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## Find topology

File: qed.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 O Al

Atom CN Sp vdW Hb Composition

O1 3 0 6 0 Al3 Al1 6 0 0 0 06

The analysis was performed with the topcryst.com<sup>1</sup>. The RCSR three-letter codes<sup>2</sup> were used to designate the network topologies. Those nets, that are absent in the RCSR, are designated with the TOPOS NDn nomenclature<sup>3</sup>, 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<sup>3</sup>, the application of which for specific structures is discussed in the article<sup>4</sup>. The TTD collection<sup>5</sup> was used to determine the topological type of the crystal structure.

#### References

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