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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I. INTRODUCTION
  o Definition of a heme protein
  o The importance of heme proteins
  o Characteristics of heme proteins
  o Common ligands and substrates (examples of enzyme models)
  o Common reaction cycles
  o The apparent effects of CO and NO binding to heme
  o The role of the axial ligand
  o The motive for studying the effects of the axial ligand on oxygen-containing complexes to heme proteins

II. METHODS
  o An explanation of B3LYP
  o Description of Density Functional Theory
  o The ability of DFT to predict geometries
  o The model molecules studied
  o Conditions of the methods

III. ANALYSIS
  o Spin state results for \( \text{O}_2 \) (low spin Fe (III))
  o Open shell singlet for Fe\(^{III}\)O\(_2\)^-
  o Coordination of \( \text{O}_2 \) to Fe through overlap
  o Axial ligand role in binding of \( \text{O}_2 \) to Fe (III) (comparison of axial ligands to bond energies)
  o Coordination of NO to Fe
  o Coordination of CO to Fe
  o Binding variances for three substrates in different metalloenzymes

IV. DISCUSSION
  o Comparison of three oxygen-containing substrates in binding patterns
  o Differences in spin states
  o Differences in electron configurations
  o Differences in geometries
  o Axial ligands’ roles in binding affinity (proposed for NO and CO)
  o Example of Cu as the metal as compared to Fe and the differences in binding
  o How this research relates to other studies
    ▪ DFT investigation of Fe-N-O in heme proteins
    ▪ Spin-dependent mechanism for diatomic ligand binding to heme
    ▪ Electronic spin transition in ligand-heme protein binding (including some kinetics)
V. REFERENCES


