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First Principles Electronic Structure Investigation of Order of Singlet and Triplet States of Oxyhemoglobin and 57mFe Nuclear Quadrupole Interactions

Singlet Triplet OxyHb

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Oral

Summary

Interest in the possibility of magnetic character for oxyhemoglobin (OxyHb) has been recently stimulated by the observations of muon spin-lattice relaxation effects studied [1] with the muon-spin rotation (μSR) technique. In view of this, we have carried out first-principles electronic structure investigations involving Hartree-Fock theory combined with many body perturbation effects for the singlet and triplet states of OxyHb. Our results indicate that using two recent x-ray structural data [2, 3] for OxyHb, for only Hartree-Fock theory without many-body effects included, the singlet state lies above the triplet state by energies of about 0.08 and 0.13 a.u. for the two structures in Refs [2] and [3]. Incorporation of many-body effects by the perturbation method reverses the order, with the triplet state located 0.18 and 0.14 a.u. above the singlet state for the structures in Refs [2] and [3]. Physical reasons for these relative orderings of the singlet and triplet states will be discussed.

It is clear that OxyHb by itself would be in a singlet state at room temperature or below, since from our calculation, the triplet state lies about KT above the singlet state with T having the value of 44098K and 56449K for the two structural data in Refs [2] and [3]. Our calculated Mössbaubar nuclear quadrupole frequency in the singlet state is in good agreement with the experimental results, supporting the ordering of the singlet and triplet states.

As regards the muon spin lattice relaxation effects obtained by recent μSR measurements[1] at room temperature, the sensitive dependence of the singlet-triplet separation on many-body effects in our investigation suggests that it is possible that the singlet–triplet separation could be reversed or reduced significantly when a muon is trapped near an oxygen atom of the oxygen molecule, allowing the triplet to be occupied at room temperature and lead to significant muon spin–lattice relaxation. Muon spin-lattice relaxation could also be produced by the trapping of muonium in the singlet state making the OxyHb with trapped muonium system paramagnetic.

References

[1] K. Nagamine et al. Proc. Acad.Ser.B 83, 120 (2007).

[2] Massimo Paoli et al. J.Mol. Biol. 256, 775 (1996).

[3] Sam-Yong Park et al. J.Mol. Biol. 360, 690 (2006)

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