

Article

Cu⁺/Ag⁺ Competition in Type I Copper Proteins (T1Cu)

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Table S1. Bond lengths used for justification of the chosen computational protocol. The experimental data are taken from the Cu⁺/Ag⁺ – Azurin structures, corresponding PDB Entries: 1JZG [21] and 3UGE [6].

Bond Length in Å/ Method		M ⁺ - N(His1)	M ⁺ - N(His2)	M ⁺ - S(Cys)	M ⁺ - S(Met)	M ⁺ - O(BKB)
Experiment	Cu ⁺	2.12	2.06	2.23	3.31	2.67
	Ag ⁺	2.45	2.35	2.37	3.09	2.89
	$\Delta(\text{Ag}^+ - \text{Cu}^+)$	0.33	0.29	0.14	0.22	0.22
B3LYP/6-31+G(3d,p)-D3	Cu ⁺	2.12	2.01	2.19	3.55	4.24
	Ag ⁺	2.19	2.85	2.37	3.55	4.79
	$\Delta(\text{Ag}^+ - \text{Cu}^+)$	0.07	0.84	0.18	0.00	0.55
M062X/6-31+G(d,p)	Cu ⁺	2.22	2.12	2.32	2.76	4.37
	Ag ⁺	2.57	2.31	2.48	3.09	4.44
	$\Delta(\text{Ag}^+ - \text{Cu}^+)$	0.35	0.19	0.16	0.33	0.07
M062X/6-311++(d,p)	Cu ⁺	2.23	2.12	2.33	2.79	4.38
	Ag ⁺	2.56	2.31	2.48	3.09	4.42
	$\Delta(\text{Ag}^+ - \text{Cu}^+)$	0.33	0.19	0.15	0.30	0.04