

## The Electronic Structure of Open-Shell Tetrahedral $\{\text{Fe}(\text{NO})_2\}_9$ Dinitrosyliron Complexes

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Electronic structure of open-shell  $\{\text{Fe}(\text{NO})_2\}_9$  dinitrosyliron complexes: The electronic structure, geometry, spectroscopy of typical open-shell tetrahedral  $\{\text{Fe}(\text{NO})_2\}_9$  dinitrosyliron complexes (DNICs) are investigated using multireference methods including NEVPT2/CASSCF and SAC-CI methods. The results were compared with the experiment, and oxidation states were assigned.

Mechanistic study on the sulfur transfer reaction catalyzed by mercaptopyruvate sulfurtransferases: The reaction mechanism of sulfur transfer in human mercaptopyruvate (mp) sulfurtransferases is investigated using a two-layer methodology combining DFT of B3LYP/6-31G(d) and Amber99sb force field. The roles of the CGSGVTA loop are discussed.

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Brief career: Dr. Yu obtained Ph.D from National Tsing Hua University, TAIWAN in 2002. He spent postdoc careers at National Tsing Hua University, National Chiao Tung University, and Kyoto University. In 2007, he became assistant professor at Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, and was promoted to associate professor in 2012. Since 2014 he serves as associate professor at Institute of Bioinformatics and Systems Biology, National Chiao Tung University, Hsinchu, Taiwan. He is also a member of Director Board in Taiwan Theoretical and Computational Molecular Science Association (T2CoMSA).