Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Hartree - Fock study of the Heme Unit of deoxy-hemoglobin for Hyperfine Interactions and Vibrational Properties. T.P. DAS[1], K. RAMANI LATA, R.H. PINK, DIP N. MAHATO, SUNY Albany, ARCHANA DUBEY, H.P. SAHA, A.F. SCHULTE, LEE CHOW, UCF, Orlando, R.H. SCHEICHER, MTU, Houghton, N.B. MAHARJAN, Tribhuvan University, Nepal, N. SAHU, U.T.M.D Anderson Cancer Center, Houston — The electronic structure of the Heme Unit of deoxy- Hemoglobin has been studied by the Hartree- Fock - Roothaan procedure for understanding the hyperfine interaction properties of the ^{57m}Fe nucleus and vibrational properties associated with Fe and proximal imidazole. Results will be presented for the ^{57m}Fe nucleus, including the isomer shift in Mossbauer spectroscopy, magnetic hyperfine and nuclear quadrupole interactions and for the Fe-N_{ε} vibrational frequency. Comparisons will be made with available experimental data and possible further investigations will be discussed.

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Date submitted: 15 Dec 2006 Electronic form version 1.4