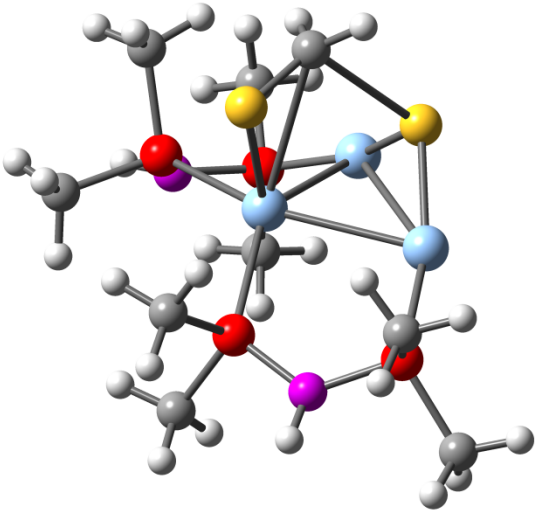
C9H28Ag3N2P4S2(1+)
E(B1) = -3071.179028 Hartrees
E(ZPE) = 0.363580 Hartrees
E(B2) = -3071.66913 Hartrees

Ag	3.099851	0.402744	1.168753
Ag	0.683987	-1.288191	2.076267
Ag	0.567148	1.724780	2.228036
P	3.777714	-1.830017	0.228384
P	0.779913	-2.288207	-0.091902
P	2.744255	2.254984	-0.589742
P	-0.143708	2.848143	0.211735

S	2.580053	1.072509	3.584873
S	2.125129	-1.963922	4.083271
N	2.412508	-2.598045	-0.494251
N	1.089980	2.609636	-0.962781
H	0.951523	3.118339	-1.840671
C	4.535604	-3.104034	1.292053
C	-0.414306	4.657776	0.246534
C	0.107791	-1.377992	-1.529950
C	1.545178	-0.333624	4.134295
C	3.369044	1.944854	-2.283733
C	3.502875	3.880567	-0.205879
C	-1.635326	2.255102	-0.657441
C	4.937439	-1.784865	-1.189586
C	0.004000	-3.930769	-0.249090
H	0.962311	-0.057713	5.016887
H	2.592712	-3.376111	-1.131124
H	0.146879	-0.015639	3.337704
H	5.492641	-2.732899	1.681342
H	3.876291	-3.295331	2.146961
H	4.710023	-4.032949	0.732221
H	5.105186	-2.789597	-1.602706
H	4.543461	-1.134477	-1.979471
H	5.905077	-1.387887	-0.857853
H	0.324956	-1.908021	-2.467360
H	-0.980146	-1.271897	-1.422799
H	0.556233	-0.374774	-1.567034
H	0.396997	-4.601943	0.522667
H	-1.080147	-3.840166	-0.110991
H	0.193553	-4.361815	-1.242188
H	-0.624582	5.042391	-0.761382
H	-1.267821	4.893451	0.894721
H	0.470519	5.164301	0.649217
H	-1.578678	1.167974	-0.784044
H	-2.524440	2.487696	-0.058269
H	-1.738182	2.732423	-1.641877
H	3.254975	4.630439	-0.970247
H	3.150120	4.227961	0.774010
H	4.594708	3.778041	-0.148912
H	4.455357	1.793914	-2.243139
H	2.905826	1.038613	-2.693773
H	3.167038	2.789562	-2.957861

Imaginary Vibrational Frequency = -967.1084 cm-1

$[Ag_3(\mu_2\text{-}S)(\kappa_2\text{-}SCH_2)(L^{Me})_2]^+$ (TS7d-8d)



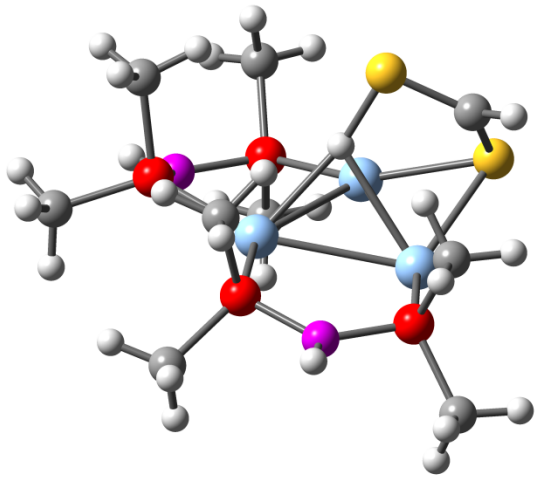
C9H28Ag3N2P4S2(1+)
E(B1) = -3071.231187 Hartrees
E(ZPE) = 0.369893 Hartrees
E(B2) = -3071.721118 Hartrees

Ag	1.763336	0.258822	0.636801
Ag	-0.047633	-2.026016	0.786829
Ag	-0.786086	1.565117	1.251588
P	3.271994	-1.725665	0.150239
P	1.051780	-3.606013	-0.678034
P	2.095696	2.390599	-0.715098
P	-0.485795	3.718163	0.221344
S	2.876071	1.217459	2.968129
S	-0.514497	-0.436102	2.464453
N	2.661015	-3.024699	-0.812100
N	0.852612	3.577030	-0.839819
H	1.097688	4.421811	-1.363325
C	3.917639	-2.519195	1.671042
C	-0.016688	5.026740	1.409046
C	0.548006	-3.902140	-2.406291
C	1.866863	0.156841	3.744767
C	2.569382	2.188289	-2.472324
C	3.533403	3.324687	-0.066949
C	-1.723194	4.552155	-0.827196
C	4.821338	-1.327505	-0.736405
C	1.239048	-5.303315	-0.024762
H	1.962814	-0.924384	3.635578
H	3.352282	-3.679383	-1.185656
H	1.216067	0.483101	4.558412
H	4.377981	-1.754219	2.312176
H	3.089114	-2.976694	2.228460
H	4.662242	-3.292759	1.437890
H	5.491468	-2.195500	-0.813724
H	4.595536	-0.956279	-1.742413
H	5.343412	-0.538291	-0.178079
H	1.271266	-4.554634	-2.914040
H	-0.436446	-4.385939	-2.425839
H	0.481741	-2.951197	-2.945307
H	1.670837	-5.264560	0.982605
H	0.258210	-5.790394	0.040734

H 1.887692 -5.908697 -0.673068
H 0.293286 5.942616 0.887008
H -0.863900 5.262442 2.065657
H 0.810841 4.668233 2.034899
H -2.022742 3.897851 -1.652537
H -2.610571 4.790008 -0.228194
H -1.319803 5.489402 -1.235169
H 3.754554 4.204980 -0.686632
H 3.333635 3.647043 0.962949
H 4.418216 2.672746 -0.050316
H 3.484483 1.584851 -2.535022
H 1.771677 1.677341 -3.022311
H 2.765646 3.160568 -2.946107

Imaginary Vibrational Frequency = -49.0669 cm-1

$[Ag_3(\mu_2\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (TS5d'-10d)



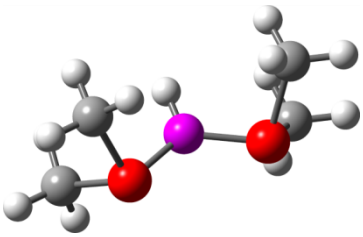
C9H28Ag3N2P4S2(1+)
E(B1) = -3071.189750 Hartrees
E(ZPE) = 0.362551 Hartrees
E(B2) = -3071.683373 Hartrees

Ag 1.868637 0.196969 -0.443940
Ag 0.034217 -1.551941 0.961693
Ag -0.596571 1.238321 0.610291
P 3.257592 -1.893664 -0.785772
P 0.915453 -3.656353 0.098957
P 2.520891 2.570856 -1.026499
P -0.114824 3.620469 0.174180
S 1.499527 0.364356 3.257934
S -1.357213 -0.272898 2.653607
N 2.334568 -3.347583 -0.821370
N 1.286283 3.750683 -0.811135
H 1.574917 4.710366 -1.019783
C 4.365840 -2.078875 0.665479
C 0.308881 4.540965 1.700958
C -0.098140 -4.641360 -1.057349
C -0.161377 0.667186 3.414850
C 3.225712 3.125098 -2.622144
C 3.833612 3.077883 0.151877
C -1.260725 4.770678 -0.661922

C	4.402770	-2.217240	-2.176939
C	1.453743	-4.919453	1.309656
H	-0.477211	1.607397	3.875531
H	2.848370	-4.179220	-1.122367
H	1.402278	0.148300	1.680910
H	5.087275	-1.250811	0.697807
H	3.765018	-2.038527	1.584534
H	4.915395	-3.030195	0.635901
H	4.922955	-3.178032	-2.053231
H	3.856187	-2.222646	-3.126229
H	5.157133	-1.421935	-2.214071
H	0.467795	-5.505429	-1.432405
H	-0.995815	-5.006228	-0.543080
H	-0.407118	-4.019306	-1.904124
H	2.167252	-4.478545	2.016371
H	0.587646	-5.279136	1.879263
H	1.925019	-5.776173	0.807089
H	0.683419	5.548714	1.471268
H	-0.581037	4.631118	2.337768
H	1.074713	3.989287	2.261446
H	-1.533533	4.381638	-1.648531
H	-2.173244	4.876525	-0.062641
H	-0.804447	5.763883	-0.778455
H	4.066532	4.147927	0.058171
H	3.504702	2.870304	1.178729
H	4.749207	2.500995	-0.037445
H	4.128661	2.543338	-2.844888
H	2.500867	2.968235	-3.428148
H	3.499712	4.189375	-2.587931

Imaginary Vibrational Frequency = -422.8989 cm-1

dmpa (L)

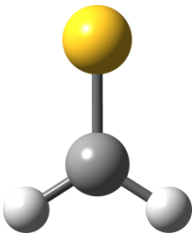


C4P2N1H13
E(B1) = -897.3386603 Hartrees
E(ZPE) = 0.166819 Hartrees
E(B2) = -897.4793544 Hartrees

P	-1.514234	0.041894	-0.566033
P	1.514234	0.041894	-0.566033
N	-0.000000	0.269670	0.234479
C	2.158726	-1.463744	0.311565
C	-2.158726	-1.463744	0.311565
C	2.525769	1.293255	0.351730
C	-2.525769	1.293255	0.351730
H	-2.218648	2.304552	0.061210

H -3.587846 1.170676 0.101551
H -2.412930 1.190167 1.441880
H -0.000000 0.261371 1.258857
H 3.205753 -1.647661 0.034952
H 2.101247 -1.355542 1.405572
H 1.571427 -2.342196 0.015456
H 2.218648 2.304552 0.061211
H 2.412929 1.190167 1.441881
H 3.587846 1.170676 0.101551
H -3.205753 -1.647661 0.034952
H -1.571427 -2.342196 0.015457
H -2.101247 -1.355541 1.405573

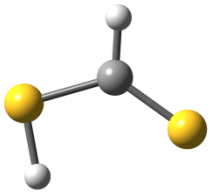
CH_2S



SCH2
E(B1) = -437.370712 Hartrees
E(ZPE) = 0.024638 Hartrees
E(B2) = -437.4122528 Hartrees

S 0.000000 -0.000000 0.586843
C 0.000000 0.000000 -1.026553
H 0.000000 0.924351 -1.615083
H -0.000000 -0.924351 -1.615083

HCS_2H



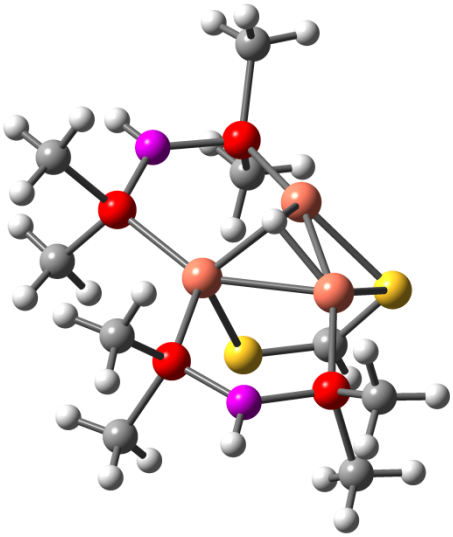
CH2S2
E(B1) = -835.545198 Hartrees
E(ZPE) = 0.026242 Hartrees
E(B2) = -835.6168508 Hartrees

S -0.380438 -0.583182 4.412376
S -1.977954 -2.220022 2.415348
C -1.623835 -1.693311 3.913300
H -2.192211 -2.027770 4.789968
H 0.108695 -0.365796 3.169653

Cartesian coordinates of DFT calculated structures associated with reductive elimination channel shown in Figure S14.[ξ]

E(B1) = energy of optimized structure for basis set 1 (M06/6-31+G(d))
E(ZPE) = zero-point energy of optimized structure for basis set 1 (M06/6-31+G(d))
E(B2) = single point energy at basis set 2 (M06/def2-TZVP)

$[Cu_3(\mu_3\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (5c')



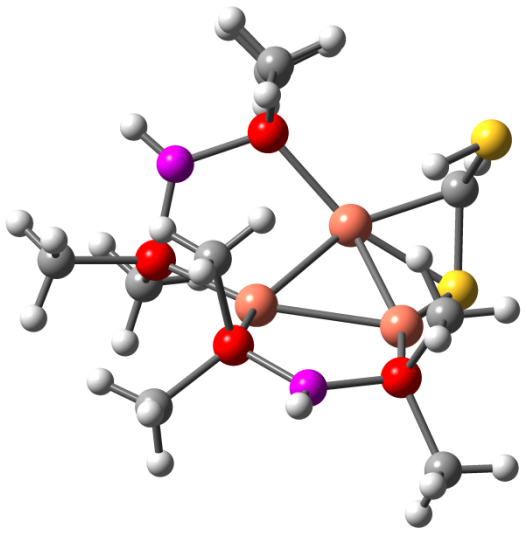
C9H28Cu3N2P4S2(1+)
E(B1) = -3222.435074 Hartrees
E(ZPE) = 0.367730 Hartrees
E(B2) = -7552.130735 Hartrees

Cu	0.001938	0.873387	0.365018
Cu	1.155608	-1.240353	1.177584
Cu	-1.250930	-1.206756	1.116622
P	2.018052	1.957048	0.235463
P	3.286377	-0.764498	0.768557
P	-1.980130	2.000843	0.121211
P	-3.347355	-0.681761	0.598358
S	-0.043083	-3.019158	0.004786
S	0.045717	-0.482084	-1.702573
N	3.367191	0.932179	0.542503
N	-3.371318	1.014254	0.356143
H	-4.275802	1.437986	0.137542
C	2.367815	3.404601	1.298172
C	-4.739560	-0.948706	1.748359
C	3.990081	-1.473206	-0.763798
C	0.013265	-2.145225	-1.447082
C	-2.237716	2.680008	-1.561441
C	2.386209	2.633259	-1.427462
C	4.612537	-1.073266	1.984468
C	-2.348342	3.461583	1.159556

[ξ] Note all structures associated with the ligand loss channels and CH_2S extrusion reaction are given in the SI associated with reference 14.

C	-3.985519	-1.387045	-0.963127
H	-3.276979	-1.165907	-1.771292
H	-4.074898	-2.477239	-0.869896
H	-4.968777	-0.970004	-1.220521
H	-3.334453	3.885437	0.924259
H	-2.320241	3.183590	2.218875
H	-1.586520	4.232325	0.981564
H	3.398341	3.058383	-1.480019
H	2.290506	1.838411	-2.178059
H	1.664826	3.424959	-1.670917
H	1.633133	4.193022	1.086718
H	2.280889	3.123455	2.353430
H	3.373612	3.807059	1.114185
H	4.292984	1.332233	0.374279
H	0.030383	-2.759903	-2.354899
H	-5.666724	-0.514108	1.349950
H	-4.895707	-2.025184	1.890327
H	-4.518648	-0.495819	2.720694
H	5.001382	-1.088463	-0.954806
H	4.036143	-2.566978	-0.681703
H	3.341814	-1.216299	-1.611277
H	-1.479802	3.447919	-1.767122
H	-2.126284	1.878974	-2.303230
H	-3.232003	3.135776	-1.669725
H	4.353211	-0.625186	2.949459
H	4.739336	-2.154152	2.121821
H	5.566817	-0.654128	1.636587
H	-0.051633	-0.182753	1.852195

$[Cu_3(\mu_2,\mu_1\text{-}HS_2CH)(L^{Me})_2]^+$ (10c)

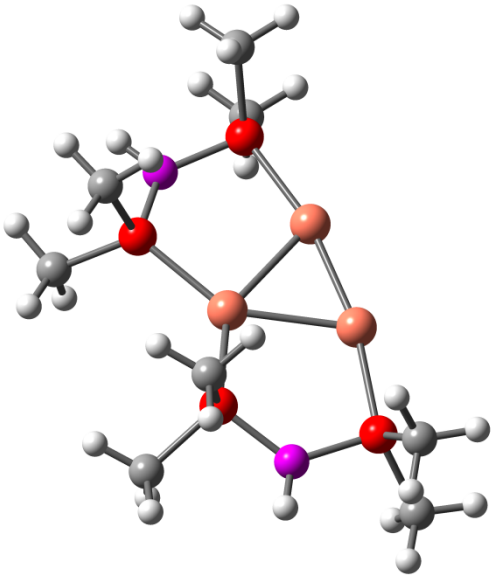


C9H28Cu3N2P4S2(1+)
E(B1) = -3222.379509 Hartrees
E(ZPE) = 0.368413 Hartrees
E(B2) = -7552.078461 Hartrees

Cu	0.007469	0.992825	-0.767003
Cu	1.122447	-1.216020	-0.670842
Cu	-1.416735	-1.179127	-0.932187

P	1.988605	2.140666	-0.909087
P	2.656147	-0.344102	0.603055
P	-1.763272	2.041948	0.191538
P	-3.386320	-0.461799	-0.200662
S	0.325095	-3.679591	1.088096
S	-0.054379	-2.694688	-1.819681
N	2.881329	1.335492	0.325840
N	-3.269035	1.218853	0.116688
H	-4.074548	1.674391	0.551079
C	2.204670	3.887017	-0.398142
C	-3.867339	-1.213057	1.396830
C	4.321932	-1.057065	0.381727
C	1.001240	-3.237528	-0.500909
C	-2.269104	3.759956	-0.181993
C	3.046326	2.049959	-2.402428
C	2.386409	-0.499485	2.398780
C	-1.373660	2.153530	1.982917
C	-4.923137	-0.590089	-1.175305
H	-4.790685	-0.112295	-2.151742
H	-5.166388	-1.647830	-1.333651
H	-5.761550	-0.111490	-0.650677
H	-2.184144	2.631476	2.550280
H	-1.208367	1.142141	2.377987
H	-0.449585	2.732040	2.127374
H	4.054772	2.435160	-2.197772
H	3.118479	1.005462	-2.732044
H	2.603240	2.633463	-3.219694
H	1.746337	4.544197	-1.147703
H	1.706815	4.054907	0.564592
H	3.264693	4.161794	-0.304289
H	3.755287	1.759639	0.643258
H	1.835081	-3.867649	-0.809704
H	-4.780122	-0.751148	1.797538
H	-4.044517	-2.287598	1.260093
H	-3.055161	-1.089598	2.124319
H	5.064712	-0.552134	1.015198
H	4.287534	-2.120015	0.654015
H	4.628178	-0.977976	-0.668224
H	-1.407999	4.425266	-0.036254
H	-2.599410	3.840616	-1.223240
H	-3.080535	4.095464	0.479358
H	1.447185	-0.005269	2.674929
H	2.316682	-1.563742	2.662263
H	3.212207	-0.041138	2.959192
H	-0.192537	-2.446323	1.369826

$[Cu_3(L^{Me})_2]^+$ (11c)

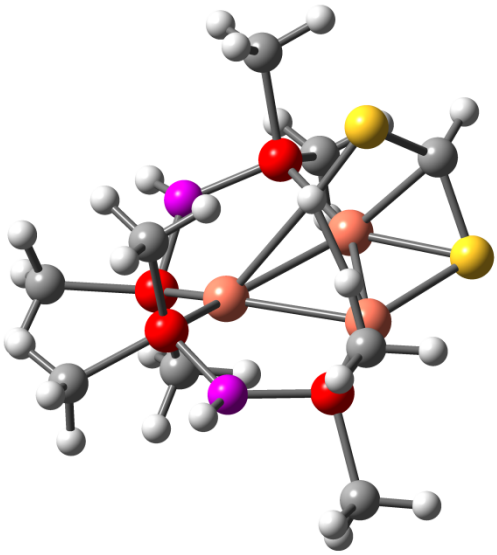


C8H26Cu3N2P4(1+)
E(B1) = -2386.795804 Hartrees
E(ZPE) = 0.341163 Hartrees
E(B2) = -6716.415477 Hartrees

Cu	-0.136520	1.070188	-0.053111
Cu	0.913254	-0.997553	0.693081
Cu	-1.453330	-0.887317	0.560179
P	1.946500	1.962752	-0.181358
P	3.184316	-0.725289	0.564348
P	-2.106228	2.191555	-0.173877
P	-3.666373	-0.395851	0.217183
N	3.244393	0.831110	-0.173648
N	-3.510554	1.216132	-0.374108
H	-4.382180	1.726373	-0.537596
C	2.253294	3.028982	1.280499
C	-4.836825	-0.230155	1.619268
C	4.298842	-1.692528	-0.515233
C	-2.433579	3.501768	-1.407593
C	2.461858	3.059312	-1.550858
C	4.206462	-0.535171	2.074344
C	-2.381360	3.087701	1.404004
C	-4.727922	-1.163788	-1.058470
H	-4.182356	-1.234323	-2.005506
H	-5.011277	-2.175318	-0.742279
H	-5.644019	-0.577177	-1.214346
H	-3.376450	3.553342	1.430718
H	-2.293458	2.383296	2.241510
H	-1.619995	3.869343	1.532625
H	3.488800	3.424378	-1.405950
H	2.402063	2.527811	-2.506728
H	1.789028	3.925503	-1.589206
H	1.586314	3.901607	1.253328
H	2.042071	2.464025	2.197738
H	3.294513	3.379632	1.308393
H	4.175473	1.230842	-0.316486
H	-5.749908	0.299950	1.313719
H	-5.118363	-1.223061	1.992159
H	-4.360351	0.320536	2.439325

H	5.276037	-1.200406	-0.619165
H	4.455396	-2.688294	-0.082170
H	3.849653	-1.810386	-1.507149
H	-1.680493	4.292841	-1.298917
H	-2.366478	3.092783	-2.421596
H	-3.427944	3.949209	-1.265238
H	3.703526	0.134702	2.782194
H	4.339541	-1.509456	2.561589
H	5.198111	-0.125331	1.836336

$[Cu_3(\mu_3\text{-}H)(\mu_2,\mu_1\text{-}S_2CH)(L^{Me})_2]^+$ (TS5c'-10c)



C9H28Cu3N2P4S2(1+)
E(B1) = -3222.376403 Hartrees
E(ZPE) = 0.364353 Hartrees
E(B2) = -7552.075555 Hartrees

Cu	-0.013559	0.909081	-0.113604
Cu	1.206343	-1.315098	-0.194730
Cu	-1.332806	-1.252611	-0.500624
P	1.910255	2.004903	-0.674452
P	3.174549	-0.500960	0.391783
P	-1.905165	1.951236	0.633155
P	-3.389060	-0.409964	-0.498477
S	0.001924	-2.067710	2.282242
S	-0.107945	-3.148224	-0.520238
N	3.199410	1.193297	0.123910
N	-3.314361	1.247151	-0.052963
H	-4.203132	1.714621	0.140370
C	2.264839	3.739884	-0.203955
C	-4.489278	-1.168045	0.751447
C	4.635755	-1.109389	-0.522965
C	0.674045	-3.038885	1.023164
C	-2.221747	3.729397	0.337488
C	2.371198	2.001473	-2.448450
C	3.685738	-0.684021	2.132471
C	-2.148836	1.833310	2.447768
C	-4.446289	-0.387910	-1.985827
H	-3.932126	0.122449	-2.806990

H	-4.665214	-1.417829	-2.293322
H	-5.395810	0.125629	-1.781285
H	-3.107216	2.277783	2.750553
H	-2.134273	0.779761	2.755995
H	-1.337375	2.353377	2.973870
H	3.390625	2.385866	-2.589814
H	2.315178	0.975991	-2.835647
H	1.674964	2.623307	-3.026093
H	1.572419	4.404864	-0.735659
H	2.121497	3.875536	0.874184
H	3.290920	4.032251	-0.468787
H	4.103297	1.667873	0.165416
H	1.556419	-3.644219	1.230503
H	-5.440031	-0.622402	0.831989
H	-4.700875	-2.208082	0.472627
H	-3.990365	-1.174757	1.728555
H	5.546565	-0.578517	-0.212654
H	4.772411	-2.180608	-0.329335
H	4.487241	-0.969439	-1.600291
H	-1.441149	4.317869	0.836679
H	-2.188447	3.944285	-0.736454
H	-3.196876	4.042735	0.736619
H	2.892807	-0.314078	2.792303
H	3.847060	-1.747430	2.353138
H	4.614796	-0.132512	2.330298
H	-0.208277	-0.887229	1.362728

Imaginary Vibrational Frequency = -519.4424 cm-1