

Multiconfigurational effects in an iron-nitrosyl (FeNO) complex.

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Nitrosyl-containing iron complexes (FeNO) have attracted many studies focusing on the mechanisms of NO binding in heme and NO release by a photoactivated nitric oxide-releasing moiety complex. M-NO and M-CO bonds form by σ -donation to an unoccupied metal orbital and the bond is strengthened by π -back donation from a filled metal d-orbital to the unoccupied π^* orbitals on the ligand. Unlike M-CO bonds which are linear, M-NO bonds are often bent, resulting from one extra electron residing in the NO π^* . Hence fluctuations between linear and bent FeNO bonds occur and are correlated to the placement of the extra electron in either the partially occupied d-orbitals or in one of the unoccupied NO π^* ligand orbitals. The understanding of the complex bonding by means of theory and computation requires a multiconfigurational approach. In the present work, we consider fluctuations in geometric and electronic properties by the sampling structures from an ab initio molecular dynamics (AIMD) simulation. Theoretical calculations (CASSCF and NEVPT2) reveal strong correlations between sampled properties and the principle Fe-N reaction coordinate. In addition to these correlations, we find that fluctuations of electronic character occur leading to a multireference description of the oxidation state of the iron metal center.

Author: COATES, Michael (Stockholms universitet)

Co-authors: BANERJEE, Ambar (Uppsala Universitet); ODELIUS, Michael (Stockholms universitet)

Presenter: COATES, Michael (Stockholms universitet)

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