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Theorectical study of FeO_2

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Abstract – Molecular oxygen (O_2) is involved in several reactions, both of biological and industrial importance, in which transition metals (TMs), especially iron, are essentials. García-Sosa and Castro (*Intern. J. of Quant. Chem*. **2000** *83(3)* 307-319.) show that the ground state (GS) for FeO_2 is a triplet (M = 3) in the C_{2v} symmetry (ReFe-O = 1.60Å and OFeO=138.1°) at GGA-B 88P86/DZP2 level. In this work, CASSCF(10,10) and MP2 calculations, using 6-31G(2d,f) basis sets, show a linear system ($D_{\infty h}$ symmetry: 1.86Å and 1.55Å, respectively). The analysis of FeO_2 illustrates that the exchange-correlation effects, level of calculation, and basis sets are important to correctly describe the structural and electronic properties.

Molecular oxygen (O_2) is involved in several reactions, both of biological and industrial importance, in which transition metals (TMs), especially iron, are essentials. It can also oxidize metal ions, and that can cause problems. Iron-containing enzymes and proteins use reduced iron, Fe(II) or Fe(I), and don't function if the iron atoms are oxidized to the stable Fe(III) form. Organisms must have means of preventing the oxidation of their iron atoms[1]. So, the knowledge of the exact nature of the iron−oxygen bond in oxy-TMs, at a molecular level, is essential for the understanding of cooperative oxygen binding to haemoglobin in biological systems[2]. García-Sosa and Castro[1] show that the ground state (GS) for FeO_2 is a triplet (M = 3) in the C_{2v} symmetry (ReFe-O = 1.60Å and OFeO=138.1°) at GGA-B88 P86/DZP2 level. In this work, CASSCF(10,10) and MP2 calculations, using 6-31G(2d,f) basis sets, show a linear system ($D_{\infty h}$ symmetry: 1.86Å and 1.55Å, respectively). The analysis of FeO_2 illustrates that the exchange-correlation effects, level of calculation, and basis sets are important to correctly describe the structural and electronic properties. All calculations in this work performed with the GAMESS computer program[3].

References

[1] García-Sosa, A. T.; Castro, M.; *Intern. J. Of. Quant. Chem.* 2000 83(3) 307-319.

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