Poster Presentations

[MS23-P01] A topological study of three-dimensional hydrogen-bonded frameworks.
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Crystallographic data on homomolecular organic crystals, i.e. containing molecular units of the same chemical composition and structure, but likely different in crystallographic symmetry and conformation, were selected from the Cambridge Structural Database (release 5.33) by means of the program package TOPOS [1]. Simplification of the crystal structure description (i.e. the representation of the framework as a simple graph, whose vertices and edges correspond to molecules and intermolecular H-bonds, respectively) as well as the topological classification of the resulting underlying net (that is the net of molecular centroids) have been performed with the ADS program of the TOPOS package. As a result, the distribution of topological types in the sample was built for 855 compounds containing three-dimensional H-bonded interpenetrating (42) and single (813) frameworks. The most frequent topologies of underlying nets are **dia** (diamondoid), **pcu** (primitive cubic lattice), sxd, hex (hexagonal primitive lattice) that conforms to the earlier results [2].

We have analyzed 63 homomolecular substances, which can crystallize in different polymorphic forms, and found relations between different topologies corresponding to these forms. The relations indicate that every pair of polymorphs can transform to each other either directly or through one intermediate net. Topological types of underlying nets alter in particular way in some homological series, e.g. in the series of α,ω-dioles with the transition **sql** (2D square lattice) → **dia** (3D diamondoid net): $C_4H_8(OH)_2$ (**sql**) → $C_5H_{10}(OH)_2$ (**dia**) → $C_6H_{12}(OH)_2$ (**sql**) → $C_7H_{14}(OH)_2$ (**dia**) → … → $C_{24}H_{48}(OH)_2$ (**sql**).

We have established a relation between the value of dielectric constant (ε) of the solvent, which is used to grow the crystal, and coordination number (CN) of a node of the underlying net; the higher is ε of the solvent, the smaller CN is. For instance, N,N'-diaminourea forms 8-coordinated **bcu** net or 6-coordinated **pcu** net when crystallizing from ethanol (ε=24) or water (ε=78), respectively.

[1] Blatov V. A. (2012). *Struct. Chem.* **23**, 955-963; www.topos.samsu.ru.
[2] Baburin I. A., Blatov V. A. (2007). *Acta Cryst*. **B63**, 791–802.

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