

LatticeMaker Input File Format

There have been several changes to the file format that was described in previous versions. The current format now allows comment lines. These comment lines start with semicolon (;). Any text between a ; and a newline character is ignored. This allows comments to be placed at the end of lines containing information. The amount of information held in the file has been expanded to include bond angles too. To indicate to LatticeMaker that it is reading a file containing bond information the first data line of the file must start with 'v2'. A sample input file is shown below to illustrate these changes to the input format. A full list of all the atom types is given in the manual distributed with this software.

v2

; This is a version 2.0 file format for LatticeMaker

2

; There are two unique atom positions in the Unit Cell

3.14 3.24

5.18

; a,b and c cell constants in Å

90

90

120

; Angles between the axes are given here

2

5

5

; number of unit cells in the x,y,z directions

0

0

0

89

; Oxygen atom at the origin

0.5

0.5

0.5 226

; Titanium atom at the centre of the cell