Theoretical Analysis of the Jahn-Teller Distortion and the Three-Dimensional Structure of Tetrathiolato Iron Complexes with a special attention to Rubredoxin

Ramon Tusell

This paper will discuss whether a Jahn Teller effect is the cause of the pseudo $D_{2d}$ symmetry of the cores of $[\text{Fe(SR)}_4]^2^-$ (where $R$ is an alkyl or aryl residue). Due to the fact that the $\beta$ carbons lower the symmetry of the Fe(II) the Jahn Teller effect is reduced to a pseudo Jahn Teller effect. Using Density Functional Theory it will be shown that the Jahn Teller distortion is completely quenched by the coordination environment. Additionally the using Density Functional Theory and the Angular Overlap model it will be shown that metal to ligand interactions are dominant and determine the symmetry of the $[\text{Fe(SR)}_4]^2^-$. 

References