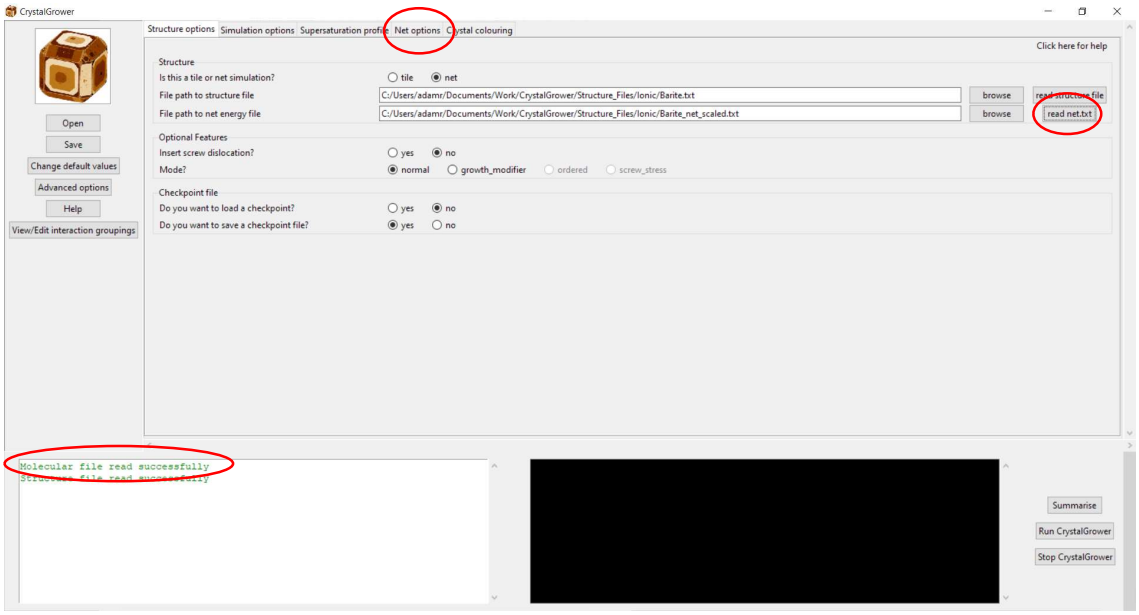
Reading a Net Energy File

File path to net energy file: this question only appears for "net" type crystals and specifies the path to the file containing the crystallisation energies associated with the structure. Once the file path is specified, press "read net.txt". Users should see the message "Net file read successfully". A box will then appear that allows you to link the energies required for different molecules. If you wish different molecules to be treated the same then enter the same letter (e.g. both A). Press "Confirm interactions".

The net energy file (or net.txt) contains the information for *CrystalGrower* to assign the free energies of crystallisation for the replacement of connected solvent species with connected neighbour molecules. This file is discussed fully in the Data Input Files section of the manual.



The interactions specified in the Interaction window will carry over to the “Net options” tab in the user interface (discussed in detail in its own manual section).