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Study of Charge and Spin Distribution Properties in Five-Liganded Helogen-Heme Systems ARCHANA DUBEY, UCF Orlando, MINAKHI PUJARI, K. RAMANI LATA, SUNY Albany, ALYSSA GARCIA, A.F. SCHULTE, UCF Orlando, S.R. BADU, R.H. PINK, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, T.P. DAS, SUNY Albany, UCF Orlando — The current emphasis in biological physics is on the study of the functions of important systems, like for instance hemoglobin and cytochromes at a quantitative level. For these studies an accurate knowledge of the electronic structures of the entire molecules as well as parts of them are very important. In the heme proteins there is great current interest in both electron transport and in attachment and detachment of O₂, CO, and NO molecules to the iron. For this purpose an in depth understanding at the electronic level of the heme units, the protein chains, and the interactions between the two, is vital. With these aims in mind, we have studied quantitatively at a first principles level the electronic structures of all four halogen five liganded heme compounds, the natures of the charge and spin distributions over them, and the associated hyperfine interactions of the nuclei of the atoms . Results and trends of these properties over the four systems and comparisons with available data will be presented and discussed.

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