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Crystal Structure Prediction and Polymorphism - Some Mutual Insights. Sarah (Sally) L. Price, Binal Patel, Pinky Pridhanani Jethani, Antonio Torrissi, Dept. of Chemistry, Univ. College London, 20 Gordon St., London, C1H 0AJ UK.

Computational crystal structure prediction seeks to predict the crystal structure of an organic molecule from the chemical diagram. The blind test of crystal structure prediction, organised by CCDC in spring 2004, will give an independent measure of the current state of development of such methods. However, the interpreting the results is complicated by the possible polymorphism of the test molecules.

Most methods of crystal structure prediction are based on a search for the structure that corresponds to the global minimum in the lattice energy. This generates a set of hypothetical crystal structures that are energetically feasible polymorphs, which usually includes many structures that are not observed. Several examples will be given, including imidazole, anthraquinone, uric acid and 2,6-diamino-3,5-dinitro pyrazine, which display a range of distributions of known and hypothetical low energy structures. A correlation with their crystallisation behavior will be attempted. Progress towards a reliable method of computational polymorph prediction raises many questions about the factors that determine polymorphism, whilst providing insight into the crystallisation options of specific molecules.