

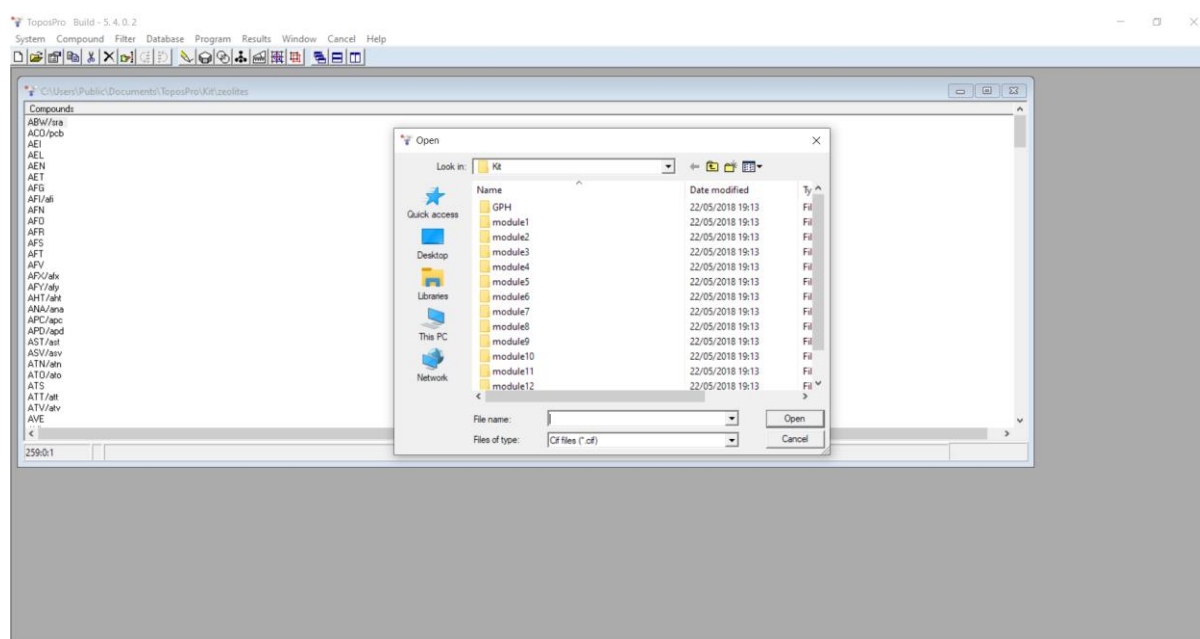
## Creating Structure Files for Tile Structures

This step-by-step guide will demonstrate how to produce a structure file for a **tile** type structure. This type of partitioning is useful for cage-based framework structures e.g. zeolites. The latter parts of the guide will discuss visualising tiles with *IsoCryst* and 3dt.

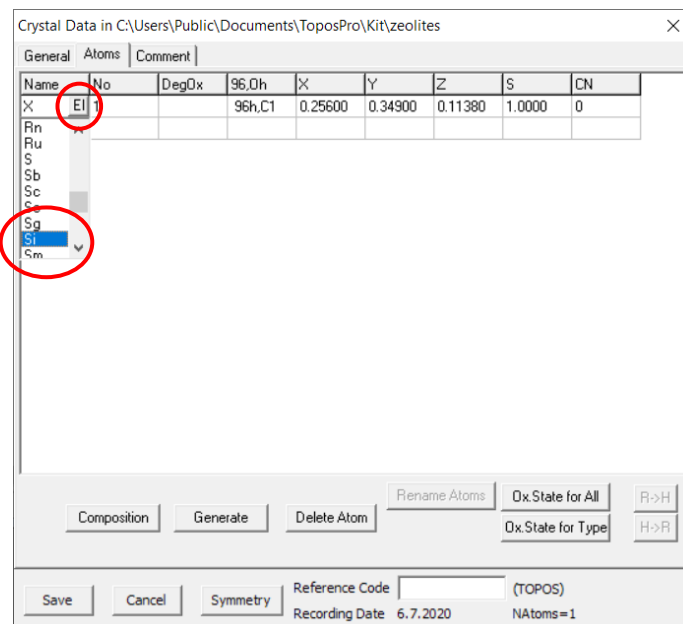
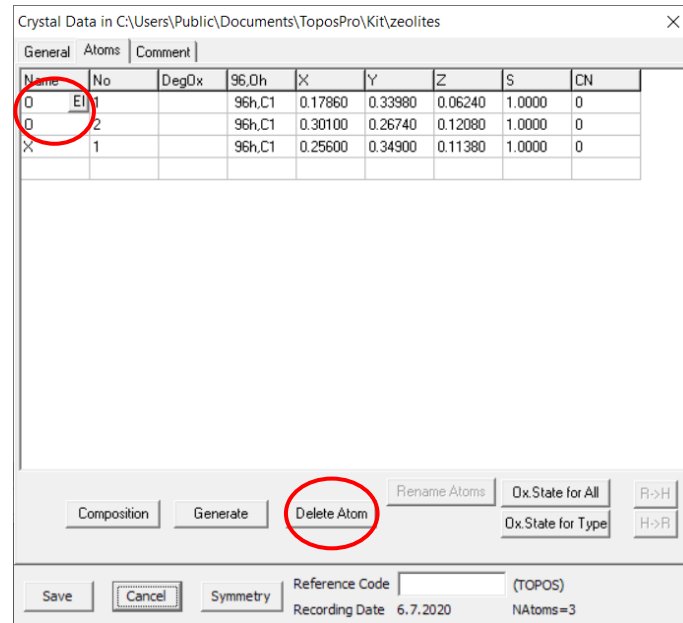
A separate procedure can be used to partition framework structures that are constructed from cages versus **net** structures. Using natural tiles – mathematically calculated units of growth that correspond to rate-determining cage formation steps – complex unit cells can be broken down into a manageable number of units for simulation. Using natural tiles allows the deconstruction of any framework material down to its composing units following regimented mathematical rules. There are some more complex cases where natural tiles may need to be split to smaller units but this again follows set rules. Examples are presented here with a focus on zeolites / zeotypes.

### Creating a Tile Structure File (Natural Tiles)

- 1.) Import a CIF for the framework structure you wish to study into an existing database in *ToposPro*. E.g. approved zeolite framework codes all have readily available CIFs on the International Zeolite Association (IZA) website: [https://europe.iza-structure.org/IZA-SC/ftc\\_table.php](https://europe.iza-structure.org/IZA-SC/ftc_table.php)

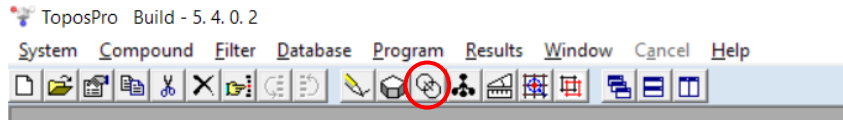


- 2.) Remove the connecting atoms between the nodes of the cage structures (e.g. bridging oxygen atoms in a zeolite framework) by double-clicking the database entry and navigating to the “Atoms” tab. Select the O atoms and press “Delete”. If required, you can set the other atoms in the structure to “Si” or “Al” (or any other element) by selecting the EI button next to each atom and selecting the required element type. *Note that the atom composition of a tile / cage e.g. Si vs. Al can be used with the “ordered” growth modification for CrystalGrower.*

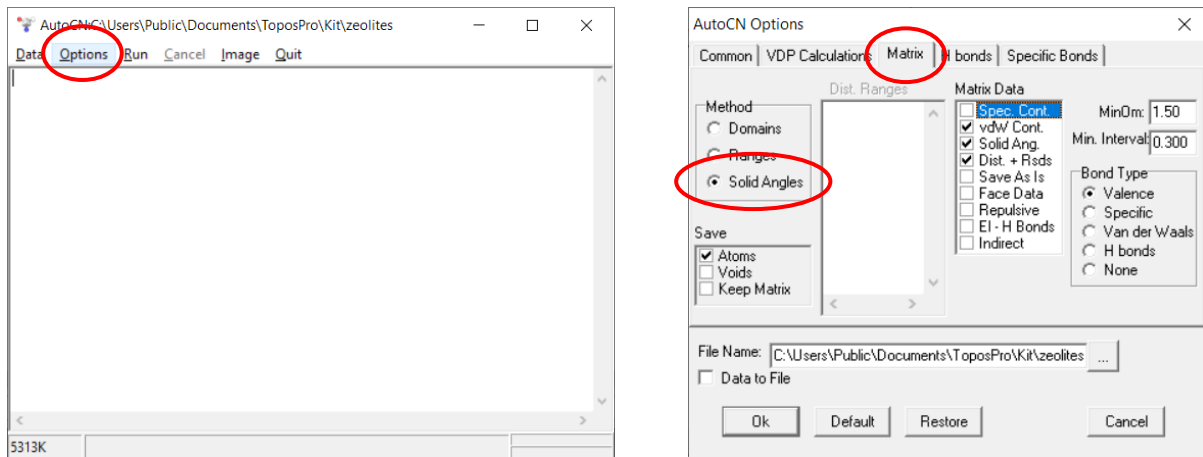


## 3.) Now the adjacency matrix will need to be calculated for the framework:

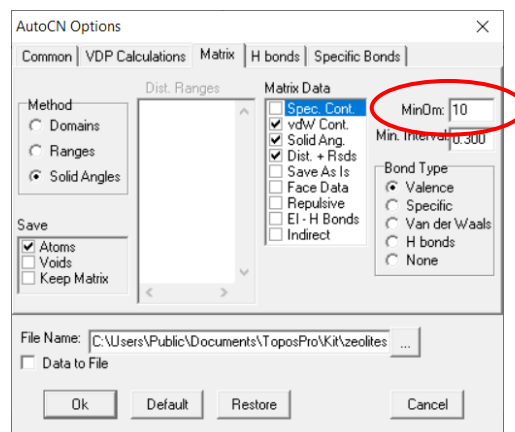
- With framework materials, we only need to consider the species bonded together directly through valence bond to assemble the tiles. Open *AutoCN* by either clicking the symbol (two overlapping circles) or pressing **CTRL + N**.



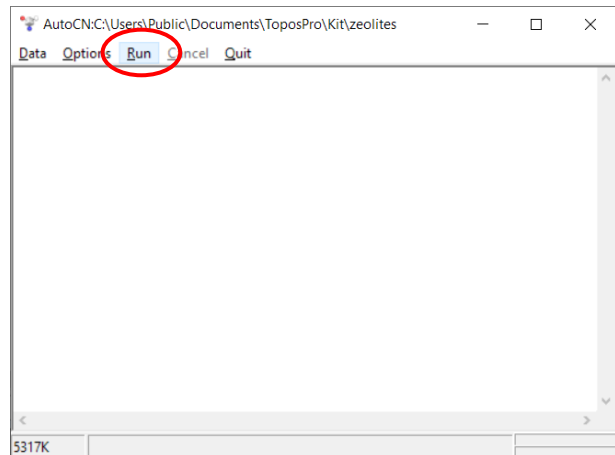
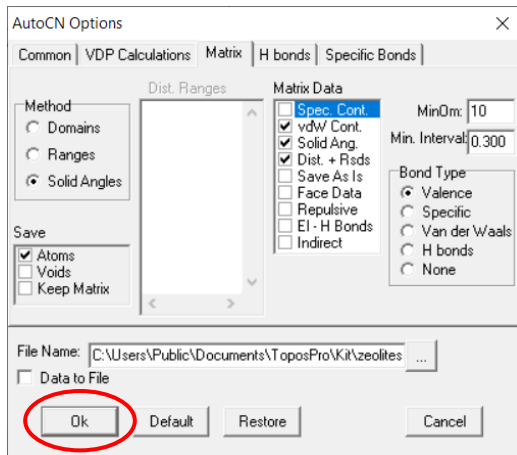
- Select "Options", navigate to the "Matrix" tab and choose the "Solid Angles" option under "Method".



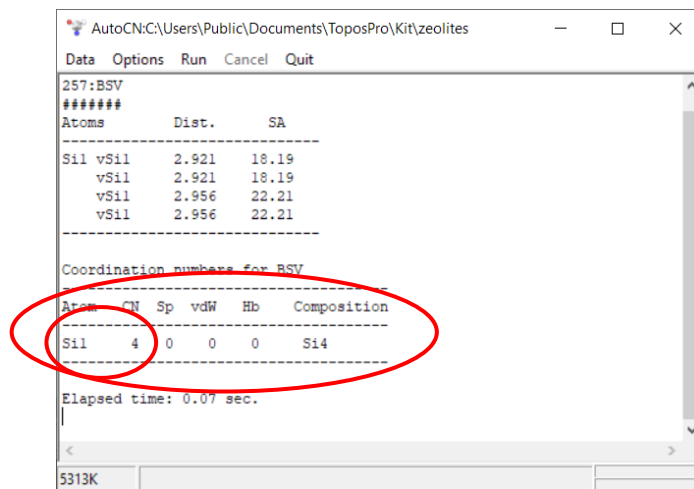
- Set a high value for minimum omega (e.g. 10 %), this will count only strong interactions when calculating the Voronoi-Dirichlet polyhedron (VDP) for each atom. This omega is the solid angle (SA), or the face contribution to the VDP – the larger the solid angle, the stronger the interaction, generally.



- Press OK, then select run.



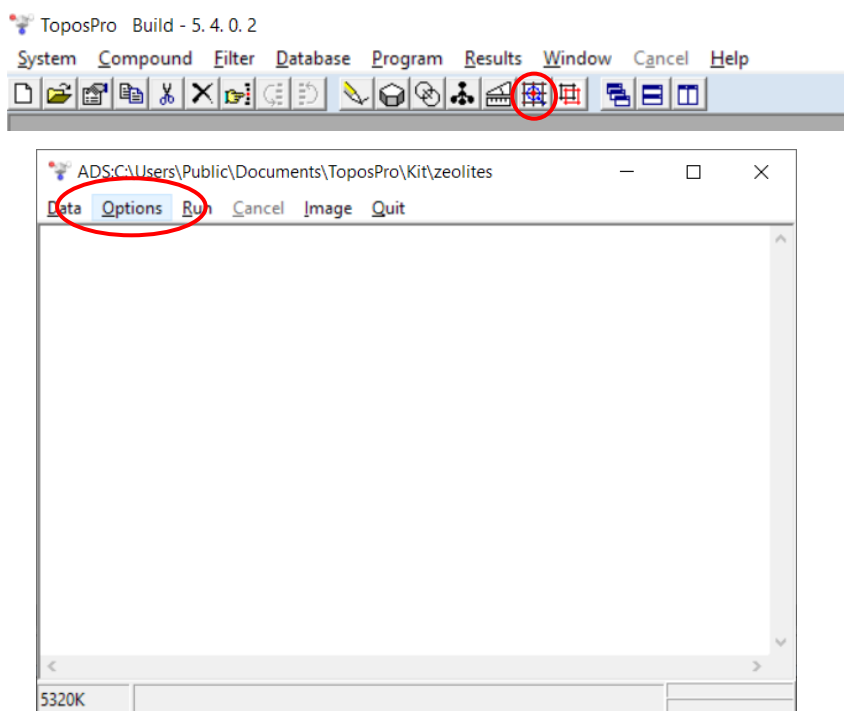
- The results window will open for verification. Check if the coordination in the system is correct, e.g. for an uninterrupted zeolite framework, the coordination for all species should be 4.



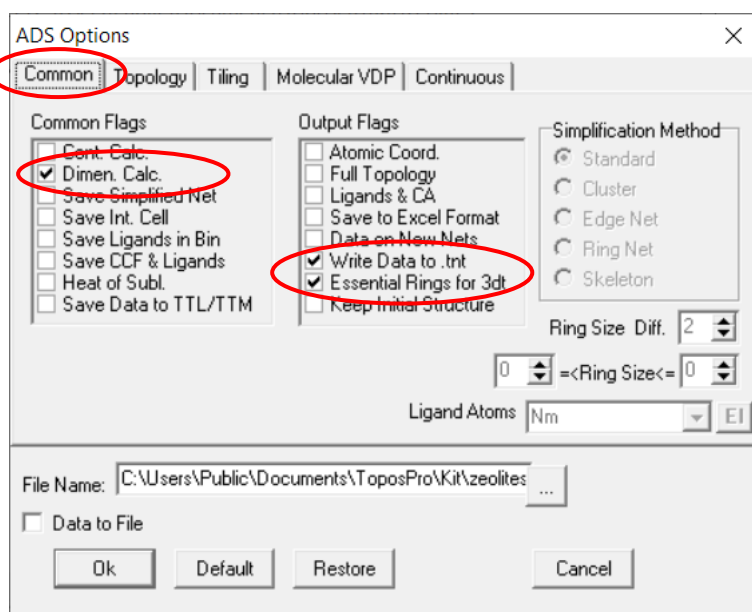
- If the coordination is overestimated (e.g. in an interrupted zeolite framework, where some species should have a lower coordination than 4) then increase the minimum omega until the correct result is obtained (i.e. some framework atoms with a coordination of 3 or 2, dependent on the structure).

4.) Now the natural tiling will be calculated for the connected framework:

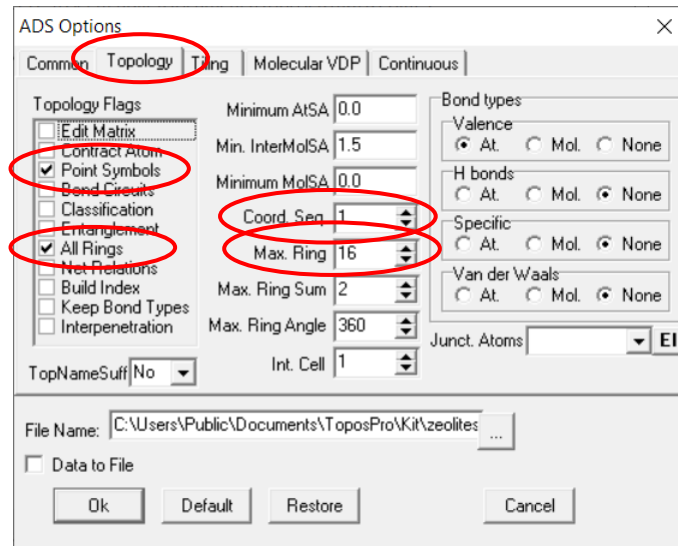
- Select the ADS module (the symbol displaying a net) and click “Options”.



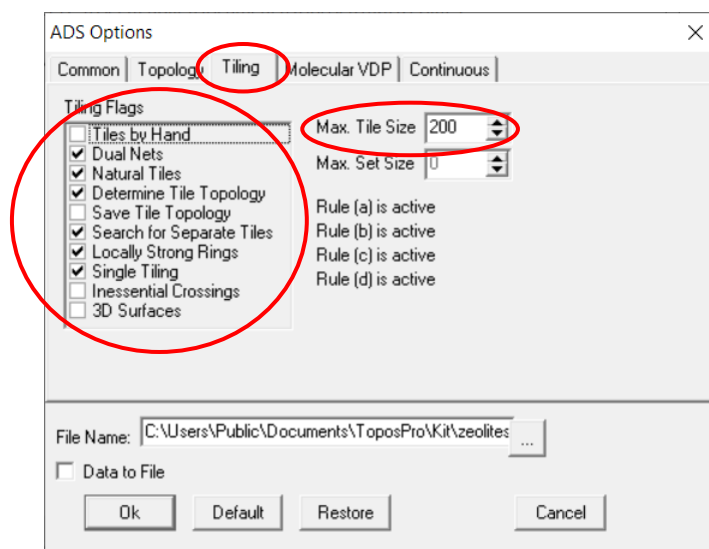
- On the “Common” tab, ensure that “Dimen. Calc”, “Write Data to .tnt” and “Essential Rings for 3dt” are selected. (The latter option is for visualising the tile structures with 3dt allowing the production of high quality raytraced images for reports and presentations).



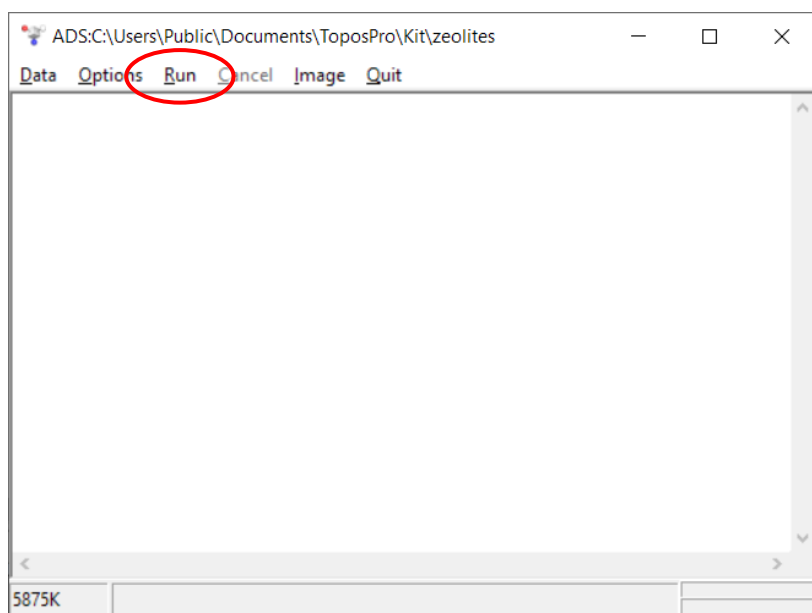
- Navigate to the “Topology” tab and ensure that “Point Symbols” and “All Rings” are enabled. Set “Coord. Seq.” to 1 (this will search for only nearest neighbours) and set “Max Ring” to the same size or larger than the biggest ring in the framework (most zeolites have 12 rings or below, 16 will capture most structures).



- Navigate to the “Tiling” tab and ensure that “Dual Nets”, “Natural Tiles”, “Determine Tile Topology”, “Search for Separate Tiles”, “Locally Strong Rings” and “Single Tiling” are selected. These options will ensure the natural tiling is calculated. Set “Max. Tile Size” to a relatively large number to capture large tiles but not so large that it slows down the calculation (100 is a good estimate, but some tiles are larger than this – 200 will catch these). Press OK.

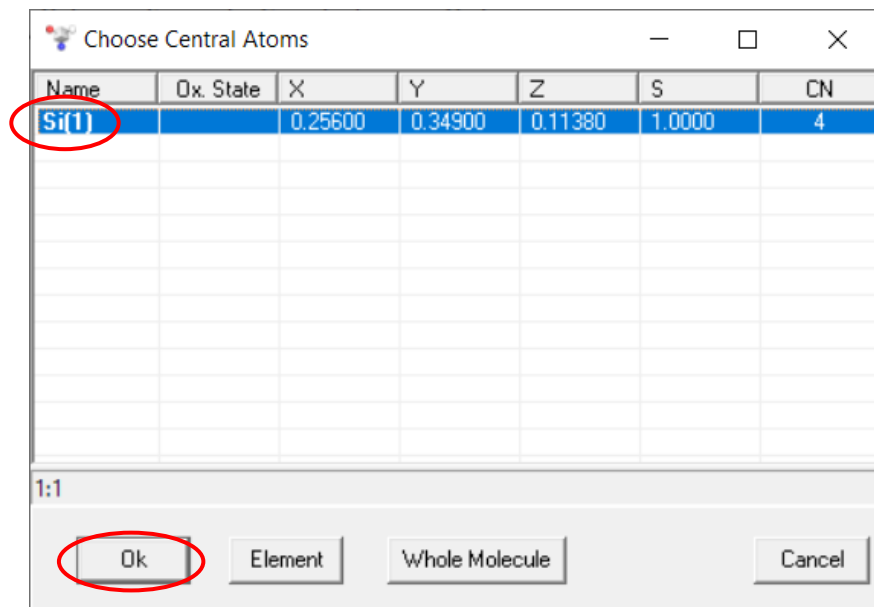
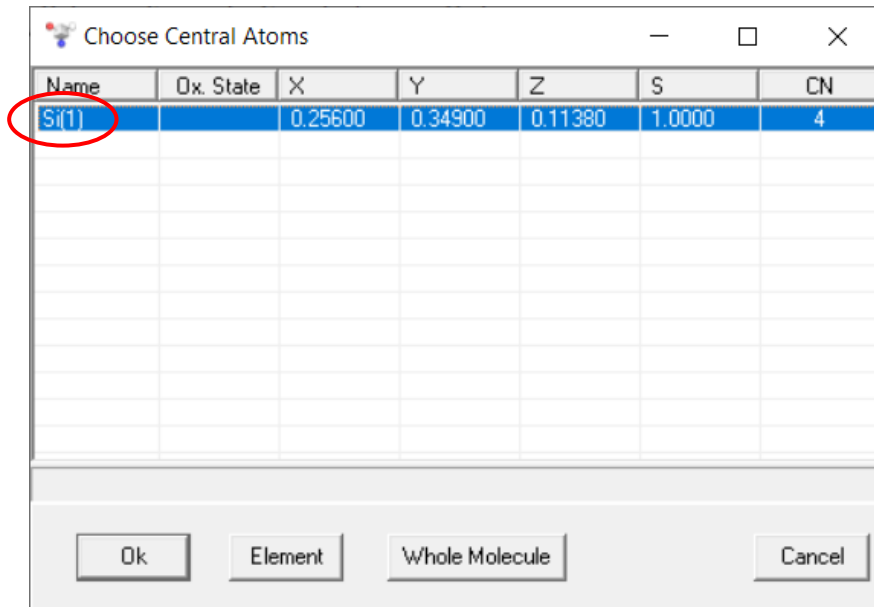


- Press run on the *ADS* window.



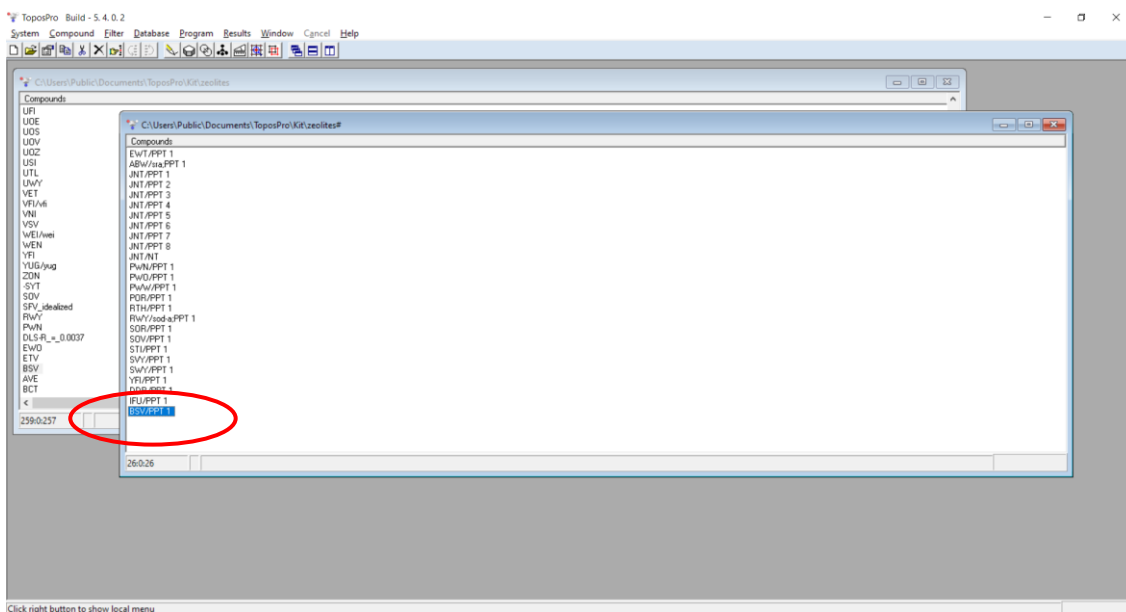
- A window will open asking to create a child database if one hasn't been created already. The naming convention for the child database created for a tiling is: `Original_Database_Name#` to differentiate from databases containing simplified nets. Select "Yes" to create a new database and type in your user code **1**.

- A window will then open to assign the central atoms for the net to be calculated for the natural tiling. Select the atoms that define the tile vertices of the system E.g. Si or Al by right clicking and pressing "Select" or use the Ins (Insert) key on the keyboard. Selected atoms will appear in bold. Then press OK.

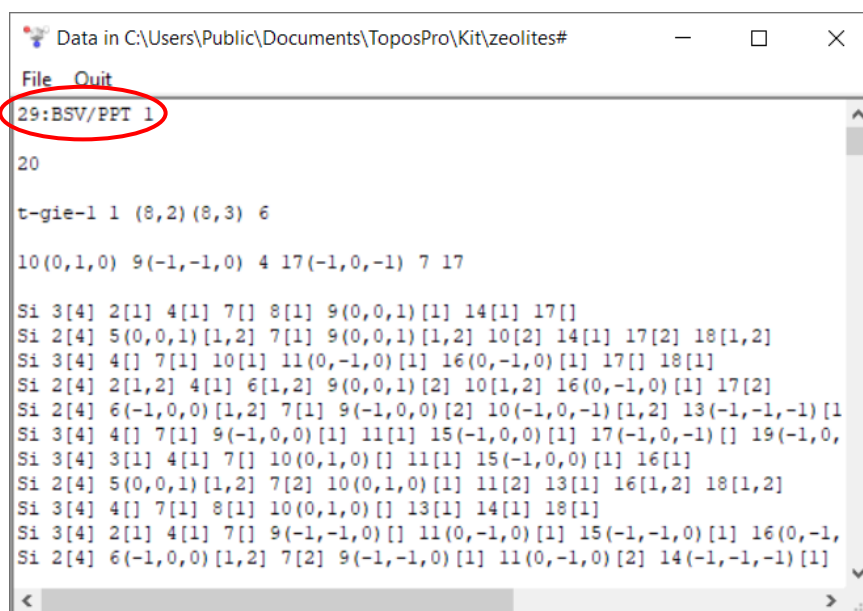




- The tiling will be calculated and the child database will be opened. If the tiling calculation fails for any reason, an error message will be displayed in the ADS calculation window. *Note that the "Program" tab in the toolbar can always be used to get back to a running module in ToposPro e.g. IsoCryst, AutoCN or ADS. Calculation results will remain as hidden open windows until they are specifically closed or the program is exited.*



- 5.) To obtain the structure file for this crystal structure: right click the newly created entry or press **F9** on the keyboard. Occasionally multiple tilings are generated, but PPT (Primitive Proper Tiling) 1 should be the natural tiling.



- Read through the structure file to check if the tiling has been calculated correctly (e.g. check the tile names are correct and not called Tile No. - this means a tile in the structure doesn't already exist in the *ToposPro* tile database). If possible (for known zeolites), verify the tiles in the structure file against the tiling shown on the IZA website for each framework code. *Note that this can be found by selecting a framework code on the IZA, then clicking PDF and selecting "Tiling".*

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern PDF

Home Codes Framework

Framework Type BOF

Framework

Cell Parameters: orthorhombic P n m a (# 62)  
 a = 7.5032 Å b = 12.7726 Å c = 13.7063 Å  
 α = 90.000° β = 90.000° γ = 90.000°  
 Volume = 1313.6 Å<sup>3</sup>  
 R<sub>OLS</sub> = 0.0012

Framework density (FD<sub>g</sub>): 18.3 T/1000 Å<sup>3</sup>  
 Topological density: TD<sub>g</sub> = 880

Ring sizes (# T-atoms): 10 6 5 4  
 Channel dimensionality: Topological (pore opening > 6-ring). 1-dimensional

Maximum diameter of a sphere:  
 that can be included: 5.58 Å  
 that can diffuse along: a: 4.67 Å b: 1.77 Å c: 1.77 Å

Accessible volume: 9.06 %  
 Composite Building Units:

Natural Tiling: t-bof t-kah t-mel

Year code assigned: 2008  
 Data last updated: Mar 26, 2014

BOF Pnma  $\{6^4\} + 14\{4.5^2.6^2\} + \{4^3.5^2.6^2.10^2\}$  3 7 8 3

TILES

Face symbol:  $\{6^4\}$   $\{4.5^2.6^2\}$   $\{4^3.5^2.6^2.10^2\}$

V, E, F: (8, 9, 3) (10, 13, 5) (22, 30, 10)

Symmetry: .m. .m. .m.

Wyckoff: 4c 4c 4c

Label: t-kah t-mel t-bof\*

TILING

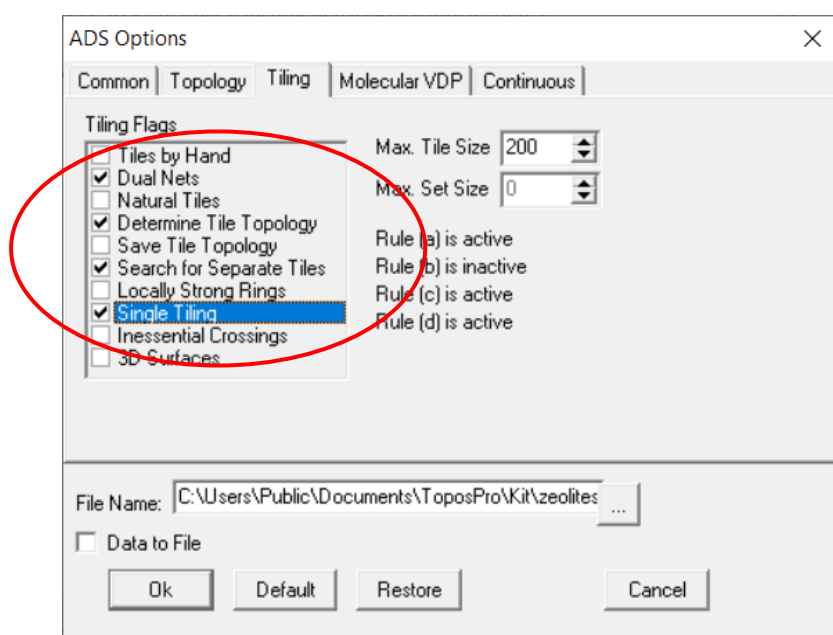
- Click File and Save As to save the structure file as a .txt which can be used with *CrystalGrower*.
- The format of the structure file for a **tile** structure is discussed in another section of the manual in detail.

- A database of the most common / industrially important zeolites is provided for free with *CrystalGrower*. There is also a full database of all currently approved zeolite structure codes (252 codes as of July 2020) which can be purchased from <https://crystalgrower.org/>.

### Creating a Modified Tile Structure File

Some structures require the calculation of a modified natural tiling. A modified natural tiling involves overruling rule b for natural tiling (i.e. all tile faces must be strong rings). There are set occasions where this can occur, namely when cages are joined together through weak ring “waists” with negative curvature. This results in large cages being split into two or more smaller cages. Some zeolite examples are DDR, LTN and UFI (although there are other examples). This should only be used if it chemically makes sense to separate large tiles into smaller tiles, or if the tiles are creating too large of an energy barrier to get any growth in *CrystalGrower*.

- The approach remains the same for the majority of the calculation, however, changes must be made to the “Topology” tab in the *ADS Options* window.
- “Natural Tiles” and “Locally Strong Rings” must be disabled to calculate a modified natural tiling, this will deactivate rule b.

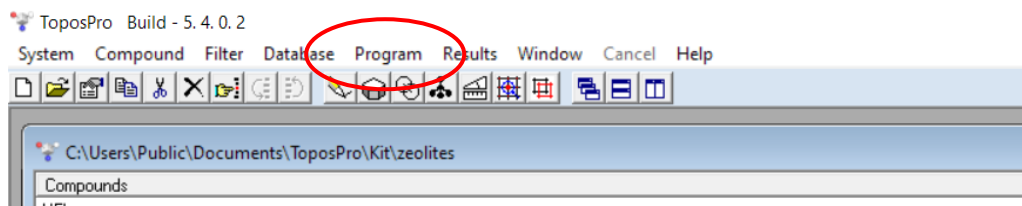


- The “Max. Ring Size” in the “Topology” tab should be reduced to try and get as close as possible to the largest ring size in the framework. This can be verified against the IZA tiling calculation if it is an approved zeolite framework.
- If this approach doesn’t work correctly, the “Tiles by Hand” option can be selected, where all rings can be defined manually as tile faces.

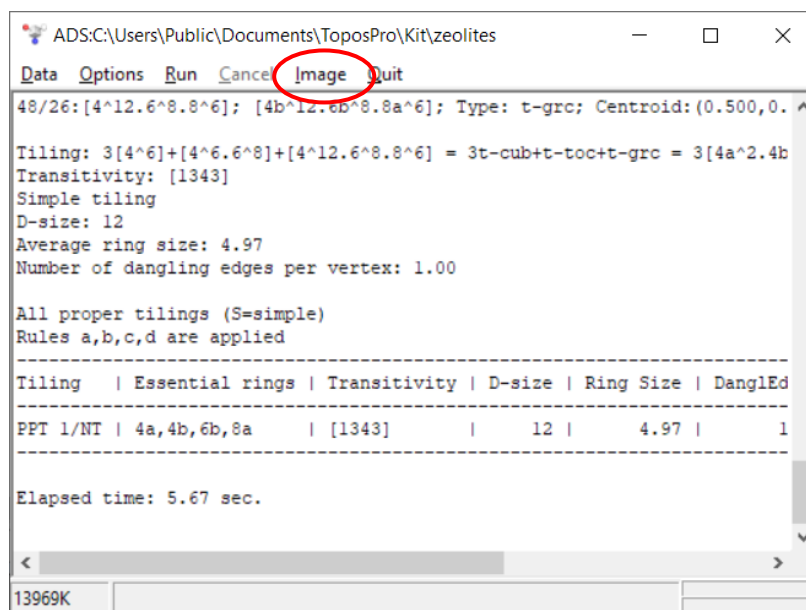
**Visualising Tiles with *IsoCryst***

Once a tiling has been calculated, the *ADS* results window can be used to show the structures of the individual tiles which assemble the crystal structure as long as the “Write Data to .tnt” was selected when calculating the tiling with *ADS*.

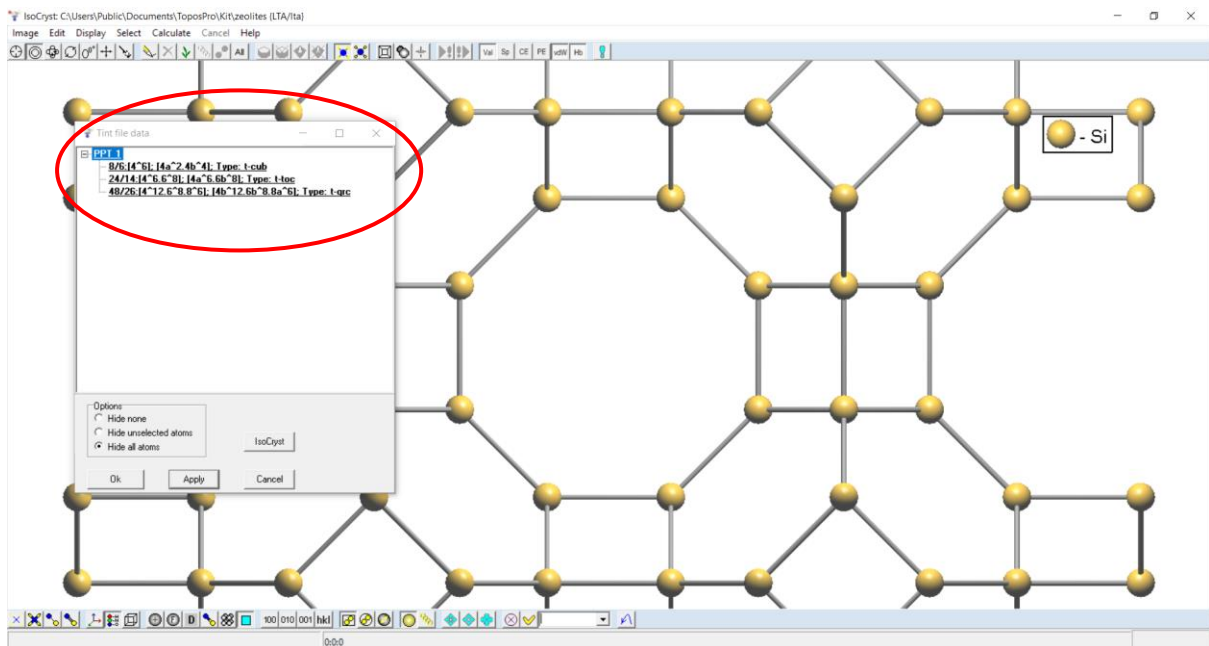
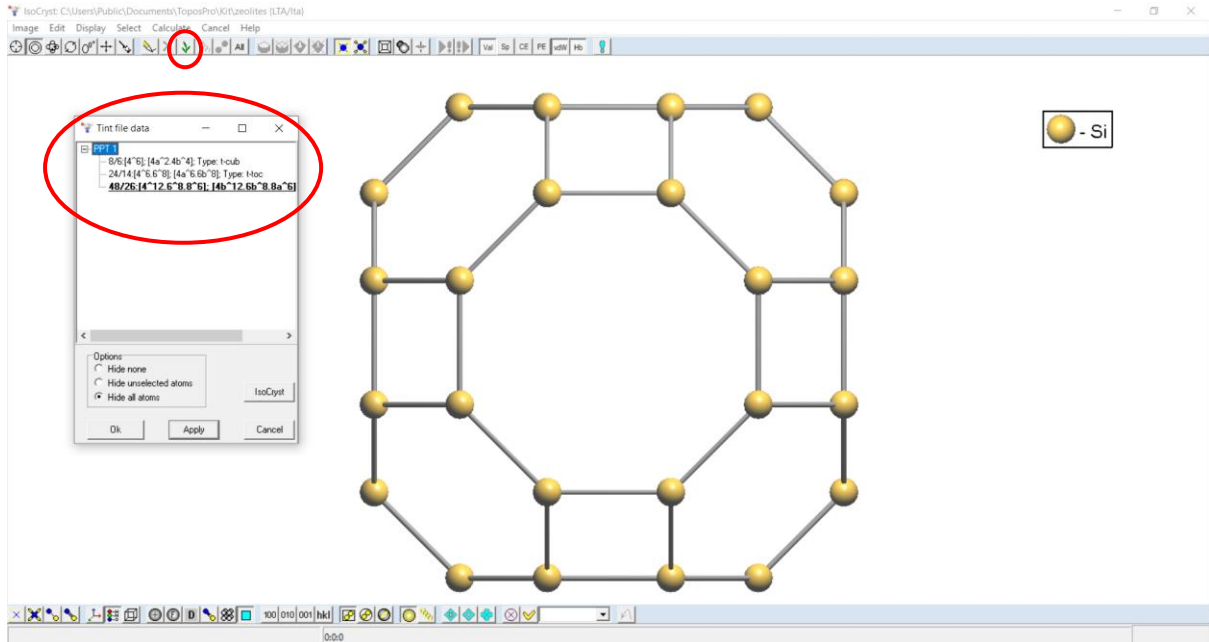
- 1.) Click Program in the main *ToposPro* toolbar and select the results window for *ADS* which was created when running the tiling calculation.



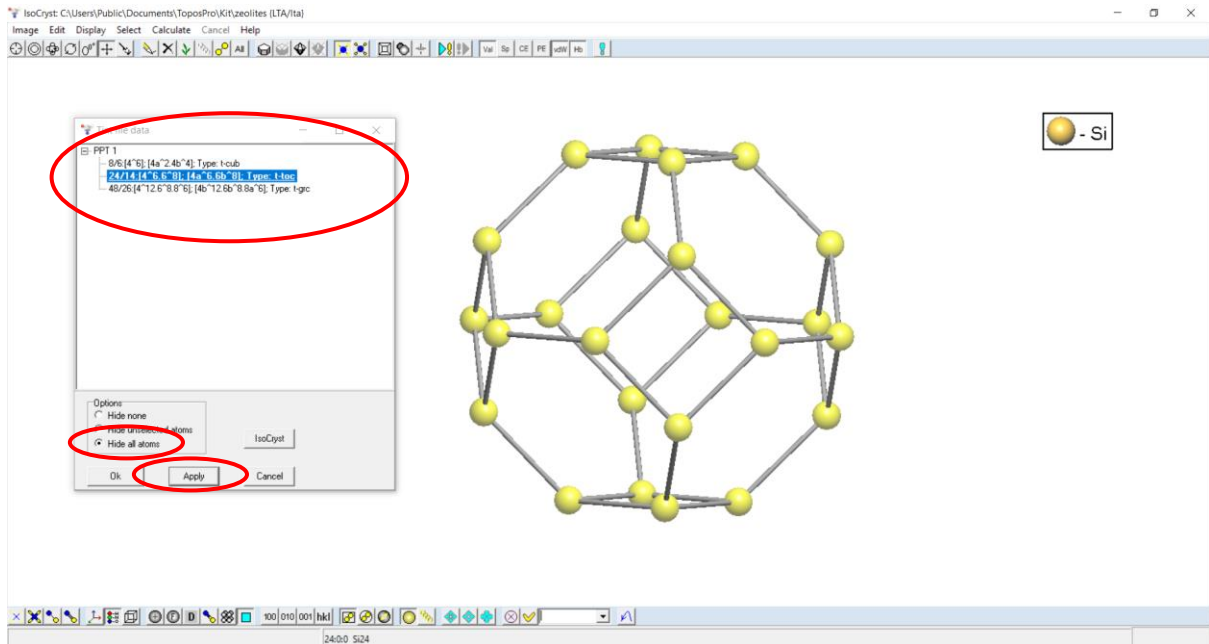
- 2.) Select “Image” and “Primitive/Natural Tiles” which will open an *IsoCryst* window.



- 3.) Grow the crystal structure with Grow or **CTRL + W** on the keyboard until all the entries in the Tint file data window become bold. This indicates the atoms that construct the tile are grown and displayed on the screen.



- 4.) Select any of the tiles in the list, select “Hide All Atoms” and click “Apply”. The selected tile will then be displayed in *IsoCryst* and can be studied like any crystal structure.



## Visualising Tiles with 3dt

Provided the “Essential Rings for 3dt” option was selected when calculating the tiling, tile structures can be displayed in 3dt to produce high quality images for reports.

- 1.) Download 3dt from <http://gavrog.org/> and install it on your PC. *Note that Java is required to run 3dt.*

# The GAVROG Project

Download the Software >>>

News

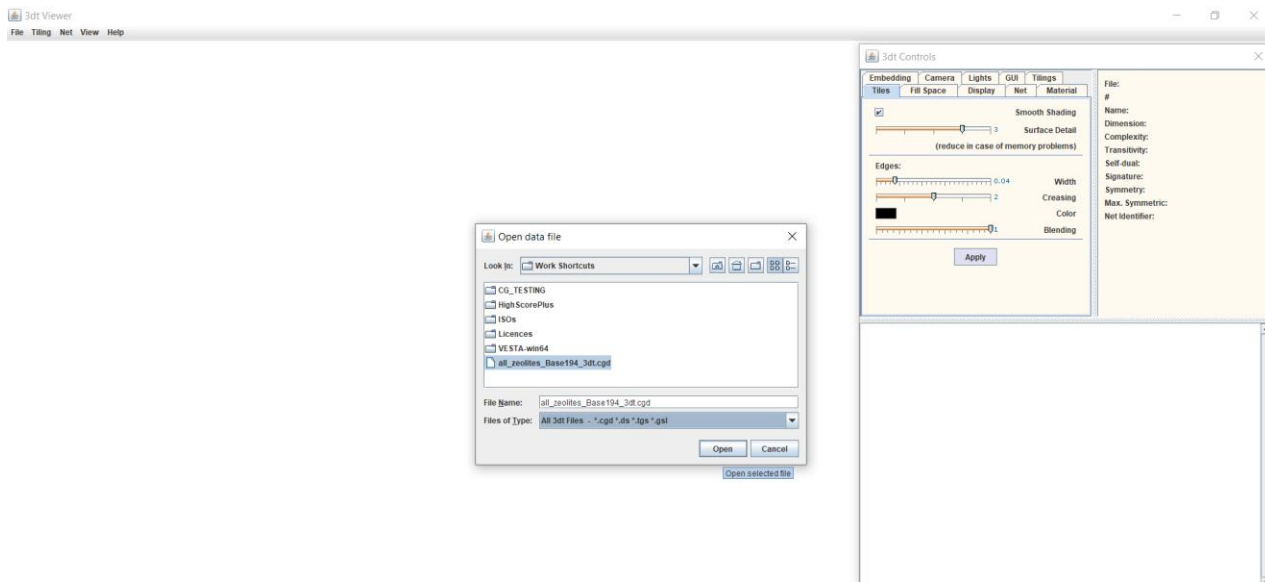
2016-05-25  
 The latest blog entry at <https://systre.wordpress.com> talks about some Gavrog "history" and new ongoing activities.

2013-09-30  
 A second beta release for 3dt 0.6.0 and SYSTRE 1.2.0 is out. For further information, please visit the [download page](#) and check the release notes.

2011-10-04  
 The source code for this project is now hosted on [GitHub](#).

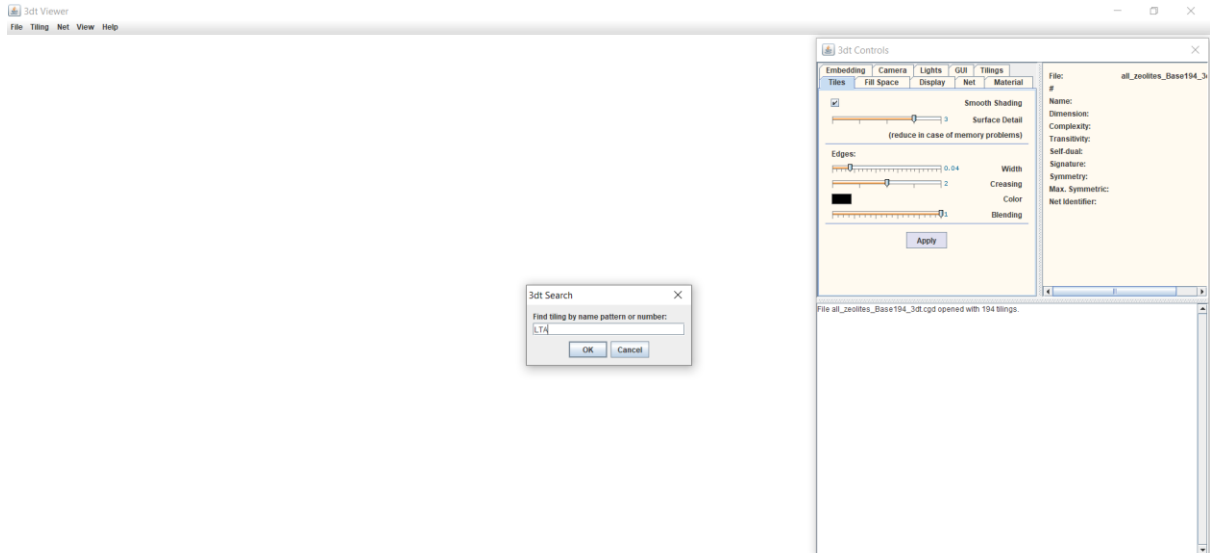
GAVROG stands for *Generation, Analysis and Visualization of Reticular Ornaments using Gavrog*. It is about pretty pictures, solid state chemistry and rather involved mathematics. Think Escher, crystals, Alhambra, soap bubbles. If you find the pictures on this page interesting, or appealing, you might like to check it out.

- 2.) Open 3dt and select Open, and navigate to the 3dt file produced when calculating the tiling. The file will be “Database\_name.cgd”.

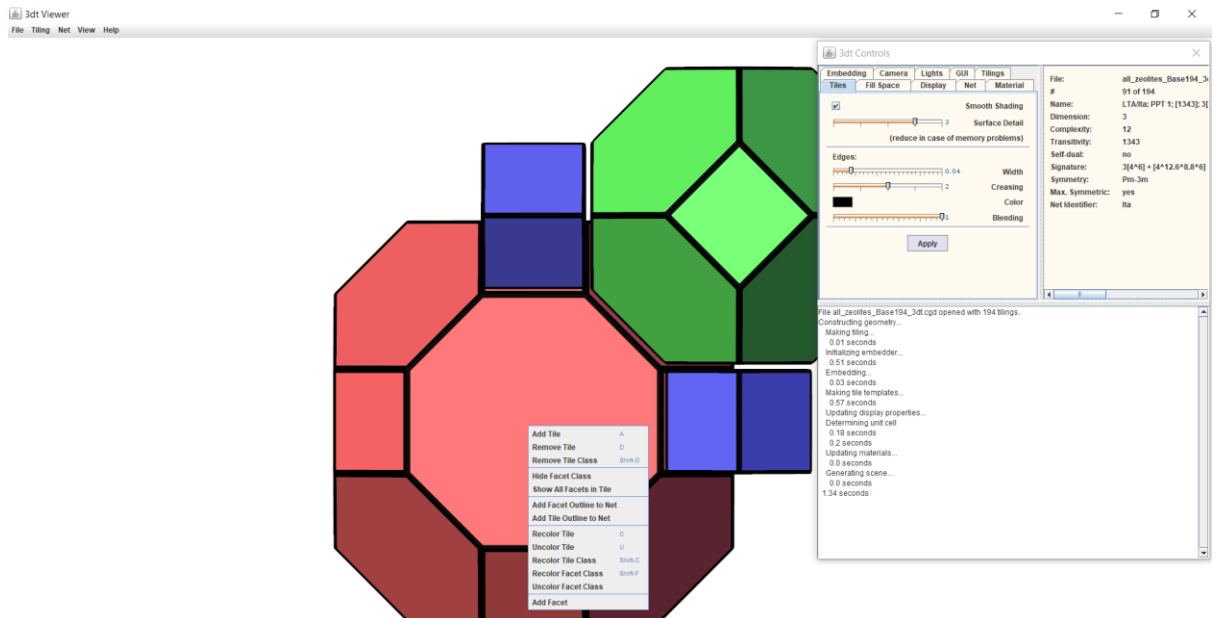




- 3.) If the .cgd file contains multiple tilings (*note that answering “no” to the question “do you want to overwrite the .cgd file” when calculating the tiling with ADS will actually append the new structure at the end of the .cgd file*) then type the name or number for the tiling you wish to visualise.



- 4.) Add or remove tiles by right clicking and selecting “Add Tile” or “Remove Tile”



- 5.) 3dt contains many options for changing the display of tiles, adding a crystal net on top of the tiles and can produce very high quality images for use in presentations and reports. Users are directed towards 3dt's existing documentation for detailed information on use of the software.
  
- 6.) Once the structure is presented in the way the user desires, a ray-traced image can be produced by selecting File, Raytraced Image (**CTRL + R**).

