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Information Package:

Introduction, Travel & Venue,
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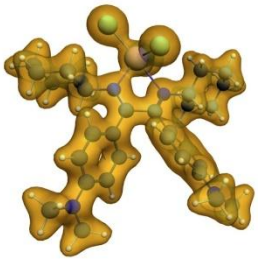

COST Action CM1305
ECOST310
Explicit Control Over Spin-states
in Technology and Biochemistry

cost
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

COMPUTATIONAL STUDY OF THE SPIN-STATE ENERGETICS IN MANGANESE PHTHALOCYANINE

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Since 3d transition metal ion complexes in different spin states usually display quite different structural, spectral and magnetic properties, and also reactivity, it is important to correctly determine the spin ground state of the system. Mn^{II} in MnPc has five d-electrons that can be distributed in a square-planar environment in three different ways: with a maximum number of unpaired electrons – the high spin state, with maximally paired electrons – the low spin state, or intermediate spin. The intermediate spin is the ground state,[1] however, different ground electronic states within this spin multiplicity are still a subject of debate in the literature.[2-6] In order to clarify these issues we performed Density Functional Theory (DFT) calculations with various Density Functional Approximations (DFAs) reliable for the spin state energetics. Moreover, lowest-lying states, ^4E_g, is the subject to the Jahn-Teller (JT) distortion.[7]

Our calculations revealed that ^4E_g is the ground state in MnPc, irrespective of level of theory employed. Intrinsic Distortion Path (IDP) model is successfully employed in the analysis of the JT distortion in MnPc.

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