

Insight into Environmental Effects on Bonding and Redox Properties of [4Fe-4S] Clusters in Proteins

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Figure S1. The calculated hydrogen bonding of terminal and bridging ligands of $[\text{Fe}_4\text{S}_4(\text{SEt})_4]^{2-}$, $[\text{Fe}_4\text{S}_4(\text{SEt})_4]^{2-}\text{-HB(t)}$ and $[\text{Fe}_4\text{S}_4(\text{SEt})_4]^{2-}\text{-HB(b)}$.

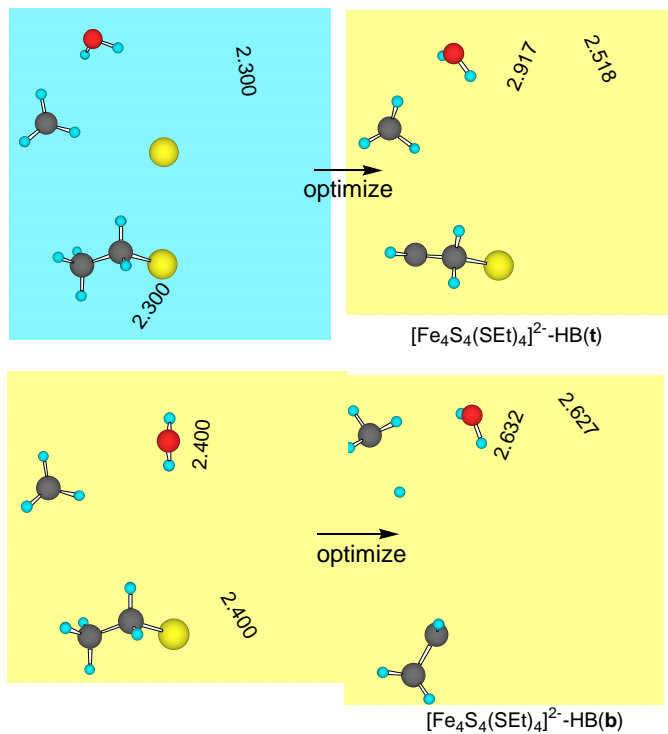


Table S1. The Conformational Parameters of the Ligands of the $[\text{Fe}_4\text{S}_4(\text{SEt})_4]^{2-}$ Analogs and Protein redox sites.

	Fe ₁ -Fe ₂ top-layer				Fe ₃ -Fe ₄ bottom-layer			
	Ligand1		Ligand2		Ligand3		Ligand4	
	χ_2	χ_3	χ_2	χ_3	χ_2	χ_3	χ_2	χ_3
$[\text{Fe}_4\text{S}_4(\text{SEt})_4]^{2-}$	87.9	50.5	87.9	49.4	87.9	49.4	87.9	50.5
SL	173.8	87.5	177.5	61.5	180.0	59.4	172.0	81.3
HB(t)	66.4	50.2	66.4	50.2	66.4	50.2	66.4	50.2
HB(b)	141.6	63.0	141.6	63.0	141.6	63.0	141.6	63.0
Fd-like	88.6	83.8	-87.6	73.9	80.5	-76.0	-87.8	66.3
HiPIP-like	81.5	-65.5	-86.4	67.7	-81.0	-153.2	-178.4	-171.9
<i>Bt</i> Fd	83.2	100.3	-68.8	66.9	64.4	-64.2	-108.8	24.0
<i>Tt</i> HiPIP	123.7	-55.9	-76.3	64.8	-66.5	-148.4	-170.8	174.2