topcryst.com

Find topology

File: scd.cif

Date analysis: 19.06.2022

Result

Standard representation of covalent and ionic compounds:

Unknown topology [3,6-c net] SBUs: C

Coordination numbers for C3

Atom CN Sp vdW Hb Composition

C1 3 0 0 0 C3 C2 3 0 0 0 C3

C3 6 0 0 0 C6

The analysis was performed with the topcryst.com¹. The RCSR three-letter codes² were used to designate the network topologies. Those nets, that are absent in the RCSR, are designated with the TOPOS NDn nomenclature³, where N is a sequence of coordination numbers of all non-equivalent nodes of the net, D is periodicity of the net (D=M, C, L, T for 0-,1-,2-,3-periodic nets), and n is the ordinal number of the net in the set of all non-isomorphic nets with the given ND sequence. To calculate the underlying nets, we used algorithms³, the application of which for specific structures is discussed in the article⁴. The TTD collection⁵ was used to determine the topological type of the crystal structure.

References

- [1] Blatov V. A., Shevchenko A. P., Proserpio D. M. Applied topological analysis of crystal structures with the program package ToposPro, Cryst. Growth Des., 2014, 14, 3576–3586. doi: 10.1021/cg500498k
- [2] O'Keeffe M., Peskov M. A., Ramsden S. J., Yaghi O. M. The reticular chemistry structure resource (RCSR) database of, and symbols for, crystal nets. Acc. Chem. Res., 2008, 41, 1782-1789. doi: 10.1021/ar800124u
- [3] Alexandrov E. V., Blatov V. A., Kochetkov A. V., Proserpio D.M. Underlying nets in three-periodic coordination polymers: topology, taxonomy and prediction from a computer-aided analysis of the Cambridge Structural Database. CrystEngComm 2011, 13, 3947-3958. doi: 10.1039/C0CE00636J

- [4] Blatov V. A., Shevchenko A. P. Simplify to understand: how to elucidate crystal structures? Struct. Chem. 2021, doi: 10.1007/s11224-020-01724-4
- [5] Alexandrov E. V., Shevchenko A. P., Blatov V. A. Topological Databases: Why Do We Need Them for Design of Coordination Polymers? Cryst. Growth Des. 2019, 19, 2604-2614. doi: 10.1021/acs.cgd.8b01721

© topcryst.com