Abstract Submitted
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Electronic Structure and the Magnetic Hyperfine Interactions in Heme Unit of Metmyoglobin N.B. MAHARJAN, Tribhuvan University, Nepal, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, R.H. PINK, SUNY Albany, LEE CHOW, A. SCHULTE, H.P. SAHA, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — The ^{14}N and ^{57m}Fe hyperfine interactions in the heme unit of metmyoglobin are available experimentally by electron-nuclear double resonance (ENDOR) and Mossbauer spectroscopic techniques. We have carried out electronic structure investigations on the heme system including the H_2O and proximal imidazole ligands by the first-principles Hartree-Fock procedure and studied the magnetic hyperfine and nuclear quadrupole coupling constants for the ^{57m}Fe nucleus and all the six ^{14}N nuclei on the four pyrrole and imidazole ligands as well as the ^{17}O nucleus on the H_2O ligand. Comparison will be made with available experimental data [1, 2] and earlier theoretical investigations [3] by the approximate self-consistent charge Extended Huckel procedure. Results will also be presented for the optical frequencies and intensities from transitions between ligand-like and iron d-like states and the Fe-N_ε vibrational frequency [1] G. Lang, Q. Rev. Biophys. 3, 1 (1970) [2] C.P. Scholes, R.A. Isaacson and G Feher, Biochim. Biophys. Acta 263,448(1972) [3] S.K. Mun, Jane C. Chang and T.P. Das J. Am. Chem. Soc. 101, 5562(1979)

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