

M11.0D Crystal Engineering

Chair: G.R. Desiraju

Co-Chair: R D. Rogers/M. Zaworotko

Attendance: 212



This well-attended microsymposium featured talks covering a wide range of topics. *Jerry Atwood* kicked off the proceedings with an exhilarating journey into the world of supramolecular synthesis. Using one of the 13 Archimedean solids, specifically the snub cube as a topological target, he described the synthesis of calixarene based structures. Hydrogen bonds and electrostatic interactions were used to construct and control complex nanoscale assemblies. The focus then shifted in *Ian Dance*'s presentation to the interactions themselves. Dance described the hexaphenyl and tetraphenyl embrace motifs which are co-operative C–H \cdots π based patterns, associated with at least 10 kcal/mol stabilisation. These motifs may be employed reliably in crystal engineering. Dance pointed out that inorganic and organometallic structures wherein the P(C₆H₅)₄⁺ cation (a hexaphenyl embrace precursor) is commonly used have greater diversity than organic molecular solids.

After witnessing the solar eclipse, the congregation reassembled to hear *Yasu Aoyama*'s thought-provoking talk on spontaneous resolution. Although this phenomenon is well-known, it is poorly understood. Aoyama addressed issues such as relationship of molecular structure to spontaneous resolution, theory of chirality and the possibility of employing spontaneous resolutions on a more general basis. *Bruce Foxman* followed with a summarising talk on reactive molecular crystals and drew from several examples in the early crystal engineering literature. Refreshingly, he showed that solid state topochemical synthesis can extend beyond 2+2 cycloaddition reactions and gave several examples of thermally induced reactions, rearrangements and isomerisations.

The two final short talks by *Maruisz Jaskolski* and *Matthew Davidson*, dealt with examples of weak or non-conventional C–H \cdots X hydrogen bonding. Jaskolski chose meaningful examples from the biomolecular world mentioning C–H/N–H synthon interchangeability, C–H group acidity and cooperativity in nucleoside structures. In a brief but informative overview, Davidson showed examples of hydrogen bonding to highly activated carbon bases. In his well-illustrated talk, he pointed out that synthons based on these weak interactions control supramolecular structure effectively.

All in all, the microsymposium showed how rapidly, and in how many directions this field is advancing, and how it offers tremendous scope to crystallographers and chemists alike. The chair and co-chairs emphasised the growth of this field which has now associated with it, two specialist journals — *Crystal Engineering* and *CrystEngComm*.

G.R. Desiraju