Coordination chemistry in heme proteins: How the axial ligand alters the binding ability of the active site to oxygen-containing complexes

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Heme proteins, which consist of an iron ion centrally coordinated to four nitrogens in a porphyrin ring, contain an axial, amino acid ligand that can alter the function of the active site, affecting the binding of the oxygen-containing complexes. Several studies have been conducted to investigate the binding abilities of O\textsubscript{2}, CO, and NO to ferrous heme. In a theoretical study, Rydberg et. al. investigated the altering effects of His, His + Asp, Tyr, Tyr + Arg, and Cys on the active sites’ interactions with O\textsubscript{2} using iron (II, III, and IV). The geometry, spin states, and electronic structure of the active site, as well as the reaction cycles’ energies were examined. Quantum chemical calculations using the density functional method B3LYP were used to model the heme proteins’ active-site coordination chemistry. In another theoretical study by Blomberg et. al., similar density functional B3LYP calculations were used to describe the binding abilities of O\textsubscript{2}, CO and NO, as well as their geometric and electronic structures. Both studies examine the binding of these molecules in myoglobin and cytochrome. This paper will provide a brief overview of the effects of axial ligands on the binding abilities of oxygen-containing complexes to ferrous heme, with a specific focus on the electronic structure and altered spin states.

References:
