Experimental and Theoretical Study of weak Interactions in Simple Molecular Solids

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The aim of this work is the study of weak intermolecular interactions in molecular crystals, by both diffraction methods and *ab initio* calculations using the new version of the *CRYSTAL* [1] program, which is designed to treat infinite periodic systems. Two molecular systems were chosen: *i) formamide* [2]: each molecule is linked to three other molecules by two types of hydrogen bonds; *ii) boric acid* [3]: each molecule forms six almost equivalent hydrogen bonds with three neighbouring molecules. The *CRYSTAL03* calculations were carried out employing the HF and DFT (B3LYP) methods with the 6-31G(d,p) basis set, also using the new geometry optimisation options. The electron density, the electrostatic potential, the binding energies and the structure factors were derived. In formamide the cooperative effects of packing on the hydrogen bond interactions leading to the formation of linear chains and on those connecting the chains were analyzed. Hydrogen bonded molecules of boric acid form layers held together by weak B---O interactions, which may play a role in dictating the inter-layer packing. The comparison of the experimental and theoretical results and the most recent results obtained using the geometry optimisation facilities in *CRYSTAL03* will be presented.

[1] Saunders V.R., et al., *CRYSTAL03:* www.crystal.unito.it . [2] Stevens E.D., *Acta Cryst*., 1978, B**34**, 544. [3] Gajhede M., Larsen S., Rettrup S., *Acta Cryst*., B**42**, 545, 1986.

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