MS46-O3 Topological collections and knowledge bases for applications in crystal engineering of coordination compounds

Eugeny V. Alexandrov[1], Alexander P. Shevchenko[1], Vladislav A. Blatov[1]

1. Samara Center for Theoretical Materials Science, Samara State Aerospace University named after academician S.P. Korolyev (National Research University), Moskovskoye Shosse 34, Samara 443086, Russia

email: aleksandrov_ev1@mail.ru

Using ToposPro program package[1] the complete database of metal coordination centers, ligands (more than 150 000) and topological types of coordination networks (more than 100 000) were created for more than 400 000 crystal structures of coordination compounds (0D-3D) presented in CSD.[2] A number of possible applications of the databases for investigation and design of coordination compounds were highlighted. The databases help in finding the relations between composition, structure, and properties of complexes in terms of structural descriptors. Consequently, the criteria for statistical analysis and estimation of the results reliability are provided. Further, we have outlined the concept of the knowledge based approach for prediction of new crystal structures using the relations in a complete set of descriptors for properties. It has been shown how knowledge based approach can be applied for finding correlations between coordination characteristics and topological parameters in cyanometallates[3,4] malonates, and other MOFs,[5-7] as well as for understanding the adsorption properties of MIL-53(Al).[8]

1 V.A. Blatov, A.P. Shevchenko, D. M. Proserpio, *Cryst. Growth Des*., **2014**, *14*, 3576.

2 Cambridge Structural Database. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK.

3 E.V. Alexandrov, A. P. Shevchenko, A. A. Asiri, V. A. Blatov, *CrystEngComm*. **2015**, *17*, 2913.

4 E.V. Alexandrov, A.V. Virovets, V.A. Blatov, E.V. Peresypkina, *Chem. Rev*., **2015**, *115*, 12286.

5 E.V. Alexandrov, V.A. Blatov, A. V. Kochetkov, D. M. Proserpio, *CrystEngComm*, **2011**, *13*, 3947.

6 E.V. Alexandrov, V.A. Blatov, D. M. Proserpio *Acta Cryst*., **2012**, *A68*, 484.

7 E.V. Alexandrov, V.A. Blatov, D. M. Proserpio, *J. Struct. Chem*., **2014**, *55*, 1308.

8 B.R. Saifutdinov, V.I. Isaeva, E.V. Alexandrov, L.M. Kustov, *Russ. Chem. Bull., Int. Ed*., **2015**, *64*, 1039.

MS46-O4 Harnessing the power of the Cambridge Structural Database in your own way: the CSD Python API

Andrew G.P. Maloney[1], Seth B. Wiggin[1], Paul C. Sanschagrin[2]

1. The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK
2. The Cambridge Crystallographic Data Centre, Piscataway, NJ, 08854, USA.

email: maloney@ccdc.cam.ac.uk

The Cambridge Structural Database (CSD) has been in existence for over 50 years and currently includes over 820,000 organic and organometallic crystal structures. The Cambridge Crystallographic Data Centre (CCDC) provides an extensive suite of desktop software to search, analyse, and make use of the data. However, the available methods and approaches in these tools are restricted to what CCDC has included. With the release of the CSD Python API, researchers and developers can now make use of CSD data and techniques in their own methods and approaches. This makes it possible to do analyses that were not possible, very difficult, or very tedious to do before in a much more effective way. Several examples of such analyses and approaches with real scientific impact will be presented. Examples of using the CSD Python API with other scientific Python tools will also be presented.