Portland State
Chemistry

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Computational study of hydrogen gas production mechanism by nickel (II) tris-pyridinethiolate catalysts

Abstract: The research focuses on the importance of intra-molecular hydrogen bonding in the thermodynamic properties and stability of the catalytic intermediates of a well-known proton reduction catalyst, nickel (II) tris-pyridinethiolate. Density Functional Theory (DFT) calculations on the catalyst and six of its derivatives demonstrate generation of geometric isomers after the protonation of the catalyst. The isomers differ in their thermodynamic stability which can be attributed to an intra-molecular hydrogen bonding stabilization, which is well-understood in case of proteins, but fairly unexplored in small molecule catalysts.