MS46-P3 DSR - Modelling Disorder with new GUIs for ShelXle and Olex2

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One of the remaining challenges in single-crystal structure refinement is the proper description of disorder in crystal structures. DSR[1] (Disordered Structure Refinement) performs semi-automatic modelling of disordered moieties using SHELXL[2]. It contains a database that includes molecular fragments and their corresponding stereochemical restraints and a fitting procedure to place these fragments on the desired position in the unit cell. The program is also suitable for speeding up model building of well-ordered crystal structures. Writing a special DSR command into the SHELXL .res file of the target structure instructs DSR on where to place and how to orient a molecular fragment from the fragment database in the unit cell (Figure 1).

Recent features to DSR such as two new Graphical user interfaces (GUIs) in ShelXle[4] and Olex2[3] as the main GUIs for SHELXL are presented. With the new GUI, the user has full control over every aspect of the model building while keeping the procedure as simple as possible. Also additional checks were added to keep restraints in the databse consistent.

The software can be downloaded at [5].

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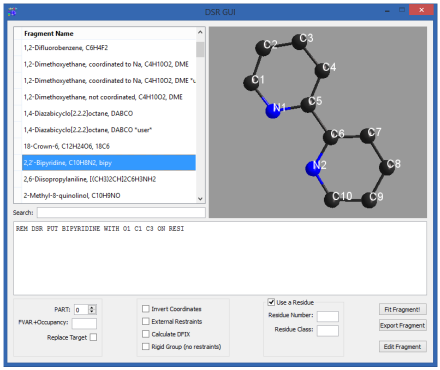

Figure 1.

Keywords: DSR, SHELXL, disorder, molecular database, computer programs, Python, C++

MS46-P4 Selection of most promising hypothetical zeolite frameworks for the synthesis of new zeolites

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Nowadays there are more than 300000 hypothetical zeolites structures in databases [1,2], whose nets are generated and optimized for energy, but only about 0.05% of them exist in nature or have been obtained in the laboratory. The aim of our work is to search for additional criteria for determination if hypothetical nets can be realized in real zeolites, and, respectively, which of them are the most likely to be synthesized.

Using the program package ToposPro [3], which implements the method of presenting zeolite framework as a packing of tiles (elementary cages) [4], we have decomposed all 230 known zeolite frameworks into tiles and found how the tiles associate to each other. A similar analysis was performed for hypothetical zeolites. According to [4], the tile packing (a way of connecting tiles without sharing atoms) features a method of the framework assembling by a polycondensation mechanism. We can expect that the most prospective hypothetical frameworks for the synthesis will be those, which have the similar method of assembling as in natural zeolites; this condition severely limits the choice. For example, the BRONZE database, which includes 274611 zeolite frameworks [1], comprises 8050 structures containing tiles of the **t-can** type (Figure 1a); 2132 of them can be built as packings of **t-can** (Fig. 1b,c). Comparative analysis allowed us to find eight hypothetical frameworks, where the arrangement of the **t-can** tiles and the way, in which they bind to each other, are the same as in real zeolites (ERI, LIO, LTL, OFF). These eight frameworks can be recommended as potential targets for synthesis.

In a similar way, we have analyzed packings of other types of tiles in hypothetical zeolite frameworks, and prepared a general list of the most prospective of them.

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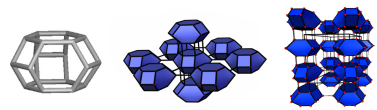

Figure 1. Tile t-can (a) local connection of t-can (b) and the ERI framework assembled as a packing of t-can (c).

Keywords: zeolites, hypothetical zeolites, tilings