

Visualisation Objects File

name_visualiser.vis: contains Cartesian coordinates and parameters required by the *CrystalGrower* visualisation software in order to know what tiles or molecules to assemble.

This visualisation file is an additional file required by the *CrystalGrower* visualisation software – the visualiser object data file. This file contains information on which objects construct the crystal structure to be displayed. Three types exist: natural tiles, molecular (average spheres) and molecular (atoms and bonds). The following sections present real and general examples of each of these files. The file format is automatically detected by the *CrystalGrower* visualisation software when reading in the data file.

Visualisation Objects – Natural TilesExample

1.000 1.000 1.000 90.000 90.000 90.000

5

26

48

96

1

8

6

1

4

8 3 4 7

1 0.18230 0.36840 0.00000

2 -0.00000 0.36840 -0.18230

3 -0.18230 0.36840 0.00000

4 -0.00000 0.36840 0.18230

5 0.18230 0.63160 0.00000

6 -0.00000 0.63160 -0.18230

7 -0.00000 0.63160 0.18230

8 -0.18230 0.63160 0.00000

General Example

Unit cell a b c (in relative units to a, 3 decimal places) α β γ (3 decimal places)

Number of different tiles in structure (tile number not type)

Maximum number of faces in a tile

Maximum number of vertices in a tile

Total number of vertices in all tiles

Tile number

Number of vertices in tile

Number of faces in tile

Face number

Number of vertices in face

Vertex order in face (by vertex number)

-Repeat for all face in tile-

Vertex number Vertex X Y Z -Coordinates scaled to unit cell a-

-Repeat for all vertices in tile-

-Repeat for all tiles in structure-

Visualisation Objects – Molecular (Average Spheres)Example

```
1.000  1.000  1.000  90.000  90.000  90.000
```

```
10
```

```
1
```

```
2
```

```
20
```

```
1
```

```
2
```

```
1
```

```
1
```

```
2
```

```
1 2
```

```
1 0.00000 0.00000 0.00000
```

```
2 0.00000 0.00000 0.00000
```

General Example

Unit cell a b c (in relative units to a, 3 decimal places) α β γ (3 decimal places)

Number of molecules in structure

Max number of faces in molecule, redundant, set to 1 in the CG visualiser after read in, placeholder to keep data consistent for read in across all operating modes

Max number of vertices in molecule, redundant, always equal to 2 to read in the two coordinates output by CG later

Total number of “vertices” in unit cell, always equal to 2 x number of molecules in unit cell

Molecule number

Number of “vertices” in molecule, redundant, always equal to 2

Number of “faces” in molecule, redundant, always equal to 1

“Face” number, redundant, always equal to 1

Number of “vertices” in face, redundant, always equal to 2

Vertex order in face, redundant, always 1 2

Vertex number Vertex X Y Z -Molecule's central coordinate scaled to unit cell a-

-Repeat for "vertex" 2-

-Repeat for all molecules in structure-

Visualisation Objects – Molecular (Atoms + Bonds)Example

1.000 1.000 3.420 90.000 90.000 120.000

4

3

4

10

1

4

3

1

2

1 4

1 C 0.00000 -0.00000 0.85497

2 O -0.12965 0.22456 0.85497

3 O 0.25930 -0.00000 0.85497

4 O -0.12965 -0.22456 0.85497

General Example

Unit cell a b c (in relative units to a, 3 decimal places) α β γ (3 decimal places)

Number of molecules in structure

Max number of bonds in molecule

Max number of atoms in molecule

Total number of atoms in unit cell

Molecule number

Number of atoms in molecule

Number of bonds in molecule

Bond number

Bond type (placeholder for now but can be manually changed to give single (2), double (3), triple (4), dashed (5) and dotted (6) bonds, always = 2 when generated)

Atom order in bond (by atom number)

-Repeat for all bonds in molecule-

Atom number Atom type Atom coordinates X Y Z -Coordinates scaled to
unit cell a-

-Repeat for all atoms in molecule-

-Repeat for all molecules in unit cell-