Poster Presentation

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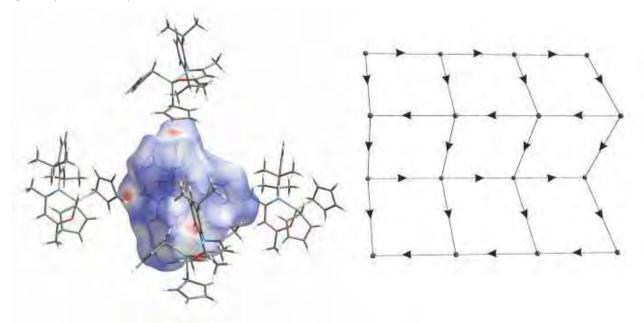
Hierarchical model of molecular crystals

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Spatial arrangement of molecules in molecular crystals depends on properties of molecules building up the crystal, and in particular on the nature of interactions occurring between them. The knowledge about primary and subsequent interactions building up the 3D structure seems to be important in many aspects, just to mention crystal engineering and crystallization processes. If the only interactions between molecules are isotropic van der Waals interactions, the observed structure will resemble a close-packing arrangement. The presence of any directional interactions leads, in accordance to Kitaigorodsky's principles,[1] to the symmetry breaking of the close-packing structure, and resulting crystal exhibits hierarchical organization. The presentation will discuss consequences of directional intermolecular interactions and their impact on generation and organization of successive levels of the hierarchical architecture in crystals. The strategy for identification, analysis and hierarchization of weak intermolecular interactions will also be presented. Selected examples will serve to illustrate usefulness of the proposed model for the discussion on molecular symmetry, supramolecular synthons' equivalency, polymorphism, isomorphism or packing.

[1] A. Kitaigorodsky, Molecular Crystals and Molecules, New-York, Academic Press, 1973.



Keywords: weak intermolecular interactions, hydrogen bonding, close-packing