

**Electronic structure studies of Fe<sub>2</sub>O<sub>4</sub>**Nelson Henrique Morgon<sup>a</sup> (PQ)<sup>a</sup>*Instituto de Química, Universidade Estadual de Campinas (UNICAMP) – morgon@iqm.unicamp.br*Keywords: Fe<sub>2</sub>O<sub>4</sub>, Electronic Structure, DFT, CASSCF

## INTRODUCTION

In the present work, we carry out a density functional theory (DFT) and complete active space SCF method (CASSCF) study on the electronic structure and chemical bonding in a series of molecular geometries and electronic states of Fe<sub>2</sub>O<sub>4</sub>. These calculations were performed to elucidate the geometric and electronic structures and the chemical bonding of this molecular system.

## METHODS

Theoretical calculations were performed at the DFT level using the B3LYP, PW91, and M06-L exchange-correlation functionals, and at the CASSCF(8,8) level of theory. A number of structural candidates including different spin states and initial geometries were evaluated (C<sub>1</sub>, C<sub>2</sub>, C<sub>2v</sub>, D<sub>2d</sub>, and D<sub>2h</sub> point groups and singlet and triplet electronic states). The search for the global minima (and fundamental electronic state) was carried out using the basis set adapted to the corresponding Stuttgart effective core potential for Fe atoms and the aug-cc-pVTZ basis set for oxygen atoms. The relativistic effects (mass velocity and Darwin effects), were taken into account via the quasi-relativistic pseudopotentials. The MP2 single point energies were employed to comparison among different methods. All calculations were performed using GAMESS program[1].

## RESULTS AND DISCUSSION

The results of the MP2 calculations for the all systems are reported in Table 1.

**Table 1.** Energies (a. u.) of the electronic states of the Fe<sub>2</sub>O<sub>4</sub> system at the DFT and CASSCF levels of theory<sup>(a)</sup>.

Electronic State	Method	Electronic Energy
D <sub>2h</sub> ( <sup>1</sup> A <sub>g</sub> )	M06-L	-547.5748
C <sub>2v</sub> ( <sup>1</sup> A <sub>1</sub> )	PW91	-547.5359
C <sub>2v</sub> ( <sup>3</sup> A <sub>1</sub> )	B3LYP	-547.3621
D <sub>2d</sub> ( <sup>3</sup> A <sub>1</sub> )	M06-L	-547.3589
C <sub>2</sub> ( <sup>3</sup> A)	B3LYP	-547.3573
C <sub>1</sub> ( <sup>3</sup> A)	M06-L	-547.3299
C <sub>1</sub> ( <sup>3</sup> A)	PW91	-547.3071
C <sub>2</sub> ( <sup>3</sup> A)	B3LYP	-547.1948
C <sub>2v</sub> ( <sup>1</sup> A <sub>1</sub> )	B3LYP	-547.1676
D <sub>2h</sub> ( <sup>3</sup> A <sub>g</sub> )	CASSCF	-547.0114

<sup>(a)</sup>The results of the structures having the 10 lowest energies are shown in the table.

## CONCLUSIONS

We report a systematic theoretical study of a series of molecular and electronic structures to Fe<sub>2</sub>O<sub>4</sub>. Extensive density functional theory (DFT) and complete active space SCF method (CASSCF) calculations were carried out to elucidate the geometric, electronic structures and chemical bonding in this system. In our calculations, the most stable molecular structure at these levels of theory was D<sub>2h</sub> (<sup>1</sup>A<sub>g</sub>) at M06-L level.

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<sup>1</sup> <http://www.msg.ameslab.gov/gamess/>