Abstract Submitted
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Hartree-Fock Investigation of Electronic Structure and Associated Properties of Heme Unit in Deoxyhemoglobin S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, K. RAMANI LATA, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, R.H. PINK, SUNY Albany, A. SCHULTE, LEE CHOW, H.P. SAHA, UCF Orlando, K. NAGAMINE, UC Riverside, T.P. DAS, SUNY Albany, UCF Orlando — Using the Hartree-Fock-Roothaan procedure and the most recent version of the Gaussian set of programs we have studied the electronic structure of the heme unit including the imidazole ligand of iron from the proximal histidine using x-ray data for the positions of all the atoms except the hydrogen. The positions of the latter have been obtained through energy optimization. The results obtained from the calculated electronic structure for the magnetic and electronic quadrupole hyperfine interactions of ^{57m}Fe and ^{14}N nuclei will be discussed. Comparison will be made with available experimental data and earlier theoretical investigations [1]. Results will also be presented for the proximal Fe-N_{ε} vibrational frequency and the frequencies and intensities of optical transitions between ligand like states and d-like states of Fe [1]. K Ramani Lata PhD Thesis SUNY Albany (1993) (Unpublished)

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