Abstract Submitted
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The Electronic Investigation of Singlet and Triplet States of Oxyhemoglobin by Hartree-Fock Procedure and Associated Hyperfine Interaction. ARCHANA DUBEY, UCF Orlando, S.R. BADU, SUNY Albany, R.H. SCHEICHER, Uppsala University,Sweden, N. SAHOO, UTMD Anderson Camcer Center, Houston, R.H. PINK, SUNY Albany, A. SCHULTE, H.P. SAHA, LEE CHOW, UCF Orlando, K. NAGAMINE, UC Riverside, T.P. DAS, SUNY Albany, UCF Orlando — The observation of paramagnetic susceptibility [1] in Oxy-Hb from measurements over a broad temperature range has stimulated interest in the occurrence of a low-lying excited triplet state close to the ground singlet state of Oxy-Hb. An earlier theoretical investigation [2] has shown the existence of such a triplet state providing support to the interpretation of the susceptibility data [1]. Support for the low-lying excited triplet state has been augmented recently [3] from microscopic relaxation rate measurements for muon attached to the heme group of Oxy-Hb. We are studying by first principles Hartree-Fock procedure the energies and the electronic wave functions of the ground and triplet states and the quantitative theoretical prediction of muon magnetic hyperfine interaction in room temperature μSR measurements on Oxy-Hb. Results will be presented for hyperfine interactions of muon and other nuclei in Oxy-Hb [1] M.Cerdonio etal. Proc. Nat. Acad. Sci USA 75, 4916(1978). [2] Zalek S. Herman and Gilda H Loew JACS 102, 1815(1980).[3] K. Nagamine etal Proc. Jpn. Acad.Ser.B 83,120(2007).

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