Supporting Material

Simulating the active sites of copper trafficking proteins. Density functional structural and spectroscopy studies on copper(I) complexes with thiols, carboxylato, amide and phenol ligands

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Table 1S. Selected computed infrared data as computed at (BS2) and {BS2W} levels of theory [uncorrected frequency (cm^{-1}) / corrected frequency (cm^{-1} , scale factor 0.96) / intensity (km/mol) / force constant ($\text{mDyne/\AA}$)] for the ternary and quaternary Cu(I) complex molecules with formato, methanethiolato, methanethiol, formato, formamide ($[\text{Cu}^{\text{I}}(\text{OOCH})]$, **5**, $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})]^-$, **6**, $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$, **7**, $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$, **8**, and $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$, **9**. Symbols for movements are: stretching ν , bending δ , symmetric sym, asymmetric asym, single bond -, double bond =, intermediate between single and double bond $\div$.

Figure 1S. The diagrams show drawings for: (a) a portion of the protein DJ-1 (Parkinsonism-associated protein) that linked a Cu(I) ion via cysteinyl sulfur, and (b) the same Cu(I) as for (a) that bridged the two cysteinyl groups at the homodimer interface. PDB Code 4BTE [3].

Figure 2S. The picture shows the Cu(I) site from the ATP7A protein associated with the Menkes disease, PDB Code 1KVJ [5].

Figure 3S. The picture shows the Cu(I) site from copper(I) loaded human metallochaperone HAH1, PDB Code 1TL4 [6].

Figure 4S. Computed spectra for selected complex species: (a) $[\text{Cu}^{\text{I}}(\text{OOCH})]$, **5** (BS2), (b) and (c) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$, **7** (BS2 and BS2W, respectively), (d) $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$, **8** (BS2), (e) and (f) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$, **9** (BS2 and BS2W, respectively).

Figure 5S. Computed spectra at BS2 or BS2W level for selected complex species: (a) and (b) $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{O}(\text{H})(\text{C}_6\text{H}_4)\text{CH}_3)]$, **10** (BS2 and BS2W, respectively), (c) and (d) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{O}(\text{H})(\text{C}_6\text{H}_4)\text{CH}_3)]^+$, **11** (BS2 and BS2W, respectively), (e) and (f) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)_2(\text{O}(\text{H})(\text{C}_6\text{H}_4)\text{CH}_3)]^+$, **13** (BS2 and BS2W, respectively).

Figure 6S. The diagrams show the ^1H -NMR spectra for selected complex molecules with thiolato and methanethiolato ligands as computed at the BS2W level of theory (reference, TMS at BS2W level of theory).

Tables SI-SLXXVI. Atomic coordinates for the optimized molecules. Standard orientations.

Table 1S. Selected computed infrared data as computed at (BS2) and {BS2W} levels of theory [uncorrected frequency (cm⁻¹) / corrected frequency (cm⁻¹, scale factor 0.96) / intensity (km/mol) / force constant (mDyne/Å)] for the ternary and quaternary Cu(I) complex molecules with formato, methanethiolato, methanethiol, formato, formamide ([Cu^I(OOCH)], **5**, [Cu^I(SCH₃)(OOCH)]⁻, **6**, [Cu^I(S(H)CH₃)(OOCH)], **7**, [Cu^I(SCH₃)(OOCH)(OC(H)NH₂)]⁻, **8**, and [Cu^I(S(H)CH₃)(OOCH)(OC(H)NH₂)], **9**. Symbols for movements are: stretching ν , bending δ , symmetric sym, asymmetric asym, single bond -, double bond =, intermediate between single and double bond $\div$.

Vibrations	Molecules				
	5	6	7	8 ^a	9
ν (<i>trans</i> to CO)N-H					(3650/3504/71.47/8.4860) {3648/3502/147.44/8.5146}
ν (<i>trans</i> to CO)N-H+				(3524/3383/240.92/8.1224)	
ν (<i>cis</i> to CO)N-H					
asym					
ν (<i>cis</i> to CO)N-H+				(3415/3278/549.80/7.1962)	{3235/3106/880.73/6.6178}
ν (<i>trans</i> to CO)N-H					
sym					
ν (CH ₃)C-H		(3074/2951/27.44/6.1575) {3114/2989/20.85/6.3256} (3068/2945/30.25/6.1203) {3110/2986/20.61/6.2984} (3006/2886/116.18/5.4786) {3035/2914/91.14/5.5839}	(3163/3036/1.53/6.5220) {3171/3044/1.22/6.5617} (3067/2944/8.65/5.6985) {3076/2953/12.80/5.7289}	(3090/2966/20.33/6.2239) (3084/2961/23.02/6.1867) (3017/2896/93.08/5.5192)	(3168/3041/0.91/6.5381) {3172/3045/2.54/6.5712} (3157/3031/3.51/6.5084) {3165/3038/3.20/6.5375} (3065/2942/18.05/5.6952) {3071/2948/18.91/5.7134}
ν (formato)C-H	(3022/2901/42.58/5.8433) {2958/2840/137.87/5.5746}				
N(CH ₃)C-H x 3H		{3035/2914/91.14/5.5839}			
sym					
ν (amide)C-H				(2900/2784/128.65/5.3566)	(3003/2883/27.03/5.7607) {3044/2922/107.94/5.9447} (2964/2845/347.74/5.6286)
ν (formato)C-H+					
ν (<i>cis</i> to CO)N-H sym					
ν (formato)C-H+					(2936/2819/184.23/5.5219)
ν (<i>cis</i> to CO)N-H					
asym					
ν (formato)C-H		(2816/2703/344.82/5.0213) {2919/2802/230.37/5.4148}	(2972/2853/129.90/5.6396) {2941/2823/191.14/5.5071}	(2870/2755/314.33/5.2300)	(2934/2817/249.50/5.4780)
ν S-H			(2636/2532/1.50/4.2529) {2657/2551/4.32/4.3193}		(2651/2545/1.46/4.3018) {2664/2557/1.09/4.3411}
ν (amide)C=O				(1755/1685/653.36/11.5022)	
ν (amide)C=O+					(1744/1674/908.77/5.1408)

$\delta(\text{scissoring})\text{NH}_2$ $\nu(\text{formato})\text{C}=\text{O}$		(1683/1616/742.10/18.6457) {1615/1550/1100.50/14.9301}	(1646/1580/419.96/16.4294) {1622/1557/1007.50/15.3031}		{1697/1629/1021.10/4.1817}
$\delta(\text{scissoring})\text{NH}_2$ $\nu(\text{formato})\text{C}=\text{O}+$ $\delta(\text{scissoring})\text{NH}_2$ $\nu(\text{formato})\text{C}=\text{O}$				(1659/1593/425.62/2.5918) (1669/1602/436.52/5.8430)	{1631/1566/393.17/2.7117} (1659/1593/322.51/2.9279)
$\delta(\text{scissoring})\text{NH}_2+$ $\nu(\text{formato})\text{C}=\text{O}+$ $\nu(\text{amide})\text{C}-\text{O}(\text{Cu})$ $\nu(\text{formato})\text{C}=\text{O}(\text{Cu})$	(1566/1503/536.70/14.6430) {1615/1550/958.93/15.8708}		{1622/1557/1007.50/15.3031}		(1615/1550/135.01/7.3971) {1583/1520/661.35/9.6673}
$\delta(\text{amide})\text{O}=\text{C}-\text{H}$				(1419/1362/22.48/1.4628)	(1415/1358/36.15/1.6152) {1414/1357/74.55/1.5848}
$\delta(\text{formato})\text{O}-\text{C}-\text{H}$		(1390/1334/4.83/1.2677) {1394/1338/19.44/1.3086}	(1366/1311/14.44/1.3646) {1391/1335/15.46/1.3091}	(1390/1334/6.49/1.2980)	(1394/1338/17.44/1.4260) {1390/1334/45.56/1.3310}
$\nu(\text{formato})\text{C}=\text{O}(\text{Cu})$	(1363/1308/47.08/10.3038) {376/1321/13.71/1.3020}				
$\nu(\text{formato})\text{C}-\text{O}(\text{Cu})$		(1329/1276/284.44/8.9828) {1321/1268/392.71/8.6386}		(1334/1281/234.03/6.8861)	(1358/1304/224.44/5.3423) {1351/1297/12.69/3.6987}
$\nu\text{C}-\text{N}$				(1300/1248/54.68/2.9257)	(1369/1314/3.47/2.6064) {1347/1293/352.46/4.7409}
$\delta(\text{formato})\text{O}-\text{C}-\text{H}$ in plane, ip $\nu(\text{formato})\text{C}-\text{O}(\text{Cu})$	(1313/1260/30.53/1.1308) {1297/1245/331.07/6.8741}		(1305/1253/188.37/4.5968) {1308/1256/408.26/3.1098} (1092/1048/9.74/0.8604) {1092/1048/21.81/0.8599}		(1095/1051/24.81/0.8663) {1091/1047/28.40/0.8585}
$\delta\text{H}-\text{S}-\text{CH}_3$				(1055/1013/4.29/0.9701)	(1078/1035/22.46/0.8599) {1064/1021/12.05/0.9481}
$\delta(\text{amide})\text{O}-\text{C}-\text{H}$ out of plane, oop $\delta(\text{formato})\text{O}-\text{C}-\text{H}$ oop $\delta(\text{amide}, \text{wagging})\text{H}-\text{N}-\text{H}$ $\delta\text{O}=\text{C}=\text{O}$	(1050/1008/1.27/1.0893) {1056/1014/0.30/1.1138}		(1057/1015/0.24/1.1163) {1060/1018/0.0282/1.1274}	(1050/1008/0.49/1.1171)	(1059/1017/1.12/1.1124) {1060/1018/0.39/1.1287}
	(806/774/12.32/4.5100) {766/735/28.57/4.1012}		(790/758/29.33/2.8240) {760/730/36.33/3.9869}	(800/768/33.96/0.4490)	{840/806/93.00/0.5088}
$\delta\text{O}-\text{C}=\text{O}$		(757/727/20.51/3.9419) {757/727/36.86/3.9700}		(762/732/25.21/4.0541)	(765/734/20.68/3.9722) {758/728/42.50/3.5368}
$\delta(\text{amide}, \text{wagging})\text{H}-\text{N}-\text{H}$ $\nu\text{C}-\text{S}$				(695/667/106.19/0.3103)	
		{675/648/4.54/1.8030}	(664/637/3.40/1.6149)	(683/656/2.73/1.8047)	(683/656/1.49/1.6775)

$\delta\text{Cu-S-H}$			{673/646/4.75/1.6411} (524/503/5.46/0.1744) {530/509/16.20/0.1789}		{678/651/2.99/1.6673}
v(formato)Cu-O+		(439/421/39.39/1.5476)	(456/438/14.81/1.6712)	(446/428/33.81/1.5921)	(399/383/21.71/0.9890)
vCu-S(sym)		{441/423/49.15/1.5832}	{449/431/23.10/1.4946}		{357/343/23.15/0.8648}
vCu-O	(329/316/26.86/1.0990) {401/385/21.20/1.1088}				
v(amide)O-Cu					(268/257/72.92/0.2223) {245/235/18.83/0.3607}
vCu-O+vCu-S(sym)		(313/300/3.14/0.7854) {316/303/5.82/0.8057}		(319/306/3.72/0.8188)	(228/219/3.52/0.2840) {233/224/21.18/0.1718}
vCu-O+vCu-S(asym)			(279/268/6.62/0.3466) {285/274/2.27/0.5761}		(196/188/5.93/0.2497) {191/183/42.80/0.1006}
$\delta\text{Cu-O(format), oop}$	(320/307/50.17/0.1510) {238/228/70.51/0.0837}	(228/219/19.84/0.0965) {227/218/48.00/0.0976}			
$\delta\text{S-Cu-O}$		(190/182/7.13/0.1488) {180/173/13.18/0.1235}	(165/158/2.05/0.0855) {161/155/3.05/0.0380}	(168/161/12.32/0.0726)	(101/97/17.11/0.0548) {102/98/9.54/0.0444}

^a The structure for $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$, **8**, when computed at the BS2W level did not strictly reach full convergence criteria in terms of forces and movements; the hessian analysis was not carried out at BS2W.

Figure 1S. The diagrams show drawings for: (a) a portion of the protein DJ-1 (Parkinsonism-associated protein) that linked a Cu(I) ion via cysteinyl sulfur, and (b) the same Cu(I) as for (a) that bridged the two cysteinyl groups at the homodimer interface. PDB Code 4BTE [3].

Figure 2S. The picture shows the Cu(I) site from the ATP7A protein associated with the Menkes disease, PDB Code 1KVJ [5].

Figure 3S. The picture shows the Cu(I) site from copper(I) loaded human metallochaperone HAH1, PDB Code 1TL4 [6].

Figure 4S. Computed spectra for selected complex species: (a) $[\text{Cu}^{\text{I}}(\text{OOCH})]$, **5** (BS2), (b) and (c) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$, **7** (BS2 and BS2W, respectively), (d) $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$, **8** (BS2), (e) and (f) $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$, **9** (BS2 and BS2W, respectively).

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Figure 6S. The diagrams show the ^1H -NMR spectra for selected complex molecules with thiolato and methanethiolato ligands as computed at the BS2W level of theory (reference, TMS at BS2W level of theory).

Table SIFile name: sch3/mes; molecule: CH₃S⁻; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.714548	-0.000005	0.000051
2	6	1.129071	-0.000002	0.000068
3	1	1.554107	-0.047266	1.016703
4	1	1.552053	0.904643	-0.468007
5	1	1.552176	-0.857281	-0.549918

Table SIIFile name: sch3++/mes++; molecule: CH₃S⁻; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.714423	-0.000026	0.000017
2	6	1.134460	-0.000041	0.000042
3	1	1.542170	-0.780069	0.657429
4	1	1.540855	0.959896	0.346741
5	1	1.540986	-0.179162	-1.004702

Table SIIIFile name: sch3pcm/messcrf; molecule: CH₃S⁻; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.716372	0.000011	-0.000004
2	6	1.139160	-0.000070	0.000027
3	1	1.542188	-1.000986	0.191982
4	1	1.542388	0.666936	0.770767
5	1	1.542424	0.334301	-0.962848

Table SIVFile name: mes++scrff; molecule: CH₃S⁻; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.715420	0.000013	0.000000
2	6	1.140532	-0.000078	0.000000
3	1	1.534328	-1.019857	-0.002262
4	1	1.534602	0.508102	0.884178
5	1	1.534597	0.512019	-0.881918

Table SVFile name: ch3s/mesh; molecule: S(H)CH₃; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.667675	-0.087080	-0.000009
2	6	1.165593	0.019653	-0.000009
3	1	1.534216	0.523365	0.894949
4	1	1.534768	0.521606	-0.895753
5	1	1.529749	-1.009195	0.001070
6	1	-0.909489	1.239581	-0.000069

Table SVIFile name: shch3++/mesh++; molecule: S(H)CH₃; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.710732	-0.052464	-0.252818
2	6	1.109817	0.041384	-0.035305
3	1	1.378464	0.112809	1.017955
4	1	1.531927	0.877162	-0.592078
5	1	1.511263	-0.888090	-0.438377
6	1	-1.001656	1.146883	0.290497

Table SVIIFile name: ch4spcm/meshscrf; molecule: S(H)CH₃; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.667344	-0.087573	-0.000006
2	6	1.168142	0.019640	-0.000006
3	1	1.527922	0.528603	0.894536
4	1	1.528421	0.527003	-0.895260
5	1	1.534308	-1.007972	0.000943
6	1	-0.922007	1.235701	-0.000087

Table SVIIIFile name: mesh++scrfl; molecule: S(H)CH₃; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	16	-0.666929	-0.087584	-0.000007
2	6	1.167752	0.019539	-0.000004
3	1	1.525152	0.528106	0.893543
4	1	1.525716	0.526242	-0.894399
5	1	1.532844	-1.006685	0.001091
6	1	-0.919365	1.236447	-0.000102

Table SIXFile name: hcoo; molecule: HCOO⁻; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	1.141660	-0.208107	0.000008
2	8	-1.141650	-0.208075	0.000008
3	6	-0.000062	0.310974	-0.000033
4	1	0.000294	1.463611	0.000061

Table SXFile name: hcoo++; molecule: HCOO⁻; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	1.137361	-0.208912	0.000005
2	8	-1.137431	-0.208852	0.000005
3	6	0.000057	0.314715	-0.000021
4	1	0.000221	1.453830	0.000039

Table SXIFile name: hcoopcm; molecule: HCOO^- ; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.135588	-0.212734	0.000006
2	8	1.135598	-0.212734	0.000006
3	6	-0.000020	0.323973	-0.000023
4	1	0.000038	1.459911	0.000044

Table SXIIFile name: hcoopcmbs2; molecule: HCOO^- ; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	2.935894	-0.916912	0.215741
2	8	1.644998	0.909080	-0.113384
3	6	2.738541	0.310596	0.039223
4	1	3.655130	0.953953	0.014245

Table SXIII

File name: hcoohss2; molecule: HCOOH; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.120394	-0.092521	0.000152
2	8	1.139004	-0.262337	0.000071
3	6	0.132566	0.400369	-0.000132
4	1	0.093332	1.499433	-0.000185
5	1	-1.037599	-1.062784	-0.000806

Table SXIV

File name: hcoohss2++; molecule: HCOOH; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.118188	-0.089169	0.000085
2	8	1.135512	-0.264452	0.000048
3	6	0.136469	0.398605	-0.000114
4	1	0.103812	1.495562	0.000012
5	1	-1.061222	-1.058222	-0.000394

Table SXV

File name: hcoohss2scrf; molecule: HCOOH; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.117661	-0.091897	0.000041
2	8	1.140911	-0.262509	0.000037
3	6	0.128893	0.400299	-0.000121
4	1	0.094946	1.498146	0.000196
5	1	-1.054304	-1.064687	-0.000098

Table SXVI

File name: hcoohss2++scrf4YES; molecule: HCOOH; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.114468	-0.089240	-0.000037
2	8	1.137117	-0.264752	0.000012
3	6	0.131441	0.399619	-0.000101
4	1	0.105219	1.494953	0.000429
5	1	-1.075052	-1.060729	0.000377

Table SXVIIFile name: hconh2; molecule: OC(H)NH₂; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.199436	-0.245355	0.000003
2	6	-0.161286	0.388023	-0.000002
3	7	1.085468	-0.158787	-0.000016
4	1	1.914135	0.413672	0.000056
5	1	-0.128255	1.496365	0.000007
6	1	1.179050	-1.163825	0.000035

Table SXVIIIFile name: hconh2++; molecule: OC(H)NH₂; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	1.196136	-0.246435	-0.000004
2	6	0.163023	0.386704	-0.000005
3	7	-1.084452	-0.157275	0.000028
4	1	-1.908522	0.420885	-0.000098
5	1	0.140514	1.492477	0.000013
6	1	-1.188060	-1.161183	-0.000050

Table SXIXFile name: hconh2pcm; molecule: OC(H)NH₂; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	1.204350	-0.242819	0.000027
2	6	0.151830	0.387397	0.000023
3	7	-1.081454	-0.160431	-0.000250
4	1	-1.910198	0.414176	0.000789
5	1	0.121045	1.492365	0.000037
6	1	-1.186444	-1.165351	0.000569

Table SXX

File name: hconh2pcmb2; molecule: OC(H)NH₂; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.201978	-0.243516	0.000021
2	6	-0.150291	0.387243	-0.000008
3	7	1.078876	-0.159930	-0.000074
4	1	1.903909	0.419527	0.000335
5	1	-0.131125	1.488564	-0.000032
6	1	1.192659	-1.163916	0.000099

Table SXXIFile name: imb; molecule: 1,4-O(H)C₆H₄CH₃; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	2.809172	-0.094578	0.004573
2	1	3.173288	0.800220	0.005809
3	6	1.442276	-0.017602	0.002099
4	6	0.727341	-1.220457	-0.000826
5	6	0.750314	1.195252	-0.000873
6	6	-0.663151	-1.196536	-0.005435
7	1	1.275601	-2.156825	-0.002232
8	6	-0.645924	1.199228	-0.005609
9	1	1.298155	2.135611	-0.002525
10	6	-1.380544	0.009912	-0.006206
11	1	-1.205579	-2.139064	-0.009862
12	1	-1.169698	2.151876	-0.009739
13	6	-2.891396	0.016248	0.007413
14	1	-3.287148	1.015834	-0.193894
15	1	-3.303672	-0.663355	-0.746479
16	1	-3.287825	-0.303940	0.978955

Table SXXIIFile name: imbss++; molecule: 1,4-O(H)C₆H₄CH₃; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	2.808549	-0.094158	0.004918
2	1	3.182199	0.793016	0.003504
3	6	1.438837	-0.017557	0.002080
4	6	0.726517	-1.217695	-0.001104
5	6	0.749306	1.193019	-0.000838
6	6	-0.662860	-1.194251	-0.005359
7	1	1.272295	-2.153646	-0.002512
8	6	-0.646058	1.197566	-0.005639
9	1	1.295491	2.132140	-0.002090
10	6	-1.379596	0.010071	-0.006052
11	1	-1.202954	-2.136046	-0.009754
12	1	-1.167573	2.149323	-0.010122
13	6	-2.889916	0.015731	0.007409
14	1	-3.284044	1.015221	-0.188822
15	1	-3.299226	-0.659236	-0.749850
16	1	-3.281963	-0.308815	0.977311

Table SXXIIIFile name: imbscrf; molecule: 1,4-O(H)C₆H₄CH₃; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	2.810548	-0.094640	0.006386
2	1	3.180465	0.799456	0.007928
3	6	1.443439	-0.017930	0.002741
4	6	0.727298	-1.221052	-0.001227
5	6	0.751458	1.196464	-0.001356
6	6	-0.665110	-1.198010	-0.007399
7	1	1.271756	-2.160209	-0.003121
8	6	-0.645229	1.199180	-0.007545
9	1	1.299864	2.135318	-0.003571
10	6	-1.381999	0.008985	-0.008283
11	1	-1.206977	-2.140704	-0.013347
12	1	-1.168295	2.152164	-0.013364
13	6	-2.893225	0.018228	0.009749
14	1	-3.288494	0.996497	-0.278111
15	1	-3.307418	-0.728315	-0.675901
16	1	-3.285080	-0.212277	1.008321

Table SXXIV

File name: imbss++scrf; molecule: 1,4-O(H)C₆H₄CH₃; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	2.810648	-0.093792	0.006360
2	1	3.188501	0.793788	0.006264
3	6	1.439217	-0.018612	0.002579
4	6	0.726013	-1.219119	-0.001490
5	6	0.750991	1.193858	-0.001320
6	6	-0.665426	-1.195996	-0.006988
7	1	1.266745	-2.158623	-0.003162
8	6	-0.644981	1.197680	-0.007310
9	1	1.298388	2.131165	-0.002978
10	6	-1.381067	0.009479	-0.007697
11	1	-1.205226	-2.137765	-0.012626
12	1	-1.165262	2.150035	-0.013179
13	6	-2.891655	0.018585	0.009304
14	1	-3.284155	1.004096	-0.249784
15	1	-3.303107	-0.706532	-0.698097
16	1	-3.279613	-0.241075	1.000202

Table SXXVFile name: cuiooch; molecule: $[\text{Cu}^{\text{I}}(\text{OOCH})]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.817656	-0.000015	-0.000005
2	8	0.799317	-1.116115	0.000041
3	8	0.799201	1.116164	0.000041
4	6	1.403400	-0.000033	-0.000100
5	1	2.503465	0.000254	0.000082

Table SXXVIFile name: cuioochss++; molecule: [Cu^I(OOCH)]; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.890181	0.000030	0.000029
2	8	0.892473	-1.111023	-0.000163
3	8	0.892733	1.111010	-0.000163
4	6	1.490486	-0.000088	0.000222
5	1	2.590668	-0.000251	0.000425

Table SXXVIIFile name: cuioochscrf; molecule: [Cu^I(OOCH)]; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.860801	-0.075514	0.000006
2	8	1.167546	-1.037356	0.000001
3	8	0.558381	1.112022	-0.000007
4	6	1.443509	0.180151	-0.000075
5	1	2.494751	0.511657	0.000324

Table SXXVIII

File name: cuioochss++scrff; molecule: [Cu^I(OOCH)]; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.046774	-0.110839	0.000043
2	8	1.738354	-0.921222	-0.000147
3	8	0.523445	0.975715	-0.000292
4	6	1.622973	0.305596	0.000211
5	1	2.524219	0.944809	0.001001

Table SXXIXFile name: cuimes; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	1.061098	0.156700	0.000000
2	16	-0.765629	-0.716439	0.000000
3	6	-1.968927	0.680847	0.000001
4	1	-2.963635	0.228860	-0.000184
5	1	-1.872168	1.302483	-0.891286
6	1	-1.872424	1.302279	0.891452

Table SXXXFile name: cuimes++; molecule: [Cu^I(SCH₃)]; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.068661	0.068249	-0.059413
2	16	-1.916757	-0.746719	-0.061144
3	6	-3.022565	0.712191	0.181528
4	1	-4.041409	0.319770	0.184265
5	1	-2.931003	1.430519	-0.632278
6	1	-2.839570	1.205740	1.135249

Table SXXXIFile name: cuimesscrf; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)]$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	1.071923	0.156244	0.000000
2	16	-0.774387	-0.715380	-0.000001
3	6	-1.989841	0.678500	-0.000001
4	1	-2.989688	0.238249	-0.000079
5	1	-1.883373	1.302938	-0.888226
6	1	-1.883460	1.302820	0.888317

Table SXXXII

File name: cuimes++scrf; molecule: [Cu^I(SCH₃)]; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	1.123128	0.146776	0.000000
2	16	-0.859760	-0.727161	0.000001
3	6	-2.008413	0.727322	0.000001
4	1	-3.025877	0.333033	-0.000577
5	1	-1.868694	1.340860	-0.889060
6	1	-1.869487	1.340253	0.889608

Table SXXXIIIFile name: cuimesh; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.135337	-0.151939	0.011188
2	16	0.780092	0.623967	-0.106789
3	6	2.075108	-0.678524	0.032666
4	1	3.034631	-0.160519	0.045114
5	1	2.007696	-1.296982	-0.862376
6	1	1.944031	-1.282381	0.928830
7	1	1.006279	1.233774	1.076601

Table SXXXIVFile name: cuimesh++; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.190400	-0.144340	0.006667
2	16	0.890602	0.665163	-0.101525
3	6	2.067020	-0.757922	0.028301
4	1	3.059803	-0.331588	0.161515
5	1	2.017846	-1.284977	-0.922390
6	1	1.807833	-1.415674	0.852984
7	1	0.984364	1.123011	1.169140

Table SXXXVFile name: cuimeshscrf; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.124821	-0.151794	0.011327
2	16	0.776721	0.631130	-0.106181
3	6	2.047670	-0.687154	0.030094
4	1	3.022741	-0.201512	0.057018
5	1	1.965363	-1.302882	-0.864671
6	1	1.888834	-1.293734	0.919448
7	1	1.029332	1.224996	1.078051

Table SXXXVI

File name: cuimesh++scrf; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.179395	-0.142536	0.006447
2	16	0.894034	0.673543	-0.100674
3	6	2.028767	-0.773256	0.026332
4	1	3.037600	-0.391246	0.165821
5	1	1.956782	-1.301910	-0.921246
6	1	1.735851	-1.420631	0.847435
7	1	0.995086	1.110187	1.173803

Table SXXXVIIFile name: cuimeshmes; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{S}(\text{H})\text{CH}_3)]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.053702	0.034110	0.182140
2	16	-1.958248	-0.578877	0.191899
3	6	-3.087229	0.574675	-0.692983
4	1	-4.111827	0.214866	-0.590136
5	1	-2.798198	0.551062	-1.743985
6	1	-2.993542	1.591493	-0.312682
7	16	2.051308	0.641441	0.174038
8	6	3.024840	-0.732447	-0.587992
9	1	2.719365	-0.920721	-1.619063
10	1	4.073322	-0.426503	-0.590089
11	1	2.937311	-1.656732	-0.013725
12	1	-2.498408	-0.397056	1.418463

Table SXXXVIII

File name: cuimeshmesss++; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{S}(\text{H})\text{CH}_3)]$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.061898	-0.027234	0.175696
2	16	-2.099689	-0.630203	0.129213
3	6	-3.026875	0.769399	-0.632407
4	1	-4.094748	0.602111	-0.502417
5	1	-2.780045	0.754464	-1.692322
6	1	-2.721910	1.718719	-0.199354
7	16	2.106740	0.641402	0.248532
8	6	3.073291	-0.658598	-0.647926
9	1	2.753371	-0.754831	-1.685703
10	1	4.118266	-0.344340	-0.636041
11	1	2.998110	-1.627341	-0.153508
12	1	-2.459402	-0.402966	1.412241

Table SXXXIX

File name: cuimeshmesscrf; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{S}(\text{H})\text{CH}_3)]$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.049275	0.081250	0.173616
2	16	-1.965723	-0.557906	0.260170
3	6	-3.096769	0.470547	-0.760032
4	1	-4.117333	0.122609	-0.601435
5	1	-2.812065	0.313234	-1.800148
6	1	-3.001977	1.524587	-0.504223
7	16	2.083041	0.639803	0.128899
8	6	3.007348	-0.818654	-0.539152
9	1	2.692717	-1.055702	-1.557063
10	1	4.070777	-0.569279	-0.553817
11	1	2.866430	-1.700591	0.088183
12	1	-2.468098	-0.212798	1.463648

Table SXL

File name: cuimeshmesss++scrff; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{S}(\text{H})\text{CH}_3)]$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.054205	0.023287	0.189112
2	16	-2.097751	-0.611608	0.196132
3	6	-3.050414	0.662704	-0.732368
4	1	-4.111347	0.483724	-0.571950
5	1	-2.805097	0.520795	-1.782652
6	1	-2.768545	1.661779	-0.412243
7	16	2.146173	0.634451	0.212081
8	6	3.055174	-0.737911	-0.643297
9	1	2.706462	-0.862595	-1.668145
10	1	4.113901	-0.475128	-0.663250
11	1	2.938868	-1.680285	-0.108531
12	1	-2.449496	-0.237849	1.445099

Table SXLIFile name: cuibismes; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2]^-$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.000169	-0.214635	-0.000022
2	16	-2.057347	-0.338720	0.501407
3	6	-2.992990	0.865285	-0.541918
4	1	-4.061572	0.774395	-0.315777
5	1	-2.855412	0.672229	-1.610113
6	1	-2.691970	1.898388	-0.341973
7	16	2.058145	-0.342109	-0.498747
8	6	2.991198	0.869651	0.537711
9	1	4.059859	0.780613	0.311222
10	1	2.687217	1.900944	0.333001
11	1	2.854965	0.681492	1.606964

Table SXLIIFile name: cuibismes++; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2]^-$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.000059	-0.286666	0.000143
2	16	-2.143961	-0.318419	0.516165
3	6	-2.912247	0.941813	-0.600265
4	1	-3.987613	0.974746	-0.400040
5	1	-2.766966	0.687503	-1.652827
6	1	-2.500631	1.938682	-0.424954
7	16	2.144340	-0.319418	-0.515570
8	6	2.911473	0.943319	0.598876
9	1	3.986997	0.976238	0.399473
10	1	2.499651	1.939678	0.421205
11	1	2.765436	0.691079	1.651822

Table SXLIIIFile name: cuibismesscrf; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2]^-$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.000025	-0.191600	0.000024
2	16	-2.051512	-0.349806	0.484775
3	6	-3.048512	0.849618	-0.513334
4	1	-4.104582	0.711791	-0.267151
5	1	-2.919470	0.682429	-1.584909
6	1	-2.773782	1.882203	-0.286632
7	16	2.051363	-0.349209	-0.485256
8	6	3.048828	0.848863	0.514035
9	1	4.104847	0.710817	0.267762
10	1	2.774540	1.881775	0.288280
11	1	2.919669	0.680734	1.585449

Table SXLIV

File name: cuibismes++scrff; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2]^-$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.000000	-0.268360	0.000010
2	16	-2.133104	-0.320623	0.518066
3	6	-2.952168	0.919436	-0.592087
4	1	-4.020765	0.924881	-0.370022
5	1	-2.816264	0.658216	-1.641850
6	1	-2.556683	1.921270	-0.422892
7	16	2.133061	-0.320468	-0.518211
8	6	2.952245	0.919235	0.592298
9	1	4.020631	0.925622	0.369271
10	1	2.555877	1.920918	0.424332
11	1	2.817438	0.656950	1.641935

Table SXLVFile name: cusmechoo; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})]^-$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.047445	0.076711	-0.060223
2	16	-1.896844	-0.752206	-0.059655
3	8	2.939804	-0.929682	0.172441
4	8	1.651240	0.934408	-0.089514
5	6	-3.020776	0.693969	0.179298
6	6	2.756651	0.279310	0.041560
7	1	-4.057295	0.338380	0.185365
8	1	-2.921123	1.428531	-0.625692
9	1	-2.834050	1.204365	1.129113
10	1	3.642471	0.961929	0.023587

Table SXLVI

File name: cusmechoo++; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})]^-$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.023557	0.048666	-0.000011
2	16	-2.005161	-0.751796	-0.000003
3	8	3.139588	-0.886290	0.000018
4	8	1.730242	0.893412	-0.000026
5	6	-3.090214	0.747655	0.000026
6	6	2.875577	0.313826	0.000020
7	1	-4.132660	0.415441	-0.000078
8	1	-2.927714	1.364253	-0.887109
9	1	-2.927850	1.364124	0.887275
10	1	3.716824	1.047727	0.000065

Table SXLVII

File name: cusmechoopcm; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})]^-$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.083868	-0.441087	0.049974
2	16	1.981156	-0.371536	-0.352563
3	8	-2.370671	1.386509	-0.390477
4	8	-1.859980	-0.699710	0.351709
5	6	2.646234	1.185196	0.396661
6	6	-2.660320	0.268556	0.044242
7	1	3.719964	1.233199	0.198199
8	1	2.494135	1.205134	1.477920
9	1	2.175451	2.070218	-0.036944
10	1	-3.726146	0.010637	0.217311

Table SXLVIII

File name: cusmechoopcmbs2; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})]^-$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.037255	-0.101677	-0.102004
2	16	1.963947	0.743089	-0.103216
3	8	-2.984177	0.952451	0.284206
4	8	-1.765248	-0.904675	-0.131332
5	6	3.090960	-0.673469	0.303485
6	6	-2.854957	-0.255963	0.064737
7	1	4.115116	-0.296859	0.316077
8	1	3.018928	-1.462528	-0.445146
9	1	2.860869	-1.091242	1.283664
10	1	-3.758278	-0.895786	0.022662

Table SXLXI

File name: cushmechoo; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.259622	-0.120700	-0.010065
2	16	-1.758468	-0.512794	-0.247950
3	8	2.096478	-0.904305	0.248003
4	8	1.738880	1.233210	-0.179611
5	6	-2.888434	0.845494	0.277733
6	6	2.528392	0.267454	0.040951
7	1	-3.921573	0.518214	0.150340
8	1	-2.691709	1.692606	-0.380053
9	1	-2.701665	1.137774	1.310953
10	1	3.614497	0.452771	0.056817
11	1	-2.215718	-1.405312	0.661772

Table SL

File name: cushmechoo++; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.183100	-0.624555	-0.033921
2	16	-2.012874	-0.386759	0.060178
3	8	1.724415	1.520483	0.195739
4	8	2.077305	-0.672081	-0.134418
5	6	-2.177504	1.435450	-0.198575
6	6	2.464031	0.549459	0.023388
7	1	-3.159195	1.751948	0.149023
8	1	-2.098679	1.593394	-1.272505
9	1	-1.375008	1.966097	0.307962
10	1	3.559721	0.681221	-0.007394
11	1	-2.163658	-0.389090	1.404315

Table SLI

File name: cushmechoopcm; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.250209	-0.113149	0.002259
2	16	-1.775184	-0.513783	-0.256873
3	8	2.112889	-0.912068	0.240924
4	8	1.773963	1.230016	-0.178310
5	6	-2.896481	0.846375	0.273570
6	6	2.554011	0.254112	0.024839
7	1	-3.928059	0.512798	0.157579
8	1	-2.706413	1.691478	-0.388041
9	1	-2.697157	1.132883	1.305214
10	1	3.642964	0.425354	0.017798
11	1	-2.204439	-1.407168	0.660555

Table SLII

File name: cushmechoopcmbs2; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})]$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-0.101122	-0.169490	-0.217901
2	16	1.996345	0.508749	-0.385336
3	8	-2.818665	1.046123	0.528304
4	8	-1.856427	-0.870552	-0.176553
5	6	2.980511	-0.468576	0.828192
6	6	-2.851120	-0.136549	0.184161
7	1	3.972229	-0.026824	0.894690
8	1	3.048716	-1.476318	0.424409
9	1	2.490654	-0.482463	1.797511
10	1	-3.817371	-0.674335	0.164973
11	1	1.921177	1.661353	0.314801

Table SLIII

File name: cusmechooonh2c2; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.015647	-0.200543	-0.497834
2	16	-1.952856	-0.930318	0.154723
3	8	0.148358	1.744190	-0.831974
4	8	1.734986	-0.969193	-0.991207
5	6	1.283882	-1.589241	0.034428
6	7	1.810126	-1.302333	1.302593
7	1	1.191607	-1.625181	2.041288
8	1	0.859056	-2.599817	-0.055881
9	1	1.949867	-0.289397	1.384274
10	6	0.871579	2.275405	0.077140
11	1	1.008791	3.376323	-0.049271
12	8	1.414309	1.737356	1.057810
13	6	-2.848604	0.641103	0.526912
14	1	-3.915871	0.521842	0.309427
15	1	-2.743158	0.911344	1.582960
16	1	-2.451591	1.459638	-0.077235

Table SLIV

File name: cusmechooonh2c2++; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.291085	0.383937	-0.195227
2	16	-1.312703	-1.765017	-0.549118
3	8	-1.180631	2.267840	0.065329
4	8	4.357729	-0.673072	0.074748
5	6	3.237339	-1.132350	-0.112838
6	7	2.074624	-0.463027	-0.097884
7	1	1.199252	-0.952859	-0.270078
8	1	3.090759	-2.211599	-0.322920
9	1	2.010406	0.540244	0.073887
10	6	-0.057778	2.859044	0.251327
11	1	-0.167291	3.957084	0.388318
12	8	1.073286	2.371151	0.293247
13	6	-1.674373	-2.507690	1.107538
14	1	-1.626477	-3.595225	1.009251
15	1	-0.945132	-2.195701	1.857424
16	1	-2.673375	-2.236026	1.454023

Table SLV

File name: cusmechooonh2c2pcm; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.216578	0.025589	-0.367328
2	16	-0.899292	-1.826053	0.048886
3	8	-0.992635	1.516866	-0.860326
4	8	1.972050	0.635190	-0.774551
5	6	2.106042	-0.515867	-0.202753
6	7	2.698769	-0.598575	1.053305
7	1	2.588057	-1.490210	1.521964
8	1	2.259807	-1.421073	-0.805651
9	1	2.495611	0.185376	1.664299
10	6	-1.144170	2.211672	0.203676
11	1	-1.809660	3.094365	0.088346
12	8	-0.629880	1.991277	1.313486
13	6	-2.644951	-1.261763	0.272578
14	1	-3.315944	-2.120077	0.182252
15	1	-2.787230	-0.813714	1.259390
16	1	-2.911920	-0.520788	-0.483261

Table SLVI

File name: cusmechooonh2c2pcmb2; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]^-$; theory level DFT-Becke3LYP/6-311++G**+PCM, partially optimized.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.981902	0.100292	-0.006670
2	16	-0.467830	1.625613	-0.200819
3	8	2.040152	-1.490544	0.203651
4	8	-3.690476	-2.088455	0.579045
5	6	-3.670070	-0.791370	0.070761
6	7	-4.765143	-0.353041	-0.499083
7	1	-4.838122	0.470436	-0.930290
8	1	-2.847714	-0.004248	-0.026991
9	1	-5.577498	-0.963689	-0.473877
10	6	3.280966	-1.715557	0.009414
11	1	3.595502	-2.743931	0.206441
12	8	4.079578	-0.969988	-0.399665
13	6	0.488540	3.039648	0.465145
14	1	-0.155208	3.921478	0.423077
15	1	0.769540	2.854122	1.501170
16	1	1.388966	3.214400	-0.135597

Table SLVII

File name: cusmechooonh2b2-shprot; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.157525	-0.306985	-0.439928
2	16	2.248703	-0.543183	-0.030555
3	8	-1.134833	-1.685441	-0.666213
4	8	-0.271588	1.561092	-0.820273
5	6	-1.213220	2.213209	-0.326254
6	7	-2.074934	1.746986	0.569484
7	1	-2.829962	2.334970	0.888215
8	1	-1.358886	3.259684	-0.631333
9	1	-2.034530	0.740784	0.856259
10	6	2.971967	0.835599	0.951391
11	1	4.038286	0.664278	1.107397
12	1	2.829882	1.741193	0.360369
13	1	2.458065	0.947855	1.906617
14	6	-1.957424	-1.725974	0.304655
15	1	-2.639343	-2.597423	0.300334
16	8	-2.065548	-0.896484	1.236086
17	1	2.481384	-1.497099	0.896991

Table SLVIII

File name: cusmechooonh2b2-shprot++; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.179638	-0.494736	-0.063171
2	16	2.465170	-0.589676	-0.404136
3	8	-1.199329	-1.831327	0.129843
4	8	0.122175	1.635429	-0.069453
5	6	-0.851717	2.406153	-0.098922
6	7	-2.126796	2.046758	-0.068937
7	1	-2.836451	2.762279	-0.096499
8	1	-0.673987	3.491076	-0.154868
9	1	-2.421491	1.043141	-0.007823
10	6	3.193556	0.715673	0.667531
11	1	4.275087	0.733358	0.544048
12	1	2.755040	1.650533	0.325408
13	1	2.922995	0.554419	1.708702
14	6	-2.452834	-1.607441	0.177811
15	1	-3.069069	-2.518468	0.291659
16	8	-3.037560	-0.514819	0.112330
17	1	2.866884	-1.662068	0.309769

Table SLIX

File name: cusmechooonh2b2-shprotpcm; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.148096	-0.304808	-0.448810
2	16	2.236537	-0.567712	-0.016261
3	8	-1.180186	-1.669237	-0.692021
4	8	-0.315161	1.539421	-0.889066
5	6	-1.184796	2.240592	-0.326185
6	7	-1.998216	1.813661	0.631164
7	1	-2.691426	2.437755	1.017386
8	1	-1.306664	3.289898	-0.620212
9	1	-1.975322	0.821736	0.917655
10	6	2.975003	0.825057	0.933278
11	1	4.024185	0.609801	1.137733
12	1	2.897419	1.710321	0.301547
13	1	2.428465	0.990734	1.861248
14	6	-1.976308	-1.725999	0.301849
15	1	-2.699495	-2.564251	0.270893
16	8	-2.014995	-0.945721	1.278708
17	1	2.430329	-1.502404	0.936651

Table SLX

File name: cusmechooochnh2b2-shprotpcmb2; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{OOCH})(\text{OC}(\text{H})\text{NH}_2)]$;
theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	0.218159	-0.476942	-0.347631
2	16	2.459929	-0.634810	-0.006255
3	8	-1.297847	-1.734745	-0.461652
4	8	-0.143687	1.564342	-0.825004
5	6	-0.996199	2.356035	-0.387392
6	7	-2.001485	2.034589	0.419373
7	1	-2.653973	2.749178	0.705113
8	1	-0.947467	3.416759	-0.664390
9	1	-2.172012	1.057157	0.697374
10	6	3.007188	0.877772	0.888064
11	1	4.045302	0.755014	1.189869
12	1	2.922198	1.697691	0.178119
13	1	2.370897	1.064778	1.749156
14	6	-2.356770	-1.606719	0.231468
15	1	-3.094122	-2.420862	0.098412
16	8	-2.634608	-0.684282	1.020684
17	1	2.537925	-1.498605	1.027061

Table SLXI

File name: cui-imb-mesb2; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.625507	0.536269	-0.149399
2	8	-0.059342	1.564059	0.076989
3	1	0.061846	2.504192	-0.110036
4	6	1.160522	0.865615	0.053629
5	6	1.070185	-0.520138	-0.023094
6	6	2.379357	1.520711	0.130844
7	6	2.244834	-1.261895	-0.020533
8	1	0.084603	-0.974106	-0.085431
9	6	3.547377	0.752452	0.124030
10	1	2.431170	2.604389	0.199616
11	6	3.503717	-0.643656	0.050475
12	1	2.182071	-2.344997	-0.080473
13	1	4.507837	1.256587	0.182241
14	6	4.768775	-1.468635	0.038531
15	1	5.654153	-0.844605	0.185558
16	1	4.757694	-2.226360	0.829386
17	1	4.889398	-1.998383	-0.913356
18	16	-3.111517	-0.870413	-0.495054
19	6	-4.273705	-0.838827	0.939322
20	1	-5.019250	-1.619393	0.770154
21	1	-3.765623	-1.048051	1.883105
22	1	-4.791558	0.119277	1.017535

Table SLXII

File name: cui-imb-mesb2ss++b; molecule: [Cu^I(SCH₃)(O(H)C₆H₄CH₃)]; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.770786	0.381957	-0.176005
2	8	0.018204	1.231403	0.046543
3	1	0.064238	2.190394	0.129398
4	6	1.300604	0.668882	0.045314
5	6	1.413023	-0.704253	-0.127276
6	6	2.423032	1.466487	0.211646
7	6	2.679934	-1.278048	-0.130775
8	1	0.522242	-1.307943	-0.260502
9	6	3.684610	0.870785	0.203765
10	1	2.326486	2.539959	0.344153
11	6	3.837731	-0.506815	0.034598
12	1	2.766158	-2.350829	-0.267910
13	1	4.560538	1.497315	0.331837
14	6	5.202138	-1.153000	0.037990
15	1	5.996427	-0.404253	0.046586
16	1	5.335695	-1.789722	0.918255
17	1	5.344848	-1.783531	-0.844002
18	16	-3.687527	-0.495282	-0.537045
19	6	-4.385261	-0.838002	1.143115
20	1	-5.361960	-1.301166	0.991927
21	1	-3.759062	-1.528901	1.708034
22	1	-4.522875	0.078982	1.716496

Table SLXIII

File name: cui-imb-mesb2scrff; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.629960	0.543227	-0.154640
2	8	-0.056130	1.535247	0.060191
3	1	0.042677	2.494129	0.146759
4	6	1.166917	0.854955	0.057018
5	6	1.091213	-0.524152	-0.112335
6	6	2.380608	1.508733	0.209154
7	6	2.267980	-1.263901	-0.126495
8	1	0.110337	-0.975235	-0.233147
9	6	3.551272	0.743841	0.190857
10	1	2.424958	2.586248	0.336269
11	6	3.520093	-0.646196	0.026529
12	1	2.213677	-2.340644	-0.261436
13	1	4.506526	1.247719	0.306945
14	6	4.790272	-1.463792	0.029312
15	1	5.672471	-0.828899	-0.086866
16	1	4.902935	-2.018313	0.968597
17	1	4.791964	-2.200278	-0.780503
18	16	-3.240829	-0.736127	-0.535289
19	6	-4.125349	-1.029661	1.063251
20	1	-4.947328	-1.723160	0.870711
21	1	-3.464849	-1.474132	1.810275
22	1	-4.540274	-0.103921	1.466279

Table SLXIV

File name: cui-imb-mesb2ss++bscrfb; molecule: [Cu^I(SCH₃)(O(H)C₆H₄CH₃)]; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.766029	0.392146	-0.198224
2	8	0.011655	1.218313	0.021679
3	1	0.046414	2.173622	0.159717
4	6	1.293462	0.659426	0.034326
5	6	1.419331	-0.705622	-0.187593
6	6	2.408266	1.454151	0.268196
7	6	2.689736	-1.276997	-0.177892
8	1	0.538273	-1.312631	-0.362769
9	6	3.671356	0.862337	0.273127
10	1	2.301295	2.518829	0.448113
11	6	3.838117	-0.507994	0.048218
12	1	2.783744	-2.344098	-0.348891
13	1	4.538994	1.486082	0.458869
14	6	5.211104	-1.135982	0.026370
15	1	5.931247	-0.534534	0.584720
16	1	5.195727	-2.139371	0.458202
17	1	5.583998	-1.228294	-0.999319
18	16	-3.727976	-0.454228	-0.510885
19	6	-4.325708	-0.918707	1.182465
20	1	-5.322290	-1.349522	1.074249
21	1	-3.672022	-1.659458	1.642127
22	1	-4.390147	-0.045396	1.830894

Table SLXV

File name: cui-imb-meshb2freq; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.544466	0.514100	-0.185904
2	8	-0.025097	1.571393	-0.041275
3	1	0.090454	2.531689	-0.038076
4	6	1.209832	0.867913	-0.001093
5	6	1.122188	-0.505743	-0.171638
6	6	2.412889	1.517217	0.211826
7	6	2.291929	-1.257949	-0.128824
8	1	0.154712	-0.971113	-0.346787
9	6	3.574445	0.741516	0.248645
10	1	2.461486	2.593476	0.352996
11	6	3.538792	-0.649307	0.079482
12	1	2.235245	-2.334017	-0.261168
13	1	4.526389	1.235805	0.416421
14	6	4.807421	-1.466282	0.094217
15	1	5.566567	-1.013479	0.737003
16	1	4.623338	-2.483449	0.449385
17	1	5.233703	-1.542380	-0.912927
18	16	-3.123162	-0.877275	-0.338611
19	1	-3.922606	-0.469848	-1.346732
20	6	-4.342319	-0.722046	1.032392
21	1	-5.144827	-1.433842	0.839325
22	1	-3.824794	-1.000890	1.950445
23	1	-4.729831	0.292500	1.109265

Table SLXVI

File name: cui-imb-meshb2ss++; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.652767	0.301976	0.251938
2	8	-0.002250	0.534999	1.218662
3	1	0.052200	0.896514	2.111748
4	6	1.306362	0.269302	0.682574
5	6	1.843079	-0.997243	0.837012
6	6	1.975904	1.284959	0.019053
7	6	3.107230	-1.248353	0.305130
8	1	1.296810	-1.768114	1.367727
9	6	3.237913	1.012203	-0.502961
10	1	1.529997	2.267552	-0.082115
11	6	3.823202	-0.254376	-0.371977
12	1	3.541877	-2.234066	0.425912
13	1	3.775436	1.800473	-1.018121
14	6	5.180701	-0.538942	-0.962661
15	1	5.857848	0.306820	-0.826141
16	1	5.638055	-1.418839	-0.507963
17	1	5.102694	-0.724583	-2.038749
18	16	-3.470209	0.022678	-0.972340
19	1	-4.112789	1.181076	-0.699899
20	6	-4.603469	-1.131228	-0.078960
21	1	-5.557764	-1.122455	-0.601786
22	1	-4.155110	-2.119939	-0.153397
23	1	-4.723186	-0.842525	0.961475

Table SLXVII

File name: cui-imb-meshb2scrf; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.576712	0.529637	-0.162979
2	8	-0.016902	1.526353	0.071176
3	1	0.073520	2.490002	0.098231
4	6	1.212105	0.850567	0.059149
5	6	1.139619	-0.534132	-0.043459
6	6	2.423789	1.517493	0.149262
7	6	2.318982	-1.269780	-0.053557
8	1	0.165763	-1.008673	-0.117749
9	6	3.597619	0.757355	0.135166
10	1	2.465100	2.599749	0.225610
11	6	3.570376	-0.638936	0.037048
12	1	2.266091	-2.351574	-0.135756
13	1	4.552337	1.270661	0.202286
14	6	4.844357	-1.450094	0.043080
15	1	5.721758	-0.813631	-0.096599
16	1	4.968764	-1.983829	0.992633
17	1	4.840203	-2.203559	-0.750949
18	16	-3.159902	-0.835491	-0.429121
19	1	-4.000135	-0.283681	-1.327860
20	6	-4.295215	-0.808721	1.015190
21	1	-5.129427	-1.475023	0.798556
22	1	-3.730977	-1.187510	1.866768
23	1	-4.644505	0.202122	1.216462

Table SLXVIII

File name: cui-imb-meshb2ss++scrfb; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**+PCM

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	29	-1.693617	0.289172	-0.183122
2	8	0.046665	1.165894	-0.039115
3	1	0.064389	2.131967	-0.023202
4	6	1.344890	0.636885	0.002225
5	6	1.498226	-0.741525	0.010611
6	6	2.443653	1.485322	0.039616
7	6	2.785116	-1.275524	0.053522
8	1	0.631930	-1.392967	-0.012806
9	6	3.721731	0.930659	0.083701
10	1	2.312521	2.562274	0.037403
11	6	3.918265	-0.454874	0.087860
12	1	2.902601	-2.353650	0.062532
13	1	4.578184	1.595308	0.116377
14	6	5.308190	-1.044151	0.103329
15	1	6.002578	-0.409138	0.657784
16	1	5.313133	-2.036577	0.558677
17	1	5.700645	-1.147543	-0.913985
18	16	-3.622027	-0.774938	-0.362836
19	1	-4.178931	-0.046146	-1.354536
20	6	-4.685700	-0.190024	1.024281
21	1	-5.693037	-0.562270	0.852124
22	1	-4.274680	-0.629942	1.929950
23	1	-4.671551	0.893950	1.087648

Table SLXIX

File name: cui-imb-bismesb; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^-$; theory level DFT-Becke3LYP/6-31G**, partially optimized.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.622839	-1.115403	0.506177
2	1	-0.009358	-0.430964	0.197735
3	6	1.909923	-0.771444	0.249009
4	6	2.903951	-1.691534	0.616876
5	6	2.294860	0.444686	-0.341864
6	6	4.249367	-1.401852	0.392124
7	1	2.599836	-2.626316	1.081500
8	6	3.647086	0.711775	-0.558415
9	1	1.521303	1.161948	-0.604897
10	6	4.652638	-0.197251	-0.202878
11	1	5.003148	-2.129803	0.688442
12	1	3.925573	1.661683	-1.015044
13	6	6.112140	0.098352	-0.476486
14	1	6.333639	1.167979	-0.374100
15	1	6.766814	-0.443055	0.216163
16	1	6.408850	-0.193113	-1.495866
17	16	-3.448422	-1.564756	0.074830
18	6	-5.129193	-1.006964	-0.463613
19	1	-5.824537	-1.851684	-0.393936
20	1	-5.513546	-0.201583	0.170828
21	1	-5.126380	-0.655798	-1.500499
22	16	-1.040960	1.909617	-0.358674
23	29	-2.238373	0.178690	-0.142433
24	6	-0.918800	2.785790	1.263777
25	1	-1.906897	2.999478	1.681906
26	1	-0.397264	3.734620	1.103587
27	1	-0.352787	2.200678	1.995671

Table SLXX

File name: cui-imb-bisnesss++b; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^-$; theory level DFT-Becke3LYP/6-311++G**, partially optimized.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	1.243343	-1.398314	-1.194101
2	1	0.758043	-1.885278	-0.504045
3	6	2.326425	-0.794687	-0.653046
4	6	3.106009	0.027530	-1.484377
5	6	2.701301	-0.951223	0.696896
6	6	4.235776	0.660248	-0.976761
7	1	2.789633	0.175346	-2.515294
8	6	3.836402	-0.307370	1.189996
9	1	2.088080	-1.562568	1.356124
10	6	4.631340	0.505348	0.368645
11	1	4.817117	1.305632	-1.635076
12	1	4.102082	-0.434852	2.241963
13	6	5.875607	1.179662	0.904024
14	1	6.773086	0.554048	0.766713
15	1	6.061199	2.133093	0.393307
16	1	5.786070	1.388966	1.979054
17	16	-3.062335	2.212601	-0.459318
18	6	-2.735162	3.023461	1.175555
19	1	-2.989625	4.085468	1.085040
20	1	-3.342822	2.592538	1.982340
21	1	-1.676828	2.947329	1.460632
22	16	-1.909178	-2.025854	-0.069691
23	29	-2.486312	0.095414	-0.264693
24	6	-2.964421	-2.821796	1.218773
25	1	-2.962995	-2.265981	2.161064
26	1	-2.582288	-3.825078	1.412839
27	1	-3.999894	-2.904153	0.870155

Table SLXXI

File name: cui-imb-bismes-scrf; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]$; theory level DFT-Becke3LYP/6-31G**+PCM, partially optimized.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0.348787	0.061900	-1.586788
2	1	0.407906	0.020743	-0.931794
3	6	-1.517603	0.103416	-0.892211
4	6	-2.691173	0.333981	-1.621044
5	6	-1.594845	-0.080651	0.493907
6	6	-3.920450	0.368986	-0.968442
7	1	-2.622343	0.494023	-2.693464
8	6	-2.837359	-0.036912	1.131953
9	1	-0.684181	-0.246804	1.062725
10	6	-4.024341	0.182086	0.419133
11	1	-4.819578	0.550283	-1.552949
12	1	-2.876764	-0.170743	2.210545
13	6	-5.369921	0.204505	1.106217
14	1	-5.264059	0.375035	2.181061
15	1	-6.016347	0.990013	0.701180
16	1	-5.901957	-0.746660	0.977907
17	16	1.861984	2.033561	0.316990
18	6	3.523372	2.547314	-0.326653
19	1	3.533726	3.635530	-0.407377
20	1	4.319617	2.241698	0.354935
21	1	3.718746	2.122176	-1.311640
22	16	1.963884	-2.171970	0.650533
23	29	1.888876	-0.059808	0.350133
24	6	1.539280	-3.002073	-0.957755
25	1	0.578892	-2.650477	-1.340666
26	1	1.477312	-4.079904	-0.792241
27	1	2.306268	-2.805042	-1.708768

Table SLXXII

File name: cui-imb-bisnesss++-scrfr; molecule: $[\text{Cu}^{\text{I}}(\text{SCH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^-$; theory level DFT-Becke3LYP/6-31G**+PCM, partially optimized.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0.826726	-0.657319	0.344525
2	1	-0.616314	-1.580415	0.147761
3	6	-2.164590	-0.400855	0.203053
4	6	-2.599936	0.910872	0.400313
5	6	-3.094006	-1.391317	-0.126605
6	6	-3.951483	1.221324	0.262659
7	1	-1.876805	1.676836	0.655515
8	6	-4.442130	-1.061981	-0.262263
9	1	-2.764867	-2.415127	-0.275960
10	6	-4.899432	0.247715	-0.075632
11	1	-4.271976	2.246341	0.421356
12	1	-5.149087	-1.845368	-0.517698
13	6	-6.357849	0.599700	-0.257481
14	1	-7.008930	-0.199137	0.106721
15	1	-6.613981	1.517032	0.277514
16	1	-6.599829	0.758790	-1.314237
17	16	2.265350	2.215124	-0.496610
18	6	3.760635	3.017349	0.243011
19	1	3.761961	4.068885	-0.050533
20	1	3.749868	2.959916	1.332498
21	1	4.680226	2.556706	-0.121473
22	16	2.354399	-2.078699	0.543370
23	29	2.309858	0.069029	0.023182
24	6	3.366087	-2.991650	-0.712734
25	1	2.902272	-2.963948	-1.700863
26	1	3.440625	-4.033038	-0.394527
27	1	4.374993	-2.580501	-0.788630

Table SLXXIII

File name: cui-imb-bismesh; molecule: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0.255793	-1.381553	-0.303001
2	1	-0.258237	-2.247162	-0.734284
3	6	-1.586764	-0.928008	-0.135666
4	6	-1.872536	-0.167491	0.990044
5	6	-2.560050	-1.228828	-1.080834
6	6	-3.172945	0.310432	1.164038
7	1	-1.106187	0.019386	1.736538
8	6	-3.855492	-0.753112	-0.880064
9	1	-2.320010	-1.822176	-1.959188
10	6	-4.185344	0.028046	0.237730
11	1	-3.403979	0.897306	2.048030
12	1	-4.621815	-0.992935	-1.611347
13	6	-5.587326	0.554546	0.425274
14	1	-6.334041	-0.206424	0.180878
15	1	-5.758601	0.878661	1.454499
16	1	-5.774913	1.414439	-0.228307
17	16	0.926293	1.883341	0.111085
18	1	-0.267454	2.132469	-0.464744
19	6	1.936340	2.948994	-0.993411
20	1	1.582143	3.975660	-0.899836
21	1	2.966158	2.891988	-0.639815
22	1	1.881531	2.613777	-2.028429
23	16	3.312693	-1.186049	-0.160238
24	29	1.340106	-0.261749	-0.104732
25	6	4.459976	-0.515502	1.111736
26	1	4.667402	0.519558	0.839362
27	1	5.386253	-1.089049	1.076002
28	1	4.016401	-0.555849	2.105747
29	1	3.249682	-2.437642	0.339504

Table SLXXIV

File name: cui-imb-bismeshss++: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0.159904	-1.329848	-0.572454
2	1	-0.109247	-1.877572	-1.365297
3	6	-1.501649	-0.979438	-0.324581
4	6	-1.883800	-0.773511	0.993941
5	6	-2.404559	-0.813716	-1.367504
6	6	-3.196212	-0.388777	1.265610
7	1	-1.174721	-0.933538	1.798328
8	6	-3.716216	-0.444109	-1.074169
9	1	-2.097637	-0.969637	-2.396973
10	6	-4.136851	-0.223101	0.242596
11	1	-3.493944	-0.232166	2.296611
12	1	-4.421055	-0.322700	-1.889387
13	6	-5.566412	0.147353	0.549951
14	1	-6.183779	-0.750107	0.660223
15	1	-5.641534	0.712479	1.480780
16	1	-6.004193	0.748095	-0.249749
17	16	0.624027	2.029556	0.443159
18	1	-0.641915	1.832681	0.012211
19	6	1.159380	3.249960	-0.831285
20	1	0.576717	4.159155	-0.697713
21	1	2.209020	3.460691	-0.635455
22	1	1.036728	2.853557	-1.835796
23	16	3.373086	-1.331210	-0.218068
24	29	1.527297	-0.005937	-0.046297
25	6	4.738062	-0.639770	0.810680
26	1	5.106703	0.235641	0.279402
27	1	5.528674	-1.384646	0.874785
28	1	4.382783	-0.359266	1.798619
29	1	3.010744	-2.344580	0.598774

Table SLXXV

File name: cui-imb-bismeshscrf: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-31G**+PCM.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0.204720	-1.158556	-0.263381
2	1	-0.103322	-1.988265	-0.752248
3	6	-1.552477	-0.808362	-0.154074
4	6	-1.883245	0.166288	0.781271
5	6	-2.526388	-1.409656	-0.944434
6	6	-3.216520	0.549352	0.917860
7	1	-1.107663	0.600990	1.403281
8	6	-3.856791	-1.016936	-0.786795
9	1	-2.257774	-2.171293	-1.670863
10	6	-4.226961	-0.030863	0.137730
11	1	-3.473627	1.307162	1.652527
12	1	-4.618516	-1.489541	-1.400486
13	6	-5.665738	0.408439	0.274222
14	1	-6.355744	-0.404288	0.030495
15	1	-5.883883	0.748701	1.290506
16	1	-5.891179	1.241211	-0.403174
17	16	1.132257	2.180345	0.018364
18	1	0.195144	2.509619	-0.892583
19	6	2.544898	2.990705	-0.828573
20	1	2.348486	4.060777	-0.891434
21	1	3.425442	2.812446	-0.211437
22	1	2.696204	2.565360	-1.819577
23	16	3.226008	-0.983407	0.629714
24	29	1.360702	0.007025	0.025119
25	6	3.491694	-2.628819	-0.143602
26	1	2.729370	-3.294111	0.262241
27	1	4.481256	-2.992639	0.132544
28	1	3.389605	-2.567391	-1.226129
29	1	4.220545	-0.345908	-0.015927

Table SLXXVI

File name: cui-imb-bismeshss++scrffbb: $[\text{Cu}^{\text{I}}(\text{S}(\text{H})\text{CH}_3)_2(\text{O}(\text{H})\text{C}_6\text{H}_4\text{CH}_3)]^+$; theory level DFT-Becke3LYP/6-311++G**+PCM.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.434040	-0.725126	1.023885
2	1	0.415887	-0.825195	1.984486
3	6	1.734230	-0.507467	0.585505
4	6	1.956298	-0.437682	-0.786349
5	6	2.791187	-0.375416	1.480322
6	6	3.249348	-0.222668	-1.257481
7	1	1.127604	-0.555800	-1.475087
8	6	4.079549	-0.164280	0.989036
9	1	2.616421	-0.437244	2.549490
10	6	4.334408	-0.078957	-0.383598
11	1	3.414230	-0.171928	-2.328676
12	1	4.898036	-0.065085	1.694183
13	6	5.726459	0.184136	-0.906497
14	1	6.486328	-0.137215	-0.191086
15	1	5.902597	-0.338572	-1.849605
16	1	5.881747	1.252377	-1.092776
17	16	-1.397613	2.199896	-0.373733
18	1	-0.531964	2.657761	0.555334
19	6	-2.927288	2.978713	0.292091
20	1	-2.830123	4.058912	0.208432
21	1	-3.744149	2.630103	-0.336213
22	1	-3.092871	2.679198	1.323128
23	16	-2.865504	-1.831432	0.250150
24	29	-1.493599	-0.009750	0.165601
25	6	-3.943207	-1.785428	-1.241539
26	1	-4.649020	-0.973170	-1.081644
27	1	-4.476337	-2.730885	-1.313655
28	1	-3.353465	-1.599618	-2.134821
29	1	-2.018907	-2.801005	-0.156604