

KN17

Intermolecular interactions 'stabilising' a crystal structure – truth or wishful thinking?

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Noncovalent intermolecular interactions are often the most discussed aspect of a crystal structure, with a common statement (particularly in students' writing) being that "the crystal structure is stabilised by XYZ interactions". But are such statements warranted? When can one say with reasonable certainty that a short distance between two atoms is genuinely indicative of an attraction, and when should one be more circumspect? For instance, when can a C–H...H interaction reasonably be considered stabilising?

In this presentation we will look at the nature of various intermolecular interactions and the ways in which crystal structures can (and should) be analysed before such broad statements regarding a "stabilising" interaction can be made.

