Structure File

Structure_Name.txt: This file contains all the information required for CrystalGrower to assemble a full description of the unit cell of the crystal structure to grow. All units are described, along with their connections to neighbouring units. The structure file can be generated through ToposPro or the CrystalGrower interaction program.

The structure file is the second file which is required for every *CrystalGrower* run. This file contains all information related to the crystal structure of the crystal to be simulated. Two main file types exist: “tile” (natural tiles) data for framework structures and “net” (atoms and bonds) data for molecular / ionic crystals. Its file path is defined in line 6 of input.txt, this can be specified using a file explorer window in the GUI version of *CrystalGrower*. Structure files can be generated either through the use of the *ToposPro* software or the *CrystalGrower* interaction program (discussed in another section of this manual).
Note that all relative unit cell coordinates here are presented in the primitive unit cell.
All visualisation coordinates are presented in the non-primitive unit cell, scaled to the unit cell a-length (aside from in simulations with screw dislocations – where all coordinates are in the primitive unit cell).

“Tile” Structure File

This section presents an example (along with a labelled example) for a “tile” structure file. The “tile” nomenclature is used as the file contains natural tile data calculated by *ToposPro*.

Example (ABW)

```
9:ABW/sra/Systre;PPT 1

2

t-kdq 1 (6,2)(8,3) 6

2(-1,0,1) 2(-2,-1,0) 2(-1,0,0) 2(0,0,1) 2(-1,-1,0) 2(-1,-1,1)

Si 3[4] 1(-1,-1,-1)[1] 1(-1,-1,0)[1] 1(0,-1,0)[1] 2(-1,-1,1)[1] 2(-2,-1,0)[1] 2(-1,-1,0)[1]
Si 3[4] 1(1,0,1)[1] 1(0,-1,0)[1] 2(-1,-1,1)[1] 2(0,-1,1)[1] 2(0,0,1)[] 2(-1,-1,0)[]
Si 3[4] 1(0,0,1)[1] 1(1,0,1)[1] 2(-1,-1,1)[1] 2(0,0,2)[1] 2(-1,0,1)[] 2(0,0,1)[]
Si 3[4] 1(-1,0,0)[1] 1(0,0,1)[1] 1(-1,-1,0)[1] 2(-1,-1,1)[1] 2(-1,0,1)[1] 2(-2,-1,0)[1]
Si 2[4] 1(1,0,0)[1,2] 1(1,0,1)[2] 1(0,-1,0)[1] 2(0,-1,1)[1,2] 2(0,0,1)[2] 2(-1,-1,0)[1]
Si 3[4] 1(0,0,-1)[1] 1(1,0,0)[1] 2(-1,-1,0)[1] 2(0,0,1)[] 2(-1,0,0)[] 2[1]
Si 2[4] 1(0,0,-1)[1,2] 1(-1,0,-1)[2] 1(-1,-1,-1)[1] 2(-1,-1,0)[1] 2(-1,0,0)[2] 2(-2,-1,-1)[1,2]
Si 3[4] 1(-1,0,-1)[1] 1(-1,-1,-1)[1] 2(-2,-1,0)[1] 2(-1,-1,0)[] 2(-1,0,0)[] 2(-2,-1,-1)[1]
Si 2[4] 1(1,1,0)[1,2] 1(0,1,0)[2] 1(1,1,1)[1] 2(0,0,1)[1] 2(0,1,1)[1,2] 2(-1,0,0)[2]
Si 3[4] 1(0,1,0)[1] 1(1,1,1)[1] 2(-1,0,1)[1] 2(0,0,1)[] 2(0,1,1)[1] 2(-1,0,0)[]
Si 2[4] 1(1,1,1)[1,2] 1(0,0,1)[1] 1(1,0,1)[2] 2(0,0,2)[1,2] 2(-1,0,1)[1] 2(0,0,1)[2]
```

Si 2[4] 1(1,1,0)[1,2] 1(0,0,-1)[1] 1(1,0,0)[2] 2(0,0,1)[2] 2(-1,0,0)[1] 2[1,2]
Si 3[4] 1(-1,0,-1)[1] 1(-1,0,0)[1] 2(-2,-1,0)[1] 2(-1,0,1)[] 2(-2,0,0)[1] 2(-1,0,0)[]
Si 2[4] 1(0,1,0)[1,2] 1(-1,0,-1)[2] 1(-1,0,0)[1] 2(-1,0,1)[1] 2(-2,0,0)[1,2] 2(-1,0,0)[2]

t-kdq 2 (6,2)(8,3) 6

1(1,1,0) 1(2,1,0) 1(1,0,0) 1(0,0,-1) 1(1,0,-1) 1(1,1,-1)

Si 3[4] 1(1,1,-1)[1] 1(2,1,0)[1] 1(1,0,-1)[1] 2(1,0,0)[1] 2(1,1,0)[1] 2(0,0,-1)[1]
Si 3[4] 1(1,1,-1)[1] 1(0,0,-2)[1] 1(0,0,-1)[] 1(1,0,-1)[] 2(-1,0,-1)[1] 2(0,0,-1)[1]
Si 3[4] 1(1,1,-1)[1] 1(0,1,-1)[1] 1(1,1,0)[] 1(0,0,-1)[] 2(0,1,0)[1] 2(-1,0,-1)[1]
Si 3[4] 1(1,1,-1)[1] 1(1,1,0)[1] 1(2,1,0)[1] 2(1,1,1)[1] 2(0,1,0)[1] 2(1,1,0)[1]
Si 2[4] 1(0,0,-2)[1,2] 1(0,0,-1)[2] 1(1,0,-1)[1] 2(-1,-1,-1)[1,2] 2(-1,0,-1)[2] 2(0,0,-1)[1]
Si 3[4] 1(1,0,-1)[1] 1(0,0,-1)[] 1(1,0,0)[] 1(0,-1,-1)[1] 2(0,-1,0)[1] 2(-1,-1,-1)[1]
Si 2[4] 1(1,0,-1)[1] 1(1,0,0)[2] 1(2,0,0)[1,2] 2(0,-1,0)[1,2] 2(1,0,1)[2] 2(1,0,0)[1]
Si 3[4] 1(2,1,0)[1] 1(1,0,-1)[] 1(1,0,0)[] 1(2,0,0)[1] 2(1,0,1)[1] 2(1,0,0)[1]
Si 2[4] 1(0,0,-1)[1] 1[1,2] 1(1,0,0)[2] 2(-1,-1,0)[1,2] 2(0,0,1)[2] 2(-1,0,0)[1]
Si 3[4] 1(1,1,0)[1] 1(0,0,-1)[] 1[1] 1(1,0,0)[] 2(0,0,1)[1] 2(-1,0,0)[1]
Si 2[4] 1(0,1,-1)[1,2] 1(1,1,0)[1] 1(0,0,-1)[2] 2(-1,0,0)[1,2] 2(0,1,0)[1] 2(-1,0,-1)[2]
Si 2[4] 1(0,0,-1)[2] 1(1,0,0)[1] 1(0,-1,-1)[1,2] 2(-1,-1,0)[1,2] 2(0,-1,0)[1] 2(-1,-1,-1)[2]
Si 3[4] 1(2,1,0)[1] 1(1,1,0)[] 1(2,1,1)[1] 1(1,0,0)[] 2(1,0,1)[1] 2(1,1,1)[1]

Si 2[4] 1(1,1,0)[1] 1(2,1,1)[1,2] 1(1,0,0)[2] 2(0,0,1)[1,2] 2(1,0,1)[2]
2(1,1,1)[1]

7.1062 7.1062 7.1062 I
91.998 136.609 103.796

Non primitive data
9.8730 5.2540 8.7700
90.000 90.000 90.000

t-kdq 1 14/6
1 -0.34930 -0.24660 0.60270
2 0.34930 -0.04800 1.10270
3 0.34930 0.24660 1.39730
4 -0.34930 0.04800 0.89730
5 0.65070 0.04800 0.89730
6 0.34930 0.24660 0.39730
7 -0.34930 0.04800 -0.10270
8 -0.65070 -0.04800 0.10270
9 0.65070 1.04800 0.89730
10 0.34930 0.95200 1.10270
11 0.65070 0.75340 1.60270
12 0.65070 0.75340 0.60270
13 -0.65070 0.24660 0.39730
14 -0.34930 0.75340 0.60270

4 13 14 10 11 3
4 13 8 1
12 6 7 8 13 14 10 9
9 10 11 3 2 5 6 12
1 2 5 6 7 8
1 2 3 4

t-kdq 2 14/6
1 1.34930 0.95200 0.10270
2 0.65070 0.75340 -0.39730

```
3  0.65070  1.04800 -0.10270
4  1.34930  1.24660  0.39730
5  0.34930  0.24660 -0.60270
6  0.65070  0.04800 -0.10270
7  1.34930  0.24660  0.39730
8  1.65070  0.75340  0.60270
9  0.34930  0.24660  0.39730
10  0.65070  0.75340  0.60270
11  0.34930  0.95200  0.10270
12  0.34930 -0.04800  0.10270
13  1.65070  1.04800  0.89730
14  1.34930  0.95200  1.10270

 4 13 14 10 11 3
 4 13 8 1
 12 6 7 8 13 14 10 9
 9 10 11 3 2 5 6 12
 1 2 5 6 7 8
 1 2 3 4
```

General Example

Structure name

Number of separate tiles in structure (tile number, not type)

Tile type Tile number (Number of vertices with Q number, Q number of said vertices) -Repeat for all Q numbers present in tile- Number of neighbouring tiles through faces

Tile number of neighbouring tile through face (unit cell X, unit cell Y, unit cell Z) – position of unit cell containing neighbouring tile relative to current tile's unit cell, absent if within the same unit cell. –Repeat for all neighbours through faces in tile-

Tile vertex atom type Vertex Q number in isolated tile [Max Q number of vertex] Neighbouring tile number (unit cell X, unit cell Y, unit cell Z) – position of unit cell containing neighbouring tile relative to current tile's unit cell, absent if within same unit cell – [Missing condensation number filled if this neighbouring tile condensates, -Repeat for all missing bonds up to total max Q number-] -Repeat for all neighbouring tiles through faces- –Repeat for all vertices in tile-

–Repeat for all tiles in unit cell–

Primitive unit cell a b c (4 decimal places) Unit cell type (e.g. I, F, P)
Primitive unit cell α β γ (3 decimal places)

Non primitive unit cell data
Unit cell a b c (4 decimal places)
Unit cell α β γ (3 decimal places)

Tile type Tile number Number of vertices in tile / Number of faces in tile
Vertex number Vertex X Y Z coordinates – scaled to unit cell a
-Repeat for all vertices in tile-

Vertex order in face listed by vertex number
-Repeat for all faces in tile-

“Net” Structure File

This section presents an example (along with a labelled example) for a structure file containing “net” (atoms and bonds) data. The “net” nomenclature is used as this file contains simplified crystal net data calculated either by *ToposPro* or the *CrystalGrower* interaction program.
The word “molecule” in the general example discussion is interchangeable with the word “ion”.

Example (Calcite)

```
25:Calcite

4

CO3 1 (3,0) 6

4(-1,0,0) 3(0,0,1) 4(0,-1,0) 3(1,0,0) 4(0,0,-1) 3(0,1,0)

O 0[2] 4(0,0,-1)[1] 3(0,1,0)[1]
O 0[2] 4(0,-1,0)[1] 3(1,0,0)[1]
O 0[2] 4(-1,0,0)[1] 3(0,0,1)[1]

CO3 2 (3,0) 6

4(1,0,0) 3(1,1,0) 4(0,1,0) 3(0,1,1) 4(0,0,1) 3(1,0,1)

O 0[2] 4(0,0,1)[1] 3(1,0,1)[1]
O 0[2] 4(0,1,0)[1] 3(0,1,1)[1]
O 0[2] 4(1,0,0)[1] 3(1,1,0)[1]

Ca 3 (1,0) 6

1(0,-1,0) 1(0,0,-1) 1(-1,0,0) 2(0,-1,-1) 2(-1,0,-1) 2(-1,-1,0)

Ca 0[6] 1(0,-1,0)[1] 1(0,0,-1)[1] 1(-1,0,0)[1] 2(0,-1,-1)[1] 2(-1,0,-1)[1]
2(-1,-1,0)[1]

Ca 4 (1,0) 6
```

1(1,0,0) 1(0,0,1) 1(0,1,0) 2(0,-1,0) 2(-1,0,0) 2(0,0,-1)

Ca 0[6] 1(1,0,0)[1] 1(0,0,1)[1] 1(0,1,0)[1] 2(0,-1,0)[1] 2(-1,0,0)[1]
2(0,0,-1)[1]

  6.3753   6.3753   6.3753 R
 46.078 46.078 46.078

Non primitive data
  4.9900   4.9900 17.0615
 90.000 90.000 120.000

CO3 1 4/3
1 C 0.25000 0.25000 0.25000
2 O 0.25000 0.50780 -0.00780
3 O 0.50780 -0.00780 0.25000
4 O -0.00780 0.25000 0.50780

 1 4
 1 3
 1 2

CO3 2 4/3
1 C 0.75000 0.75000 0.75000
2 O 0.75000 0.49220 1.00780
3 O 0.49220 1.00780 0.75000
4 O 1.00780 0.75000 0.49220

 1 4
 1 3
 1 2

Ca 3 1/0
1 Ca 0.00000 0.00000 0.00000

Ca 4 1/0
1 Ca 0.50000 0.50000 0.50000

General Example

Structure name

Number of separate molecules in structure

Molecule type Molecule number (Number of atoms in molecule that can form connections to neighbours, Starting coordination number of atoms excluding intramolecular coordination -always 0-) Number of neighbouring molecules

Molecule number of neighbouring molecule (unit cell X, unit cell Y, unit cell Z) – position of unit cell containing neighbouring molecule relative to current molecule's unit cell, absent if within the same unit cell.
–Repeat for all neighbours to molecule-

Atom type Atom starting coordination number excluding intramolecular coordination -always 0- [Max coordination number of atom excluding intramolecular coordination] Neighbouring molecule number (unit cell X, unit cell Y, unit cell Z) – position of unit cell containing neighbouring molecule relative to current molecule's unit cell [Number of coordination sites filled if this neighbouring molecule is grown] -Repeat for all neighbouring molecules connected to this atom-
–Repeat for all intermolecularly bonding atoms in molecule-

THIS LOCALISED BONDING INFORMATION ONLY APPEARS IN STRUCTURE FILES GENERATED THROUGH TOPOSPRO, IT IS ABSENT IN STRUCTURE FILES GENERATED THROUGH THE *CrystalGrower* INTERACTION PROGRAM, IT WILL BE REPLACED WITH:
C 0[0]

–Repeat for all molecules in unit cell–

Primitive unit cell a b c (4 decimal places) Unit cell type (e.g. I, F, P)

Primitive unit cell α β γ (3 decimal places)

Non primitive unit cell data
Unit cell a b c (4 decimal places)
Unit cell α β γ (3 decimal places)

Molecule type Molecule number Total number of atoms in molecule / Number of bonds in molecule
Atom number Atom type Atom X Y Z coordinates – scaled to unit cell a
-Repeat for all atoms in molecule-

Atom order in bond listed by atom number
-Repeat for all bonds in molecule-

For files generated with the *CrystalGrower* interaction program, the atomic structure of molecules is absent. It is replaced with central coordinates for each molecule to place a sphere at the desired position.
