Find topology

File: sed.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 [3,6-c net] SBUs: Al, O

Standard representation of coordination compounds and valence-bonded MOFs:

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

Coordination numbers for Al O

Atom	CN	Sp	vdW	Hb	Composition
Al1	6	0	0	0	O6
O1	3	0	5	0	Al3

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

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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

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