Neutron Diffraction Structure of the β-Cyclodextrin Ibuprofen Complex at 15K

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The structure of the inclusion complex of β-cyclodextrin (β-CD) with ibuprofen has been determined as part of a study of β-CD complexes with non steroidal anti-inflammatory drug molecules and similar organic compounds. Ibuprofen is a hydrophobic molecule but becomes soluble in water by complexation with β-CD. This complex forms dimers in the crystalline state. Very often β-CD complexes crystallize as dimers linked head to head by hydrogen bonds between secondary hydroxyls. These dimers form infinite two dimensional layers in a C2 unit cell. The extended crystal structure is built up by linking together the layers in different packing modes. As well as the substantial pharmaceutical interest of describing the interaction between the drug and the CD molecule in the crystalline complex, one of our goals was to investigate how the nature of the guest and the solvent molecules influences the packing mode in the crystal, how the hydrogen bonding interactions are important in the supramolecular structure, and how order-disorder phenomena observed in analogous compounds can be explained. In these studies, we have used X-ray and neutron diffraction data, as well as X-ray diffuse scattering patterns. The results of the X-ray diffuse scattering analyses will not be described here. Here we report the first neutron diffraction structure of a dimeric β-CD complex (at 15K) and the comparison with the Synchrotron X-ray structure (at 300K).

Keywords: β-cyclodextrin-ibuprofen, neutron diffraction, order-disorder