

Poster Presentation

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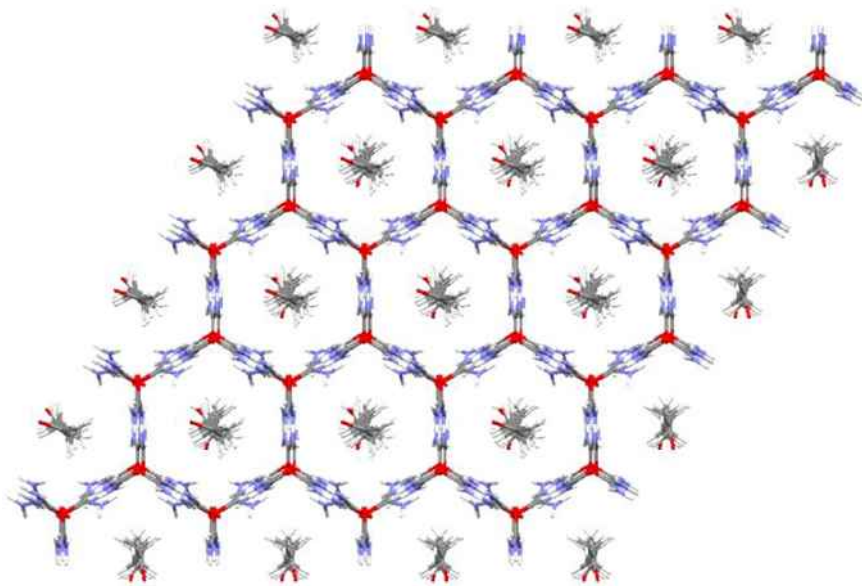
The changeable nature of urea inclusion compounds.

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Urea inclusion compounds (UICs), the β -phase of urea, have been known only since 1949 and have revealed various structural and behavioural characteristics of interest, largely influenced by the type of guest molecule present in the crystal. These structures have a hexagonally symmetrical honeycomb structure of a hydrogen-bonded urea network encapsulating the guest molecules, a defining motif of these clathrates. The simplest of this class contains an alkane guest (C7-C20), creating an incommensurate relationship between host and guest and a significantly disordered crystal structure with respect to the guest. As a result, diffuse scattering is typical in the diffraction patterns of UICs. As the guest molecules are altered, so too is the behaviour of the host network. With certain dihaloalkanes for example, the guest may coil into an atypical conformation in order to present a commensurate relationship with the host. This increase in guest order creates a distortion of the host network away from hexagonal symmetry, creating an internal stress which causes domain switching within the system. A number of different effects such as this can be seen on changing the guest molecule, ferroelasticity being an example for certain diketone guests. In this work we are exploring examples of UICs which, due to unusual interaction between the host and guest, display atypical structural features, symmetry or behaviour. These crystal structures are under investigation at a range of temperatures and pressures, by both X-ray and neutron diffraction techniques in order to fully understand the nature and bonding of UICs.

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