Poster Presentation

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Tuning colour in multi-component complexes: Molecular disorder as a design tool

C. Jones[1], C. Wilson[1], L. Thomas[1]

[1]*University of Bath, Department of Chemistry, Bath, UK*

The key aim of multi-component crystallisation is modification of the physicochemical properties for a specific task.[1] Tuning colour using molecular components is a relatively unexplored area, which is surprising given the possible advantages in pigment development. In crystalline materials, the optical characteristics are not solely dependent on the molecules but also on the crystal packing;[2] it follows that the optical properties could be modified using crystal engineering techniques. We have systematically investigated co-crystallising haloanilines with dinitrobenzoic acids to build an understanding of the intermolecular interactions. Molecular disorder of one or more of the components tends to lead to layered crystal structures that include stacking interactions and therefore strong colour, indicating that molecular disorder is desirable. Defects in inorganic systems are routinely exploited as a route to enhancing or introducing physical properties but similar effects in organic systems are yet to be properly exploited. We will discuss the methods by which disorder can be designed into molecular complexes, and the local ordering effects which give rise to strong diffuse scattering. Additionally we have identified a pair of thermochromic molecular complexes, 2-iodoaniline/2-bromoaniline 3,4-dinitrobenzoic acid, where disorder appears to be crucial in lending the materials their properties. Both complexes undergo a temperature-induced colour change from red to yellow corresponding to a significant molecular rearrangement. The thermochromic transition is a single-crystal to single-crystal effect; the role of molecular disorder as a facilitator for the molecular rearrangement, maintaining the crystal integrity, will be discussed. Despite the complexes being isostructural, only the bromoaniline complex shows reversible thermochromic behaviour; subtleties in the manifestation of this disorder can explain the differences in the reversibility of the transition.

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