conference abstracts

s9'.m2.p3 **Insights into Crystal Structure Prediction using the Cambridge Structural Database and other related methods**. S.J. Borwick, D.J. Watkin, *Chemical Crystallography Laboratory, University of Oxford, 9 Parks Road, Oxford, OX1 3QS, United Kingdom*; W.D.S. Motherwell, *Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, United Kingdom.*.
Keywords: database, structure prediction, neural networks.

Significant progress has been made in the field of crystal structure prediction using computer simulation methods involving energy calculations and powder diffraction patterns[1], but there still remains the important problem that these methods often produce a selection of possible structures of very similar energy (within kT of the lowest energy polymorph), of which the observed crystal structure is only one.

Clearly the solution to the problem of successful crystal structure prediction lies not only in these calculations of intermolecular interaction energies, but also in some other factor which as yet eludes computational crystallographers.

There exists in the Cambridge Structural Database[2] a wealth of information on over 200,000 structures[3] which may provide insight into the more subtle factors at work in the crystallization process. We have begun investigating this packing information with a view to determining the reason why only one polymorph of a compound is found in nature despite energetic considerations indicating the likelihood of several.

Initial results are presented from these studies, exploring the dominant packing arrangements – independent of spacegroup – and linking these motifs with molecular properties through the use of Neural Networks as a means of pattern recognition.

s9'.m2.p4 **Crystallographic Computing Of The High Energy Material Hmxp**. B. Kempa, V. Thome, M. Herrmann, W. Engel *Fraunhofer Institut für Chemische Technologie (ICT), Joseph-von-Fraunhofer-Str. 7 D-76327 Pfinztal*
Keywords: computing, morphology, surface.

The crystal morphologies of energetic materials used in explosives and propellants depend on polymorphs and crystallization conditions. Crystallographic computing on a Silicon Graphics Octane workstation, equipped with the program Cerius 4.0 from MSI, is used to study the morphologies of HMX.

HMX ($C_4H_8N_8O_8$), a cyclic nitramine, crystallizes in four polymorphs with different morphologies[1]. The crystal structures of the HMX polymorphs were generated from the crystal data reported in literature and the morphologies were approximated in a first step by a geometric calculation after Bravais Friedel Donnay Harker[2]. In a second step the morphologies were refined with an attachment energy method, which takes inter- and intramolecular energies (Coulomb and van der Waals) of the system into account, applying the Universal Forcefield[3] and a spline function with a real space spline off distance of 8.5 Å. An Ewald summation is not recommendable for HMX, as Coulomb interactions are overestimated.

Comparing the calculated morphologies with SEM photographs of recrystallized polymorphs[1] shows a good agreement. The attachment energy and the growth rate, calculated for a series of suitable faces, indicate, that the (011) face is the predominated one in HMX. Therefore the surface of (011) was simulated separately for investigating surface chemistry and interactions with different solvents.

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