ELECTRONIC STRUCTURE ASPECTS OF THE COMPLETE O2 TRANSFER REACTION BETWEEN NI(II) AND MN(II) COMPLEXES WITH CYCLAM LIGANDS

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Abstract

This work explores the electronic structure aspects involving the complete intermolecular O2 transfer between Ni (II) and Mn (II) complexes, both containing Ntetramethylated cyclams (TMC). The energy of the low-lying states of reactants, intermediates and products is established at the CASSCF level and also the DDCI level when possible. The orthogonal valence bond analysis of the wave functions obtained from CASSCF and DDCI calculations indicates the dominant superoxide nature of all the adducts participating in the reaction, and consequently that th whole reaction can be described as the transfer of the superoxide O2− between Ni (II) and Mn (II) complexes, without any additional change in the electronic structure of the fragments.

Keywords

Ni (II) and Mn(II); Electronic structure; CASSCF and DDCI; Electronic structure