

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Unrestricted Hartree-Fock Investigation of the Electron Distribution on the Heme System in Azidohemoglobin- ^{57m}Fe and ^{14}N Hyperfine Interactions. ARCHANA DUBEY, H.P. SAHA, LEE CHOW, UCF, Orlando, R.H. SCHEICHER, MTU, Houghton, N. SAHOO, R.H. PINK, DIP N. MAHATO, M.B. HUANG, T.P. DAS*, SUNY Albany — We have a program of investigations in progress on the electronic structure of azidohemoglobin by the first-principles Unrestricted Hartree-Fock procedure to understand the substantial amount of magnetic (g-tensor), magnetic hyperfine, and nuclear quadrupole interaction, data available [1] from electron paramagnetic resonance, Mosbauer and electron-nuclear double resonance measurements. Earlier semi-empirical Self-Consistent Charge Extended Huckel investigations have provided semiquantitative results [2] with different degrees of agreement for the available properties and suggested the need for more accurate and quantitative investigations. Results of our investigations will be presented for the ^{57m}Fe and ^{14}N nuclear quadrupole and magnetic hyperfine interaction properties and compared with experimental data. *Also UCF Orlando [1] See Refs. 2-4 listed in Ref.[2]. [2] Santosh K. Mishra, J.N. Roy, K.C. Mishra and T.P. Das, Theo. Chim. Acta 75, 195(1989).

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Date submitted: 29 Nov 2005

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