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Histidine protonation and its influence on the electronic and vibrational properties of a "Rieske-like"iron-sulfur protein

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Iron-sulfur (Fe-S) clusters play a central role in energy transduction and electron transport. Unlike "ferredoxin-like"Fe-S clusters, Rieske centers contain a 2Fe2S cluster with one Fe coordinated by two histidines (Fe_N) and one Fe coordinated by two cysteines (Fe_S). A special feature of the Rieske centers is the pH dependence of their reduction potentials. Protonation of the N^{ε2} atoms of the two imidazole rings coordinated to the Fe-S cluster is coupled with cluster reduction (electron transfer) in the *Thermus thermophilus* Rieske protein. Here, we present a nuclear forward scattering (NFS) and nuclear inelastic scattering (NIS) study on a "Rieske-like"Fe-S protein from *Saccharomyces cerevisiae* in order to investigate the influence of protonation on the electronic structure of the Fe-S cluster and on the Fe-ligand vibrations. NIS data sets of ⁵⁷Fe enriched "Rieske-like"Fe-S protein at three different pH values (6.4, 8.5 and 10.4) reveal pH dependent vibrational bands in an area where the Fe_N-histidine modes occur. In order to explain this effect and to get a deeper understanding of the coupling of the electron transfer to the protonation state of the coordinating histidines, NIS data have been simulated by means of combined quantum chemical and molecular mechanics (QM/MM) calculations based on a model for a 2Fe2S "Rieske-like"cluster with different His-ligand protonation states.

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