# Self-Compression in Urea Inclusion Compounds

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In urea inclusion compounds (UICs) linear guest molecules crystallize within a within a hexagonal honeycomb lattice of hydrogen-bonded urea molecules [1]. The majority of UICs are incommensurate crystals, with the guest repeat being defined as an irrational number of host repeats, $\gamma = c_h/c_g$ (Fig. 1).

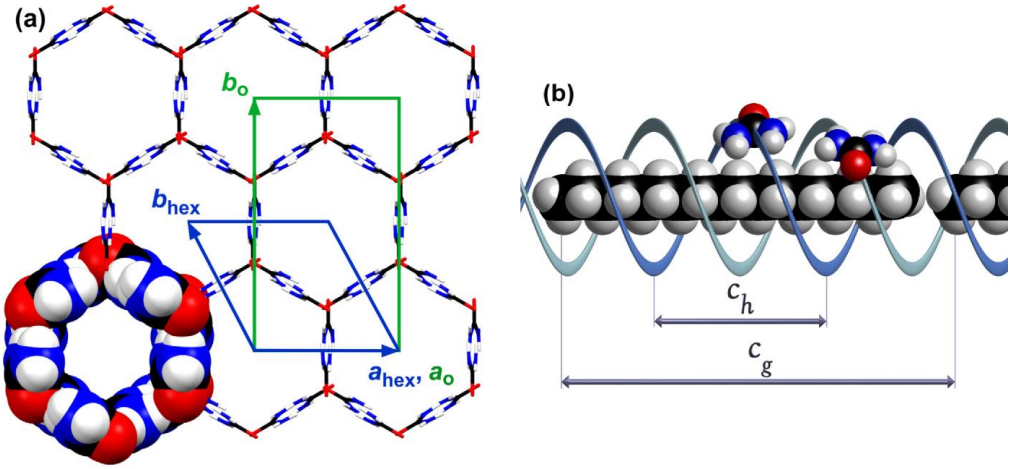


**Figure 1**. (a) Channel axis view of the host structure of a urea inclusion compound, showing the unit-cell axes for an undistorted hexagonal form (blue) and the orthorhombic form (green). An undistorted (orthohexagonal) channel will have $b_o = \sqrt{3}a_o$. (b) Schematic structure of n-octadecane/urea viewed perpendicular to the channel axis, showing the definitions of the host repeat, $c_h$, and guest repeat, $c_g$. Figures taken from [2].

A novel phase transition has been observed in several UICs in which the guest repeat length, $c_g$, increases on cooling to lock-in to a commensurate structure with the host. Because of the confinement provided by the urea host channels, nearby guest molecules are pushed further down the channel as the commensurate phase grows. It was found that instead of being forced from the ends of the crystal, these guests were increasingly compressed, leading to a self-compression mechanism. In one case, further lock-in phase transitions to different commensurate structures were observed in this compressed incommensurate phase, leading to even more compression.

Urea inclusion compounds provide a good model system for observing stress propagation in crystals, which is an important factor in many solid-state reactions. The structure of the rigid host network restricts motion to one dimension, making it easier to study. Furthermore, by changing the initial incommensurate guest repeat length it is possible to affect the amount of generated compression.

1. M. D. Hollingsworth, K. D. M. Harris, *Compr. Supramol. Chem.*, **6**, (1996), 177.

2. C. Mariette, I. Frantsuzov, B. Wang, L. Guérin, P. Rabiller, M. D. Hollingsworth, B. Toudic, *Phys. Rev. B*, **94**, (2016), 184105.