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.

	are options simulation options supersatura	ation profile. Net options: Cystal colouring	Click here
The A	ucture		Click here
	his a tile or net simulation?	⊖ tile	
	path to structure file	C:/Users/adamr/Documents/Work/CrystalGrower/Structure_Files/Ionic/Barite.txt	
-			browse read struc
n File	path to net energy file	C:/Users/adamr/Documents/Work/CrystalGrower/Structure_Files/Ionic/Barite_net_scaled.txt	browse read n
	tional Features		\sim
Inse	ert screw dislocation?	O yes 🔘 no	
ult values Mo	de?	formal Ogrowth_modifier Ordered Screw_stress	
options	ckpoint file		
	you want to load a checkpoint?	⊖yes	
	you want to save a checkpoint file?	⊛yes ⊖ no	
file read succes	effally	~	
file read succes	sfully	~	Â
	ofully	<u>^</u>	
	ofully		^ Sum
	ofully		^ Sum
	stuliy	^	
	etully		∩ Sumi Run Crys
	sfully -5		Run Crys
	sfully	^	

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).

