**Copper(I)-Alkyl Sulfide and -Cysteine Tri-nuclear Clusters as Models for Metallo Proteins. A
Structural Density Functional Analysis**

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SUPPORTING INFORMATION

Basis sets abbreviations (see text for details)

BS1, B3LYP/6-31G** for all the atoms

BS1W, B3LYP/6-31G** for all the atoms and solvent treatment PCM (water)

BS2, B3LYP/6-311++G** for all the atoms

BS2W, B3LYP/6-311++G** for all the atoms and solvent treatment PCM (water)

Figure S.1. Computed structures for (a) H_2S and (b) SH^- (BS2).

Table S.1. Average bond distances ($\text{\AA}$) and angles ($^\circ$) for fully optimized H_2S and HS^- free ligands as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details).

Vector(s)	H_2S	HS^-
S-H	1.347 (1.348) [1.346] {1.347}	1.357 (1.355) [1.352] {1.351}
H-S-H	92.7 (92.5) [93.9] {93.1}	

Figure S.2. Selected computed models for $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_n]^+$ (a-c) and $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_n]^{1-n}$ (d-f) ($n=1-3$) structures as calculated at BS2 level of theory (see text for details).

Table S.2. Selected average bond distances (Å) and angles (°) for fully optimized $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_n]^+$ and $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_n]^{1-n}$ ($n=1-3$) models as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details).

Vector(s)	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_n]^+$			$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_n]^{1-n}$		
	n=1	n=2	n=3	n=1	n=2	n=3
Cu-S	2.078	2.145	2.219	2.029	2.130	2.304
	(2.250)	(2.255)	(2.345)	(2.146)	(2.209)	(2.396)
	[2.065]	[2.143]	[2.218]	[2.049]	[2.121]	[2.244]
	{2.242}	{2.248}	{2.337}	{2.170}	{2.200}	{2.330}
S-H	1.353	1.351	1.349	1.354	1.355	1.360
	(1.356)	(1.354)	(1.351)	(1.353)	(1.353)	(1.353)
	[1.351]	[1.350]	[1.347]	[1.353]	[1.352]	[1.355]
	{1.352}	{1.351}	{1.349}	{1.351}	{1.351}	{1.351}
S-Cu-S		169.5	119.8		174.5	120.0
		(175.7)	(119.9)		(178.5)	(120.0)
		[169.9]	[119.8]		[173.3]	[120.0]
		{177.0}	{120.0}		{178.0}	{120.0}
Cu-S-H	107.3	107.4	109.9	100.6	104.8	106.5
	(98.6)	(99.6)	(102.9)	(94.1)	(96.8)	(98.8)
	[107.7]	[106.3]	[108.3]	[103.1]	[106.2]	[109.9]
	{98.1}	{98.6}	{101.1}	{95.5}	{98.0}	{103.0}

Figure S.3. Computed structures for $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_4]^+$, obtained by starting from a *pseudo*-tetrahedral arrangement.

Table S.3. Selected average bond distances (Å) and angles (°) for fully optimized $[\text{Cu}^{\text{I/II}}(\underline{\text{S}}\text{-SH}_2)_4]^{+/2+}$, $[\text{Cu}^{\text{I/II}}(\underline{\text{S}}\text{-SH})_4]^{3-/2-}$ models as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_4]^+$	$[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH}_2)_4]^{2+}$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_4]^{3-}$	$[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH})_4]^{2-}$
Cu-S	2.328	2.401	dnc	2.396
	(2.327)	(2.437)	(dnc)	(2.410)
	[2.286/2.319/2.388]	[2.394]	[2.449]	[2.349]
	{2.428}	{2.417}	{2.503}	{2.367}
S-H	1.349	1.352	dnc	1.351
	(1.349)	(1.355)	(dnc)	(1.350)
	[1.347]	[1.348]	[1.354]	[1.349]
	{1.349}	{1.351}	{1.351}	{1.349}
S-Cu-S	109.6	97.5/138.3	dnc	96.6/140.4
	(109.5)	(95.2/144.3)	(dnc)	(95.2/144.9)
	[109.5]	[96.7/140.0]	[105.1/118.6]	[97.1/138.6]
	{109.5}	{94.0/149.0}	{107.2/114.1}	{95.9/142.4}
Cu-S-H	109.5	105.7	dnc	99.0
	(109.4)	103.0	(dnc)	(96.8)
	[107.4]	[100.8]	[111.6]	[102.5]
	{101.3}	{98.9}	{103.0}	{100.4}

Figure S.4. Computed structures for (a) CH_3SH and (b) CH_3S^- (BS2).

Table S.4. Average bond distances ($\text{\AA}$) and angles ($^\circ$) for fully optimized CH_3SH and CH_3S^- free ligands as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details).

Vector(s)	CH_3SH	CH_3S^-
S-C	1.839	1.844
	(1.836)	(1.849)
	[1.838]	[1.855]
	{1.837}	{1.858}
S-H	1.348	
	(1.348)	
	[1.348]	
	{1.348}	
C-S-H	96.1	
	(96.9)	
	[97.5]	
	{97.4}	

Table S.5. Average bond distances (Å) and angles (°) for fully optimized $[\text{Cu}(\underline{\text{S}}\text{-S(H)CH}_3)_n]^+$ ($n=1$ -4) models as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details).

Vector(s)	$[\text{Cu}(\underline{\text{S}}\text{-S(H)CH}_3)_n]^+$			
	n=1	n=2	n=3	n=4
Cu-S	2.069	2.137	2.210	2.319
	(2.235)	(2.243)	(2.329)	(2.419)
	[2.060]	[2.137]	[2.211]	[2.318]
	{2.231}	{2.241}	{2.324}	{2.344}
S-C	1.842	1.841	1.838	1.838
	(1.851)	(1.847)	(1.842)	(1.841)
	[1.836]	[1.837]	[1.835]	[1.835]
	{1.843}	{1.842}	{1.840}	{1.838}
S-H	1.350	1.349	1.347	1.347
	(1.354)	(1.352)	(1.350)	(1.349)
	[1.349]	[1.348]	[1.346]	[1.347]
	{1.351}	{1.350}	{1.349}	{1.348}
Cu-S-C	112.4	113.8	115.6	114.0
	(108.0)	(108.8)	(111.6)	(111.0)
	[111.2]	[110.8]	[112.8]	[112.1]
	{106.3}	{106.7}	{108.3}	{108.7}
Cu-S-H	106.0	106.0	108.5	107.2
	(98.1)	(99.5)	(102.2)	(103.4)
	[106.9]	[105.2]	[107.4]	[105.5]
	{98.2}	{98.8}	{101.3}	{101.3}
S-Cu-S		167.0	118.5	109.5
		(173.7)	(119.6)	(109.4)
		[169.6]	[119.0]	[109.5]
		{175.8}	{119.9}	{109.4}
C-S-H	97.7	98.0	97.0	97.1
	(98.6)	(98.5)	(98.1)	(97.7)
	[97.0]	[97.5]	[96.8]	[97.0]
	{98.2}	{98.3}	{97.9}	{97.7}

Table S.6. Average bond distances (Å) and angles (°) for fully optimized $[\text{Cu}(\text{S-SCH}_3)_n]^{1-n}$ (n=1-4) models as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}(\text{S-SCH}_3)_n]^{1-n}$			
	n=1	n=2	n=3	n=4
Cu-S	2.024	2.121	2.274	dnc
	(2.147)	(2.205)	(2.369)	(dnc)
	[2.042]	[2.114]	[2.233]	[2.433]
	{2.166}	{2.196}	{2.320}	{2.504}
S-C	1.846	1.848	1.849	dnc
	(1.848)	(1.851)	(1.849)	(dnc)
	[1.850]	[1.852]	[1.854]	[1.850]
	{1.854}	{1.855}	{1.853}	{1.854}
S-Cu-S		173.2	120.0	dnc
		(178.3)	(120.0)	(dnc)
		[171.4]	[120.0]	[105.8/117.0]
		{177.3}	{120.0}	{107.8/112.8}
Cu-S-C	103.8	108.6	107.9	dnc
	(104.7)	(104.6)	(103.6)	(dnc)
	[105.8]	[110.5]	[112.8]	[114.0]
	{104.5}	{105.8.}	{108.5}	{107.6}

Table S.7. Average bond distances (Å) and angles (°) for H₂Cys(NH₂,SH,COOH), HCys⁻(NH₂,S⁻,COOH) and Cys²⁻(NH₂,S⁻,COO⁻) free ligands (selected conformations) as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details). Data compared to X-ray structure for H₂Cys(NH₃⁺,SH,COO⁻) (Moggach, Clark, & Parsons, 2005).

Vector(s)	H ₂ Cys X-Ray	H ₂ Cys ^a	H ₂ Cys ^b	H ₂ Cys ^c	HCys ⁻ (NH ₂ ,S ⁻ ,COOH) ^b	HCys ⁻ (NH ₂ ,S ⁻ ,COOH) ^c	Cys ²⁻ (NH ₂ ,S ⁻ ,COO ⁻) ^b
S-C	1.824(1)	1.839 (1.837) [1.841] {1.836}	1.843 (1.941) [1.844] {1.842}	1.851 (1.849) [1.854] {1.853}	1.849 (1.850) [1.853]	1.848 (1.846) [1.855] {1.853}	1.867 (1.877) [1.864] {1.861}
C-O	1.244(1)	1.211 (1.204) [1.247] {1.245}	1.210 (1.204) [1.243] {1.242}	1.208 (1.201) [1.216] {1.210}	1.237 (1.238) [1.246]	1.227 (1.221) [1.223] {1.218}	1.261 (1.257) [1.261] {1.261}
C-O(H) or C-O(...H)	1.262(1)	1.338 (1.339) [1.266] {1.259}	1.337 (1.336) [1.267] {1.259}	1.342 (1.343) [1.335] {1.335}	1.2779 (1.268) [1.269]	1.320 (1.320) [1.330] {1.329}	1.268 (1.267) [1.266] {1.261}
S-H or S...H	1.31(3)	1.348 (1.348) [1.360] {1.352}	1.349 (1.349) [1.349] {1.349}	1.350 (1.349) [1.348] {1.348}			
O...S		3.246 (3.278) [3.140] {3.219}	3.543 (3.652) [3.602] {3.740}			2.931 (2.936) [2.956] {2.949}	
S-H...O or S...H-O		126.3 (123.6) [138.8] {130.9}	115.3 (112.7) [116.2] {112.4}			160.3 (159.7) [159.6] {159.1}	

N...O	2.589 (2.610) [2.469] {2.528}	2.596 (2.609) [2.501] {2.556}	2.612 (2.636) [2.559] {2.575}	2.457 (2.537) [2.518]	2.683 (2.691) [2.695] {2.707}	2.722 (2.734) [2.729] {2.767}
O-H...N or N-H...O	124.7 (123.5) [130.6] {123.5}	125.5 (125.0) [127.0] {119.7}	123.4 (121.8) [127.1] {125.7}	133.7 (123.0) [125.5]	113.7 (110.4) [105.6] {101.8}	123.3 (103.3) [118.1] {108.7}
N...S		2.855 (3.277) [3.216] {3.173}		2.855 (2.878) [2.970]		3.202 (3.287) [3.243] {3.229}
N-H...S		113.1 (113.3) [114.1] {116.3}		137.4 (133.3) [129.3]		129.0 (108.5) [122.7] {119.6}

^a Fully optimized structure from input structure reported in [Figure 3a](#), gas phase treatment optimized a not-zwitterionic form, solvent treatments optimized a zwitterionic form.

^b Fully optimized structure from input structure as reported in [Moggach, Clark, & Parsons, 2005](#), X-ray experimental structures for H₂Cys(NH₃⁺,SH,COO⁻).

^c Fully optimized structure having conformation similar to the complexes

Table S.8. Average bond distances (Å) and angles (°) for the models $[\text{Cu}(\underline{\text{S}}\text{-H}_2\text{Cys})_n]^+$ ($n=1,4$) and $[\text{Cu}(\underline{\text{S}},\underline{\text{O}}\text{-H}_2\text{Cys})_n]^+$ ($n=1,2$) as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details).

Vector(s)	$[\text{Cu}(\underline{\text{S}}\text{-H}_2\text{Cys})_n]^+$				$[\text{Cu}(\underline{\text{S}},\underline{\text{O}}\text{-H}_2\text{Cys})_n]^+$	
	n=1	n=2	n=3	n=4	n=1	n=2
Cu-S	2.040	2.133	2.228	2.340	2.103	2.256
	(2.219)	(2.241)	(2.344)	(2.453)	(2.262)	(2.290)
	[2.055]	[2.135]	[2.218]	[2.325]		[2.259]
	{2.231}	{2.244}	{2.330}	{2.426}		
Cu-O					1.839	2.001
					(1.980)	(2.244)
						[2.001]
S-C	1.855	1.856	1.854	1.851	1.876	1.851
	(1.872)	(1.865)	(1.860)	(1.853)	(1.873)	(1.860)
	[1.849]	[1.850]	[1.853]	[1.847]		[1.849]
	{1.856}	{1.858}	{1.860}	{1.849}		
C-O	1.270	1.221	1.216	1.218	1.245	1.228
	(1.220)	(1.208)	(1.210)	(1.210)	(1.231)	(1.218)
	[1.221]	[1.216]	[1.219]	[1.213]		[1.231]
	{1.212}	{1.210}	{1.212}	{1.208}		
C-O(H)	1.274	1.318	1.324	1.333	1.291	1.311
	(1.310)	(1.325)	(1.325)	(1.333)	(1.298)	(1.316)
	[1.326]	[1.332]	[1.329]	[1.344]		[1.313]
	{1.329}	{1.331}	{1.330}	{1.344}		
S-H	1.923	1.381	1.348	1.349	1.351	1.349
	(1.404)	(1.357)	(1.352)	(1.350)	(1.352)	(1.351)
	[1.356]	[1.349]	[1.347]	[1.347]		[1.348]
	{1.353}	{1.351}	{1.351}	{1.349}		
S-Cu-S		169.8	117.5	99.2/99.4/102.1/106.2/116.7/134.2		124.1
		(176.4)	(118.5)	(92.5/102.7/106.7/110.7/114.4/129.0)		(156.4)
		[171.0]	[119.0]	[104.4/108.2/109.3/110.8/111.1/112.9]		[114.3]
		{177.1}	{119.9}	{105.9/107.0/108.3/108.1/112.0/114.6}		

O-Cu-O						111.0 (86.4) [105.6]
S-Cu-O					128.1 (107.6)	94.6/116.8 (90.1/107.2) [97.8/121.3]
Cu-S-C	109.5 (108.9) [109.4] {105.7}	111.1 (107.2) [107.3] {106.0}	121.2 (116.3) [115.7] {109.2}	110.5/113.4/113.6/128.7 (108.3/110.5/112.2/125.8) [112.4/112.4/112.5/114.4] {108.8/108.8/110.5/112.4}	84.6 (94.5)	101.7 (99.3) [103.6]
Cu-O-C					112.1 (125.2)	135.7 (132.4) [132.3]
O...S	2.894 (2.929) [3.087] {3.171}	3.004 (3.171) [3.383] {3.532}	3.178 (3.282) [3.262] {3.445}	*		
S-H...O or S...H-O	153.9 (145.2) [133.7] {123.0}	128.2/149.1 (123.2) [117.0] {112.3}	139.0 (144.9) [130.5] {145.3}	*		
N...O	2.506 (2.615) [2.553] {2.580}	2.611 (2.665) [2.580] {2.589}	2.601 (2.617) [2.558] {2.576}	*	2.520 (2.556)	2.557 (2.577) [2.514]
O-H...N or O...H-N	128.3 (122.1) [127.1] {125.3}	122.3 (119.3) [125.7] {125.4}	123.4 (122.3) [127.0] {125.7}	*	127.6 (125.0)	125.8 (124.5) [129.5]

*Orientations of the four H₂Cys ligand are not symmetry related to each other; the averaging of intra-molecular H-bonds interaction is not applicable.

Table S.9. Average bond distances (Å) and angles (°) for the models $[\text{Cu}(\underline{\text{S}}\text{-HCys})_n]^{1-n}$ ($n=1,4$), $[\text{Cu}(\underline{\text{S}},\underline{\text{Q}}\text{-HCys})_n]^{1-n}$ ($n=1,2$), $[\text{Cu}(\underline{\text{S}}\text{-Cys})]^-$ and $[\text{Cu}(\underline{\text{S}},\underline{\text{Q}}\text{-Cys})]^-$ as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}(\underline{\text{S}}\text{-HCys})_n]^{n-1}$				$[\text{Cu}(\underline{\text{S}},\underline{\text{Q}}\text{-HCys})_n]^{n-1}$		$[\text{Cu}(\underline{\text{S}},\underline{\text{N}}\text{-HCys})_2]^-$	$[\text{Cu}(\underline{\text{S}}\text{-Cys})]^-$	$[\text{Cu}(\underline{\text{S}},\underline{\text{Q}}\text{-Cys})]^-$
	n=1	n=2	n=3	n=4	n=1	n=2			
Cu-S	2.027	2.115	2.224	dnc	2.085	2.185	2.315	2.030	2.101
	(2.160)	(2.202)	(2.331)	(2.503)	(2.174)	(dnc)	(dnc)	(2.158)	(2.177)
	[2.042]	[2.113]	[2.211]	[2.384]	[2.092]	[2.226]	[2.367]	[2.039]	[2.731]
	{2.176}	{2.200}		{2.464}	{2.187}	{2.213}	{2.296}	{2.165}	{2.190}
Cu-O/Cu-N					1.865	2.359	2.096		1.833
					(2.036)	(dnc)	(dnc)		(1.937)
					[1.865]	[2.146]	[2.055]		[2.190]
					{2.042}	{3.006}	{2.402}		{1.963}
S-C	1.857	1.854	1.852	dnc	1.872	1.837	1.839	1.855	1.888
	(1.861)	(1.856)	(1.849)	(1.844)	(1.857)	(dnc)	(dnc)	(1.860)	(1.880)
	[1.857]	[1.859]	[1.856]	[1.852]	[1.878]	[1.840]	[1.843]	[1.862]	[1.878]
	{1.863}	{1.862}		{1.852}	{1.862}	{1.853}	{1.847}	{1.862}	{1.875}
C-O	1.210	1.218	1.225	dnc	1.242	1.212	1.218	1.255	1.307
	(1.204)	(1.212)	(1.219)	(1.225)	(1.227)	(dnc)	(dnc)	(1.253)	(1.296)
	[1.216]	[1.217]	[1.220]	[1.222]	[1.248]	[1.227]	[1.217]	[1.266]	[1.322]
	{1.212}	{1.212}		{1.217}	{1.231}	{1.210}	{1.212}	{1.259}	{1.294}
C-O(H)	1.345	1.335	1.325	dnc	1.307	1.349	1.367	1.261	1.234
	(1.349)	(1.334)	(1.325)	(1.312)	(1.315)	(dnc)	(dnc)	(1.254)	(1.234)
	[1.341]	[1.340]	[1.336]	[1.332]	[1.300]	[1.331]	[1.350]	[1.259]	[1.240]
	{1.340}	{1.339}		{1.330}	{1.312}	{1.339}	{1.348}	{1.260}	{1.239}
S-Cu-S		179.0	119.5	dnc		159.5	144.9		
		(179.9)	(120.0)	(109.3)		(dnc)	(dnc)		
		[175.5]	[119.7]	[109.5]		[135.1]	[125.6]		
		{178.3}		{111.2}		{168.1}	{146.2}		

O-Cu-O/N-Cu-N					71.7 (dnc) [86.0] {80.2}	123.6 (dnc) [113.7] {94.0}			
S-Cu-O/S-Cu-N					135.4 (115.6) [135.3] {113.9}	92.7/104.0 (dnc) [97.5/115.4] {85.7/103.5}	91.0/105.4 (dnc) [90.7/118.9] {85.6/118.2}		141.9 (126.0) [141.0] {121.5}
Cu-S-C	103.7 (105.4) [103.9] {105.2}	105.4 (105.3) [107.3] {105.8}	110.6 (105.7) [112.7]	dnc (103.1) [112.9] {107.5}	80.6 (92.2) [80.9] {93.6}	98.8 (dnc) [105.6] {107.6}	93.0 (dnc) [91.3] {98.2}	95.0 (103.4) [97.7] {103.8}	79.1 (87.9) [84.6] {91.3}
Cu-O-C/Cu-N-C					106.0 (116.8) [105.9] {117.7}	126.7 (dnc) [116.8] {121.2}	107.7 (dnc) [109.9] {106.5}		101.2 (109.8) [84.8] {110.6}
O...S	3.074 (3.132) [3.004] {3.040}	3.002 (3.025) [3.000] {3.018}	2.937 (2.973) [2.959]	dnc (2.934) [2.939] {2.969}					
S-H...O or S...H-O	152.6 (143.0) [156.4] {154.6}	157.2 (156.1) [156.0] {155.0}	159.4 (158.0) [158.1]	dnc (159.1) [159.9] {158.7}					
N...O	2.767 (2.789) [2.785] {2.798}	2.755 (2.766) [2.742] {2.754}	2.746 (2.751) [2.754]	dnc (2.737) [2.698] {2.707}	2.500 (2.528) [2.460] {2.498}	2.546 (dnc) [2.531] {2.553}	2.840 (dnc) [2.796] {2.842}	2.672 (2.682) [2.818] {2.935}	2.721 (2.731) [2.848] {2.777}
O-H...N or O...H-N	98.1 (91.1) [95.8] {87.8}	106.2 (103.6) [93.0] {88.3}	112.7 (111.5) [96.6]	dnc (114.6) [104.9] {101.8}	131.0 (128.9) [133.2] {130.5}	128.7 (dnc) [129.1] {126.9}	104.5 (dnc) [103.5] {98.0}	121.4 (118.5) [111.3] {101.7}	107.7 (106.3) [105.7] {100.1}

Table S.10. Average bond distances (Å) and angles (°) for fully optimized CopZ dimer models: $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_2^{2+}$, $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_2^{2-}$, as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}(\underline{\text{S}}\text{-S(H)Et})_2]_2^{2+}$	$[\text{Cu}(\underline{\text{S}}\text{-SEt})_2]_2^{2-}$
Cu...Cu	dnc	2.294
	(dnc)	(2.912)
	[3.268]	[2.273]
	{3.591} ^a	{2.717}
Cu-S	dnc	2.185, 2.813, 2.202
	(dnc)	(2.415, 2.281)
	[2.307, 2.266, 2.185]	[2.176, 2.785, 2.173]
	{2.547, 2.348, 2.268} ^a	{2.254, 2.405, 2.377}
S-C	dnc	1.845
	(dnc)	(1.848)
	[1.847]	[1.853]
	{1.857} ^a	{1.859}
S-H	dnc	---
	(dnc)	---
	[1.346]	---
	{1.349} ^a	---
S-Cu-S	dnc	98.0, 102.4, 157.9
	(dnc)	(93.4, 129.9, 136.7)
	[87.8, 129.1, 140.5]	[94.7, 103.3, 161.4]
	{85.7, 124.1, 149.7} ^a	{93.9, 127.0, 139.0}
Cu-S-Cu	dnc	52.8
	(dnc)	(74.1)
	[91.3]	[52.8]
	{94.2} ^a	{69.2}
Cu-S-C	dnc	108.5
	(dnc)	(108.4)
	[115.6]	[110.7]
	{114.1} ^a	{110.9}

^a Structure partially optimized

Table S.11. Average bond distances (Å) and angles (°) for fully optimized CopZ trimer models: $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_3]$, $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_2]_3^{3-}$, $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_2]_3^{3+}$ as calculated via DFT methods at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_3]$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_2]_3^{3-}$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_2]_3^{3+}$
Cu...Cu	2.300	3.869	3.925
	(2.700)	(4.073)	(dnc)
	[2.296]	[2.366] ^a	[3.735] ^a
	{2.693}	{3.493}	{4.279} ^a
Cu-S	2.185	2.228, 2.263, 2.304	2.274/2.238
	(2.248)	(2.351, 2.393, 2.362)	(dnc)
	[2.192]	[2.296, 2.334] ^a	[2.224/2.231] ^a
	{2.252}	{2.347, 2.300}	{2.388/2.305} ^a
S-H	1.351	1.358	1.353
	(1.353)	(1.353)	(dnc)
	[1.350]	[1.352] ^a	[1.348] [†]
	{1.352}	{1.351}	{1.348} [†]
Cu...Cu...Cu	60.0	60.0	60.0
	(60.0)	(60.0)	(dnc)
	[60.0]	[60.0] ^a	[60.0] ^a
	{60.0}	{60.0}	{60.0} ^a
S-Cu-S	170.2	108.6, 123.6, 127.3	107.6/125.0
	(165.9)	(109.8, 123.1, 126.8)	(dnc)
	[170.1]	[112.6, 116.8, 124.8] ^a	[109.5/125.1] ^a
	{166.2}	{111.7, 122.1, 126.1}	{107.7/126.1} ^a
Cu-S-Cu	63.5	119.0	119.3
	(73.8)	(117.8)	(dnc)
	[63.2]	[62.0] ^a	[114.2] ^a
	{73.4}	{96.1}	{127.3} ^a

^a Structure partially optimized.

Table S.12. Average bond distances (Å) and angles (°) for fully optimized CopZ trimer models: $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_3^{3+}$, $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_3^{3-}$, $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]_3^{3+}$ ($\text{NH}_2, \text{SH}, \text{COOH}$), $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-}$ ($\text{NH}_2, \text{S}^-, \text{COOH}$), $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys})_2]_3^{6-}$ ($\text{NH}_2, \text{S}^-, \text{COO}^-$) as calculated via DFT methods at BS1 and [BS1W] levels of theory (see text for details; dnc, did not converge).

Vector(s)	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_3^{3+}$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_3^{3-}$	
Cu...Cu	3.736 [3.632] ^a	2.412 [2.407]	
Cu-S	2.245/2.215 [2.220/2.225] ^a	2.308/2.384 [2.299/2.295]	
S-C	1.872 [1.850] ^a	1.848 [1.854]	
S-H	1.349 [1.348] ^a		
Cu...Cu...Cu	60.0 [60.0] ^a	60.0 [60.0]	
S-Cu-S	107.8/121.1/130.0 [109.0/123.1/127.7] ^a	110.7/119.4/123.5 [117.5/111.1/126.1]	
Cu-S-Cu	112.5 [109.8] ^a	63.0 [63.1]	
Cu-S-C	117.1 [115.1] ^a	108.3 [112.0]	
Vector(s)	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]_3^{3+}$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-}$	$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys})_2]_3^{6-}$
Cu...Cu	4.035/4.747/4.831 [3.573] ^a	2.458 [2.429]	dnc [2.417] ^a
Cu-S	2.221-2.909/2.209-2.373 [2.221/2.234] ^a	2.282 [2.298]	dnc [2.306] ^a
S-C	1.857 [1.848] ^a	1.844 [1.849]	dnc [1.857] ^a
S-H	1.351 [1.346] ^a		
Cu...Cu...Cu	49.8/64.0/66.2 [60.0] ^a	60.0 [60.0]	dnc [60.0] ^a
S-Cu-S	227.1/106.5/77.8 [109.0/125.2] ^a	135.6/107.0/113.2 [110.6//116.0/116.9]	dnc [111.8/126.4/116.5] ^a
Cu-S-Cu	125.9/141.7 [107.2] ^a	64.4 [64.1]	dnc [63.2] ^a
Cu-S-C	87.8/119.2/133.2 [128.2] ^a	112.2 [111.5]	dnc [112.0] ^a

^a Structure partially optimized.

Table S.13. Total electronic energies (Eel, Hartrees) for selected structures fully optimized via DFT method at BS1, (BS2), [BS1W] and {BS2W} levels of theory (see text for method details; dnc, did not converge).

Structure	Eel, Hartrees
Cu(I) ⁺	-1639.86090 (-1640.17691) [-1639.99681] {-1640.31454}
Cu(II) ²⁺	-1639.21380 (-1639.41060) [-1639.75742] {-1639.95476}
H ₂ S	-399.39163 (-399.42265) [-399.39547] {-339.42627}
[Cu ^I (<u>S</u> -SH ₂) ⁺	-2039.36284 (-2039.67345) [-2039.47690] {-2039.78235}
[Cu ^I (<u>S</u> -SH ₂) ₂] ⁺	-2438.83133 (-2439.16024) [-2438.92497] {-2439.25067}
[Cu ^I (<u>S</u> -SH ₂) ₃] ⁺	-2838.25775 (-2838.60442) [-2838.34422] {-2838.68872}
[Cu ^I (<u>S</u> -SH ₂) ₄] ⁺	-3237.66177 (-3237.66242) [-3237.74341] {-3238.1215} †
HS ⁻	-398.80956 (-398.85896) [-398.92451] {-398.96561}
[Cu ^I (<u>S</u> -SH)]	-2039.03089 (-2039.34473) [-2039.04953] {-2039.36151}
[Cu ^I (<u>S</u> -SH) ₂] ⁻	-2437.97281 (-2438.31202) [-2438.05541] {-2438.39261}
[Cu ^I (<u>S</u> -SH) ₃] ²⁻	-2836.69069 (-2837.07543) [-2836.99174] {-2837.36135}

$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_4]^{3-}$	dnc dnc [-3235.89619] † {-3236.31316} †
$[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH})_3]^-$	-2836.78293 (-2837.12957) † {-2837.20656} †
$[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH})_4]^{2-}$	-3235.54209 (-3235.91269) [-3235.82604] {-3236.18448}
$[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH}_2)_4]^{2+}$	-3237.24341 (-3237.59068) [-3237.5485] † {-3237.8888} †
CH_3SH	-438.70527 (-438.74350) [-438.70951] {-438.74723}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)]^+$	-2078.69369 (-2079.00636) [-2078.80019] {-2079.10790}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)_2]^+$	-2517.48524 (-2517.82043) [-2517.56818] {-2517.90091}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)_3]^+$	-2956.23124 (-2956.58791) [-2956.30658] {-2956.66207} †
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)_4]^+$	-3394.95254 (-3395.34707) [-3395.02180] {-3395.41614}
CH_3S^-	-438.11411 (-438.16829) [-438.22508] {-438.27345}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)]$	-2078.34323 (-2078.65978) [-2078.36060] {-2078.67547}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_2]^-$	-2516.58869 (-2516.93593) [2516.67223] {-2517.01776}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_3]^{2-}$	-2954.61877 (-2955.01309) [-2954.91303] {-2955.29536}

$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_4]^{3-}$	dnc dnc [-3393.1189] † {-3393.553} †
$\text{H}_2\text{Cys}(\text{NH}_2, \text{SH}, \text{COOH})$	-721.94180 (-722.06701) [-721.948774]* {-722.07938} -721.94525 (-721.07100) [-721.95047]* {-722.08310} -721.93652 (-722.06212) [-721.95410] {-722.08027}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}, \underline{\text{O}}\text{-H}_2\text{Cys})]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-2362.00247 (-2362.36353)
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-2361.95132 (-2362.33669) [-2362.04865] {-2362.44193}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}, \underline{\text{O}}\text{-H}_2\text{Cys})_2]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-3084.02370 (-3084.49497) [-3084.10081]
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-3083.96888 (-3084.47022) [-3084.06092] {-3084.56863}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_3]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-3805.96563 † (-3806.57565) [-3806.04762] {-3806.660} †
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_4]^+(\text{NH}_2, \text{SH}, \text{COOH})$	-4527.90930 (-4528.64059) [-4527.96271] {-4528.71825}
$\text{HCys}^-(\text{NH}_2, \text{S}^-, \text{COOH})$ and $\text{HCys}^-(\text{NH}_2, \text{SH}, \text{COO}^-)$	-721.39098 (-721.53134) [-721.48106] {-721.61921}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})](\text{NH}_2, \text{S}^-, \text{COOH})$	-2361.57964 (-2361.98294) [-2361.60808] {-2362.01046}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}, \underline{\text{O}}\text{-HCys})](\text{NH}_2, \text{S}^-, \text{COOH})$	-2361.63854 (-2362.00304) [-2361.65790] {-2362.02293}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2](\text{NH}_2, \text{S}^-, \text{COOH})$	-3083.10176

	(-3083.62207)
	[-3083.17001]
	{-3083.69272}
$[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{Q}}\text{-HCys})_2]^- (\text{NH}_2,\text{S}^-, \text{COOH})$	-3083.06784
	(-3083.62412)
	[-3083.18093]
	{-3083.68382}
$[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{N}}\text{-HCys})_2]^- (\text{NH}_2,\text{S}^-, \text{COOH})$	-3083.08356
	[-3083.18705]
	{-3083.68288}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_3]^{2-} (\text{NH}_2,\text{S}^-, \text{COOH})$	-3804.45673
	(-3805.1036) †
	[-3804.67627]
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_4]^{3-} (\text{NH}_2,\text{S}^-, \text{COOH})$	(-4526.49533)
	[-4526.14687]
	{-4526.93194}
$\text{Cys}^{2-} (\text{NH}_2,\text{S}^-, \text{COO}^-)$	-720.66612
	(-720.84277)
	[-720.97973]
	{-721.14270}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys})]^- (\text{NH}_2,\text{S}^-, \text{COO}^-)$	-2361.00900
	(-2361.42864)
	[-2361.11669]
	{-2361.54402}
$[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{Q}}\text{-Cys})]^- (\text{NH}_2,\text{S}^-, \text{COO}^-)$	-2361.11316
	(-2364.48441)
	[-2361.19556]
	{-2361.56938}
EtSH	-478.02382
	(-478.06994)
	[-478.02761]
	{-478.07341}
EtS^-	-477.43479
	(-477.49757)
	[-477.54227]
	{-477.59932}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]^{2+}$	-5192.19864 †
	(-5192.88928) †
	[-5192.43493]
	{-5193.10203} †
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]^{2-}$	-5190.39504
	(-5191.08736)
	[-5190.65647]
	{-5191.33525}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})]_3$	-6117.40169
	(-6118.22528)
	[-6117.41340]
	{-6118.23356}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_2]_3^{3-}$	-7313.70045
	(-7314.68514)

	[-7314.25378] † {-7315.17935}
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_3^{3+}$	-7788.22151 [-7788.695] †
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_3^{3-}$	-7785.50139 [-7786.01294]
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]_3^{3+} (\text{NH}_2, \text{SH}, \text{COOH})$	-9251.80804 [-9252.22288] †
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-} (\text{NH}_2, \text{S}^-, \text{COOH})$	-9249.21214 [-9249.61946]
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-} (\text{NH}_2, \text{SH}, \text{COO}^-)$	-9249.18086 [-9249.39128]
$[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys})_2]_3^{9-} (\text{NH}_2, \text{S}^-, \text{COO}^-)$	-9244.24095 [-9246.61908] †

* Fully optimized zwitterionic form.

† Structure partially optimized.

Table S.I. Computed Cartesian coordinates (in Å) of H₂S at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.000000	0.000000	0.103360
H	0.000000	0.974823	-0.826879
H	0.000000	-0.974823	-0.826879
BS2			
S	0.000000	0.000000	0.103569
H	0.000000	0.973198	-0.828548
H	0.000000	-0.973198	-0.828548
BS1W			
S	0.000000	0.000000	0.102679
H	0.000000	0.979349	-0.821432
H	0.000000	-0.979349	-0.821432
BS2W			
S	0.000000	0.000000	0.102949
H	0.000000	0.977849	-0.823593
H	0.000000	-0.977849	-0.823593

Table S.II. Computed Cartesian coordinates (in Å) of HS⁻ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.000000	0.000000	0.079848
H	0.000000	0.000000	-1.277566
BS2			
S	0.000000	0.000000	0.079689
H	0.000000	0.000000	-1.275021
BS1W			
S	0.000000	0.000000	0.079506
H	0.000000	0.000000	-1.272101
BS2W			
S	0.000000	0.000000	0.079470
H	0.000000	0.000000	-1.271521

Table S.III. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})]$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.028925	1.273952	0.000000
Cu	0.028925	-0.755425	0.000000
H	-1.301632	1.524080	0.000000
BS2			
S	0.029330	1.350855	0.000000
Cu	0.029330	-0.795205	0.000000
H	-1.319839	1.447268	0.000000
BS1W			
S	0.028650	1.285015	0.000000
Cu	0.028650	-0.763867	0.000000
H	-1.289235	1.591906	0.000000
BS2W			
S	0.029248	1.365229	0.000000
Cu	0.029248	-0.804759	0.000000
H	-1.316159	1.494344	0.000000

Table S.IV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_2]^-$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-2.126483	-0.077948	0.060786
Cu	-0.000003	0.025950	0.000923
H	-2.542660	0.864776	-0.819299
S	2.126433	-0.073167	-0.066369
H	2.543551	0.800503	0.881858
BS2			
S	2.208190	-0.043379	-0.060151
Cu	0.000000	-0.014598	0.000008
H	2.406065	0.905772	0.883209
S	-2.208192	-0.043445	0.060076
H	-2.406029	0.906758	-0.882234
BS1W			
S	-2.117247	-0.085503	0.062852
Cu	0.000067	0.038014	0.000699
H	-2.573886	0.817169	-0.834983
S	2.116944	-0.085340	-0.064146
H	2.576795	0.813902	0.835419
BS2W			
S	-2.199063	-0.048582	0.060059
Cu	-0.000047	-0.008786	0.000078
H	-2.429513	0.904379	-0.870133
S	2.199078	-0.047880	-0.060850
H	2.430622	0.893806	0.880525

Table S.V. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_3]^{2-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.174515	2.296171	-0.000367
Cu	-0.000719	-0.004631	0.000148
S	1.907255	-1.295137	0.000002
H	2.956076	-0.429998	-0.000007
S	-2.079705	-0.993331	-0.000192
H	-1.871872	-2.336957	0.000455
H	-1.096391	2.778000	0.004162
BS2			
S	-0.033718	2.396135	-0.000110
Cu	0.000154	-0.003050	0.000008
S	2.093985	-1.166639	-0.000073
H	2.923813	-0.097901	0.001201
S	-2.060070	-1.224210	-0.000109
H	-1.557294	-2.480748	0.001487
H	-1.374169	2.582541	0.001755
BS1W			
S	-2.144573	-0.663360	-0.000168
Cu	-0.000556	-0.001391	0.000111
S	0.496575	2.187556	-0.000062
H	-0.643180	2.920762	0.000366
S	1.649062	-1.522043	-0.000100
H	2.851865	-0.898072	0.000269
H	-2.209587	-2.016789	0.001430
BS2W			
S	-0.181881	2.318169	-0.000136
Cu	-0.000124	-0.006363	0.000010
S	-1.928708	-1.311592	0.000064
H	-2.914531	-0.387705	-0.000260
S	2.109426	-0.996399	0.000005
H	1.831107	-2.318572	-0.000699
H	1.105618	2.727941	0.001742

Table S.VI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-1.260902	-0.000149	-0.107298
Cu	0.813518	-0.000022	0.010512
H	-1.707430	0.985519	0.704750
H	-1.710160	-0.982500	0.707169
BS2			
S	1.376312	-0.000067	-0.108688
Cu	-0.871280	-0.000026	0.005932
H	1.624155	-0.989389	0.784269
H	1.621977	0.991224	0.782703
BS1W			
S	-1.252368	-0.000077	-0.107557
Cu	0.808862	-0.000010	0.010773
H	-1.708886	0.978719	0.703634
H	-1.710233	-0.977192	0.704865
BS2W			
S	-1.371513	-0.000029	-0.108461
Cu	0.867494	-0.000012	0.005685
H	-1.606059	0.987285	0.784912
H	-1.607042	-0.986473	0.785607

Table S.VII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_2]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-2.134724	0.079561	-0.117305
Cu	0.000018	-0.005037	0.073492
H	-2.660585	0.169513	1.124299
S	2.134569	-0.062486	-0.127283
H	2.661487	-0.326382	1.088818
H	2.562959	1.219039	-0.130785
H	-2.561888	-1.189303	-0.300198
BS2			
S	-2.251767	0.000041	-0.108095
Cu	0.000000	0.006053	0.005897
H	-2.529688	0.989747	0.772845
S	2.251773	-0.108140	0.001824
H	2.529924	0.788631	0.977177
H	2.515912	0.763427	-1.000097
H	-2.516242	-0.987755	0.779405
BS1W			
S	2.134767	-0.044631	-0.128930
Cu	-0.000013	-0.000079	0.059441
S	2.612499	-0.587089	1.010817
S	-2.134738	0.044778	-0.128916
H	-2.612435	0.586943	1.010990
H	-2.560925	-1.195057	0.189775
H	2.560785	1.195153	0.190156
BS2W			
S	-2.246018	-0.064923	-0.076812
Cu	-0.000016	-0.006287	-0.000076
H	-2.481273	1.264298	-0.141649
S	2.246048	-0.064420	0.077397
H	2.481541	1.265151	0.133481
H	2.489122	-0.142955	-1.249754
H	-2.489406	-0.134699	1.250757

Table S.VIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_3]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-2.010583	-0.933853	-0.120547
Cu	-0.002172	-0.009265	0.043768
S	0.192228	2.204602	0.088632
H	-0.755817	2.757533	-0.695289
S	1.825027	-1.254384	-0.120470
H	2.797635	-0.729563	0.652842
H	-2.100920	-2.016132	0.678919
H	-2.892972	-0.231699	0.619935
H	1.190176	2.584213	-0.735360
H	1.718137	-2.357491	0.647847
BS2			
S	-2.126822	-0.988218	-0.109596
Cu	-0.001664	-0.005949	0.012077
S	0.198597	2.329548	0.104960
H	-0.763229	2.746752	-0.747323
S	1.933341	-1.324651	-0.109454
H	2.746209	-0.738257	0.796650
H	-2.024616	-2.050618	0.718535
H	-2.839651	-0.261500	0.778917
H	1.196829	2.578451	-0.770955
H	1.650857	-2.369167	0.699366
BS1W			
S	-2.000793	-0.947543	-0.119672
Cu	-0.001626	-0.006389	0.038520
S	0.178600	2.208393	0.092519
H	-0.762196	2.721747	-0.723958
S	1.825621	-1.251451	-0.119852
H	2.780247	-0.688905	0.647181
H	-2.048032	-2.010068	0.707449
H	-2.860952	-0.235842	0.635022
H	1.185507	2.561639	-0.730027
H	1.697747	-2.313660	0.699309
BS2W			
S	0.661240	2.239247	-0.100110
Cu	-0.001383	-0.000890	-0.007306
S	1.614396	-1.685528	0.114332
H	2.543610	-1.218473	-0.745330
S	-2.269803	-0.557264	-0.099887
H	-2.328240	-1.546003	0.816490
H	-0.238996	2.813693	0.724729
H	1.646354	2.251100	0.821787
H	1.123552	-2.583121	-0.765546

H	-2.799512	0.365325	0.730395
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Table S.IX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)(\underline{\text{S}}\text{-SH})_2]^-$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	1.249204	2.001628	0.002720
Cu	-0.368950	-0.526720	0.013973
S	-2.287930	0.413231	-0.000640
S	1.521312	-1.557369	-0.093380
H	2.227226	1.077873	-0.056341
H	2.105115	3.064841	0.031575
H	-3.133530	-0.639978	-0.097978
H	1.779367	-1.947689	1.178329
BS2			
S	4.209203	-0.473333	0.033954
Cu	-1.223115	0.146896	-0.028873
S	-0.444250	2.215434	-0.025352
S	-2.001221	-1.922057	-0.032915
H	4.543857	-1.655787	-0.519361
H	5.492359	-0.057316	0.031848
H	-1.471988	2.732764	0.686190
H	-1.313620	-2.400332	1.027666
BS1W			
S	-0.860910	2.187730	0.004817
Cu	0.243681	-0.568690	0.014198
S	2.278899	0.097500	-0.029662
S	-1.689426	-1.447814	-0.078013
H	-2.089257	1.680805	-0.199753
H	-1.317673	3.468652	0.032875
H	3.001147	-0.981489	0.340636
H	-2.317962	-1.074617	1.060212
BS2W			
S	-5.458805	-0.442590	-0.011327
Cu	1.590143	0.140682	-0.015024
S	0.608058	2.109178	-0.030552
S	2.541151	-1.843350	-0.052768
H	-5.884229	-1.716778	0.096553
H	-6.708123	0.057514	0.062974
H	1.494979	2.765321	0.749444
H	1.936776	-2.357633	1.041086

Table S.X. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_4]^{3-}$ at BS1W and BS2W levels of theory.

Atom	x	y	z
BS1W			
Cu	0.002112	0.000667	-0.002055
S	-1.034767	-1.822102	1.262702
S	-1.844887	1.031677	-1.244360
S	1.050406	1.830951	1.241544
S	1.826584	-1.043201	-1.255807
H	-0.114457	-2.499232	1.989559
H	-2.552841	0.115695	-1.946609
H	0.139091	2.543476	1.944634
H	2.509582	-0.136476	-1.993256
BS2W			
Cu	0.000636	0.003201	-0.000451
S	0.176069	-2.061157	1.403928
S	-2.116244	-0.190979	-1.331443
S	-0.140742	2.124466	1.316446
S	2.074627	0.122159	-1.389725
H	1.405194	-1.945907	1.952113
H	-1.991792	-1.399474	-1.922178
H	-1.317048	2.003801	1.969758
H	1.985855	1.336948	-1.973902

Table S.XI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH})_3]^-$ at BS1, BS2 and BS2W levels of theory.

Atom	x	y	z
BS1			
S	1.538359	-1.654665	0.000002
Cu	-0.033288	-0.007920	-0.000028
S	0.717533	2.138669	0.000020
H	2.049217	1.919000	0.000017
S	-2.200006	-0.466277	0.000010
H	-2.726529	0.777519	0.000066
H	0.748493	-2.750473	0.000230
BS2			
S	-2.193625	-0.787493	-0.074506
Cu	-0.029182	-0.222184	-0.011488
S	0.205966	2.060180	0.030880
H	-1.068294	2.345351	-0.310189
S	2.093371	-0.989172	0.050459
H	2.686617	-0.011562	-0.666484
H	-2.463431	-0.426708	1.200500
BS2W			
S	-2.257496	-0.613052	-0.073479
Cu	-0.077995	-0.178254	-0.012176
S	0.489207	2.034315	0.007594
H	-0.759300	2.545766	-0.030518
S	1.937805	-1.211299	0.011160
H	2.770419	-0.151352	-0.002030
H	-2.461534	-0.584484	1.261243

Table S.XII Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH})_4]^{2-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.000762	0.000680	-0.000988
S	1.209046	-1.899987	0.812835
S	-1.902117	-1.211908	-0.810949
S	1.904681	1.207267	-0.811496
S	-1.213581	1.903229	0.809973
H	-1.349309	-2.442693	-0.884318
H	2.439246	-1.349114	0.902033
H	-2.444457	1.350875	0.878880
H	1.363945	2.443608	-0.873737
BS2			
Cu	-0.000384	-0.001753	-0.001162
S	0.810086	-2.148379	-0.726805
S	2.151452	0.808512	0.727973
S	-2.153679	-0.807832	0.726022
S	-0.807767	2.151391	-0.725846
H	2.777081	-0.388027	0.738216
H	-0.380999	-2.783398	-0.723548
H	0.389943	2.773525	-0.737319
H	-2.776373	0.389664	0.734839
BS1W			
Cu	0.007822	-0.001063	-0.000262
S	1.389514	-1.711287	-0.825971
S	1.591521	1.511437	0.831017
S	-1.612830	-1.500561	0.826089
S	-1.497121	1.601843	-0.829865
H	2.670165	0.732364	1.055485
H	2.577973	-1.085284	-0.947150
H	-0.705508	2.676326	-1.031025
H	-2.706797	-0.715504	0.909976
BS2W			
Cu	-0.005292	0.008240	-0.000616
S	1.600379	1.570291	-0.760595
S	-1.688467	1.470981	0.760356
S	1.689811	-1.478918	0.759994
S	-1.481447	-1.682625	-0.758438
H	-0.976121	2.602524	0.941163
H	0.836577	2.675619	-0.880562
H	-2.616807	-0.964937	-0.891123
H	0.985417	-2.627837	0.827325

TableS.XIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_4]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.001533	0.005649	-0.008253
S	1.696364	-0.676421	-1.441700
S	-0.466644	2.271137	-0.261254
S	0.820298	-0.265172	2.130183
S	-1.950584	-1.289658	-0.297757
H	-1.112121	2.469733	-1.428266
H	1.350681	-0.423822	-2.720224
H	-2.388794	-1.194536	-1.569574
H	-0.206232	-0.383286	2.997066
H	2.668350	0.258916	-1.443043
H	1.201651	-1.547712	2.299029
H	-1.549027	2.602870	0.472431
H	-1.599901	-2.584154	-0.439621
BS2			
Cu	0.001517	-0.000028	-0.000524
S	1.372490	1.805795	0.523206
S	-1.316518	-0.575151	1.830199
S	1.372163	-1.780906	-0.601867
S	-1.432078	0.551164	-1.750362
H	-2.140545	-1.594365	1.511436
H	0.689357	2.648666	1.324261
H	-2.246235	1.562856	-1.385658
H	0.654621	-2.643996	-1.349667
H	2.238549	1.465327	1.499693
H	2.164324	-1.431645	-1.636308
H	-0.581963	-1.336232	2.666820
H	-0.759011	1.315779	-2.634212
BS1W			
Cu	-0.030430	-0.001924	-0.042918
S	0.467530	2.208777	-0.537840
S	1.283483	-1.451705	-1.288048
S	-2.238105	-0.392476	-0.489502
S	0.418232	-0.373668	2.272750
H	2.554246	-1.297396	-0.867656
H	1.807718	2.338685	-0.491018
H	1.681587	0.037233	2.496263
H	-2.587013	-1.551347	0.103178
H	0.431157	2.342782	-1.878122
H	-2.968547	0.345023	0.369917
H	1.180432	-2.681435	-0.746244
H	-0.115357	0.667418	2.940565

BS2W			
Cu	0.009074	0.005239	-0.016265
S	-1.198069	-1.783249	-1.127815
S	-1.133812	2.118692	-0.337129
S	2.212426	0.175424	-1.012451
S	0.202189	-0.488346	2.360951
H	-2.263140	1.906352	0.368797
H	-2.450900	-1.559983	-0.680892
H	-1.074190	-0.783115	2.682369
H	2.833194	0.992684	-0.136836
H	-1.442588	-1.237532	-2.336942
H	2.804808	-0.933936	-0.524392
H	-0.577942	2.885209	0.623473
H	0.583880	-1.781930	2.339213

Table S.XIV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{II}}(\underline{\text{S}}\text{-SH}_2)_4]^{2+}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.034805	0.010305	0.049964
S	-2.123411	0.733146	0.859474
S	0.782830	2.090502	-0.883429
S	-0.942918	-1.965457	-0.926301
S	2.120290	-0.919120	0.712557
H	1.091812	2.897008	0.156388
H	-1.907217	1.882361	1.536580
H	2.619021	-0.024199	1.594223
H	0.068804	-2.804946	-1.239144
H	-2.707109	1.337070	-0.200401
H	-1.400649	-2.712538	0.103014
H	2.067137	1.908951	-1.265769
H	1.770194	-1.807690	1.669362
BS2			
Cu	-0.046672	0.001263	-0.057589
S	2.007997	1.133275	-0.760252
S	-1.171306	1.993257	0.780929
S	1.349549	-1.825842	0.810011
S	-1.984050	-1.316233	-0.590538
H	-1.670701	2.577404	-0.335400
H	1.586573	2.297379	-1.310276
H	-2.595236	-0.511663	-1.493878
H	0.478260	-2.783304	1.210083
H	2.419329	1.706418	0.397175
H	1.737859	-2.487410	-0.307166
H	-2.375991	1.542133	1.208497
H	-1.461620	-2.128882	-1.541360
BS1W			
Cu	0.004071	-0.013287	-0.006177
S	-1.031218	1.957107	0.893266
S	1.940791	1.040841	-0.916321
S	-2.075314	-0.975227	-0.724434
S	1.010204	-2.051141	0.739368
H	2.639114	1.373050	0.188370
H	1.897080	-1.536935	1.615099
H	-2.381282	-0.085100	-1.690327
H	-1.052836	2.794244	-0.163594
H	-1.610504	-1.890118	-1.599521
H	2.741783	0.003381	-1.232025
H	0.127410	-2.389812	1.701319
BS2W			
Cu	0.011203	-0.016491	-0.005266

S	-1.689931	1.569797	0.711044
S	1.562032	1.677297	-0.737435
S	-1.698338	-1.637853	-0.552629
S	1.685417	-1.644528	0.565572
H	2.046061	2.082368	0.457669
H	-0.912470	2.481966	1.333582
H	2.216932	-0.935360	1.585922
H	-2.218303	-0.956327	-1.597947
H	-1.831822	2.305430	-0.413514
H	-0.962748	-2.447983	-1.345497
H	2.649305	0.933838	-1.036720
H	0.941280	-2.421101	1.384355

Table S.XV. Computed Cartesian coordinates (in Å) of CH₃SH at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.669340	-0.088784	-0.000021
C	-1.166435	0.015404	-0.000029
H	0.888786	1.241380	0.000353
H	-1.591006	-0.989531	-0.002885
H	-1.504143	0.540904	-0.894438
H	-1.504466	0.535364	0.897490
BS2			
S	0.667273	-0.087063	0.000000
C	-1.165348	0.019629	0.000001
H	0.907697	1.239791	-0.000003
H	-1.527816	-1.008077	-0.000021
H	-1.532081	0.521772	-0.894460
H	-1.532084	0.521744	0.894475
BS1W			
S	-0.667248	-0.087549	-0.000001
C	1.167925	0.019659	-0.000001
H	-0.921751	1.235791	0.000010
H	1.533515	-1.008168	-0.000162
H	1.528322	0.527456	0.895003
H	1.528326	0.527754	-0.894834
BS2W			
S	-0.666814	-0.087563	-0.000001
C	1.167485	0.019562	-0.000001
H	-0.919171	1.236516	0.000012
H	1.532111	-1.006850	-0.000170
H	1.525588	0.526828	0.894068
H	1.525595	0.527142	-0.893889

Table S.XVI. Computed Cartesian coordinates (in Å) of CH₃S⁻ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.714598	-0.000015	0.000001
C	-1.129056	0.000083	-0.000004
H	-1.552855	1.018175	-0.017903
H	-1.553204	-0.493702	0.890471
H	-1.553178	-0.524727	-0.872559
BS2			
S	0.714452	-0.000019	0.000005
C	-1.134361	0.000118	-0.000017
H	-1.541417	1.018942	-0.057165
H	-1.541881	-0.460128	0.910662
H	-1.541767	-0.559212	-0.853467
BS1W			
S	0.716210	-0.000009	0.000004
C	-1.138623	0.000069	-0.000032
H	-1.542436	0.997031	-0.210947
H	-1.542622	-0.315898	0.968901
H	-1.542561	-0.681407	-0.757835
BS2W			
S	0.715965	-0.000001	0.000026
C	-1.142107	0.000005	-0.000090
H	-1.534750	-0.025269	1.019761
H	-1.534034	-0.870739	-0.531697
H	-1.534019	0.895999	-0.487948

Table S.XVII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.779580	-0.623785	-0.106792
C	2.074604	0.678202	0.032682
Cu	-1.134969	0.151940	0.011220
H	3.034484	0.160681	0.039533
H	1.947029	1.278713	0.931613
H	2.004267	1.300251	-0.859693
H	1.007428	-1.234553	1.075748
BS2			
S	0.890536	-0.665704	-0.101506
C	2.066154	0.758636	0.028224
Cu	-1.190062	0.144392	0.006658
H	3.059216	0.333286	0.162106
H	1.805653	1.416145	0.852622
H	2.016866	1.285468	-0.922537
H	0.984554	-1.122811	1.169463
BS1W			
S	0.776714	-0.631129	-0.106180
C	2.047660	0.687119	0.030075
Cu	-1.124822	0.151792	0.011327
H	3.022740	0.201495	0.057022
H	1.888842	1.293705	0.919450
H	1.965457	1.303040	-0.864579
H	1.029420	-1.224866	1.078048
BS2W			
S	0.894111	-0.673667	-0.100661
C	2.028495	0.773473	0.026314
Cu	-1.179346	0.142528	0.006442
H	3.037405	0.391704	0.165873
H	1.735330	1.420782	0.847375
H	1.956409	1.302064	-0.921291
H	0.995158	-1.110026	1.173909

Table S.XVIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S}(\text{H})\text{CH}_3)_2]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	-0.000101	-0.205479	-0.001525
S	2.119817	-0.447059	0.116615
C	3.065137	1.092955	-0.237936
S	-2.120345	-0.447414	-0.114035
C	-3.063534	1.094519	0.237985
H	4.119693	0.875887	-0.068608
H	2.730677	1.919670	0.386499
H	2.908531	1.324466	-1.291628
H	-4.118770	0.877615	0.072732
H	-2.730463	1.918765	-0.390445
H	-2.903481	1.329687	1.290347
H	2.409095	-0.547897	1.430633
H	-2.413520	-0.552572	-1.426865
BS2			
Cu	0.000057	-0.318421	-0.000788
S	2.239965	-0.441541	-0.019938
C	2.929900	1.271207	-0.080754
S	-2.239689	-0.441450	0.021226
C	-2.930325	1.271026	0.080842
H	4.001301	1.199218	0.094850
H	2.455611	1.916960	0.652975
H	2.750278	1.638674	-1.089209
H	-4.001971	1.198246	-0.092927
H	-2.457539	1.916013	-0.654531
H	-2.749256	1.639949	1.088507
H	2.460356	-0.699267	1.289142
H	-2.462300	-0.701110	-1.287093
BS1W			
Cu	-0.000013	-0.223159	-0.000138
S	2.110541	-0.416892	0.275598
C	2.997491	1.028344	-0.432053
S	-2.110618	-0.417038	-0.275216
C	-2.997256	1.028706	0.431819
H	4.053790	0.930914	-0.184199
H	2.589458	1.960365	-0.045660
H	2.865029	0.980127	-1.512392
H	-4.053621	0.931274	0.184240
H	-2.589201	1.960482	0.044874
H	-2.864595	0.981035	1.512159
H	2.324094	-0.135418	1.576493
H	-2.324732	-0.136586	-1.576234

BS2W			
Cu	-0.000110	-0.334069	-0.007626
S	-2.229988	-0.414977	-0.211788
C	-2.876259	1.200255	0.394603
S	2.226679	-0.412360	0.228059
C	2.884364	1.190362	-0.399170
H	-3.929895	1.260934	0.132122
H	-2.315570	2.024838	-0.035653
H	-2.762373	1.187375	1.476218
H	3.933383	1.256048	-0.119952
H	2.316840	2.023535	0.004754
H	2.789054	1.155854	-1.482120
H	-2.325630	-0.177324	-1.537782
H	2.301704	-0.149590	1.550644

Table S.XIX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)_3]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	-0.001662	-0.000136	0.001124
S	1.919991	-1.057614	-0.266832
S	-1.879670	-1.133662	-0.268569
S	-0.039703	2.192417	-0.273724
C	1.979373	-2.779058	0.374525
C	-3.394371	-0.319955	0.380873
C	1.419168	3.096773	0.383545
H	2.996454	-3.154515	0.260693
H	1.308980	-3.370990	-0.249675
H	1.663214	-2.827316	1.416029
H	-4.233882	-1.004422	0.257698
H	-3.563264	0.565645	-0.232869
H	-3.277137	-0.035595	1.426056
H	1.248836	4.165964	0.256085
H	2.274663	2.796984	-0.222908
H	1.598564	2.855805	1.430871
H	-1.873900	-2.176363	0.584499
H	-0.951365	2.716499	0.568461
H	2.822126	-0.532550	0.584791
BS2			
Cu	0.000052	-0.000463	-0.020766
S	-0.739775	2.203356	-0.171280
S	2.277999	-0.462278	-0.175154
S	-1.540156	-1.740812	-0.178347
C	0.611280	3.398087	0.204450
C	2.638731	-2.226875	0.212208
C	-3.247706	-1.170039	0.211981
H	0.184880	4.397738	0.257983
H	1.305863	3.346551	-0.632228
H	1.117331	3.143111	1.132381
H	3.717842	-2.356578	0.263979
H	2.245068	-2.808756	-0.619418
H	2.167351	-2.531252	1.143511
H	-3.901095	-2.038841	0.259334
H	-3.553668	-0.533383	-0.616396
H	-3.274644	-0.614276	1.146094
H	2.757261	0.083540	0.962727
H	-1.307164	-2.432721	0.957114
H	-1.443437	2.347031	0.971802
BS1W			
Cu	0.002922	-0.000524	-0.105877
S	-1.350707	1.735752	-0.328122
S	2.181266	0.298439	-0.330190

S	-0.832855	-2.035010	-0.328592
C	-0.771242	3.211262	0.596719
C	3.167033	-0.939317	0.600133
C	-2.400743	-2.268858	0.596684
H	-1.524984	3.994500	0.518637
H	0.151532	3.538951	0.117834
H	-0.577448	2.961880	1.638977
H	4.222024	-0.675917	0.527150
H	2.993725	-1.902702	0.120458
H	2.848977	-0.982816	1.640744
H	-2.703603	-3.312730	0.517442
H	-3.145040	-1.632137	0.118279
H	-2.281066	-1.977436	1.639102
H	2.519260	1.366187	0.417305
H	-0.080005	-2.862719	0.420347
H	-2.441671	1.494697	0.423417

BS2W

Cu	-0.000383	-0.000554	-0.246772
S	-0.139478	2.318783	-0.325551
S	2.075947	-1.041614	-0.331850
S	-1.939312	-1.279660	-0.327618
C	1.197500	3.014714	0.728882
C	2.018315	-2.537069	0.738006
C	-3.210711	-0.472077	0.728680
H	1.027850	4.081893	0.854468
H	2.127851	2.850387	0.188950
H	1.230122	2.509117	1.690339
H	3.028063	-2.924106	0.856611
H	1.403688	-3.264893	0.212093
H	1.575193	-2.301921	1.702069
H	-4.050149	-1.152946	0.852163
H	-3.533243	0.417318	0.191059
H	-2.789709	-0.193864	1.691222
H	2.802236	-0.255376	0.488944
H	-1.622909	-2.292216	0.505542
H	-1.173045	2.549119	0.509828

Table S.XX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)CH}_3)_4]^+$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	-0.022963	-0.070740	-0.017881
S	-1.569928	-1.291235	-1.252953
S	1.301079	-1.437069	1.269653
S	-1.296804	1.458365	1.182794
S	1.358137	1.087843	-1.478030
C	-2.980730	-1.920528	-0.258820
H	-3.525996	-1.045176	0.095732
H	-3.631419	-2.517014	-0.898294
H	-2.636228	-2.504847	0.594229
C	2.179005	-0.586309	2.641856
H	2.707711	-1.327199	3.241835
H	2.903252	0.087159	2.182037
H	1.488552	-0.013535	3.260972
C	-1.363428	3.125263	0.411445
H	-1.983530	3.031509	-0.481073
H	-1.838492	3.820589	1.103645
H	-0.367558	3.471737	0.135240
C	2.618155	0.038394	-2.307362
H	2.156913	-0.815858	-2.802263
H	3.174058	0.645516	-3.021878
H	3.296305	-0.313749	-1.529320
H	-0.563218	1.806942	2.257465
H	-1.019352	-2.485544	-1.545768
H	0.627566	1.364462	-2.576095
H	0.479633	-2.180913	2.035919
BS2			
Cu	0.075779	-0.079049	-0.081635
S	2.030323	-1.146523	-0.992377
S	0.439437	0.907797	2.094052
S	-1.623261	-1.812014	0.193965
S	-0.831774	1.636748	-1.508856
C	3.418622	-1.227021	0.213397
H	3.124738	-1.948970	0.973699
H	4.310288	-1.588606	-0.294826
H	3.602287	-0.256869	0.669793
C	-1.132007	0.864962	3.051613
H	-0.925402	1.134731	4.085270
H	-1.782743	1.616646	2.607728
H	-1.601063	-0.114252	2.990060
C	-2.936351	-1.706795	-1.091160
H	-2.505819	-1.660265	-2.088900
H	-3.596497	-2.566491	-0.996430
H	-3.497267	-0.796543	-0.886254
C	0.178192	3.169913	-1.377204

H	1.239060	2.953954	-1.480771
H	-0.149942	3.877861	-2.135521
H	-0.017529	3.583521	-0.389461
H	-1.003260	-2.916732	-0.269522
H	2.557153	-0.208191	-1.805940
H	-0.442858	1.267365	-2.747107
H	1.084924	-0.067196	2.767192
<hr/>			
BS1W			
Cu	0.107504	0.014371	-0.093472
S	2.381278	0.299999	-0.498591
S	-0.316688	0.184258	2.206180
S	-0.398500	-2.088089	-0.926352
S	-1.100657	1.612663	-1.191950
C	3.442682	-0.833801	0.479637
H	3.255805	-1.838616	0.099666
H	4.489918	-0.574215	0.324355
H	3.187407	-0.789670	1.537860
C	-2.050989	-0.281864	2.583281
H	-2.183055	-0.351073	3.662992
H	-2.677945	0.517912	2.188150
H	-2.313699	-1.223004	2.101215
C	-2.118199	-2.188168	-1.560684
H	-2.144201	-1.604903	-2.481614
H	-2.360888	-3.227619	-1.781431
H	-2.822914	-1.770056	-0.842766
C	-0.699227	3.307693	-0.613916
H	0.377640	3.472810	-0.610272
H	-1.199666	4.033099	-1.255344
H	-1.086589	3.389677	0.401917
H	-0.578294	-2.869717	0.155608
H	2.728175	1.437583	0.132173
H	-0.549785	1.723661	-2.415601
H	0.267955	-0.907087	2.735272
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BS2W			
Cu	0.110874	0.017065	-0.079399
S	2.456876	0.532192	-0.433026
S	-0.381974	0.256857	2.270185
S	-0.262901	-2.203526	-0.945524
S	-1.223896	1.588447	-1.327216
C	3.484255	-0.750682	0.390834
H	3.390411	-1.651301	-0.213220
H	4.522972	-0.427091	0.405121
H	3.124458	-0.942562	1.398721
C	-2.024877	-0.490642	2.616482
H	-2.177601	-0.544010	3.692447
H	-2.762763	0.175800	2.173776
H	-2.101296	-1.477369	2.166304
C	-1.991891	-2.314354	-1.561352
H	-2.019148	-1.759771	-2.497487

H	-2.240707	-3.357060	-1.747484
H	-2.683218	-1.871340	-0.848884
C	-0.968662	3.258514	-0.601232
H	0.088189	3.443844	-0.425982
H	-1.389123	4.008120	-1.268355
H	-1.507802	3.266663	0.344287
H	-0.430486	-2.910186	0.190697
H	2.652560	1.522215	0.461686
H	-0.462617	1.751264	-2.428510
H	0.378213	-0.722625	2.800368

Table S.XXI. Computed Cartesian coordinates (in Å) of [Cu^I(S-SCH₃)] at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	0.767397	-0.727881	-0.000032
C	1.947858	0.691954	0.000088
Cu	-1.053172	0.157395	0.000010
H	2.975388	0.325461	-0.024506
H	1.816837	1.288610	0.904287
H	1.784270	1.315838	-0.880110
BS2			
S	0.847639	-0.723353	0.000002
C	2.000409	0.721113	0.000008
Cu	-1.114922	0.147481	0.000002
H	3.008272	0.301555	-0.001232
H	1.880761	1.333597	0.892834
H	1.879033	1.334875	-0.891717
BS1W			
S	0.774342	-0.715394	0.000004
C	1.990012	0.678512	0.000002
Cu	-1.071943	0.156261	0.000001
H	2.989740	0.238039	-0.000279
H	1.883777	1.302732	0.888391
H	1.883290	1.302895	-0.888204
BS2W			
S	-0.859486	-0.727468	0.000000
C	-2.008040	0.727772	0.000001
Cu	1.122812	0.146842	0.000000
H	-3.025358	0.333355	-0.000210
H	-1.867959	1.340664	-0.889346
H	-1.868204	1.340421	0.889558

Table S.XXII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_2]^-$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.000119	-0.215027	0.000235
S	-2.056982	-0.337471	-0.502625
C	-2.992486	0.864284	0.543472
S	2.058150	-0.342790	0.498177
C	2.990259	0.870943	-0.537057
H	-4.060961	0.775209	0.316068
H	-2.690236	1.897673	0.346892
H	-2.856130	0.667743	1.611161
H	4.059475	0.779239	-0.314235
H	2.688717	1.901995	-0.327544
H	2.850338	0.686754	-1.606483
BS2			
Cu	0.000016	-0.286932	0.000046
S	-2.144099	-0.318651	-0.515859
C	-2.911726	0.942664	0.599802
S	2.144378	-0.319716	0.514909
C	2.911231	0.944126	-0.598418
H	-3.987516	0.974018	0.401593
H	-2.501592	1.939698	0.421928
H	-2.764138	0.690404	1.652531
H	3.987152	0.975057	-0.400851
H	2.501193	1.940746	-0.418027
H	2.762946	0.694234	-1.651614
BS1W			
Cu	0.000165	-0.191111	0.000502
S	-2.050519	-0.345892	-0.488481
C	-3.050787	0.843868	0.517908
S	2.051976	-0.352220	0.483020
C	3.047959	0.851688	-0.510656
H	-4.106223	0.706888	0.268565
H	-2.776888	1.878681	0.300530
H	-2.923571	0.667772	1.588277
H	4.104211	0.713323	-0.265566
H	2.772899	1.883238	-0.279664
H	2.918451	0.688782	-1.582838
BS2W			
Cu	0.000024	-0.268747	0.000041
S	-2.132959	-0.319734	-0.518606
C	-2.951982	0.918903	0.593203
S	2.133392	-0.321696	0.516951
C	2.951214	0.921480	-0.590669
H	-4.020323	0.925920	0.369963

H	-2.555256	1.920662	0.426527
H	-2.817498	0.655332	1.642562
H	4.019758	0.927761	-0.368380
H	2.554502	1.922509	-0.419645
H	2.815803	0.662063	-1.640946

Table S.XXIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_3]^{2-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.001213	-0.001369	0.016794
S	-0.803740	-2.128648	0.007441
S	-1.442795	1.756208	0.005202
S	2.244824	0.370985	0.002140
C	-2.649652	-2.034503	-0.027983
C	-0.444747	3.312169	-0.023110
C	3.093446	-1.271279	-0.023023
H	-3.100857	-3.038873	-0.101441
H	-3.002437	-1.443151	-0.881497
H	-3.045272	-1.555189	0.876366
H	-1.092705	4.202748	-0.092053
H	0.243429	3.329322	-0.876804
H	0.167913	3.413521	0.881618
H	4.188808	-1.155506	-0.090051
H	2.765746	-1.876429	-0.876839
H	2.873293	-1.851769	0.881842
BS2			
Cu	0.001530	0.000297	-0.006865
S	-0.174122	2.362802	-0.007310
S	-1.959752	-1.328955	-0.001927
S	2.133844	-1.032063	-0.001292
C	-1.999033	2.661041	0.016208
C	-1.313187	-3.061683	0.008809
C	3.307709	0.396976	0.012426
H	-2.212812	3.739309	0.040521
H	-2.461593	2.198242	0.893614
H	-2.478809	2.234793	-0.870519
H	-2.143221	-3.781920	0.044763
H	-0.668625	-3.235187	0.876177
H	-0.719165	-3.266266	-0.887668
H	4.347324	0.041027	0.051931
H	3.131000	1.041932	0.878820
H	3.189091	1.012895	-0.884765
BS1W			
Cu	-0.001469	-0.000630	-0.000066
S	-0.069607	2.232486	0.000139
S	1.967364	-1.052206	0.000155
S	-1.900534	-1.177563	-0.000899
C	1.617144	3.000808	-0.000236
C	1.803791	-2.898702	0.000396
C	-3.412107	-0.104576	0.001004
H	1.531809	4.092618	-0.000259
H	2.189106	2.704538	-0.884844

H	2.189486	2.704605	0.884149
H	2.795839	-3.362560	0.001599
H	1.265034	-3.250771	-0.884622
H	1.263077	-3.250349	0.884382
H	-4.313373	-0.726711	0.000873
H	-3.443953	0.540016	-0.882720
H	-3.442965	0.538239	0.886047
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BS2W			
Cu	0.002896	-0.005260	-0.000137
S	-1.136935	2.016633	-0.000081
S	2.321102	-0.022935	-0.000272
S	-1.190555	-1.994497	-0.000086
C	0.103412	3.393822	0.000373
C	2.897850	-1.784626	0.000487
C	-2.999694	-1.592055	0.000256
H	-0.413317	4.356575	0.000905
H	0.741148	3.346860	-0.884731
H	0.741416	3.346022	0.885238
H	3.990101	-1.815958	0.000346
H	2.538995	-2.314457	-0.884363
H	2.539247	-2.313592	0.885955
H	-3.583633	-2.515580	-0.000177
H	-3.272635	-1.013246	-0.884511
H	-3.272516	-1.014152	0.885648
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Table S.XXIV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SCH}_3)_4]^{3-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1 planar input			
Cu	1.170836	2.064948	0.344145
S	0.448043	0.262526	1.173819
S	24.747745	-4.325230	-0.514644
S	2.000871	3.594943	-0.864705
S	-28.059867	-3.076354	-0.255665
C	-1.108022	0.171076	0.117302
H	-0.899671	0.548372	-0.890667
H	-1.418981	-0.877834	0.047785
H	-1.967970	0.736932	0.501741
C	23.566020	-3.100086	0.226160
H	23.194592	-3.417416	1.220929
H	24.022242	-2.086887	0.352531
H	22.663978	-2.974244	-0.405220
C	1.582628	5.367800	-0.442806
H	0.671531	5.656194	-1.029228
H	1.379551	5.583997	0.605960
H	2.373881	6.069491	-0.726105
C	-26.188313	-3.002008	-0.188836
H	-25.770197	-3.948627	0.220444
H	-25.747232	-2.891662	-1.196841
H	-25.758507	-2.196677	0.426661
BS1 tetrahedral input			
Cu	-12.601009	-0.005043	0.022580
S	53.342653	-0.018882	0.173965
S	-11.346445	1.386942	-1.276006
S	-14.128750	0.879243	1.464216
S	-12.456633	-2.257598	-0.227789
C	-15.054993	-0.517498	2.244302
C	-11.895187	3.113144	-0.928928
C	-11.202675	-2.594431	-1.542921
C	51.515074	0.031361	-0.055113
H	-15.418704	-1.222110	1.487466
H	-14.420421	-1.089671	2.934279
H	-15.924592	-0.152021	2.817139
H	-12.988568	3.182069	-0.942239
H	-11.568676	3.428210	0.070980
H	-11.491462	3.837411	-1.656546
H	-11.406613	-2.003897	-2.443605
H	-10.190330	-2.334618	-1.209595
H	-11.194506	-3.660515	-1.827794
H	50.969956	0.157566	0.893575
H	51.194468	0.860224	-0.705585
H	51.122191	-0.887132	-0.527104

BS2 tetrahedral input			
Cu	1.298645	0.236719	-0.487595
S	-5.304788	-0.850694	0.727769
S	0.593613	2.407766	-0.989441
S	2.006649	-0.085322	1.881152
S	1.052099	-1.737629	-1.709556
C	3.039151	-1.646526	1.709499
C	0.513282	3.416863	0.569445
C	0.050299	-2.840223	-0.566273
C	-4.866941	0.777424	-0.087896
H	2.811962	-2.353096	2.527378
H	2.803529	-2.135853	0.758107
H	4.122206	-1.420143	1.734136
H	1.051113	4.371548	0.461728
H	-0.516885	3.642055	0.865819
H	0.991245	2.837735	1.362549
H	0.603569	-3.015754	0.370318
H	-0.961638	-2.464265	-0.321741
H	-0.103535	-3.808730	-1.069387
H	-5.334377	0.822230	-1.084124
H	-5.297522	1.612838	0.494799
H	-3.806296	1.055417	-0.266766

BS2 planar input			
Cu	0.004232	-0.050429	-0.043303
S	-0.632271	2.210222	0.080753
S	2.247461	0.638826	-0.096063
S	0.800275	-2.256597	0.096286
S	-2.297984	-0.635662	0.005231
C	-2.424298	2.646790	0.133799
H	-2.933421	2.221801	1.016423
H	-2.512309	3.748233	0.184556
H	-2.950849	2.295402	-0.770816
C	2.662457	2.435745	-0.104740
H	2.252527	2.959668	-0.983512
H	2.294864	2.946754	0.800609
H	3.770556	2.525772	-0.130242
C	2.622287	-2.549300	0.144527
H	3.109508	-2.143749	-0.758175
H	3.114592	-2.095775	1.022451
H	2.805872	-3.639934	0.168355
C	-3.060271	-2.314593	-0.175070
H	-3.056008	-2.880965	0.777078
H	-4.115212	-2.160469	-0.495114
H	-2.583615	-2.934782	-0.946238

BS1W			
Cu	0.000119	-0.003894	-0.001841
S	1.270443	0.793657	1.909241
S	-1.259290	1.928923	-0.801265
S	1.272563	-0.808858	-1.912726

S	-1.280573	-1.905889	0.795606
C	2.381254	-0.477684	2.665486
H	3.104252	-0.863681	1.938459
H	2.946920	-0.052658	3.502752
H	1.811724	-1.331429	3.048028
C	-2.379778	2.667074	0.471290
H	-3.085044	1.924787	0.860781
H	-1.814827	3.062744	1.322607
H	-2.964110	3.491408	0.046177
C	2.392722	0.467698	-2.645416
H	1.825650	1.305290	-3.065690
H	3.076165	0.878927	-1.894106
H	3.001799	0.039613	-3.450151
C	-2.399596	-2.658089	-0.471532
H	-1.835769	-3.040488	-1.328857
H	-2.966959	-3.493460	-0.044998
H	-3.121161	-1.927426	-0.854251
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BS2W			
Cu	0.004166	-0.012983	0.002463
S	1.383243	-1.749402	1.173448
S	-1.395817	1.164792	1.698844
S	1.391644	1.687891	-1.190276
S	-1.372313	-1.206095	-1.729294
C	2.594092	-2.410050	-0.065646
H	3.144811	-1.596830	-0.545040
H	3.317097	-3.071242	0.418869
H	2.085852	-2.979408	-0.848307
C	-2.430955	-0.107450	2.562985
H	-3.026824	-0.679287	1.846759
H	-1.805932	-0.810550	3.119690
H	-3.115062	0.370580	3.268824
C	2.306113	2.675027	0.084855
H	1.614045	3.240223	0.714900
H	2.898546	2.024317	0.733561
H	2.985237	3.384965	-0.394674
C	-2.492096	0.045285	-2.514101
H	-1.929997	0.727293	-3.165553
H	-3.260549	-0.452350	-3.123000
H	-2.999067	0.646950	-1.749574

Table S.XXV. Computed Cartesian coordinates (in Å) of H₂Cys (NH₂,SH,COOH) or (NH₃⁺,SH,COO⁻) (selected conformations) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1 – input from X-Ray			
S	-2.027180	-0.270623	-0.536257
C	-1.040833	0.099408	0.975647
C	0.379428	0.603425	0.683082
C	1.250571	-0.522390	0.077801
N	0.492779	1.792760	-0.168469
O	1.095794	-1.692043	0.347669
O	2.204451	-0.072001	-0.743506
H	-1.348601	-1.385736	-0.875200
H	-1.609939	0.864710	1.510024
H	-0.992729	-0.795955	1.596266
H	0.849393	0.842011	1.647862
H	2.030598	0.897569	-0.818608
H	-0.206368	1.742067	-0.910119
H	0.326124	2.645673	0.356677
BS2 – input from X-Ray			
S	-2.036298	-0.285385	-0.538678
C	-1.033573	0.014493	0.976318
C	0.366799	0.579038	0.698536
C	1.281969	-0.494291	0.062870
N	0.419569	1.804867	-0.105098
O	1.225961	-1.659776	0.358960
O	2.161608	-0.002688	-0.814862
H	-1.356035	-1.372450	-0.957940
H	-1.613236	0.732194	1.559473
H	-0.957917	-0.912417	1.541952
H	0.831174	0.795654	1.668653
H	1.947179	0.954113	-0.891092
H	-0.319286	1.799602	-0.805740
H	0.320180	2.639669	0.460103
BS1W – input from X-Ray			
S	-1.999813	-0.269690	-0.540664
C	-1.030374	0.034385	0.997847
C	0.389952	0.521949	0.746185
C	1.312936	-0.516800	0.006640
N	0.456950	1.758318	-0.102690
O	1.183762	-1.708005	0.335755
O	2.094294	0.015942	-0.836006
H	-1.248703	-1.299591	-0.981107
H	-1.612634	0.760216	1.570008
H	-0.965171	-0.891458	1.568326
H	0.856694	0.764355	1.705693
H	1.331189	1.540407	-0.664620
H	-0.342153	1.797231	-0.745618

H	0.519612	2.634947	0.414743
BS2W – input from X-Ray			
S	-2.020902	-0.301486	-0.533234
C	-1.008906	-0.093153	0.992096
C	0.380268	0.485189	0.746587
C	1.368426	-0.458648	-0.025603
N	0.326893	1.772040	-0.029608
O	1.360740	-1.653320	0.316207
O	2.081594	0.122428	-0.884901
H	-1.272978	-1.273995	-1.093974
H	-1.599521	0.562976	1.632840
H	-0.899775	-1.053652	1.489236
H	0.842475	0.712561	1.709946
H	1.196378	1.751092	-0.600008
H	-0.471379	1.756683	-0.675921
H	0.273576	2.610630	0.547954
BS1 – Zwitterionic input and Not- Zwitterionic output			
N	-1.417328	1.664430	-0.019098
H	-2.624208	0.217815	-0.241809
C	-0.403839	0.624824	-0.279235
H	-0.186404	0.648892	-1.354286
C	0.915659	0.807418	0.488446
C	-1.058332	-0.750837	-0.010255
H	1.221317	1.855476	0.421093
H	0.778938	0.565231	1.546896
S	2.344627	-0.136820	-0.180875
O	-2.392482	-0.732302	-0.113822
O	-0.435204	-1.757333	0.245070
H	-1.217248	2.512607	-0.540504
H	1.772070	-1.346188	-0.015676
H	-1.436633	1.912942	0.968243
BS2 – Zwitterionic input and Not-Zwitterionic output			
N	-1.389480	1.684626	-0.026475
H	-2.647589	0.227527	-0.234971
C	-0.399354	0.620424	-0.270609
H	-0.174147	0.630784	-1.342483
C	0.919685	0.779832	0.503582
C	-1.074082	-0.746048	-0.009482
H	1.225273	1.826966	0.458466
H	0.785869	0.513316	1.554379
S	2.353477	-0.140023	-0.184475
O	-2.409288	-0.716146	-0.109171
O	-0.466777	-1.756766	0.233404
H	-1.194756	2.513252	-0.576616
H	1.820562	-1.365805	-0.008243
H	-1.413445	1.959992	0.951590

BS1W – Zwitterionic input and output			
N	-1.519933	1.548196	-0.098098
H	-2.318620	0.844953	0.048335
C	-0.400769	0.568430	-0.361330
H	-0.181946	0.607782	-1.430733
C	0.852973	0.921695	0.441088
C	-1.042142	-0.831734	-0.024461
H	1.131809	1.964805	0.273218
H	0.676152	0.781935	1.511301
S	2.312828	-0.073673	-0.076733
O	-2.290565	-0.781227	0.180071
O	-0.290975	-1.826581	-0.007834
H	-1.699739	2.187719	-0.871673
H	1.603058	-1.233424	-0.076771
H	-1.384478	2.099757	0.751061
BS2W – Zwitterionic input and output			
N	-1.453220	1.606076	-0.090593
H	-2.331718	1.038300	-0.032987
C	-0.397662	0.549254	-0.336114
H	-0.172033	0.576509	-1.402860
C	0.865323	0.847533	0.473275
C	-1.097976	-0.821475	-0.021534
H	1.142233	1.896903	0.359812
H	0.701752	0.649661	1.533959
S	2.338447	-0.084826	-0.103796
O	-2.346938	-0.749469	0.122166
O	-0.365293	-1.826206	0.029518
H	-1.509565	2.303709	-0.831857
H	1.734376	-1.292073	-0.035648
H	-1.327929	2.095203	0.797250
BS1 – input and output as in the complexes			
N	-1.451238	1.654996	0.000158
H	-1.497427	1.861214	0.996325
C	-0.424370	0.636350	-0.278461
H	-0.221594	0.670735	-1.356243
C	0.899887	0.823649	0.475296
C	-1.039694	-0.752317	-0.006548
H	1.223457	1.861559	0.374124
H	0.758242	0.609872	1.538571
S	2.255584	-0.262029	-0.164781
O	-0.384101	-1.722540	0.291186
O	-2.373019	-0.784641	-0.153942
H	-1.248399	2.526332	-0.480519
H	-2.639655	0.152192	-0.293250
H	3.136726	0.736940	-0.383297
BS2 – input and output as in the complexes			
N	-1.398898	1.687305	0.008076
H	-1.467394	1.903125	0.998922

C	-0.407720	0.631154	-0.255596
H	-0.191775	0.657636	-1.329105
C	0.915624	0.766484	0.512472
C	-1.071524	-0.739334	-0.003473
H	1.241986	1.805416	0.481041
H	0.777402	0.480728	1.556656
S	2.280030	-0.274357	-0.176635
O	-0.461630	-1.722350	0.319099
O	-2.400124	-0.741724	-0.202197
H	-1.175832	2.545835	-0.482366
H	-2.655774	0.191950	-0.346332
H	3.058954	0.756641	-0.564822

BS1W – input and output as in the complexes

N	-1.470925	1.628570	-0.037326
H	-1.437934	1.937399	0.932410
C	-0.431171	0.625297	-0.310307
H	-0.233219	0.642426	-1.388795
C	0.887409	0.867636	0.436536
C	-1.031511	-0.763747	-0.020779
H	1.207951	1.892513	0.248051
H	0.740925	0.742977	1.512568
S	2.257305	-0.251654	-0.119456
O	-0.370631	-1.769460	0.152127
O	-2.366431	-0.768815	-0.009187
H	-1.353576	2.450278	-0.621957
H	-2.607071	0.192650	-0.107280
H	3.210656	0.699317	-0.178628

BS2W – input and output as in the complexes

N	-1.434476	1.652978	-0.042076
H	-1.409203	1.976780	0.921223
C	-0.419238	0.621066	-0.297277
H	-0.207851	0.628754	-1.371426
C	0.896526	0.829209	0.465060
C	-1.053392	-0.754686	-0.020905
H	1.218922	1.857853	0.318642
H	0.749087	0.661034	1.532826
S	2.274419	-0.261736	-0.122743
O	-0.422450	-1.772070	0.156241
O	-2.388460	-0.738270	-0.025505
H	-1.304320	2.459675	-0.641900
H	-2.627528	0.218374	-0.120981
H	3.175415	0.723639	-0.307120

Table S.XXVI. Computed Cartesian coordinates (in Å) of HCys⁻(NH₂,S⁻,COOH) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1 - input and output as in the complexes			
N	-1.508496	1.669518	0.028120
H	-2.406376	1.190671	-0.040824
C	-0.477272	0.671852	-0.305929
H	-0.231970	0.656347	-1.383516
C	0.846499	0.968272	0.431603
C	-1.054683	-0.730829	-0.018948
H	1.091609	2.019892	0.236991
H	0.661953	0.888560	1.511030
S	2.246295	-0.116147	-0.096820
O	-2.262496	-0.904145	0.110661
O	-0.195880	-1.731981	0.028482
H	-1.497648	2.409116	-0.668936
H	0.780930	-1.359621	-0.055972
BS2 - input and output as in the complexes			
N	-1.499308	1.675588	0.018256
H	-2.417075	1.245776	-0.063106
C	-0.476513	0.666617	-0.303279
H	-0.231457	0.648849	-1.377873
C	0.844187	0.959329	0.438078
C	-1.060796	-0.730789	-0.019258
H	1.091974	2.008422	0.248561
H	0.665970	0.864223	1.514776
S	2.245665	-0.116453	-0.098001
O	-2.262001	-0.903830	0.114386
O	-0.202336	-1.732101	0.024269
H	-1.443508	2.454440	-0.627545
H	0.772060	-1.371071	-0.057082
BS1W - input and output as in the complexes			
N	-1.487008	1.676914	0.031945
H	-2.405193	1.306269	-0.203543
C	-0.484534	0.667113	-0.321980
H	-0.251677	0.645814	-1.402441
C	0.839255	0.962038	0.417782
C	-1.069677	-0.721470	-0.021016
H	1.094985	2.006783	0.212857
H	0.657614	0.887679	1.496177
S	2.255635	-0.125652	-0.083092
O	-2.268453	-0.900485	0.140665
O	-0.217446	-1.741545	0.006601
H	-1.342091	2.505169	-0.539518
H	0.742184	-1.389534	-0.084512

BS2W - input and output as in the complexes			
N	-1.485745	1.681564	0.016877
H	-2.410080	1.359540	-0.253394
C	-0.486136	0.662612	-0.318352
H	-0.252716	0.638650	-1.395545
C	0.833541	0.958240	0.425535
C	-1.069997	-0.723475	-0.019444
H	1.089766	2.000324	0.222738
H	0.658526	0.871388	1.501577
S	2.250165	-0.123265	-0.081985
O	-2.260775	-0.908548	0.156929
O	-0.214866	-1.740866	-0.009101
H	-1.293483	2.535016	-0.497197
H	0.746242	-1.392579	-0.093602
BS1 - input from X-Ray			
S	-2.305254	-0.107297	-0.435041
C	-0.888726	-0.938354	0.414697
C	0.300479	0.031440	0.738583
C	1.608829	-0.194285	-0.116834
N	-0.081283	1.447118	0.452401
O	2.105242	-1.327055	-0.098403
O	2.008790	0.868479	-0.702925
H	-1.236869	-1.388215	1.351878
H	-0.477159	-1.747314	-0.193772
H	0.582818	-0.059327	1.792178
H	0.762544	1.687462	-0.188523
H	-1.055359	1.331382	-0.050740
H	-0.158676	2.038734	1.274768
BS2 - input from X-Ray			
S	-2.489380	-0.158826	-0.118218
C	-0.785358	-0.865647	-0.256406
C	0.253456	-0.026215	0.531235
C	1.716005	-0.162878	-0.015332
N	-0.128446	1.417134	0.357785
O	2.318684	-1.203291	0.281809
O	2.090220	0.822903	-0.719578
H	-0.746909	-1.883857	0.130188
H	-0.486995	-0.902431	-1.308464
H	0.204042	-0.277348	1.590607
H	0.563124	1.726180	-0.365983
H	-1.177451	1.368417	0.081084
H	-0.002455	1.961873	1.204737
BS1W - input from X-Ray			
S	-2.065552	-0.264401	-0.599863
C	-0.969018	-0.575236	0.860802
C	0.318135	0.268863	0.821636
C	1.444047	-0.304207	-0.108001
N	0.030060	1.640686	0.293835

O	1.729974	-1.507943	0.038801
O	1.967268	0.549307	-0.888239
H	-1.517309	-0.364553	1.785681
H	-0.643271	-1.617098	0.896680
H	0.738363	0.371894	1.827253
H	0.846065	1.791541	-0.351199
H	-0.855726	1.526948	-0.267109
H	-0.066626	2.369452	0.998543

Table S.XXVII. Computed Cartesian coordinates (in Å) of Cys²⁻(NH₂,S⁻,COO⁻) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1 - input from X-Ray			
S	-2.279840	-0.201589	-0.533435
C	-0.947576	-0.599947	0.712093
C	0.339039	0.288640	0.743219
C	1.533858	-0.258484	-0.139611
N	0.064696	1.718663	0.501339
O	1.853181	-1.464401	0.044708
O	2.117491	0.587265	-0.882445
H	-1.410578	-0.553943	1.712291
H	-0.590236	-1.626659	0.576788
H	0.734018	0.170031	1.774100
H	-0.814138	1.700745	-0.035369
H	0.788196	1.940450	-0.194537
BS2 - input from X-Ray			
S	2.616332	-0.128728	-0.158143
C	0.881357	-0.656677	0.324414
C	-0.230311	0.251490	-0.207469
C	-1.708970	-0.271765	-0.068145
N	-0.127184	1.588906	0.412017
O	-1.892675	-1.501284	0.114765
O	-2.600467	0.613680	-0.227669
H	0.700447	-1.666545	-0.044262
H	0.812759	-0.682709	1.417686
H	-0.073954	0.316757	-1.301965
H	-0.889805	2.149986	0.044070
H	0.772213	1.982358	0.141084
BS1W - input from X-Ray			
S	-2.078048	-0.337999	-0.583327
C	-0.985851	-0.255918	0.924856
C	0.353756	0.482537	0.743614
C	1.394886	-0.343946	-0.083965
N	0.165558	1.854550	0.240258
O	1.562706	-1.544962	0.262820
O	2.023014	0.277952	-0.989785
H	-1.549346	0.229085	1.733032
H	-0.740659	-1.267403	1.258015
H	0.798303	0.539978	1.755608
H	-0.639444	1.785830	-0.390488
H	0.958510	1.978689	-0.396048
BS2W - input from X-Ray			
S	-2.049901	-0.385173	-0.580054
C	-0.985928	-0.227438	0.938790
C	0.352169	0.504392	0.734195

C	1.387305	-0.331705	-0.083713
N	0.124846	1.863344	0.220032
O	1.614693	-1.499992	0.333937
O	1.959856	0.232310	-1.055780
H	-1.555836	0.310801	1.702752
H	-0.766305	-1.220716	1.329227
H	0.806078	0.589245	1.733555
H	-0.626184	1.787340	-0.468327
H	0.949083	2.122654	-0.317445

Table S.XXVIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})]^+$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	2.823100	1.483261	-0.167111
H	2.578054	1.991153	-1.013929
C	1.718016	0.669818	0.347390
H	1.730453	0.698473	1.445292
C	0.304708	1.064808	-0.126367
C	2.082864	-0.775965	-0.027565
H	0.129476	2.107799	0.143797
H	0.229314	0.968171	-1.212934
S	-0.927408	-0.016989	0.742332
O	1.288646	-1.759869	0.090801
O	3.263296	-0.964673	-0.469433
H	3.177727	2.146060	0.515241
Cu	-2.683192	-0.019307	-0.296234
H	3.642259	-0.014877	-0.498574
H	0.353028	-1.403515	0.372680
BS2			
N	2.875032	1.428353	-0.355470
H	2.668522	1.707297	-1.309748
C	1.810074	0.661529	0.281178
H	1.916298	0.780723	1.365103
C	0.393584	1.113166	-0.135730
C	2.045345	-0.847940	0.011594
H	0.267351	2.177497	0.056605
H	0.217561	0.912120	-1.192125
S	-0.904512	0.241177	0.893515
O	1.180612	-1.690453	0.187048
O	3.252804	-1.159502	-0.390684
H	3.157683	2.244674	0.173605
Cu	-2.702010	-0.108593	-0.359473
H	3.750647	-0.315127	-0.485315
H	-0.234135	-0.976181	0.695494
BS1W			
N	2.704501	1.614358	-0.116119
H	2.495520	1.947210	-1.055095
C	1.717216	0.633709	0.343994
H	1.721173	0.647981	1.440609
C	0.291205	0.916012	-0.152694
C	2.227732	-0.769052	-0.057273
H	0.020796	1.947299	0.078267
H	0.208933	0.763412	-1.230039
S	-0.960557	-0.134986	0.711919
O	1.531864	-1.772040	-0.085970
O	3.523093	-0.793969	-0.339159

H	2.747135	2.421305	0.498156
Cu	-2.760852	0.003637	-0.268686
H	3.796797	0.164784	-0.290768
H	-0.344801	-1.294155	0.369761
BS2W			
N	2.689468	1.649061	-0.135503
H	2.448719	1.985299	-1.064093
C	1.757732	0.624127	0.342528
H	1.796497	0.626957	1.436443
C	0.308243	0.860052	-0.111768
C	2.294124	-0.759154	-0.080344
H	0.030903	1.892493	0.094733
H	0.184182	0.663390	-1.175032
S	-0.932497	-0.143317	0.835715
O	1.626823	-1.771290	-0.088310
O	3.582419	-0.756003	-0.407042
H	2.726170	2.447076	0.488230
Cu	-2.837349	0.005559	-0.316886
H	3.854671	0.195628	-0.369470
H	-0.498887	-1.354205	0.416299

Table S.XXIX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]^+$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-5.150500	-0.781234	0.677390
H	-5.357252	-1.325638	1.508291
C	-4.154458	0.254009	0.911591
H	-4.415633	0.742292	1.861403
C	-2.678482	-0.157694	1.064960
C	-4.322279	1.353557	-0.163735
H	-2.091652	0.680637	1.440821
H	-2.583440	-1.001712	1.750665
S	-1.932904	-0.702069	-0.546448
O	-3.389176	2.024428	-0.562138
O	-5.564735	1.498517	-0.598901
H	-4.886736	-1.416378	-0.072231
Cu	0.167868	-0.987117	-0.284919
S	2.177275	-1.641157	-0.011487
C	3.401087	-0.674262	-1.016812
C	3.613552	0.773463	-0.537891
H	3.068404	-0.683990	-2.055904
H	4.334279	-1.241702	-0.954616
N	4.603894	1.511982	-1.322313
H	2.660230	1.312763	-0.612181
C	4.022178	0.872391	0.957416
H	5.376079	0.925108	-1.629808
O	3.559357	0.148013	1.832983
O	4.878094	1.831265	1.220810
H	4.204470	1.967691	-2.135973
H	5.112805	2.226851	0.341814
H	-6.087609	0.764392	-0.204092
H	2.652635	-1.012296	1.149223
H	-2.096358	0.518184	-1.118546
BS2			
N	-5.308541	-0.899918	0.995698
H	-5.454240	-1.351434	1.890526
C	-4.341862	0.186662	1.044559
H	-4.526369	0.737440	1.976040
C	-2.843313	-0.161678	1.076252
C	-4.649887	1.207695	-0.076923
H	-2.252293	0.724277	1.296101
H	-2.643990	-0.931276	1.821490
S	-2.240786	-0.866363	-0.542032
O	-3.791490	1.899480	-0.570450
O	-5.924734	1.263460	-0.433663
H	-5.096510	-1.605732	0.297368
Cu	-0.000536	-0.812686	-0.494932
S	2.239665	-0.874029	-0.527388

C	2.834141	0.891389	-0.614196
C	4.335124	1.023443	-0.300938
H	2.246849	1.477217	0.088996
H	2.624612	1.220073	-1.631768
N	5.295607	0.505192	-1.263459
H	4.515556	2.103160	-0.218856
C	4.658434	0.468328	1.107235
H	5.085230	-0.434006	-1.586618
O	3.808233	0.325310	1.953173
O	5.936578	0.178932	1.303011
H	5.430546	1.109767	-2.064758
H	6.397388	0.287706	0.445821
H	-6.393745	0.545110	0.038528
H	2.458394	-1.007948	0.805211
H	-2.451933	0.270405	-1.252503

BS1W

N	-4.954130	1.688152	-0.091138
H	-4.992158	2.465228	-0.743072
C	-4.535168	0.452054	-0.749501
H	-5.014419	0.428065	-1.737491
C	-3.038332	0.253709	-1.010688
C	-5.146611	-0.737268	0.019149
H	-2.865305	-0.652933	-1.589192
H	-2.631971	1.107466	-1.554191
S	-2.054999	0.138748	0.552667
O	-4.711113	-1.871058	-0.038784
O	-6.218233	-0.403958	0.736095
H	-4.316856	1.943122	0.660985
Cu	0.000047	-0.029400	-0.000431
S	2.055166	0.138572	-0.553122
C	3.037959	0.253610	1.010577
C	4.534874	0.452072	0.749889
H	2.864893	-0.653116	1.588948
H	2.631331	1.107285	1.553993
N	4.953984	1.688195	0.091657
H	5.013795	0.428111	1.738030
C	5.146629	-0.737213	-0.018626
H	4.316960	1.943136	-0.660685
O	4.711154	-1.871021	0.039021
O	6.218507	-0.403789	-0.735135
H	4.991786	2.465269	0.743604
H	6.268503	0.585567	-0.652795
H	-6.268408	0.585395	0.653843
H	2.470139	-1.097465	-0.898287
H	-2.469913	-1.097243	0.898091

BS2W

N	-5.242621	-1.438298	0.154922
H	-5.444138	-2.151154	0.846191
C	-4.646450	-0.246704	0.756911

H	-5.094489	-0.122423	1.749745
C	-3.130989	-0.256686	0.986475
C	-5.107544	0.999460	-0.027124
H	-2.805051	0.646626	1.495254
H	-2.850132	-1.125179	1.579601
S	-2.163484	-0.417627	-0.591457
O	-4.573325	2.081724	0.058471
O	-6.178873	0.784071	-0.787358
H	-4.648497	-1.849100	-0.560001
Cu	0.000033	-0.360191	-0.000160
S	2.163523	-0.417752	0.591377
C	3.131250	-0.257299	-0.986510
C	4.646672	-0.246842	-0.756707
H	2.805182	0.645748	-1.495678
H	2.850675	-1.126092	-1.579325
N	5.243047	-1.438165	-0.154387
H	5.094796	-0.122665	-1.749509
C	5.107272	0.999637	0.027137
H	4.648752	-1.849231	0.560238
O	4.572766	2.081733	-0.058873
O	6.178421	0.784736	0.787754
H	5.445231	-2.150939	-0.845545
H	6.359582	-0.185341	0.706954
H	-6.359672	-0.186053	-0.706231
H	2.306756	0.857577	1.014664
H	-2.306711	0.857538	-1.015225

Table S.XXX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_3]^+$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-0.062391	-2.201260	-0.611945
C	0.672184	-3.386768	0.609204
C	1.927651	-4.094589	0.073018
H	-0.103123	-4.131391	0.797962
H	0.890435	-2.866373	1.544705
N	2.363183	-5.253432	0.857006
H	1.723469	-4.445470	-0.946284
C	3.115169	-3.119933	-0.047053
H	2.251298	-5.106190	1.857550
O	2.962831	-1.943239	-0.313347
H	1.864366	-6.100602	0.605332
O	4.302487	-3.673474	0.146046
H	4.116538	-4.607888	0.409958
Cu	0.000061	-0.001483	-0.262415
S	1.933768	1.045981	-0.615363
C	2.600159	2.273632	0.602890
C	2.583334	3.714952	0.067391
H	3.633538	1.973705	0.785880
H	2.044281	2.202350	1.540724
N	3.380129	4.669619	0.842504
H	2.977420	3.713289	-0.956678
C	1.145440	4.258455	-0.036498
H	3.317753	4.499810	1.843792
O	0.198340	3.539317	-0.289845
S	-1.873689	1.150067	-0.616138
C	-3.269027	1.113270	0.603533
C	-4.510347	0.380672	0.067967
H	-3.524037	2.158388	0.787865
H	-2.929853	0.666515	1.540931
N	-5.733667	0.590013	0.847009
H	-4.708315	0.727575	-0.953975
C	-4.263412	-1.136290	-0.043158
H	-5.554032	0.615304	1.848237
O	-3.167827	-1.597640	-0.298970
O	-5.340283	-1.883380	0.146850
O	1.035561	5.564156	0.154767
H	-6.055932	-1.251287	0.401840
H	-6.213809	1.446682	0.591186
H	4.360798	4.657826	0.581437
H	1.941464	5.869430	0.405786
H	2.853416	0.086739	-0.389047
H	-1.352020	-2.516943	-0.378486
H	-1.501695	2.425218	-0.386962

BS2			
S	0.726401	2.208466	-0.902260
C	0.437751	3.361315	0.528435
C	-0.610835	4.443614	0.218040
H	1.397304	3.844977	0.706517
H	0.160433	2.788300	1.413494
N	-0.605253	5.578849	1.144484
H	-0.417871	4.840193	-0.784713
C	-2.036040	3.858065	0.157349
H	-0.426199	5.305557	2.106277
O	-2.258896	2.739786	-0.246978
H	0.064243	6.293789	0.885201
O	-2.992475	4.680861	0.561600
H	-2.540703	5.490878	0.888860
Cu	0.000289	-0.002638	-0.617800
S	-2.277799	-0.476012	-0.909097
C	-3.137594	-1.298618	0.520177
C	-3.546668	-2.749878	0.213217
H	-4.038412	-0.710598	0.690908
H	-2.507838	-1.247640	1.408572
N	-4.535530	-3.311221	1.137187
H	-3.982396	-2.785511	-0.791239
C	-2.325328	-3.689849	0.160632
H	-4.391343	-3.018415	2.099112
O	-1.243138	-3.322813	-0.236775
S	1.551350	-1.736516	-0.899448
C	2.694762	-2.058080	0.531434
C	4.156096	-1.692682	0.217097
H	2.633355	-3.130079	0.714216
H	2.338822	-1.527282	1.414582
N	5.139686	-2.264552	1.140138
H	4.400232	-2.058825	-0.786152
C	4.362396	-0.165598	0.155079
H	4.819734	-2.276378	2.104144
O	3.501260	0.588312	-0.237102
O	5.559305	0.249238	0.543164
O	-2.560472	-4.929352	0.564991
H	6.037224	-0.547283	0.866001
H	5.418395	-3.204372	0.883881
H	-5.488608	-3.089084	0.874676
H	-3.489509	-4.944017	0.887165
H	-2.761119	0.767489	-0.689757
H	2.044616	2.007288	-0.679985
H	0.717789	-2.777026	-0.675301
BS1W			
S	0.026772	-2.203924	-0.588674
C	0.903772	-3.134856	0.752615
C	2.133367	-3.902831	0.248689
H	0.179086	-3.848048	1.146089
H	1.178374	-2.441257	1.549497

N	2.700155	-4.832353	1.232533
H	1.848464	-4.487669	-0.633797
C	3.263435	-2.966782	-0.218734
H	2.618453	-4.468745	2.179882
O	3.071819	-1.913380	-0.800734
H	2.232914	-5.733153	1.207159
O	4.480021	-3.431437	0.044656
H	4.308249	-4.261357	0.570340
Cu	-0.003535	0.002110	-0.364894
S	1.894946	1.127794	-0.598591
C	2.275459	2.348080	0.743397
C	2.316625	3.798638	0.243749
H	3.260913	2.078447	1.123880
H	1.547389	2.234386	1.548899
N	2.844017	4.752754	1.226129
H	2.957725	3.849049	-0.644192
C	0.935555	4.305619	-0.211096
H	2.580509	4.495925	2.175252
O	0.118139	3.611487	-0.789990
S	-1.927486	1.081731	-0.590384
C	-3.173758	0.790085	0.749840
C	-4.449883	0.103018	0.244889
H	-3.433164	1.775470	1.137492
H	-2.710386	0.210675	1.550732
N	-5.539956	0.073625	1.227037
H	-4.814383	0.639151	-0.639150
C	-4.195796	-1.342944	-0.219688
H	-5.185856	-0.033347	2.175440
O	-3.185847	-1.697762	-0.802200
O	-5.200893	-2.170106	0.046554
O	0.727452	5.590465	0.055875
H	-5.837410	-1.608641	0.570398
H	-6.091197	0.925488	1.198558
H	3.857224	4.802372	1.191032
H	1.535987	5.859060	0.574363
H	2.849602	0.234393	-0.275385
H	-1.221486	-2.586948	-0.258440
H	-1.633899	2.353470	-0.258876
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BS2W			
S	-2.284165	0.442465	-0.963373
C	-3.060969	-0.073929	0.647265
C	-4.146392	-1.145003	0.473074
H	-3.521839	0.823658	1.054224
H	-2.282770	-0.412744	1.329550
N	-4.966278	-1.352459	1.672113
H	-4.817307	-0.842687	-0.337631
C	-3.566503	-2.504319	0.039743
H	-4.432096	-1.229065	2.528166
O	-2.648732	-2.625381	-0.742899
H	-5.756264	-0.718351	1.702489

O	-4.186717	-3.551215	0.575978
H	-4.845419	-3.159446	1.204779
Cu	0.003408	0.000826	-0.896730
S	0.759574	-2.201556	-0.966826
C	1.591789	-2.613595	0.645172
C	3.065383	-3.013717	0.475257
H	1.047917	-3.463691	1.051616
H	1.489268	-1.769814	1.326506
N	3.655541	-3.612393	1.677727
H	3.143220	-3.748831	-0.331751
C	3.953211	-1.834588	0.034568
H	3.279752	-3.206958	2.530269
O	3.602074	-0.987377	-0.758458
S	1.529247	1.759792	-0.960509
C	1.460695	2.678688	0.655231
C	1.077054	4.156256	0.485641
H	2.464747	2.625936	1.070124
H	0.772857	2.168242	1.327471
N	1.291816	4.968450	1.688497
H	1.682473	4.590129	-0.316078
C	-0.382507	4.337206	0.030971
H	1.117227	4.445364	2.542470
O	-0.935802	3.606064	-0.762049
O	-0.983992	5.398534	0.560454
O	5.165040	-1.837640	0.581761
H	-0.323278	5.773294	1.196782
H	2.237331	5.331459	1.732455
H	3.503472	-4.613986	1.715378
H	5.155147	-2.601791	1.213400
H	-0.417704	-2.813021	-0.709276
H	-2.231936	1.767594	-0.703588
H	2.648792	1.048468	-0.699057

Table S.XXXI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_4]^+$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-1.325746	-1.859109	-1.104910
C	-2.322354	-0.641275	-2.085495
C	-3.807716	-1.024564	-2.218385
H	-1.866709	-0.629346	-3.077747
H	-2.212310	0.348088	-1.636040
N	-4.535414	-0.177616	-3.171425
H	-3.886046	-2.063085	-2.564117
C	-4.581487	-0.970400	-0.875461
H	-4.196248	0.782120	-3.157681
O	-4.114919	-1.341742	0.194543
H	-4.476153	-0.523641	-4.123428
O	-5.811418	-0.510815	-0.983128
H	-5.899745	-0.242444	-1.937363
Cu	0.306604	-0.746041	0.183248
S	1.433911	-2.579048	1.029415
C	3.240573	-2.785223	1.325843
C	4.137337	-2.662376	0.089176
H	3.403927	-3.756272	1.795039
H	3.497803	-2.001511	2.042500
N	5.508486	-2.947035	0.492570
H	3.839825	-3.418163	-0.648742
C	4.000439	-1.254553	-0.505266
H	5.885902	-2.184025	1.049703
O	4.131431	-0.259449	0.185418
S	0.893394	1.008342	-1.191965
C	1.102004	2.614425	-0.297484
C	2.494858	2.871537	0.310939
H	0.356154	2.605960	0.495674
H	0.855512	3.408384	-1.006127
N	2.358432	4.025607	1.194508
H	2.796928	2.002101	0.904940
C	3.495631	3.139327	-0.838294
H	2.370719	4.863559	0.612724
O	3.530321	4.216288	-1.385930
S	-0.426205	0.229414	2.229004
C	-2.211460	-0.114582	2.611129
C	-3.151546	1.061754	2.295654
H	-2.261973	-0.325422	3.680846
H	-2.536568	-0.998998	2.061845
N	-4.563738	0.752538	2.521234
H	-2.880433	1.915688	2.929552
C	-3.013745	1.562727	0.846327
H	-4.796893	-0.174761	2.167504
O	-1.951388	1.595616	0.250155
O	4.272201	2.120035	-1.247453

O	3.786296	-1.122674	-1.824286
O	-4.151703	1.967669	0.298833
H	-4.845650	1.772750	0.983283
H	4.217905	1.344418	-0.649287
H	3.709465	-1.982708	-2.264253
H	3.175499	4.093951	1.797130
H	-4.836852	0.826495	3.495123
H	6.122307	-3.088558	-0.304548
H	1.271413	-3.646477	0.221559
H	-2.312238	-2.058950	-0.200562
H	2.148864	0.888076	-1.665217
H	0.062264	-0.590290	3.183265
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BS2			
S	-1.513272	-2.041525	-1.050028
C	-2.612169	-0.865521	-1.970439
C	-4.103071	-1.249872	-1.949051
H	-2.251298	-0.905424	-2.998409
H	-2.457546	0.139259	-1.578015
N	-4.906540	-0.536060	-2.947720
H	-4.202617	-2.322150	-2.150390
C	-4.758177	-1.030624	-0.562947
H	-4.596227	0.421776	-3.086073
O	-4.185540	-1.231431	0.490353
H	-4.919641	-1.002783	-3.846874
O	-6.013418	-0.623757	-0.611821
H	-6.215447	-0.478811	-1.566976
Cu	0.344790	-0.754265	-0.060181
S	1.554387	-2.838338	0.651044
C	3.289001	-2.920145	1.274726
C	4.382134	-2.538137	0.271641
H	3.473961	-3.930516	1.635423
H	3.310009	-2.236326	2.124455
N	5.677326	-2.712986	0.917312
H	4.340414	-3.229692	-0.576906
C	4.178795	-1.097669	-0.217773
H	5.859601	-1.994949	1.611239
O	3.978578	-0.178424	0.543872
S	0.987333	0.877956	-1.677841
C	0.951193	2.574613	-0.936221
C	2.089982	2.928252	0.033340
H	0.001509	2.609247	-0.407482
H	0.926865	3.282775	-1.765112
N	1.662564	4.102674	0.794056
H	2.238885	2.104983	0.736717
C	3.383045	3.211576	-0.768618
H	1.721305	4.929507	0.204005
O	3.480460	4.194727	-1.454515
S	-0.189534	0.308654	2.072502
C	-1.953174	0.005803	2.585476
C	-2.870545	1.220848	2.370634

H	-1.922532	-0.219852	3.650568
H	-2.345524	-0.854800	2.048665
N	-4.239097	1.006104	2.839303
H	-2.458579	2.080432	2.911756
C	-2.933673	1.660978	0.897505
H	-4.590625	0.087467	2.578208
O	-1.995821	1.562001	0.136010
O	4.389358	2.327848	-0.671036
O	4.278114	-0.854645	-1.537051
O	-4.097587	2.174108	0.524560
H	-4.701352	2.067041	1.297107
H	4.164268	1.557288	-0.115540
H	4.468568	-1.656888	-2.040837
H	2.279721	4.261135	1.584549
H	-4.346921	1.142607	3.836927
H	6.450449	-2.742718	0.262470
H	1.688833	-3.676130	-0.398756
H	-2.300781	-2.116736	0.044268
H	2.308395	0.769724	-1.935754
H	0.361787	-0.501868	3.001916
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BS1W			
S	2.352064	-0.830955	-0.517819
C	2.355125	-2.605139	-1.031542
C	3.594970	-3.034473	-1.847952
H	1.478126	-2.738607	-1.665017
H	2.233467	-3.225646	-0.141383
N	3.358384	-4.394177	-2.316832
H	3.676612	-2.374674	-2.718284
C	4.878896	-2.919520	-1.002887
H	3.585873	-5.035401	-1.557524
O	5.339502	-3.852965	-0.383031
H	4.016520	-4.609192	-3.062839
O	5.479920	-1.712690	-0.944901
H	5.011025	-1.061306	-1.491492
Cu	0.247070	-0.084748	0.054087
S	-0.893602	0.121463	-2.023411
C	-2.490756	1.033931	-1.863182
C	-3.191782	1.352778	-3.205016
H	-2.297970	1.967411	-1.334274
H	-3.125953	0.412178	-1.229032
N	-4.252865	2.309827	-2.917525
H	-2.432827	1.736404	-3.908288
C	-3.811575	0.125272	-3.896069
H	-4.988128	2.197467	-3.611189
O	-4.946637	0.124896	-4.323843
S	-0.815410	-1.605829	1.439389
C	-2.566154	-1.176103	1.844974
C	-3.282339	-2.191326	2.767322
H	-3.119318	-1.099463	0.909170
H	-2.533847	-0.184869	2.302123

N	-4.700073	-1.852594	2.757379
H	-3.071288	-3.206455	2.390687
C	-2.783220	-2.179123	4.223290
H	-5.107866	-2.136267	3.644882
O	-3.540076	-2.118630	5.169228
S	0.428187	1.912097	1.178370
C	1.034001	3.281206	0.094020
C	1.271404	4.624200	0.824128
H	0.300818	3.433124	-0.697882
H	1.954696	2.916073	-0.365450
N	1.453729	5.643025	-0.202223
H	0.409566	4.816388	1.485469
C	2.506559	4.622806	1.741861
H	2.052938	6.375827	0.169684
O	3.344178	5.499253	1.706889
O	-1.461196	-2.285173	4.431220
O	-3.035495	-0.957800	-4.058862
O	2.619667	3.624904	2.633217
H	1.885024	2.984118	2.553466
H	-0.963260	-2.308836	3.589409
H	-2.151110	-0.832719	-3.659425
H	-5.173678	-2.363399	2.018428
H	0.558828	6.060894	-0.438604
H	-3.894663	3.257249	-2.992355
H	-0.209735	1.088991	-2.665377
H	2.996524	-0.978347	0.654079
H	-1.078989	-2.686106	0.678925
H	-0.820156	2.380466	1.370500
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BS2W			
S	2.620731	-0.274152	-0.755880
C	2.885206	-1.974895	-1.424975
C	4.293263	-2.192392	-1.982692
H	2.167400	-2.086510	-2.235553
H	2.655223	-2.696925	-0.643363
N	4.345512	-3.527193	-2.590190
H	4.477052	-1.460361	-2.772937
C	5.358906	-2.047179	-0.881382
H	4.344483	-4.255258	-1.881486
O	5.178066	-2.383924	0.265214
H	5.175542	-3.649127	-3.161044
O	6.569947	-1.586670	-1.253389
H	6.583095	-1.310513	-2.180661
Cu	0.335687	-0.059196	-0.072063
S	-1.023690	-0.094532	-2.101198
C	-2.558618	0.923017	-1.939967
C	-3.432038	0.986153	-3.214657
H	-2.264999	1.934558	-1.670372
H	-3.112796	0.493104	-1.106163
N	-4.424867	2.035765	-3.008427
H	-2.775987	1.184567	-4.075662

C	-4.157748	-0.326502	-3.547035
H	-5.240851	1.861552	-3.586313
O	-5.342479	-0.378775	-3.775148
S	-0.370618	-1.909947	1.353741
C	-2.169681	-1.768126	1.757696
C	-2.747685	-2.938559	2.587360
H	-2.718519	-1.702144	0.821223
H	-2.278366	-0.822464	2.288172
N	-4.200747	-2.803852	2.569041
H	-2.402497	-3.884345	2.142950
C	-2.269854	-2.977221	4.046676
H	-4.604279	-3.269459	3.375545
O	-3.028968	-3.073696	4.980860
S	0.094805	1.946329	1.271173
C	0.611462	3.407529	0.260953
C	0.360687	4.780572	0.926260
H	0.071217	3.371190	-0.682035
H	1.671395	3.259444	0.055142
N	0.547256	5.799865	-0.101277
H	-0.655965	4.783589	1.348204
C	1.291813	5.090854	2.108543
H	0.790553	6.686445	0.328722
O	1.893799	6.132913	2.208907
O	-0.945446	-2.951161	4.266243
O	-3.415276	-1.442265	-3.626859
O	1.387536	4.171317	3.081853
H	0.883442	3.361676	2.871177
H	-0.439949	-2.833986	3.438648
H	-2.482006	-1.277704	-3.389258
H	-4.585522	-3.227803	1.731898
H	-0.306263	5.928149	-0.633765
H	-4.043225	2.940576	-3.261806
H	-0.355330	0.717024	-2.947083
H	3.224817	-0.456220	0.436503
H	-0.458794	-2.944123	0.491148
H	-1.235234	2.175082	1.256485

Table S.XXXII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}, \underline{\text{O}}\text{-H}_2\text{Cys})]^+$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-2.402356	1.418438	-0.190456
H	-2.502655	1.946352	0.672959
C	-1.105328	0.750866	-0.319086
H	-0.820198	0.765665	-1.379146
C	0.002928	1.449102	0.522377
C	-1.361859	-0.753946	0.019469
H	-0.167939	2.525613	0.472768
H	-0.041118	1.138057	1.569183
S	1.736252	1.157301	-0.133037
O	-0.464908	-1.615426	0.087376
O	-2.605191	-1.067622	0.171488
H	-2.617577	2.029779	-0.971493
Cu	1.214778	-0.877775	-0.045233
H	-3.098700	-0.199703	0.042453
H	2.402424	1.592095	0.959342
BS2			
N	-2.743946	1.056684	-0.139922
H	-2.930353	1.484827	0.762091
C	-1.353680	0.634278	-0.315888
H	-1.113296	0.717637	-1.381899
C	-0.360997	1.499242	0.500233
C	-1.289925	-0.889499	-0.003322
H	-0.674582	2.539444	0.421683
H	-0.346197	1.207444	1.550799
S	1.390914	1.458634	-0.160123
O	-0.249599	-1.540843	0.087812
O	-2.445289	-1.468226	0.123063
H	-3.070428	1.678830	-0.870162
Cu	1.579237	-0.790954	-0.023308
H	-3.123376	-0.750446	0.011896
H	2.000063	1.933420	0.949815

Table S.XXXIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{Q}}\text{-H}_2\text{Cys})_2]^+$ ($\text{NH}_2,\text{SH},\text{COOH}$) at BS1, BS2 and BS1W levels of theory.

Atom	x	y	z
BS1			
N	4.713273	0.913117	0.027280
H	4.734143	1.526589	0.838768
C	3.479976	0.123017	-0.043014
H	3.708571	-0.802956	-0.587597
C	2.893319	-0.244822	1.333149
C	2.488526	0.895646	-0.944854
H	3.695679	-0.645614	1.955931
H	2.467618	0.636621	1.821029
S	1.596670	-1.558302	1.191257
O	1.291145	0.634401	-1.025661
O	3.036174	1.845730	-1.662794
H	5.546532	0.334287	0.045459
Cu	0.000031	-0.499169	-0.000356
S	-1.596542	-1.556191	-1.194003
C	-2.892951	-0.242254	-1.333864
C	-3.480053	0.122994	0.042791
H	-3.695134	-0.641734	-1.957715
H	-2.466968	0.640078	-1.819889
N	-4.713123	0.913548	-0.026318
H	-3.709157	-0.804005	0.585417
C	-2.488792	0.893497	0.946633
H	-5.546479	0.334931	-0.046783
O	-1.291388	0.632222	1.026940
O	-3.036631	1.841735	1.666877
H	-4.733198	1.529238	-0.836150
H	-3.991495	1.857001	1.383201
H	3.991116	1.860238	-1.379281
H	-1.316684	-1.610279	-2.512685
H	1.316881	-1.614427	2.509871
BS2			
N	3.953985	1.801642	-0.057339
H	3.750915	2.322930	0.790620
C	3.099219	0.622393	-0.225363
H	3.658613	-0.106190	-0.823225
C	2.690327	-0.031404	1.109235
C	1.891500	1.024329	-1.107185
H	3.576230	-0.108403	1.738887
H	1.924402	0.552720	1.621193
S	2.064507	-1.767222	0.874782
O	0.896365	0.336867	-1.247021
O	2.034164	2.171123	-1.736739
H	4.942023	1.577480	-0.067378
Cu	-0.000095	-1.299548	0.000189
S	-2.064168	-1.766968	-0.875596

C	-2.689837	-0.031061	-1.109603
C	-3.099210	0.622186	0.225127
H	-3.575508	-0.107744	-1.739622
H	-1.923702	0.553259	-1.621026
N	-3.953842	1.801571	0.057312
H	-3.658851	-0.106622	0.822480
C	-1.891812	1.023697	1.107587
H	-4.941894	1.577442	0.066885
O	-0.896785	0.336102	1.247599
O	-2.034637	2.170263	1.737500
H	-3.750448	2.323191	-0.790368
H	-2.903799	2.535752	1.439547
H	2.903437	2.536473	-1.438947
H	-1.819222	-2.016894	-2.180373
H	1.820120	-2.017651	2.179568
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BS1W			
N	4.823036	0.482419	-0.081007
H	5.062365	0.891830	0.819136
C	3.460336	-0.065982	-0.090836
H	3.453312	-0.952452	-0.736650
C	2.956651	-0.455297	1.310566
C	2.568114	0.976044	-0.799294
H	3.736214	-1.034810	1.806612
H	2.736803	0.433985	1.905230
S	1.442228	-1.513483	1.234868
O	1.340149	0.919838	-0.863870
O	3.241504	1.943754	-1.376653
H	5.516792	-0.225581	-0.297728
Cu	-0.000028	-0.288947	0.000034
S	-1.442341	-1.513953	-1.234139
C	-2.956611	-0.455607	-1.310420
C	-3.460370	-0.065659	0.090762
H	-3.736203	-1.035227	-1.806299
H	-2.736607	0.433408	-1.905422
N	-4.823357	0.482135	0.080449
H	-3.453228	-0.951894	0.736898
C	-2.568014	0.976728	0.798802
H	-5.516840	-0.226094	0.297310
O	-1.340059	0.920338	0.863485
O	-3.241085	1.944541	1.376310
H	-5.062694	0.890965	-0.819961
H	-4.197221	1.725602	1.137751
H	4.197618	1.724915	-1.137968
H	-1.170289	-1.449230	-2.552977
H	1.170158	-1.447993	2.553663

Table S.XXXIV. Computed Cartesian coordinates (in Å) of [Cu^I(S-HCys)] (NH₂,S⁻,COOH) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	2.634042	1.702315	-0.143533
H	2.830558	1.524390	-1.128210
C	1.729059	0.663049	0.331859
H	1.720050	0.701852	1.430121
C	0.297517	0.986289	-0.149377
C	2.194845	-0.759432	-0.070276
H	0.150777	2.060626	-0.035831
H	0.184835	0.731223	-1.206119
S	-0.967549	0.091180	0.873479
O	3.239985	-0.949239	-0.650054
O	1.392806	-1.783567	0.272250
H	3.535711	1.570684	0.310530
Cu	-2.562654	-0.069008	-0.366641
H	0.546661	-1.439620	0.640354
BS2			
N	-2.954897	-1.113085	-0.513392
H	-3.089364	-0.569335	-1.361755
C	-1.792431	-0.612446	0.208785
H	-1.876837	-0.927848	1.254120
C	-0.525927	-1.282733	-0.373505
C	-1.699386	0.930254	0.193967
H	-0.723001	-2.353431	-0.410966
H	-0.351728	-0.944220	-1.394874
S	1.008447	-1.084714	0.661543
O	-2.416247	1.623723	-0.480046
O	-0.763052	1.476581	0.996188
H	-3.796061	-0.979090	0.037844
Cu	2.209853	0.383893	-0.370355
H	-0.158756	0.775168	1.320375
BS1W			
N	2.617100	1.741423	-0.099125
H	2.597759	1.771361	-1.118592
C	1.734096	0.666210	0.347044
H	1.749873	0.653941	1.446903
C	0.290903	0.975502	-0.092819
C	2.230103	-0.731174	-0.092136
H	0.105192	2.032185	0.104439
H	0.175931	0.806312	-1.166153
S	-0.943041	-0.045972	0.846080
O	3.336820	-0.908194	-0.564851
O	1.405577	-1.768832	0.112179
H	3.574005	1.472839	0.125430
Cu	-2.600916	-0.027507	-0.345685

H	0.522963	-1.440371	0.438263
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BS2W			
N	-2.794380	-1.547581	-0.361716
H	-2.794978	-1.419265	-1.370574
C	-1.808226	-0.666292	0.255180
H	-1.876357	-0.801634	1.341438
C	-0.393654	-1.098068	-0.185700
C	-2.092639	0.832299	0.002350
H	-0.352550	-2.184555	-0.134412
H	-0.207057	-0.796136	-1.216066
S	0.932635	-0.418711	0.932873
O	-3.098374	1.228354	-0.544913
O	-1.186555	1.708288	0.457386
H	-3.726900	-1.294454	-0.048842
Cu	2.552403	0.168880	-0.395856
H	-0.376798	1.230191	0.783573
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Table S.XXXV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]^-$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	5.171872	1.909613	0.074599
H	4.886927	2.177428	-0.868401
C	4.396916	0.720337	0.445681
H	4.536499	0.548143	1.523873
C	2.898070	0.980080	0.220032
C	4.936397	-0.554354	-0.251182
H	2.674379	1.970250	0.624270
H	2.681759	1.001983	-0.853649
S	1.830343	-0.281476	1.059733
O	6.016510	-0.557965	-0.814075
O	4.198957	-1.663237	-0.160616
H	6.135696	1.595844	-0.046430
Cu	0.000193	-0.263091	-0.000145
S	-1.830210	-0.280523	-1.059574
C	-2.898346	0.980513	-0.219684
C	-4.397124	0.720371	-0.445432
H	-2.674999	1.970835	-0.623732
H	-2.682099	1.002313	0.854019
N	-5.172386	1.909369	-0.074084
H	-4.536643	0.548428	-1.523676
C	-4.936355	-0.554602	0.251061
H	-6.136207	1.595418	0.046471
O	-6.016554	-0.558614	0.813801
O	-4.198804	-1.663397	0.160092
H	-4.887802	2.176814	0.869129
H	-3.323849	-1.453495	-0.282735
H	3.324001	-1.453593	0.282450
BS2			
N	5.259928	1.879893	0.106481
H	4.946712	2.233122	-0.794704
C	4.472156	0.692814	0.452756
H	4.629435	0.483630	1.519349
C	2.974765	0.989965	0.261154
C	4.970161	-0.572576	-0.290407
H	2.781359	1.977356	0.681426
H	2.735841	1.021079	-0.805263
S	1.895199	-0.250738	1.121592
O	6.023894	-0.585239	-0.889568
O	4.218486	-1.670723	-0.197657
H	6.223824	1.591016	-0.042393
Cu	0.000000	-0.248327	0.000284
S	-1.895101	-0.250979	-1.121264
C	-2.974744	0.989931	-0.261250
C	-4.472135	0.692816	-0.453043

H	-2.781224	1.977240	-0.681665
H	-2.736009	1.021244	0.805205
N	-5.259920	1.879920	-0.106880
H	-4.629272	0.483611	-1.519651
C	-4.970223	-0.572521	0.290101
H	-6.223787	1.591003	0.042121
O	-6.023990	-0.585106	0.889222
O	-4.218613	-1.670709	0.197358
H	-4.946648	2.233277	0.794237
H	-3.357028	-1.465312	-0.268663
H	3.357084	-1.465368	0.268597

BS1W

N	5.238385	1.820420	0.364795
H	5.097291	2.160462	-0.586637
C	4.411857	0.628620	0.553251
H	4.544445	0.288767	1.590971
C	2.926568	0.997902	0.374285
C	4.865542	-0.554287	-0.331694
H	2.756505	1.932277	0.912585
H	2.706501	1.176353	-0.682255
S	1.785811	-0.304337	1.046457
O	5.909409	-0.536972	-0.957954
O	4.080941	-1.640329	-0.348364
H	6.214674	1.528750	0.382625
Cu	-0.017848	-0.183474	-0.048421
S	-1.824510	-0.227009	-1.146071
C	-2.972077	1.017421	-0.372570
C	-4.462461	0.605531	-0.497524
H	-2.845314	1.967325	-0.898075
H	-2.708524	1.179476	0.676327
N	-5.407638	1.685781	-0.228713
H	-4.614324	0.264972	-1.532403
C	-4.805034	-0.584980	0.410361
H	-5.421287	1.879262	0.770280
O	-5.714570	-0.570544	1.217518
O	-4.037852	-1.674924	0.268697
H	-5.085496	2.533535	-0.689952
H	-3.248955	-1.459871	-0.308518
H	3.236242	-1.451514	0.154670

BS2W

N	5.291294	1.758017	0.366257
H	5.148704	2.148445	-0.562049
C	4.436762	0.587895	0.552224
H	4.621275	0.199581	1.561541
C	2.956621	1.015722	0.479198
C	4.785475	-0.573790	-0.406439
H	2.854653	1.930845	1.060588
H	2.677038	1.235437	-0.552527
S	1.806934	-0.263999	1.188990

O	5.762348	-0.562047	-1.125371
O	3.978826	-1.641464	-0.385823
H	6.267636	1.479970	0.402196
Cu	-0.016990	-0.175165	-0.038245
S	-1.839172	-0.149802	-1.270151
C	-2.999698	1.047588	-0.436611
C	-4.477283	0.576006	-0.488747
H	-2.938451	1.996801	-0.969293
H	-2.692190	1.218544	0.596223
N	-5.447604	1.628408	-0.196251
H	-4.667995	0.217220	-1.507708
C	-4.732286	-0.615088	0.444285
H	-5.405069	1.893798	0.783402
O	-5.597640	-0.631734	1.292414
O	-3.936083	-1.678024	0.274626
H	-5.235316	2.455290	-0.745749
H	-3.176095	-1.449815	-0.334173
H	3.171343	-1.454362	0.174933

Table S.XXXVI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_3]^{2-}$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1, BS2 and BS1W levels of theory.

Atom	x	y	z
BS1			
S	0.349929	2.186166	-0.918168
C	2.140696	2.578378	-0.660032
C	2.374957	4.053475	-0.291880
H	2.698394	2.369794	-1.578142
H	2.552746	1.931271	0.124334
N	3.807179	4.394202	-0.364247
H	1.839288	4.658619	-1.040282
C	1.769852	4.473009	1.071222
H	3.934759	5.163744	0.296630
O	2.368132	5.240280	1.815923
H	4.316331	3.617839	0.060629
O	0.559241	4.021926	1.365712
H	0.260931	3.344525	0.650638
Cu	-0.002351	-0.005177	-0.768700
S	1.723071	-1.398401	-0.933337
C	1.181226	-3.149518	-0.670056
C	2.346773	-4.077280	-0.287254
H	0.733780	-3.537938	-1.589947
H	0.407888	-3.184597	0.107424
N	1.936498	-5.491532	-0.352347
H	3.141732	-3.917292	-1.032621
C	3.003483	-3.748140	1.077379
H	2.558753	-5.982061	0.293724
O	3.379783	-4.642500	1.825589
S	-2.077156	-0.790641	-0.910308
C	-3.304260	0.568348	-0.635174
C	-4.706254	0.036809	-0.291804
H	-3.388060	1.175906	-1.541379
H	-2.952124	1.228796	0.167156
N	-5.709287	1.115025	-0.353017
H	-4.960589	-0.713108	-1.057461
C	-4.785011	-0.722624	1.056353
H	-6.447064	0.833646	0.296431
O	-5.755676	-0.597321	1.793501
O	-3.795668	-1.555161	1.346018
O	3.197833	-2.470411	1.368779
H	-3.051264	-1.464298	0.641169
H	-5.289536	1.933422	0.090311
H	1.021395	-5.552737	0.096645
H	2.758658	-1.882495	0.646595
BS2			
S	-1.208070	1.982344	-0.679733
C	0.050135	3.337471	-0.672962
C	-0.561415	4.727440	-0.423469

H	0.549332	3.364502	-1.643654
H	0.811050	3.127658	0.085987
N	0.412283	5.788432	-0.733532
H	-1.414328	4.828766	-1.108912
C	-1.165035	4.913660	0.988207
H	0.219393	6.574686	-0.115838
O	-1.030499	5.957217	1.604543
H	1.340089	5.457311	-0.481006
O	-1.885567	3.914308	1.475998
H	-1.821220	3.099572	0.863763
Cu	0.004198	-0.008501	-0.586359
S	2.331816	0.053714	-0.671863
C	2.883457	-1.710927	-0.676876
C	4.392395	-1.869970	-0.422286
H	2.665143	-2.149634	-1.652573
H	2.319615	-2.273472	0.074451
N	4.834772	-3.238007	-0.742303
H	4.906509	-1.173919	-1.099778
C	4.848833	-1.450505	0.994616
H	5.608048	-3.464066	-0.119401
O	5.685977	-2.090490	1.607990
S	-1.123751	-2.045455	-0.672796
C	-2.923664	-1.618573	-0.666028
C	-3.830538	-2.837512	-0.423471
H	-3.193207	-1.194310	-1.635301
H	-3.118089	-0.855646	0.095351
N	-5.233934	-2.514765	-0.732099
H	-3.496876	-3.626475	-1.112011
C	-3.695592	-3.462115	0.984806
H	-5.819706	-3.061612	-0.103946
O	-4.669784	-3.857813	1.602328
O	-2.469460	-3.607579	1.466806
O	4.337854	-0.331781	1.488835
H	-1.793294	-3.146609	0.855205
H	-5.403021	-1.540910	-0.493300
H	4.086970	-3.884282	-0.502555
H	3.600455	0.021015	0.876479
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BS1W			
S	2.194332	0.328185	-1.074320
C	3.214876	-1.194213	-0.778036
C	4.595763	-0.881068	-0.170277
H	3.384516	-1.709426	-1.727009
H	2.667738	-1.882203	-0.124094
N	5.461448	-2.058924	-0.262639
H	5.047313	-0.082242	-0.777435
C	4.524664	-0.311972	1.264992
H	6.293023	-1.873453	0.297322
O	5.281134	-0.680722	2.147904
H	5.001815	-2.828343	0.225076
O	3.626494	0.650481	1.492901

H	3.041989	0.762357	0.672725
Cu	0.022436	-0.059389	-0.983689
S	-0.760153	-2.127925	-1.084992
C	-2.604787	-2.203940	-0.864433
C	-3.069507	-3.492171	-0.135767
H	-3.073925	-2.196186	-1.853057
H	-2.956327	-1.316779	-0.327105
N	-4.507332	-3.750987	-0.211164
H	-2.542911	-4.332065	-0.612840
C	-2.645006	-3.495975	1.339566
H	-4.993006	-3.109544	0.412169
O	-3.424048	-3.675942	2.258705
S	-1.391265	1.636696	-1.111935
C	-0.563808	3.275950	-0.840298
C	-1.508252	4.333476	-0.237090
H	-0.206037	3.665730	-1.796738
H	0.309659	3.143312	-0.192449
N	-0.905180	5.663663	-0.347988
H	-2.430100	4.329881	-0.837755
C	-1.958730	4.008535	1.205021
H	-1.469832	6.304152	0.209227
O	-1.996384	4.857072	2.080363
O	-2.361791	2.758075	1.447890
O	-1.344499	-3.290841	1.574260
H	-2.180408	2.185113	0.632208
H	-0.005966	5.644433	0.133882
H	-4.830803	-3.544241	-1.153762
H	-0.895096	-2.982471	0.720830

Table S.XXXVII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_4]^{3-}$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	2.876985	-1.404387	-1.444424
C	2.953896	-3.056291	-0.621092
C	4.176017	-3.892662	-1.055796
H	2.053515	-3.621935	-0.878062
H	2.961504	-2.942941	0.470642
N	4.081043	-5.281630	-0.565493
H	4.168392	-3.905394	-2.157361
C	5.536690	-3.262562	-0.671957
H	5.044093	-5.558334	-0.358121
O	6.454119	-3.947064	-0.227262
H	3.614125	-5.252926	0.341328
O	5.683715	-1.968163	-0.905719
H	4.761441	-1.557229	-1.131452
Cu	1.519329	-0.067361	-0.192561
S	0.193441	-1.149929	1.285411
C	-1.160922	0.111758	1.399498
C	-2.356965	-0.311965	2.280741
H	-1.555642	0.293036	0.397727
H	-0.777773	1.067190	1.783879
N	-3.538596	0.579991	2.188261
H	-2.677333	-1.316704	1.995011
C	-1.930945	-0.357058	3.735322
H	-3.204067	1.536097	2.311691
O	-1.697983	0.602032	4.445206
S	1.724579	2.127002	-0.549845
C	3.466351	2.330538	-1.156036
C	3.957027	3.780949	-1.044647
H	3.535137	2.018537	-2.202219
H	4.130858	1.671988	-0.583200
N	5.226929	3.968324	-1.758290
H	3.187741	4.416160	-1.516489
C	4.054720	4.308583	0.415046
H	5.695197	4.740239	-1.274580
O	4.957830	5.077581	0.735777
S	-5.084415	1.133434	-1.109726
C	-5.820214	-0.541568	-0.881036
C	-7.342960	-0.527853	-0.656501
H	-5.348157	-1.033250	-0.023990
H	-5.599739	-1.167229	-1.761659
N	-7.852613	-1.885039	-0.397681
H	-7.525977	0.094246	0.236155
C	-8.152233	0.172390	-1.795016
H	-8.775318	-1.894628	-0.843708
O	-9.221106	-0.334097	-2.168945
O	3.100946	3.966740	1.259240

O	-1.836083	-1.623623	4.231559
O	-7.677756	1.291479	-2.241619
H	-6.523131	1.439603	-1.773475
H	2.456179	3.266658	0.818772
H	-1.479863	-1.500153	5.127599
H	5.809499	3.154670	-1.552871
H	-7.294277	-2.530337	-0.959922
H	-3.895958	0.522048	1.231275
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BS2			
S	-0.611694	-1.678288	-1.650201
C	-1.633139	-0.743947	-2.868766
C	-2.227434	-1.636929	-3.975377
H	-1.008322	0.012615	-3.349538
H	-2.443073	-0.220141	-2.347264
N	-2.813492	-0.836053	-5.070292
H	-1.394357	-2.230549	-4.377706
C	-3.241882	-2.682660	-3.464741
H	-3.713012	-1.252194	-5.304406
O	-4.275450	-2.921634	-4.077560
H	-3.001484	0.100067	-4.722985
O	-2.916534	-3.347341	-2.373311
H	-2.071997	-2.921672	-1.932932
Cu	0.134603	0.024643	-0.012459
S	1.135303	1.924108	-1.356676
C	1.550499	3.138342	-0.031320
C	2.071124	4.483281	-0.572909
H	2.328322	2.708541	0.604379
H	0.669229	3.306763	0.597558
N	2.615668	5.327641	0.511082
H	2.882550	4.247463	-1.276199
C	1.043070	5.270003	-1.415971
H	2.310500	6.282874	0.332810
O	0.931050	6.486260	-1.313614
S	-1.435014	1.012018	1.631310
C	-1.527784	-0.232604	2.989180
C	-2.482311	0.180111	4.126459
H	-0.531943	-0.363814	3.419089
H	-1.841772	-1.201028	2.582023
N	-2.333394	-0.692944	5.309166
H	-2.207294	1.206340	4.408032
C	-3.963597	0.273887	3.701491
H	-3.269103	-0.911744	5.646321
O	-4.862748	-0.140105	4.423225
S	2.061259	-0.942188	1.297630
C	3.149131	-1.552892	-0.061024
C	4.391979	-2.310058	0.445213
H	3.489966	-0.695365	-0.646068
H	2.570068	-2.198481	-0.731005
N	5.359192	-2.557385	-0.644519
H	4.866674	-1.666964	1.199979

C	4.069558	-3.620188	1.195962
H	5.688762	-3.515959	-0.546656
O	4.734869	-4.635253	1.026170
O	-4.219336	0.873791	2.555199
O	0.338456	4.582586	-2.292478
O	3.085374	-3.577854	2.072815
H	2.567165	-2.673048	1.984511
H	-3.332150	1.046891	2.035509
H	0.489460	3.556114	-2.146969
H	-1.913493	-1.570000	5.014315
H	4.864867	-2.505166	-1.530852
H	2.182704	5.042907	1.385565
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BS1W			
S	0.822837	0.045972	-2.059765
C	0.797395	-1.766368	-2.444332
C	2.189578	-2.334493	-2.796015
H	0.140741	-1.946897	-3.301486
H	0.394029	-2.332124	-1.598906
N	2.057251	-3.715265	-3.268235
H	2.638369	-1.659001	-3.547696
C	3.172890	-2.316442	-1.615107
H	2.967475	-4.164359	-3.192250
O	3.926294	-3.248751	-1.379400
H	1.806394	-3.708539	-4.253413
O	3.207583	-1.204519	-0.883244
H	2.462787	-0.572558	-1.192778
Cu	-0.695740	0.712457	-0.414458
S	-2.879534	0.589554	-1.249374
C	-4.170953	1.324471	-0.141989
C	-5.550400	0.646705	-0.279281
H	-4.297128	2.384276	-0.386138
H	-3.851083	1.272720	0.904247
N	-6.552837	1.396413	0.483068
H	-5.778204	0.591834	-1.360156
C	-5.570333	-0.813892	0.198897
H	-7.359428	0.791724	0.623618
O	-6.509522	-1.279657	0.826772
S	-0.750126	-0.804352	1.556982
C	0.920642	-0.905348	2.346365
C	1.245779	-2.296703	2.929800
H	0.980995	-0.183363	3.167099
H	1.697750	-0.635254	1.623690
N	2.496897	-2.236317	3.690669
H	0.377975	-2.602911	3.543123
C	1.377454	-3.393394	1.862763
H	2.840768	-3.186336	3.812762
O	2.249619	-4.247553	1.909061
S	0.023064	2.846376	0.319629
C	1.396556	3.506144	-0.734295
C	2.436378	4.325587	0.058662

H	0.979085	4.163995	-1.503608
H	1.899143	2.682520	-1.251438
N	3.382645	4.955388	-0.866473
H	1.876220	5.057020	0.670743
C	3.233214	3.495550	1.077493
H	4.205608	5.232645	-0.335644
O	4.431394	3.657955	1.253937
O	0.454046	-3.408275	0.902995
O	-4.533664	-1.572905	-0.147358
O	2.545316	2.620276	1.806902
H	1.575768	2.589319	1.474213
H	-0.140734	-2.576804	0.987563
H	-3.830935	-0.994268	-0.619124
H	2.304420	-1.865501	4.617603
H	2.967360	5.804408	-1.241233
H	-6.866200	2.190380	-0.069365
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BS2W			
S	1.149909	-0.083085	-1.848173
C	0.536116	-1.715761	-2.471541
C	1.620550	-2.544800	-3.189904
H	-0.271251	-1.543976	-3.186185
H	0.124060	-2.300743	-1.645675
N	1.008698	-3.707935	-3.839881
H	2.121087	-1.875590	-3.909357
C	2.745991	-3.028606	-2.266891
H	1.729058	-4.378243	-4.091080
O	3.228201	-4.142793	-2.353469
H	0.544570	-3.419080	-4.694808
O	3.218708	-2.151504	-1.385382
H	2.661778	-1.297574	-1.405697
Cu	-0.396475	0.700285	-0.124923
S	-2.602774	1.127850	-1.183836
C	-3.760279	1.602981	0.181588
C	-5.249829	1.482662	-0.199323
H	-3.577347	2.643388	0.458340
H	-3.562251	0.989547	1.063831
N	-6.080960	2.074026	0.854454
H	-5.381685	1.986568	-1.171366
C	-5.713806	0.041851	-0.446244
H	-7.046976	1.785446	0.733013
O	-6.790753	-0.373732	-0.059858
S	-0.844578	-0.869929	1.711326
C	0.772798	-1.257715	2.526828
C	0.763501	-2.587326	3.308236
H	1.014270	-0.463659	3.236255
H	1.570542	-1.283208	1.779989
N	1.994513	-2.710263	4.095564
H	-0.141193	-2.589452	3.938769
C	0.616348	-3.829770	2.421434
H	2.107080	-3.669600	4.409037

O	1.247035	-4.852074	2.618265
S	0.582345	2.771170	0.801523
C	1.646817	3.525290	-0.514667
C	2.828427	4.345557	0.041526
H	1.039281	4.198927	-1.122618
H	2.027753	2.741475	-1.173091
N	3.491319	5.064511	-1.051166
H	2.422716	5.026458	0.808262
C	3.873917	3.506564	0.787566
H	4.399071	5.397970	-0.741353
O	5.070402	3.697810	0.668877
O	-0.280814	-3.764303	1.441374
O	-4.901040	-0.737265	-1.154785
O	3.414077	2.579586	1.622546
H	2.397120	2.510729	1.544375
H	-0.665822	-2.821444	1.379065
H	-4.020345	-0.254381	-1.337580
H	1.934896	-2.121528	4.919945
H	2.939024	5.873684	-1.315594
H	-6.050885	3.086212	0.787915

Table S.XXXVIII. Computed Cartesian coordinates (in Å) of [Cu^I(S,Q-HCys)] (NH₂,S⁻,COOH) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-2.305607	1.470014	-0.267627
H	-2.303485	2.145339	0.492430
C	-1.013497	0.744399	-0.337703
H	-0.668035	0.724664	-1.377890
C	0.096887	1.416800	0.522560
C	-1.349793	-0.727966	0.036628
H	-0.070818	2.496102	0.441322
H	-0.049067	1.153638	1.576592
S	1.871055	1.115717	0.008045
O	-0.518177	-1.650651	0.067117
O	-2.615714	-0.951863	0.270321
H	-2.499104	1.975804	-1.125903
Cu	1.154739	-0.840610	-0.083369
H	-3.025010	-0.038704	0.127420
BS2			
N	-2.639641	1.144185	-0.264416
H	-2.741695	1.809157	0.495732
C	-1.247733	0.640646	-0.358964
H	-0.918877	0.681870	-1.401525
C	-0.256741	1.485868	0.483272
C	-1.294916	-0.864454	0.017007
H	-0.551543	2.528371	0.337174
H	-0.384683	1.254661	1.545625
S	1.540377	1.412088	0.021988
O	-0.328666	-1.620775	0.040470
O	-2.498097	-1.316942	0.295787
H	-2.933582	1.603923	-1.117966
Cu	1.512394	-0.759615	-0.071278
H	-3.087146	-0.522480	0.169196
BS1W			
N	-2.319926	1.442930	-0.243346
H	-2.348659	2.084555	0.545109
C	-1.021105	0.745076	-0.338231
H	-0.704982	0.726036	-1.387071
C	0.088767	1.434902	0.504908
C	-1.346423	-0.730892	0.036422
H	-0.078773	2.510426	0.405068
H	-0.045219	1.187339	1.562253
S	1.871121	1.124597	-0.000762
O	-0.509835	-1.655399	0.084578
O	-2.610523	-0.951023	0.242932
H	-2.532844	1.969782	-1.084318
Cu	1.160219	-0.841720	-0.077842

H	-2.998900	-0.005443	0.093316
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BS2W			
N	-2.672013	1.089137	-0.251332
H	-2.803991	1.718742	0.534241
C	-1.272050	0.628878	-0.360103
H	-0.967270	0.664739	-1.409592
C	-0.298503	1.505147	0.465609
C	-1.283689	-0.873035	0.022561
H	-0.604393	2.538917	0.296684
H	-0.423563	1.293624	1.530223
S	1.509195	1.435466	0.022652
O	-0.300635	-1.612481	0.070577
O	-2.481381	-1.346158	0.272934
H	-2.978485	1.567736	-1.090249
Cu	1.544488	-0.749390	-0.072986
H	-3.073902	-0.539692	0.135696
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Table S.XXXIX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{Q}}\text{-HCys})_2]^-$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-3.634849	1.928076	-0.005333
H	-3.368841	2.270027	-0.928510
C	-2.855055	0.683985	0.273813
H	-3.444314	0.075521	0.971212
C	-2.576695	-0.169520	-0.976653
C	-1.589183	1.106244	1.045318
H	-3.516746	-0.189741	-1.546646
H	-1.827391	0.344140	-1.590181
S	-2.057572	-1.896672	-0.626144
O	-0.620114	0.403893	1.233909
O	-1.657903	2.360266	1.539010
H	-4.624122	1.702607	-0.062834
Cu	-0.000773	-1.507664	0.000273
S	2.056138	-1.897733	0.625077
C	2.576917	-0.171168	0.975857
C	2.855685	0.682639	-0.274392
H	3.517143	-0.192395	1.545522
H	1.828277	0.342995	1.589801
N	3.637216	1.925577	0.005090
H	3.443746	0.073807	-0.972458
C	1.589843	1.106959	-1.044737
H	4.626178	1.698667	0.062524
O	0.620198	0.405553	-1.233831
O	1.659313	2.361573	-1.536927
H	3.371744	2.267349	0.928516
H	2.531609	2.689599	-1.200570
H	-2.529503	2.689456	1.201944
BS2			
N	-3.925654	-1.230928	0.353529
H	-3.308190	-1.789190	-0.241934
C	-3.488600	0.172471	0.246790
H	-2.766397	0.449853	1.020874
C	-2.839178	0.440694	-1.131415
C	-4.712791	1.090194	0.398119
H	-3.604467	0.369393	-1.910780
H	-2.455826	1.460138	-1.133076
S	-1.517560	-0.763395	-1.592190
O	-4.648879	2.277462	0.601712
O	-5.884103	0.445228	0.239363
H	-3.803500	-1.571285	1.301798
Cu	0.000131	-0.662580	0.000461
S	1.517329	-0.759837	1.593779
C	2.839342	0.443012	1.130842
C	3.488371	0.172438	-0.247096

H	3.604757	0.372593	1.910158
H	2.456378	1.462605	1.131024
N	3.924452	-1.231400	-0.351962
H	2.766215	0.449222	-1.021440
C	4.713169	1.089120	-0.399890
H	3.801875	-1.573004	-1.299726
O	4.650114	2.276159	-0.605095
O	5.884055	0.443539	-0.240417
H	3.306783	-1.788417	0.244457
H	5.614619	-0.503557	-0.136228
H	-5.615303	-0.502189	0.136510

BS1W

N	-4.207288	1.447948	0.289396
H	-4.885914	1.191147	-0.421926
C	-3.183686	0.394745	0.454441
H	-3.393603	-0.276292	1.293986
C	-3.087970	-0.454580	-0.839459
C	-1.857244	1.107711	0.740371
H	-4.092083	-0.851525	-1.028235
H	-2.842971	0.216087	-1.671621
S	-1.905897	-1.863088	-0.775733
O	-0.857171	0.555823	1.189080
O	-1.866322	2.400687	0.422582
H	-4.719907	1.599868	1.154028
Cu	-0.000365	-1.013037	-0.000242
S	1.905143	-1.863825	0.775014
C	3.087566	-0.455599	0.839314
C	3.183643	0.394111	-0.454274
H	4.091550	-0.852884	1.028026
H	2.842683	0.214781	1.671745
N	4.208276	1.446447	-0.289595
H	3.392762	-0.276783	-1.294114
C	1.857679	1.108372	-0.739573
H	4.722295	1.596374	-1.153725
O	0.856397	0.557041	-1.186315
O	1.868656	2.401642	-0.423415
H	4.885556	1.190228	0.423215
H	2.826790	2.553321	-0.164736
H	-2.823835	2.553479	0.162906

BS2W

N	-4.696339	1.176487	-0.266563
H	-4.572142	1.826501	-1.038356
C	-3.473527	0.381907	-0.031199
H	-3.787164	-0.549469	0.450742
C	-2.674665	0.026026	-1.302035
C	-2.639177	1.122647	1.031669
H	-3.392535	-0.042396	-2.121118
H	-1.973176	0.826622	-1.544007
S	-1.794131	-1.604709	-1.275443

O	-1.467923	0.923059	1.262754
O	-3.346956	2.020108	1.729650
H	-5.481367	0.578307	-0.498546
Cu	-0.000016	-1.376032	-0.000027
S	1.794109	-1.604740	1.275387
C	2.674663	0.025980	1.302039
C	3.473505	0.381888	0.031200
H	3.392554	-0.042490	2.121100
H	1.973199	0.826583	1.544059
N	4.696409	1.176327	0.266553
H	3.787039	-0.549485	-0.450817
C	2.639165	1.122793	-1.031562
H	5.481382	0.578052	0.498476
O	1.467941	0.923150	-1.262747
O	3.346991	2.020227	-1.729535
H	4.572313	1.826318	1.038383
H	4.236545	2.024109	-1.288699
H	-4.236531	2.023964	1.288868

Table S.XL. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}, \underline{\text{N}}\text{-HCys})_2]^-$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
Cu	0.014552	0.167547	-0.472303
S	1.158203	-1.534218	-1.563533
N	1.737187	0.695679	0.580237
N	-1.618788	-0.838434	0.395773
S	-1.250155	2.076612	-0.756259
C	2.624229	-1.375842	-0.461806
C	-2.673853	1.398629	0.188768
H	3.517983	-1.779657	-0.952916
H	2.488243	-1.932774	0.475940
H	-3.607407	1.884246	-0.118434
H	-2.556951	1.567122	1.269338
C	2.904624	0.105722	-0.105362
C	-2.830210	-0.131312	-0.035629
C	-4.051254	-0.632916	0.704214
C	4.176981	0.242797	0.700253
O	4.024083	-0.165074	2.002073
O	5.256695	0.634785	0.299170
O	-5.201035	-0.487223	-0.010808
O	-4.067870	-1.085680	1.835818
H	-5.908291	-0.786269	0.585380
H	4.904479	-0.059190	2.398352
H	-2.962259	-0.287254	-1.108629
H	1.757268	0.418709	1.561433
H	1.783150	1.711607	0.565147
H	-1.678619	-0.971177	1.406598
H	-1.571754	-1.768745	-0.013428
H	3.056504	0.648595	-1.040031
BS2			
Cu	0.484042	-1.917521	-0.076552
S	2.686953	-1.859548	0.219522
N	0.904604	0.738844	-0.667670
N	-1.647651	0.592344	1.319716
S	-1.716996	-2.255100	-0.125433
C	2.905292	-0.064099	0.573523
C	-2.439022	-0.643976	-0.667024
H	3.979028	0.125181	0.671437
H	2.439330	0.198738	1.527348
H	-3.339319	-0.851915	-1.245942
H	-1.729987	-0.111465	-1.304123
C	2.351406	0.867096	-0.526659
C	-2.825829	0.264018	0.526952
C	-3.505982	1.538777	0.064393
C	2.793853	2.302836	-0.272379
O	2.273978	2.824002	0.874407

O	3.526361	2.961118	-0.979862
O	-4.629236	1.276019	-0.666917
O	-3.171917	2.674909	0.302936
H	-4.995318	2.138270	-0.910749
H	2.595290	3.735450	0.930481
H	-3.594389	-0.286963	1.095595
H	0.370940	1.036759	0.147732
H	0.559099	1.241863	-1.476902
H	-1.892875	1.132183	2.142596
H	-1.229059	-0.290471	1.610108
H	2.810266	0.580228	-1.474669

BS1W

Cu	0.007001	-0.492582	0.037247
S	1.409079	-1.525981	1.632232
N	1.588850	0.615002	-0.674386
N	-1.576674	0.646983	0.677965
S	-1.392499	-1.621930	-1.509992
C	2.799165	-0.372226	1.258979
C	-2.747223	-0.399814	-1.250566
H	3.754905	-0.827298	1.537831
H	2.693100	0.552376	1.839616
H	-3.709757	-0.829390	-1.543556
H	-2.579796	0.488225	-1.873398
C	2.857756	-0.003337	-0.238879
C	-2.846990	0.056555	0.222908
C	-3.990230	1.048486	0.367627
C	4.076287	0.866547	-0.502912
O	3.849702	2.170364	-0.222466
O	5.154746	0.455262	-0.884770
O	-5.188850	0.438649	0.443014
O	-3.859900	2.258881	0.376832
H	-5.869383	1.133668	0.485901
H	4.678055	2.653582	-0.387222
H	-3.060389	-0.821691	0.838045
H	1.570287	1.575983	-0.331700
H	1.598514	0.700779	-1.689139
H	-1.557358	1.611418	0.340469
H	-1.609758	0.738637	1.691815
H	2.999866	-0.921253	-0.813537

BS2W

Cu	0.005166	-1.029003	0.021497
S	1.678204	-1.683189	1.450376
N	1.593008	0.586288	-0.796798
N	-1.549923	0.630733	0.776182
S	-1.673097	-1.710119	-1.391816
C	2.837181	-0.272653	1.167275
C	-2.800692	-0.265076	-1.166294
H	3.835905	-0.566433	1.497364
H	2.528789	0.589193	1.766185

H	-3.803092	-0.544696	-1.494766
H	-2.465073	0.568584	-1.791085
C	2.907858	0.149191	-0.317019
C	-2.869619	0.214799	0.302491
C	-3.906308	1.329825	0.399448
C	4.016527	1.182943	-0.483904
O	3.625886	2.429609	-0.145818
O	5.145357	0.930313	-0.846459
O	-5.159719	0.845015	0.504992
O	-3.664499	2.516245	0.355964
H	-5.780790	1.591350	0.513038
H	4.383639	3.028091	-0.243397
H	-3.210805	-0.619626	0.917968
H	1.346721	1.484452	-0.389702
H	1.597893	0.708193	-1.804854
H	-1.309665	1.533693	0.373677
H	-1.555055	0.755466	1.783997
H	3.212524	-0.717044	-0.905912

Table S.XLI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys)}]^- (\text{NH}_2, \text{S}^-, \text{COO}^-)$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-2.270842	1.881113	0.031578
H	-3.221188	1.517637	0.172181
C	-1.517102	0.674912	-0.337464
H	-1.288075	0.639367	-1.415501
C	-0.185587	0.633103	0.420361
C	-2.366328	-0.605154	-0.025300
H	0.368833	1.555940	0.239659
H	-0.382833	0.561839	1.493517
S	0.857477	-0.808616	-0.103890
O	-3.600248	-0.434849	0.126929
O	-1.711259	-1.681198	0.024206
H	-2.311960	2.518935	-0.759801
Cu	2.617849	0.196123	0.005396
BS2			
N	-2.329777	1.890208	0.006103
H	-3.299300	1.592666	0.138917
C	-1.596005	0.654900	-0.312655
H	-1.325404	0.609484	-1.376844
C	-0.293287	0.601152	0.502620
C	-2.490021	-0.606484	-0.039239
H	0.215025	1.560061	0.415485
H	-0.520735	0.427201	1.556059
S	0.843597	-0.752407	-0.077318
O	-3.720215	-0.401973	0.088658
O	-1.866640	-1.692927	0.007903
H	-2.308450	2.536225	-0.775336
Cu	2.793809	0.170456	-0.015199
BS1W			
N	-2.356066	1.864833	-0.304666
H	-2.641884	1.799630	0.675962
C	-1.654470	0.582050	-0.551041
H	-1.653794	0.384312	-1.629067
C	-0.209319	0.768885	-0.070659
C	-2.344603	-0.606543	0.187404
H	0.205685	1.667297	-0.531130
H	-0.224954	0.918337	1.012407
S	0.886840	-0.682675	-0.466793
O	-2.670414	-0.366519	1.386735
O	-2.515369	-1.676106	-0.454167
H	-3.237877	1.835056	-0.817932
Cu	2.641119	0.108241	0.208150
BS2W			

N	-2.521194	1.834330	-0.161598
H	-2.672727	1.856450	0.844956
C	-1.747711	0.613030	-0.480307
H	-1.788246	0.472940	-1.563400
C	-0.294608	0.862666	-0.059059
C	-2.349245	-0.650973	0.201982
H	0.043052	1.796265	-0.508747
H	-0.248817	0.958829	1.026469
S	0.835307	-0.515176	-0.600621
O	-2.443824	-0.611030	1.459119
O	-2.721660	-1.593873	-0.546793
H	-3.445964	1.764628	-0.579060
Cu	2.761014	0.042906	0.215400

Table S.XLII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}},\underline{\text{Q}}\text{-Cys})]^-$ ($\text{NH}_2, \text{S}^-, \text{COO}^-$) at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
N	-2.164312	1.638537	-0.491522
H	-2.751693	1.278388	-1.245148
C	-0.988723	0.747609	-0.412718
H	-0.579812	0.637553	-1.423866
C	0.093476	1.450781	0.465098
C	-1.414207	-0.682305	0.107845
H	-0.023355	2.522850	0.286453
H	-0.131245	1.274803	1.523293
S	1.907393	1.038210	0.143657
O	-0.614110	-1.679057	-0.166406
O	-2.492425	-0.786036	0.699169
H	-2.714643	1.401861	0.338702
Cu	1.018678	-0.847322	-0.122784
BS2			
N	-2.464443	1.353764	-0.522861
H	-2.973627	0.962862	-1.311709
C	-1.168060	0.649234	-0.422364
H	-0.741274	0.587482	-1.428019
C	-0.205298	1.520059	0.436057
C	-1.363120	-0.819913	0.116187
H	-0.435112	2.556736	0.185472
H	-0.426525	1.374671	1.497661
S	1.646736	1.324817	0.177158
O	-0.429056	-1.682386	-0.134091
O	-2.406433	-1.075984	0.723802
H	-3.009719	1.061176	0.287977
Cu	1.296289	-0.801575	-0.134581
BS1W			
N	-2.435881	1.258997	-0.527354
H	-3.017283	0.725191	-1.173038
C	-1.095740	0.650304	-0.501945
H	-0.746216	0.554356	-1.535420
C	-0.152737	1.612452	0.260218
C	-1.122377	-0.768344	0.162513
H	-0.295280	2.616197	-0.147039
H	-0.462732	1.630843	1.310168
S	1.681897	1.215359	0.190535
O	-0.502755	-1.755028	-0.463235
O	-1.777630	-0.901848	1.206656
H	-2.845423	1.081299	0.391254
Cu	1.033653	-0.778554	-0.126727
BS2W			

N	-2.555866	1.195282	-0.599185
H	-3.071231	0.693204	-1.317777
C	-1.225285	0.582276	-0.448645
H	-0.778636	0.516791	-1.444479
C	-0.345780	1.533113	0.408001
C	-1.304902	-0.866716	0.136949
H	-0.609781	2.548837	0.111345
H	-0.599889	1.419477	1.465401
S	1.515577	1.405013	0.223425
O	-0.342676	-1.685104	-0.143649
O	-2.288127	-1.172557	0.826384
H	-3.078586	1.032622	0.259232
Cu	1.382144	-0.747892	-0.154963

Table S.XLIII. Computed Cartesian coordinates (in Å) of S(H)Et at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
C	1.651064	-0.351996	-0.054027
C	0.505252	0.644834	0.091698
S	-1.174835	-0.098575	-0.079576
H	0.541551	1.397882	-0.700987
H	0.559125	1.178063	1.044686
H	1.621233	-1.108581	0.736711
H	1.604192	-0.868584	-1.016387
H	2.615040	0.165544	0.015279
H	-1.081675	-0.944161	0.967889
BS2			
C	1.650958	-0.351378	-0.053397
C	0.504834	0.643948	0.091287
S	-1.173892	-0.099414	-0.080630
H	0.540412	1.395856	-0.699865
H	0.555350	1.174369	1.043645
H	1.622302	-1.106351	0.736885
H	1.604878	-0.868258	-1.014245
H	2.613578	0.166528	0.014562
H	-1.088999	-0.926952	0.981758
BS1W			
C	1.650548	-0.354184	-0.053761
C	0.508917	0.645993	0.091745
S	-1.175066	-0.097913	-0.080161
H	0.544981	1.401584	-0.697721
H	0.556896	1.169552	1.049311
H	1.613285	-1.114994	0.732048
H	1.613721	-0.860921	-1.022138
H	2.612247	0.165036	0.026652
H	-1.096867	-0.944511	0.966518
BS2W			
C	1.650399	-0.353267	-0.053265
C	0.508315	0.644800	0.091432
S	-1.174102	-0.098692	-0.081178
H	0.543632	1.399549	-0.696008
H	0.552519	1.165094	1.048592
H	1.613710	-1.113365	0.731309
H	1.614754	-0.859071	-1.020877
H	2.610660	0.166155	0.027045
H	-1.101924	-0.928492	0.979778

Table S.XLIV. Computed Cartesian coordinates (in Å) of SEt^- at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
C	1.619036	-0.354449	0.000015
C	0.452836	0.643566	0.000002
S	-1.206175	-0.154369	-0.000019
H	0.569540	1.301838	-0.877553
H	0.569067	1.301316	0.877946
H	1.560710	-1.004651	0.880893
H	1.560230	-1.004928	-0.880639
H	2.608021	0.141629	-0.000442
BS2			
C	1.620210	-0.353518	0.000019
C	0.453555	0.642635	0.000003
S	-1.205073	-0.154777	-0.000019
H	0.553651	1.293895	-0.879813
H	0.553188	1.293442	0.880172
H	1.566304	-1.000733	0.881603
H	1.565576	-1.001318	-0.881110
H	2.599858	0.156445	-0.000679
BS1W			
C	1.627719	-0.353438	0.000004
C	0.463577	0.639674	0.000007
S	-1.214941	-0.154104	-0.000015
H	0.556025	1.294094	-0.876447
H	0.555784	1.293527	0.876861
H	1.591339	-1.000565	0.883415
H	1.589916	-1.001794	-0.882440
H	2.598220	0.162984	-0.001221
BS2W			
C	1.625805	-0.353856	0.000008
C	0.465215	0.640943	0.000005
S	-1.213154	-0.154385	-0.000015
H	0.546880	1.289891	-0.877489
H	0.546613	1.289368	0.877880
H	1.589932	-0.997846	0.883987
H	1.588160	-0.999545	-0.882658
H	2.592764	0.165768	-0.001561

Table S.XLV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_2^{2+}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	3.930733	-1.472944	-0.348475
S	-3.040107	0.603769	-0.186072
S	1.316358	2.565591	0.723454
S	-2.865331	-0.794647	-1.032621
Cu	0.843970	0.316983	-0.320009
Cu	0.443866	-0.419094	0.634160
C	4.051434	3.862378	-0.513056
H	3.831269	3.558593	-1.617987
H	4.660785	5.019361	-0.480884
H	4.848310	2.903128	0.129877
C	2.605272	4.314670	0.144322
H	2.804014	4.716553	1.167892
H	1.826210	5.317635	-0.479569
C	-6.604084	-0.214096	-1.226334
H	-7.585618	0.454564	-0.834932
H	-6.471724	-0.326526	-2.957094
H	-7.323740	-1.292792	-0.597300
C	-4.564719	0.451343	-0.283142
H	-3.803830	1.489155	-0.928859
H	-4.640521	0.696359	1.511547
C	5.628778	-3.802255	0.252976
H	5.090814	-4.235312	1.108834
H	6.088781	-4.640213	-0.334008
H	6.480436	-3.075924	0.569956
C	-4.643930	-0.969321	0.404947
H	-4.449768	-1.693087	-0.857233
H	-6.084059	-0.538461	0.338931
C	-4.215920	-1.722761	2.524470
H	-5.489532	-2.387122	2.886986
H	-2.938628	-2.341842	2.643213
H	-4.150086	-1.048940	3.717223
C	4.723492	-3.152464	-0.839629
H	5.257684	-2.759995	-1.733505
H	3.796557	-3.695559	-1.116703
H	4.797302	-0.418445	0.602907
H	2.351273	1.862823	1.548896
H	-3.864951	-2.031970	-0.424728
H	-3.726579	0.395947	-2.261744
BS2			
S	-1.217039	-2.066105	-0.021232
S	-3.623600	1.707064	-0.179363
S	1.135814	2.181457	-0.094694
S	3.565642	-1.555047	0.286618
Cu	-2.421979	-0.177910	-0.098601

Cu	2.362261	0.322419	0.090643
C	3.524295	3.759775	-0.117173
H	4.165376	2.876867	-0.163235
H	4.049435	4.579310	-0.615426
H	3.389725	4.043919	0.927719
C	2.198377	3.536034	-0.821286
H	1.561067	4.419855	-0.798604
H	2.322576	3.238191	-1.862680
C	6.266448	-2.317725	0.220012
H	7.307104	-2.011539	0.347879
H	6.052068	-3.092884	0.954009
H	6.171467	-2.740304	-0.780343
C	5.381733	-1.098471	0.410142
H	5.468504	-0.682279	1.412339
H	5.582816	-0.317759	-0.317873
C	-3.598737	-3.618196	-0.390981
H	-4.206773	-2.733764	-0.594401
H	-4.041954	-4.457696	-0.933576
H	-3.655946	-3.849974	0.674664
C	-5.430240	1.322270	0.060925
H	-5.713075	0.547447	-0.645797
H	-5.938562	2.247731	-0.203976
C	-5.703418	0.925508	1.502097
H	-6.776675	0.780842	1.620457
H	-5.211931	-0.010501	1.773610
H	-5.395845	1.699583	2.204059
C	-2.165365	-3.443698	-0.858325
H	-1.558336	-4.331492	-0.679739
H	-2.095188	-3.195151	-1.917991
H	-1.436115	-2.432295	1.262341
H	1.155339	2.597258	1.192516
H	3.562628	-1.947427	-1.004631
H	-3.637514	1.910413	-1.514284
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BS1W			
S	0.491265	-1.439414	0.112364
S	3.590998	1.229251	-0.810405
S	-0.353892	1.613071	-0.008385
S	-3.430525	-1.072673	-0.909753
Cu	1.658659	0.486546	-0.106575
Cu	-1.505118	-0.328002	-0.195892
C	-2.162922	3.312726	1.294193
H	-2.901977	2.508537	1.334504
H	-2.328906	3.975558	2.148905
H	-2.323694	3.892607	0.381323
C	-0.744941	2.769222	1.366385
H	0.008262	3.557961	1.328591
H	-0.575847	2.173943	2.266350
C	-6.182576	-0.713895	-0.520248
H	-6.976313	-0.075235	-0.119961
H	-6.341918	-0.825723	-1.595959

H	-6.274241	-1.697370	-0.050044
C	-4.832815	-0.077408	-0.219744
H	-4.728792	0.900197	-0.695547
H	-4.663897	0.042762	0.851142
C	2.132097	-2.962859	1.805842
H	2.855624	-2.145374	1.858540
H	2.188395	-3.532289	2.738653
H	2.413469	-3.629551	0.986111
C	5.000693	0.163085	-0.242869
H	4.880786	-0.014320	0.826345
H	5.904557	0.751574	-0.411016
C	5.024256	-1.137374	-1.034049
H	5.867518	-1.746184	-0.695440
H	4.108286	-1.715225	-0.881189
H	5.145857	-0.953637	-2.105189
C	0.714118	-2.440289	1.639008
H	-0.025041	-3.241639	1.590344
H	0.429628	-1.757881	2.442889
H	0.809581	-2.359169	-0.816594
H	-0.571696	2.426757	-1.057177
H	-3.663097	-2.192519	-0.195772
H	3.857783	2.295457	-0.030482
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BS2W			
S	0.288698	-1.639267	-0.346716
S	3.910574	0.945082	-0.510429
S	-0.286194	1.644586	-0.340138
S	-3.906115	-0.955929	-0.516380
Cu	1.785399	0.172360	-0.338779
Cu	-1.790027	-0.156906	-0.347628
C	-1.941194	3.589558	0.884150
H	-2.708366	2.839039	1.082449
H	-2.005179	4.356604	1.661352
H	-2.153443	4.064770	-0.075581
C	-0.547040	2.986569	0.913855
H	0.231820	3.721985	0.716894
H	-0.327424	2.493896	1.860873
C	-6.444121	-0.369291	0.539456
H	-7.071172	0.360941	1.058962
H	-6.881402	-0.554718	-0.443835
H	-6.467022	-1.299068	1.112333
C	-5.031483	0.183909	0.426556
H	-5.003482	1.109006	-0.149386
H	-4.580027	0.367518	1.399571
C	1.935819	-3.584439	0.886698
H	2.706677	-2.835462	1.075737
H	1.998637	-4.345072	1.670159
H	2.142631	-4.068880	-0.069592
C	5.033516	-0.209638	0.416951
H	5.000880	-1.127254	-0.170488
H	4.584402	-0.402760	1.389018

C	6.448446	0.337794	0.532346
H	7.075135	-0.400841	1.040392
H	6.883185	0.534421	-0.449906
H	6.475970	1.260003	1.117140
C	0.544826	-2.974184	0.914898
H	-0.238493	-3.706913	0.725817
H	0.330902	-2.473355	1.858815
H	0.483855	-2.344509	-1.480322
H	-0.469051	2.345408	-1.478527
H	-3.853407	-1.959938	0.385252
H	3.874528	1.943789	0.397826

Table S.XLVI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_2^{2-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-0.902822	1.672625	-1.527485
S	-2.135796	-1.616561	0.963399
S	0.896632	-1.668733	-1.534128
S	2.147276	1.623656	0.943695
Cu	-1.136710	-0.141411	-0.331449
Cu	1.139023	0.144322	-0.338887
C	2.275078	-3.245635	0.382717
H	2.336484	-2.374278	1.042591
H	2.295085	-4.157277	1.003071
H	3.169454	-3.239786	-0.251928
C	1.003468	-3.165103	-0.462484
H	0.946102	-4.040693	-1.124504
H	0.124465	-3.196717	0.188884
C	4.809746	0.717344	0.581494
H	5.726050	0.289061	1.023958
H	4.476947	0.062544	-0.230209
H	5.062604	1.687496	0.137885
C	3.693865	0.875506	1.617182
H	3.470605	-0.103393	2.058015
H	4.049671	1.518047	2.436475
C	-2.286316	3.247796	0.386694
H	-2.354175	2.374307	1.043136
H	-2.306925	4.157340	1.010121
H	-3.177152	3.247066	-0.252959
C	-3.698179	-0.880130	1.612943
H	-3.490993	0.105289	2.047180
H	-4.055649	-1.519265	2.434201
C	-4.804337	-0.744099	0.563780
H	-5.730419	-0.322822	0.992418
H	-4.470205	-0.092491	-0.249961
H	-5.040817	-1.720974	0.125951
C	-1.010276	3.166026	-0.451733
H	-0.946276	4.043594	-1.110478
H	-0.134853	3.192523	0.204645
BS2			
S	0.813417	-1.557808	-0.979259
S	2.984997	1.710594	0.932715
S	-0.813378	1.557738	-0.978900
S	-2.985134	-1.711021	0.932184
Cu	1.290616	0.673793	-0.188092
Cu	-1.290636	-0.673825	-0.187901
C	-2.740703	3.423057	-0.107063
H	-3.506486	2.642498	-0.123093
H	-3.043473	4.187406	0.625817

H	-2.720851	3.887207	-1.098832
C	-1.373338	2.830760	0.239796
H	-0.618555	3.623015	0.264719
H	-1.403244	2.380399	1.234432
C	-5.089286	-0.331671	-0.375023
H	-5.933777	0.373855	-0.304617
H	-4.378510	0.051922	-1.111775
H	-5.468006	-1.290304	-0.745388
C	-4.395920	-0.517581	0.976876
H	-4.038712	0.451671	1.338310
H	-5.123315	-0.887882	1.711513
C	2.740856	-3.422722	-0.106750
H	3.506564	-2.642092	-0.122773
H	3.043580	-4.186931	0.626294
H	2.721189	-3.887021	-1.098452
C	4.396028	0.517449	0.976741
H	4.039088	-0.452024	1.337857
H	5.123455	0.887612	1.711418
C	5.089249	0.332195	-0.375325
H	5.933868	-0.373216	-0.305312
H	4.378439	-0.051223	-1.112136
H	5.467753	1.291041	-0.745353
C	1.373353	-2.830518	0.239787
H	0.618676	-3.622880	0.264732
H	1.403024	-2.379964	1.234338
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BS1W			
S	-0.975708	1.552961	-1.603625
S	-1.868989	-1.677940	1.077854
S	0.974934	-1.554574	-1.602152
S	1.867922	1.678231	1.077157
Cu	-1.116476	-0.212939	-0.345089
Cu	1.116292	0.212767	-0.345722
C	2.815451	-3.083224	-0.058622
H	2.942218	-2.256771	0.649033
H	3.014082	-4.022487	0.473471
H	3.572223	-2.970269	-0.842254
C	1.407284	-3.080236	-0.647702
H	1.291213	-3.922060	-1.338913
H	0.665786	-3.211238	0.146229
C	4.671898	1.205692	0.921405
H	5.586096	0.890949	1.441607
H	4.545023	0.563605	0.042885
H	4.820697	2.231075	0.566555
C	3.459625	1.114410	1.845679
H	3.338680	0.086048	2.200398
H	3.622183	1.740618	2.730077
C	-2.812031	3.084576	-0.058271
H	-2.938823	2.258455	0.649772
H	-3.008791	4.024231	0.473825
H	-3.570010	2.972321	-0.840836

C	-3.460950	-1.113284	1.845305
H	-3.339859	-0.084763	2.199503
H	-3.624149	-1.738948	2.729973
C	-4.672802	-1.204732	0.920490
H	-5.587167	-0.889477	1.440088
H	-4.545368	-0.563150	0.041678
H	-4.821690	-2.230267	0.566123
C	-1.404666	3.079660	-0.649277
H	-1.288511	3.921035	-1.341021
H	-0.661895	3.210024	0.143559
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BS2W			
S	0.855856	-1.532395	-1.163307
S	2.649069	1.717582	1.095134
S	-0.857661	1.513409	-1.140824
S	-2.677247	-1.744073	1.057434
Cu	1.189773	0.629369	-0.234442
Cu	-1.196353	-0.670193	-0.258224
C	-2.927481	3.325542	-0.480330
H	-3.655110	2.509732	-0.461710
H	-3.289700	4.116910	0.186238
H	-2.899745	3.728144	-1.496947
C	-1.547532	2.843799	-0.040710
H	-0.838696	3.675316	-0.053843
H	-1.585721	2.462742	0.980945
C	-5.114838	-0.578315	0.165636
H	-5.971252	0.066462	0.398277
H	-4.620507	-0.176391	-0.723200
H	-5.497900	-1.571975	-0.084237
C	-4.148354	-0.644641	1.345591
H	-3.793873	0.357247	1.597011
H	-4.667132	-1.034003	2.226198
C	2.990972	-3.220009	-0.385933
H	3.637656	-2.353337	-0.224744
H	3.342960	-4.030115	0.263347
H	3.113241	-3.542860	-1.423793
C	4.179016	0.685426	1.316823
H	3.881960	-0.335889	1.565115
H	4.708267	1.087177	2.185539
C	5.107216	0.680829	0.104510
H	5.999626	0.073285	0.298807
H	4.601902	0.268852	-0.773529
H	5.435575	1.694568	-0.142652
C	1.534197	-2.882882	-0.081022
H	0.905080	-3.763447	-0.233143
H	1.424733	-2.579373	0.961265

Table S.XLVII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})]_3$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	1.347335	-2.123053	-0.134904
Cu	1.326678	0.055398	0.034647
S	-2.512139	-0.104983	-0.137081
Cu	-0.615509	-1.176669	0.037501
S	1.165249	2.228316	-0.134649
Cu	-0.711372	1.121058	0.037160
H	1.404823	2.684797	1.113765
H	-3.032540	-0.126186	1.109195
H	1.626481	-2.556920	1.113255
BS2			
S	2.411791	-0.907194	-0.064122
Cu	1.204791	0.988657	-0.008326
S	-1.991333	-1.634767	-0.063859
Cu	0.254011	-1.537296	-0.008214
S	-0.419739	2.541760	-0.063702
Cu	-1.459246	0.548826	-0.008575
H	-0.460598	2.790198	1.265453
H	-2.186646	-1.795050	1.265110
H	2.648576	-0.997345	1.264719
BS1W			
S	2.460119	-0.555114	-0.141413
Cu	0.899208	0.973473	0.040464
S	-1.710756	-1.853077	-0.136939
Cu	0.393908	-1.265379	0.039299
S	-0.748480	2.408087	-0.137951
Cu	-1.293569	0.291931	0.035192
H	-0.904051	2.898319	1.110122
H	-2.061584	-2.227739	1.111584
H	2.964650	-0.669665	1.105444
BS2W			
S	-2.107346	-1.491876	-0.061607
Cu	-1.413179	0.649928	-0.009573
S	-0.238391	2.570452	-0.062231
Cu	1.269674	0.898487	-0.009082
S	2.345757	-1.079044	-0.062098
Cu	0.143496	-1.548132	-0.009712
H	2.578012	-1.186228	1.265715
H	-0.262812	2.825270	1.265602
H	-2.315229	-1.639772	1.266318

Table S.XLVIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_2]_3^{3-}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	3.619088	-2.518198	0.694223
S	1.915311	0.878506	-0.632003
Cu	1.809493	-1.308882	-0.060760
S	-3.989668	-1.876573	0.696088
S	-0.196995	-2.096128	-0.626798
Cu	-2.040457	-0.910519	-0.062346
S	0.368758	4.391062	0.700074
S	-1.715778	1.217542	-0.634145
Cu	0.230452	2.221672	-0.063055
H	-2.728272	1.964116	-0.123969
H	-0.922453	4.778331	0.870416
H	3.064289	1.382665	-0.113940
H	4.605626	-1.597776	0.856507
H	-0.334774	-3.342686	-0.107330
H	-3.681028	-3.189892	0.857967
BS2			
S	2.019195	4.080432	0.784889
S	-1.233890	1.892754	-0.692053
Cu	1.080615	2.092514	-0.084170
S	2.528996	-3.786470	0.783896
S	2.253982	0.122347	-0.694504
Cu	1.271370	-1.982135	-0.083526
S	-4.544087	-0.293817	0.783979
S	-1.022311	-2.016055	-0.689759
Cu	-2.353169	-0.109968	-0.084729
H	-1.528961	-2.991010	0.097102
H	-4.606021	-1.642649	0.873680
H	-1.827338	2.819395	0.092555
H	0.882689	4.808887	0.879915
H	3.355307	0.171967	0.087200
H	3.728500	-3.165552	0.866707
BS1W			
S	-0.068476	2.737551	1.639507
S	-2.096923	1.059415	-1.292851
Cu	-0.073387	1.361536	-0.245408
S	2.408013	-1.310527	1.643692
S	1.967338	1.288329	-1.294044
Cu	1.221339	-0.619531	-0.241818
S	-2.356351	-1.423059	1.628140
S	0.138090	-2.342519	-1.290547
Cu	-1.142856	-0.746672	-0.246937
H	0.193637	-3.364442	-0.407159
H	-1.830888	-2.612327	1.992385

H	-3.006790	1.522941	-0.407204
H	-1.368211	2.841060	1.993253
H	2.824759	1.851980	-0.413754
H	3.172638	-0.250901	1.990856
BS2W			
S	1.889815	-3.094229	1.444841
S	2.244215	0.102082	-1.175950
Cu	1.094456	-1.691333	-0.194916
S	-3.657675	-0.087218	1.418734
S	-1.029389	-1.990058	-1.154580
Cu	-2.019762	-0.090817	-0.194995
S	1.742904	3.176040	1.448251
S	-1.205558	1.891370	-1.154635
Cu	0.933519	1.783527	-0.194154
H	-1.809552	2.850794	-0.420745
H	0.683532	3.983381	1.673231
H	3.384589	0.153178	-0.454138
H	3.122639	-2.591723	1.674094
H	-1.550413	-2.996612	-0.420271
H	-3.817957	-1.406728	1.659141

Table S.XLIX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH}_2)_2]_3^{3+}$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	-3.762340	-1.351647	1.216074
S	-0.374292	-2.085003	-0.791574
Cu	-2.132469	-0.768660	-0.202285
S	0.707966	3.931608	1.217758
S	-1.618939	1.367782	-0.790974
Cu	0.401136	2.229330	-0.202384
S	3.051847	-2.579190	1.218300
S	1.994553	0.717861	-0.793459
Cu	1.731888	-1.461595	-0.202072
H	3.232510	1.164639	-0.472468
H	4.327691	-2.361663	0.830037
H	-0.607048	-3.379927	-0.468759
H	-4.212644	-2.565464	0.829155
H	-2.623050	2.217971	-0.468049
H	-0.114636	4.929794	0.826798
H	-4.883957	-0.712451	0.816948
H	-1.821691	1.540296	-2.118831
H	1.825002	4.581577	0.823299
H	2.243492	0.806887	-2.121688
H	3.059917	-3.870473	0.820415
H	-0.422385	-2.346911	-2.119400
BS2			
S	-5.774928	-2.022630	0.296048
S	-3.414213	1.783189	-0.330202
Cu	-4.582783	-0.131209	0.006782
S	4.633740	-4.028975	0.283212
S	0.150862	-3.756022	-0.303380
Cu	2.397772	-3.877241	0.013909
S	1.145721	5.986689	0.316117
S	3.261617	2.036303	-0.337377
Cu	2.187522	4.008536	0.014242
H	4.127678	2.427481	-1.294156
H	1.794693	6.730749	-0.654622
H	-4.178560	2.343810	-1.291597
H	-6.761723	-1.806021	-0.650886
H	0.005470	-4.701083	-1.259022
H	4.906116	-4.997157	-0.665947
H	-6.589496	-1.626096	1.347246
H	-0.255812	-4.574264	0.690994
H	4.675854	-4.935644	1.332780
H	4.180404	2.121030	0.645972
H	1.925999	6.501762	1.342643
H	-3.948226	2.536080	0.652857

BS1W			
S	-0.344310	3.971523	1.091768
S	-1.901746	0.885752	-0.830916
Cu	-0.188932	2.151158	-0.188763
S	3.629667	-1.681632	1.078150
S	1.710934	1.199550	-0.839291
Cu	1.957400	-0.910504	-0.180258
S	-3.290155	-2.282849	1.067559
S	0.186053	-2.097685	-0.813460
Cu	-1.761674	-1.235044	-0.174965
H	0.299740	-3.413489	-0.539575
H	-2.594200	-2.991907	1.977711
H	-3.103713	1.442091	-0.577053
H	-1.309007	3.693843	1.990699
H	2.795709	1.961225	-0.587522
H	3.878163	-0.712820	1.980886
H	0.644469	3.855058	1.999796
H	1.851789	1.292131	-2.176337
H	3.053396	-2.491908	1.987542
H	0.201579	-2.285559	-2.147779
H	-3.704650	-1.376237	1.974120
H	-2.057380	0.950374	-2.167811

BS2W			
S	-1.367722	4.390600	0.701188
S	-2.165340	0.492010	-0.573669
Cu	-0.721378	2.338019	-0.115843
S	4.489908	-1.015423	0.693295
S	1.513021	1.633270	-0.559122
Cu	2.387342	-0.543179	-0.118726
S	-3.131160	-3.371494	0.697633
S	0.658519	-2.128242	-0.549115
Cu	-1.664084	-1.795069	-0.117543
H	1.034904	-3.346733	-0.107574
H	-2.350218	-3.969943	1.622129
H	-3.419540	0.777686	-0.165136
H	-2.288195	4.008041	1.611569
H	2.384072	2.572375	-0.133840
H	4.618054	-0.033386	1.610776
H	-0.403788	4.596106	1.623801
H	1.716123	1.853524	-1.875508
H	4.186576	-1.958813	1.610108
H	0.751174	-2.430994	-1.861574
H	-3.798592	-2.629313	1.606805
H	-2.440715	0.556549	-1.893664

Table S.L. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SH})_{\text{b}}(\underline{\text{S}}\text{-SH}_2)_{\text{p}}]_3$ at BS1, BS2, BS1W and BS2W levels of theory.

Atom	x	y	z
BS1			
S	2.983094	-1.440831	1.545991
S	1.976335	1.607529	-0.755519
Cu	1.241144	-0.463813	-0.563771
S	-2.752294	-1.811455	1.551037
S	0.393705	-2.497145	-0.707394
Cu	-1.041595	-0.822506	-0.552425
S	-0.206216	3.170855	1.635826
S	-2.376015	0.922513	-0.750514
Cu	-0.211001	1.338185	-0.523644
H	-0.455636	3.251929	2.961555
H	3.550703	-1.557733	2.767122
H	-3.077423	-2.206220	2.802336
H	2.479140	-2.688453	1.562056
H	0.464390	-2.717095	-2.036543
H	-3.590857	-0.759047	1.570456
H	-2.560976	0.955430	-2.086317
H	1.128936	3.234095	1.794136
H	2.096079	1.759536	-2.090292
BS2			
S	3.707794	-0.726414	1.569131
S	1.699608	1.949952	-0.716188
Cu	1.559382	-0.306519	-0.573547
S	-2.477471	-2.838474	1.580102
S	0.836040	-2.448856	-0.712401
Cu	-1.048648	-1.199600	-0.572152
S	-1.217685	3.566889	1.581605
S	-2.540874	0.498899	-0.718308
Cu	-0.516837	1.504830	-0.576111
H	-2.049782	2.996256	2.475912
H	3.637218	0.288005	2.454667
H	-1.554820	-3.278760	2.459163
H	3.254396	-1.632426	2.458877
H	0.866336	-2.539019	-2.060959
H	-3.030051	-1.992642	2.472812
H	-2.631538	0.516009	-2.067103
H	-0.197118	3.627194	2.460787
H	1.763747	2.020857	-2.064740
BS1W			
S	-0.223299	2.677755	1.621484
S	-2.199293	1.035811	-1.177247
Cu	-0.112497	1.352128	-0.333357
S	2.449339	-1.135745	1.619987
S	1.998450	1.382722	-1.176786

Cu	1.228407	-0.580344	-0.332186
S	-2.226360	-1.522911	1.621653
S	0.201888	-2.435153	-1.150048
Cu	-1.115729	-0.775105	-0.332524
H	-1.319215	-2.024564	2.482718
H	-1.146652	2.156519	2.453318
H	2.467284	-0.071226	2.446507
H	0.807026	2.359625	2.430436
H	1.752705	1.212072	-2.492405
H	1.669371	-1.865429	2.441688
H	0.183820	-2.158215	-2.470404
H	-2.499847	-0.457721	2.400458
H	-1.931363	0.905631	-2.493067
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BS2W			
S	2.452664	-1.597711	1.716446
S	2.220737	1.128701	-1.126020
Cu	1.386515	-0.900691	-0.408069
S	-2.616674	-1.320671	1.711308
S	-0.130218	-2.484634	-1.127480
Cu	-1.475103	-0.749090	-0.410463
S	0.156769	2.911895	1.719882
S	-2.084749	1.358457	-1.127854
Cu	0.089986	1.651812	-0.409362
H	-0.859262	2.397112	2.441268
H	2.527465	-0.462277	2.440152
H	-1.670406	-1.936053	2.449478
H	1.435996	-2.096684	2.448673
H	-0.112142	-2.157000	-2.437281
H	-2.562680	-0.184328	2.435650
H	-1.808929	1.177973	-2.437489
H	1.103693	2.282973	2.444554
H	1.929239	0.982757	-2.436609

Table S.LI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}_3(\underline{\text{S}}\text{-SH})_b\{(\underline{\text{S}}\text{-SH}_2)_2\}_b\{(\underline{\text{S}}\text{-SH}_2)_3\}_p]^{+2}$ at BS1 and BS2 levels of theory.

Atom	x	y	z
BS1			
S	2.657410	-1.472991	1.277563
S	2.024552	1.843207	-0.920263
Cu	1.211600	-0.899738	-0.359824
S	-2.670546	-1.388229	1.338194
S	-0.026890	-1.398691	-2.039337
Cu	-1.218918	-0.911524	-0.325400
S	0.216519	1.504703	2.334098
S	-2.105157	1.830484	-0.827077
Cu	-0.017558	1.079970	0.011741
H	-2.280970	3.135574	-0.523957
H	-0.931302	1.161459	2.954142
H	2.214358	3.158166	-0.671196
H	3.806632	-0.821022	0.995033
H	-2.687687	-2.738301	1.359989
H	3.118685	-2.661974	0.830114
H	-0.039569	-0.335848	-2.873573
H	-3.886952	-1.284104	0.758549
H	-1.990085	2.049951	-2.152129
H	0.011063	2.829270	2.488533
H	1.852988	2.018545	-2.245339
BS2			
S	6.106885	-2.543215	-1.073739
S	-3.506220	-2.173369	-0.230214
Cu	4.540527	-1.068040	0.440212
S	3.014277	3.486723	-0.979646
S	2.655827	-0.292478	1.437757
Cu	2.920443	1.525937	0.187524
S	-7.483789	-0.390434	-0.501320
S	-4.231990	1.838673	0.520004
Cu	-5.198516	-0.369303	-0.060857
H	-4.999823	2.687687	-0.209835
H	-8.000694	-0.183482	0.739055
H	-4.291349	-2.833006	-1.127663
H	7.164149	-2.789714	-0.027826
H	4.378196	3.565268	-1.171624
H	6.989420	-1.573075	-1.623983
H	2.128376	-1.201577	0.446612
H	2.772108	3.058781	-2.265515
H	-4.737174	2.334165	1.678541
H	-7.763390	-1.722623	-0.488354
H	-4.130803	-2.726041	0.845612

Table S.LII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}_3\{(\underline{\text{S}}\text{-SH})_2\}_b(\underline{\text{S}}\text{-SH}_2)_b\{(\underline{\text{S}}\text{-SH}_2)_3\}_p]^+$ at BS1 and BS2 levels of theory.

Atom	x	y	z
BS1			
S	3.278879	-0.501895	1.402082
S	1.640625	1.780501	-1.153613
Cu	1.447064	-0.296374	-0.324672
S	-2.429563	-1.616606	1.652147
S	0.725282	-2.344513	-0.701928
Cu	-0.841615	-0.814602	-0.451081
S	-1.358172	2.127738	1.730063
S	-2.462815	0.226955	-1.635967
Cu	-0.152282	1.371102	0.015328
H	-3.253154	-0.715524	-2.197158
H	-2.668472	1.887688	1.507255
H	4.172081	0.446140	1.054593
H	0.865890	-2.995090	0.472931
H	-1.490891	-2.287147	2.345730
H	4.006691	-1.497235	0.859332
H	-2.924632	-2.733516	1.085573
H	-1.891772	0.554629	-2.812141
H	-1.479250	3.448255	1.472522
H	1.213910	1.593295	-2.420880
BS2			
S	-0.658304	3.714887	-1.020143
S	2.433852	1.669589	0.061040
Cu	0.145421	1.802608	0.345493
S	-3.671008	-1.678984	-1.403641
S	-1.450256	0.760575	1.604580
Cu	-2.435456	-0.565064	0.140276
S	3.195649	-2.656131	-0.617698
S	-0.509565	-2.958229	0.773216
Cu	2.777693	-0.473863	-0.233843
H	-0.901748	-4.243460	0.648512
H	3.105888	-3.135532	0.642954
H	0.434254	4.502917	-1.099040
H	-2.427426	1.692890	1.659062
H	-4.460270	-2.417581	-0.591023
H	-1.260457	4.503339	-0.105522
H	-4.645920	-0.780648	-1.669409
H	-0.756848	-2.926170	2.098074
H	4.548946	-2.648679	-0.616755
H	2.775607	1.678873	1.369619

Table S.LIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}_3\{(\underline{\text{S}}\text{-SH})_3\}_b(\underline{\text{S}}\text{-SH})_p\{(\underline{\text{S}}\text{-SH}_2)_2\}_p]^-$ at BS1 and BS2 levels of theory.

Atom	x	y	z
BS1			
S	-5.283290	-0.722511	0.297764
S	1.116048	2.333174	0.682579
Cu	1.086383	0.261489	1.400356
S	-1.693225	-1.268945	-0.831345
S	1.085767	-1.819432	1.934195
Cu	0.457373	-1.152816	-0.305550
S	-2.626725	2.418421	-0.466722
S	2.060058	-0.841290	-2.127432
Cu	1.624523	0.777414	-0.781794
H	-2.287207	1.095546	-0.603273
H	-4.890386	0.529963	0.607777
H	-4.029718	-1.067085	-0.122616
H	2.400648	-2.110245	1.816896
H	-1.699108	-1.022141	-2.159340
H	3.226585	-1.296631	-1.618267
H	-1.431893	2.739140	0.074716
H	2.292868	2.844228	1.102122
BS2			
S	5.992621	-0.122384	-0.709037
S	-3.099516	0.000632	-1.353791
Cu	-1.486579	-1.437963	-0.758843
S	2.394466	0.792254	0.011887
S	0.169459	-2.700707	0.015747
Cu	0.652308	-0.504380	0.846579
S	-0.424486	2.864432	-0.860132
S	-0.870626	0.611195	2.324541
Cu	-1.715661	1.034590	0.238042
H	0.770145	2.170674	-0.613171
H	6.066969	1.013333	-1.430946
H	4.671894	0.095453	-0.400086
H	-0.550954	-3.163272	1.063591
H	2.617435	1.550836	1.106873
H	-1.700028	-0.404849	2.647920
H	-0.480787	2.471280	-2.148702
H	-4.037313	-0.535388	-0.540466

Table S.LIV. Computed Cartesian coordinates (in Å) of $[\text{Cu}_3\{(\underline{\text{S}}\text{-SH})_3\}_b\{(\underline{\text{S}}\text{-SH})_2\}_b(\underline{\text{S}}\text{-SH}_2)_p]^{2-}$ at BS1 and BS2 levels of theory.

Atom	x	y	z
BS1			
S	3.930948	0.125165	-1.287834
S	-1.637070	2.115718	-1.284882
Cu	-1.161985	-0.025346	-1.136890
S	1.759239	-2.316182	0.634557
S	-1.434887	-2.199945	-1.316821
Cu	-0.218406	-1.205085	0.625874
S	1.581151	2.432158	0.620017
S	-1.325219	-0.061058	2.263078
Cu	-0.300774	1.175273	0.651357
H	2.312921	1.860799	1.602014
H	3.100019	1.084259	-0.762652
H	3.168952	-0.881091	-0.743070
H	-2.717480	-2.250300	-0.886567
H	2.426060	-1.697562	1.634258
H	-2.617109	-0.102180	1.855299
H	-2.906188	2.051977	-0.819042
BS2			
S	-0.000682	0.074480	2.626430
S	-2.148300	1.892331	-0.241450
Cu	0.000222	1.497311	0.526974
S	2.769546	-1.886096	0.807353
S	2.148393	1.892597	-0.242104
Cu	1.654133	-0.483147	-0.665004
S	-2.770551	-1.885545	0.805941
S	0.000418	-0.906562	-2.285138
Cu	-1.653599	-0.482767	-0.665555
H	-2.078982	-3.024026	0.577221
H	-1.003484	-0.735240	2.148563
H	1.002372	-0.735236	2.148970
H	1.761230	2.445638	-1.413243
H	2.077026	-3.023973	0.578533
H	0.000739	0.317358	-2.859864
H	-1.761995	2.445684	-1.412727

Table S.LV. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-S(H)Et})_2]_3^{3+}$ at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
C	-5.671568	-2.023473	2.596043
C	-4.332925	-2.149531	1.883348
S	-4.072574	-0.720522	0.703400
C	-2.401277	-4.001499	-1.870349
C	-1.164307	-3.780033	-1.018759
S	-0.625413	-1.987140	-1.018367
Cu	-2.102154	-0.482771	-0.272067
C	1.218087	6.093541	2.258272
C	0.557783	5.198698	1.220172
S	1.205356	3.443901	1.343432
C	-2.354875	4.086180	-1.805698
C	-2.725007	2.902886	-0.929772
S	-1.431191	1.551600	-0.991672
Cu	0.633839	2.056732	-0.297246
C	4.589422	-3.843545	2.593975
C	3.995733	-2.627576	1.897621
S	2.715102	-3.145503	0.634902
C	4.670066	-0.060883	-1.903879
C	3.865893	0.889387	-1.034711
S	2.042538	0.465699	-1.036894
Cu	1.478033	-1.578231	-0.315911
H	-0.300276	-4.343191	-1.378293
H	-1.325514	-4.015456	0.036249
H	-4.297047	-3.030647	1.237594
H	-3.487889	-2.175716	2.573196
H	-0.516266	5.093308	1.393009
H	4.743075	-2.091483	1.306985
H	3.522198	-1.932399	2.592684
H	3.925379	1.924124	-1.379355
H	4.154396	0.851053	0.018769
H	-2.224264	-3.765618	-2.923614
H	-2.666570	-5.062287	-1.816239
H	-3.260919	-3.425120	-1.515852
H	5.362103	-3.498482	3.288286
H	3.840514	-4.384910	3.178785
H	5.054735	-4.532567	1.885575
H	5.722794	0.234379	-1.848138
H	4.597526	-1.098813	-1.566006
H	4.374172	-0.007776	-2.955531
H	0.724447	5.544754	0.198787
H	2.293141	6.194045	2.085380
H	0.778448	7.092837	2.177874
H	1.052201	5.731021	3.275212
H	-5.710737	-1.139142	3.238178
H	-6.506280	-1.990582	1.892286

H	-5.803356	-2.901154	3.236732
H	-2.797056	3.163691	0.129137
H	-3.657539	2.426332	-1.240040
H	-1.421383	4.561103	-1.490653
H	-3.151931	4.832224	-1.723851
H	-2.277709	3.809818	-2.861167
H	-4.198971	0.272096	1.606345
H	-0.611573	-1.860059	-2.362512
H	-1.391131	1.482366	-2.339652
H	2.508605	3.734181	1.154172
H	1.929017	0.434149	-2.382211
H	1.918585	-3.835748	1.474955
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BS1W			
C	-4.895482	0.577049	3.235578
C	-4.007021	0.062025	2.111727
S	-3.556455	1.403488	0.919628
C	-4.201652	-2.068028	-1.968269
C	-2.995278	-2.546879	-1.179583
S	-1.600739	-1.333367	-1.232791
Cu	-1.969102	0.727295	-0.483905
C	2.953818	3.901454	3.258886
C	2.055824	3.381345	2.145539
S	3.003206	2.393178	0.896184
C	0.304452	4.689537	-1.933975
C	-0.716015	3.868928	-1.165683
S	-0.356958	2.057661	-1.226715
Cu	1.613095	1.343470	-0.487857
C	1.912051	-4.515711	3.251428
C	1.930139	-3.493851	2.123349
S	0.560687	-3.779997	0.908167
C	3.903737	-2.612084	-1.945289
C	3.705583	-1.322899	-1.165524
S	1.961374	-0.718240	-1.230758
Cu	0.362634	-2.060397	-0.489532
H	-2.590128	-3.484032	-1.564570
H	-3.212684	-2.669325	-0.115633
H	-4.522735	-0.681818	1.498624
H	-3.084436	-0.382948	2.484575
H	1.243417	2.759868	2.526669
H	2.838854	-3.567183	1.522638
H	1.845997	-2.470543	2.490577
H	4.316689	-0.506279	-1.553172
H	3.916344	-1.439471	-0.101368
H	-3.964447	-1.926361	-3.026474
H	-4.986326	-2.827758	-1.898872
H	-4.597831	-1.130130	-1.570203
H	2.760723	-4.326157	3.916035
H	0.996936	-4.440993	3.846558
H	1.996553	-5.536360	2.869047
H	4.956166	-2.904073	-1.874462

H	3.297665	-3.428377	-1.544629
H	3.660367	-2.483451	-3.003582
H	1.623385	4.197777	1.561588
H	3.759685	4.525565	2.863519
H	2.353719	4.508268	3.943956
H	3.395410	3.084351	3.837102
H	-4.381726	1.333109	3.836354
H	-5.821369	1.009851	2.847638
H	-5.157334	-0.255901	3.895902
H	-0.732207	4.112021	-0.101464
H	-1.726500	3.986534	-1.561189
H	1.312534	4.571731	-1.528911
H	0.027503	5.745257	-1.858077
H	0.317592	4.422468	-2.994415
H	-2.907466	2.190729	1.799332
H	-1.517619	-1.258779	-2.576024
H	-0.329547	1.955279	-2.570228
H	3.432703	1.430275	1.735653
H	1.868399	-0.688197	-2.574406
H	-0.459277	-3.614506	1.770921

Table S.LVI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_2]_3^{3-}$ at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
C	-3.388507	-1.238313	3.198177
C	-2.209543	-0.565339	2.488292
S	-2.740689	0.638542	1.193514
C	-3.998606	-2.563601	-0.797427
C	-2.507536	-2.892219	-0.879029
S	-1.572854	-1.686418	-1.923260
Cu	-1.403788	0.299224	-0.757928
C	1.211299	2.391131	3.780964
C	0.709977	2.554616	2.343179
S	1.970460	2.032109	1.100701
C	-0.282103	4.797211	-0.598422
C	-1.332959	3.686255	-0.622705
S	-0.877126	2.307044	-1.767713
Cu	0.856935	1.136986	-0.784697
C	2.781060	-2.600251	2.927099
C	1.553682	-1.899182	2.337201
S	0.838148	-2.793514	0.888905
C	4.265808	-2.039814	-1.057237
C	3.738915	-0.614546	-0.888080
S	2.257465	-0.284604	-1.943868
Cu	0.444221	-1.240087	-0.891683
H	-2.358603	-3.894990	-1.305786
H	-2.057056	-2.896599	0.117169
H	-1.563693	-1.321868	2.031513
H	-1.596832	-0.042561	3.235996
H	-0.199435	1.963648	2.193565
H	1.811167	-0.878625	2.036399
H	0.785617	-1.809917	3.118649
H	4.516688	0.116826	-1.150552
H	3.460948	-0.431455	0.152892
H	-4.451971	-2.538699	-1.798193
H	-4.547219	-3.309856	-0.195252
H	-4.128183	-1.578501	-0.336792
H	3.173825	-2.069429	3.812418
H	2.538614	-3.629400	3.226993
H	3.583573	-2.659683	2.183270
H	5.175296	-2.212205	-0.454541
H	3.496653	-2.749794	-0.736723
H	4.513113	-2.245941	-2.107911
H	0.432795	3.607199	2.180362
H	2.129729	2.972195	3.945085
H	0.460961	2.721447	4.520982
H	1.450254	1.341311	3.982065
H	-4.048429	-0.489262	3.657707
H	-3.993035	-1.808721	2.483633

H	-3.052875	-1.930030	3.990975
H	-1.472593	3.263281	0.375625
H	-2.304528	4.089354	-0.944737
H	0.674872	4.388596	-0.256572
H	-0.576370	5.622019	0.074602
H	-0.132372	5.217835	-1.602442
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BS1W			
C	-3.785103	-1.623342	3.274394
C	-2.819366	-1.771208	2.099889
S	-2.762932	-0.250198	1.040547
C	-2.509705	-4.205994	-1.150968
C	-1.079981	-3.780338	-0.827630
S	-0.554142	-2.262722	-1.754315
Cu	-1.318919	-0.365191	-0.726987
C	-0.224805	3.853448	3.361507
C	-0.552879	3.247713	1.997713
S	0.945868	2.551341	1.155780
C	-2.296802	4.206310	-1.539512
C	-2.607639	2.751561	-1.198397
S	-1.424468	1.563975	-1.990809
Cu	0.443596	1.275291	-0.696821
C	4.050992	-1.602839	2.529916
C	2.567433	-1.255912	2.647706
S	1.476672	-2.154974	1.447700
C	5.058664	0.068787	-1.099194
C	3.826180	0.868187	-0.685840
S	2.326988	0.392227	-1.666784
Cu	0.978918	-1.058321	-0.506276
H	-0.381523	-4.583495	-1.087955
H	-0.967154	-3.585284	0.241467
H	-3.112677	-2.629482	1.485539
H	-1.809507	-1.979232	2.469426
H	-1.291859	2.447573	2.109200
H	2.420090	-0.179785	2.516076
H	2.217079	-1.502466	3.657014
H	4.002738	1.938768	-0.835856
H	3.607871	0.723124	0.374449
H	-2.632355	-4.402995	-2.221646
H	-2.778274	-5.120811	-0.607398
H	-3.223326	-3.423381	-0.871558
H	4.643818	-1.058993	3.277849
H	4.218760	-2.674422	2.683602
H	4.439294	-1.344390	1.539423
H	5.938995	0.374797	-0.520040
H	4.901752	-1.003214	-0.938094
H	5.286540	0.215317	-2.160533
H	-1.006031	4.010374	1.354715
H	0.499518	4.670227	3.268463
H	-1.125530	4.256322	3.843184
H	0.208044	3.102416	4.031176

H	-3.497717	-0.783987	3.916795
H	-4.806684	-1.437373	2.924948
H	-3.800211	-2.530920	3.892052
H	-2.580649	2.591977	-0.118414
H	-3.615106	2.491285	-1.541601
H	-1.299119	4.486712	-1.184985
H	-3.025429	4.882683	-1.074667
H	-2.325313	4.374407	-2.621633

Table S.LVII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-SEt})_b(\underline{\text{S}}\text{-S(H)Et})_p]_3$ at BS1 levels of theory.

Atom	x	y	z
BS1			
C	0.441922	-1.892727	4.103054
C	0.380316	-1.443588	2.648078
S	0.348513	-2.842995	1.445618
C	3.345628	-3.712073	-0.878871
C	3.210871	-2.202445	-0.703704
S	1.851865	-1.530532	-1.767974
Cu	-0.119410	-1.663491	-0.679185
C	-4.718366	3.263405	0.953183
C	-3.819004	2.253082	0.251908
S	-2.652144	1.382564	1.390569
C	-4.745069	-2.000372	0.195525
C	-3.243130	-2.218541	0.353588
S	-2.302013	-1.536983	-1.090697
Cu	-1.313413	0.389995	-0.602592
C	5.192621	2.959490	1.310360
C	4.173545	2.008588	1.928856
S	2.996686	1.267360	0.705452
C	1.118850	4.478558	-0.824289
C	0.111288	3.480067	-0.262755
S	-0.251397	2.147070	-1.495771
Cu	0.959532	0.357349	-1.158932
H	4.136024	-1.700835	-1.006104
H	3.024530	-1.947007	0.342728
H	1.266216	-0.869790	2.360544
H	-0.487318	-0.808319	2.450969
H	-4.398479	1.443023	-0.198873
H	3.525453	2.534673	2.635981
H	4.662012	1.198101	2.476641
H	-0.834792	3.981678	-0.031192
H	0.491877	3.033342	0.659930
H	3.518314	-3.970297	-1.927744
H	4.186585	-4.094757	-0.288174
H	2.436388	-4.224868	-0.551940
H	5.831193	3.389391	2.090776
H	5.840478	2.438131	0.598703
H	4.698436	3.777168	0.779030
H	1.301841	5.287888	-0.106770
H	2.068885	3.980983	-1.037326
H	0.752624	4.923186	-1.754300
H	-3.230256	2.705746	-0.550249
H	-4.135542	4.073930	1.402063
H	-5.407723	3.710117	0.228098
H	-5.308820	2.791347	1.743043
H	-0.447564	-2.465639	4.383464

H	1.319960	-2.517083	4.289218
H	0.496376	-1.018372	4.761424
H	-2.885267	-1.755065	1.278097
H	-3.025176	-3.290304	0.408630
H	-4.987694	-0.933403	0.170220
H	-5.294021	-2.453780	1.029477
H	-5.108409	-2.444551	-0.735661
H	3.918891	0.631380	-0.040411
H	-1.893638	2.454319	1.690952
H	-0.866939	-3.316472	1.784603

Table S.LVIII. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-H}_2\text{Cys})_2]_3^{3+}$ ($\text{NH}_2, \text{SH}, \text{COOH}$) at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
N	-6.943592	-0.370888	3.998818
C	-6.280187	-0.070086	2.735027
C	-6.257181	-1.367152	1.907397
O	-5.500851	-1.510924	0.941274
C	-4.874763	0.554419	2.866587
S	-4.305350	1.421023	1.314896
N	-4.289633	-0.726398	-1.446086
C	-3.877465	-2.079015	-1.927249
C	-5.056659	-3.070356	-2.184483
O	-5.092867	-3.666025	-3.227726
C	-2.870437	-2.765875	-0.999117
S	-1.339999	-1.736187	-0.839979
Cu	-3.117618	0.528195	-0.421124
N	2.386460	6.045618	3.288098
C	2.458407	5.167876	2.123331
C	1.424867	5.673996	1.101074
O	1.034919	4.978394	0.156765
C	2.290086	3.664848	2.417787
S	2.766092	2.601182	0.971713
N	1.353408	3.087928	-1.975307
C	0.047125	3.481538	-2.583979
C	0.041436	4.923801	-3.174805
O	-0.183616	5.073387	-4.346395
C	-1.113517	3.300825	-1.603331
S	-1.220782	1.530570	-1.078275
Cu	1.514903	1.519400	-0.730284
N	4.489644	-6.179655	2.080012
C	3.730987	-5.792996	0.904362
C	4.576302	-5.076848	-0.155306
O	4.481613	-3.880656	-0.421002
C	2.568099	-4.913216	1.380946
S	1.396040	-4.490145	-0.008474
N	5.711448	-1.065925	-0.961127
C	4.864650	-0.264948	-0.094691
C	5.634050	0.126986	1.207157
O	5.068699	0.705764	2.121844
C	3.556014	-0.936116	0.350678
S	2.099843	-0.640258	-0.756201
Cu	0.712313	-2.414406	-0.330727
O	5.461439	-5.892130	-0.708372
H	6.021273	-5.411330	-1.343561
O	6.903327	-0.193427	1.206821
O	1.001897	6.890219	1.293998
O	0.284446	5.935840	-2.339983
O	-7.092312	-2.289228	2.286941

O	-5.954503	-3.238598	-1.212236
H	2.029802	3.037656	-2.738595
H	1.669585	3.864772	-1.387385
H	3.291762	6.230050	3.708343
H	1.753477	5.713754	4.011468
H	5.137163	-5.465723	2.399121
H	4.995878	-7.049218	1.949849
H	-7.523560	0.387418	4.343158
H	-6.309926	-0.664128	4.738178
H	5.503693	-2.062332	-0.947355
H	5.796588	-0.726303	-1.911062
H	-4.709399	-0.250201	-2.246617
H	-5.056073	-0.852335	-0.780542
H	-3.422306	-1.959057	-2.913547
H	-2.606657	-3.744682	-1.402732
H	-3.254479	-2.883751	0.017234
H	-6.922689	0.624626	2.178607
H	-4.131260	-0.188038	3.162988
H	-4.916959	1.340918	3.621586
H	2.966221	3.378764	3.225003
H	3.435869	5.319945	1.648439
H	1.266342	3.428700	2.716026
H	3.335101	-6.704342	0.444314
H	2.930818	-3.980391	1.812822
H	1.998827	-5.453042	2.136483
H	3.236045	-0.549625	1.319466
H	3.690500	-2.017787	0.405440
H	4.657950	0.699092	-0.578238
H	-5.786441	-2.740827	-0.383007
H	-7.529028	-1.935990	3.111174
H	1.431843	7.188894	2.144348
H	7.070223	-0.649207	0.342646
H	0.432212	5.678404	-1.403953
H	-0.972312	3.879698	-0.688073
H	-2.054940	3.588891	-2.074057
H	-0.117302	2.843905	-3.456256
H	0.334713	-5.173982	0.457786
H	-1.241277	-1.471427	-2.157229
H	-1.088584	1.069003	-2.339432
H	2.706172	-0.997523	-1.910616
H	3.616682	1.749930	1.619413
H	-3.599958	2.383597	1.936842

BS1W

N	1.489820	4.303719	4.274240
C	2.369935	3.993785	3.136730
C	2.215547	5.104695	2.091141
O	1.574686	4.974377	1.065574
C	1.922944	2.654498	2.551507
S	2.930794	2.179705	1.072392
N	1.649493	4.838915	-1.983225

C	0.219282	4.697219	-2.235680
C	-0.404775	6.115376	-2.329171
O	-1.598215	6.332592	-2.286804
C	-0.603698	3.877824	-1.235648
S	-0.247730	2.071828	-1.314311
Cu	1.660813	1.272581	-0.524798
N	3.176728	-3.448760	4.262083
C	2.440214	-4.009357	3.127932
C	3.377319	-4.485441	2.003259
O	3.627506	-3.809580	1.020103
C	1.484638	-2.934173	2.602821
S	0.506661	-3.552182	1.154306
N	3.452528	-3.798204	-1.988479
C	4.023830	-2.484124	-2.267824
C	5.561527	-2.635781	-2.423058
O	6.335697	-1.700990	-2.412620
C	3.748341	-1.364724	-1.258037
S	2.003469	-0.780264	-1.307156
Cu	0.377760	-2.037922	-0.484801
N	-5.242663	-0.664081	3.967654
C	-5.112173	0.082998	2.719580
C	-5.896020	-0.662776	1.636940
O	-5.363557	-1.257523	0.704861
C	-3.654987	0.310941	2.292791
S	-3.512498	1.384448	0.781669
N	-4.720546	-1.001047	-2.330194
C	-4.059481	-2.296373	-2.277897
C	-5.113882	-3.412455	-2.105813
O	-5.170146	-4.369397	-2.847595
C	-2.972506	-2.520972	-1.200342
S	-1.567537	-1.334361	-1.320267
Cu	-1.875904	0.744922	-0.594172
O	-7.205230	-0.614606	1.823035
H	-7.650143	-1.116186	1.116098
O	-5.978198	-3.291851	-1.090139
O	3.984020	-5.668345	2.158129
O	5.938379	-3.896305	-2.610829
O	2.805192	6.277265	2.359499
O	0.508034	7.064173	-2.514354
H	2.533727	-3.927741	-2.399199
H	3.408165	-3.986061	-0.987291
H	3.647118	-4.173465	4.797292
H	3.888936	-2.794523	3.944959
H	-4.646562	-1.489201	3.958523
H	-4.944328	-0.086528	4.748877
H	1.701869	3.663366	5.036865
H	1.683004	5.234254	4.637671
H	-4.938544	-0.629603	-1.410535
H	-4.169704	-0.315401	-2.836093
H	1.855277	4.868146	-0.985982
H	2.208665	4.118349	-2.425829

H	0.088992	4.272103	-3.239342
H	-1.667124	4.003743	-1.436879
H	-0.386234	4.169851	-0.206664
H	3.438262	3.929459	3.400992
H	0.880248	2.714105	2.244735
H	2.032498	1.860365	3.290388
H	0.784428	-2.644440	3.384889
H	1.856412	-4.862418	3.490699
H	2.041612	-2.055541	2.277216
H	-5.609624	1.049188	2.855416
H	-3.164538	-0.635444	2.066079
H	-3.107222	0.810478	3.091897
H	-2.551414	-3.524710	-1.289242
H	-3.366699	-2.384718	-0.192311
H	-3.618785	-2.491234	-3.258277
H	1.376951	6.574576	-2.460709
H	3.363734	6.236832	3.153167
H	3.679774	-6.125951	2.958150
H	-5.833686	-2.493315	-0.536642
H	5.087843	-4.411050	-2.528328
H	3.915768	-1.699285	-0.232480
H	4.380746	-0.503067	-1.469677
H	3.678606	-2.164867	-3.259593
H	-3.062169	2.489885	1.401489
H	-0.244150	1.971188	-2.657644
H	1.894371	-0.724536	-2.649126
H	-1.450791	-1.355671	-2.661570
H	-0.702503	-3.545063	1.744123
H	3.580135	1.140235	1.626289

Table S.LIX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-}$ ($\text{NH}_2, \text{S}^-, \text{COOH}$) at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
N	-3.460856	-1.617206	4.155904
C	-3.742884	-1.084508	2.817094
C	-4.956148	-1.848778	2.250179
O	-5.728934	-2.454446	2.980106
C	-2.477967	-1.126059	1.937297
S	-2.728622	-0.216210	0.349731
N	-2.783583	-3.590241	-0.472662
C	-2.038868	-4.510702	-1.338465
C	-2.167848	-5.929407	-0.755745
O	-1.908780	-6.950514	-1.366457
C	-0.555595	-4.094355	-1.364153
S	-0.279638	-2.514512	-2.278197
Cu	-1.203392	-0.691207	-1.284362
N	-1.331141	4.047964	3.654494
C	-0.269347	3.935157	2.639890
C	-0.148889	5.239086	1.812169
O	-0.717882	6.266694	2.156130
C	-0.451394	2.651576	1.807512
S	0.985413	2.297462	0.703127
N	-1.445225	4.007824	-1.171081
C	-2.323275	3.726173	-2.310697
C	-3.606628	4.560384	-2.148614
O	-4.412671	4.762524	-3.037942
C	-2.680303	2.226847	-2.314616
S	-1.238556	1.157034	-2.738614
Cu	0.444805	1.155101	-1.199858
N	3.060302	-0.374580	4.414970
C	3.031351	-1.313764	3.276943
C	4.234926	-1.069755	2.398884
O	4.606694	0.085906	2.145767
C	1.766541	-1.134367	2.377242
S	1.572492	-2.297849	0.963707
N	4.637545	-1.531198	-0.670044
C	5.009786	-0.260744	-1.342363
C	6.392416	0.228004	-0.878293
O	7.297088	0.423297	-1.674593
C	3.903532	0.792222	-1.130133
S	2.410381	0.348570	-2.125878
Cu	1.167391	-1.188747	-1.009798
O	4.769432	-2.134068	1.842748
H	4.952147	-1.881498	0.842659
O	6.580160	0.456459	0.423677
O	0.666659	5.219520	0.761685
O	-3.768113	5.027669	-0.901413
O	-5.167760	-1.760033	0.941259

O	-2.578252	-5.930628	0.520809
H	-0.807815	4.780152	-1.344710
H	-0.854261	3.188868	-0.985515
H	-1.480757	5.050374	3.784731
H	-2.193364	3.717494	3.219970
H	3.258892	0.542609	4.012630
H	2.107014	-0.304594	4.771386
H	-3.044687	-0.886029	4.725823
H	-4.351620	-1.883572	4.570697
H	3.606354	-1.584781	-0.607869
H	4.913471	-2.322682	-1.246839
H	-2.359801	-2.656245	-0.522783
H	-3.749057	-3.474556	-0.768981
H	-2.406493	-4.547453	-2.372530
H	0.016209	-4.880202	-1.865576
H	-0.187416	-3.993728	-0.336886
H	-4.077000	-0.028549	2.835912
H	-2.179364	-2.160475	1.753129
H	-1.661948	-0.651426	2.489810
H	-0.573693	1.818941	2.505625
H	0.699783	3.846361	3.157184
H	-1.370351	2.712413	1.217159
H	3.068509	-2.345214	3.642363
H	1.750058	-0.102312	2.012478
H	0.904538	-1.265185	3.045972
H	4.270440	1.765902	-1.470693
H	3.645563	0.876212	-0.071246
H	5.116596	-0.412838	-2.420808
H	-2.736904	-4.955138	0.691643
H	-4.415953	-1.207093	0.511797
H	0.958834	4.248694	0.584479
H	5.774984	0.288520	0.997162
H	-2.923557	4.726613	-0.453237
H	-3.078770	1.952007	-1.331875
H	-3.459527	2.058231	-3.062937
H	-1.886789	3.979960	-3.285656

BS1W

N	2.593833	-3.197214	4.050435
C	1.795195	-3.612993	2.896075
C	2.716045	-4.333325	1.902091
O	3.831207	-4.724739	2.196132
C	1.074637	-2.383574	2.299983
S	-0.144042	-2.805245	0.970926
N	3.920594	-3.833254	-1.879404
C	4.430656	-2.466464	-1.685667
C	5.797054	-2.574159	-0.974817
O	6.391757	-1.633654	-0.483265
C	3.497194	-1.491132	-0.961559
S	2.022256	-1.081220	-1.999155
Cu	0.058215	-1.514390	-0.944234

N	-4.899149	-0.398740	3.668609
C	-4.452196	0.555771	2.653532
C	-5.589909	0.985149	1.699043
O	-6.743672	0.620112	1.854211
C	-3.216757	-0.013471	1.926388
S	-2.364738	1.213105	0.831934
N	-4.789988	-0.814728	-1.054891
C	-4.561894	-2.180901	-1.542330
C	-5.533366	-3.126096	-0.809006
O	-5.675371	-4.301303	-1.090920
C	-3.122837	-2.651393	-1.266148
S	-1.872439	-1.632628	-2.162074
Cu	-1.482786	0.335944	-1.060993
N	1.494265	4.595709	3.457922
C	2.143799	3.478561	2.746884
C	3.434809	4.044358	2.166851
O	3.476683	4.965767	1.371704
C	1.282495	2.864183	1.630282
S	2.088609	1.437478	0.774298
N	1.833134	4.020471	-1.629234
C	0.530956	4.527921	-2.077331
C	0.305809	5.913642	-1.439679
O	-0.627284	6.643881	-1.721637
C	-0.640870	3.614333	-1.667526
S	-0.497425	1.925042	-2.394300
Cu	0.943254	0.730929	-1.075068
O	4.543004	3.451646	2.646874
H	5.307381	3.882426	2.223358
O	1.216379	6.228806	-0.515000
O	-5.268688	1.836487	0.719613
O	-6.188810	-2.537952	0.196847
O	2.209979	-4.564216	0.682902
O	6.293734	-3.815021	-0.985947
H	-5.354775	-0.274789	-1.704064
H	-3.900562	-0.321631	-0.949453
H	-5.767311	-0.046989	4.069916
H	-5.176267	-1.258635	3.194725
H	1.237327	5.299946	2.766663
H	0.617296	4.259233	3.851784
H	1.986804	-3.109086	4.861211
H	3.267253	-3.931121	4.257863
H	1.756049	3.061876	-1.280191
H	2.509028	4.013525	-2.386619
H	3.318317	-4.105182	-1.100653
H	3.367846	-3.896491	-2.728176
H	4.658607	-2.053441	-2.677146
H	4.045130	-0.575277	-0.732361
H	3.168464	-1.929049	-0.015891
H	1.015792	-4.355973	3.146874
H	1.806240	-1.662477	1.927011
H	0.535507	-1.895738	3.117539

H	-2.515419	-0.353479	2.691734
H	-4.138730	1.475644	3.167846
H	-3.512222	-0.888121	1.341764
H	2.402300	2.708959	3.479585
H	1.061360	3.656261	0.909766
H	0.331643	2.537742	2.064204
H	-1.569760	4.077261	-2.008260
H	-0.688521	3.527163	-0.578823
H	0.496066	4.665865	-3.164063
H	5.565754	-4.338930	-1.432689
H	1.309641	-4.095919	0.590696
H	-4.263499	1.861127	0.625712
H	1.855925	5.455607	-0.538919
H	-5.872227	-1.589227	0.146345
H	-2.907909	-2.619514	-0.193834
H	-3.034915	-3.689682	-1.593826
H	-4.760069	-2.285110	-2.615688

Table S.LX. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-HCys})_2]_3^{3-}$ ($\text{NH}_2, \text{SH}, \text{COO}^-$) at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
N	-4.191511	-3.813072	-1.208269
C	-3.970132	-2.411640	-1.548920
C	-4.834600	-2.065310	-2.774073
O	-5.789239	-2.742983	-3.106193
C	-2.459149	-2.176238	-1.744880
S	-1.986991	-0.388627	-1.874709
N	3.013949	3.725351	-0.561232
C	3.046728	3.366776	-1.990200
C	3.099039	4.682956	-2.808637
O	3.067635	4.738062	-4.023618
C	1.909158	2.451297	-2.466678
S	2.085597	0.757804	-1.756533
Cu	0.201211	-0.301045	-1.359029
N	-2.699700	-4.422727	1.678790
C	-1.918695	-3.318312	2.257684
C	-1.641822	-3.583518	3.747173
O	-1.956831	-4.625231	4.295845
C	-2.629778	-1.963431	2.037033
S	-1.527970	-0.493276	2.260512
N	-3.561681	4.000196	2.544698
C	-3.761413	4.478305	1.162761
C	-5.211400	5.075233	0.903459
O	-5.559112	5.161665	-0.296028
C	-3.413443	3.386673	0.164924
S	-1.641563	2.825272	0.381219
Cu	-1.467425	0.522940	0.131162
N	4.669033	-4.082717	-1.086409
C	3.223803	-3.888503	-1.253873
C	2.814403	-3.977729	-2.744846
O	3.573430	-4.429155	-3.584670
C	2.776351	-2.610371	-0.522030
S	0.941138	-2.515412	-0.318820
N	4.908284	1.814235	0.821389
C	4.746212	1.317030	2.205919
C	6.134591	0.839672	2.827405
O	6.055616	0.234643	3.920043
C	3.708968	0.212393	2.326862
S	1.974755	0.769089	1.943307
Cu	0.313342	-0.792568	0.980180
O	1.565435	-3.630515	-3.068062
O	7.146573	1.175510	2.157041
O	-1.037675	-2.606426	4.431175
O	-5.807076	5.437332	1.951987
O	-4.532880	-0.944153	-3.441600
O	3.221229	5.757615	-2.022665

H	-4.127460	3.153213	2.639470
H	-4.096130	4.680180	3.094055
H	-2.104263	-4.952289	1.047948
H	-2.939712	-5.053585	2.443685
H	4.981150	-4.604652	-1.906407
H	5.118904	-3.171488	-1.173773
H	-3.963742	-3.972871	-0.225832
H	-5.171734	-4.027987	-1.370464
H	5.927249	1.954438	0.774635
H	4.721327	1.044559	0.176626
H	3.694725	3.162855	-0.017393
H	3.206125	5.319400	-1.105322
H	3.995939	2.854740	-2.196428
H	1.939097	2.399821	-3.557605
H	0.943934	2.883092	-2.180177
H	-4.306408	-1.701110	-0.766708
H	-2.116546	-2.694549	-2.645174
H	-1.927575	-2.620636	-0.902173
H	-3.027062	-1.960779	1.024294
H	-0.943853	-3.242346	1.755991
H	-3.477551	-1.851859	2.722154
H	2.704060	-4.733305	-0.773420
H	3.127066	-1.718342	-1.051612
H	3.237206	-2.625604	0.468282
H	3.706438	-0.146250	3.356527
H	3.945394	-0.630065	1.669483
H	4.415345	2.156006	2.835949
H	-4.060702	2.513135	0.291497
H	-3.529188	3.755842	-0.852849
H	-3.061413	5.313968	1.006549
H	1.104577	-3.237729	-2.277857
H	2.092872	3.530679	-0.174149
H	-1.697901	3.002030	1.724612
H	2.217079	1.145491	0.653697
H	-0.936895	-1.798315	3.861412
H	-3.734898	-0.505268	-3.049528
<hr/>			
BS1W			
N	0.819956	0.713176	3.893307
C	-0.610819	0.389894	3.804721
C	-1.172604	-0.214221	5.134634
O	-0.314141	-0.695287	5.924959
C	-0.765271	-0.585373	2.618895
S	-2.494979	-0.991550	2.101499
N	-3.557018	-3.281688	-0.381810
C	-2.796279	-4.510134	-0.732431
C	-3.323542	-5.744907	0.090978
O	-2.835060	-6.849914	-0.230606
C	-1.300107	-4.366954	-0.428035
S	-0.653926	-2.767335	-1.062355
Cu	-2.506028	-1.580547	-0.148344

N	0.827241	3.909258	3.568210
C	0.883391	4.275635	2.138943
C	0.262400	5.682133	1.857257
O	-0.671791	6.017396	2.636936
C	0.114641	3.167343	1.396819
S	0.102042	3.343107	-0.443658
N	-2.799617	3.243814	-2.776765
C	-3.962433	2.384996	-2.581712
C	-5.268382	3.250867	-2.392890
O	-6.345444	2.612923	-2.475341
C	-3.899672	1.454384	-1.365036
S	-2.452714	0.298507	-1.409706
Cu	-0.502003	1.371426	-1.332124
N	5.290860	0.433627	2.757515
C	4.818547	-0.841406	2.196494
C	5.808024	-1.271165	1.066227
O	5.883583	-0.443446	0.108292
C	3.412772	-0.671972	1.605337
S	2.773583	-2.239554	0.823772
N	4.150241	-1.319250	-2.443970
C	3.660700	-0.284176	-3.342879
C	4.830318	0.548335	-4.001534
O	4.449718	1.370591	-4.874995
C	2.714533	0.748393	-2.713499
S	1.124915	0.005430	-2.117239
Cu	1.307498	-1.760446	-0.768295
O	6.409259	-2.361580	1.195753
O	5.989520	0.324333	-3.583607
O	0.726609	6.318061	0.877755
O	-5.087046	4.470208	-2.145326
O	-2.421431	-0.179929	5.279525
O	-4.147910	-5.464924	1.001484
H	-1.973261	2.838745	-2.343267
H	-3.021825	4.115748	-2.292080
H	1.627727	4.328405	4.038332
H	0.012553	4.421700	3.918680
H	5.447086	1.055038	1.964013
H	4.562136	0.862335	3.327192
H	0.928170	1.729070	3.965978
H	1.125469	0.284077	4.769286
H	4.849086	-0.923582	-1.809241
H	3.384029	-1.663168	-1.866835
H	-4.286915	-3.157813	-1.080895
H	-4.066367	-3.579724	0.464205
H	-2.914778	-4.719275	-1.799465
H	-0.732618	-5.192713	-0.853210
H	-1.109378	-4.321811	0.647685
H	-1.188620	1.293562	3.575482
H	-0.312415	-1.551592	2.860925
H	-0.247520	-0.177586	1.749256
H	0.527652	2.191417	1.649635

H	1.924929	4.267804	1.801179
H	-0.941593	3.187920	1.680007
H	4.811721	-1.603114	2.983733
H	3.476934	0.043769	0.784544
H	2.661919	-0.337138	2.329151
H	2.445526	1.516776	-3.438300
H	3.156004	1.213566	-1.828046
H	3.119030	-0.756568	-4.174928
H	-3.778298	2.013360	-0.433004
H	-4.798077	0.839130	-1.306826
H	-4.124605	1.753551	-3.466977
H	2.058053	-2.698617	1.867308
H	-0.911726	-2.966480	-2.369020
H	-2.628623	-0.076755	-2.694464
H	0.732879	-0.460215	-3.320139
H	1.437643	3.389507	-0.615580
H	-2.965073	0.270361	2.105008

Table S.LXI. Computed Cartesian coordinates (in Å) of $[\text{Cu}^{\text{I}}(\underline{\text{S}}\text{-Cys})_2]_3^{6-}$ ($\text{NH}_2, \text{S}^-, \text{COO}^-$) at BS1 and BS1W levels of theory.

Atom	x	y	z
BS1			
N	4.132320	-6.074159	4.645289
C	4.942355	-6.627733	3.543706
C	5.992542	-7.635613	4.163770
O	7.122444	-7.744308	3.613917
C	5.474835	-5.498310	2.652400
S	4.057151	-4.719342	1.683678
N	6.901901	-3.624243	-1.234946
C	6.393645	-2.844890	-2.370887
C	7.367745	-3.019220	-3.614323
O	7.523333	-2.032426	-4.379672
C	6.171619	-1.395756	-1.942008
S	4.757195	-1.204383	-0.712390
Cu	4.407705	-2.929410	0.533371
N	-25.434057	0.634136	-0.487933
C	-25.209283	0.747747	1.049771
C	-26.403591	1.562347	1.770432
O	-27.073031	2.362598	0.958107
C	-23.853782	1.502554	1.402681
S	-22.277459	0.694086	0.794384
N	-1.720613	-1.061352	-3.267341
C	-1.888276	-2.478132	-2.881324
C	-3.374164	-2.951633	-3.196208
O	-3.525970	-4.176597	-3.507962
C	-1.592365	-2.736499	-1.383079
S	0.096575	-2.226509	-0.741958
Cu	0.507404	-0.156375	-1.022988
N	10.132987	7.332970	3.777423
C	10.890111	7.198654	2.504207
C	11.799710	8.481819	2.296284
O	11.316256	9.597754	2.689282
C	9.955057	6.947413	1.266155
S	8.660227	5.568657	1.392520
N	1.104457	4.026468	-3.197092
C	0.356730	3.916799	-1.883041
C	-0.122569	5.354244	-1.374146
O	-1.167527	5.384117	-0.571708
C	1.203026	3.242090	-0.733352
S	1.836913	1.542755	-1.258917
Cu	3.700835	0.646051	-0.619969
O	12.926894	8.313723	1.731975
O	0.616598	6.329186	-1.811850
O	-26.586751	1.344461	3.083839
O	-4.281944	-2.068333	-3.067796
O	5.545934	-8.317415	5.143237
O	7.854819	-4.176611	-3.746480

H	-0.954786	-0.666306	-2.697770
H	-2.600687	-0.614027	-2.968354
H	-25.960373	1.525672	-0.715463
H	-24.503462	0.716422	-0.922756
H	9.833107	8.319707	3.755031
H	9.286239	6.758316	3.613412
H	3.300318	-5.646555	4.231370
H	3.866735	-6.885447	5.201917
H	1.677896	4.886393	-3.090589
H	1.758283	3.229311	-3.271000
H	6.151351	-3.699483	-0.537437
H	7.095427	-4.551897	-1.607297
H	5.410791	-3.219722	-2.733720
H	5.930992	-0.798286	-2.821190
H	7.082192	-1.001707	-1.476705
H	4.328362	-7.269559	2.872581
H	6.221025	-5.904562	1.967235
H	5.960401	-4.743603	3.278378
H	-23.950951	2.505244	0.916087
H	-25.181287	-0.318231	1.521721
H	-23.791295	1.725290	2.529840
H	11.559556	6.324539	2.581605
H	10.607423	6.760604	0.388742
H	9.449126	7.913172	1.067718
H	0.565687	3.160382	0.192381
H	2.119897	3.839831	-0.484428
H	-0.578438	3.309642	-2.031876
H	-2.370254	-2.226148	-0.794152
H	-1.677427	-3.813494	-1.186952
H	-1.195365	-3.108662	-3.470497
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BS1W			
N	-1.302934	3.625564	4.004843
C	-0.079776	3.647815	3.164488
C	0.546795	5.071311	3.340298
O	0.868960	5.728268	2.319622
C	-0.432150	3.244085	1.728124
S	0.978877	2.474375	0.799196
N	-1.574772	4.864440	-2.161436
C	-2.846105	4.127148	-2.206161
C	-4.003079	5.030969	-1.651376
O	-5.078360	4.450845	-1.350721
C	-2.759279	2.791409	-1.466367
S	-1.596201	1.598292	-2.290895
Cu	0.353279	1.324845	-1.083812
N	4.897942	-1.338473	3.236990
C	3.929105	-2.223761	2.533131
C	4.664049	-3.362755	1.766668
O	5.567816	-2.982047	0.963505
C	3.106787	-1.336765	1.591278
S	1.711810	-2.190007	0.722224

N	5.159284	-0.888849	-1.795180
C	5.059718	0.572928	-1.856750
C	6.214404	1.243763	-1.041496
O	6.516636	2.418653	-1.384301
C	3.728352	1.168014	-1.347939
S	2.220731	0.569505	-2.255871
Cu	0.965986	-0.997057	-1.115396
N	-3.116060	-3.327530	3.769375
C	-3.406547	-2.090571	3.006607
C	-4.926642	-2.127621	2.662041
O	-5.317095	-3.182787	2.081719
C	-2.522929	-1.988536	1.749947
S	-2.691552	-0.420399	0.771723
N	-3.514277	-3.245881	-1.494647
C	-2.474596	-4.219771	-1.858105
C	-2.727840	-5.614617	-1.193341
O	-2.035268	-6.568142	-1.640723
C	-1.056430	-3.754516	-1.492086
S	-0.580127	-2.165189	-2.327214
Cu	-1.375811	-0.375305	-1.119976
O	-5.632663	-1.140568	2.991777
O	-3.576604	-5.658319	-0.257966
O	4.336744	-4.553057	2.023693
O	6.708384	0.578770	-0.088047
O	0.667273	5.437776	4.548291
O	-3.771233	6.273027	-1.612736
H	4.234501	-1.282479	-1.968777
H	5.416903	-1.137181	-0.838670
H	5.397848	-1.910422	3.920013
H	5.606909	-1.129055	2.528982
H	-3.537981	-4.074166	3.214871
H	-2.109922	-3.499944	3.751872
H	-1.536282	2.658837	4.228777
H	-1.025975	4.068771	4.880336
H	-3.973132	-3.647734	-0.674574
H	-3.065632	-2.381464	-1.186554
H	-0.986766	4.589193	-2.942871
H	-1.830415	5.845169	-2.275461
H	-3.146917	3.898204	-3.247094
H	-3.755968	2.346766	-1.432737
H	-2.422271	2.953795	-0.439027
H	0.677912	2.935307	3.540173
H	-0.791248	4.123438	1.187206
H	-1.243751	2.509881	1.753342
H	2.708299	-0.488350	2.159690
H	3.272155	-2.675385	3.285867
H	3.792099	-0.924469	0.844593
H	-3.217803	-1.224433	3.653040
H	-2.754202	-2.840834	1.105563
H	-1.472063	-2.082382	2.050946
H	-0.343079	-4.526839	-1.792070

H	-0.972851	-3.609109	-0.410940
H	-2.484047	-4.395211	-2.946188
H	3.593011	0.946975	-0.286838
H	3.774376	2.255934	-1.457129
H	5.175483	0.894523	-2.902898

Table S.LXII. Computed Cartesian coordinates (in Å) of tri-nuclear Cu(I)-cluster having as ligands six di-amidate cysteine molecules (HS-CH₂-C(H)-(C(=O)-N(H)-CH₃)-N(H)-C(=O)-CH₃), at BS1 level of theory.

Atom	x	y	z
BS1			
N	1.769015	-2.411867	3.795756
C	1.099854	-2.900913	2.599574
C	2.075328	-3.432633	1.536629
O	1.840603	-3.232295	0.336872
C	0.158618	-1.852731	1.985166
S	-1.021715	-2.645004	0.798624
N	0.667219	-4.467557	-2.548339
C	1.476864	-3.582423	-3.369718
C	2.711431	-4.447271	-3.768969
C	2.034368	-2.340762	-2.642065
S	0.808830	-0.979461	-2.372202
Cu	-1.077380	-1.722081	-1.297487
N	-3.745715	-0.253638	4.263583
C	-3.802170	0.995241	3.502913
C	-5.173638	1.193781	2.807317
O	-5.306658	2.039223	1.891038
C	-2.564026	1.092828	2.572688
S	-2.502749	2.619135	1.516443
N	-5.462317	1.736986	-1.118765
C	-5.390548	0.462452	-1.813921
C	-6.813811	-0.155356	-1.668637
C	-4.396942	-0.560909	-1.222467
S	-2.621172	-0.120572	-1.498293
Cu	-2.156304	2.012056	-0.692973
N	5.375871	1.197192	3.203426
C	5.056583	0.675461	1.884902
C	6.232547	0.754138	0.889651
O	6.008489	0.721629	-0.328903
C	3.773211	1.312853	1.305833
S	3.075662	0.177470	0.026138
N	1.993994	4.492159	-2.831220
C	1.514682	4.914443	-1.500151
C	2.723738	5.468808	-0.676091
C	0.824304	3.873110	-0.603428
S	-0.100496	2.507707	-1.430962
Cu	1.629261	0.940718	-1.568052
O	3.441627	4.692465	-0.052514
O	-7.454063	0.080232	-0.647555
O	3.126492	-5.278222	-2.967017
H	-6.239447	1.793138	-0.463101
H	-3.588001	-0.194014	5.260705
H	2.629884	-1.875293	3.726052
H	1.190616	-5.272681	-2.211354
H	0.899059	-3.281865	-4.251728

H	2.852961	-1.904492	-3.219206
H	2.383491	-2.619120	-1.644430
H	0.475176	-3.741083	2.926700
H	0.720935	-1.079377	1.461563
H	-0.439140	-1.417282	2.784130
H	-2.536638	0.217944	1.930757
H	-3.742807	1.810009	4.233955
H	4.847431	-0.388402	2.045301
H	3.948860	2.299524	0.871221
H	3.026245	1.384089	2.098017
H	0.126669	4.392884	0.056229
H	1.585575	3.384987	0.003583
H	0.800084	5.715777	-1.711830
H	-4.527199	-0.659716	-0.141863
H	-4.552280	-1.539595	-1.682466
H	-5.146415	0.644323	-2.867092
H	4.272182	0.205160	-0.641964
H	0.432957	-0.890592	-3.666842
H	-2.794517	0.165369	-2.805844
H	-0.182911	3.083927	-2.649224
H	-3.913911	2.642487	1.536349
H	-2.173029	-2.286666	1.424108
N	3.119979	-4.142989	1.994072
H	3.209437	-4.248325	2.995998
N	3.268365	-4.173402	-4.964546
H	2.772923	-3.570676	-5.606160
C	4.431906	-4.902693	-5.474238
H	4.133663	-5.629402	-6.235250
H	5.149236	-4.201570	-5.906091
H	4.892101	-5.430668	-4.640477
C	4.080078	-4.820258	1.126986
H	3.683459	-4.839655	0.112009
H	5.044277	-4.302329	1.125047
H	4.231835	-5.844890	1.473694
N	7.466010	0.813638	1.418100
H	7.551944	0.763024	2.423723
N	2.911861	6.800560	-0.763640
H	2.232798	7.363930	-1.255767
C	8.684181	0.800588	0.610167
H	8.403305	0.956397	-0.430230
H	9.354082	1.601023	0.932158
H	9.201538	-0.158676	0.703815
C	4.023144	7.494927	-0.112205
H	4.597937	8.062486	-0.848211
H	3.651222	8.177598	0.656499
H	4.663718	6.744929	0.348873
N	-6.209693	0.517331	3.288789
H	-6.035590	-0.156372	4.020326
N	-7.218042	-0.953664	-2.673027
H	-6.666380	-0.992975	-3.518516
C	-7.577240	0.703329	2.792788

H	-7.664075	0.353849	1.761387
H	-8.252774	0.135249	3.431337
H	-7.846176	1.760991	2.835611
C	-8.523405	-1.618430	-2.679706
H	-9.196913	-1.140680	-3.396478
H	-8.403283	-2.671505	-2.943247
H	-8.949911	-1.537593	-1.681194
C	1.042961	-2.337535	4.968573
O	-0.138539	-2.674902	4.997343
C	1.798279	-1.878691	6.193716
H	2.703881	-1.322731	5.945980
H	1.135277	-1.275458	6.816518
H	2.076539	-2.762499	6.778053
C	-0.636835	-4.341660	-2.272302
O	-1.285056	-3.309095	-2.582490
C	-1.305996	-5.506202	-1.590658
H	-0.632073	-6.344536	-1.407641
H	-1.731373	-5.173561	-0.640497
H	-2.131221	-5.846028	-2.223271
C	4.807407	0.630281	4.320534
O	4.082848	-0.361632	4.227876
C	5.146647	1.270159	5.645998
H	5.774307	2.159173	5.555341
H	4.221483	1.534602	6.164446
H	5.666302	0.534401	6.266470
H	5.792547	2.115502	3.283884
C	-4.660706	2.797658	-1.298142
O	-3.602317	2.725186	-1.976785
C	-5.123472	4.101417	-0.700913
H	-4.261658	4.706294	-0.414542
H	-5.673230	4.654204	-1.471072
H	-5.781713	3.960563	0.158057
C	-3.655554	-1.490237	3.669208
O	-3.724952	-1.600882	2.438189
C	-3.452120	-2.659448	4.597950
H	-2.376790	-2.822659	4.742492
H	-3.904261	-2.498293	5.580139
H	-3.882985	-3.551692	4.142276
H	2.066894	5.265598	-3.479568
C	2.702540	3.385425	-3.200266
O	2.745931	2.349147	-2.520951
C	3.425593	3.472462	-4.522252
H	3.117927	4.318599	-5.140314
H	4.498136	3.562961	-4.318734
H	3.276639	2.544058	-5.076662
H	-1.672206	1.102116	3.201983