Net Interaction File

net.txt: This file contains the interaction types for each neighbour interaction within the primitive unit cell. It is explicitly linked to the structure file with the neighbour interactions following the same order in each file. Also specified within this file are the interaction strengths in kcal / mol for each interaction type from each species.

This section presents an example (along with a labelled example) for a net interaction file containing energy values and interaction types with neighbouring species. This file is required when running *CrystalGrower* in net crystal mode. It is paired with the structure file, with the order of neighbour interactions in the structure file corresponding to the interaction order in the net interaction file. By changing the interaction types and strengths, users will change the crystal growth rates along interaction directions, resulting in different crystal morphologies. When using the GUI version of *CrystalGrower*, any file path can be specified for the net interaction file via a file explorer window. The interactions strengths can then be changed from within the GUI. Note that all relative unit cell coordinates in the symmetry labels here are presented in the non-primitive unit cell.

When using the command line version of *CrystalGrower*, the file must be manually altered. (Note that the filename for this file must always be net.txt and must be located in the same directory as the *CrystalGrower* executable for the command line version of *CrystalGrower*).

Example (MOF-5)
```
1:[1A][C8H4(1)-O(1)](z,-y,x) R=5.680
1:[1A][C8H4(1)-O(1)](-y,z,-x)(1/2,1/2,0) R=5.680
1:[1A][C8H4(1)-O(1)](-z,y,x)(1/2,1/2,0) R=5.680
1:[1A][C8H4(1)-O(1)](y,-z,-x) R=5.680
2:[1A][C8H4(1)-O13Zn4(1)](y,-x,z) R=6.458
2:[1A][C8H4(1)-O13Zn4(1)](x,-y,-z) R=6.458
6.000
10.000
1:[1A][C8H4(1)-O(1)](z,y,-x) R=5.680
1:[1A][C8H4(1)-O(1)](-z,x,-y)(1/2,0,1/2) R=5.680
1:[1A][C8H4(1)-O(1)](x,-z,y)(0,1/2,1/2) R=5.680
1:[1A][C8H4(1)-O(1)](y,z,x) R=5.680
2:[1A][C8H4(1)-O13Zn4(1)](y,x,-z) R=6.458
```

2:[1A][C8H4(1)-O13Zn4(1)] R=6.458

6.000

10.000

General Example

Interaction type : [Number identifying symmetry position of origin species Origin species molecule / ion type] [Origin species chemical formula (Origin species number for species with multiple symmetry positions) – Destination species chemical formula (Destination species number for species present in multiple symmetry positions)] (Space group symmetry information) (unit cell translation information) R = Interaction length in angstroms.
-Repeat for all interactions with neighbours-
Free energy of crystallisation for interaction type (kcal/mol)
-Repeat for all interaction types from molecule / ion-
-Repeat for all molecules in unit cell-

Note: the free energy of crystallisation for interaction types first generated here will be equal to the solid angle of the molecular Voronoi Dirichlet polyhedron (VDP) face calculated in *ToposPro*. This is strictly related to the bond strength and not the free energy of crystallisation and will likely not be correct, but it is a good first approximation.