

Influence of Ag⁺ on the Magnetic Response of [2.2.2]Paracyclophane: NMR Properties of a Prototypical Organic Host for Cation Binding Based on DFT Calculations

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The complexation of metal cations into a host-guest situation is particularly well exemplified by [2.2.2]paracyclophane and AgI, which leads to a strong cation- π interaction with a specific face of the host molecule. Through this study we sought a deeper understanding of the effects the metal center has on the NMR spectroscopic properties of the prototypical organic host, generating theoretical reasons for the observed experimental results with an aim to determine the role of the cation- π interaction in a host-guest scenario. From an analysis of certain components of the induced magnetic field and the ¹³CNMR shielding tensor under its own principal axis system (PAS), the local and overall magnetic behavior can be clearly described. Interestingly, the magnetic response of such a complex exhibits a large axis-dependent behavior, which leads to an overall shielding effect for the coordinating carbon atoms and a deshielding effect for the respective uncoordinated counterparts, evidence that complements previous experimental results. This proposed approach can be useful to gain further insight into the local and overall variation of NMR shifts for host-guest pairs involving both inorganic and organic hosts. Magnetic personality: Deeper insight into the NMR spectroscopic properties of host-guest systems formed through cation- π interactions is provided by using information from experimentally determined NMR chemical shift values to guide DFT calculations. This approach can be useful for gathering further information regarding local and global variations in NMR shifts for host-guest pairs that involve both inorganic and organic hosts. © 2015 The Authors. Published by Wiley-VCH Verlag GmbH & Co. KGaA.

cation- π interactions

host-guest systems

NMR spectroscopy

shielding

silver