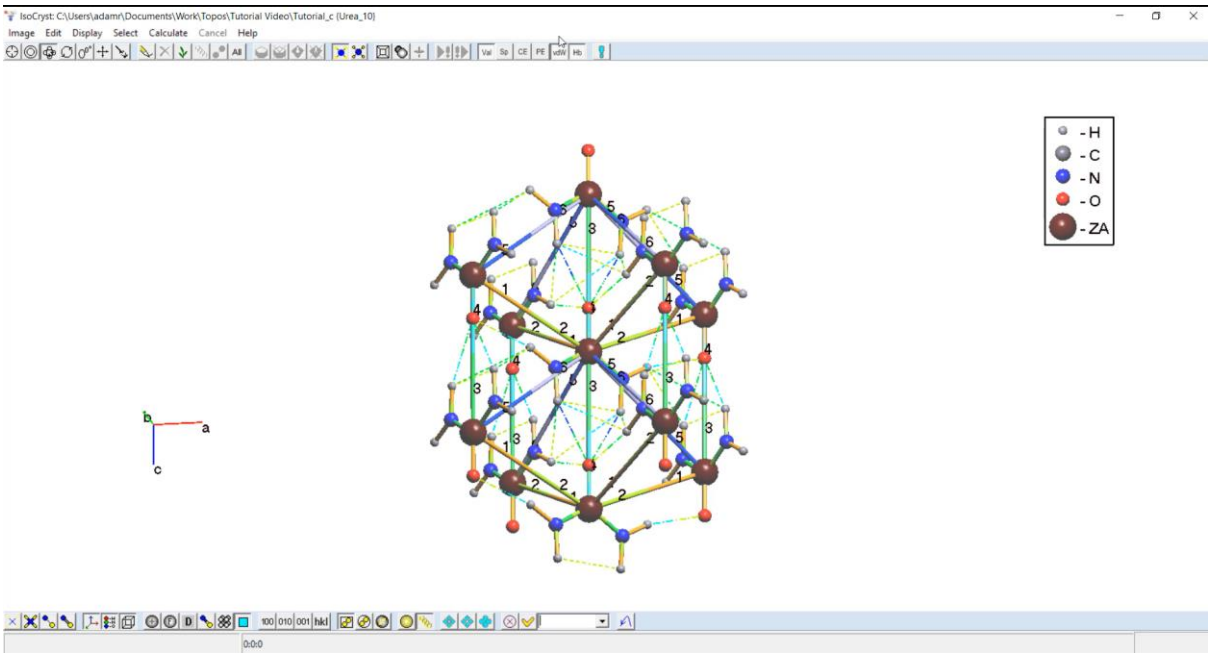


Using *ToposPro* with *CrystalGrower*

ToposPro is a software package for the topological analysis of crystal structures. This software can be used to partition any crystal structure into units of growth (e.g. natural tiles or Voronoi-Dirichlet polyhedra - VDP). An interface between *CrystalGrower* and *ToposPro* has been developed over a number of years to produce the input files required for *CrystalGrower* to grow the crystal structure from its units of growth. Due to the advanced nature of the *ToposPro* software, guides are provided here to familiarise CrystalGrower users with the operation of this software.

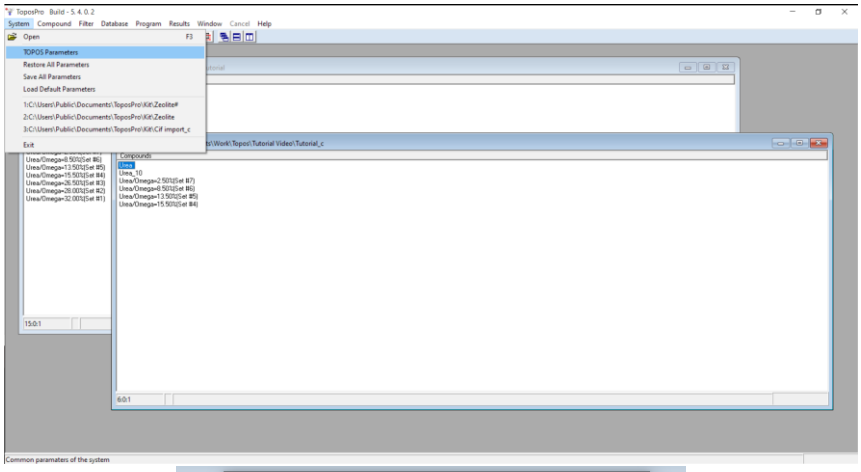
Creating Structure and Interaction Files for Net Structures

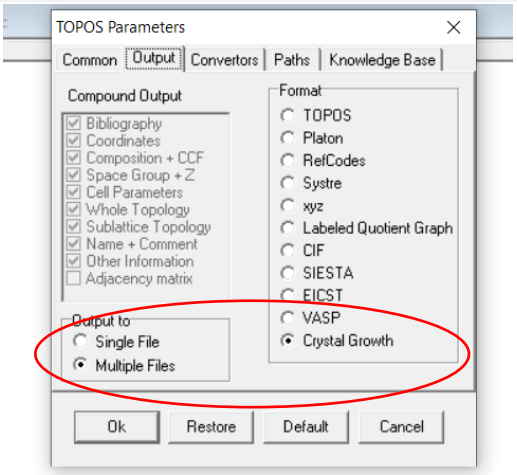
This step-by-step guide will demonstrate how to produce a structure file for a **net** type structure, along with its corresponding interaction energy file (net.txt). These files are required as inputs for *CrystalGrower*, therefore care must be taken to ensure the structures and interactions are chosen correctly to make sense chemically.

1.) Download *ToposPro* from https://topospro.com/ and find the version which matches your operating system (64 bit or 32 bit). Install and run the software (*ToposPro* requires administrator rights on your machine to run, even after installation). A light version of *ToposPro* is bundled with *CrystalGrower.*

2.) First check: System > TOPOS Parameters > Output > Format is set to Crystal Growth.

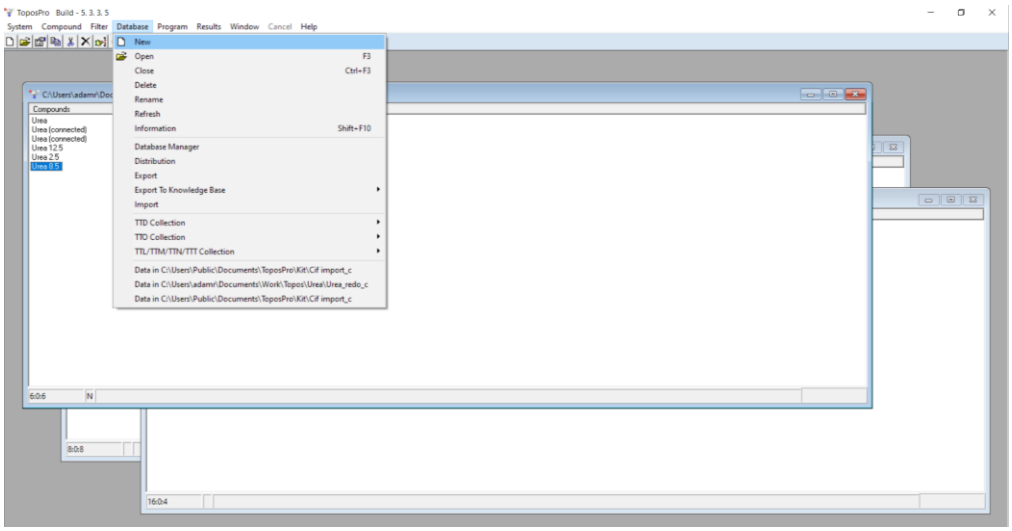
- If you are writing multiple structure files (e.g. a whole database) select: Output to > Multiple Files, otherwise select Single File. This will create separate structure and bonds / net.txt files for all the selected structures (including natural tile structures where the bonds files are redundant).

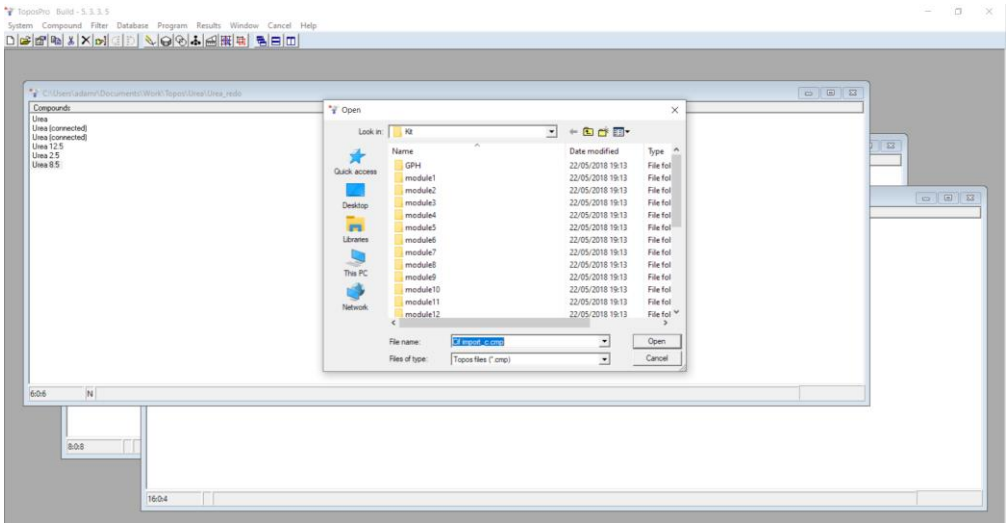




3.) Creating a database (.cmp):

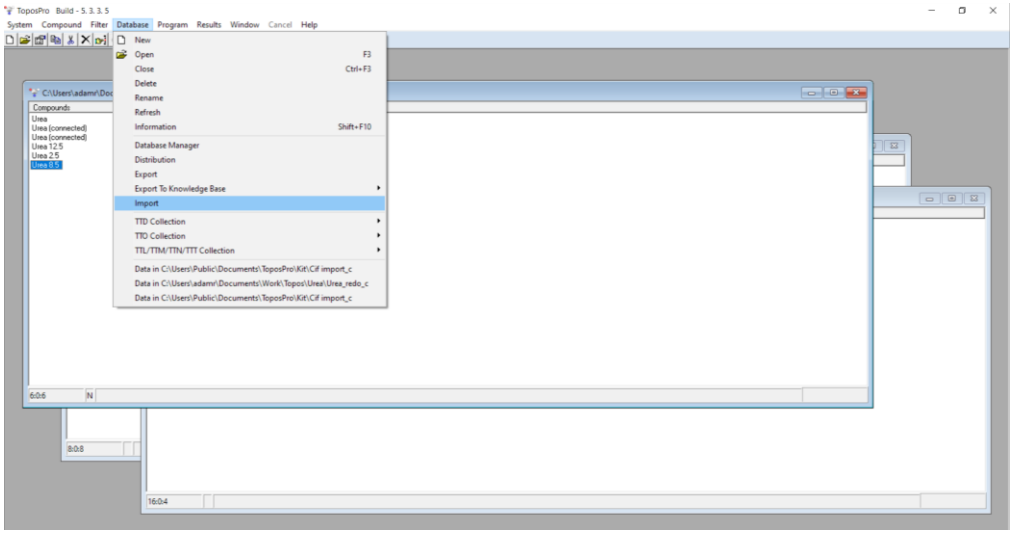
- Click Database > New and browse to a location to save the database. When the prompt appears for your user code, enter the number **1** . *Note: If you want to copy a database to another machine, you must also copy the corresponding .adm and .cd files which are also generated when creating a database.*

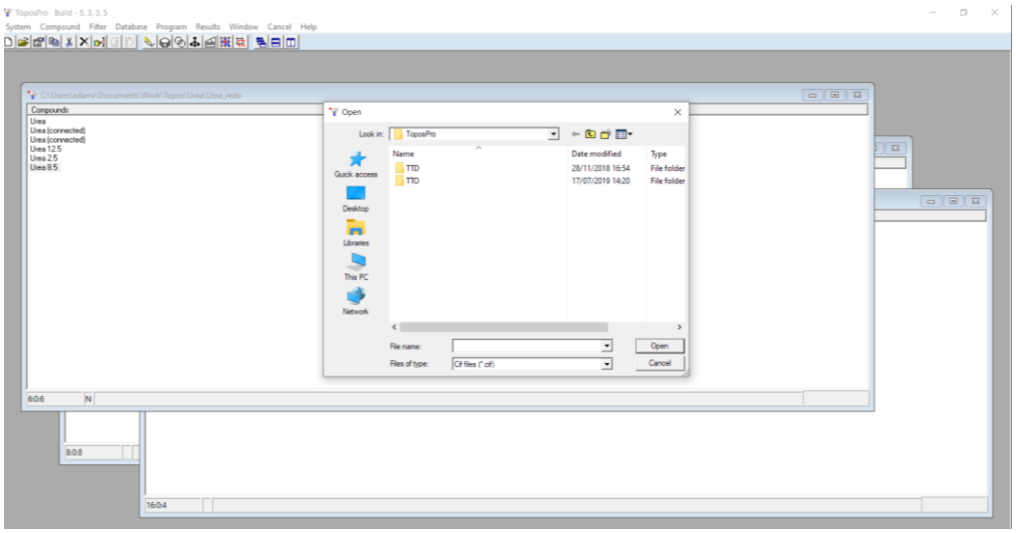




4.) Importing a CIF

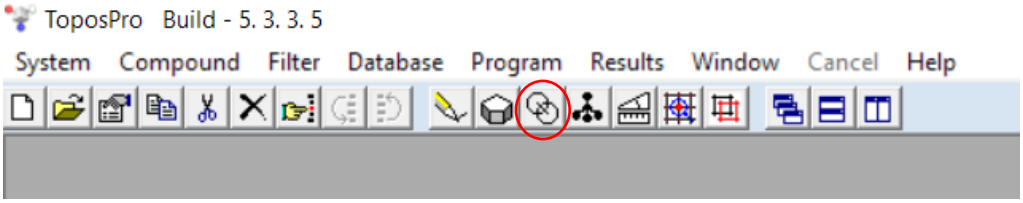
- <u>Close the newly created database first.</u>
- Click Database > Import and select the CIF (.cif) to import. Then select the database (.cmp) to import the CIF into.

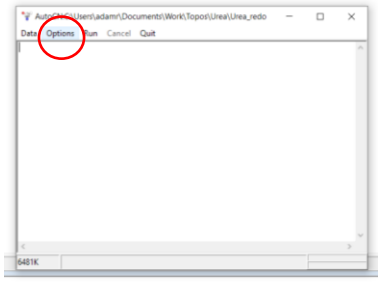


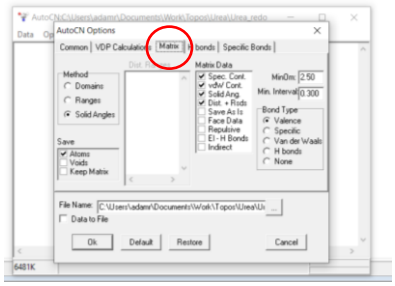


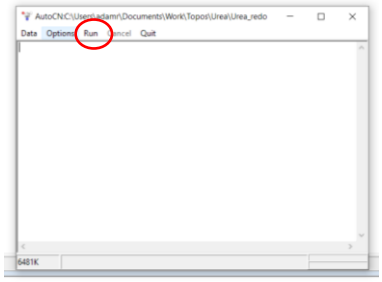
5.) Creating an adjacency matrix:

- Click *AutoCN* (symbol with two intersecting circles) then navigate to Options > Matrix to change the settings and generate the required set of interactions for crystal structure. Starting with the default “Domains” option is a good first approximation for most structures. This is a **crucial step** and can be difficult to perform correctly – a full guide is presented later in this manual. Click Run – The adjacency matrix is now generated. Further info on *AutoCN* can be found here: https://topospro.com/software/topospro/manual/details-of-the-autocn-algorithms/



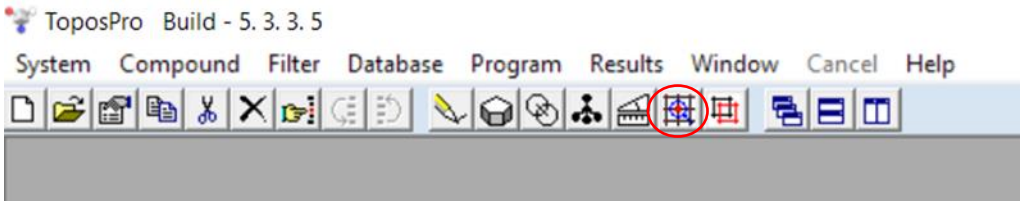


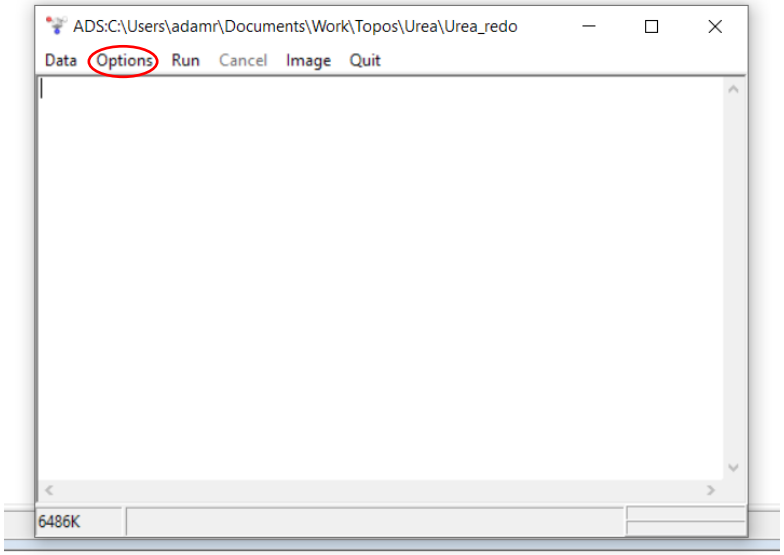




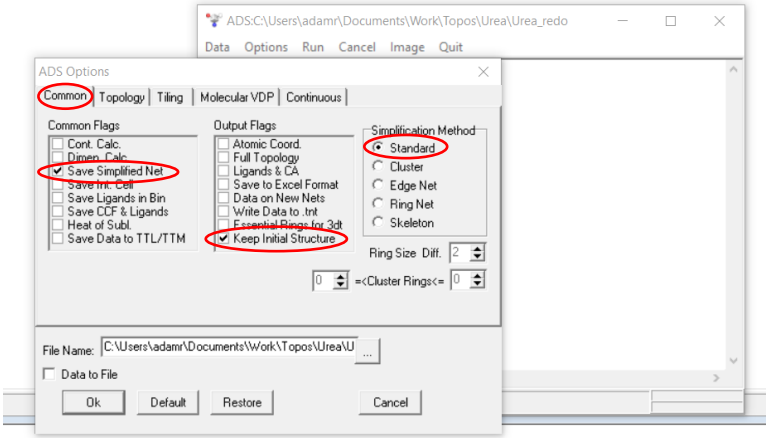
6.) Creating a simplified net with *ADS*:

- Click the *ADS* button (net symbol) and select “Options”

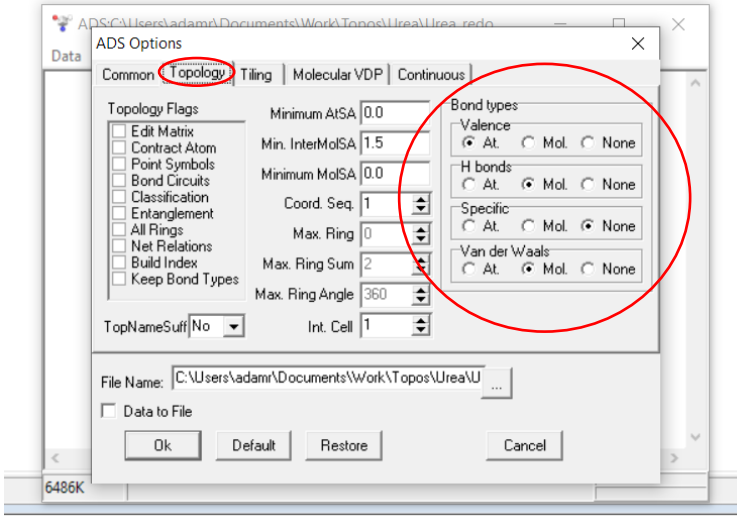


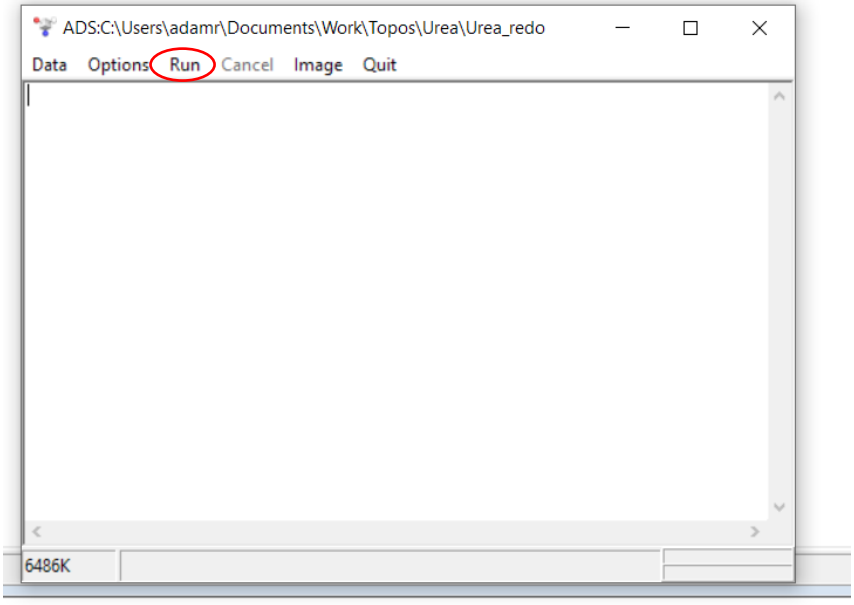


- Navigate to the “Common” tab and select save simplified net. Tick Keep Initial Structure to retain local bonding information. Click standard simplification method.

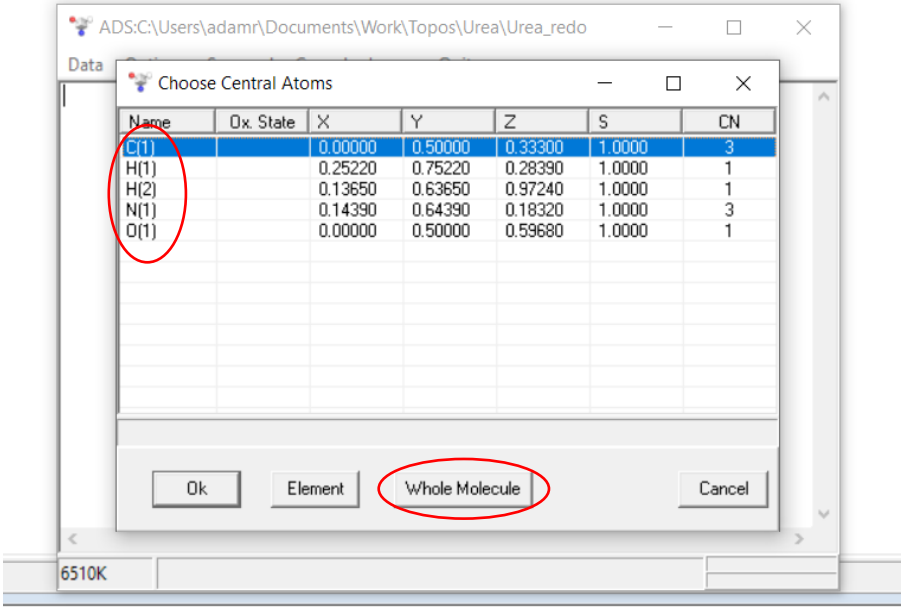


- Navigate to the Topology tab and use the Bond Type options to control how bond types are treated during simplification.
- The available bond types are: Valence Bonds, Hydrogen Bonds (H bonds), Van der Waals (vdW) interactions and Specific Bonds. The options for treating bonds are: “Atomic (At.)”, “Molecular (Mol.)” and “None”. The options selected here will define how the net is partitioned into nodes and edges.
- Setting a bond type to “Atomic (At.)” will result in all the atoms within the same molecule linked by the selected bond type being treated as separate nodes in the net. Setting a bond type as “Molecular (Mol.)” will result in separate molecules linked by the selected bond type being treated as separate nodes in the net. Setting a bond type to “None” will result in it being ignored entirely during simplification. The “Molecular (Mol.)” option is generally used for molecular crystals, whereas the “Atomic (At.)” option is usually used for ionic crystals (e.g. NaCl).
- Click OK, then run.





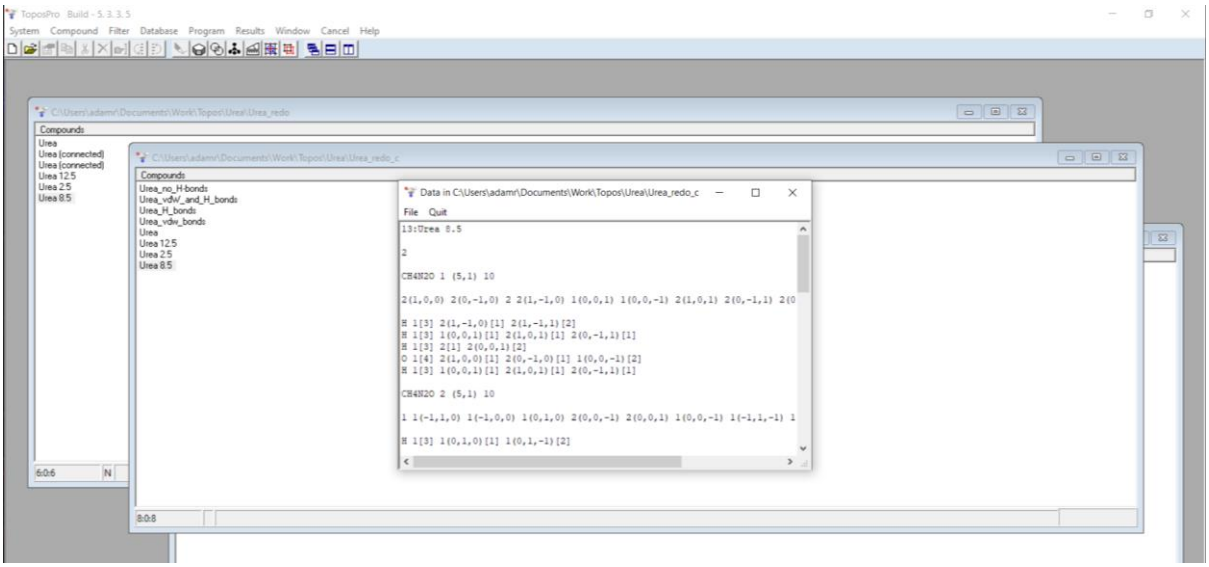
- A window will appear to select central atoms.
- For ionic crystals, select the atoms that define the nodes of the crystal net (e.g. Na^+ and Cl^- in NaCl) or atoms at the centres of the ionic species (e.g. C in CO_3^{2-} in calcite) by using the Insert key or by right clicking and choosing “Select”. Selected atoms will appear in **bold**. Then press OK.
- For molecular crystals (e.g. urea) select the “**Whole Molecule**” option to consider the centroid of the molecule as the nodes of the crystal net. This option also applies to ionic crystals made up of molecular ions linked by vdW or H-Bonds (e.g. ammonium nitrate).



- The simplified net will now be calculated, and a child database will open (xxx_c.cmp).

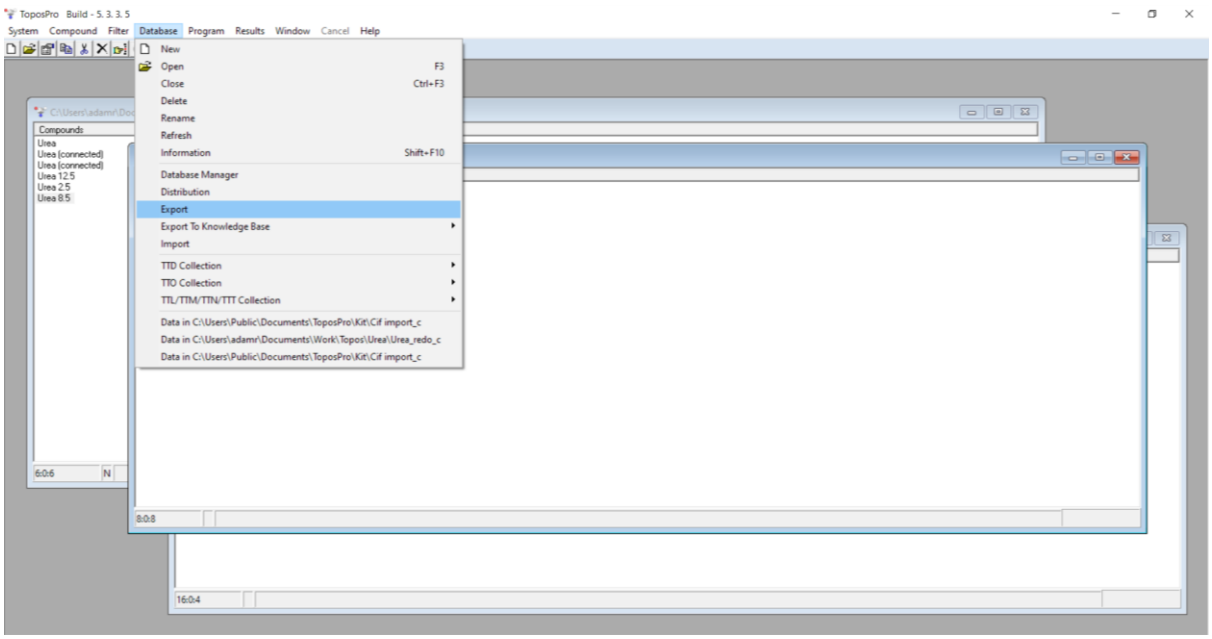
7.) To obtain the structure file only:

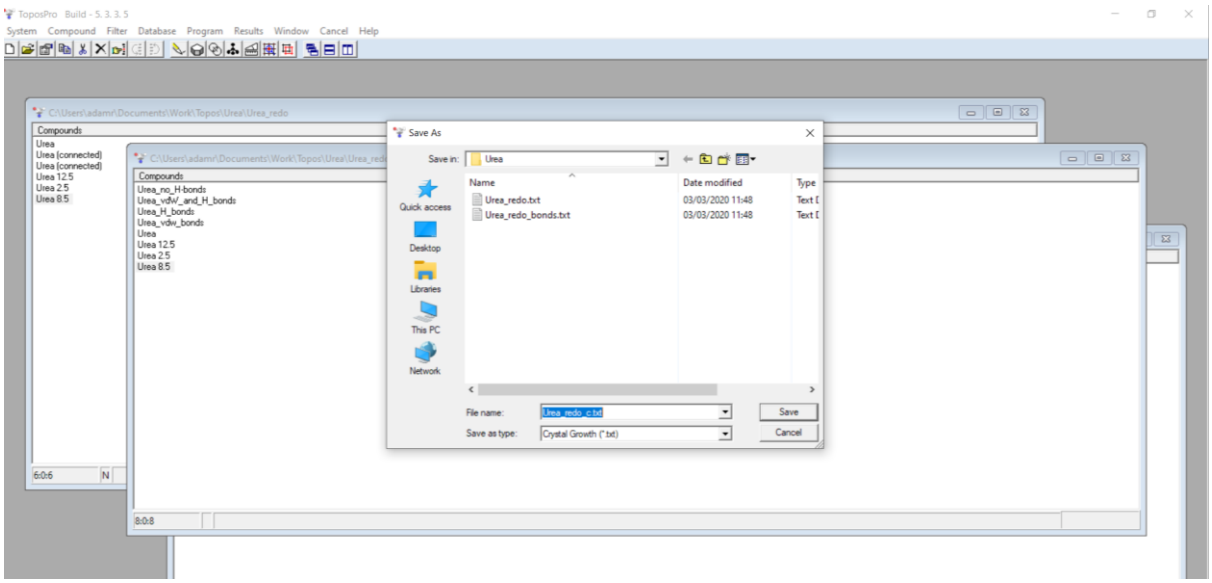
- Select the newly created entry.
- Press F9 or right-click and select “view” to view the structure file.
- Select File > Save As to save the structure file as a text file.



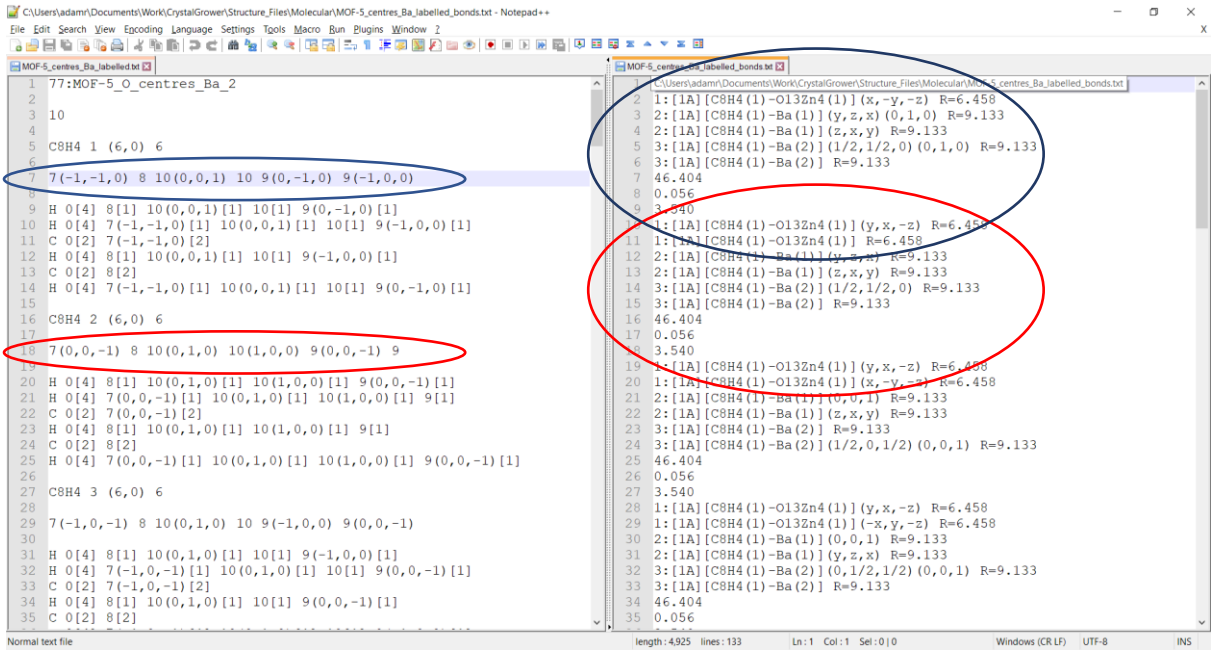
8.) To obtain the net.txt / interaction energy information and structure file simultaneously:

- Select the newly created database entry. Or hold CTRL / SHIFT to select multiple entries (selected entries appear in bold).
- Select Database > Export and choose where to save the output.
- This will save the structure file, along with a companion file called XXX_bonds.txt which is the automatically generated net energy / interaction data for *CrystalGrower*.





9.) Both files will be related to each other: i.e. neighbour 1 for molecule 1 in the structure file will correspond to interaction 1 on molecule 1 in the “bonds” file.



10.) The file format for a bonds / net interaction energy file (net.txt) is the following (delimiting characters are highlighted in **bold**):

- Interaction (bond) type**: [**Origin species symmetry position Origin species type e.g. A, B or C etc.**][**Origin species chemical formula **(**Origin species symmetry position e.g. 1, 2 or 3 for the same species in different coordination environments**) –** Destination species chemical formula **(**Destination species symmetry position**)] (**Symmetry transformation for destination species**)(**Translation for destination species, if required**) R =** Interaction length in angstroms

  This repeats for all interactions to neighbours
- Energy for each interaction type (kcal/mol) – Default is solid angle / size of Voronoi face. These will require changing to match the free energies of crystallisation for the units of growth that compose the crystal structure.

  This repeats for all interaction <u>types</u> to neighbours

  All of the above is then repeated for all molecules in <u>primitive</u> cell