

## Visualisation Coordinates File

**name\_ovito\_CGvisualiser.XYZ:** this is a 6 column file containing the simulation output. Column 1 is the structure group / type; column 2 is the structure number; column 3 is the layer for facet colouring; columns 4, 5 and 6 contain x, y and z Cartesian coordinates that can be read into the *CrystalGrower* visualisation software or an open source visualisation program such as Ovito. This can be a single frame or multiple frames for a movie, consequently the file can become quite large.

This file contains the XYZ coordinate data for the centres of species to be drawn using the *CrystalGrower* visualisation software and Ovito. There is one general file type shared between the two programs. One key difference is the “LAYERS” vs. “TILES” option on the second line of the file. “LAYERS” denotes that the simulation was performed with the facet colouring mode activated in *CrystalGrower*, whereas “TILES” denotes that only colouring by species is available. The following sections present a real and general example for this file type. It is also worth noting at this point that “TILES” data does not exclusively apply to natural tile structures, but rather refers to natural tiles / molecules / ions coloured by species type alone. Species type in this context is the same as species group for molecular structures.

### Example

```
368728
LAYERS // 1 // 4 // 16:AFI/afi/Systre;PPT 1
1 24 2 21.500 -0.866 32.578
```

### General Example

```
Number of grown species to display in frame
“LAYERS” or “TILES” // Number of frames in file // Number of species
types in structure (species type, not species number) // Structure
Title
Species type Species number Layer number Species central X Y Z
coordinates (3 decimal places)
-Repeat for all grown species in frame-
-Repeat for all frames-
```

**Some notes on layer colouring:**

The third column titled “Layer number” will only be useful in simulations run with the “LAYERS” colouring method enabled by using the crystal facet find / colour mechanism in *CrystalGrower*.

The layer colouring pattern follows the following format, denoted by the value in the layer number column:

1 – 4 – Layers 1 through 4, the colour cycle then restarts if more than 4 layers were defined when running *CrystalGrower*.

15 – species that do not fit into any of the defined facet, or are in layers below the number of layers coloured. These are assigned a different colour to allow them to be identified easily.

If this mode is invoked along with a second defect sweep in *CrystalGrower*, the values seen will differ slightly:

1 – 4 – Layers 1 through 4, the colour cycle then restarts.

15 – species that do not fit into any of the defined facet, or are in layers below the number of layers coloured.

101-999 – Internal defects grouped by species type (e.g. 101 is an internal defect for species type 1).

> 1000 – Indirect internal defects grouped by species type (e.g. 1001 is an indirect internal defect for species type 1). These are currently not displayed in the *CrystalGrower* visualisation software but can be chosen to display or hide in Ovito.