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The computational investigation of a
dinuclear manganese complex with
Jahn-Teller compression and elongation

MSc Thesis

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15 August 2017

Acknowledgements

I would like to express my sincere gratitude to my supervisor, Assoc. Prof. Paul Plieger, for his help, support and enthusiasm throughout this project. I would also like to acknowledge Prof. John McGrady from Oxford University for his specialist knowledge in modelling manganese complexes. I am grateful to Dist. Prof. Peter Schwerdtfeger and Mike Yap for allowing me to use the CTCP cluster for my calculations. A special thanks goes to David Nixon and Tyson Dais for their help in using Gaussian 09.

Abstract

Complexes that possess both Jahn-Teller compression and elongation effects at metal centres within the same molecule are extremely rare with only 11 examples known in the literature. Only two of these examples exist as discrete compounds. Jahn-Teller distortions influence metal-ligand bond lengths as well as the energy levels of the e_g and t_{2g} orbitals on the metal centre. The orientation of the Jahn-Teller axes have also been found to be an influential parameter in determining the exchange interactions in Mn^{III} dimers. X-ray crystallographic analysis of a di-manganese coordination compound serendipitously synthesised by Willoughby suggested that the complex possessed both Jahn-Teller compression and elongation. Willoughby's complex was synthesised in a very low yield and analysis of the crystals obtained by X-ray diffraction gave a structural determination of only moderate quality.

In this research project, the complex was computationally modelled in order to investigate the Jahn-Teller distortions and the coupling between the manganese centres. The bond lengths, molecular orbitals and spin density plot were explored in order to investigate these properties. The computational results gave strong evidence that Jahn-Teller compression and elongation were present in the di-manganese complex. The modelled ferromagnetic complex was found to be lower in energy than the modelled antiferromagnetic complex. Attempts were also made to re-synthesise the di-manganese complex in suitable quantity for complete structural and magnetic characterisation. Several different routes were trialled but after exhaustive attempts it was not possible to repeat the synthesis of the dinuclear complex.

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