The programme CASTEP\_gen\_cutoff.py will take a .cell and .param input and generate a set of inputs for different plane wave energy cutoff. The range of cutoff values can be set by editing the CASTEP\_gen\_curoff.py file.

Graphical user interface, text, application

Description automatically generated

Text

Description automatically generated

The file CASTEP\_total\_energy\_convergence.py will read a single geometry optimisation .castep output file and plot the SCF convergence per geometry optimisation step. This is mainly a sanity check the calculation has run correctly.

Graphical user interface

Description automatically generated

The CASTEP\_multiple\_file\_convergence.py will read the total energy and bond length from a series of .castep files and generate a text file for plotting with some programme. The .castep files should first all be copied to a single directory and CASTEP\_multiple\_file\_convergence.py should be run from in that directory. The energy should work for any calculation, but the bond-length probably only works properly for the primitive unit cell. This could be modified also to extract other parameters.

Text

Description automatically generated with medium confidence

The programme CASTEP\_gen\_supercell.py reads in a unit cell and generates a new larger one depending on the integers supplied in the input:

**Graphical user interface

Description automatically generated**

The file CASTEP\_reorder\_coords.py reorders the cell coordinates by z, then y, then z. This is useful after generating a larger cell from a smaller one, for example, and will be useful when working with surfaces.

Table

Description automatically generated