

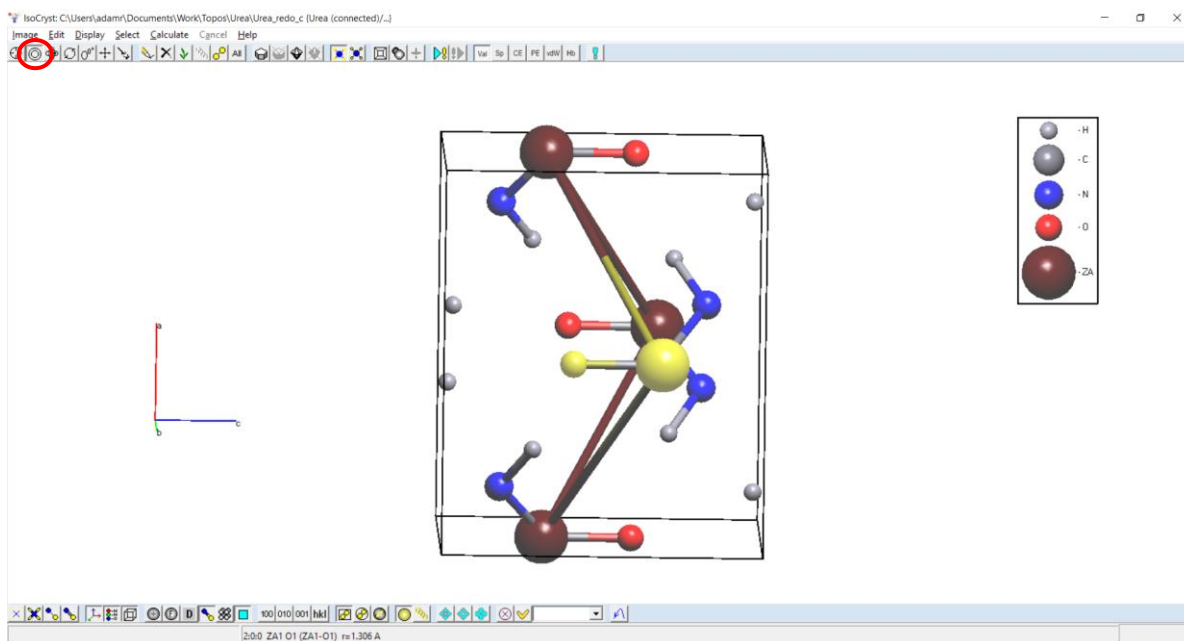
Matching Interaction Types Using *ToposPro*

This step-by-step guide will demonstrate how to relate the interaction types used in *CrystalGrower* to their real chemical counterparts. Using *Isocryst* within *ToposPro*, interactions can be visualised and labelled to allow their identification within the context of the crystal structure.

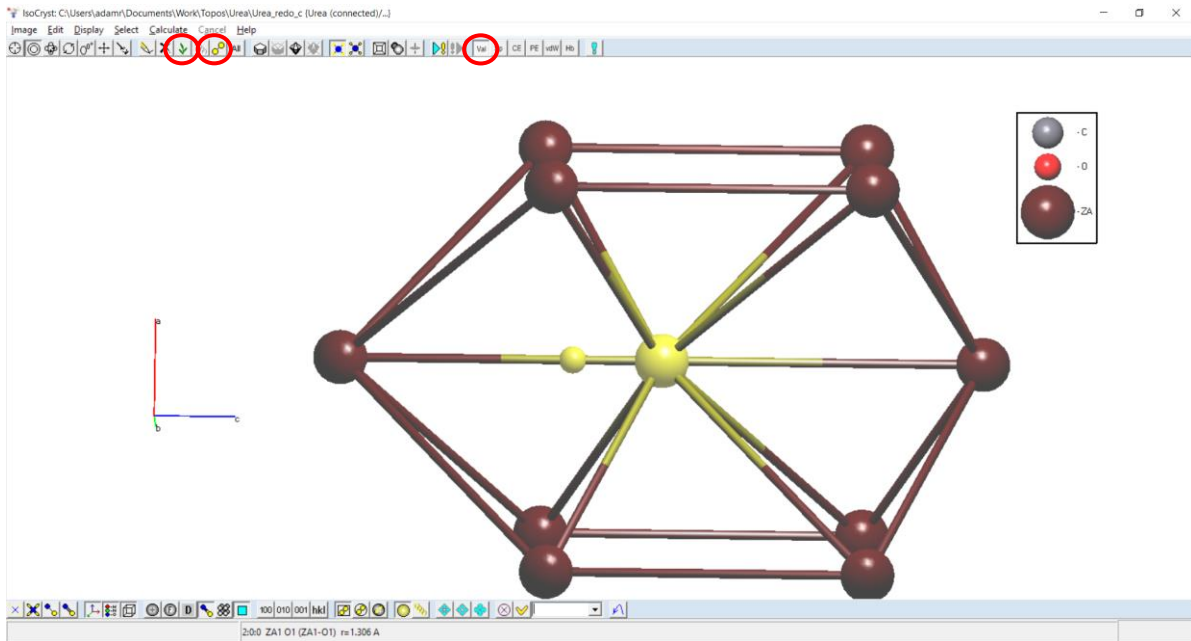
After calculating the simplified net with *ADS*, the generated database entry in the child database can be studied using *Isocryst*. By employing the previously discussed techniques for visualising connected species through bonds, it is possible to correlate interaction types in *CrystalGrower* with real-life chemical interactions (e.g. hydrogen bond donors and acceptors). Understanding the makeup of the interspecies interactions will allow more accurate approximations of the free energies of crystallisation required to obtain desired crystal morphologies. For example, knowing that an interaction between two molecules is composed solely of hydrogen bonds will have important implications for systems crystallising in solvents which form strong hydrogen bonds vs. solvents with weak or no hydrogen bonds.

Using urea for which the simplified net has been calculated as an example, all interactions originating from a central molecule to its neighbours can be displayed and labelled:

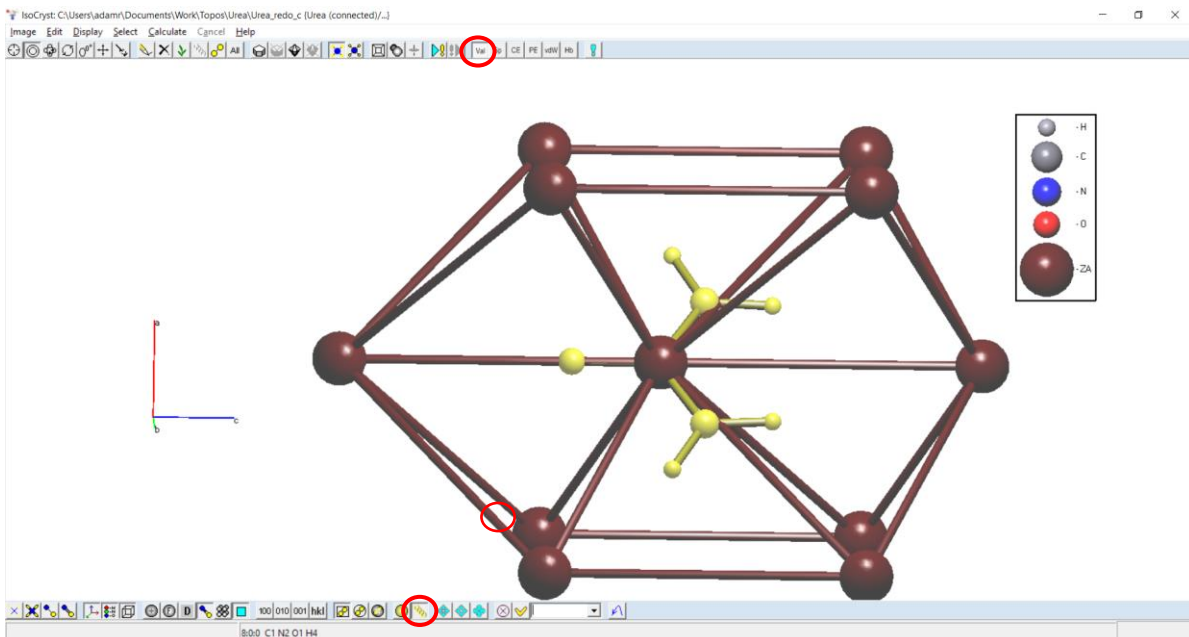
- 1.) Use the Select tool to select the urea molecule and its central atom (usually ZA or another dummy atom type, the simplified net nodes are linked through valence bonds and are a separate net to the urea molecules in the underlying net).



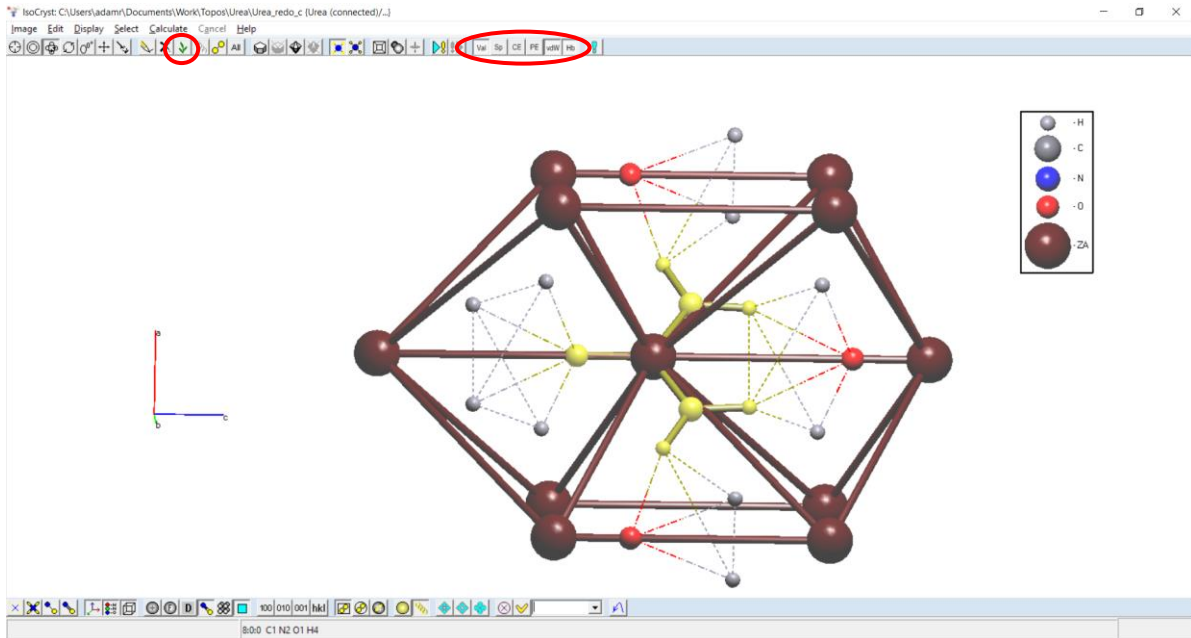
- 2.) Show the selected atoms only by clicking “Show Selection Only”. Restrict the growth to only grow via valence bonds and press grow once.



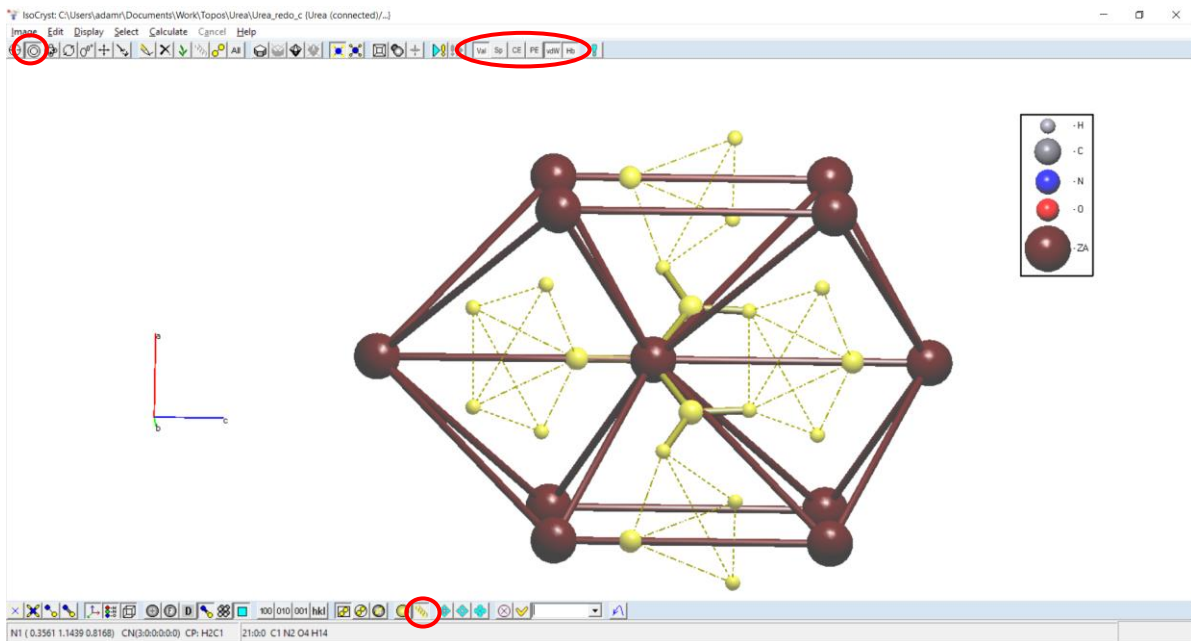
- 3.) Deselect (right click) the central dummy atom as the first nearest neighbours are already displayed for the simplified net. Use the Polymeric Chain selection tool and fully grow the central urea molecule via valence bonds only to begin constructing the underlying crystal net.



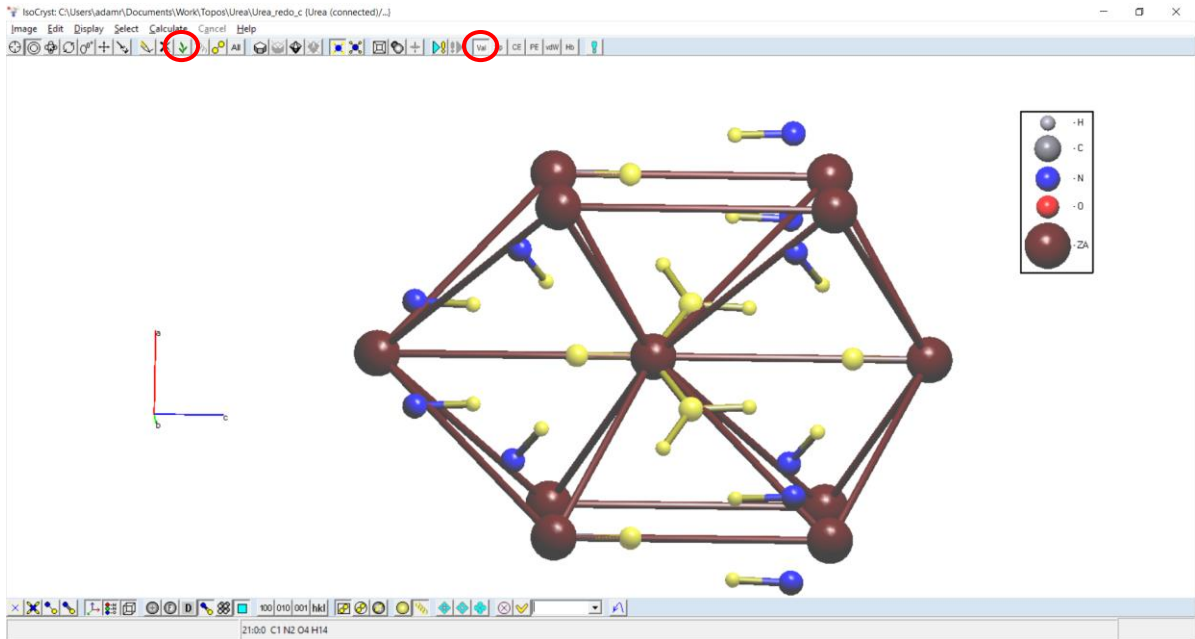
- 4.) Activate Hb and vdW bonds and press Grow once to grow the closest neighbouring molecules.



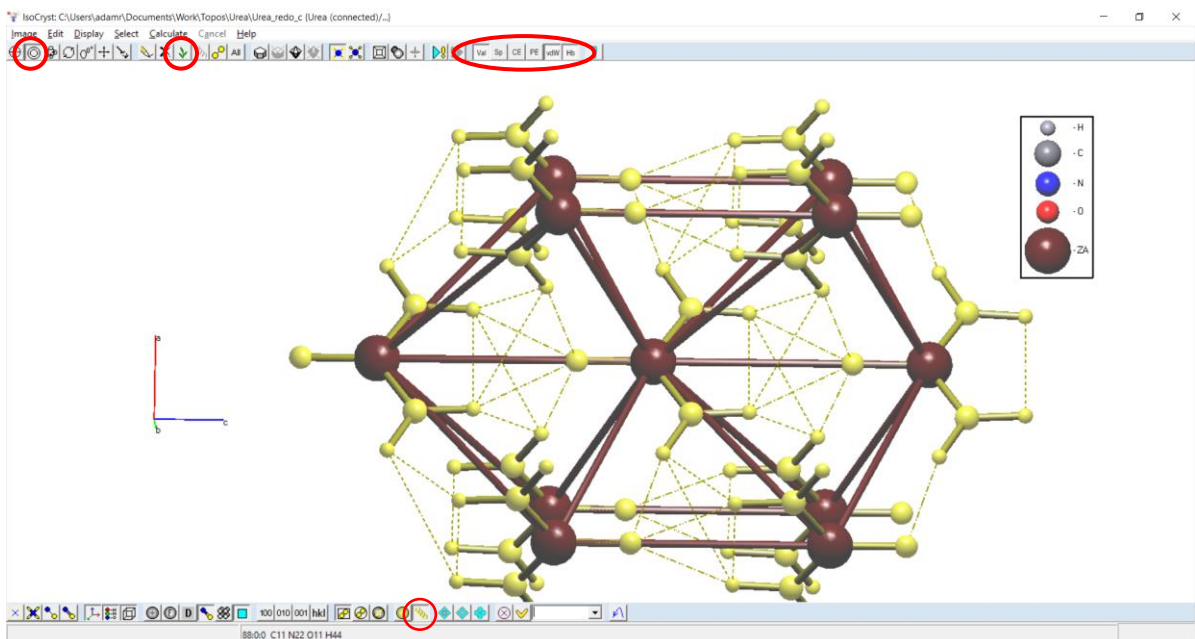
- 5.) Select the polymeric chain option and click any of the atoms in the underlying net to select all the atoms connected by H-bonds, vdW bonds and valence bonds.



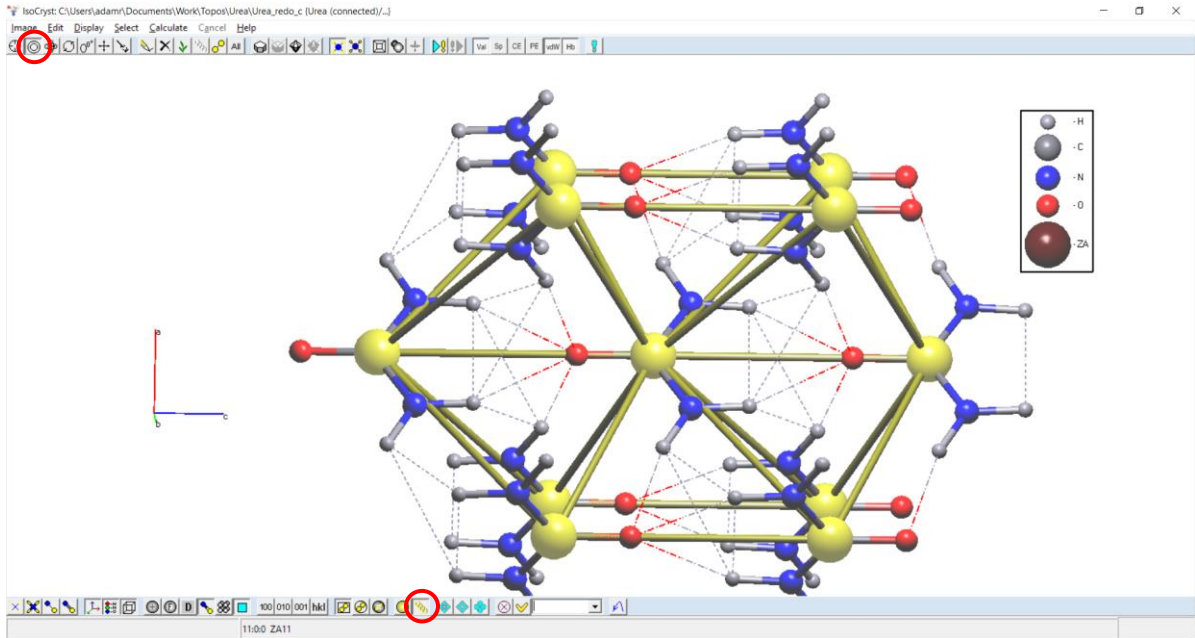
6.) Turn off Hb and vdW to only allow growth by valence bonds again, and press Grow.



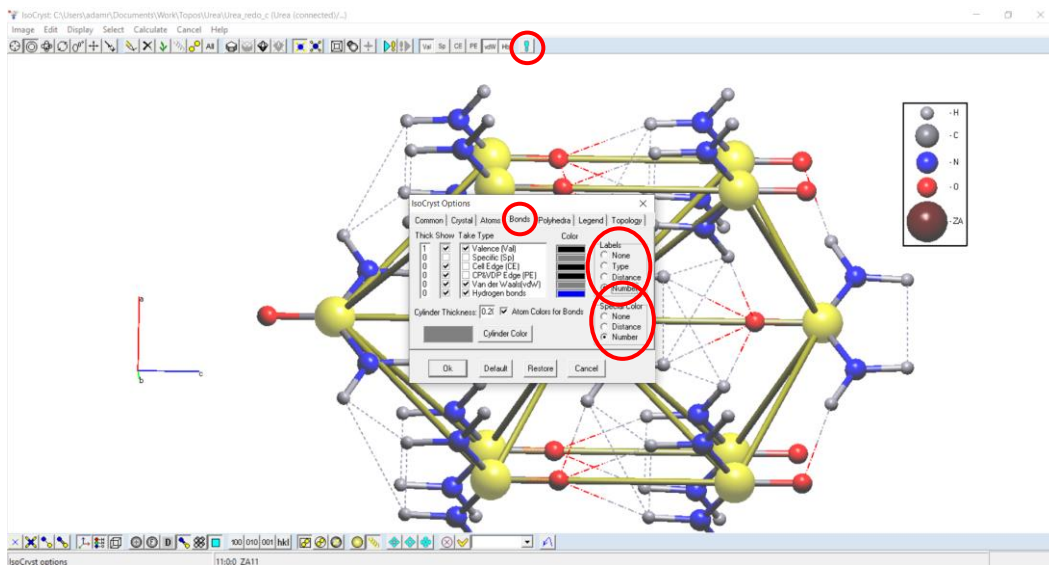
7.) Turn Hb and vdW back on, ensure Select Polymeric Chain is switched on and select one of the urea molecules, this will again select all the connected atoms through valence, Hbonds and vdW bonds. Then turn off Hb and vdW again to restrict growth to valence bonds and press Grow. Repeat this procedure several times to grow the neighbouring molecules in full.



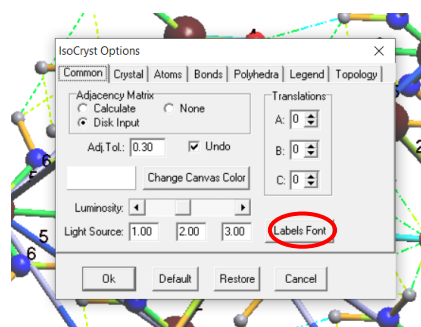
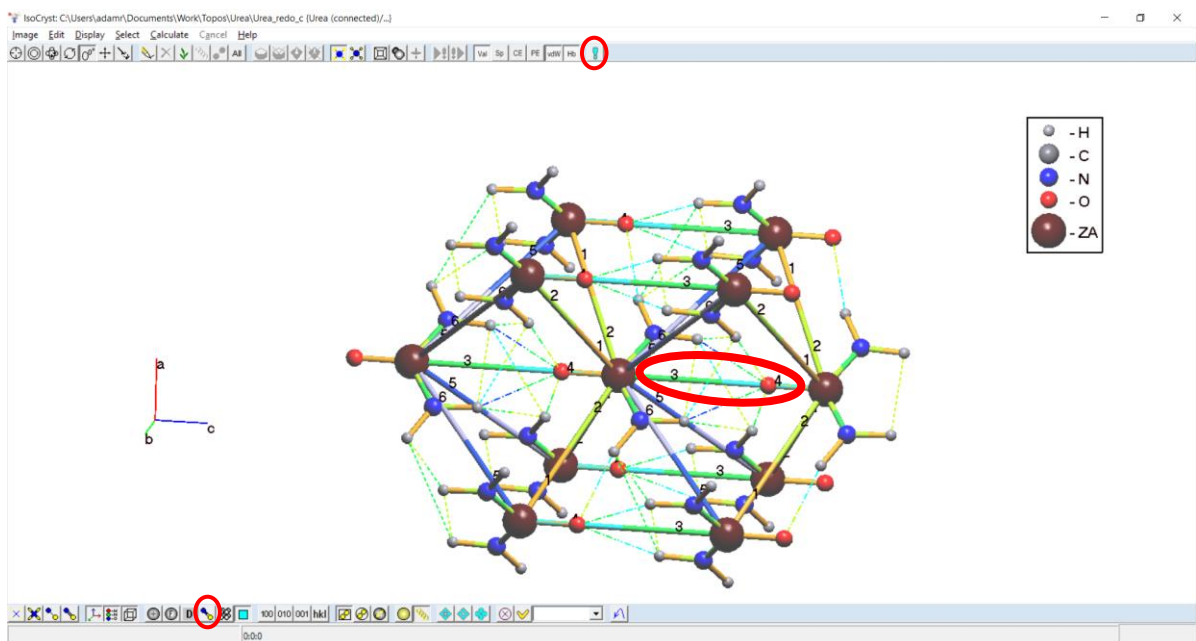
- 8.) Now the fully connected neighbouring molecules are displayed. To show the interaction types, deselect the molecules (right click anywhere except on an atom) and select one of the central dummy atoms with “Select Polymeric Chain” engaged.



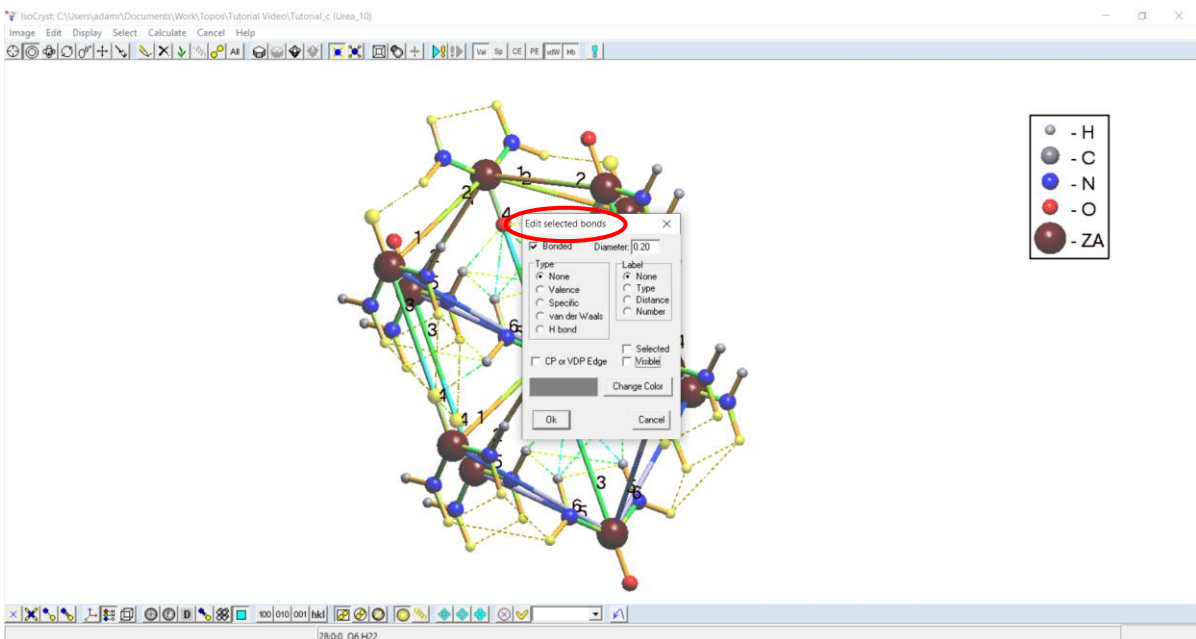
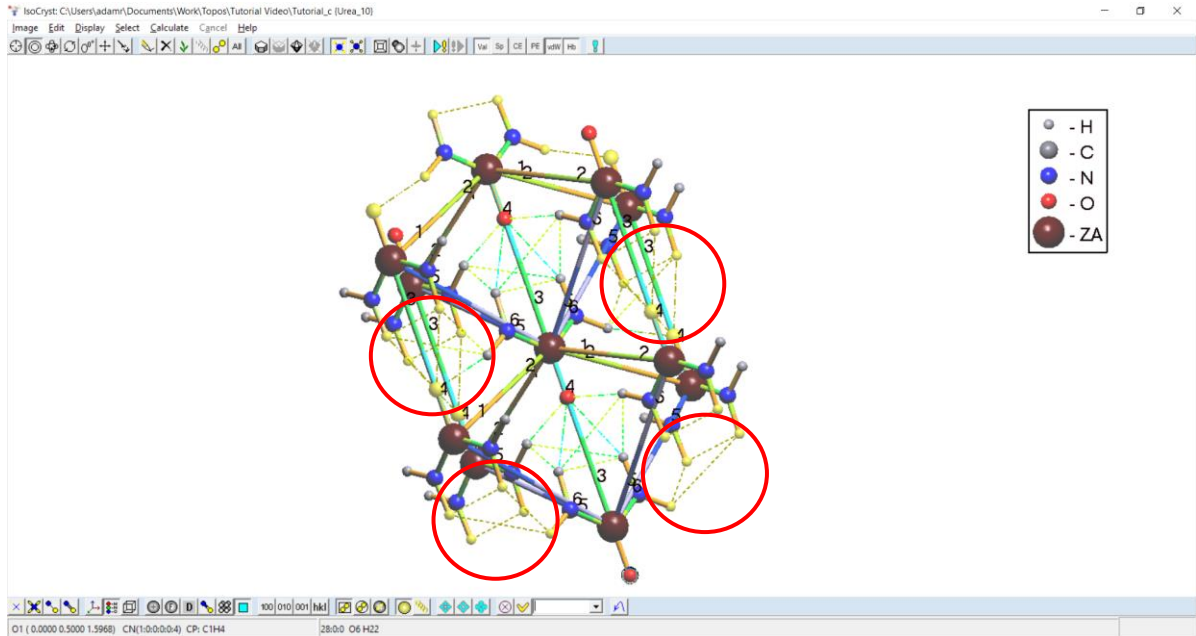
- 9.) Select *IsoCryst* options and navigate to the “Bonds” tab. Under “Labels” select “Number” and under “Special Color” select “Number”.

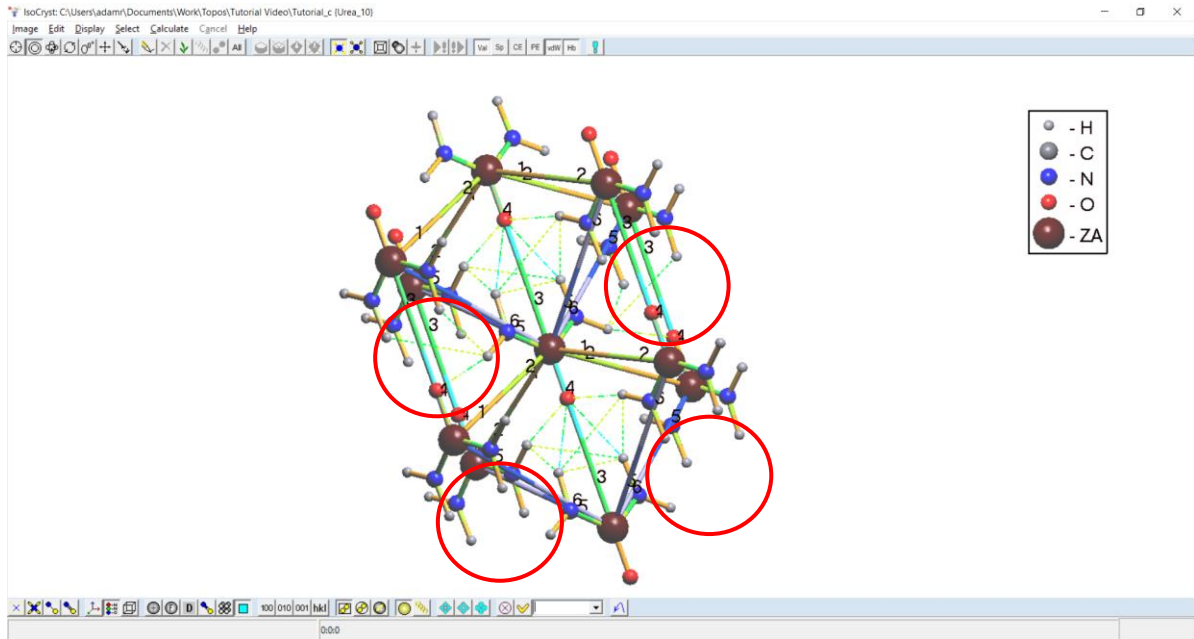


- 10.) Ensure that the “Show Bonds Coloured” option is disabled (this is specifically for bonds coloured by atom components). If the displayed labels are too small, change their font size under the “Common” tab of *IsoCryst* options (blue exclamation mark). The numbers assigned to each half bond will correspond to the interaction types in the net interaction / bonds file. The numbers are defined by the species from which the half bond originates, and will always follow the origin species’ point group symmetry. This means that if a species is coordinated in exactly the same way, but in a different symmetry position, the interaction types will still correspond to the same chemical interactions. Half bond colours will also differ between interaction types to allow easy identification.

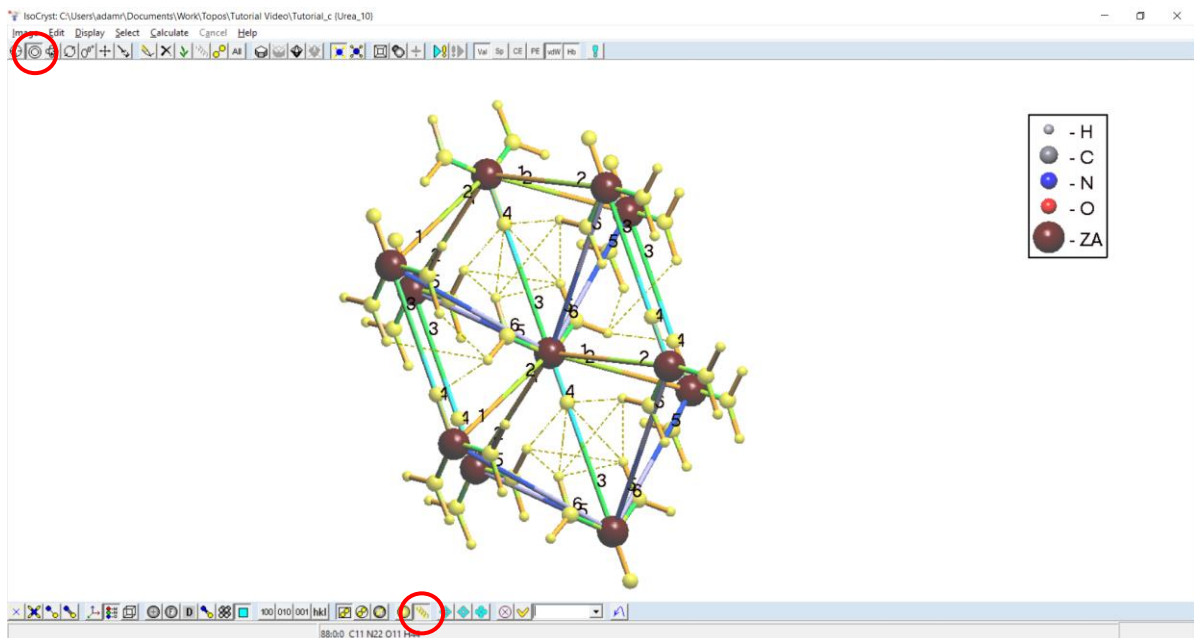


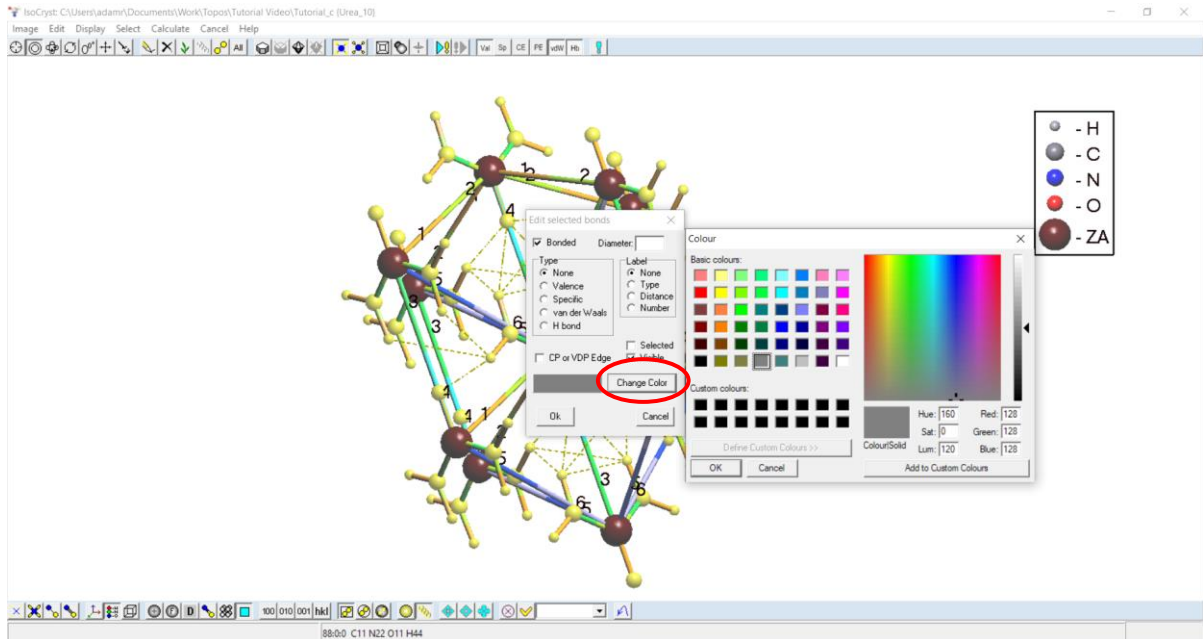
- 11.) Remember that individual bonds can be made invisible to tidy up the presentation of the neighbours using the Edit Bond tool (**CTRL + B**). If you only wish to see bonds to and from the central neighbour, use the Select tool to select the atoms that connect between the neighbours and set the bonds to invisible.



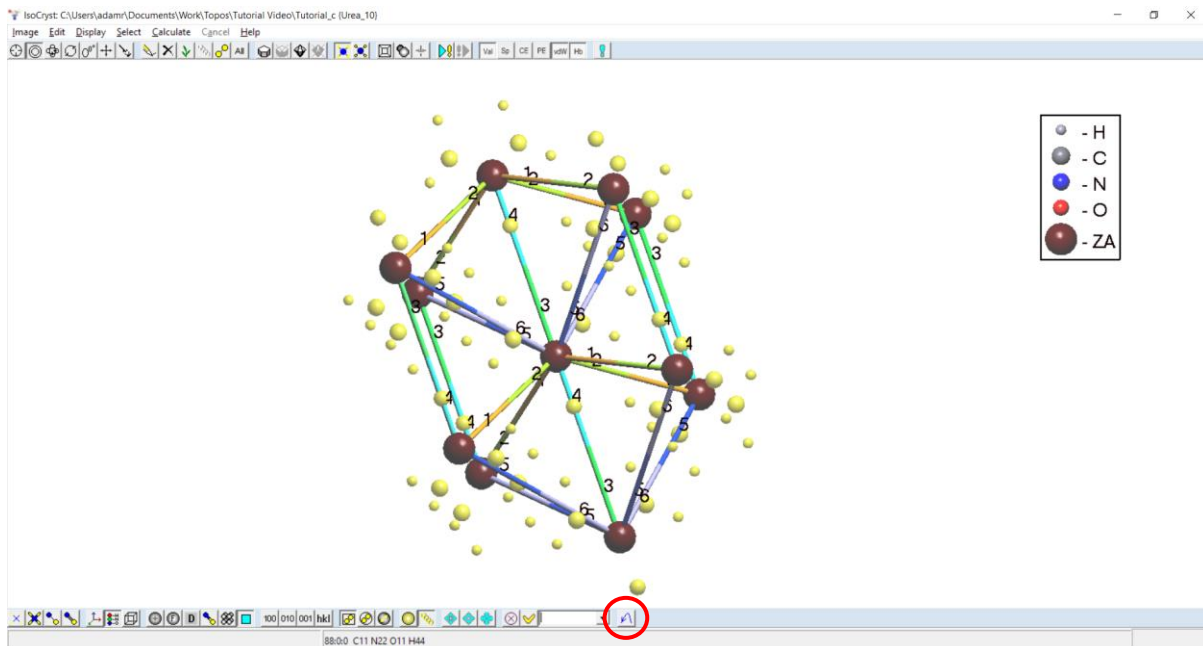


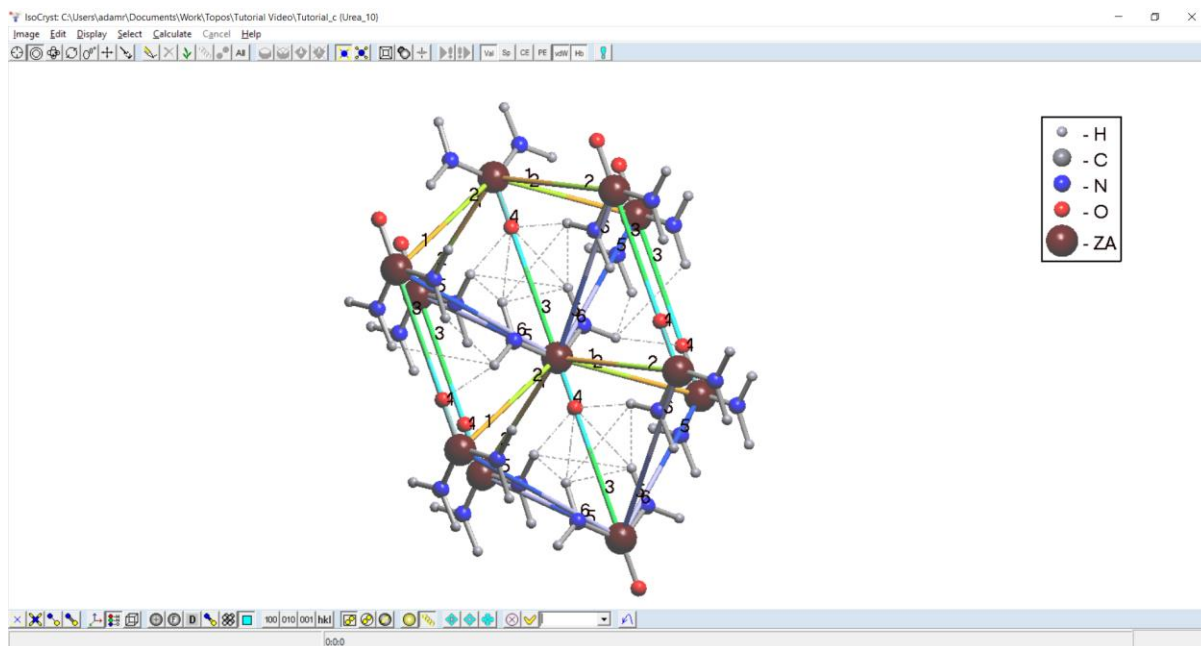
- 12.) If the colouring of the underlying net bonds is distracting from the half-bond interaction colouring, these bonds can be recoloured exclusively to a single colour. Select the underlying net by using the Select Polyhedral Chain tool and clicking an atom that is part of the underlying net. Then select Edit Bond and choose a colour to replace the existing colouring.





- On some occasions this can cause the original bonds to disappear. But pressing Undo (**CTRL + Z**) will bring the bonds back with the assigned colour.





- This method is useful for producing high quality graphics to clearly present what each interaction corresponds to in *CrystalGrower* and *ToposPro*. Minimising the number of bonds displayed and colouring only the intermolecular interactions makes it far easier to identify the important interactions, equivalent interactions and the components of each interaction.