FOUNDATIONS
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Supporting information for article:

Hierarchical topological analysis of crystal structures: the skeletal net concept

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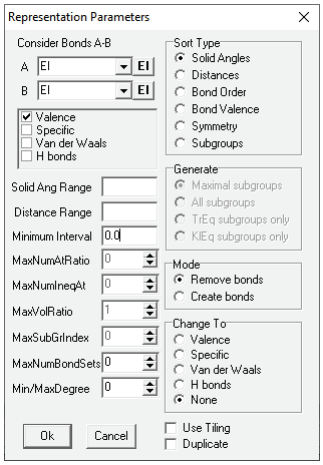
S1. Algorithm of constructing skeletal net in *ToposPro*

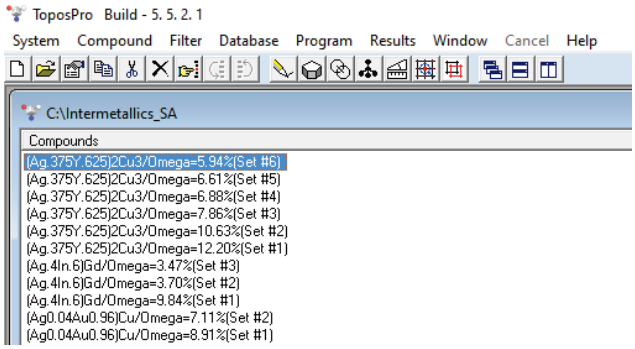
Below it is intended that the user has learnt the *ToposPro* Practical Manual 1.1.4, Modules 1, 2 and 5. All program windows are given for the *ToposPro* version 5.5.2.1.

1. Download a database with the crystal structures for which the skeletal nets should be constructed. All records should contain unique **Reference Codes**, which usually correspond to the unique keys of the records in external databases like Reference Codes of the CSD or Collection Codes of the ICSD. Compute adjacency matrices for the structures using the default set of the *AutoCN* program options.

2. Construct all representations for each crystal structure using the **Generate Representations** procedure with the parameters specified below. The specification of **Minimum Interval** = 0.0 enables to discriminate all values of solid angles without merging them into groups and to generate all possible nets for a particular structure by the subsequent removal of weak valence bonds, which are characterized by small solid angles.

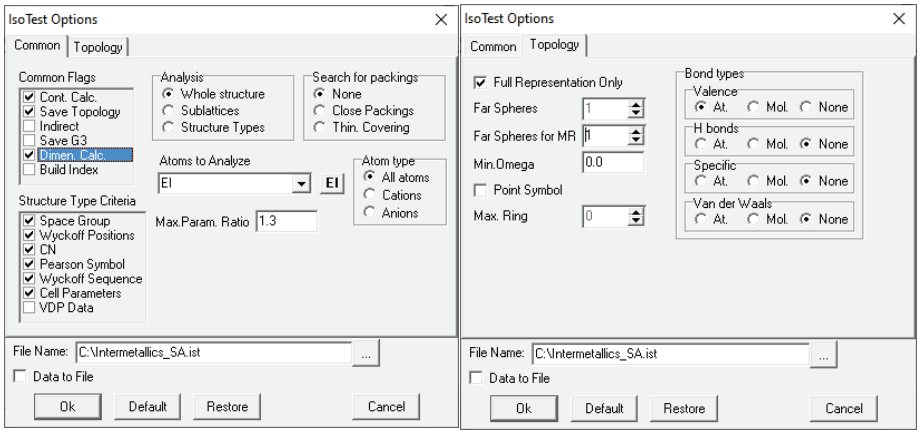


After clicking '**Ok**' create a new database which will contain all generated representation. The content of the database looks like in the example below (the database name is **Intermetallics_SA**):



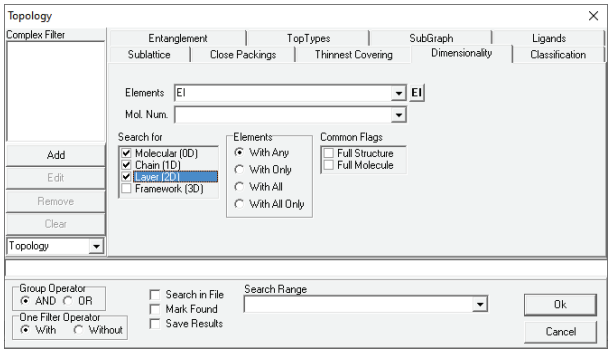
where the representations of each structure are numbered '**Set #X**' and the **Omega** value shows the minimal solid angle, which was considered as an interatomic bond in a given representation or an edge in the corresponding net. Thus, in the example above the first record corresponds to the 6th representation of the $(Ag_{0.375}Y_{0.625})Cu_3$ crystal structure where all interatomic contacts with solid angles 5.94% or higher are considered as edges of the net.

3. Select all records in the database and run the *IsoTest* program with the following set of options:



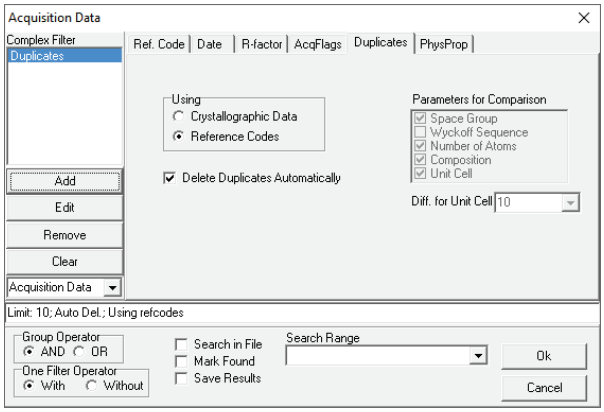
As a result, the periodicity (0D–3D) will be determined for each net in the representations.

4. Find all low-periodic (0D–2D) representations using **Filter/Topology/Dimensionality**:



and remove them from the database. After this, the database contains only three-periodic representations.

5. Remove all three-periodic representations besides the simplest representation for each structure using **Filter/Acquisition Data/Duplicates** with the following options:



As a result, only skeletal nets, *i.e.* the simplest three-periodic nets, remain in the database.