MS32-P05 | Insights into Weak C-H…F-C Interactions in C_6F_6:C_6H_{6-N}Men Co-crystals using Variable Temperature Crystallography to follow Molecular Dynamics

Cockcroft, Jeremy (UCL, London, GBR)

The development of modern X-ray instrumentation (new sources and detectors) combined with modern software is enabling problems to be tackled in the laboratory that were inconceivable several years ago. One can now solve structures from tiny single-crystals selected from polycrystalline sample in a matter of minutes, e.g. routinely using a "What is This?" approach in CrysAlisPro on a Supernova diffractometer. Combining this with variable temperature PXRD and DSC data has permitted structures to be solved from "single-crystals" that no "self-respecting crystallographer" would have dared touch in the past, for example, structures from broken crystals or ones with high mosaic spread as a consequence of phase transitions.

This talk will present examples of how a daring and patient approach to in-situ crystallography has enabled a detailed understanding of co-crystal adducts formed from C_6F_6 with a variety of methyl-substituted benzenes across a wide range of temperature and through several phase transitions. In terms of the parent adduct C_6F_6:C_6H_6, it enabled 25 year old powder neutron data to be analysed extensively. Earlier this year, we solved the structures of both the toluene and p-xylene adducts from SXD data despite PXRD data showing the existence of an apparently highly-destructive transition from 6-fold disorder to 2-fold disorder and then to an ordered state for the former. The talk will demonstrate how software such as CrysAlisPro and ShelXT can be used to tackle these challenging systems in order to enable a deeper understanding of these systems and their phase transitions.