Electronic Supplementary Material (ESI) for Dalton Transactions.

Extending the chemistry of weakly basic ligands: solvates of Ag^+ and Cu^+ stabilized by $[Al\{OC(CF_3)_3\}_4]^-$ anion as model examples in the screening for useful weakly-interacting solvents.

Electronic Supplementary Information

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1. Experimental methods

1.1. Synthetic procedures

Typically, all manipulations have been performed in argon atmosphere in MBraun gloveboxes (<1 ppm O_2, <1 ppm H_2O) or in Schlenk-type glassware. The previously described H-shaped vessels with P4 frit were used as reactors in all solvent-mediated processes.[S1] Unless stated otherwise, all the solvents were dried over P_2O_5 prior to use. We want to stress, that it may happen that the time of pumping of the samples under high vacuum given here may vary depending on the vacuum achieved in the vacuum line, which is difficult to control in the region below 10^{-3} mbar, especially when the sensor is exposed to various chemicals present in the line. Therefore we suggest to treat these values only as a suggestion.

1.1.1. $Cu(SO_2)[Al(OR^F)_4]$ (**IIa**)

The compound was synthesized from the $Cu[Al(OR^F)_4]$ prepared according to the literature procedure.[S2] After obtaining crude $Cu[Al(OR^F)_4]$ contaminated with Cu powder and AgI, the remaining C_6F_{14} has been removed and SO_2 has been condensed on the sample, which resulted in immediate formation of a yellow solution. Removal of SO_2 followed by extraction with C_6F_{14} yielded a yellow solid, which has been further identified as $Cu(SO_2)[Al(OR^F)_4]$. Yield of the recovered product: 40 %.

It has to be noted, that the compound is highly reactive towards traces of moisture. We have observed, that it decomposed (by turning into sticky pulp) upon contact with agate mortar or borosilicate glass capillaries which were not dried via heating under vacuum. This has not been the case for similar Ag compounds including highly reactive Ag^+-I_2 complexes.

In order to obtain the compound without significant Ag impurity, the SO_2 has to be removed before extraction with C_6F_{14} to prevent formation of $Ag(SO_2)[Al(OR^F)_4]$, which we have found to be fairly well soluble in C_6F_{14}, alike its Cu counterpart. However, very poor solubility of the neat $Ag[Al(OR^F)_4]$ in perfluorinated hexane minimizes contamination of the final Cu salt.

$Cu(SO_2)[Al(OR^F)_4]$ can be also obtained in the metathetic reaction between $Ag[Al(OR^F)_4]$ and CuBr in SO_2, though yield and purity are inferior to the product of the previous method.

Upon prolonged pumping of $Cu(SO_2)[Al(OR^F)_4]$ below 10^{-3} mbar the sample turns brown. The product dissolves in C_6F_{14} and it was possible to grow single crystals suitable for structure determination (though their quality was rather poor). Structure solution proved the crystal to be bridged $[Cu\text{-}SO_2\text{-}Cu][Al(OR^F)_4]_2$ (**IIb**). Noteworthy, its solution in C_6F_{14} left for couple of hours turned yellow and white precipitate formed. This is indicative of dissociation of $[Cu\text{-}SO_2\text{-}Cu][Al(OR^F)_4]_2$ into $Cu(SO_2)[Al(OR^F)_4]$ (dissolved in C_6F_{14}) and $Cu[Al(OR^F)_4]$ (precipitate).

1.1.2. $Ag(CH_2Cl_2)[Al(OR^F)_4]$ (**Ia**) and crystals of $[Ag(CH_2Cl_2)_3][Al(OR^F)_4]$(**Ib**) and $[Ag(CH_2Cl_2)_4][Al(OR^F)_4]$ x 0.5 CH_2Cl_2 (**Ic**)

$Ag(CH_2Cl_2)[Al(OR^F)_4]$ can be obtained by dissolving $Ag[Al(OR^F)_4]$ in CH_2Cl_2 followed by drying for 1 hour at 10^{-2} mbar. The sample is homogenous as based on XRDP analysis.

Crystals of $[Ag(CH_2Cl_2)_3][Al(OR^F)_4]$ were obtained from the solution of $Ag[Al(OR^F)_4]$ in the mixture of CH_2Cl_2 and n-C_6H_{14}. Crystals of $[Ag(CH_2Cl_2)_4][Al(OR^F)_4]$ x 0.5 CH_2Cl_2 were grown from the saturated solution of $Ag[Al(OR^F)_4]$ in CH_2Cl_2 slowly cooled to −78°C (dry ice). Handling of crystals of the latter was extremely difficult, as even slight warming of the sample resulted in their immediate dissolution. The microscope plate used to investigate them under microscope was cooled down to −100°C, similarly to all accessories which had contact with these crystals. These conditions provided only several minutes to select and try the crystals on the diffractometer.

1.1.3. $Cu(CH_2Cl_2)_3[AlFAl]$ (**V**)

We have attempted to obtain Cu^+-CH_2Cl_2 complexes *via* ligand exchange between $Cu(N_2O)[Al(OR^F)_4]$[S2] (usually *ca.* 100 mg) and excess of CH_2Cl_2 (typically > 0.5 ml). Upon contact immediate gas evolution ensued and the solution turned cloudy. Crystallization of the product was difficult and only crystals of $Cu(CH_2Cl_2)_3[AlFAl]$ were obtained. The homogeneity of the product could not be confirmed by XRDP owing poor diffraction (probably caused by low crystallinity). However, IR points at the presence of $[AlFAl]^-$ anion.

1.1.4. $[Ag(Cl_3CCN)_2][Al(OR^F)_4]$ (**III**) and $[Cu(Cl_3CCN)_3][Al(OR^F)_4]$ (**IV**)

$[Ag(Cl_3CCN)_2][Al(OR^F)_4]$ has been obtained from $Ag[Al(OR^F)_4]$ dissolved in an excess of Cl_3CCN. Removal of all volatiles from the sample (which required *ca.* 6 hours of pumping below 10^{-2} mbar for 100 mg of the sample) resulted in white crystalline powder well soluble in SO_2. Slow removal of SO_2 yielded crystals suitable for SC-XRD structure determination. Yield of recovered product: 80% for ca. 100 mg of the sample.

$[Cu(Cl_3CCN)_3][Al(OR^F)_4]$ was obtained in metathetic reaction of CuBr (5-fold excess) and $Ag[Al(OR^F)_4]$ performed in Cl_3CCN. 1 hour of enhancement with ultrasounds afforded yellowish solution above solid residues. Double extraction with Cl_3CCN and subsequent removal of the solvent resulted in off-white powder, well soluble in SO_2 (the solution is yellowish). XRDP pattern matches the structure of $[Cu(Cl_3CCN)_3][Al(OR^F)_4]$ with no signs of any contamination. After 1 hour of sonication the yield of the recovered product is 65%. Single crystals were obtained by crystallization in SO_2 in which the compound is well soluble.

1.2. Analytical procedures

1.2.1. FTIR spectroscopy

The FTIR spectra of the solid samples were measured either in transmission or in reflection geometry. For the measurements in transmission mode a Vertex 80v FTIR spectrometer (Bruker) has been used. The samples were placed between the windows made of AgCl. The measurements in reflection geometry were conducted using Nicolet Magna-IR spectrometer with a Diamond-ATR module with ATR corrections applied.

1.2.2. Raman spectroscopy

Raman spectra have been recorded on a Bruker VERTEX 70 spectrometer with RAM II module at 1064 nm (Nd-YAG laser). Samples were closed in a flame-sealed glass capillaries. Samples of solvates including $Cu(SO_2)[Al(OR^F)_4]$ were recorded on a Horiba-Yvon LabRam-HR Raman micro-spectrometer with use of 514.5 nm He-Ar laser (5 mW).

1.2.3. Powder X-ray diffraction

Powder X-ray diffraction (XRDP) patterns of the samples sealed inside quartz capillaries (diameter of 0.5–1 mm) were measured on three diffractometers: Bruker D8 Discover diffractometer (parallel beam; the $CuK_{\alpha1}$ and $CuK_{\alpha2}$ radiation), Panalytical X'Pert Pro diffractometer (parallel beam; the $CoK_{\alpha1}$ and $CoK_{\alpha2}$ radiation) and Stoe Stadi P powder diffractometer using monochromated Mo $K_{\alpha1}$ radiation and PSD or Mythen 1K microstrip X-ray detector. They are marked according to the radiation used.

1.2.4. Single crystal diffraction

The single crystals suitable for structure determination were grown in various ways. The crystals of $Ag(CH_2Cl_2)[Al(OR^F)_4]$, $Cu(SO_2)[Al(OR^F)_4]$, $[Cu\text{-}SO_2\text{-}Cu][Al(OR^F)_4]_2$ were obtained from the solutions in C_6F_{14} by slow removal of the solvent (slow condensation in the other arm of H-vessel). During the measurements the crystals were immersed in the protective perfluorinated oil (Krytox 1531).

Data collection and reduction was performed with one of the two setups: Agilent Supernova X-ray diffractometer with Cu-Kα radiation (microsource) with data reduction performed by CrysAlisPro software (v. 38.43)[S3] or Bruker Smart Apex II Quazar single crystal diffractometer, graphite-monochromated Mo-Kα radiation from microsource, data collection and reduction: APEX v2013.10-0 and SAINT V8.34A; absorption correction: TWINABS 2012/1. Structure solution: SHELXT[S4], refinement against F^2 in Shelxl-2013,[S4] with ShelXle as GUI software.[S5] The disorder of the $–OC(CF_3)_3$ groups was resolved using DSR.[S6] Graphical presentation of crystal structures has been performed with Vesta.[S7]

1.2.5. TGA/DSC

Thermal decomposition was investigated using a combined thermogravimeter (TGA) and differential scanning calorimeter (DSC) from Netzsch – STA 409 PG. The samples were placed inside Al_2O_3 crucibles, and were heated at $5^oC\ min^{-1}$ rate under a constant Ar (99.9999%) flow. The evolved gases were analyzed with a quadrupole mass spectrometer (MS) QMS 403 C (Pfeiffer Vacuum), connected to the TGA/DSC device by a quartz capillary preheated to 200^oC to avoid condensation of low-boiling volatiles. Range of M/Z from 1 to at least 120 was studied.

1.2.6. NMR spectra

NMR spectra were recorded on Bruker AVANCE III HD 300 MHz or 500 MHz. Samples highly susceptible to traces of water (Li, Na, N-compounds, Cl_3CCN solvates) were placed in 4mm air-tight NMR tubes equipped with PTFE valve and dissolved in SO_2. Deuterated solvents (acetone, $CDCl_3$ or CD_2Cl_2) for these compounds were placed in outer, 5mm tube.

It was observed, that in every 19F measurement there is a weak signal ca. 0.8 ppm less negative the main one. We assign it as experimental artifact, since it is present for samples obtained in different ways, with different batches of chemicals with other analyses (IR, XRDP) showing pure products. The position of the signal is not in agreement with e.g. $MOC(CF_3)_3$ which all show higher shifts as compared to $[Al(OR^F)_4]^-$.[S8]

2. Supplementary analytical results

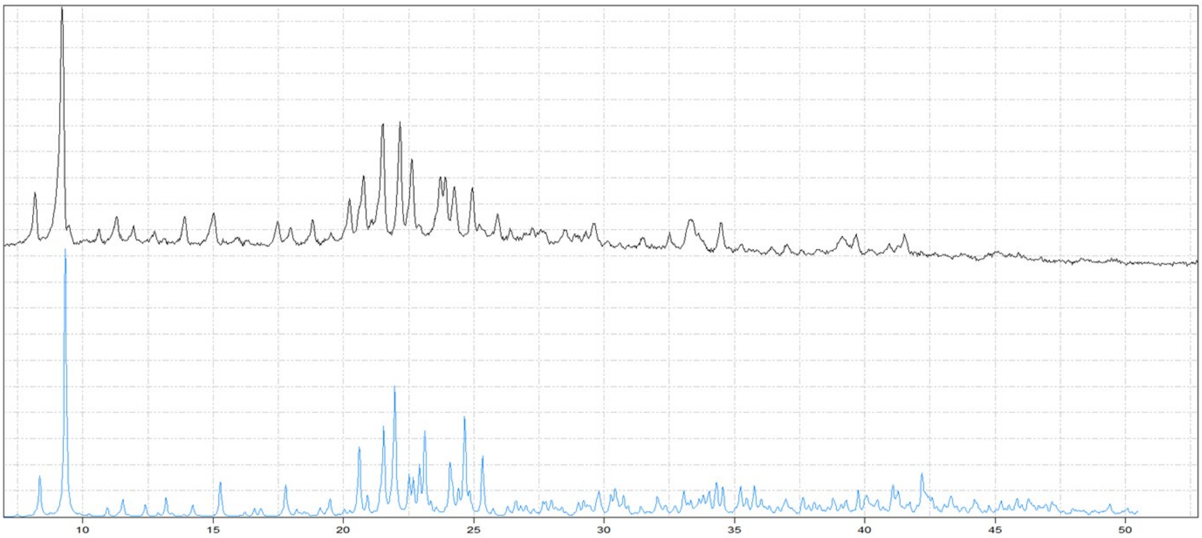


Figure S1. XRDP patterns of $[Ag(Cl_3CCN)_2][Al(OR^F)_4]$: experimental (RT, top) and generated from crystal structure (for 100 K). The shift in positions of reflexes is the result of different measurement temperature. Co Kα.

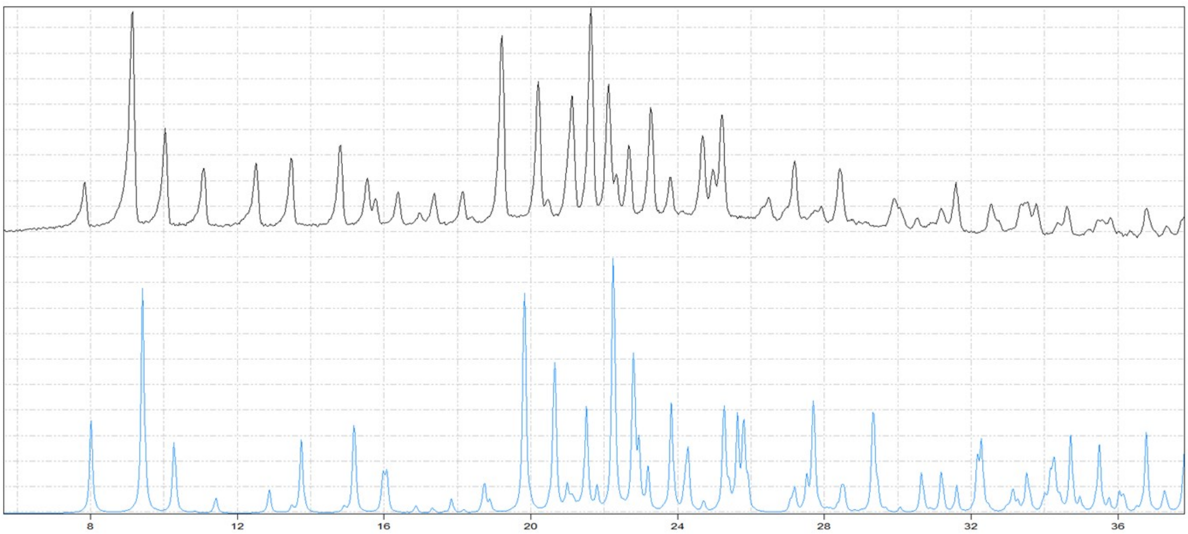


Figure S2. XRDP patterns of $[Cu(Cl_3CCN)_3][Al(OR^F)_4]$: experimental (RT, top) and generated from crystal structure (for 100 K). The shift in positions of reflexes and differences in intensities are the result of different measurement temperatures. Co Kα.

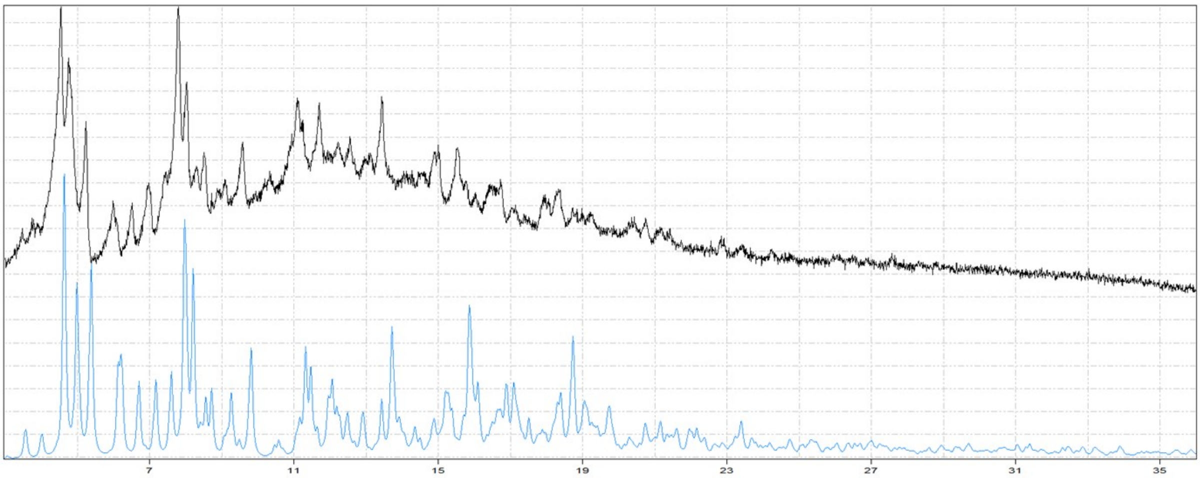


Figure S 3. XRDP patterns of $Ag(CH_2Cl_2)[Al(OR^F)_4]$: experimental (RT, top) and generated from crystal structure (for 100 K). The shift in positions of reflexes and differences in intensities are the result of different measurement temperatures. Mo Kα

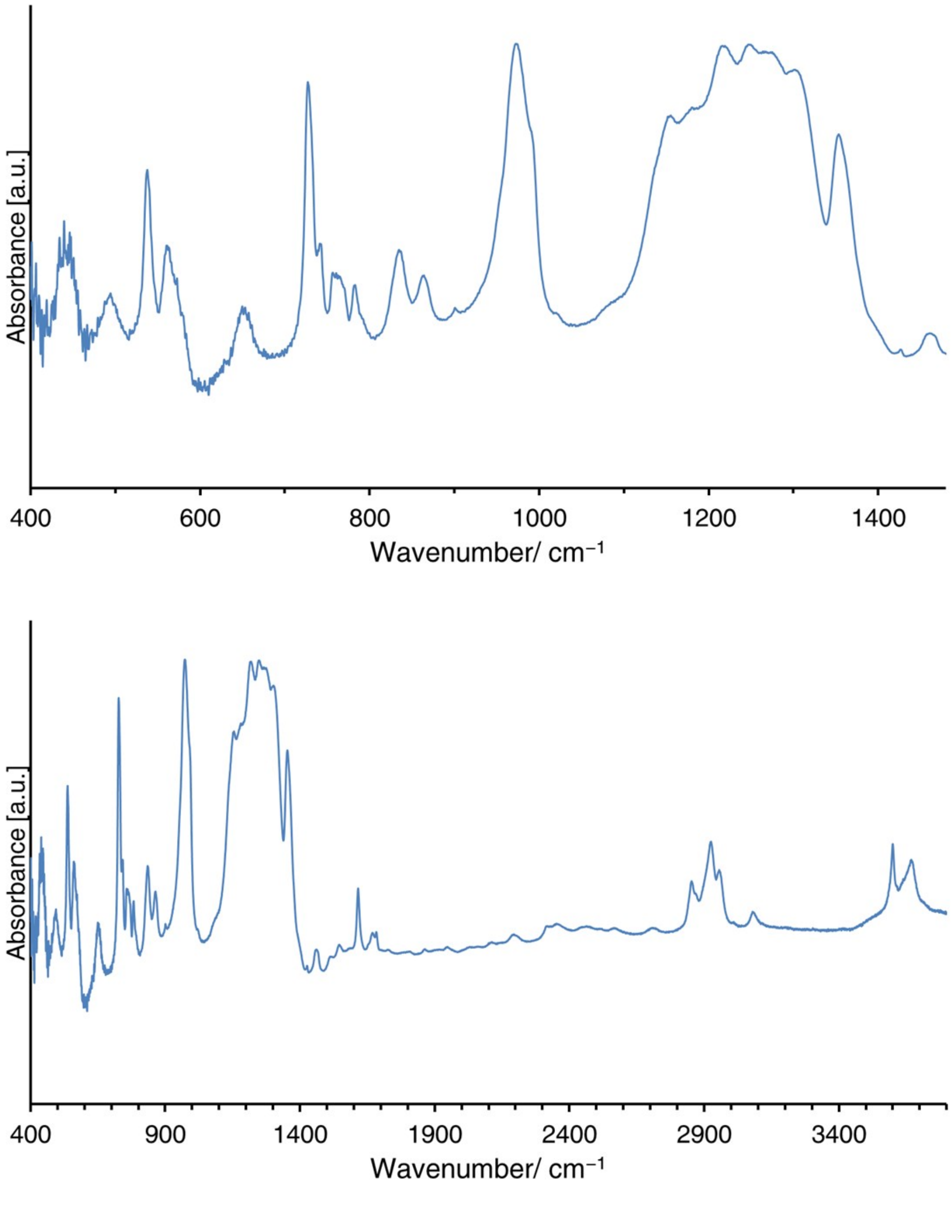


Figure S 4. IR spectra of $Cu(CH_2Cl_2)_3[AlFAl]$ (**V**) shown in narrower (top) and broader (bottom) range.

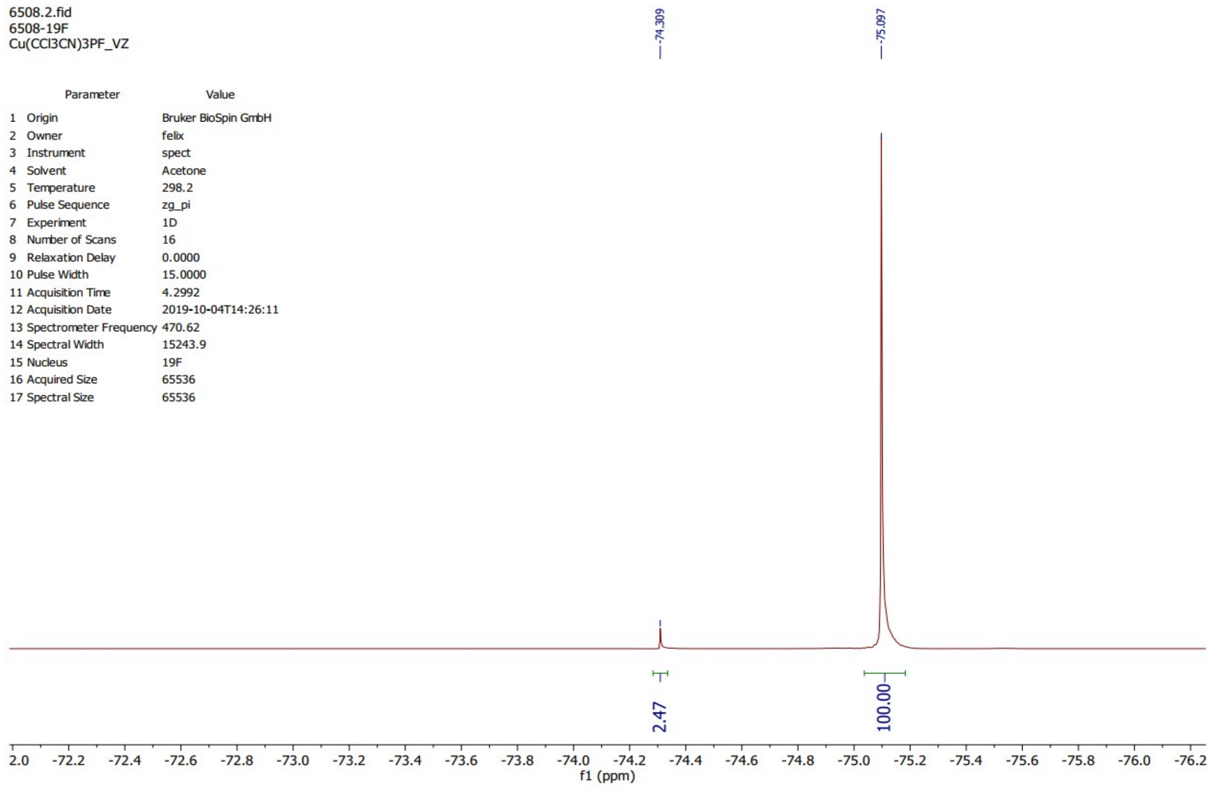
Table S 1. List of vibrational bands.

$Cu(SO_2)[Al(OR^F)_4]$ (**IIa**)		$[Ag(Cl_3CCN)_2][Al(OR^F)_4]$ (**III**)	$[Cu(Cl_3CCN)_3][Al(OR^F)_4]$ (**IV**)	$[Cu(CH_2Cl_2)_3]$[*AlFAl*] (**V**)
IR	R	448 s, br	448 m, br	440 m, br
		505 m	500 w	495 m
524 w	526 vw		506 w	
538 m	537 vw	536 m	536 m	538 m
561 m, br	570 w, br	560 m	561 m	562 m
		572 w	571 w	
				652 w
728 s	742 w	727 s	727 s	728 s
742 w	756 vw	755 w	755 w	742 w
760 w	794 w	800 s, br	797 s, br	762 w, br
784 w,br		834 m	834 w	783 w
839 w, br				834 m
862 w				864 m
				903 w
971 vs		972 vs	974 vs	976 vs
		988 w, sh		990 w, sh
		1028 w	1004 vw	1021 vw
			1030 w	1085 vw, sh
1125 w, sh	1125 vs	1132 w, sh	1131 w	1153 s
1150 w			1166 m	1180 s
1177 w		1172 m		
1214 m				1218 vs
1221 s		1223 vs	1220 vs	1248 vs
1243 s	1249 vw	1242 vs	1242 s	
1275 s		1266 m, sh	1266 w, sh	
		1275 s	1277 s	1274 s
1303 s		1300 s	1300 s	1302 vs
1331 w, sh	1331 vw			
1354 m		1353 m	1355 m	1353 s
				1425 vw
				1460 w, br
				1513 w
				1547 w
				1673 w, br
				1684 w
		2326 vvw, br*	2285 w	
				2855 m
				2868 w, sh
				2924 s
				2955 s

NMR spectra

$[Cu(Cl_3CCN)_3][Al(OR^F)_4]$

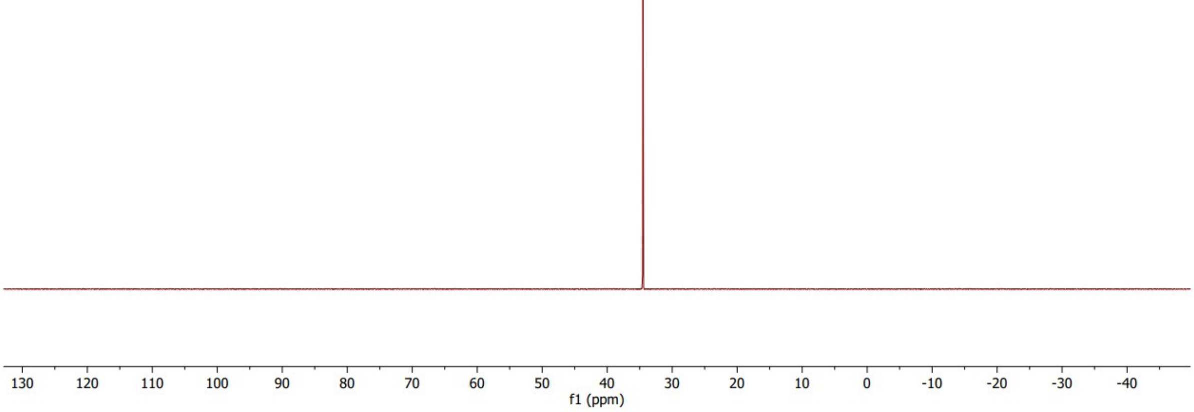
19F



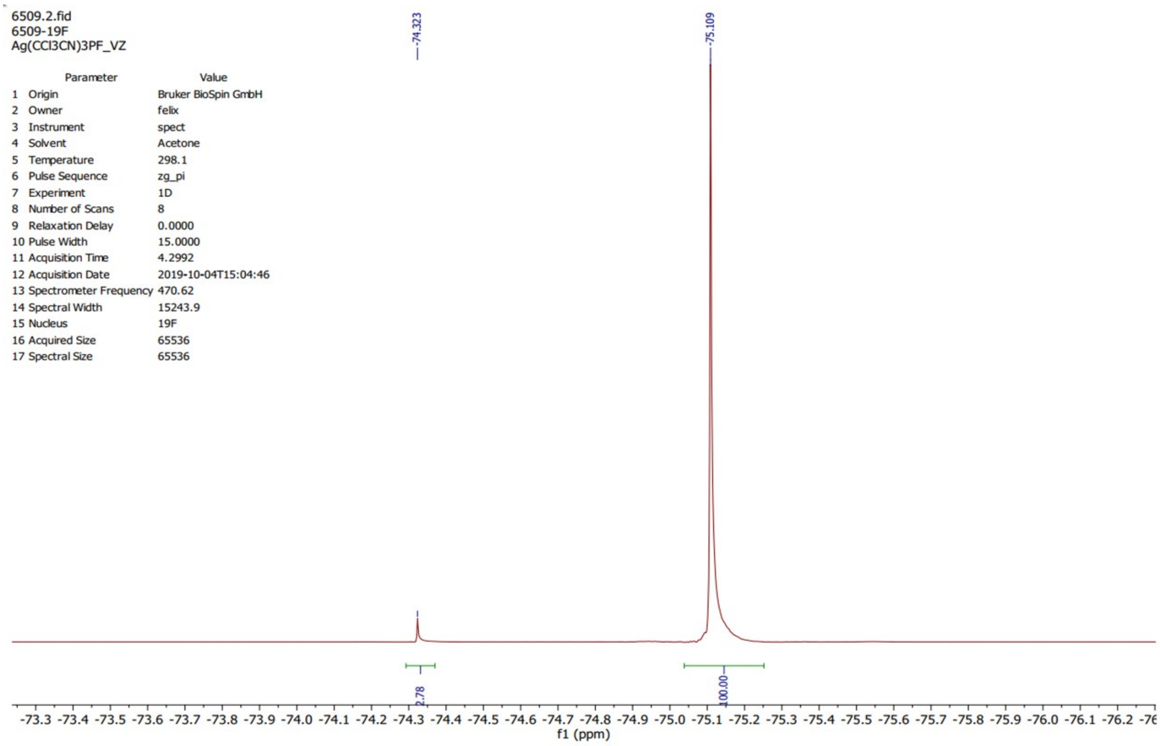
27Al

6508.3.fid
6508-27Al
Cu(CCl3CN)3PF_VZ

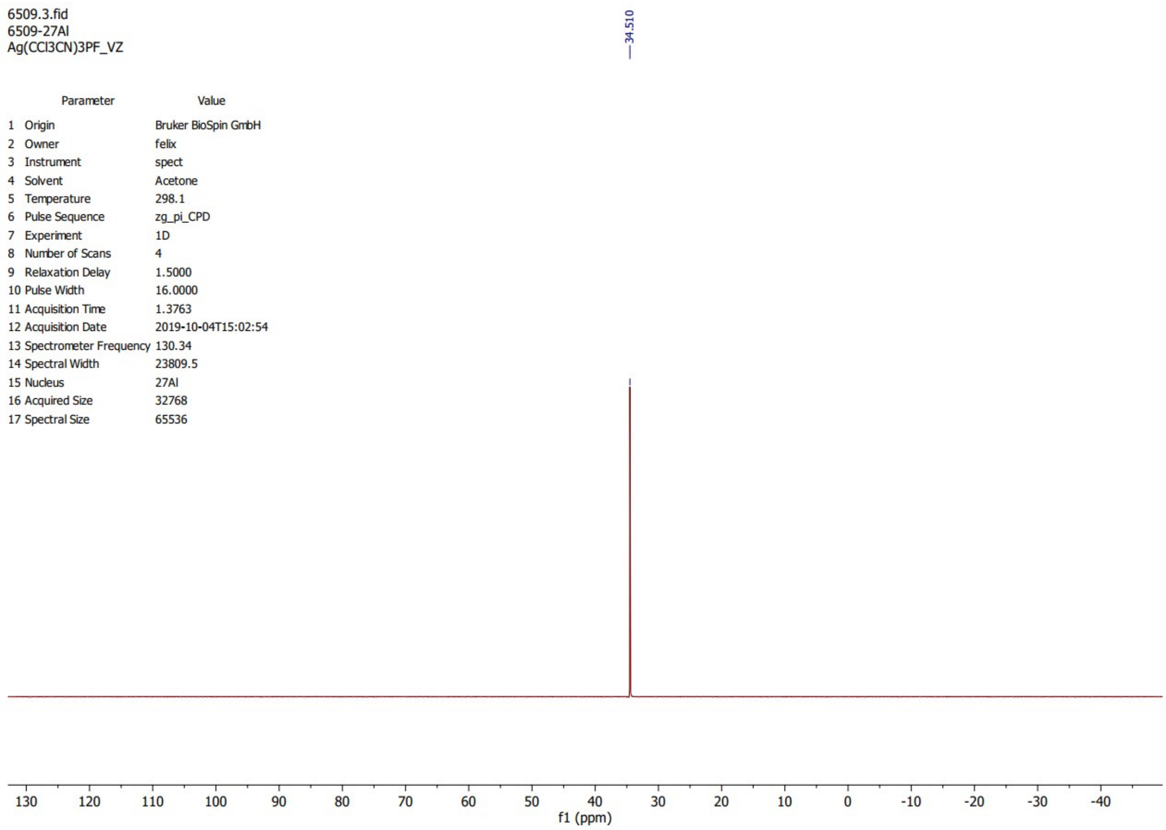
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	felix
3	Instrument	spect
4	Solvent	Acetone
5	Temperature	298.2
6	Pulse Sequence	zg_pi_CPD
7	Experiment	1D
8	Number of Scans	4
9	Relaxation Delay	1.5000
10	Pulse Width	16.0000
11	Acquisition Time	1.3763
12	Acquisition Date	2019-10-04T14:47:08
13	Spectrometer Frequency	130.34
14	Spectral Width	23809.5
15	Nucleus	27Al
16	Acquired Size	32768
17	Spectral Size	65536



$[Ag(Cl_3CCN)_2][Al(OR^F)_4]$



27Al



Note on thermal decomposition of examined samples:

In the case of solvates of Ag and Cu, the thermal stability is related to the basicity of the ligands and the coordination number. Indeed, the stability of $Ag(SO_2)[Al(OR^F)_4]$ is very poor and low-temperature techniques have to be used to manipulate the compound.[S9] For the solvates containing CH_2Cl_2 – a molecule that binds Ag^+ stronger than SO_2 – it is possible to isolate $Ag(CH_2Cl_2)_4^+$ and $Ag(CH_2Cl_2)_3^+$, which are stable only in the presence of the solvent at –78°C and room temperature, respectively. However, the stability of **Ia** is much higher and prolonged pumping under HV at room temperature is required to remove the solvent completely.[22] Heating the latter compound will cause decomposition starting above 75°C, *i.e.* close to the point where the plain $Ag[Al(OR^F)_4]$ starts to decompose.[S10] In the evolved gases CH_2Cl_2 is detected aside to other products (probably C_4F_8O as indicated by the MS spectrum) of anion decomposition.[§] Above 150°C the profile of TG and DSC curves match those recorded for $Ag[Al(OR^F)_4]$ suggesting formation of the same decomposition product.

While Cl_3CCN binds silver more strongly than CH_2Cl_2 (*cf.* DFT calculations section), thermal decomposition of **III** starts already at 50°C, what is probably linked to higher number of ligands bound to Ag^+. This is an endothermic process accompanied by the mass loss of *ca.* 10 wt.%. However, *no* Cl_3CCN is detected in the evolved gases according to the MS results. Above 75°C the decomposition continues in several endothermic steps, leaving around 15 wt. % of residual mass above 300°C. The endothermic peak observed at 455°C matches the melting point of AgCl indicating its formation in the sample. These data are consistent with the composition of the final product as a mixture of AgCl and AlF_3, which together would correspond to 16.5 wt.% of initial mass. This also points at the non-inert character of Cl_3CCN, which acts as a chloride donor to Ag^+, all being in accord with the absence of Cl_3CCN in the MS spectra. This feature of the ligand is in line with fairly high reactivity of chlorine atoms in the molecule and is responsible for lower decomposition temperature of this compound as compared to plain $Ag[Al(OR^F)_4]$ and its CH_2Cl_2 adduct.

The behavior of copper solvates is different from their silver congeners. Firstly, copper binds SO_2 strong enough to make **IIa** stable and isolable at room temperature, also under reduced pressure. Upon heating the mass loss starts at 55°C, where SO_2 is evolved as indicated by the signal m/z = 64 visible in the MS spectrum. However, concomitant decomposition of the anion is observed (signal m/z = 69 corresponding to CF_3), what is in accord with previous findings that $Cu[Al(OR^F)_4]$ – which most probably forms after loss of SO_2 – is unstable at this temperature.[18] Further decomposition processes are multistep in character, but at 310°C the mass becomes constant at 16.5% of the initial weight. This corresponds to the mixture of AlF_3+0.5Cu+0.5CuF_2 (theor. 17%), which would suggest, that there is a fluoride abstraction in the course of decomposition of the salt.

Alike for Ag, when Cu is ligated with Cl_3CCN, the stability of the complex is greater than for SO_2 adduct. Although there are three ligands around Cu in the compound **IV**, its decomposition starts only at 90°C and is followed by almost constant mass loss achieved at 280°C with remaining 14 wt.%. Very complex DSC curve points at a multistep character of the process with numerous intermediate steps. However, an endothermic peak around 410°C suggests that CuCl is present in the sample (mp. 426°C). The residual mass at 300°C corresponds well with the composition AlF_2Cl+CuCl (theor. 13.5 wt.%). Similar mixed halides of Al have been reported[23] and they could form in the system owing to the non-innocent character of Cl_3CCN and the fact that it is not observed in the MS spectrum, what indicates that all Cl_3CCN molecules are engaged in unknown reactions in the course of thermal decomposition of **IV**.

§ The exact identity of evolved gases is hard to determine as there are plenty of signals present in the mass spectra of limited resolution. However, the dominating m/z = 69 points at presence of CF_3 groups. Most probably the dominating gas is C_4F_8O – previously reported in that class of compounds.[S11]

Note on the origin of **V**

As mentioned in the main text, observations suggest that V is formed as a result of partial decomposition of $[Al(OR^F)_4]^-$ into more resistant $[$*AlFAl*$]^-$ triggered by highly reactive carbocationic species derived form CH_2Cl_2 via Cl^- abstraction. Such scenario is backed by the observation for old **Ia** samples, where AgCl was detected in powder XRD patterns what points at the potential of $Ag[Al(OR^F)_4]$ to abstract Cl^- from Ag-bound CH_2Cl_2 molecule. However, with much higher affinity of Cu(I) to chlorides, the decomposition seems to occur faster in this case. Moreover, the chloride ion affinity (ClA) of $Cu[Al(OR^F)_4]$ is estimated at *ca.* 310 kJ mol^{-1} which is comparable to CIA of SbF_5 (333 kJ mol^{-1}) - the compound reported as causing decomposition of CH_2Cl_2.[S12] As shown above, the behavior of $Cu[Al(OR^F)_4]$-CH_2Cl_2 system is much more complicated than its silver relative and deems separate study and analyzes which is beyond the scope of this paper.

3. Crystallographic data

Table S2. Crystallographic data for refined structures.

Compound	$Ag(CH_2Cl_2)[Al(OR^F)_4]$ (**Ia**)	$[Ag(CH_2Cl_2)_3][Al(OR^F)_4]$ (**Ib**)	$[Ag(CH_2Cl_2)_4][Al(OR^F)_4]$x 0.5 CH_2Cl_2 (**Ic**)	$Cu(SO_2)[Al(OR^F)_4]$ (**IIa**)	$[Cu(SO_2)Cu][Al(OR^F)_4]_2$ (**IIb**)	$[Ag(Cl_3CCN)_2][Al(OR^F)_4]$ (**III**)	$[Cu(Cl_3CCN)_3][Al(OR^F)_4]$ (**IV**)	$[Cu(CH_2Cl_2)_3]$[*AlFAl*] (**V**)
K_α	0.71073 (Mo)	0.71073 (Mo)	0.71073 (Mo)	1.54184 (Cu)	1.54184 (Cu)	1.54184 (Cu)	1.54184 (Cu)	1.54184 (Cu)
Temperature (K)	100	100	100	100	100	100	100	100
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$I2/a$	$P2_1/n$	$P2_1/n$	$P\bar{1}$
Z	8	2	1	4	4	4	4	2
a (Å)	17.8865(12)	9.9840(4)	9.7789(3)	10.7624(4)	18.5302(5)	15.8763(3)	11.2034(5)	10.30957(13)
b (Å)	17.8859(12)	13.2483(4)	15.2594(4)	17.9916(8)	19.5531(6)	23.2524(4)	15.9579(5)	10.30942(13)
c (Å)	20.2655(13)	15.0662(4)	15.3111(4)	15.7057(7)	33.2117(9)	32.6565(7)	26.0862(7)	25.3144(4)
α (°)	90.027(3)	86.439(2)	79.397(2)	90	90	90	90	86.0419(12)
β (°)	89.997(3)	87.425(3)	80.251(2)	98.206(4)	90.005(3)	94.580(2)	101.111(4)	86.0626(12)
γ (°)	101.127(3)	79.209(3)	86.321(2	90	90	90	90	83.4930(10)
V ($Å^3$)	6361.4(7)	1952.68(11)	2212.00(11)	3010.0(2)	12033.4(6)	12017.0(4)	4576.3(3)	2661.82(6)
$\rho_{calc.}$ (g cm^{-3})	2.422	2.258	2.195	2.416	2.346	2.261	2.125	2.248
$\mu_{exp.}$ (mm^{-1})	1.072	1.155	1.208	4.498	4.130	9.901	7.472	5.935
ϑ_{max} (°)	25.194	25.242	25.203	76.140	67.555	74.042	73.516	75.551
R_1	2.94%	6.14%	6.76%	6.45%	6.57%	6.54%	8.67%	6.14%
wR_2	6.95%	14.78%	15.83%	14.78%	17.32%	15.46%	22.99	16.77%
GooF	1.037	1.122	1.034	1.021	1.027	1.045	1.071	1.043
Crystal size (mm×mm×mm)	0.16x0.25x0.32	0.09 x 0.15 x 0.19	0.20x0.20x0.10	0.10x0.16x0.21	0.09x0.18x0.29	0.06x0.15x0.32	0.06x0.09x0.20	0.16x0.30x0.47
Crystal colour	colorless	colorless	colorless	yellow	brown	colorless	colorless	colorless
CCDC No.	1960208	1960202	1945481	1960200	1960201	1960203	1960458	2033578

4. Supplementary data and figures for description of the crystal structures

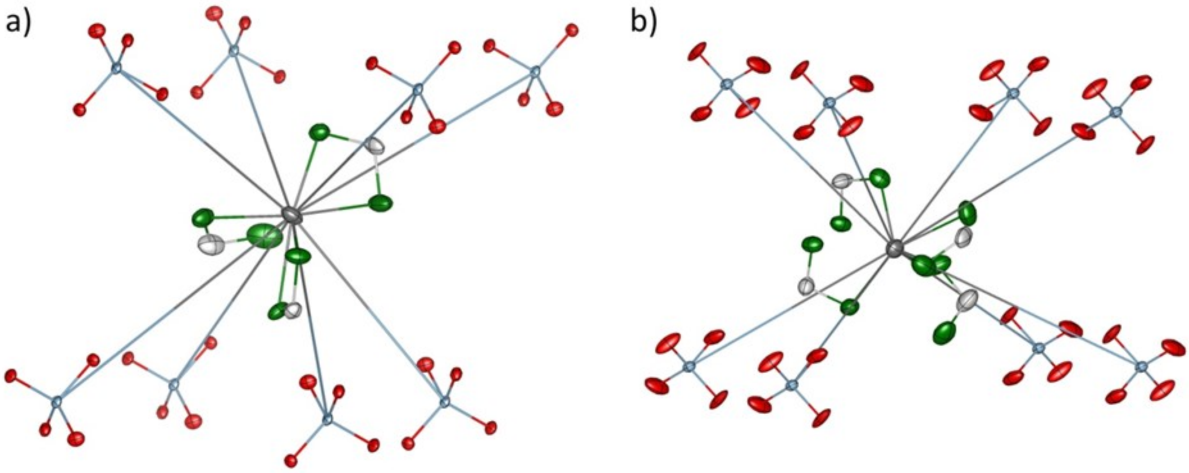


Figure S5. The arrangement of anions (only the AlO_4 units shown for clarity) and (a) $[Ag(CH_2Cl_2)_3]^+$ or (b) $Ag(CH_2Cl_2)_4]^+$ cations in the crystal structures.

5. DFT calculations details and results

All calculations were performed with the use of Orca [S13] (v. 4.0.1.2) using BP86,[S14] B3LYP [S15] and PBE0 [S16] functionals with def2-TZVP [S17] (with ECP Ag [S18]) and D3BJ dispersion correction. [S19] RI-J [S20] or RIJCOSX [S21] approximation was used to increase the speed of calculations (with auxiliary basis set by Weigend [S22]) . Thermal contributions to *ab initio* reaction energies were calculated with inclusion of zero point energy, thermal contributions to the enthalpy/entropy. Graphical presentation of the calculated structures and molecular orbitals has been performed with Avogadro [S23] or Vesta. [S7]

5.1. Vibrational modes for the selected cationic complexes

Below are given vibrational modes for three Ag^+ and Cu^+ complexes together with calculated and experimental modes for isolated ligands. Values are obtained with B3LYP/def2-TZVP/D3BJ method.

$[Cu(Cl_3CCN)_3]^+$

Vibrational frequency [cm^{-1}] (not scaled)	Relative intensity [a.u.]	Overall band intensity [a.u.]	Vibrational frequency [cm^{-1}] Cl_3CCN (calc.) (not scaled)	Vibrational frequency [cm^{-1}] Cl_3CCN (exp.)[S24]	Assignment
510.87	0.7	113.8	504.2 504.4	485 (s) 488 (s)	Cl_3CCN
512.52	1.0				
516.15	0.1				
519.58	2.3				
521.84	29.1				
522.63	3.4				
522.96	2.5				
523.26	37.0				
525.38	37.7				
756.16	12.2	719	754 754.1	789 (m)	CCl_3
757.76	181.7				
758.4	82.4				
759.49	116.2				
759.84	30.4				
761.06	296.1				
1024.75	91.9	193.2	1035.7	1028 (w)	ν(CC)
1025.69	100.9				
1030.73	0.4				
2372.98	2.1	5.3	2358.4	2249 (s)	ν(CN)
2373.59	3.1				
2380.67	0.1				

$[Ag(Cl_3CCN)_2]^+$

Vibrational frequency [cm^{-1}] (not scaled)	Relative intensity [a.u.]	Overall band intensity [a.u.]	Vibrational frequency [cm^{-1}] Cl_3CCN (calc.) (not scaled)	Vibrational frequency [cm^{-1}] Cl_3CCN (exp.)[20]	Assignment
519.5	0.0	63.7	504.2 504.4	485 (s) 488 (s)	Cl_3CCN
525.9	1.1				
526.1	0.5				
527.4	27.4				
527.6	27.1				
530.7	7.6				
760.7	45.5	474.5	754 754.1	789 (m)	CCl_3
761.3	171.8				
762.5	34.6				
762.9	222.7				

1018.4 1018.7	5.8 111.0	116.8	1035.7	1028 (w)	ν(CC)
2392.2 2393.3	22.1 40.7	62.8	2358.4	2249 (s)	ν(CN)

[Cu(SO$_2$)]$^+$

Vibrational frequency [cm^{-1}] (not scaled)	IR intensity [a.u.]	Raman activity [a.u.]	Vibrational frequency [cm^{-1}] SO$_2$ (calc.) (not scaled)	SO$_2$ (exp.)	Assignment
529.12	29	3	522	518	δ(OSO)
1124.23	137	71	1180	1152	ν_{sym}(SO)
1355.32	181	11	1375	1360	ν_{asym}(SO)

[Cu(CH$_2$Cl$_2$)$_3$][*AlFAl*]

Vibrational frequency [cm^{-1}] (not scaled)	IR intensity [a.u.]	Assignment
632.87	82.05	ν(C-Cl)
643.61	51.41	
669.31	53.30	
711.62	49.51	
728.35	53.53	
739.21	63.45	
898.19	2.48	δ, ρ (CH$_2$)
900.82	1.04	
904.19	0.54	
1155.55	0.01	
1163.29	0.04	
1163.55	0.35	
1280.56	9.53	
1283.69	28.22	
1287.43	24.39	
1451.07	2.59	
1453.81	3.00	
1458.53	0.40	
3127.26	0.95	ν(C-H)
3127.44	0.29	
3130.22	0.23	
3213.69	7.32	
3215.51	6.79	
3218.46	6.86	

5.2. Coordinates of optimized structures

$Ag(C_6H_5CH_3)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-1.53618275108758	1.66155350650598	0.07085672125979	C	-1.55665047111780	1.67911646833269	0.04011164953158
C	-0.18921985660128	2.02754982099078	0.00993173082076	C	-0.20973786825831	2.03513050085341	-0.00433687947470
C	0.81925267330716	1.07145989807396	-0.04606140728738	C	0.79835943336160	1.07933875381024	-0.00422950899275
C	0.52208463264126	-0.28955008276613	-0.02097440394397	C	0.49496140620970	-0.27369776737230	0.04397193224419
C	-0.80436209987977	-0.69747013224459	0.04639393741644	C	-0.84462451376590	-0.67275708987309	0.07218533670414
C	-1.84157334909596	0.27411196039288	0.09829235758065	C	-1.87122342502735	0.30669307041189	0.07874462011847
C	-2.62682986815594	2.69068817733452	-0.00172470085802	C	-2.63442065019724	2.71133463750396	-0.03541547075079
H	0.06949603829640	3.07839645272693	-0.02370453905460	H	0.05455653577111	3.08566547157537	-0.05475016617808
H	-1.06304689368538	-1.74745309527570	-0.00549644593824	H	-1.10531577405768	-1.72255027822963	-0.01798838486505
H	-2.87162157245927	-0.04220302467369	-0.03538468435876	H	-2.90700440264287	-0.00620081774822	-0.01783392182044
H	1.85047678441083	1.39171806338461	-0.11718357211171	H	1.83359293328121	1.39534180146249	-0.05133101969153
H	1.31347392063378	-1.02406083901033	-0.07772752212350	H	1.28090814375656	-1.01819615053492	0.01938231939564
H	-3.59111640940358	2.28732997654842	0.30519224537483	H	-3.59531767135472	2.32395239930946	0.30335426973549
H	-2.72979754340146	3.04371501508432	-1.03115010583454	H	-2.75907008207305	3.04099722541430	-1.07102249594614
H	-2.39787377981053	3.56039411540201	0.61427149085044	H	-2.38434705442908	3.59373361026081	0.55490240553882
Ag	-1.71466992570869	0.08455018752604	2.39391889820784	Ag	-1.38617653945620	-0.18717183517645	2.32370531445118

$Ag(C_6H_5F)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
F	0.51183442185124	-1.74455503010835	-0.38912553648306	F	0.50665329650927	-1.73080502928932	-0.36670727950640
H	-1.98470102439921	-1.15593138482739	-0.24334167078393	H	-1.98646758887439	-1.14802840413081	-0.22585177867280
C	-1.79330740569249	0.97572515335699	0.04439506212579	C	-1.79155855221342	0.98527556648205	0.04342364243691
C	-0.88807040831108	2.06240588522438	0.16565745619061	C	-0.89057504929892	2.07067558876135	0.14973473633321
C	0.50773285261738	1.81451877901378	0.09307762360668	C	0.50037171502857	1.82092900271195	0.09095243206188
C	0.97911383919653	0.52436934471770	-0.08591698830922	C	0.97223589252614	0.53012984558385	-0.07561822095325
C	0.05865089115157	-0.51279357528609	-0.20306127513211	C	0.05617365135012	-0.50679802729264	-0.19051593885415
C	-1.31636620255209	-0.31313562695531	-0.13251920984719	C	-1.31544761184325	-0.30456670128937	-0.12198293184593
H	-2.85877779918084	1.16495821480794	0.03502196894952	H	-2.85906552598255	1.17320528637130	0.02923039815704
H	1.20047695671766	2.64535765129525	0.12231355183908	H	1.19629388182995	2.65161724523331	0.11583823590119
H	2.03641816425401	0.31075923006577	-0.16137928841565	H	2.03178100532391	0.31757871424348	-0.14368881647681
H	-1.25681135462078	3.07961011187065	0.07984186125068	H	-1.26036372944228	3.08988936412835	0.07438391954359
Ag	-0.92419293103191	1.99313124682467	2.46198644500880	Ag	-0.88803138491316	1.89531754848648	2.40775160187551

$Ag(o\text{-}C_6H_4F_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
F	0.58677747609099	-1.73186985898321	0.36293587644352	F	0.58170638478192	-1.71996575270140	0.33184038652279
F	-2.05973825495155	-1.40498985606072	0.39653503413823	F	-2.05356002796339	-1.39342234419519	0.40685654171545
C	-1.85560374982227	0.89523597971832	-0.02243884948960	C	-1.85995257236784	0.89849119180317	-0.00996853441278
C	-1.01156633933906	2.00258300559073	-0.22490836418097	C	-1.02466654340318	2.00445951191683	-0.21511413153316
C	0.39805551732895	1.82572810943419	-0.23563489062728	C	0.38066197841991	1.83179468696563	-0.24473002262654
C	0.94437709903296	0.54903949194570	-0.04910909486680	C	0.93065958516407	0.55419846855208	-0.07294244348120
C	0.09867094642763	-0.52049589214875	0.16678452739514	C	0.09261843772666	-0.51658586466187	0.14880585964227
C	-1.29525727084685	-0.34837825052994	0.18136577136371	C	-1.29771438527807	-0.34448565529447	0.18457333055965
H	-2.93057579936041	1.00718383159951	0.02202061448159	H	-2.93633483709952	1.00695500142325	0.04536776307663
H	1.05103180892168	2.68952476713298	-0.25691744855811	H	1.03363641589924	2.69877290866798	-0.25128105375645
H	2.01398408972824	0.38974289091653	-0.03114674116949	H	2.00230893754748	0.39691622465291	-0.06418568197441
H	-1.43034544354613	3.00209351420846	-0.20416055957908	H	-1.44760944400225	3.00389481461370	-0.20640127396212
Ag	-0.45801007966416	1.96185226717620	-2.54462587535088	Ag	-0.34995392942501	1.89622680825739	-2.49212073977016

$Ag(o\text{-}C_6H_2F_4)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
F	1.53206305318367	5.21566490048877	-1.21448781447717	F	1.47518276637938	5.16073835909447	-1.30863278077450
F	2.98321064558153	3.03591643020909	-0.59175489312609	F	2.95909096228554	3.01152884880463	-0.65088367760426
C	1.05336875758096	1.77354011513687	-0.20549599738330	C	1.04529849794618	1.76735139282159	-0.17511471392982
C	-0.33346827032737	1.70102694555415	-0.17479839322682	C	-0.34019456981354	1.68381196434136	-0.11111101839573
C	-1.11847470463389	2.82337498634206	-0.49639914475217	C	-1.13087834851415	2.78057446848490	-0.44433958652229
C	-0.47371067105290	4.04387601452632	-0.84267007354363	C	-0.50836936764604	3.98518126014019	-0.86683385941748
C	0.90725171072907	4.09620989374124	-0.88442563024393	C	0.88075920403860	4.04850977515776	-0.94077915477042
C	1.67311977744530	2.97394641945413	-0.55889701888607	C	1.65626860379251	2.94982903464873	-0.59175092462593
F	1.78776932225283	0.72512535514205	0.10281152726063	F	1.78681943038218	0.74334162387010	0.15194167152258
H	-2.16506180851847	2.81693999235307	-0.20921721703952	H	-2.18919000433819	2.75501915002427	-0.20536499286374
H	-1.04432903353381	4.95196300269665	-0.98576502303453	H	-1.07784941992231	4.90457409922364	-0.95811921734766
F	-0.91341653726835	0.57471245583696	0.20579027781355	F	-0.89428577253459	0.56649535543436	0.30051949229606
Ag	-1.50249224143858	2.48924348851857	-2.77297059936093	Ag	-1.27682198205558	2.86458466795395	-2.82781123756679

$Ag(C_6H_5CF_3)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-1.47719186366424	1.62108440838008	0.02648434685358	C	-1.48444338907066	1.61981922233308	0.01172495822346
C	-0.16928569210015	1.99001207253328	0.28672850801482	C	-0.17879002743120	1.98560181346784	0.28320579892205
C	0.83742061203308	1.02148917296470	0.28458110283663	C	0.82452510070310	1.01893848302203	0.28587087641694
C	0.54798875825733	-0.30629262813196	0.00280675535758	C	0.53561680275359	-0.30447187950159	-0.00268594123527
C	-0.76945012858766	-0.69720461110617	-0.24023547768683	C	-0.77935358451463	-0.69289720866381	-0.25399943399979
C	-1.80007146546690	0.26367355147399	-0.21830068130962	C	-1.80757193890276	0.26628425107246	-0.23098120534400
C	-2.59489871429382	2.63658967459865	-0.02441800444040	C	-2.60288812381340	2.63429360848041	-0.02155207096308
H	0.06738703488656	3.02443649206161	0.49248964468002	H	0.05650021208822	3.02100432742480	0.49456577989637
H	-1.01704622373333	-1.74240111698253	-0.37298451138210	H	-1.02607565042165	-1.73969508396796	-0.39061833495886
H	-2.83927076578432	-0.05240749965902	-0.20973990939691	H	-2.84945920027235	-0.04701792029399	-0.24541762105178
H	1.85527491744486	1.31642295816861	0.50149097478343	H	1.84283339518198	1.31130036288384	0.51137058078573
H	1.33637251278406	-1.04634744207658	0.00115968834264	H	1.32392645257766	-1.04696517005165	-0.00324840067808
F	-3.59587867130604	2.31476237288476	0.79856033725738	F	-3.53450976456490	2.36409152671913	0.88265599857367
F	-3.11783159047007	2.65536698474158	-1.29432439408729	F	-3.20473912270748	2.58921807022148	-1.23889572942951
F	-2.18390474965368	3.86865798432444	0.25216323728204	F	-2.16730430136729	3.86790780223186	0.16378700000418
Ag	-1.71877397034568	0.48959762582457	-2.54452161710498	Ag	-1.58742686023822	0.51002779462209	-2.50384225516203

$Ag(m\text{-}C_6H_4(CF_3)_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-0.00367116796229	2.40598752536634	-0.03758924210499	C	-0.00213417649262	2.40173195910288	-0.04734084761352
C	-0.83685880480139	1.29000370878219	-0.00694881983794	C	-0.83246260679172	1.28783471986322	-0.01297466727487
C	1.37772501545999	2.24967425433619	-0.00229770501323	C	1.37561873649578	2.24409480150202	-0.01213075887368
C	1.94247261005242	0.97980777898934	0.09646084947018	C	1.93934848151431	0.97575304501011	0.09410863421155
C	1.10030129839181	-0.15398017520092	0.14705777793588	C	1.09961203460163	-0.15437654347365	0.15600190143517
C	-0.30113631983941	0.01062400684602	0.08530059269816	C	-0.29739160987935	0.01057992701120	0.08627185468931
H	-0.43241221134098	3.39736901618304	-0.08936629615097	H	-0.43106704063581	3.39511534254075	-0.10233821908705
H	-0.95172244299265	-0.84993606167831	0.16674349973898	H	-0.95147032986599	-0.84936432619088	0.17248308345536
H	1.51756133100355	-1.12405124567657	0.39526376251284	H	1.51743204330392	-1.12671829754833	0.40113764580055
H	3.01375276449334	0.86436221095162	0.19784477748982	H	3.01254099318558	0.86311650580251	0.20048503756710
C	-2.33854498203283	1.46017701219170	-0.13650931401863	C	-2.33210454625919	1.45501542801905	-0.13935390229281
F	-2.74511594674940	2.64178545251580	0.33043731612598	F	-2.73443637792862	2.62456141233347	0.33520053976742
F	-2.99669322516655	0.49258854516392	0.51356667038708	F	-2.97944219579560	0.48697370172261	0.50146244593542
F	-2.68236593183162	1.38539408483911	-1.44064000645880	F	-2.67377534314298	1.38980999101429	-1.43334191965762
C	2.28817212696423	3.45644955597484	-0.12702245021414	C	2.28751714220608	3.44665619425808	-0.13440804321740
F	1.67951552687870	4.58015670876338	0.25365575363451	F	1.67628847773899	4.56340401885947	0.22987857066403
F	2.66127309670063	3.60025680151775	-1.41843362392846	F	2.67338691587069	3.57908555716012	-1.41209444087221
F	3.40044531828045	3.30286552191329	0.60173786407842	F	3.38134950756090	3.29546176524338	0.60515836629536
Ag	1.27140194449199	-0.30892470177868	-2.18821140634470	Ag	1.23528989431399	-0.20812520223025	-2.14715528093212

$Ag(CH_2Cl_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-2.29428400203219	1.19039774127866	0.14118752102674	C	-2.28548995626066	1.19173364266236	0.13177027324522
Cl	-0.51847572511365	1.04797264589611	0.37186904321381	Cl	-0.53008120426069	1.03869059414890	0.35548551740490
H	-2.66728285536967	1.92932350368234	0.84059466403144	H	-2.65418460260542	1.93812920647396	0.82911213222746
H	-2.73231303145514	0.20808585394696	0.27483830700079	H	-2.73541343823448	0.21434652392701	0.28025070448150
Cl	-2.67714046008393	1.75070316233579	-1.52222426753757	Cl	-2.66375156831103	1.73317873206215	-1.51721382946160
Ag	-0.07097392594543	2.07065709286014	-2.07144526773520	Ag	-0.09154923032773	2.08106130072562	-2.04458479789748

$Ag(C_2H_4Cl_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-3.17004930829769	1.66755195876166	-0.08343942288953	C	-3.16915291245486	1.66214301798732	-0.07495277311383
C	-1.67514513734165	1.49903431783660	-0.11688789132036	C	-1.67746387520243	1.49872823080586	-0.10463914726295
Cl	-4.00431238101238	0.42412325302966	0.96238230581330	Cl	-3.99026068179883	0.44185185404581	0.96460279010174
H	-3.57718345301560	1.49948555255328	-1.07922926634415	H	-3.57029891648175	1.49101173649827	-1.07437171759502
H	-3.48174830511929	2.63956241505772	0.28785304301582	H	-3.48000840551052	2.64161516715389	0.28281675306356
H	-1.36493353856745	0.48446577159738	-0.35034689541998	H	-1.36757675198878	0.48425166072978	-0.34796708525098
Cl	-0.87278772791180	1.93346506527434	1.46628535786208	Cl	-0.89211110232568	1.92512799442441	1.46030747401781
H	-1.24647017382681	2.19606136124644	-0.83507757896986	H	-1.25215379768192	2.19699426335319	-0.82596367172354
Ag	-2.44003997490735	0.58720030464293	3.03034034825269	Ag	-2.43364355655525	0.58922607500147	3.00204737776323

$Ag(CCl_2FCClF_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-1.14557668259787	1.58721789289809	-0.04090469413822	C	-1.14159150120373	1.58517333289753	-0.03160748878022
C	-0.25207782762845	0.29300112237663	-0.12154478008484	C	-0.25362643636998	0.29476249390031	-0.11452590869473
F	-1.12053628578956	2.14668998847840	-1.24105863416918	F	-1.12123420972157	2.13933590430340	-1.22622802714696
Cl	-0.48301532684174	2.74709612119606	1.15814418174432	Cl	-0.48182248158482	2.72896544168529	1.15450089823630
Cl	-2.83434297006143	1.16529586418903	0.38320069224171	Cl	-2.81204246374165	1.16313984258361	0.39596644718180
F	0.97039728265973	0.64291503929286	-0.47865570820275	F	0.95818691757227	0.64377610295778	-0.48093230301894
F	-0.76767865153829	-0.52407081277955	-1.02320261709638	F	-0.77416133835055	-0.51756333004515	-1.00677362170658
Cl	-0.14572521950061	-0.60606379445864	1.46072812595673	Cl	-0.14276292852564	-0.58354246616313	1.45286536679731
Ag	-1.69310431870178	0.98091857880712	2.99174343374860	Ag	-1.70260555807434	0.97895267788036	2.94518463713202

$Ag(CH_2ClF)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-5.20134698286143	2.67783428914096	-0.08747441894149	C	-5.19178193080126	2.68509175508953	-0.08554292163004
Cl	-3.39295575702412	2.82698405028930	-0.34903712667981	Cl	-3.40832019008159	2.83405053670979	-0.34290050166563
H	-5.65377259565816	2.63858381783364	-1.07334613141257	H	-5.64929011881474	2.63985232693898	-1.07114706593918
F	-5.61178984998823	3.79419440209097	0.57836722648425	F	-5.60604781852499	3.79251187810666	0.57546380736618
H	-5.35200038095599	1.79403627894470	0.52465480174225	H	-5.34708640188158	1.79768125444477	0.52399517262947
Ag	-3.20167443351207	5.07885716170042	0.82051564880736	Ag	-3.21101353989583	5.06130224871027	0.81381150923918

$Ag(MeOEt)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-3.29301387361549	-0.04851901609797	0.15834706151119	C	-3.27348869845256	-0.03419665293069	0.17999119538551
C	-2.12224556812773	0.77479992527067	-0.31381687313266	C	-2.10418077321926	0.76566997245880	-0.31824093269374
H	-4.19273570367642	0.20804190954828	-0.40272874508406	H	-4.17459406924827	0.19626072462414	-0.39161392851665
H	-3.52775237471487	0.16531016508646	1.21257895903373	H	-3.51571290446771	0.22377296043036	1.22404605797784
H	-3.11260757685932	-1.11652586599591	0.02033011742457	H	-3.09603368601605	-1.10905126236194	0.07755278471660
O	-0.95458616358591	0.41051939577382	0.46700284919319	O	-0.95086360204957	0.41107402439031	0.45926644325052
H	-1.89057591484933	0.57155954714196	-1.36159897358466	H	-1.88683609651153	0.54019833169802	-1.36643665883461
H	-2.30179950701139	1.84542056935964	-0.18927074911896	H	-2.27978331846688	1.84145541841945	-0.21869635676673
C	0.23710737030848	1.14634955477796	0.11585438679748	C	0.22213833072881	1.15456350512026	0.11795802903763
H	1.05366441609482	0.74834388514882	0.71207787112201	H	1.04657291517072	0.76320914268418	0.70994265150133
H	0.09816554420227	2.20818184602636	0.32474921267078	H	0.07517017196042	2.21527957814976	0.33462461461813
H	0.45057536994148	0.99538425713839	-0.94266728171319	H	0.44207223485255	1.01767879441367	-0.94274484905681
Ag	-1.36842601810660	-0.53019617317851	2.41821216488058	Ag	-1.42869050428069	-0.60724453709635	2.35342094938097

$Ag(C_4H_8O)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-2.66244465457677	-0.71118969513299	-0.16615342596713	C	-2.64910080481598	-0.71013046021868	-0.16839716450525
C	-2.26628976202173	0.70119454473255	0.22049734812156	C	-2.26025513278821	0.69600071663001	0.22387741481793
C	-0.79554995023552	0.77722794874383	-0.21020050453156	C	-0.80095294890207	0.77210044325741	-0.21326851812009
H	-2.36036706539215	0.84422471076111	1.29765606721167	H	-2.34759258452450	0.83163434843904	1.30378237781611
H	-2.88736252696454	1.44240206187362	-0.27945362690838	H	-2.88788175061142	1.43913471139904	-0.26692449273553
C	-0.26414334825075	-0.59758473530796	0.14901901290175	C	-0.27771146240183	-0.59806769611263	0.14894984978188
H	-0.24915374152666	1.56511329401331	0.30529881895243	H	-0.24831160330666	1.56166605100038	0.29487092251361
H	-0.71640139340154	0.95042565168422	-1.28413067602016	H	-0.72765997143723	0.93951781096242	-1.28975359526845
O	-1.42260577965859	-1.49246477661390	-0.01694275581040	O	-1.42279126776251	-1.48384865281507	-0.02070750017555
H	-2.97614094756067	-0.78858837910309	-1.20779673166286	H	-2.96407547184338	-0.77806877669340	-1.21241559774114
H	-3.41265254084467	-1.15721672708790	0.48413195676269	H	-3.40716023643161	-1.15619092962659	0.47590422647010
H	0.05576247172055	-0.66478708894887	1.18951303570334	H	0.04047308052178	-0.65805596636635	1.19256769224016
H	0.52591869809931	-0.95567053346784	-0.50844517484139	H	0.52148833393833	-0.95392854120992	-0.50179742578796
Ag	-1.31435945938626	-3.64733627614607	-0.05680334391157	Ag	-1.31425817963472	-3.63601305864566	-0.05049818930581

$Ag(MeOC_2F_5)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-3.35098320401120	0.01921874218115	0.16956825413742	C	-3.34044006689005	0.02531011034164	0.17465374734990
C	-2.08924810306314	0.78119542766987	-0.32992607897411	C	-2.08259347563696	0.77936080187432	-0.32993508888784
F	-4.40080316426782	0.29553280355519	-0.55793542369733	F	-4.38365951635653	0.29932211094829	-0.55081357518632
F	-3.58503126198303	0.34100340207008	1.46239255780314	F	-3.57037163617529	0.35142430586121	1.45611060309119
F	-3.10857799868059	-1.31260320949619	0.14109296630847	F	-3.10116587488259	-1.29797197692740	0.15032807376459
O	-1.02929385140415	0.47420746646615	0.50110306343870	O	-1.03194550033215	0.47456634411019	0.50255414534057
F	-1.82979679687714	0.41343649334362	-1.59124909426730	F	-1.82470084562990	0.40254720207116	-1.57882934841026
F	-2.34267975676411	2.09549452876650	-0.31755133109517	F	-2.33110645538052	2.08476708016737	-0.32571698642314
C	0.23162407430258	1.16862746486375	0.18387214568680	C	0.21152702651616	1.16579394237981	0.18646979367169
H	0.94806045824993	0.81981076912487	0.91968728969059	H	0.93777031354341	0.82628555008445	0.91910876478989
H	0.07744891654064	2.23987103598464	0.27698730705659	H	0.05918105938730	2.23916141209701	0.27710237018086

H 0.54605743290831 0.89306018196474 -0.81906955286073	H 0.53244299851863 0.89364532824414 -0.81718682684504
Ag -1.30876674495030 -1.08627510649435 2.22538789677292	Ag -1.31692802668153 -1.10163221125218 2.20051432756388

$Ag(O(C_2F_5)_2)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
O 0.22829390297514 -0.60831763338551 0.50998473397174	O 0.22753549154249 -0.60930461151214 0.51611556633627
C -0.90530142946444 -1.04054480152515 -0.21003495639908	C -0.89613898267046 -1.04009091532520 -0.20305785185526
C 1.51781374147934 -0.82244000784127 -0.01992058538944	C 1.50658740403405 -0.82102918741316 -0.01695161985775
C 2.50785939996678 -0.76223294339570 1.18262756541717	C 2.49618263687017 -0.75983880895047 1.17803200734799
C -2.09707425535141 -0.15060515866362 0.25897908554945	C -2.08368301866973 -0.15148454551277 0.25961350552694
F 1.61063356449538 -2.00903295861982 -0.60489578193192	F 1.59790262685647 -2.00096230038446 -0.59710653519122
F 1.81590794511855 0.13548196426557 -0.89132218893096	F 1.79976091362975 0.13095587052017 -0.88376546928242
F 3.74797598888000 -0.78204645444026 0.76979857387327	F 3.72749336513117 -0.77662328655895 0.76039830148751
F 2.29298560062871 0.41306486061295 1.86444361141487	F 2.28216883459637 0.40364755135700 1.85613313224079
F 2.27120217034812 -1.75740880169059 2.02631116607678	F 2.26675177715772 -1.75331483458791 2.01318155004117
F -1.86249983930710 1.12314263770097 -0.04118429745481	F -1.84514125956121 1.11352019359458 -0.03903472639555
F -3.22378917317805 -0.55585730800577 -0.26503589389378	F -3.20174301129939 -0.55239084178692 -0.26937090552971
F -2.19344301331300 -0.23204674176248 1.62677049885315	F -2.18588643362555 -0.23390259365012 1.61481529629245
F -0.73501385017913 -0.88961530855179 -1.51642075019315	F -0.72251846910738 -0.89075906656850 -1.50081661162807
F -1.16041163489750 -2.31331709410753 0.06940892612301	F -1.15210543603747 -2.30406811448930 0.07582590671839
Ag -0.07746911820137 0.68567574941001 2.71944029291370	Ag -0.07949643884698 0.67954549126815 2.71493845374846

$Ag(C_4F_8O)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
F -3.88312570572073 3.92508351741119 -0.62247345766754	F -3.87668292475464 3.91184806389124 -0.61479850117855
F -2.89569445750606 -0.20408730168725 0.54969567897697	F -2.89294553936597 -0.19101450922968 0.54398050683856
F -3.45015189056119 3.46911860404392 1.44385303452651	F -3.43865038793660 3.45919975929733 1.43837640122557
F -0.27314124101800 1.16132083809290 -0.56382831190113	F -0.28406377706302 1.16462630473353 -0.55659637642603
F -1.07201482960157 1.41721085871429 1.46179995703908	F -1.08201656613775 1.42435953404557 1.45533849597565
F -1.47475405484945 3.35377246691321 -1.41662584954173	F -1.48385821108487 3.34240424576981 -1.41161888913618
F -0.97983912379714 3.92537494504552 0.64198293186148	F -0.98677004537600 3.91736959522867 0.63243536007983
O -3.66199851858445 1.79836995745987 -0.02309692815736	O -3.65445267872678 1.79958846943252 -0.01923362950293
C -2.62208918540322 0.84003599948086 -0.22089853930690	C -2.62273844311763 0.84965415652300 -0.21935709400885
C -1.30217188954394 1.58858644866789 0.15397334364112	C -1.30697553717646 1.59143761953695 0.15526367848323
C -1.66058823315129 3.07999228731225 -0.11913391403277	C -1.66394238620525 3.07504701658873 -0.12118175721911
C -3.19324292664334 3.13128639155585 0.18705887007383	C -3.18917939321730 3.12212769447767 0.18850273995662
F -2.64550036472992 0.45544519096200 -1.49095209630192	F -2.64419444615805 0.47093509770589 -1.48275743088386
Ag -5.90184757888970 1.25730919602747 -0.11076471920963	Ag -5.88968966367968 1.26123695199874 -0.11776350420395

$Ag(SO_2)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
S -0.20095703945735 0.18867987112298 -0.01278186399490	S -0.20467323029703 0.19052036156836 -0.01308918977339
O 0.29690654562778 1.52586073365804 0.00311629857675	O 0.31857371802426 1.51032807579068 0.00446179788029
O -1.65959828101555 0.03927941833372 -0.07308636983333	O -1.65696998897547 0.06898625273121 -0.07328558854100
Ag -3.37589997088731 1.48378170159891 -0.16966105293545	Ag -3.39647924448419 1.46776703462340 -0.17050000775283

$Ag(SO_2Cl_2)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
S -0.20235993680010 0.24999417501384 -0.01469336851088	S -0.20682428641013 0.24272423817857 -0.01533384036827
O 0.17058684509548 1.62139435857105 -0.00192753040376	O 0.15510514528030 1.61106013668007 -0.00255874418053
O -1.62820916831497 -0.06812639651531 -0.05998335125141	O -1.62321824061053 -0.08004726147299 -0.06159862666612
Cl 0.65007443173251 -0.69754288026677 -1.55216408426765	Cl 0.64257301661703 -0.68489268770310 -1.52952209583469
Cl 0.55059466859374 -0.70204871756481 1.57008423331298	Cl 0.54357113489715 -0.68824605573698 1.54746907080142
Ag -3.23164684030666 1.49156946076200 -0.17116589887927	Ag -3.20216676977382 1.49464163005442 -0.16830576375180

$Ag(SO_2ClF)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
S -0.16898722069972 -0.04970949031739 -0.06909704196619	S -0.16532509887796 -0.04884183062785 -0.06767246028486
O -0.05474242239310 1.38282591603005 -0.26469806335796	O -0.05451265978051 1.37685466301784 -0.25944933538403
O -1.43754209816090 -0.66600041629069 -0.12227976924145	O -1.42833120851069 -0.66338268317942 -0.12235401020378
Cl 1.15390308322770 -0.92993448340227 -1.23904533906405	Cl 1.13674987768899 -0.91550715452361 -1.22897647016669
F 0.47357394485426 -0.31452701990424 1.30851389818550	F 0.47074079016103 -0.31500430036065 1.29651090702606
Ag -1.61808528682824 2.98431549388454 -0.43242368455585	Ag -1.61120170068086 2.97285130567369 -0.43708863098670

$Ag(CH_3NO_2)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-6.92470204841086	3.51766186142320	0.01055141570651	C	-6.91486868852168	3.50794812910686	0.01159960762466
N	-5.90115386639668	2.43462552416606	0.04301621064301	N	-5.90146346294179	2.43549727414672	0.04430777347745
H	-7.41157394341682	3.43999746816259	-0.96243141865480	H	-7.40404554265851	3.43013602919322	-0.96148961420401
H	-6.40475888591826	4.46494490386244	0.10592886138654	H	-6.39835292238839	4.45871042701252	0.10313967083817
H	-7.63215138364836	3.32464098470888	0.81015899998878	H	-7.62622094834639	3.31826646238968	0.81002972259712
O	-4.77006531516298	2.67386107500840	-0.36510558494681	O	-4.77783484113971	2.67429906375291	-0.35892274895271
O	-6.22429523733796	1.32571015301492	0.45275627328592	O	-6.22345625333071	1.33413837478119	0.44963224953599
Ag	-3.97325931970811	0.37140802965350	0.04618524259084	Ag	-3.99571734067285	0.39385423961688	0.04276333908331

$Ag(CH_3CN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
Ag	-0.18057649228905	-0.00156861540177	-0.00012951587599	Ag	-0.16474793983261	-0.00159617012479	-0.00026746080433
N	1.94069808905497	0.00066788605680	0.00010535082729	N	1.94319032998868	0.00076456042558	0.00018824988894
C	3.08659649488644	0.00136043973079	0.00013177612538	C	3.08849909711747	0.00131318851425	0.00025914179782
C	4.53189934960512	0.00018305715906	-0.00000307561884	C	4.52746806625297	0.00015056420032	-0.00000478986885
H	4.89831605097468	1.02749291963616	0.03360571304908	H	4.89300764307242	1.02842816909983	0.03360459103911
H	4.89657676270564	-0.48483081557823	-0.90689959412436	H	4.89128275020181	-0.48525929237596	-0.90775534437132
H	4.89648974506219	-0.54329487160282	0.87318934561743	H	4.89130005319926	-0.54379101973922	0.87397561231861

$Ag(CH_2FCN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
Ag	-0.21346647279182	0.04720798754454	0.00197038104997	Ag	-0.19810159879870	0.04084707118020	0.00196694601534
N	1.92086751299370	-0.04318253325405	-0.00164414369801	N	1.92301025292034	-0.04312121739022	-0.00179261480650
C	3.06481300083898	-0.05777296539459	-0.00224751918916	C	3.06642184389489	-0.05100359461869	-0.00215703683062
C	4.53868375882730	-0.05162729377474	-0.00186105043447	C	4.53586313211564	-0.04413283652712	-0.00165449270998
F	4.97012302598328	1.24408122752932	0.04114307481399	F	4.97077702435779	1.23724909827736	0.04101147277172
H	4.89463502404044	-0.54027890586423	-0.91290021658255	H	4.88623767779617	-0.54092562937432	-0.91241243064644
H	4.89434415010814	-0.59841751678626	0.87553947404022	H	4.88579166771388	-0.59890289154722	0.87503815620647

$Ag(CHF_2CN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
N	1.85383095579752	0.02176309795300	0.02998251182454	N	1.85575847884084	0.02277134942413	0.03218911299912
C	2.99616129057092	0.00370247240416	0.03155474985584	C	2.99740388852295	0.00673588815469	0.03352340750176
C	4.50065775493748	-0.02958275588546	0.04669545653554	C	4.49909975380149	-0.02700128692903	0.04372403577778
F	4.93732828102095	1.23774600287170	0.07878268003206	F	4.93453291193442	1.22997934951440	0.07621729732489
F	4.90470537092367	-0.63222217137542	-1.08147766594075	F	4.89578262607365	-0.62707137222579	-1.07660150524396
H	4.86009517775923	-0.57717667256707	0.92208535297782	H	4.85432808737108	-0.57717372469651	0.92175134584027
Ag	-0.29139883100976	0.11064002659910	-0.04068308528504	Ag	-0.27552574654442	0.10662979675812	-0.04386369419985

$Ag(Cl_3CCN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
Ag	-0.25702542978361	0.00553619577558	0.00050137956261	Ag	-0.24059042634221	0.00701998181427	0.00082378680432
N	1.87743095928889	-0.00305314791999	-0.00014855122458	N	1.88032634583220	-0.00320647774168	-0.00024712148505
C	3.02213856118213	-0.00336300609928	-0.00041528645327	C	3.02438472408837	-0.00413855742914	-0.00057634167855
C	4.48821615416427	-0.00046342413324	-0.00017758610545	C	4.49014161184516	-0.00101489755843	-0.00032578337369
Cl	5.01004698809207	1.69576752019842	0.05580804322454	Cl	5.00065634382129	1.67992349984708	0.05534665664993
Cl	5.01814072874861	-0.79923574842766	-1.49467941479381	Cl	5.01126774000786	-0.79180251620670	-1.48032723875464
Cl	5.01763653598057	-0.89518468079982	1.43911334925142	Cl	5.01039815842026	-0.88677732413139	1.42530797529915

$[Ag(Cl_3CCN)_2]^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
Ag	3.23264322021467	12.18360133571137	3.91857389900388	Ag	3.23290196047555	12.18386369577256	3.91731944890869
Cl	4.33665432153771	6.97668513937395	5.26337853635370	Cl	4.33232136770287	7.00665770913948	5.25080826143659
Cl	0.15465324797759	16.73552040761789	3.55434514934458	Cl	0.17710901945887	16.70744705651326	3.55950657143720
Cl	1.96560753189510	17.16900878956006	5.82363517373862	Cl	1.97095946798424	17.14322761716976	5.80741206738804
Cl	3.82633667877892	6.95211483554356	2.37454460229452	Cl	3.82904717472298	6.97981234689032	2.38784953283155
Cl	6.45309621321514	7.77725967742457	3.39224862996839	Cl	6.43053884903010	7.79250386125504	3.39774238803493
Cl	2.92524914697107	17.57860473277702	3.08112040723912	Cl	2.91694553883504	17.55752260332858	3.09056396033501
N	3.88971812187292	10.21625135271964	3.82045492684600	N	3.87847311040311	10.22805777004484	3.81885723154207
N	2.58519068547568	14.15458741367799	4.01728750738985	N	2.59664632273216	14.14276282847245	4.01722321276838
C	4.70347091788344	7.74081884287893	3.70253892645162	C	4.69959168198079	7.75605477377544	3.70339322327797

C	1.83271674793440	16.64944149635496	4.13043836532123	C	1.83856731294486	16.63511424937300	4.12934987234130
C	4.24464061031648	9.12972773813062	3.77009982889435	C	4.23902455211108	9.14419578533529	3.76938261509646
C	2.25205202841882	15.24787224459025	4.06652963034161	C	2.26272705300695	15.23520346841896	4.06511442933338

$[Ag(Cl_3CCN)_3]^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
Ag	3.21846815514731	12.05028170951074	3.93042990812418	Ag	3.20033440240579	12.05076533764411	3.92830751253573
Cl	-1.38629043311067	11.98278689747459	7.30482930238309	Cl	-1.36616766382779	11.98117393314542	7.28055602783225
Cl	-2.31542512832377	13.08305865399238	4.75065442579535	Cl	-2.28632184147123	13.07180947384284	4.75061744662638
Cl	-2.00069823121127	10.18551187411553	5.07042999170856	Cl	-1.97509060746474	10.20139234712678	5.06676016643723
Cl	5.41152824669445	17.19917498022448	4.32086623622950	Cl	5.39895289176260	17.16974925106632	4.31087023356804
Cl	6.54529946639025	7.50642807602473	3.37538819505618	Cl	6.52205475828836	7.52718798651598	3.37989389873440
Cl	3.90615295273884	6.72939694147298	2.36127110974321	Cl	3.90762644443870	6.75910173583562	2.37626406499722
Cl	3.47340403755829	17.31841458177340	2.12310675374619	Cl	3.47970181341382	17.28908297538835	2.13443000353945
Cl	6.15971861200437	16.24435690481503	1.64919564645507	Cl	6.13933634643029	16.22409856817822	1.66431894974882
Cl	4.41837416713005	6.75158051195451	5.24858164865546	Cl	4.41649564014686	6.77769951615937	5.23539755495266
N	1.08225755980402	11.96050343981167	4.70617552492285	N	1.09825056944750	11.96006166022279	4.70866088248137
N	3.99046827298971	14.03333126936100	3.43719543183005	N	3.98783058201433	14.01784566320408	3.45122149178523
N	4.01409616654687	10.00026404588778	3.80732455565577	N	4.00544947340072	10.01566974588029	3.80158400331231
C	0.00045120289105	11.88632283133445	5.07494991888340	C	0.01526909336492	11.88611607154340	5.07143902491242
C	-1.38332652643439	11.78813177591761	5.53725444395144	C	-1.36883769893402	11.78822147734367	5.53132780667237
C	4.36418713165882	15.08266889403362	3.17278467330068	C	4.35897015052777	15.06553819226273	3.17919684641194
C	4.35726655936548	8.90929516514294	3.75325503514257	C	4.35122275301754	8.92571907181275	3.75434219043458
C	4.83945793149547	16.42203769284809	2.82714535728337	C	4.83355721547391	16.40448249554482	2.83015117541794
C	4.79528985666512	7.51561375430444	3.68647184113309	C	4.79026970061667	7.53209947615361	3.68909278777087

$Ag(C_6F_5CN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
N	-3.43785770079900	3.40891016554067	0.10298499307476	N	-3.43329253196624	3.40273585712470	0.10105858428844
C	-2.60329145976152	2.61900314718901	0.08033747664534	C	-2.59823033539731	2.61436380980196	0.08175518107810
C	-1.90640314699803	0.28334954732485	0.03274678448268	C	-1.90590568000156	0.28545993088322	0.03602971962515
C	-0.91091115450506	-0.67392120271448	-0.00910943160827	C	-0.91265815448958	-0.67027176348610	-0.00874296236397
C	0.42444817830032	-0.26950591386194	-0.03276075694590	C	0.41947220795116	-0.26494295685362	-0.03478791116338
C	0.76688462503142	1.08345659377724	-0.01018543631054	C	0.76353075475366	1.08481345586677	-0.00977413008869
C	-0.23439311657460	2.03503913169798	0.03166880782316	C	-0.23537307746779	2.03507004002036	0.03496825774305
C	-1.58350261892050	1.64903165967151	0.05143132075069	C	-1.57986168765904	1.64653210819517	0.05524937269664
F	1.37277536456520	-1.17684056250257	-0.07830107900922	F	1.36111727988212	-1.16650008846563	-0.08506599046112
F	2.03693523622338	1.44400862527311	-0.03133133554458	F	2.02539313389011	1.44057440940730	-0.03226238215284
F	-3.17762798647231	-0.08434234103316	0.05364764819535	F	-3.16814639908032	-0.07767000478096	0.05836885679752
F	-1.21287914607311	-1.95942023212558	-0.02898653578362	F	-1.21107697899106	-1.94722720990333	-0.02990881841388
F	0.07485789249238	3.32205775986527	0.05128536816890	F	0.07049027397326	3.31278713113997	0.05590544792210
Ag	-4.97077496650858	4.87016362189812	0.12898217606124	Ag	-4.95719880539742	4.85526528105022	0.11961677449289

$Ag(C_6H_5CN)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-1.64243248163808	1.57365014616566	-0.08301394814694	C	-1.64003213306147	1.57124560725113	-0.08166421142411
C	-0.32087143796426	2.04439325745331	-0.05531626024515	C	-0.32348421490860	2.04326545861031	-0.05450639430825
C	0.71465675255442	1.12959572434350	0.01436791789658	C	0.70994135113823	1.13034836370739	0.01404533784365
C	0.43943187224147	-0.23505759492439	0.05516109850423	C	0.43469372565246	-0.23095577601202	0.05406421835612
C	-0.87358626253684	-0.69817481470069	0.02778551522889	C	-0.87485752844699	-0.69391452668563	0.02745870084169
C	-1.92406694042782	0.19955164337867	-0.04178228849871	C	-1.92329946103873	0.20189716550132	-0.04098606977593
C	-2.70848264593690	2.49925682515919	-0.15415492496505	C	-2.70481482894451	2.49600776690844	-0.15241226212767
H	-0.12071266621728	3.10643828618750	-0.08790314908744	H	-0.12420046881096	3.10694991880178	-0.08676152620715
H	-1.07630271208350	-1.75974358527170	0.06072736713749	H	-1.07734520448999	-1.75688143310981	0.06014789550074
H	-2.94816646257778	-0.14649978124297	-0.06417675958894	H	-2.94908219990696	-0.14369219682517	-0.06305697574053
H	1.73773546847771	1.47878116716745	0.03701243928194	H	1.73433710174510	1.47981237287186	0.03640374361743
H	1.25533541693632	-0.94360313470578	0.10891322462873	H	1.25181666665839	-0.94034232952258	0.10702996348879
N	-3.57776397141446	3.25318832039831	-0.20154445111535	N	-3.57298905913229	3.24948833178235	-0.20178390404416
Ag	-5.15911392941298	4.63380354059197	-0.33852578103029	Ag	-5.14502374645369	4.62235127672065	-0.34042851602064

$Ag(NH_3)^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
N	-2.38781048769524	0.96241811944982	0.84242138104377	N	-2.38923321383580	0.95664150116004	0.84194859001956
H	-1.38316941215153	1.11660432907804	0.79835233373709	H	-1.38643590333303	1.11514298420661	0.79844059341877
H	-2.81270855589274	1.49689479602747	0.08823535852575	H	-2.81160757483879	1.49464394157695	0.09046654301502
H	-2.71905788171147	1.35609687988142	1.72010698641221	H	-2.71822661949010	1.35414396855639	1.71738379992927
Ag	-2.87686366254901	-1.17727412443675	0.68627394028119	Ag	-2.87410668850227	-1.16583239549998	0.68715047361737

$Ag(N(CH_3)_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N -6.43923874522003 3.01133963897018 -0.12031466841891	N -6.44076307728038 3.01017975767291 -0.12482832619008
C -4.95379373868689 3.02134418918087 -0.11061494006224	C -4.96670063864857 3.02158991858738 -0.10969506117195
C -6.94760238276402 4.33939437561863 0.30931883842853	C -6.94253742411485 4.32754143021213 0.30661345276961
C -6.93790036926664 1.96404429195665 0.80759699423163	C -6.93310797241142 1.97368143514023 0.80050114964752
H -6.58108412073921 5.11212461401763 -0.36318673135795	H -6.57591784614517 5.10576907128508 -0.36187571551075
H -6.59669709548780 4.55618234537417 1.32293767418562	H -6.59039502807989 4.54229853124545 1.32199582962560
H -8.03563057273551 4.33884754984144 0.30619825039654	H -8.03204658198901 4.33202812042239 0.30731597633669
H -4.58447176029744 3.78996231267893 -0.78623572240112	H -4.59169145796384 3.79148897831630 -0.78310093309449
H -4.57416572087099 2.04985629031544 -0.42026129843648	H -4.58074053645149 2.05006100645908 -0.41657644593127
H -4.59475168489189 3.23619042728381 0.90056759683669	H -4.60919799545082 3.23726744689877 0.90362487313645
H -6.56469336404301 0.98895833870251 0.50155214202669	H -6.56040443098549 0.99496194513448 0.50023873266616
H -8.02589460824194 1.95533074390654 0.80602899914437	H -8.02255916462735 1.96242383096337 0.80471575798121
H -6.58689431101507 2.17503796045494 1.82236225133437	H -6.58058067377748 2.18688901665959 1.81602341043372
Ag -7.15559152573952 2.58040692169826 -2.16589938590774	Ag -7.15176717207419 2.58283951100283 -2.15490270069843

$Ag(NF_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N 0.14799085346251 -0.20087254167763 0.15681032867585	N 0.14845148596725 -0.20061908982195 0.15632179735556
F 1.37888666885714 0.14553086650443 -0.29392194483128	F 1.36489806013084 0.14164591183194 -0.28882658827236
F -0.42810993146389 -0.83407582785037 -0.89536623170939	F -0.42151923348705 -0.82761677463888 -0.88228980004010
F -0.51909609139587 0.97679541954376 0.24542915034010	F -0.51140091102505 0.96255720669224 0.24572328432888
Ag 0.14948850054013 -1.46992791652019 2.16954869752472	Ag 0.14873059841401 -1.45851725406334 2.15157130662802

$Ag(N(CF_3)_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N -6.39105633213742 3.05322923441230 0.02383207620482	N -6.39094280879472 3.05381435036179 0.02401164113225
C -4.89702528133826 3.00672791530691 -0.08496166788361	C -4.90739371304839 3.00639230980439 -0.08455661970823
C -6.93290225875720 4.41120951767838 0.35456701662718	C -6.92878388552033 4.40256184451944 0.35279845791267
C -6.96591965158499 1.95572999254256 0.86724952682068	C -6.96187937441615 1.96452111859222 0.86240682941716
F -6.86156363871139 5.15808186910600 -0.75093658803191	F -6.85577947971207 5.14752387217741 -0.74338664873046
F -6.25682522284470 4.98736886544629 1.32489674058343	F -6.25902657058805 4.97329043091959 1.32056411278894
F -8.20417690730940 4.28824237088171 0.69482184133894	F -8.19329413382141 4.27843526036507 0.68817960845674
F -4.46542325215121 4.15757860773543 -0.56796760332414	F -4.47837072706029 4.15136635848255 -0.56282451459041
F -4.58657658874968 2.03989393595407 -0.95554459764757	F -4.59881662382918 2.04689549507922 -0.95092927487242
F -4.32809892881620 2.75857057041424 1.07427161531729	F -4.34174156526236 2.75792053751669 1.06752674254323
F -6.23086584450447 0.86854088983032 0.71194466091391	F -6.23000037892382 0.88426169176116 0.70859477480725
F -8.19778105084302 1.70135127547286 0.41440077930692	F -8.18601688169951 1.71054920095184 0.41380411080922
F -7.02110398494892 2.29006973207001 2.13766284502823	F -7.01621271856359 2.29780539036270 2.12528760059799
Ag -7.18808105730317 2.57961522314890 -2.20453664525420	Ag -7.17914113876015 2.58087213910590 -2.18177682056397

$Ag(I_2)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
I -2.27012812878730 -0.20072681451288 -0.26696063883497	I -2.26836463957186 -0.20704048634364 -0.26177540349338
I 0.31441427147564 0.60512277357351 -0.31551435144489	I 0.27033911952400 0.62409776666852 -0.33956156161188
Ag -3.19272143558835 1.73636205753936 -1.94111549252014	Ag -3.15040977285214 1.72370073627512 -1.92225351769473

$Cu(C_6H_5CH_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
C -1.61995395194671 1.61580734527456 -0.05549408897082	C -1.61964798044481 1.61592307394747 -0.05617664509431
C -0.27179911352361 1.97036781944038 0.17871852653178	C -0.27286829962496 1.96971232761551 0.17572171019508
C 0.74406539853389 0.99897562102036 0.20013563474613	C 0.74216885194281 0.99963695775560 0.19484099564176
C 0.43537795513348 -0.35409983246140 -0.02555835267126	C 0.43365044453574 -0.35145146554472 -0.03164858001625
C -0.89742929719431 -0.72179264398394 -0.28177962112391	C -0.89754874630769 -0.71857810719406 -0.28676522571704
C -1.90943913105947 0.25444219613568 -0.30237292392448	C -1.90818020242217 0.25670881823832 -0.30508019223472
C -2.71316457578518 2.64013070782992 0.00994548446859	C -2.70760235063428 2.63607091283730 0.00338480111253
H -0.02095351460341 3.00662396868784 0.36532427172366	H -0.02095827679048 3.00848233535378 0.35474931644155
H -1.14918879756153 -1.75950632922383 -0.45453331449902	H -1.14822637877235 -1.75574629882621 -0.47200412854845
H -2.93316807299703 -0.04429233693881 -0.48755709731692	H -2.93217117869684 -0.04045284290351 -0.49917908755366
H 1.76541185992495 1.29482129026520 0.39875197203355	H 1.76639575184039 1.29736552154889 0.38253589881503
H 1.21293462952383 -1.10467775366811 0.00468176010389	H 1.21428397514777 -1.10118499527214 -0.01553397661842
H -3.07993768121571 2.71342102316990 1.03761021147724	H -3.07335075428027 2.71444054512902 1.03172784314409
H -3.55832823604290 2.36735424527261 -0.62083630521456	H -3.55469278745426 2.36005173048117 -0.62421957145847

H -2.35784090359562 3.62762538681771 -0.28215952134412	H -2.35366436269388 3.62343392155786 -0.29262387733951
Cu -0.28574656759066 0.85223929236194 -1.94293663601978	Cu -0.30674770534470 0.84302756527574 -1.81778928076925

$Cu(C_6H_5F)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
F 0.48326727873858 -1.74930636123089 -0.26209587872253	F 0.44632018833891 -1.71302756681631 -0.10858325922331
H -2.00375523539443 -1.10787954439747 -0.07001934597258	H -2.04762927457573 -1.05985176101809 -0.03349588607588
C -1.76749962785014 1.04278544161600 0.08842651064626	C -1.80659826648250 1.10126762532102 0.00423823448675
C -0.83515588402499 2.11901251047310 0.12203070298898	C -0.88349185406354 2.16638427270218 0.01596592177862
C 0.54668662907256 1.83513113854703 0.04346425284025	C 0.49533141332859 1.88516486908538 0.02657127594812
C 0.98783522293430 0.52882018432483 -0.09010637554654	C 0.95187292601572 0.56449128790381 -0.00524227636409
C 0.05111675346285 -0.50327217858867 -0.12661985575787	C 0.01976297151861 -0.47208827911271 -0.04661760848668
C -1.31354419971235 -0.27680802109510 -0.02189888688336	C -1.35459569737484 -0.22752997826824 -0.00914792493204
H -2.82980540734564 1.25010663579154 0.04285771416293	H -2.87090009513790 1.30270540909850 0.00575925543175
H 1.25999349452448 2.64827647928896 0.04522147815238	H 1.21144265578419 2.69754738097597 0.04408794937524
H 2.03998141912323 0.29350428238604 -0.17668103998962	H 2.00958173950115 0.33097644098200 -0.01882163155357
H -1.18498867179180 3.14242247779772 0.05180022590324	H -1.23217966301203 3.19110955976693 0.01801653239736
Cu -1.16213177173664 1.62162695508690 2.14057049817846	Cu -0.66691704384061 1.07727073937954 1.89421941721775

$Cu(o\text{-}C_6H_4F_2)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
F 1.55880748918865 5.23196908807514 -1.06777032612401	F 1.53629927110073 5.20976547564389 -1.10378543850421
F 2.95179738639739 2.99048070803509 -0.66137128596495	F 2.92549116907382 2.97086021859642 -0.72152284522561
C 0.99590189187296 1.73742375349948 -0.36016773744278	C 0.97508417594730 1.73371610713344 -0.36325190273968
C -0.40699593537525 1.71017921268104 -0.27235682651558	C -0.42406554975098 1.71262765842346 -0.24359490308028
C -1.15130315056341 2.90696020809685 -0.46984674056786	C -1.16421327491360 2.90523281351144 -0.43772247238855
C -0.47855335311020 4.10994153738630 -0.75849664645568	C -0.49203586294892 4.09879281984271 -0.75091653353323
C 0.90147624087242 4.11552895381663 -0.81617304276160	C 0.88773035634159 4.10366323376147 -0.83232008922281
C 1.63511472477227 2.93514596309267 -0.61428083694581	C 1.61881799727272 2.92570421381390 -0.63515890622408
H 1.58851109967764 0.84834654203851 -0.19191985520819	H 1.56779047884945 0.84155975610210 -0.20004619870690
H -2.21379027085515 2.92685663398473 -0.25679252729078	H -2.23094558286805 2.92305617492822 -0.24308551788221
H -1.01804519343350 5.03837264166202 -0.88981830763820	H -1.03126325673211 5.02916100261694 -0.88424620296309
H -0.90301121449599 0.81375544094423 0.07968996361130	H -0.92116186625951 0.81047159804279 0.09533188091049
Cu -1.07406818938638 1.85657617244696 -2.33283885076121	Cu -0.86168652955098 1.95692578334288 -2.30795066623519

$Cu(o\text{-}C_6H_2F_4)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
F 1.48588019198954 5.16822647792620 -1.30171072780408	F 1.50041832012967 5.15018664938273 -1.29134374561634
F 2.96314094603184 2.99796471050541 -0.66137128596833	F 2.94779771110078 2.96904903289638 -0.67465500282818
C 1.03366458870091 1.75341319728676 -0.20301820280323	C 1.01711842238928 1.74582537744443 -0.21575025188647
C -0.35555954903058 1.67465024890899 -0.14385754362916	C -0.37152079843481 1.68356338378031 -0.15048875325825
C -1.14644211989911 2.78121585519676 -0.46647265332230	C -1.14841417484720 2.80062431287307 -0.46176727006032
C -0.51362998962762 3.99499155993210 -0.87729795212128	C -0.50540844761695 4.00611906037737 -0.86567797289441
C 0.88150471249599 4.04901878882458 -0.94619147221829	C 0.88675839858308 4.04479567622243 -0.94294206656854
C 1.65256084408638 2.94028334753484 -0.60625074000900	C 1.64554170349606 2.92540028707569 -0.61378989824563
F 1.77317491124726 0.71637374659570 0.11716849137526	F 1.74052746839986 0.70537403521867 0.09424218429310
H -2.20233389576904 2.75810171865205 -0.22245513955109	H -2.20707245474706 2.78684425636695 -0.22110811936462
H -1.07532179058087 4.91932744389526 -0.94915074532486	H -1.06105098823498 4.93527995023832 -0.94613614947075
F -0.91833498281086 0.54955447895786 0.25724599158617	F -0.93972940354843 0.56941998963755 0.24304400498387
Cu -1.19247386683385 2.91841896578342 -2.62491802020979	Cu -1.11913575666931 2.89905798848606 -2.58190695908345

$Cu(C_6H_5CF_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
C -1.48170924734261 1.61281950565736 0.00996579839689	C -1.47620878254531 1.55109771305596 0.07052115483352
C -0.17151857131403 1.98071747863376 0.27830932412549	C -0.15558423974598 1.95413566927718 0.23059243315830
C 0.83287917444903 1.01081933157284 0.28020700287581	C 0.84999055182719 0.99749814590730 0.21086840722782
C 0.54378833017241 -0.31605999244968 -0.01167279018864	C 0.54352405364255 -0.34196121025545 0.01449602110365
C -0.77187851597856 -0.70713437374574 -0.26441537427576	C -0.77645655004559 -0.74509954919131 -0.14889429488583
C -1.80668453274450 0.25006801658276 -0.23185295166479	C -1.79718875495387 0.19791126314888 -0.11700854758083
C -2.60265418492319 2.62868250665587 -0.04655288582049	C -2.57592321752512 2.56312079859881 -0.05340902739899
H 0.06565680553405 3.01499342063827 0.48459553176352	H 0.08017818156409 3.00124553296659 0.37571786263012
H -1.01461351819153 -1.75126020955120 -0.41228914158485	H -1.01746664082386 -1.79394171766914 -0.27172769743543
H -2.84592358822374 -0.06845071183077 -0.22930701495396	H -2.83754863461172 -0.11461963668971 -0.16218007101471
H 1.85014059441182 1.30292451880413 0.50395767098372	H 1.88014175051715 1.30322146475181 0.34614011711218
H 1.33304858147952 -1.05539724760230 -0.01808678973939	H 1.33663178164658 -1.07946543735770 -0.00043633478891
F -3.58657394262605 2.33517159384271 0.80259424778173	F -3.71178881510217 2.20229536303133 0.49411734115367
F -3.14851441533377 2.60179618472943 -1.31212182114585	F -2.85067430180142 2.65059442356133 -1.45245979942099
F -2.18551295143454 3.86803917693068 0.17791713930601	F -2.25170419960077 3.76996852682733 0.32429955520009

B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
Cu -1.64909001793428 0.64971080113184 -2.26930794585944	Cu -1.87908218244173 1.24143865003674 -2.11869711989364

$Cu(m\text{-}C_6H_4(CF_3)_2)^+$	
B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
C 0.00076523245378 2.39615991075351 -0.04871464690805	C 0.00461170678591 2.37874596233839 -0.06776001303083
C -0.83199524629780 1.27918069163376 -0.02051946243721	C -0.82534775255080 1.26203620638328 -0.01985849174343
C 1.38261711477835 2.23917384830902 -0.01935812445815	C 1.38466996402684 2.21777215635119 -0.02537749156578
C 1.95035184987452 0.96657395950899 0.07874644388824	C 1.94955666409853 0.94257608754341 0.10701757935451
C 1.10757951645527 -0.16933658161440 0.14269898217980	C 1.10677540726126 -0.18558162636173 0.19160715017727
C -0.29579084391971 -0.00349443856749 0.07212596358528	C -0.28835745764737 -0.01926073504099 0.10112883706137
H -0.42804136254015 3.38765369903132 -0.09853541740005	H -0.42281443471173 3.37138580483957 -0.14369271175790
H -0.94752337729773 -0.86335275303608 0.15205241260631	H -0.94383183449287 -0.87901083769251 0.17377251121080
H 1.52620845691669 -1.14199443152924 0.37738571271434	H 1.52748638842808 -1.16668052172638 0.38087371302478
H 3.02215671217449 0.85307160194172 0.17698296649462	H 3.02308346327646 0.83013472838247 0.20644173094204
C -2.33562057219815 1.44906837144579 -0.14894040463478	C -2.32549769846058 1.42884215232995 -0.16251110603575
F -2.74002538434053 2.62760369521449 0.32582791696024	F -2.72890937255750 2.59691437111022 0.31381459399390
F -2.99027108476655 0.47725505069584 0.49678286381640	F -2.97670959892851 0.45822149393922 0.46699673559297
F -2.67787956496145 1.38162815652658 -1.45258863407159	F -2.64986028402503 1.37117060631872 -1.46084756921490
C 2.29537875230396 3.44672579824472 -0.14158766817435	C 2.30066485796079 3.41783395715920 -0.16795582875972
F 1.68107404546727 4.56969647631887 0.22996313640981	F 1.69184079547526 4.53761131800030 0.18807576230341
F 2.67912259632200 3.58350911876349 -1.42922140585461	F 2.67530976322623 3.53291507203756 -1.45060983569549
F 3.39916482537270 3.29421995365862 0.59883340482230	F 3.39660290609632 3.26980908884025 0.56590843606329
Cu 1.16682833420302 -0.09273212729948 -1.95088403953855	Cu 1.06482651673869 0.31517471524790 -1.85597400192053

$Cu(CH_2Cl_2)^+$	
B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
C -2.26554223680170 1.20362015735629 0.11319679289672	C -2.25644926595597 1.20465706669445 0.10317137457874
Cl -0.48010108561014 1.09060946229561 0.32865600499591	Cl -0.49181165591993 1.07918109866628 0.31372060137874
H -2.65048800620155 1.92936377598615 0.82005902103533	H -2.63622042402405 1.93871935732190 0.80778309236430
H -2.68807787135569 0.21199522284945 0.22695200769974	H -2.69259431641063 0.21842231756518 0.23388249086559
Cl -2.62533172503772 1.78952718528627 -1.55223078046143	Cl -2.61523330415168 1.77020652364093 -1.54740408322689
Cu -0.25092907499320 1.97202419622624 -1.90181304616627	Cu -0.26816103353774 1.98595363611125 -1.87633347596048

$Cu(C_2H_4Cl_2)^+$	
B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
C -3.16906378583789 1.65370280264238 -0.05821576089221	C -3.16770722605253 1.64784126054648 -0.04843491959583
C -1.67291692403121 1.49451048268935 -0.09543356614394	C -1.67454089554670 1.49364068704816 -0.08368648686898
Cl -3.98551207693101 0.44243405097990 1.05282761372615	Cl -3.96977868431488 0.45480382854454 1.04930904350843
H -3.58349036238666 1.44230723215496 -1.04278169330620	H -3.57813487396810 1.43995087598763 -1.03722288858069
H -3.48946262196258 2.63326895870111 0.28410989467072	H -3.48665281557890 2.63281653691855 0.28612545807878
H -1.35206037085353 0.49483002372906 -0.37330994179257	H -1.35489276575847 0.49381336327906 -0.37036752170360
Cl -0.88047195505803 1.84368510003752 1.52323899445350	Cl -0.89672209988290 1.83658302568262 1.51332594308877
H -1.24476971890714 2.23209086070147 -0.77272843353640	H -1.24998285903860 2.23025331235347 -0.76695501525473
Cu -2.45492218403197 0.69412048836425 2.76417289282098	Cu -2.45425777985891 0.70124710963949 2.73978638732789

$Cu(CCl_2FCClF_2)^+$	
B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
C -1.31130205217567 1.54402023116975 -0.10168937345374	C -1.15783869845986 1.58336693552778 -0.01323389510443
C -0.36183887526111 0.28726761430188 -0.04885862643268	C -0.26606294247001 0.29249670293683 -0.08368835657901
F -1.02797362579485 2.17925924074315 -1.23158953674184	F -1.13395414933795 2.14164400427000 -1.20152583875553
Cl -0.85668953575035 2.72827488486507 1.25640992560059	Cl -0.50721550167192 2.71884498146570 1.19843113255425
Cl -2.98866091498475 1.11238454445454 -0.00697372503857	Cl -2.82313062424709 1.15858244910277 0.43589839180879
F 0.89901399599952 0.67605600757662 -0.08866793427543	F 0.95400002942566 0.63672834422550 -0.41620389166941
F -0.63333849682022 -0.49404419731946 -1.07057394755704	F -0.76700354824948 -0.52250136207358 -0.98052017725722
Cl -0.60032031029001 -0.72069192498523 1.47866167610016	Cl -0.20561609146674 -0.57579773509254 1.50500068915481
Cu -0.59055018492255 1.12047359919368 2.90173154179856	Cu -1.56483847352261 0.99963567963756 2.64429194584775

$Cu(CH_2ClF)^+$	
B3LYP/def2-TZVP/D3BJ	PBE0/def2-TZVP/D3BJ
C -5.22104122705466 2.66015770110121 -0.09522081842610	C -5.21110900098979 2.66680742498828 -0.09357854928831
Cl -3.40498412804367 2.83116711905802 -0.35500914346638	Cl -3.42113737381197 2.83560170502075 -0.35034195402337
H -5.67102142888423 2.61413523256311 -1.08189223000129	H -5.66652197220559 2.61539876075300 -1.07985050193837
F -5.62389230851746 3.78231901580709 0.56445075472385	F -5.61707393979457 3.78046212832810 0.56152763472883
H -5.36224601088427 1.78008257962563 0.52439010709397	H -5.35798968561325 1.78363761735055 0.52412476940482
Cu -3.30820489661571 4.81279835184494 0.76395133007595	Cu -3.31755802758483 4.79875236355931 0.75878860111640

Cu(MeOEt)$^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-3.29672144768960	-0.04866187109635	0.18833075102251	C	-3.27369828356325	-0.01235991675244	0.23229893866305
C	-2.12940304729418	0.76206851817689	-0.31366876301392	C	-2.11807640440787	0.78465404659456	-0.30557094611195
H	-4.19684346024579	0.18186029710169	-0.38344210226758	H	-4.17987212734572	0.15334795458244	-0.35343036529171
H	-3.53129447547549	0.20206394702812	1.23346940955925	H	-3.51876126858954	0.29084263119222	1.26061377769347
H	-3.11271814285446	-1.12098064854671	0.08589634647632	H	-3.07197129397368	-1.09215834725153	0.17478562115003
O	-0.96829869591298	0.43755833938321	0.50584324853808	O	-0.98285948391981	0.50085336321651	0.53073028447016
H	-1.87811067094172	0.51518425661137	-1.34654503947339	H	-1.87210767090200	0.50158925399518	-1.33271722453436
H	-2.31047512087094	1.83571723223711	-0.23297055707696	H	-2.31431468327525	1.85973783588148	-0.26909264501654
C	0.23897610879101	1.15138813461027	0.14308981106784	C	0.22679614779640	1.16877099203695	0.15161439554998
H	1.03884060744299	0.78475796869029	0.77989558400135	H	0.99863131758842	0.88544496303566	0.86307053043422
H	0.09222026196322	2.22090992350775	0.29486798714866	H	0.07235983906977	2.24872851995268	0.18436065165469
H	0.47160141895345	0.94151704984430	-0.90054799151438	H	0.51688674808087	0.85766496528649	-0.85372049033937
Cu	-1.34200333586550	-0.48471314754796	2.16485131553222	Cu	-1.40724283655835	-0.76844626177022	1.93612747167832

Cu(C_4H_8O)$^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-2.66778661728058	-0.72516689473628	-0.16568486872863	C	-2.65421161632025	-0.72437997801668	-0.16712989198991
C	-2.26257282273318	0.68400351769744	0.21956514225239	C	-2.25667977269324	0.67923163526326	0.22248469940275
C	-0.79272078907743	0.75589604862146	-0.21413397372758	C	-0.79795186172027	0.75089855889287	-0.21711877503623
H	-2.35512481395655	0.82890267321643	1.29653094594142	H	-2.34305566843955	0.81795408772889	1.30200025006217
H	-2.88194144539822	1.42629704985684	-0.28087416776502	H	-2.88239931275995	1.42292132667317	-0.26988592669535
C	-0.25891307947688	-0.61445861788727	0.15277028255758	C	-0.27280099720574	-0.61514084460278	0.15304382540969
H	-0.24532205524401	1.54581508758582	0.29719934193041	H	-0.24440984390754	1.54234159640506	0.28711191581466
H	-0.71403935054052	0.92344121760142	-1.28894241970168	H	-0.72462726909228	0.91272592429478	-1.29440371538179
O	-1.42301238912303	-1.51293921230561	-0.01822194710435	O	-1.42340017875373	-1.50338955294639	-0.02065404773388
H	-2.97900640834982	-0.80579045531022	-1.20706347059843	H	-2.96700636126925	-0.79640760915643	-1.21079126620114
H	-3.41494015717756	-1.17097836854040	0.48742275651692	H	-3.40902927667629	-1.17003539860992	0.48046079513635
H	0.05014159652979	-0.68183317646807	1.19583278907809	H	0.03505503576488	-0.67491283172950	1.19908371800073
H	0.53228543814199	-0.97781299726692	-0.49952232329905	H	0.52712116936825	-0.97705139562464	-0.49260573951715
Cu	-1.33283710631401	-3.40962587206466	-0.05868808735207	Cu	-1.33239404629501	-3.39900551857170	-0.0554058412709

Cu($MeOC_2F_5$)$^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
C	-3.37107907030450	0.10049073767520	0.28075831193058	C	-3.36068785263435	0.10060290390478	0.28029099693032
C	-2.08933401014240	0.75420168458614	-0.32676583545416	C	-2.08382581472013	0.75379666491933	-0.32276167021102
F	-4.33539996097733	-0.02175978967696	-0.58432126077458	F	-4.31758342691448	-0.01589110032322	-0.58481675810886
F	-3.76536418521186	0.73748416469798	1.36224011503184	F	-3.75428724386885	0.73588397552382	1.35422247247813
F	-2.99632844601636	-1.19404840904975	0.68988917657174	F	-2.99209428394635	-1.18098825356876	0.68280778326152
O	-1.03075655798981	0.43231929655512	0.50969709070721	O	-1.03418316684366	0.43392269861661	0.51461205959680
F	-1.88164565195573	0.26347546638580	-1.55645663593580	F	-1.87256392849956	0.26596728399015	-1.54266683538268
F	-2.26253609169432	2.06935945908434	-0.41318766737055	F	-2.25664804070146	2.06036211277688	-0.40761694983880
C	0.22083638279060	1.18133477176376	0.27712350551424	C	0.20162141568009	1.17449516812114	0.27565576217673
H	0.92265912339969	0.79768223057823	1.01042071262245	H	0.91641747820568	0.79569297885312	1.00090964073355
H	0.03251461188551	2.23667183458160	0.44561983165212	H	0.02025104583057	2.23252687314233	0.44569253846655
H	0.56717544467126	0.98829803380615	-0.73482668140035	H	0.54591057350893	0.98580920137797	-0.73964639954107
Cu	-1.25273158845476	-1.20292948098760	1.30416933690527	Cu	-1.25431675509643	-1.19960050733415	1.30767735943882

Cu($O(C_2F_5)_2$)$^+$							
B3LYP/def2-TZVP/D3BJ				**PBE0/def2-TZVP/D3BJ**			
O	0.22665329661004	-0.61057827598873	0.51260853949452	O	0.22522292163371	-0.61389465733162	0.52103887335290
C	-0.92279784768609	-1.04233518799222	-0.19635391088267	C	-0.91368188709599	-1.03436773255049	-0.19464215017091
C	1.52770547599310	-0.80316216033781	-0.01383384311104	C	1.51534835909967	-0.81249049101763	-0.00671251157843
C	2.49943647490253	-0.77508842311392	1.21226512071500	C	2.48854759910398	-0.77247892479616	1.21021409154509
C	-2.08952657633395	-0.10196765570297	0.25126959692211	C	-2.07470178885737	-0.09734009991731	0.25082886665917
F	1.62785572631870	-1.96887548031771	-0.63161800308719	F	1.60932760065328	-1.97888258875176	-0.60678503438077
F	1.82197266111497	0.18359995099213	-0.84845111341706	F	1.80657405362880	0.15780751960163	-0.84856808825286
F	3.73981843209399	-0.63327995382033	0.83380423271181	F	3.71949429952519	-0.62994258799937	0.82322202619745
F	2.16290638017157	0.31555662000143	2.00370917536895	F	2.15548183848067	0.31000061931171	1.98986466841662
F	2.33934533437680	-1.85625601553845	1.95290308813679	F	2.33828714404254	-1.84627577345867	1.95055973519105
F	-1.90002983523170	1.12111240699261	-0.20924790100716	F	-1.87213753013433	1.12445704459518	-0.18730852030337
F	-3.24918538361030	-0.57582066667957	-0.11301920258012	F	-3.22482832093591	-0.55649437574575	-0.13797725346820
F	-2.06884027186637	-0.02376403626519	1.63786726253020	F	-2.07107228920428	-0.04248782914093	1.62488943047789
F	-0.74893261922217	-0.94027704796323	-1.50355222532940	F	-0.73084347096836	-0.92431013939254	-1.49148826695550
F	-1.19869831082833	-2.29549794619301	0.13372735262195	F	-1.19644383123156	-2.28040655782305	0.12367915580650
Cu	-0.03001293680277	0.44053387192697	2.45687183091331	Cu	-0.03690469774004	0.43100657441672	2.45813497746337

$Cu(C_4F_8O)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
F	-3.90303672855075	3.93282825052005	-0.61085070399860	F	-3.89664911427772	3.91932942907507	-0.60485658824491
F	-2.91676568433419	-0.21218592357968	0.54074796416649	F	-2.91676658685147	-0.19730143976559	0.53516669117827
F	-3.46353580035308	3.45726081085606	1.44894620716535	F	-3.45382816902894	3.44600893721728	1.44211283432194
F	-0.29025917563248	1.15659771133529	-0.54955761687903	F	-0.30081741174161	1.15996028337646	-0.54254712187373
F	-1.10944177460704	1.41769216853604	1.46759449619997	F	-1.11939577875739	1.42405012686345	1.46092224538010
F	-1.50455137631867	3.33765883932370	-1.42426074348708	F	-1.51120545892751	3.32774329609870	-1.41830597258869
F	-0.99626769846520	3.92148118513563	0.62817160705007	F	-1.00344573662170	3.91328152811477	0.62073052377388
O	-3.68934205495996	1.79394671633918	-0.03229696760716	O	-3.68007244089936	1.79615623369899	-0.03149213886352
C	-2.63707926812219	0.82708467226025	-0.22809891613122	C	-2.63797475264851	0.83776940380447	-0.22735048952026
C	-1.32569478638363	1.58421362491201	0.15744138857377	C	-1.33012784546465	1.58706671842753	0.15855212875418
C	-1.68258717988954	3.07397544949821	-0.12421568596668	C	-1.68517721234129	3.06945299174800	-0.12576505853717
C	-3.21247165835015	3.13751202526018	0.19006632372260	C	-3.20825437024207	3.12776701297692	0.18986312835576
F	-2.65729410796557	0.45142777431071	-1.49664067277941	F	-2.65519679822978	0.46603195964222	-1.48898852106689
Cu	-5.62783270606753	1.31932669529234	-0.09645668002907	Cu	-5.61724832396797	1.32150351872169	-0.09745166106896

$Cu(SO_2)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
Cu	-3.23004098973146	1.18202444292625	-0.13311759880929	Cu	-3.24666059713308	1.16788124954049	-0.13371403167848
S	-0.19537346526200	0.18952465431550	-0.01547972603249	S	-0.19861463349370	0.19195375407560	-0.01551298930144
O	-1.66296491516991	0.04317554800949	-0.07032309846716	O	-1.65792117459465	0.06676405816018	-0.07025039250155
O	0.30335937016336	1.52354535474876	0.00459042330895	O	0.31817640522142	1.51167093822372	0.00514741348148

$Cu(SO_2Cl_2)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
S	-0.19783379567339	0.30464729374970	-0.02009754726715	S	-0.20229173993023	0.29603863733281	-0.02105554704923
O	0.25912449953590	1.64629645734876	-0.00492834838388	O	0.24485455250047	1.63483292098189	-0.00653470466089
O	-1.64677212475492	0.06483411127893	-0.07358286984742	O	-1.64201069066801	0.05250913762644	-0.07546866707783
Cl	0.58463751947987	-0.69923686528499	-1.55384823365333	Cl	0.58047065364457	-0.68800195300645	-1.53103185629211
Cl	0.46402850689510	-0.69694554513189	1.57068685963934	Cl	0.45937271611517	-0.68384438517699	1.54841665168311
Cu	-3.15414460548254	1.27564454803949	-0.14807986048755	Cu	-3.13135549166197	1.28370564224230	-0.14417587660305

$Cu(SO_2ClF)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
S	-0.16327835746441	0.29501276386764	-0.01114466942667	S	-0.16369688548617	0.29063061593835	-0.01121497420530
O	0.37175834265525	1.59613282272297	0.05876180107527	O	0.36997945749010	1.58629857259572	0.05644815142914
O	-1.60382064582345	0.10771643646339	-0.11996601129063	O	-1.59673031208254	0.10634786500041	-0.11738606625662
Cl	0.67634008984582	-0.81077867760403	-1.40650477873171	Cl	0.66511451737061	-0.79734303359413	-1.39227992497255
F	0.22800440762693	-0.50164948543943	1.24847119377436	F	0.22647011318661	-0.49705966276568	1.23741813130306
Cu	-3.19996383684013	1.20880613998946	0.00053246459938	Cu	-3.19209689047859	1.20636564282534	-0.00283531729772

$Cu(CH_3NO_2)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
C	-6.90318023332250	3.49472581342386	0.01048077673020	C	-6.89356873819052	3.48546771535559	0.01192638098284
N	-5.88251919458993	2.41436067000133	0.04341817479789	N	-5.88325951861104	2.41548416849643	0.04393087371881
H	-7.38954729698009	3.41628581534601	-0.96328980589270	H	-7.38291778159835	3.40816061068809	-0.96182528484782
H	-6.38170847488694	4.44148424423611	0.10650433778663	H	-6.37589245045055	4.43586244152625	0.10417465724365
H	-7.61022671340081	3.30045353490590	0.81061490775804	H	-7.60481001253572	3.29425071468902	0.81053221363809
O	-4.74453191953012	2.63857576699570	-0.36225760856876	O	-4.75317572088521	2.63940733649241	-0.35794014093544
O	-6.19142594851113	1.29831827437770	0.45200260147017	O	-6.19204478144973	1.30732726116852	0.44818652715444
Cu	-4.13882021877852	0.54864588071337	0.04358661591850	Cu	-4.15629099627891	0.56688975158367	0.04207477304541

$Cu(CH_3CN)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
Cu	0.03561077489215	-0.00136281811585	-0.00027623109719	Cu	0.04697211758419	-0.00150692782298	-0.00021846851252
N	1.90575730818679	0.00063098424285	0.00016568085950	N	1.90885143260254	0.00068890647896	0.00016640783062
C	3.05214047950600	0.00119914020310	0.00027065342443	C	3.05457039727223	0.00130749010889	0.00021145466529
C	4.49589742583420	0.00012239109920	0.00001347199701	C	4.49197781691238	0.00016117331880	-0.00000470169953
H	4.86123059260624	1.02814527724693	0.03360317315622	H	4.85704509428755	1.02893858006916	0.03362576542798
H	4.85962199552117	-0.48511157537352	-0.90750449814155	H	4.85530768039373	-0.48550716447814	-0.90819226740812
H	4.85974142345344	-0.54361339930269	0.87372774980158	H	4.85527546094737	-0.54407205767468	0.87441180969627

$Cu(CH_2FCN)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N 1.84648927573934 -0.04081179642730 -0.00152348882035	N 1.84944922839762 -0.04247319034263 -0.00175839235777
C 2.99082794527532 -0.05588659026093 -0.00212820186863	C 2.99318871501353 -0.05074717382333 -0.00216044485403
C 4.46472019874851 -0.05091746457372 -0.00183308164848	C 4.46249200845391 -0.04408972480230 -0.00166955512978
F 4.89634653993546 1.24334304511053 0.04110762220269	F 4.89551632959492 1.23684235876224 0.04101843889881
H 4.81842697844730 -0.54134063210244 -0.91322238125922	H 4.81168726131525 -0.54165265591705 -0.91287370395210
H 4.81817564755605 -0.59950903363695 0.87577169550014	H 4.81120037657835 -0.59963408931779 0.87544869492439
Cu -0.03035658570198 0.00864247189080 0.00063783589385	Cu -0.01890391935357 0.00527447544086 0.00080496247047

$Cu(CHF_2CN)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N 1.81585988726541 0.02730030650536 0.02633596946771	N 1.81853273141656 0.02910230826464 0.02668793655984
C 2.95849278309651 0.00797241413818 0.03058599883136	C 2.96043254283817 0.01113342133540 0.03069082823156
C 4.46490604683491 -0.02860020831262 0.04684201268423	C 4.46419343657465 -0.02600982716827 0.04360634464186
F 4.90098205483914 1.23780271072177 0.07903280267989	F 4.89931992837564 1.22993517220751 0.07679900070073
F 4.86471850143797 -0.63202826401595 -1.08127304438884	F 4.85808205988593 -0.62697016043639 -1.07608795519465
H 4.82148666429049 -0.57737202955810 0.92286423281503	H 4.81488273958515 -0.57742958680038 0.92291903784352
Cu -0.06506593776441 0.09979507052137 -0.03744797208938	Cu -0.05406343867608 0.09510867259750 -0.03767519278287

$Cu(Cl_3CCN)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
Cu -0.00470724343702 0.01504044925045 0.00120207691018	Cu 0.00661214839269 0.01476091385806 0.00128716124215
N 1.86949604968414 -0.00193375953475 -0.00011798966416	N 1.87320345406618 -0.00116420820645 -0.00016434393498
C 3.01474161910712 -0.00276188797895 -0.00043943618115	C 3.01770919359510 -0.00280978247447 -0.00050931185393
C 4.48045067841755 -0.00086457670733 -0.00026696623137	C 4.48314792849746 -0.00082240833540 -0.00028290346403
Cl 4.99810062321010 1.69650625212440 0.05580549156606	Cl 4.99077454583945 1.68047280903853 0.05535326559014
Cl 5.00636102882355 -0.79963300522231 -1.49519970633457	Cl 4.99968687895896 -0.79236403204947 -1.48092274498835
Cl 5.00558724419456 -0.89567347193152 1.43963652993501	Cl 4.99889585065015 -0.88739329183082 1.42585887740900

$[Cu(Cl_3CCN)_2]^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
Cu 3.24224581416446 12.19185314609138 3.91407615365413	Cu 3.24026036473195 12.19112200353798 3.91341816807349
Cl 4.26594693952557 7.19026721097817 5.27559174509210	Cl 4.26145917525914 7.21680322985605 5.26203792541491
Cl 0.22444651122752 16.51151280118606 3.54478044753622	Cl 0.24498282750540 16.49185865856796 3.55014453733606
Cl 2.03150943736547 16.96173317550546 5.81540786710592	Cl 2.03620520024273 16.94197593225733 5.79843536812328
Cl 3.75800184196596 7.16000056283759 2.38480759846106	Cl 3.76168022592156 7.18420918381108 2.39851098263030
Cl 6.37913997874958 7.99950470544778 3.40487821572671	Cl 6.35960737928140 8.01031406585993 3.40985801135469
Cl 2.98575963703027 17.38979089849959 3.07158565066999	Cl 2.97757935264092 17.36764702332060 3.08116333851801
N 3.81042379980653 10.42619998938495 3.82761907735139	N 3.80327736645226 10.43476012432365 3.82444325622197
N 2.67678694039596 13.95892667994580 4.00330047566406	N 2.68656896265692 13.95072118026687 4.00422788960955
C 4.62987210822440 7.95279328747441 3.71343997815247	C 4.62844955808374 7.96409215096980 3.71383034881492
C 1.90397597559909 16.44731319239699 4.11971671749710	C 1.90723075325679 16.43624155441289 4.11953704334818
C 4.16540281596890 9.33902906244167 3.77901709971856	C 4.16436621172485 9.35010800292966 3.77715399122460
C 2.33698200652077 15.05103822914227 4.05352312074634	C 2.34355993234478 15.04103305596685 4.05379342648846

$[Cu(Cl_3CCN)_3]^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
Cu 2.78653663850404 12.00506933933714 4.07513296529373	Cu 2.80123184443231 11.91871456614657 4.07531763311859
Cl -1.46733591897071 12.07403295440910 7.39022162973758	Cl -1.42499248235517 12.28442739068907 7.34197964264063
Cl -2.38150095432518 13.20377143427616 4.84211778539820	Cl -2.28021952099914 13.29832734007156 4.75702912675283
Cl -2.16383355908375 10.29645855895704 5.16171490224503	Cl -2.21020333345374 10.43604261025877 5.24122247363029
Cl 5.09314405689075 16.86416043414104 4.29337998191953	Cl 4.96345551332708 16.80115100602299 4.34126167974002
Cl 6.65571717391900 8.39949096090975 2.98649449027071	Cl 6.69937276248380 8.40305419205373 2.99010262130021
Cl 4.10361352975273 7.17793286743506 2.21455970500669	Cl 4.20338842193109 7.15894724069431 2.17869376993679
Cl 4.05019996081914 16.60364488196707 1.56285866165634	Cl 3.93229380987870 16.55387350910529 1.63520715537921
Cl 6.57587910597688 15.30701631872137 2.29750872485844	Cl 6.47988103911040 15.34703780622818 2.33406090490027
Cl 4.95129975242437 7.15573763678126 5.02363555728653	Cl 5.00987930598844 7.11342038631289 4.96999058414732
N 0.97480007477891 11.96559780389705 4.77749691126717	N 0.99852938718169 11.91970094491826 4.76536011532783
N 3.66716590032946 13.66239032946855 3.56518255782413	N 3.65052949375448 13.58240422748551 3.57765347357168
N 3.75674648943946 10.32398079606445 3.85889845113803	N 3.77624432619157 10.26248274328574 3.85005133950753
C -0.10737106235578 11.92872015195080 5.15154837088137	C -0.08409144615984 11.94678166193944 5.13668704574680
C -1.48924201140431 11.87725513185056 5.62297332951952	C -1.46675108957450 11.98883570358121 5.60730134064718
C 4.23376775694742 14.60992771530292 3.25933456750368	C 4.18454853976200 14.55129959391818 3.28331221213281
C 4.30073157099048 9.32833864496059 3.69958457596949	C 4.33723527981186 9.27856520332607 3.68249038095447
C 4.96601596612208 15.81153113030127 2.86594813610716	C 4.87321906839631 15.78390604721216 2.90761584623654
C 4.98434552924500 8.05410290926882 3.48871869611668	C 5.04712908029263 8.02018782675011 3.46197265432902

$[Cu(CH_2Cl_2)_3]^+$
B3LYP/def2-TZVP/D3BJ
Cu 11.28799857454763 9.51055835545927 12.02994641194003
C 10.19968963182621 9.76133086091946 9.04186039523212
H 10.99300290907736 10.19218707325898 8.44426933623615
H 9.40043305721934 9.33269572980310 8.44939012352789
C 9.67856842233430 8.02317399157652 14.30624522668739
H 9.34297390389233 7.02193850192850 14.06511341025315
H 9.46829304254573 8.30998270914219 15.32956275273957
Cl 12.32694989092784 11.47286458752343 12.74462354942827
C 12.87473783068799 12.33049813930647 11.23501144772708
H 13.68626686014361 12.97824297600053 11.54507674962113
H 12.01768028216229 12.87554763334639 10.85969506194091
Cl 13.44542479125353 11.19709008780011 10.01422162188463
Cl 10.93670211753207 8.39457230286991 9.98517799656875
Cl 11.46784646365747 8.07424881996661 14.07572512381837
Cl 9.54052118979248 11.00680596388291 10.11148675687721
Cl 8.87864530709905 9.17267338311503 13.20637656881666

$Cu(C_6F_5CN)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N -3.45029088016364 3.41971356846008 0.10161602776561	N -3.44537858289427 3.41346880100516 0.09941670314639
C -2.61374773527539 2.63047804747403 0.08046481553270	C -2.60911606268976 2.62509168943881 0.08312998390685
C -1.92028730713209 0.29596171322841 0.03388948457253	C -1.91947463001376 0.29709534609218 0.03749012522997
C -0.92523892153870 -0.66119564580180 -0.00855416194723	C -0.92640900989667 -0.65814365633039 -0.00847317874216
C 0.41058922621252 -0.25653096537238 -0.03266391413102	C 0.40604980387954 -0.25214638539704 -0.03513575628902
C 0.75455110536095 1.09656979764528 -0.00965036566112	C 0.75107916413338 1.09786539858252 -0.00945604333256
C -0.24563068341529 2.04878390820208 0.03279023740007	C -0.24713014115813 2.04818729792836 0.03644412706336
C -1.59591478518557 1.66256568287368 0.05264935767137	C -1.59273326277664 1.65921744438468 0.05703806235359
F 1.35787264794361 -1.16366285439513 -0.07908160960309	F 1.34688647767204 -1.15319046852270 -0.08626138263398
F 2.02454202251553 1.45535710146225 -0.03112750366555	F 2.01270816184699 1.45243968414143 -0.03238725840073
F -3.19145505790422 -0.06956419144771 0.05506211749835	F -3.18154666159506 -0.06434598102614 0.06051736561588
F -1.22680010191676 -1.94622866392258 -0.02874353369128	F -1.22392830915711 -1.93476130443904 -0.03002638711238
F 0.06285738048529 3.33527632188959 0.05265330781257	F 0.05738805177857 3.32558636057626 0.05794843500361
Cu -4.80278690998622 4.70346617970422 0.12310574044611	Cu -4.79013499912912 4.69462577356593 0.11216520419119

$Cu(C_6H_5CN)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
C -1.63292295255129 1.56515173479244 -0.08171840321232	C -1.63006480867292 1.56251163818233 -0.08154471078052
C -0.31069438440292 2.03698800531327 -0.05444302405662	C -0.31289602711408 2.03553944788131 -0.05444829200332
C 0.72415746526082 1.12203054115670 0.01468548792555	C 0.71989106972650 1.12243357638841 0.01450755509300
C 0.44833234244160 -0.24276377525239 0.05548275914794	C 0.44403924142766 -0.23903319195132 0.05508187391690
C -0.86468393504685 -0.70667190731967 0.02811797308303	C -0.86554889620871 -0.70273877879599 0.02793442194096
C -1.91533338781257 0.19022812943192 -0.04086999297669	C -1.91409925687606 0.19237684019256 -0.04088304557792
C -2.69667815180238 2.48873586415564 -0.15083114180273	C -2.69312473542678 2.48519134188616 -0.15030912790594
H -0.11068386932261 3.09904734176394 -0.08689875490959	H -0.11367218221027 3.09922046533024 -0.08691980510610
H -1.06687866374794 -1.76832362512061 0.06083851739207	H -1.06755408271060 -1.76576329111235 0.06085301545672
H -2.93939631779327 -0.15590502355511 -0.06312484330690	H -2.93987456688456 -0.15319963877693 -0.06317328070462
H 1.74734462229699 1.47083430722582 0.03712484749436	H 1.74441243601410 1.47142814838735 0.03713139603663
H 1.26427736322215 -0.95127982050572 0.10934052317275	H 1.26114930987849 -0.94838088101786 0.10902234455053
N -3.56647889604748 3.24345278751272 -0.20018300062802	N -3.56207687432217 3.23895072390901 -0.20102105501870
Cu -4.97077123469424 4.44970544040107 -0.32599094732281	Cu -4.96099062662058 4.44269359949709 -0.32470128989759

$Cu(NH_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N -2.39955231794248 0.91077166473914 0.83866619728392	N -2.40062734795166 0.90653390547562 0.83832161605850
H -1.39408212588804 1.07179493647431 0.79491257045754	H -1.39703754486453 1.07121503741454 0.79516148240607
H -2.82264173246672 1.45167770775511 0.08549110866976	H -2.82134204628478 1.45039704900517 0.08772719668645
H -2.72926965334856 1.31091843006576 1.71615315081588	H -2.72818088477039 1.30985753480726 1.71364804575830
Cu -2.83406417035421 -0.99042273903432 0.70016697277290	Cu -2.83242217612863 -0.98326352670259 0.70053165909068

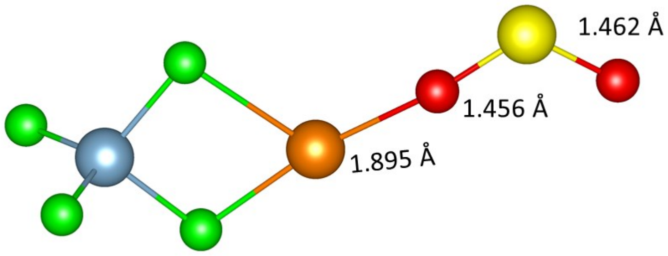
$Cu(N(CH_3)_3)^+$	
B3LYP/def2-TZVP/D3BJ	**PBE0/def2-TZVP/D3BJ**
N -6.44772166324951 3.00712010080648 -0.14337649034655	N -6.44822833589432 3.00660684131199 -0.14492627438832
C -4.95775568410847 3.01747457858442 -0.12887806681079	C -4.97020715403174 3.01788393329136 -0.12744349667758
C -6.95322921146829 4.33824093769679 0.29592167673558	C -6.94812743611833 4.32677993125448 0.29380543894070
C -6.94490111804763 1.95850607035023 0.79121882683047	C -6.94007982082387 1.96804359412065 0.78480217783940

H	-6.58644920313887	5.11340160484735	-0.37358146559368	H	-6.58136969728068	5.10624045119544	-0.37317772204874
H	-6.59733655804476	4.54548105051993	1.30896456770294	H	-6.59205378418897	4.53411872642905	1.30859710072390
H	-8.04122062481714	4.33990072328279	0.29628003151602	H	-8.03762586456793	4.33225793485700	0.29660059181763
H	-4.58689288007485	3.78754303473241	-0.80195045381215	H	-4.59514042413360	3.78898724688657	-0.79945475404047
H	-4.57723218688506	2.04641845366378	-0.43865765519594	H	-4.58479054788586	2.04655190100724	-0.43565408116642
H	-4.60564143974440	3.23084543601275	0.88419886645824	H	-4.61732422555793	3.23194553860477	0.88705561295494
H	-6.57345825367566	0.98280792576566	0.48513633423259	H	-6.56950960597614	0.98914904327014	0.48249084980110
H	-8.03286518976927	1.95119512450265	0.79416248241890	H	-8.02953424408257	1.95894474465429	0.79196578410114
H	-6.58808074003257	2.17370146812373	1.80221470660232	H	-6.58256910968007	2.18329256373949	1.79736744525196
Cu	-7.08562524694350	2.62638349111106	-1.96160336073796	Cu	-7.08184974977795	2.62821754937755	-1.95197867310925

$Cu(NF_3)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
N	0.14770145964801	-0.23430438161233	0.20945979661164	N	0.14835733010389	-0.23270145729223	0.20676728714241
F	1.39019371627153	0.08369026005278	-0.22595523474937	F	1.37619451079473	0.08152450942714	-0.22328172493085
F	-0.42847754043295	-0.86616510478197	-0.84130748502138	F	-0.42185149748842	-0.85846891476549	-0.83043321822640
F	-0.49808993853687	0.95401506522231	0.28674053777419	F	-0.49059347693544	0.94099883138520	0.28513323168999
Cu	0.11783230305030	-1.31978583888079	1.95356238538492	Cu	0.11705313352524	-1.31390296875461	1.94431442432485

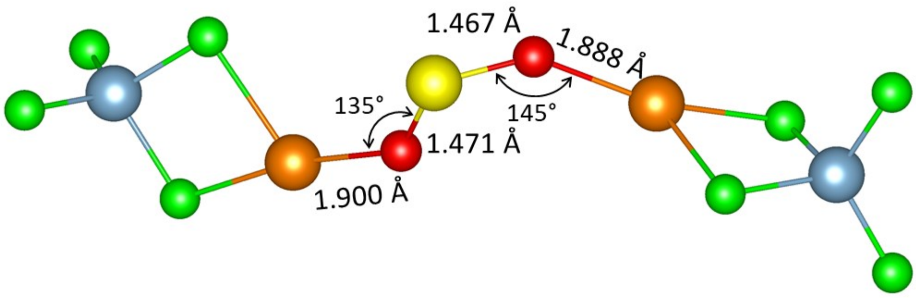
$Cu(N(CF_3)_3)^+$							
B3LYP/def2-TZVP/D3BJ				PBE0/def2-TZVP/D3BJ			
N	-6.41133120645015	3.04041024312309	-0.03109357548508	N	-6.40993495866442	3.04231938410246	-0.02568392681654
C	-4.89836435919738	3.00447464582096	-0.10972966500745	C	-4.90998364915256	3.00466919050891	-0.10780541936096
C	-6.94657577304197	4.41001810814768	0.33444141926582	C	-6.94179497412401	4.40102732311530	0.33409732552606
C	-6.97487025414942	1.94224994261613	0.84758998709376	C	-6.97042493818508	1.95236954795155	0.84335794352826
F	-6.86478220285497	5.16951804352823	-0.75711912624166	F	-6.86141799806411	5.15488079321273	-0.75166144283114
F	-6.26106987891326	4.95051553993051	1.31517620118026	F	-6.26190418761873	4.94138645272566	1.30899010638239
F	-8.21627372598609	4.28733805696617	0.67245444057136	F	-8.20407686996491	4.27796712963207	0.66986704055243
F	-4.47151243267709	4.15313121677026	-0.59735417885077	F	-4.48490021542403	4.14751443394243	-0.58981634962037
F	-4.57356732961488	2.03036918595408	-0.96028159320320	F	-4.59048844887822	2.03900123690158	-0.95853140285367
F	-4.36021638067108	2.77729549026820	1.06568778544043	F	-4.37078529214061	2.77319938801297	1.05769624572551
F	-6.24284771339902	0.85634337754422	0.68639980235695	F	-6.24105157551616	0.87353425532807	0.68387696897728
F	-8.21309033910146	1.69238004028066	0.42248018048180	F	-8.19998376889179	1.70240749607115	0.41786552670834
F	-6.99490004030269	2.30011500562231	2.11005876030976	F	-6.99399913058495	2.30619087846411	2.09903433036957
Cu	-7.09799836364052	2.64205110342749	-1.95901043791199	Cu	-7.08665399279039	2.63974249003100	-1.94158694628719

AlF_4–Cu–SO_2 – B3LYP/def2-TZVP/D3BJ



Cu	-3.38236451420000	0.70599973230000	-0.21767139260000
S	-0.63827511640000	-0.28342873130000	1.41168609050000
Al	-6.21428808440000	1.13072750110000	-0.19410969680000
F	-7.12904816830000	-0.19790095080000	-0.56235827490000
F	-5.14121319610000	0.80954391570000	1.12137786330000
F	-6.95779592280000	2.59996921330000	-0.07155378030000
F	-4.88049735870000	1.22850618960000	-1.34938315960000
O	-1.82468952780000	0.04360922930000	0.63355930610000
O	0.61207825030000	-0.26667369900000	0.65415135900000

AlF_4–Cu–OSO–Cu–AlF_4 – B3LYP/def2-TZVP/D3BJ



Cu	-3.24363103717725	0.08348228046221	-0.24128110515111
Al	-5.78635332997382	1.31796798707469	-0.16832045710279
F	-4.60591310367029	0.90326769497046	-1.41450147312319
F	-6.26550949948939	2.89095345607121	-0.28291400432028
F	-4.59102240671082	1.04659868509982	1.06806571459893
F	-6.92625489718409	0.12022577995251	-0.10937401126878
Cu	2.20538010018794	0.35553902021095	0.38494970156871
F	4.10516595527228	0.82805096785843	0.25342787832136
F	5.68086661214002	-0.96599602943589	-1.24820944138212
Al	4.81945164851816	-0.78548574966987	0.14703432031158
F	5.58580873897312	-1.13812792866663	1.56836975429776
F	3.23562609480775	-1.50519428208993	0.07028587563509
O	0.35096964776348	0.16496935432218	0.75450740806428
O	-1.80363454852178	-0.97018081087834	0.37564348587619
S	-0.53805224186025	-0.94979518875716	1.11739942221012

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