

Understanding the Effects of Crystal Packing on NMR Chemical Shift Tensors

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Abstract

Solid-state NMR spectroscopy is one of the most powerful techniques used for the characterization of solid samples. This method is nowadays routinely used for the study of the structure and dynamics of pharmaceutical compounds, biomolecules, polymers and nanomaterials. However, the relationship between the NMR observables and the supramolecular structure of any system is not straightforward. In this work we examine the influence of the crystal packing for three purine derivatives (hypoxanthine, theobromine, and 6-(2-methoxy)benzylaminopurine) on the principal components of the NMR chemical shift tensors (CSTs). We employ density functional calculations to obtain various molecular properties (the ground-state electron density, the magnitudes and orientations of the components of NMR chemical shift tensor, and the spatial distribution of the isotropic magnetic shielding) for the isolated molecules and for the molecules embedded in supramolecular clusters modeling the crystal environment and evaluate their differences. The concept has enabled us to rationalize the effect of the crystal packing on the NMR CSTs in terms of the redistribution of the ground-state electron density induced by intermolecular interactions in the solid state.