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First-Principles Hartree-Fock Investigation of Electronic Structure and Hyperfine Properties of Deoxyhemoglobin K. RAMANI LATA, R. H. SCHEICHER (*), N. SAHOO (**), T. P. DAS (***), Dept. of Physics, SUNY at Albany, NY, S. BYAHUT, Central Dept. Of Physics, Tribhuvan University, Kathmandu, Nepal — The electronic structure of Deoxyhemoglobin is studied using the Unrestricted Hartree–Fock Cluster Procedure considering as representative the entity involving the porphyrin ring, the Fe^{2+} ion and the proximal histidine. The positions of the atoms are taken from X-ray data. The calculated electronic structure of the spin S=2 system is used to derive the magnetic hyperfine fields, nuclear quadrupole interaction parameters and the Mossbauer isomer shifts for the ^{57m}Fe. The results are in good agreement with experiment, providing support for the accuracy of the calculated isotropic and anisotropic components of the spin density and electronic charge density near the ^{57m}Fe nucleus. Results for the hyperfine properties of ^{14}N, ^{13}C, ^{1}H and ^{2}H nuclei will also be discussed. (*) Present Address: Dept. of Physics, Uppsala University, Sweden (**) Present Address: M. D. Anderson Center, Houston, Texas (***) Also: Dept. of Physics, University of Central Florida, Orlando, Florida

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