BuildCell - A tool for super-cell creation

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BuildCell is a perl script that creates a super-cell file from crystallographic unit cell data.

Usage

BuildCell is a command line driven program. A command has the general form

$ BuildCell [OPTIONS]

Options

Options can be given in a long form (--option[=value]) or (for almost all options) in a short form of a single character (-o [=value]). Note that the equal sign = is not mandatory, a space will do also.

Full list of options

--helplh --ciflc=<filename> --spacegroupls=<number> --latticell=< a,b,c,α,β,γ >
--symmetryly=<value> --atomla=<value> --override --debug --outputlo=<ofilename>

--helplh	display a help page
--ciflc	parse a CIF file with the name 'filename'
--spacegroupls	create a crystal with space group number 'number'
--latticell	the lattice parameters a,b,c,α,β,γ
--symmetryly	add a symmetry operation (see examples below)
--atomla	add an atom to the base (symbol,x,y,z,occupancy,Debye-Waller-factor)
--override	replace an existing output file without prompting
--debug	provide chatty output
--outputlo	write EMS cell to a file with name 'ofilename'

Examples

✦ Create an EMS super cell from a CIF file containing a hexagonal unit cell of bismuth iodine:

```
BuildCell --cif=icsd_BiI3.cif --output=BiI3.cel
```

- Create an EMS super cell containing a tetragonal unit cell of barium titanate using the space group number, the atom base and the lattice parameters:

```
BuildCell --spacegroup=99 --lattice=3.9998,3.9998,4.018,90.,90.,90. --atom=Ba,0.,0.,0.,1.0,0.45 --atom=Ti,0.5,0.5,0.482,1.0,0.5 --atom=O,0.5,0.5,0.016,1.0,0.55 --atom=O,0.50,0.,0.515,1.0,0.55  --output=BaTiO3.cel
```

- Create an EMS super cell containing an orthorhombic unit cell of calcium titanate using symmetry operations and the atom base:

```
BuildCell --symmetry=x,y,z --symmetry=x+1/2,-y+1/2,-z --symmetry=-x,-y,z+1/2 --symmetry=-x+1/2,y+1/2 ,-z+1/2 --symmetry=-x,-y,-z --symmetry=-x+1/2,y+1/2,z --symmetry=x,y,-z+1/2 --symmetry=x+1/2,-y+1/2,z+1/2  --lattice=5.37,5.44,7.64,90.,90.,90. --atom=Ca,0.,0.03,0.25,1.0,0.45 --atom=Ti,0.5,0.,0.,1.0,0.5 --atom=O,0.037,0.482,0.25,1.0,0.55 --atom=O,0.732,0.268,0.026,1.0,0.55 --output=CaTiO3.cel
```