Poster

Noncovalent interactions – an obscure aspect of the definition of isostructurality

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The attempt to fine-tune the structural properties requires mastering the supramolecular packing architecture [1-3], while isostructurality of the crystals may be preserved. The investigation of isostructurality leads to a deeper understanding of the close packing principles, the role of molecular conformation, supramolecular interactions and symmetries [4-5]. In isostructural crystals, both the placement of the molecules and the conformation of flexible molecules may adjust to the supramolecular features [6-7].

Notwithstanding*, the definition of isostructurality is not explicit about the supramolecular interactions* , whether it requires the compared structures to have identical intermolecular systems. There are crystals whose cell parameters are similar, space groups are the same, and arrangements of the molecules are analogous, the only difference is in the preference of the intermolecular interactions (Fig. 1). Can we consider them to be isostructural? The definition of isostructurality is not explicit about the symmetry restrictions, whether it requires the compared structures to have the same symmetry elements. It is a question, what the extent of differences is the limit to consider the structures being isostructural.

To fit the state-of-the-art of crystallography *the definition of isostructurality needs reconsideration* involving the aspects of symmetry, measure of similarity and formation of supramolecular interactions [8].

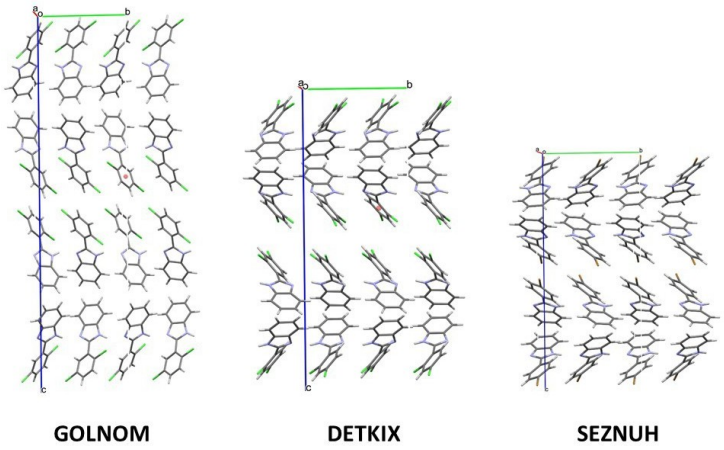

Figure 1. Are these structures isostructural? All three benzimidazole derivative compounds crystallize in the *Pbca* space group. N- H…N strong hydrogen bonds arranges the molecules into chains. In GOLNOM the X…π intermolecular interactions are decisive, in SEZNUH the X…X interactions govern the further arrangement, while in DETKIX both supramolecular interactions are responsible for close packing.

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