Find topology

File: bed-2.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 [3^2,8-c net] SBUs: N, Tb

Standard representation of coordination compounds and valence-bonded MOFs:

Unknown topology [3^2,8-c net] SBUs: C4N (98266), C6N, Tb

Coordination numbers for N2 C6 Tb

Atom	CN	Sp	vdW	Hb	Composition
N1	3	0	3	0	C2Tb1
C1	2	0	6	0	C1N1
C2	2	0	7	0	C1Tb1
C3	2	0	4	0	C1Tb1
C4	2	0	3	0	C1N1
C5	2	0	7	0	C1Tb1
C6	2	0	4	0	C1N1
Tb1	8	0	0	0	C6N2
N2	3	0	0	0	C3

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

[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

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