MS44-P08 | UTILISING MAXRD IN THE STUDY OF INCLUSION COMPOUNDS

Ramsnes, Stian (University of Stavanger, Stavanger, NOR); Larsen, Helge Bøvik (University of Stavanger, Stavanger, NOR); Thorkildsen, Gunnar (University of Stavanger, Stavanger, NOR); Nicholson, David Graham (Norwegian University of Science and Technology, Trondheim, NOR)

The *Mathematica* X-ray diffraction package *MaXrd* has now been expanded with the capability to compose custom crystal structures, particularly aimed at facilitating the embedment of a guest phase into a host lattice. After importing the required crystallographic information from a cif file, one can extend the asymmetric unit to a desired number of unit cells while inserting atoms, molecules or other structures in the process. The embedded phase can also be distorted and/or rotated by a specified or random amount when placed into the host. The resulting structure can be visualised in three dimensions in direct space and the information may be utilised automatically by *DISCUS* to obtain a simulated diffraction pattern. A consequence of this technique is that the space group of the guest phase becomes independent of that of the host (essentially having *P1* symmetry). This gives the means to test hypotheses on the crystal structure and simultaneously investigate reciprocal space for any implied characteristics in a relatively swift and easy manner. This functionality is used in our ongoing study of a thiourea-ferrocene clathrate, which has proven challenging with regard to its phase transitions and the five-fold symmetry of the cyclopentadienyl rings.