Find topology

File: aed.cif
Date analysis: 19.06.2022

Result

Warning: Atomic connectivity is not found. The connectivity will be calculated with default settings.

Standard representation of covalent and ionic compounds:

Unknown topology [6^3-c net] SBUs: Al, O

Standard representation of coordination compounds and valence-bonded MOFs:

ana; 4/4/c5; sqc11218; ANA SBUs: O4

Coordination numbers for Al O2

Atom	CN	Sp	vdW	Hb	Composition
Al1	6	0	0	0	O6
O1	6	0	1	0	O3Al3
O2	6	0	0	0	O3Al3

The analysis was performed with the topcryst.com[1]. The RCSR three-letter codes[2] were used to designate the network topologies. Those nets, that are absent in the RCSR, are designated with the TOPOS NDn nomenclature[3], 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 algorithms[3], the application of which for specific structures is discussed in the article[4]. The TTD collection[5] 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

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[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