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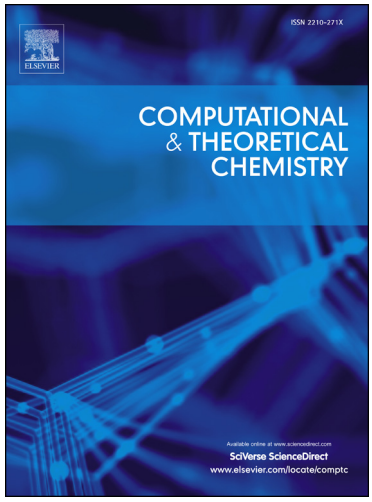

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Electronic structure of phosphorus and arsenic-bridged cyclopentadienyl-manganese(II) dimers

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Abstract

Electronic structure of recently reported phosphorus and arsenic-bridged cyclopentadienyl-manganese(II) dimers $[(\eta^5\text{-Cp})Mn\{\mu\text{-}E(SiMe_3)_2\}]_2$ (E=P,As) in the ground and five excited electronic states has been studied using density functional theory. Computational data for the gas phase species indicate that the undecaplet state is the ground state for both compounds, with the first excited (nonet) state lying by more than 80 kJ mol^{-1} higher in energy. These theoretical findings question the interpretation of the experimentally observed magnetic susceptibility - temperature dependence as reversible transition between distinct electronic states.

Keywords: manganese(II), phosphorus, arsenic, dimers, electronic structure, DFT

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