

# ATOMS

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Generate atom lists from crystallographic data

Version 2.50

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# 1 Introduction

## 1.1 Overview

ATOMS writes a list of atomic coordinates for any crystal given its crystallographic information. The list will be sorted by radial distance from an atom chosen as the central atom. ATOMS also estimates the bulk absorption and density of the material and various corrections to XAFS data due to experimental effects.

ATOMS runs from an input file, which uses keywords to specify the input parameters. The code requires a file called `atoms.inp`. Because some operating systems are case sensitive the code will search for `ATOMS.INP` if `atoms.inp` is not found. The output is a text file that can serve as the input file for FEFF. This file is appropriate for versions of FEFF from 5 through 8, but not FEFF3 or FEFF4.

`atoms.inp` must contain all the data necessary to uniquely specify the crystal. The information that the program requires is:

1. The Hermann-Maguin or Schoenflies notation for the crystal space group. The notation conventions are slightly modified to work with a keyboard. This document lists all 230 groups as recognized by the program.
2. The non-redundant, non-default cell axis lengths and angles between the axes.
3. The two letter symbol and cell coordinates of each unique atom. The definition of unique atom is an atom occupying a unique crystallographic site. Sodium chloride (NaCl) has two unique atoms that must be specified. In Lead Titanate (PbTiO<sub>3</sub>), for example, there are two unique oxygen sites, so four unique atoms must be specified. One of the atoms must be chosen as the central atom.

Usually this data can be taken directly from the crystallography literature. When confusion arises, consult *The International Tables of X-Ray Crystallography*. This is the standard by which the program was written.

Chapter 3 should be read carefully. That chapter explains all of the conventions necessary to specify crystallographic information in ATOMS. This is a wonderful program in that it quickly generates a list of atomic coordinates for an arbitrarily complicated crystal. It is an awful program in that it requires you, the user, to speak its language. There are numerous quirks and limitations to the algorithms that interpret unit cell structure. Much error checking is included in the code. If ATOMS finds something in the input file that it does not like, it should give a useful run-time message.

The output is a file that can be used to run FEFF, the *ab initio* multiple scattering XAFS code written by Rehr and Zabinsky. The atom positions are organized into a list in the format read by FEFF. ATOMS makes reasonable guesses for several other inputs to FEFF. The `feff.inp` file generated by ATOMS will run FEFF to completion.

ATOMS has been extensively tested, but is not guaranteed to be free of bugs. If you are displeased with the result of a run and you have followed all of the instructions and hints in this document, then you may have found a bug. To report your bug, first capture to a file all screen messages from the run with the suspect input file. Send the screen messages, the input file, and any output files to the author. Also tell what kind of computer you are using and which Fortran compiler you used to make the executable. You will find the author's e-mail address on the title page of this document.

## 1.2 About Version 2.50

Version 2.50 of ATOMS is almost identical to the last version – 2.46b. The most important change is that, by default, it writes input files which are suitable for FEFF8. If you want ATOMS to write input files using the syntax of FEFF6 or FEFF7, set `feff8=false` in the ‘atoms.inp’ file.

There have also been a number of bug fixes and general code maintenance incorporated into ATOMS. A few new keywords have been added. See Chapter 2 for details regarding keywords.

Take particular note of the SCF card in the FEFF8 input file. It’s first argument determines the size of the cluster used to calculate self-consistent atomic potentials. See the FEFF document for a discussion of sensible values for this number and always be sure to edit your FEFF8 input file accordingly. A poor choice for this number can result either in poor potentials or in needlessly lengthy calculations.

For the latest information about the status of ATOMS, please see the ATOMS web site at <http://feff.phys.washington.edu/~ravel/atoms>.

## 2 Keywords

### 2.1 General Format

Take a peek at Appendix B. Included there are many examples of input files for ATOMS. Each one specifies lattice parameters, a space group, positions of atoms within the unit cell, and a few other pieces of information. The purpose of this chapter is teach you how to construct input files, thus to communicate with ATOMS.

`atoms.inp` uses keywords to describe the inputs. With only a few exceptions, the keywords are allowed to occur in any order in the file, and usually have transparent meanings. This structure allows the input file to be easily read and modified. All keywords use the syntax:

```
keyword delimiter value(s) delimiter ...
```

The delimiter can be:

1. one or more white spaces (blanks and/or TABs)
2. one equal sign and any number of white spaces
3. one comma and any number of white spaces

Most keywords take only one value. Many keywords can be put on one line (though some keywords require their own line). Internal comments can be written anywhere in `atoms.inp`, which help remind you what the keywords mean, or how you chose the input values. Keywords can be in upper, lower, or mixed case. ATOMS is not sensitive to the case of keywords or their values.

### 2.2 List of Keywords

Here is a summary of keywords and their meanings. The following sections give more detailed explanations for each keyword. Where appropriate, default values are given in brackets.

* or % or !	Indicates a comment.	
Title	Title line to write to output file.	no lines
Space	The space group designation.	no default
A	The first lattice constant.	no default
B	The second lattice constant.	[equal to A]
C	The third lattice constant.	[equal to A]
Alpha	The angle between B and C.	[90.0 deg]
Beta	The angle between C and A.	[90.0 deg]
Gamma	The angle between A and B.	[90.0 deg]
Core	Specifies absorbing atom.	no default
Rmax	Radial size of the cluster.	[5.0 A]
Index	Flag controlling indexing of atom list.	[False]
Shift	Shift coordinates of all atoms.	[0,0,0]
Out	Output file name.	[feff.inp]
Edge	Specifies absorption edge.	[K for Z>=57]
Nitrogen	Flag for fluorescence calculations.	[0.0]

Argon	Flag for fluorescence calculations.	[0.0]
Krypton	Flag for fluorescence calculations.	[0.0]
Feff	Flag for writing feff.inp.	[True]
Feff8	Flag for writing feff.inp for feff8.	[True]
Corrections	Flag for turning off McMaster corrections	
Geom	Flag for writing geom.dat file.	[False]
Unit	Flag for output file with full unit cell	[False]
P1	Flag for output file as space group p 1	[False]
Dopant	Symbols of dopant and site replaced + %	[no dopants]
Atom	Begin atom list on next line.	
Basis	Begin basis list on next line.	

---

## 2.3 Explanations of Keywords

### \* or % or ! /

Everything after one of these characters on a line in the input file will be ignored by ATOMS.

**Title** Indicates a user-chosen title line which will be written to `feff.inp`. 9 title lines of 72 characters each can be used. Everything on a line after the keyword title will be included in the title. If keywords are on the line following title, they will be read as part of the title, not as separate keywords. The word `comment` is synonymous with `title`.

**Space** This keyword is followed by the Hermann-Maguin or Schoenflies designation for the space group. Complete lists of these designations are found in Appendix A. Because the Hermann-Maguin designation, as adapted for the keyboard, includes spaces, this keyword is handled specially by ATOMS. `space` should be on its own line or at the end of a line.

**A** This specifies the first lattice constant. A must always be specified. In a cubic or rhombohedral space groups, where only one lattice parameter is needed, A is the one to specify.

**B** This specifies the second lattice constant. It is set equal to A unless specified.

**C** This specifies the third lattice constant. It is set equal to A unless specified. In tetragonal, or hexagonal space groups, this is the second lattice constant that must be specified.

**Alpha** This specifies the angle between B and C. Specify the angle in degrees. This is the angle that must be specified for rhombohedral space groups. The default value is 90 deg.

**Beta** This specifies the angle between C and A. Specify the angle in degrees. The default value is 90 deg. This is the angle that must be specified for monoclinic space groups.

**Gamma** This specifies the angle between A and B. Specify the angle in degrees. The default value is 90 deg for orthogonal groups and 120 deg for hexagonal and trigonal groups.

- Core** This specifies the absorbing atom. The value of this keyword must be a site tag. This atom will be placed at the center of the cluster and will be used as the central atom in the McMaster and fluorescent correction calculations. The central atom must be specified by this keyword. This is a change from early versions of ATOMS. This keyword has no default. A central atom must be specified. The keyword `central` is synonymous with `core`.
- Rmax** This specifies the maximum radial distance in the cluster of calculated atomic coordinates.
- Index** This is a logical flag, thus takes a value of true or false. Along with the coordinates, the atom list in `feff.inp` contains the symbol of each atom. With the index feature turned off, only the two letter symbol of each atom is printed. With it turned on, atoms of the same type will be numbered sequentially according to distance. To enable this feature, the syntax is
- ```
index true
```
- An example: in pure copper, the 12 nearest neighbors will be labeled Cu01, the 6 next neighbors will be labeled Cu02, and so on. Without indexing, all the atoms will be labeled Cu.
- Shift** Moves all atoms in the atom list by the specified amount. This keyword takes three real numbers as its values. The syntax is:
- ```
shift xvalue yvalue zvalue
```
- The value of the shift vector is simply added to all fractional atomic coordinates in the atom list. Read the section on Multiple Origins in section 3.6 for a discussion of the usefulness of this keyword.
- Out** This specifies an output file name other than `feff.inp`. It can be up to 72 characters, so can include a directory path as well as the file name. If `out = list` is specified then a file called `atoms.lis` will be written instead of `feff.inp`. `atoms.lis` will contain the title lines and the coordinate list but none of headers or FEFF keywords. This option is useful for applications other than FEFF that require a list of atomic coordinates.
- Edge** This specifies the absorption edge of the central atom. If edge is not specified, the default value is determined from the Z of the central atom. For central atoms with  $Z \leq 57$ , the K edge is chosen. For heavier atoms, the L3 edge is chosen. K, L1, L2, and L3 are the only values for edge recognized by ATOMS.
- Nitrogen** This number specifies the percentage by pressure of nitrogen gas in the I0 chamber in a fluorescence XAFS experiment. Specifying either this keyword or the argon or krypton keywords tells ATOMS to estimate the corrections to the data due to the energy response of the I0 chamber and the self-absorption of the sample. These calculations are described in detail in chapter 4. This keyword takes a real number between 0 and 1 as its value. The default is that the fluorescence calculations are turned off.
- Argon** This number specifies the percentage by pressure of argon gas in the I0 chamber in a fluorescence XAFS experiment. Specifying either this keyword or the nitrogen or krypton keywords tells ATOMS to estimate the corrections to the

data due to the energy response of the I0 chamber and the self-absorption of the sample. These calculations are described in detail in chapter 4. This keyword takes a real number between 0 and 1 as its value. The default is that the fluorescence calculations are turned off.

- Krypton** This number specifies the percentage by pressure of krypton gas in the I0 chamber in a fluorescence XAFS experiment. Specifying either this keyword or the nitrogen or argon keywords tells ATOMS to estimate the corrections to the data due to the energy response of the I0 chamber and the self-absorption of the sample. These calculations are described in detail in chapter 4. This keyword takes a real number between 0 and 1 as its value. The default is that the fluorescence calculations are turned off.
- Geom** This is a logical flag, thus takes a value of true or false. If true, ATOMS will write a file called `geom.dat` for use in the path finder module of FEFF. If `geom.dat` is written, the NOGEOM card will be written to `feff.inp`.
- Unit** This is a logical flag, thus takes a value of true or false. If true, ATOMS will write a file called `unit.dat` containing the atomic coordinates of all atoms in the unit cell as well as all atoms on the walls, edges, and corners of the unit cell.
- P1** This is a logical flag, thus takes a value of true or false. If true, ATOMS will write a file called `p1.inp`. This file is a valid input file for ATOMS. It contains the entire contents of the unit cell in the atoms list and has the space keyword set to `p 1`, the monoclinic space group of no internal symmetries. All axes and angles are explicitly specified in `p1.inp`, as are `core`, `edge`, `rmax`, and all of the title lines.
- Feff** This is a logical flag, thus takes a value of true or false. By default it is true and will write out `feff.inp`. If it is false, ATOMS will not calculate the cluster of atoms, thus will not write out either `feff.inp` or `geom.dat`.
- Dopant** This keyword specifies the type and percent substitution of a dopant material. The syntax is:
- ```
dopant dp tag percentage
```
- Where `dp` is the atomic symbol of the doping atom, `tag` is the site tag of the site where the dopant resides, and the percentage is a real number between 0 and 1 specifying the amount of substitution. If `tag` is an atomic symbol rather than a site tag, then all sites containing that atomic species will be affected.
- Atom** This must be the last keyword in the input file. If it is not the program will almost certainly stop running. This keyword tells the program to go to the next line and begin reading in the unique atom coordinates. The atom list is a five column, structured list. Column one is the two letter atomic symbol (**not** the Z number). Columns two through four contain the x, y, and z coordinates of each atom. These numbers are entered as fractions of the a, b, and c axes respectively. The fifth column contains the site tag. See section 2.4 for an explanation of the site tags. The keywords `atom` and `basis` are incompatible. If both are specified in an input file, the program will stop running.
- Basis** This must be the last keyword in the input file. If it is not the program will almost certainly stop running. This keyword tells the program to go to the



next line and begin reading in the basis atom coordinates. The basis list is a five column, structured list. Column one is the two letter atomic symbol (**not** the Z number). Columns two through four contain the x, y, and z coordinates of each atom. These numbers are entered as fractions of the a, b, and c axes respectively. The fifth column contains the site tag. See section 2.4 for an explanation of the site tags. A basis may be constructed around an empty site. Specify that site with the word `null` rather than an atomic symbol. The keywords `atom` and `basis` are incompatible. If both are specified in an input file, the program will stop running.

## 2.4 Specifying Site Tags and the Central Atom

The central atom of the cluster written to `feff.inp` must be explicitly specified with the keyword `core`. To avoid ambiguity in a situation involving inequivalent crystallographic sites containing the same atomic species, the value of this keyword must be a site tag. The site tags are the user supplied character strings which appear in the fifth column of the atom or basis list.

**Users of Atoms 2.41 and prior versions:** This is the most important difference between ATOMS 2.42 and versions numbered 2.41 and lower. Previously the fifth column of the atom or basis list was used to specify the central atom. The addition of site tags used to label the different sites requires specification of the central atom by keyword.

The fifth column of the atom list contains the site tag. The user may label the sites in any way desired and these labels may be up to 10 characters long. The sites must be labeled uniquely or else ATOMS will become confused if one of the sites labeled redundantly is chosen as the core atom. If a tag is not specified for a site then the default tag will be used. The default for a site tags is to label that site with the atomic symbol of the occupying atom. Remember that ATOMS is insensitive to case, thus the tag `THISATOM` is the same as `thisatom` and `ThisAtom`.

Here is an example. Note that the the value of `core` is a tag, not an element symbol.

```

title YBCO: Y Ba2 Cu3 O7
title  a 3.817  b 3.882  c 11.671
space P M M M
rmax=7.2          a 3.817  b 3.882  c 11.671
core= cu1
atom
! At.type  x      y      z      tag
  Y      0.5    0.5    0.5
  Ba     0.5    0.5    0.1839
  Cu     0      0      0      cu1
  Cu     0      0      0.3546  cu2
  O      0      0.5    0      01
  O      0      0      0.1589  02
  O      0      0.5    0.3780  03
  O      0.5    0      0.3783  04

```

This is the `atoms.inp` for superconducting Y Ba2 Cu3 O7. Notice that the copper and oxygen sites are tagged with unique labels. The central atom is specified with one of these

labels – the Cu1 site will be at the center of the cluster written to `feff.inp`. The yttrium and barium sites are tagged with the atomic symbol by default. Since each of these species occupies only one site, there is no ambiguity in using the atomic symbol as the tag.

In `feff.inp` each atom will be identified by its tag, not by its atomic symbol. Assignment of unique potentials, however, is based on atomic species. If you wish to assign unique potentials based on crystallographic considerations, you will need to edit `feff.inp`.

## 2.5 Basis List v. Atom List

ATOMS has the ability to recognize basis vectors. For some lattice types this is a somewhat nicer way of describing the structure. In introductory solid state physics texts, the diamond structure is often described as face centered cubic with a two atom basis. For example, silicon might be specified as a diamond structure crystal with a unique atom at position  $(1/8, 1/8, 1/8)$ . It might also be specified as an FCC structure with a basis of  $(0,0,0)$  and  $(1/4, 1/4, 1/4)$ .

ATOMS handles a basis list slightly differently from an atom list. When given an atom list, the code translates each point in the list by the symmetry operations specified in the space group name. When given a basis list, the code only performs these symmetry operations on one of the points listed. It then constructs the basis at each of the points so generated. The keyword `core` may select any atom in the basis as the central atom of the cluster.

The best use of this feature would be to generate an atom list for a structure that is described by a periodic repetition of some large, complex local structure. Clathrates are an excellent example of this.

One very important rule must be followed when using a basis list. The first atom in the list must correctly represent the desired translation symmetry. In the case of silicon, the basis must be translated like the point  $(0,0,0)$  in space group  $Fm\bar{3}m$  (the space group of FCC crystals) to yield the diamond structure. Thus the first atom in the basis list for silicon **must** be at  $(0,0,0)$  or else the basis will not be expanded correctly.

A basis can be constructed around an empty site, by specifying the coordinates of the empty site as the first entry in the basis list and entering the word `null` instead of an atomic symbol. The null site will not appear in the atom list in `feff.inp`. The keyword `core` may not take `null` as a value.

To finish the example of silicon, here are two input files that give the same output:

```

title Si, fcc with a two atom basis
a = 6.485 space F m 3 m ! space group of fcc
rmax=6.5 core=si1
basis
  Si 0.0  0.0  0.0  si1
  Si 0.25 0.25 0.25 si2
-----

title Si, diamond structure
a = 6.485 space F d 3 m ! space group of diamond
rmax 6.5
atom
  Si 0.125 0.125 0.125

```

-----

See section 3.7 for an explanation of why the silicon atom in the second example must be at  $(1/8, 1/8, 1/8)$  rather than at  $(0,0,0)$ .

## 2.6 Dopants

ATOMS handles dopants in the simplest possible fashion. It assumes all dopants are substitutional and that there are no correlations between cells regarding which lattice sites are occupied by doping atoms. Furthermore, ATOMS makes no assumptions about which physical sites are occupied by dopants. Thus the atom list written to `feff.inp` is the list for the undoped structure. ATOMS uses information about the dopants in the following ways:

1. For calculating the density, the absorption, and the experimental corrections.
2. A dopant may be the central atom in the atom list, thus the calculations mentioned above will be performed at the absorption edge of the dopant.

The syntax is:

```
dopant dp tag percentage
```

where `dp` and `tag` are character strings and `percentage` is a number between 0 and 1. The value of `dp` is the atomic symbol of the dopant. The value of `tag` is the site tag of the site where the dopant resides. If the value of `tag` is an atomic symbol then all sites containing that atomic species will be doped.

ATOMS allows up to 3 dopants per site and no more than 9 in the entire crystal. If this is insufficient, then you have a mess on your hands. You also have my sympathy – contact me and I will help you alter the code to accommodate your horrid problem.

The atomic species specified for a site by the dopant keyword need not be the minority component. This might be useful for uniquely specifying the core atom. Vacancies may be introduced by doping sites with `null`.

Analyzing a doped material in fine structure spectroscopies is complicated. The simple scheme that I describe in this section is useful for several of the calculations in the code, but is clearly insufficient for the task of resolving the local structure of a doped material. That ATOMS writes the atom list in `feff.inp` using the undoped structure is indicative of this.

## 2.7 geom.dat

The path finder in FEFF has an option to use crystal symmetries in order to speed the determination and computation of all paths. This is done by providing a file called `geom.dat` containing special flags specifying the relevant symmetries. Setting `geom = true` in `atoms.inp` will tell ATOMS to write a `geom.dat` file and to place the card `NOGEOM` in `feff.inp`. This leads to a large reduction of computation time only in crystals of high symmetry. In an fcc structure, the reduction in time can be as high as a factor of about 50. In a structure of lower symmetry, the savings will rarely be more than a factor of about 4. Use of the `geom.dat` generated by ATOMS will not effect the computation time of the potentials and phase shifts calculation of the first module of FEFF, nor will it effect the computation time of the individual paths in the third module. The `geom.dat` file has the same atom list as the `feff.inp` file.

To use the `geom.dat` file, it must be located in the directory in which `FEFF` is run. Since the `NOGEOM` card is in `feff.inp`, `FEFF` will know to access at the appropriate time the `geom.dat` file written by `ATOMS`. The `geom.dat` file and the atom list in `feff.inp` should both remain unmodified, or else `FEFF` might get confused. The `FEFF` card `RMAX` can be changed to limit the extent of the `FEFF` calculation without needing to change `geom.dat`. See the `FEFF` document for more details about this.

## 3 Space Groups

### 3.1 Notation Conventions

The two most commonly used standards for the designation of three dimensional space groups are the Hermann-Maguin and Schoenflies conventions. ATOMS recognizes both conventions. Each of the 230 space groups as designated in each convention is listed in appendix A.

The Hermann-Maguin system uses four symbols to uniquely specify the group properties of each of the 230 space groups. The first symbol is a single letter (P, I, R, F, A, B or C) which refers to the Bravais lattice type. The remaining three letters refer to the point group of the crystal.

Some modifications to the notation convention are made for use with a keyboard. Spaces must separate each of the four symbols. Subscripted numbers are printed next to the number being modified (e.g. 6<sub>3</sub> is printed as 63). A bar above a number is entered with a minus sign.

Occasionally there are variations in how space groups are referenced. For example, the hausmannite structure of Mn<sub>3</sub>O<sub>4</sub> is placed in space group I 41/A M D by the conventions laid out in *The International Tables*. In *Crystal Structures* v. 3, Wyckoff denotes this space group as I 4/A M D. This sort of incongruity is unfortunate. The list of Hermann-Maguin space group designations as recognized by ATOMS is included in appendix A. If you cannot resolve the incongruity using this list, try using the Schoenflies notation.

The Schoenflies conventions are also recognized by ATOMS. In the literature there is less variation in the application of these conventions. The Schoenflies convention is, in fact, less precise than the Hermann-Maguin in that the complete symmetry characteristics of the crystal are not encoded in the space group designation. Adaptations to the keyboard have been made here as well. Subscripts are denoted with an underscore (\_) and superscripts are denoted with a caret (^). Spaces are not allowed in the keyboard designation. A couple of examples: d<sub>4</sub><sup>8</sup>, and O<sub>5</sub>. The underscore does not need to precede to superscript. C<sub>2</sub><sup>V9</sup> can also be written C<sup>V9</sup><sub>2</sub>. Each of the 230 space groups as designated by the Schoenflies notation is listed in Appendix A in the same order as the listing of the Hermann-Maguin notation. The two conventions are equally supported in the code.

### 3.2 Unique Crystallographic Positions

The atom or basis list in `atoms.inp` is a list of the unique crystallographic sites in the unit cell. A unique site is one (and only one) of a group of equivalent positions. The equivalent positions are related to one another by the symmetry properties of the crystal. ATOMS determines the symmetry properties of the crystal from the name of the space group and applies those symmetry operations to each unique site to generate all of the equivalent positions.

If you include more than one of a group of equivalent positions in the atom or basis list, then a few odd things will happen. A series of run-time messages will be printed to the screen telling you that atom positions were found that were coincident in space. This is because each of the equivalent positions generated the same set of points in the unit cell. ATOMS removes these redundancies from the atom list. The atom list and the potentials

list written to `feff.inp` will be correct and FEFF can be run correctly using this output. However, the site tags and the indexing of the atoms will certainly make no sense. Also the density of the crystal will be calculated incorrectly, thus the absorption calculation (section 4.1) and the self-absorption correction (section 4.3) will be calculated incorrectly as well. The McMaster correction (section 4.2) is unaffected.

### 3.3 Specially Recognized Lattice Types

For some common crystal types it is convenient to have a shorthand way of designating the space group. For instance, one might remember that copper is an fcc crystal, but not that it is in space group  $F M \bar{3} M$  (or  $O_H^5$ ). In this spirit, ATOMS will recognize the following words for common crystal types. These words may be used as the value of the keyword `space` and ATOMS will supply the correct space group. Note that several of the common crystal types are in the same space groups. For copper it will still be necessary to specify that an atom lies at (0,0,0), but it isn't necessary to remember that the space group is  $F M \bar{3} M$ .

|                      |                   |                 |
|----------------------|-------------------|-----------------|
| cubic                | cubic             | $P M \bar{3} M$ |
| body-centered cubic  | bcc               | $I M \bar{3} M$ |
| face-centered cubic  | fcc               | $F M \bar{3} M$ |
| halite               | salt or nacl      | $F M \bar{3} M$ |
| zincblende           | zincblende or zns | $F \bar{4} 3 M$ |
| cesium chloride      | cscl              | $P M \bar{3} M$ |
| perovskite           | perovskite        | $P M \bar{3} M$ |
| diamond              | diamond           | $F D \bar{3} M$ |
| hexagonal close pack | hex or hcp        | $P 63/M M C$    |
| graphite             | graphite          | $P 63 M C$      |

When `space` is set to hex or graphite, `gamma` is automatically set to 120.

### 3.4 Bravais Lattice Conventions

ATOMS assumes certain conventions for each of the Bravais lattice types. Listed here are the labeling conventions for the axes and angles in each Bravais lattice.

- Triclinic: All axes and angles must be specified.
- Monoclinic: B is the perpendicular axis, thus `beta` is the angle not equal to 90.
- Orthorhombic: A, B, and C must all be specified.
- Tetragonal: The C axis is the unique axis in a tetragonal cell. The A and B axes are equivalent. Specify A and C in `atoms.inp`.
- Trigonal: If the cell is rhombohedral then the three axes are equivalent as are the three angles. Specify A and `alpha`. If the cell has hexagonal axes, specify A and C. `gamma` will be set to 120 by the program.
- Hexagonal: The equivalent axes are A and B. Specify A and C in `atoms.inp`. `Gamma` will be set to 120 by the program.
- Cubic: Specify A in `<tt /atoms.inp/`. The other axes will be set equal to A and the angles will all be set to 90.

### 3.5 Low Symmetry Space Groups

In three dimensional space there is an ambiguity in choice of right handed coordinate systems. Given a set of mutually orthogonal axes, there are six choices for how to label the positive  $x$ ,  $y$ , and  $z$  directions. For some specific physical problem, the crystallographer might choose a non-standard setting for a crystal. The choice of standard setting is described in detail in *The International Tables*. The Hermann-Maguin symbol describes the symmetries of the space group relative to this choice of coordinate system.

The symbols for triclinic crystals and for crystals of high symmetry are insensitive to choice of axes. Monoclinic and orthorhombic notations reflect the choice of axes for those groups that possess a unique axis. Tetragonal crystals may be rotated by 45 degrees about the  $z$  axis to produce a unit cell of doubled volume and of a different Bravais type. Alternative symbols for those space groups that have them are listed in Appendix A.

ATOMS recognizes those non-standard notations for these crystal classes that are tabulated in *The International Tables*. `atoms.inp` may use any of these alternate notations so long as the specified cell dimensions and atomic positions are consistent with the choice of notation. Any notation not tabulated in chapter 6 of the 1969 edition of *The International Tables* will not be recognized by ATOMS.

This resolution of ambiguity in choice of coordinate system is one of the main advantages of the Hermann-Maguin notation system over that of Schoenflies. In a situation where a non-standard setting has been chosen in the literature, use of the Schoenflies notation will, for many space groups, result in unsatisfactory output from ATOMS. In these situations, ATOMS requires the use of the Hermann-Maguinn notation to resolve the choice of axes.

Here is an example. In the literature reference, La<sub>2</sub> Cu O<sub>4</sub> was given in the non-standard `b m a b` setting rather than the standard `c m c a`. As you can see from the axes and coordinates, these settings differ by a 90 degree rotation about the A axis. The coordination geometry of the output atom list will be the same with either of these input files, but the actual coordinates will reflect this 90 degree rotation.

```

title La2CuO4 structure at 10K from Radaelli et al.
title standard setting
space c m c a
a= 5.3269 b= 13.1640 c= 5.3819
rmax= 8.0 core= la
atom
  la 0      0.3611  0.0074
  Cu 0      0      0
  O  0.25  -0.0068 -0.25   o1
  O  0      0.1835 -0.0332 o2
-----

```

```

title La2CuO4 structure at 10K from Radaelli et al.
title non standard setting, rotated by 90 degrees about A axis
space b m a b
a= 5.3269 b= 5.3819 c= 13.1640
rmax= 8.0 core= la

```

```

atom
  la  0      -0.0074   0.3611
  Cu  0        0        0
  O   0.25    0.25    -0.0068   o1
  O   0        0.0332   0.1835   o2
-----

```

### 3.6 Rhombohedral Space Groups

There are seven rhombohedral space groups. Crystals in any of these space groups that may be represented as either monomolecular rhombohedral cells or as trimolecular hexagonal cells. These two representations are entirely equivalent. The rhombohedral space groups are the ones beginning with the letter R in the Hermann-Maguin notation. ATOMS does not care which representation you use, but a simple convention must be maintained. If the rhombohedral representation is used then the keyword **alpha** must be specified in `atoms.inp` to designate the angle between the rhombohedral axes and the keyword **a** must be specified to designate the length of the rhombohedral axes. If the hexagonal representation is used, then **a** and **c** must be specified in `atoms.inp`. **Gamma** will be set to 120 by the code. Atomic coordinates consistent with the choice of axes must be used.

### 3.7 Multiple Origins and the Shift Keyword

Some space groups in *The International Tables* are listed with two possible origins. The difference is only in which symmetry point is placed at (0,0,0). ATOMS always wants the orientation labeled “origin-at-centre”. This orientation places (0,0,0) at a point of highest crystallographic symmetry. Wyckoff and other authors have the unfortunate habit of not choosing the “origin-at-centre” orientation when there is a choice. Again Mn<sub>3</sub>O<sub>4</sub> is an example. Wyckoff uses the “origin at -4m<sup>2</sup>” option, which places one Mn atom at (0,0,0) and another at (0,1/4,5/8). ATOMS wants the “origin-at-centre” orientation which places these atoms at (0,3/4,1/8) and (0,0,1/2). Admittedly, this is an arcane and frustrating limitation of the code, but it is not possible to conclusively check if the “origin-at-centre” orientation has been chosen.

Twenty one of the space groups are listed with two origins in *The International Tables for X-Ray Crystallography*. ATOMS knows which groups these are and by how much the two origins are offset, but **cannot** know if you chose the correct one for your crystal. If you use one of these groups, ATOMS will print a run-time message warning you of the potential problem and telling you by how much to shift the atomic coordinates in `atoms.inp` if the incorrect orientation was used. This warning will also be printed at the top of the `feff.inp` file. If you use the “origin-at-center” orientation, you may ignore this message.

If you use one of these space groups, it usually isn’t hard to know if you have used the incorrect orientation. Some common problems include atoms in the atom list that are very close together (less than 1 angstrom), unphysically large densities (see section 4.1), and interatomic distances that do not agree with values published in the crystallography literature. Because it is tedious to edit the atomic coordinates in the input file every time this problem is encountered and because forcing the user to do arithmetic (any good scientist’s bugaboo!) invites trouble, there is a useful keyword called **shift**. For the Mn<sub>3</sub>



O4 example discussed above, simply insert this line in `atoms.inp` if you have supplied coordinates referenced to the incorrect origin:

```
shift = 0.0 0.25 -0.125
```

This vector will be added to all of the coordinates in the atom list after the input file is read.

Here is the input file for Mn3 O4 using the shift keyword:

```
title Mn3O4, hausmannite structure, using the shift keyword
a      5.75    c      9.42 core   Mn2
rmax   7.0     Space  i 41/a m d
shift  0.0 0.25 -0.125
atom
! At.type  x    y    z    tag
Mn        0.0 0.0  0.0   Mn1
Mn        0.0 0.25 0.625 Mn2
O         0.0 0.25 0.375
```

---

The above input file gives the same output as the following. Here the shift keyword has been removed and the shift vector has been added to all of the fractional coordinates. These two input files give equivalent output.

```
title Mn3O4, hausmannite structure, no shift keyword
a      5.75    c      9.42 core   Mn2
rmax   7.0     Space  i 41/a m d
atom
! At.type  x    y    z    tag
Mn        0.0 0.25 -0.125 Mn1
Mn        0.0 0.50  0.50   Mn2
O         0.0 0.50  0.25
```

---

## 4 Absorption Calculation and Experimental Corrections

Included in ATOMS is data from *Compilation of X-Ray Cross Sections* by McMaster, et al. Using this and the crystallographic information from `atoms.inp`, ATOMS is able to make several calculations useful for XAFS analysis. It approximates the absorption depth and edge step size of the material at the edge energy of the core atom and estimates three corrections needed for the analysis of XAFS data. These corrections are the “McMaster correction”, the energy response of the I0 chamber in a fluorescence experiment, and the self-absorption of a thick material in a fluorescence experiment. All of these numbers are written at the top of the output file. For more information on these calculations consult Chapter 10 of *Handbook of Synchrotron Radiation, v.1*.

### 4.1 Absorption Calculation

Proper sample preparation for an XAFS experiment requires knowledge of the absorption depth and edge step size of the material of interest. The statistics of data collection can be optimized by choosing the correct sample thickness. It is also necessary to avoid distortions to the data due to thickness and large particle size effects.

ATOMS calculates the total cross section of the material above the edge energy of the central atom and divides by the unit cell volume. The number obtained,  $\mu_{total}$ , has units of  $\text{cm}^{-1}$ . Thus, if  $x$  is the thickness of the sample in cm, the x-ray beam passing through the sample will be attenuated by  $\exp(-\mu_{total} * x)$ .

ATOMS also calculates the change in cross section of the central atom below and above the absorption edge and divides by the unit cell volume. This number,  $\Delta\mu$ , multiplied by the sample thickness in cm gives the approximate edge step in a transmission experiment.

The density of the material is also reported. This number assumes that the bulk material will have the same density as the unit cell. It is included as an aid to sample preparation.

### 4.2 McMaster Correction

Typically, XAFS data is normalized to a single number representing the size of the edge step. While there are compelling reasons to use this simple normalization, it can introduce an important distortion to the amplitude of the  $\chi(k)$  extracted from the absorption data. This distortion comes from energy response of the bare atom absorption of the central atom. This is poorly approximated away from the edge by a single number. Because this affects the amplitude of  $\chi(k)$  and not the phase, it can be corrected by including a Debye-Waller factor and a fourth cumulant in the analysis of the data. These two “McMaster corrections” are intended to be additive corrections to any thermal or structural disorder included in the analysis of the XAFS.

ATOMS uses data from McMaster to construct the bare atom absorption for the central atom. ATOMS then regresses a quadratic polynomial in energy to the natural logarithm of the constructed central atom absorption. Because energy and photo-electron wave number are simply related,  $E$  is proportional to  $k^2$ , the coefficients of this regression can be related to the XAFS Debye-Waller factor and fourth cumulant. The coefficient of the term linear in energy equals  $2 * \sigma_M M^2$  and the coefficient of the quadratic term equals  $4/3 * \sigma_M M^4$ . The values of  $\sigma_{MM^2}$  and  $\sigma_{MM^4}$  are written at the top of the output file.

### 4.3 I0 Correction.

The response of the I0 chamber varies with energy during an XAFS experiment. In a fluorescence experiment, the absorption signal is obtained by normalizing the IF signal by the I0 signal. There is no energy response in the IF signal since all atoms fluoresce at set energies. The energy response of I0 is ignored by this normalization. At low energies this can be a significant effect. Like the McMaster correction, this effect attenuates the amplitude of  $\chi(k)$  and is well approximated by an additional Debye-Waller factor and fourth cumulant.

ATOMS uses the values of the nitrogen, argon and krypton keywords in `atoms.inp` to determine the content of the I0 chamber by pressure. It assumes that the remainder of the chamber is filled with helium. It then uses McMaster's data to construct the energy response of the chamber and regresses a polynomial to it in the manner described above. `sigma_I0^2` and `sigma_I0^4` are also written at the top of the output file and intended as additive corrections in the analysis.

### 4.4 Self-Absorption Correction.

If the thickness of a sample is large compared to absorption length of the sample and the absorbing atom is sufficiently concentrated in the sample, then the amplitude of the  $\chi(k)$  extracted from the data taken on it in fluorescence will be distorted by self-absorption effects in a way that is easily estimated. The absorption depth of the material might vary significantly through the absorption edge and the XAFS wiggles. The correction for this effect is well approximated as

$$1 + \mu_{\text{abs}} / (\mu_{\text{background}} + \mu_{\text{fluor}})$$

where `mu_background` is the absorption of the non-resonant atoms in the material and `mu_fluor` is the total absorption of the material at the fluorescent energy of the absorbing atom. ATOMS constructs this function using the McMaster tables then regresses a polynomial to it in the manner described above. `sigma_self^2` and `sigma_self^4` are written at the top of the output file and intended as additive corrections in the analysis. Because the size of the edge step is affected by self-absorption, the amplitude of  $\chi(k)$  is attenuated when normalized to the edge step. Since the amplitude is a measure of  $S0^2$ , this is an important effect. The number reported in `feff.inp` as the amplitude factor is intended to be a multiplicative correction to the data or to the measured  $S0^2$ .

## 5 A Worked Example

Here is an example of ATOMS in action. The material is Lead Titanate,  $\text{PbTiO}_3$ . The crystallographic literature places this material in the tetragonal space group  $P4mm$ . The data was taken in fluorescence at the titanium K-edge. Since the edge energy is around 5 KeV and the sample was very thick, the I0 and self-absorption corrections are expected to be significant. That titanium is the central atom is indicated by the keyword `core`. ATOMS assumes the K-edge of the titanium was probed because the atomic number of titanium is less than 57 and the edge was not otherwise chosen with the `edge` keyword. The I0 chamber was filled with 92% helium and 8% nitrogen by pressure. This is indicated by the `nitrogen` keyword. The indexing feature is engaged with the `index` keyword. The size of the cluster to be printed in `feff.inp` is chosen with the `rmax` keyword.

```

title PbTiO3 10K,a=3.885,c=4.139
space P 4 m m
a=3.885          c=4.139          nitrogen = 0.08
index=true      rmax=4.2          core=ti
atom
! At.type x      y      z      tag
  Pb    0.0  0.0  0.0
  Ti    0.5  0.5  0.5377
  O     0.5  0.5  0.1118 axial
  O     0.0  0.5  0.6174 planar

```

ATOMS produces the output reproduced below. The absorption and correction calculations are at the top of the file. All the CONTROL cards are set to 1 and the PRINT cards are set to 0. This will run all four modules of FEFF and produce the default output files. Several other useful FEFF cards are printed but commented out by an asterisk (\*). The unique potential list is constructed in a simple fashion – the core atom is potential 0 and each different atomic species has a single potential. The atom list is printed in the format required by FEFF. The atom list has two comment columns. The indexed atomic symbol and radial distance are written by ATOMS for your use when reading `feff.inp` and are ignored by FEFF.

FEFF will run to completion using the input file generated by ATOMS. It is still likely that the user will want to edit `feff.inp`. Several assumptions are made by ATOMS that might not hold true. The assignment of unique potentials is made by a simple algorithm and may not adequately reflect the physics of the problem. The CONTROL cards are such that all four modules of FEFF will be run. The FEFF user might want to run the modules separately. Values for other cards have been assumed and might not be desired. Other cards have been left out entirely. Always check your `feff.inp` file to be sure it is just what you want.

```

* This feff.inp file generated by ATOMS, version 2.50
* ATOMS written by and copyright (c) Bruce Ravel, 1998

* -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- *
*      total mu =      5269.6 cm^-1, delta mu =      772.6 cm^-1
*      specific gravity = 8.057, cluster contains 21 atoms.

```

```

* -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- *
*      mcmaster corrections:  0.00093 ang^2 and  0.165E-05 ang^4
*      self-abs. corrections: amplitude factor =  1.087
*                               0.00004 ang^2 and  0.461E-07 ang^4
*      i0 corrections:        0.00118 ang^2 and  0.122E-05 ang^4
* -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- *
*      sum of corrections:    0.00216 ang^2 and  0.292E-05 ang^4
* -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- * -- *

TITLE  PbTiO3 10K,a=3.885,c=4.139

EDGE   K
S02    1.0

*      pot      xsph  fms   paths  genfmt  ff2chi
CONTROL  1      1     1     1     1     1
PRINT   1      0     0     0     0     0

RPATH   0
*      r_scf    [ l_scf  n_scf  ca ]
SCF     3.5     0     15    0.1

*      ixc     [ Vr  Vi ]
EXCHANGE 0      0     0

EXAFS
*      kmax    [ delta_k  delta_e ]
*XANES  4.0     0.5     0.5
*      r_fms    [ l_fms ]
*FMS    3.87816  0.00000
*      emin    emax  resolution
*LDOS   -20    20     0.1

POTENTIALS
*      ipot    z  label  l_scm  l_fms  stoichiometry
        0     22  Ti    -1     -1     0
        1     8   0     -1     -1     1
        2    82  Pb    -1     -1     1
        3    22  Ti    -1     -1     1

ATOMS
  0.00000  0.00000  0.00000  0  Ti_00  0.00000
  0.00000  0.00000 -1.76280  1  axial_01  1.76280
-1.94250  0.00000  0.32988  1  planar_01  1.97031
  0.00000 -1.94250  0.32988  1  planar_01  1.97031
  1.94250  0.00000  0.32988  1  planar_01  1.97031
  0.00000  1.94250  0.32988  1  planar_01  1.97031

```

|          |          |          |   |          |         |
|----------|----------|----------|---|----------|---------|
| 0.00000  | 0.00000  | 2.37620  | 1 | axial_02 | 2.37620 |
| 1.94250  | 1.94250  | 1.91346  | 2 | Pb_01    | 3.34783 |
| -1.94250 | -1.94250 | 1.91346  | 2 | Pb_01    | 3.34783 |
| 1.94250  | -1.94250 | 1.91346  | 2 | Pb_01    | 3.34783 |
| -1.94250 | 1.94250  | 1.91346  | 2 | Pb_01    | 3.34783 |
| 1.94250  | 1.94250  | -2.22554 | 2 | Pb_02    | 3.53548 |
| 1.94250  | -1.94250 | -2.22554 | 2 | Pb_02    | 3.53548 |
| -1.94250 | -1.94250 | -2.22554 | 2 | Pb_02    | 3.53548 |
| -1.94250 | 1.94250  | -2.22554 | 2 | Pb_02    | 3.53548 |
| 3.88500  | 0.00000  | 0.00000  | 3 | Ti_01    | 3.88500 |
| 0.00000  | -3.88500 | 0.00000  | 3 | Ti_01    | 3.88500 |
| -3.88500 | 0.00000  | 0.00000  | 3 | Ti_01    | 3.88500 |
| 0.00000  | 3.88500  | 0.00000  | 3 | Ti_01    | 3.88500 |
| 0.00000  | 0.00000  | -4.13900 | 3 | Ti_02    | 4.13900 |
| 0.00000  | 0.00000  | 4.13900  | 3 | Ti_02    | 4.13900 |

END

## 6 Program Notes

### 6.1 Acknowledgments

I would like to thank my many colleagues who have been a source of help and inspiration. The support of Profs. Ed Stern and John Rehr has always been appreciated. I would like to thank Chuck Bouldin, Boyan Boyanovich, Julie Cross, Tim Elam, Matt Newville, Hans Stragier, Kalle Voss, Steve Zabinsky, and Yanjun Zhang for their contributions, helpful criticism and useful suggestions as I have developed this program.

The essential calculation in this program is handled in the routine `equipt`, which decodes the Hermann-Maguin notation and performs the proscribed symmetry operations on the input atomic coordinates. This routine was written by H. Burzlaff and A. Hountas and is in the public domain. Several parts of this program were inspired by the program `SEXIE` by Bernhard Rupp. `SEXIE` uses input files that are similar to `atoms.inp` and its database is a good resource for composing `atoms.inp` files. The original version of the routine `mucal` was written by P. Bandyopadhyay using data from *Compilation of X-Ray Cross Section* by McMaster et. al. Several of the character string manipulation routines (`triml`, `istrln`, `upper`, `lower`, `bwords`) were written by S.I. Zabinsky and M. Newville and released for this use.

### 6.2 Comments on the Fortran Code

Every routine used by `ATOMS` has been written in ANSI standard Fortran-77. At the time of this writing the code has been found to compile and run under many different operating systems. Presently, the code is developed on an Intel 486 laptop which runs Linux using F2C and GCC for compilation. The code is thus easily ported to any machine with a Fortran compiler. The author has run `ATOMS` under four different unices, MS-DOS, Macintosh System 7.5, Vax-VMS, and Open-VMS on an DEC Alpha. At this time, there are four caveats for the user:

1. In the main program, the unit for the output files are opened with status `unknown`. On VMS machines, it is more convenient, but not necessary, to open files with `new` status to take advantage of multiple versions of files. To change this for use on a Vax-VMS machine, search for the line in the main program where the variable `vaxflg` is defined and change it to `.true`.
2. All run-time messages are written by the subroutine `messag`. Thus if your machine has particular requirements for writing to standard output, `messag` should be the only routine that you need to alter.
3. Tab characters are allowed in the input file, even though the handling of tab characters might be machine specific. This is done by reading a line from the input file and filtering it through a subroutine called `untab`, which replaces tab characters with blank spaces. `untab` is written assuming tab is ASCII character 9. If your machine handles this differently, you only need to edit `untab` or simply don't use tabs.
4. The character string manipulation assumes the ASCII character set. If your machine does not use ASCII, then you are probably familiar with how to alter code for use on your machine. Contact the author for which subroutines need to be altered.

If you ever have a problem with carriage-control while using ATOMS or FEFF with a `feff.inp` file generated by ATOMS, please contact the author.

ATOMS is delivered with the following parameter values:

1. `iat` = 20, maximum number of unique atoms
2. `natx` = 800, maximum number of atoms in cluster
3. `ntitx` = 9, maximum number of title lines
4. `maxln` = 800, maximum number of atoms in `feff.inp`

FEFF limits the size of the cluster in its calculation to 400 atoms. In ATOMS these values are imposed by parameter statements, thus are easy to change. Global parameters such as these are set in the main program and passed as arguments to the rest of the program. Find these near the beginning of the main program and change them to whatever value you want. If you do not know exactly how to do this but still think you need to, consult your local Fortran guru or, if you must, the author.

The source code for ATOMS is written in a style with mostly lower case characters. All executable statements are written in lower case. This is a departure from strict adherence to the ANSI standard. Care has been taken to make the code insensitive to case. That is, the source may be placed in all upper case or all lower case without damaging its functionality. The algorithm that parses the input file is certainly insensitive to case.

### 6.3 What is new since version 2.42

1. Correct handling of hexagonal space groups. This is the most important new feature. My chagrined thanks to the **many** people who discovered this little problem and took the time to tell me about it. I also improved handling of trigonal and rhombohedral space groups.
2. Support for notations of all settings of orthorhombic, tetragonal, and monoclinic space groups. `<sl/atoms/` is now fully compliant with all Hermann-Maguin short notations as specified in `<it/The International Tables of X-Ray Crystallography/`, 1969 edition.
3. Better recognition of Schoenflies notation.
4. Improved error messages. Hopefully my error messages are now more informative and spelled correctly.
5. Improvements to the calculations using the McMaster tables. I have also corrected a few incorrect values that have been found in the electronic version of the McMaster tables.
6. Addition of `p1` and `krypton` keywords.
7. Improved writing of `geom.dat` files.
8. Improved handling of input and output filenames.
9. Allow L1 and L2 edges for `feff.inp`.
10. Writing of five digits after the decimal places in `feff.inp`. This matches the precision of `<sl/feff/`'s degeneracy checker.
11. Writing of edge energy in the HOLE line of `feff.inp`. This is for informational purposes only, it serves no purpose in `<sl/feff/`.



## 6.4 Naming Conventions

Between versions 2.41 and 2.42, my program had a name change. Earlier versions were called ATOM, while later versions are called ATOMS, with an s. The reason for this change was to avoid confusion with the subroutine `atom` that is an important part of FEFF. Hopefully this reduces confusion rather than adds to it! For now, the version number is incremented by 0.01 when minor functionality is added and by 0.1 when major functionality is added. Bug corrections have been denoted with an incrementing letter appended to the version number.

## 6.5 Obtaining New Copies of Feff or of the UWXAFS Analysis Programs

If you do not have a license to use the UWXAFS analysis programs or FEFF and are interested in obtaining one contact:

Ed Stern  
c/o UWXAFS Project  
University of Washington  
Department of Physics, FM-15  
Seattle WA, 98195, USA  
phone: (206) 543-2023  
fax: (206) 543-0635  
electronic mail: [stern@phys.washington.edu](mailto:stern@phys.washington.edu)

or

John Rehr  
c/o Feff Project  
University of Washington  
Department of Physics, FM-15  
Seattle WA, 98195, USA  
phone: (206) 543-8593  
fax: (206) 543-0635  
electronic mail: [jjr@phys.washington.edu](mailto:jjr@phys.washington.edu)

You should request copies of the licensing agreements for FEFF and the UWXAFS programs. These are licensed separately. ATOMS is distributed with both packages.

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## Appendix A Denoting Space Groups

This appendix is my attempt to demystify the crazy symbolism used by the Hermann-Maguin and Schoenflies conventions. This is by no means an adequate explanation of the rich and beautiful field of crystallography. For that, I recommend one of the books in the bibliography.

An important part of the demystification process is to define some of the important terms used to describe crystal symmetries. The words *system*, *Bravais lattice*, *crystal class*, and *space group* have well-defined meanings. The symbols used in each of the notation conventions specifically relate the various symmetries of crystals. In crystallography, a symmetry operation is defined as a sequence of reflections, translations, and/or rotations that map the crystal back onto itself in such a way that the crystal after the mapping is indistinguishable from the crystal before the mapping.

### A.1 A Quick Review of Crystallography

To start, here are some definitions. These will be elaborated below.

- System: The undecorated shape of the unit cell.
- Bravais Lattice: An undecorated lattice of equivalent points.
- Crystal Class: The description of the symmetries about a point.
- Space Group: The complete description of three dimensional crystal symmetries.

There are seven systems of crystals. The system refers to the shape of the undecorated unit cell. They are:

- Triclinic:  $a \neq b \neq c$ ,  $\alpha \neq \beta \neq \gamma \neq 90$  deg
- Monoclinic:  $a \neq b \neq c$ ,  $\alpha = \gamma = 90$  deg,  $\beta \neq 90$  deg
- Orthorhombic:  $a \neq b \neq c$ ,  $\alpha = \beta = \gamma = 90$  deg
- Tetragonal:  $a = b \neq c$ ,  $\alpha = \beta = \gamma = 90$  deg
- Hexagonal:  $a = b \neq c$ ,  $\alpha = \beta = 90$  deg,  $\gamma = 120$  deg
- Trigonal: (rhombohedral axes):  
 $a = b = c$ ,  $\alpha = \beta = \gamma < 120$  deg  $\neq 90$  deg (hexagonal axes):  
 $a = b \neq c$ ,  $\alpha = \beta = 90$  deg,  $\gamma = 120$  deg
- cubic:  $a = b = c$ ,  $\alpha = \beta = \gamma = 90$  deg

There are fourteen Bravais lattices. The Bravais lattices are constructed from the simplest translational symmetries applied to the seven crystal systems. A **P** lattice has decoration only at the corners of the unit cell. An **I** lattice has decoration at the body center of the cell as well as at the corners. An **F** lattice has decoration at the face centers as well as at the corners. A **C** lattice has decoration at the center of the (001) face as well as at the corners. Likewise **A** and **B** lattices have decoration at the centers of the (100) and (010) faces respectively. **R** lattices are a special type in the trigonal system which possess rhombohedral symmetry.

All seven crystal systems have **P** lattices, but not all the classes have the other type of Bravais lattices. This is because there is degeneracy when all the Bravais lattice types are applied to all the crystal systems. For example, a face centered tetragonal cell can be

expressed as a body centered tetragonal cell by rotating the two equivalent axes by 45 deg and shortening them by a factor of square root of 2. Considering such degeneracies reduces the possible decorations of the seven systems to these 14 unique three dimensional lattices:

|              |            |
|--------------|------------|
| Triclinic    | P          |
| Monoclinic   | P, C       |
| Orthorhombic | P, C, I, F |
| Tetragonal   | P, I       |
| Hexagonal    | P          |
| Trigonal     | P, R       |
| Cubic        | P, I, F    |

For historic reasons, hexagonal cells are sometimes called C lattices. ATOMS will recognize hexagonal P cells denoted in `atoms.inp` by the letter C. Modern literature usually uses the P designation.

The decorations placed on the Bravais lattices come in 32 flavors called classes or point groups which represent the possible symmetries within the decorations. Each type of symmetry is defined either by a reflection plane, a rotation axis, or a rotary inversion axis. A reflection plane can either be a simple mirror plane or a glide plane, which defines the symmetry operation of reflecting through a mirror followed by translating along a direction in the plane. A rotation axis can either define a simple rotation or a screw rotation, which is the symmetry operation of rotating about the axis followed by translating along that axis. A rotary inversion axis defines the symmetry operation of reflecting through a plane followed by rotating about an axis in that plane.

These three symmetry types, reflection plane, rotation axis, and rotary inversion axis, can be combined in 32 non-degenerate ways. (An example degeneracy: the symmetry operation of combining a 180 deg rotary inversion with a mirror reflection is identical to the operation of a simple 180 deg rotation.) It would seem that the 32 classes could decorate the 14 Bravais lattices in 458 ways. In fact, the number might be larger as there are numerous types of screw axes and glide planes. Again, considering degeneracies reduces the total number of combinations, leaving 230 unique decorations of the Bravais lattices. These are called space groups. The 230 space groups are a rigorously complete set of descriptions of crystal symmetries in three dimensional space. That is, there may be new crystals but there are no new space groups. Here I am only considering space-filling crystals with translational periodicity. 3-D Penrose structures and quasi-crystals are outside the realm of this appendix and of the code.

## A.2 Decoding the Hermann-Maguin Notation

The Hermann-Maguin notation uses a set of two to four symbols to completely specify the symmetries of a space group. The first symbol is always a single letter specifying the Bravais lattice. The next three symbols specify the class of the space group. These three symbols are some combination of the following characters:

1 2 3 4 5 6 A B C D M N / -

These are sufficient to completely specify the various planar and axial symmetries of the classes and sub-classes. The following is a discussion of the most important rules of this convention. Some details are neglected but sufficient information is provided to appreciate the information contained in the notation.

The second symbol in the Hermann-Maguin notation, i.e. the one after the Bravais lattice symbol, tells about symmetries involving the primary axis of the cell and/or of the plane normal to the primary axis. The primary axis is defined as follows:

- Triclinic: none
- Monoclinic: the B axis
- Orthorhombic: the C axis
- Tetragonal: the C axis
- Hexagonal: the C axis
- Trigonal: the A axis
- Cubic: the A axis

In cubic or rhombohedral lattices the axes are equivalent, thus the primary axis is arbitrary. For orthorhombic lattices the third and fourth symbols specify the symmetries of the a and b axes respectively. In other lattices, the last two symbols encode the remaining symmetries as described below.

A space filling crystal will always show a symmetry when rotated through  $(360/n)$  degrees, where n is one of {1,2,3,4, or 6}. The second symbol often tells the rotational symmetry properties of the primary axis. Notice that all trigonal, tetragonal, and hexagonal groups have a 3, 4, or 6 respectively in their designations. Many orthorhombic and monoclinic groups have a 2, which is the highest degree of rotational symmetry available to those lattices. Cubic groups may possess 2- or 4-fold rotational symmetry about the cell axes, thus have 2 or 4 in the second symbol.

Many second symbols contain a second number. This is the subscripted number when the Hermann-Maguin notation is typeset. This refers to the type of screw symmetry associated with the axis. A screw symmetric lattice is mapped onto itself by an anti-clockwise rotation through  $m * (360/n)$  degrees and a translation of  $1/n$  up the primary axis. Here n is the degree of rotational symmetry, m is the type of screw, and the definition of rotation and direction is right-handed. Two types of screw symmetry that are different only in handedness of rotation are called enantiomorphous. The enantiomorphous pairs are 31 and 32, 41 and 43, 61 and 65, and 62 and 64.

Several of the second symbols are one or two numbers followed by a slash and a letter, e.g. P 63/M M C. The letter specifies the type of reflection plane that is normal to the rotation axis.

There are several types of reflection planes. The simplest is a mirror plane, denoted by the letter M. This says the crystal is mapped onto itself by reflecting all atoms through a mirror placed in an appropriate plane in the crystal. The letters A, B, or C denote glide planes. These map the crystal onto itself by reflecting through the plane then translating elements of the crystal by half the length of the cell axis normal to the reflection plane. A D glide plane is similar but involves translations of a quarter of the cell axis length. Finally, the letter N denotes a diagonal glide plane, which is a reflection through a plane followed by a translation in the same plane of half the length of both cell axes in that plane.

The symbol  $\bar{\phantom{x}}$  before a number indicates a rotary inversion axis. This maps the crystal back onto itself by rotating through  $(360/n)$  deg then reflecting through a plane parallel to the rotation axis.

A final word about the Hermann-Maguin notation. All cubic space groups have four three-fold rotational axes through the body diagonals. Thus all cubic groups have the number 3 as the third symbol.

### A.3 Decoding the Schoenflies Notation

The Schoenflies notation uses a set of three symbols to classify sets of space groups by their dominant symmetry features. The letters C, D, S, T, and O denote the character of the center of symmetry. The symbol after the underscore (the subscript when typeset) indicates the presence of symmetry planes and additional symmetry axes. The number after the caret (the superscript when typeset) is simply an indexing of all the distinct space groups that share major symmetry properties. In the older literature, D symmetry centers are occasionally referred to as V. ATOMS will probably understand a space group referred to by the letter V, but using the D notation is recommended.

The letter C indicates an rotation axis where the crystal is mapped onto itself when rotated by  $(360/n)$  deg, where n is the number after the underscore. An H after the underscore indicates the presence of a plane of symmetry normal to the rotation axis. A V after the underscore indicates one or two planes of symmetry parallel to the rotation axis. The letter S after the underscore indicates a normal plane of symmetry in a crystal where the degree of rotational symmetry is 1. The letter I after the underscore indicates the presence of a point center of symmetry.

The letter S indicates a rotary inversion axis. The degree of rotation is the number after the underscore.

The letter D denotes a primary rotation axis with another rotation axis normal to it. The degree of rotation of both axes is the number after the underscore. The letters H and V have the same meanings as they did in groups beginning with the letter C. The letter D indicates the presence of a diagonal symmetry plane.

Cubic groups are all specified by the letters T and O. T indicates tetrahedral symmetry, that is, the presence of the four three-fold axes and three two-fold axes. O indicates octahedral symmetry, i.e. four three-fold axes with three four-fold axes. H and D after the underscore carry the same meaning as before.

## A.4 The Hermann-Maguin Notation

### A.4.1 Notation for the Standard Settings

#### 2 Triclinic and 13 Monoclinic Space Groups

|       |             |       |       |        |       |
|-------|-------------|-------|-------|--------|-------|
| P 1   | P $\bar{1}$ | P 2   | P 21  | C 2    | P M   |
| P C   | C M         | C C   | P 2/M | P 21/M | C 2/M |
| P 2/C | P 21/C      | C 2/C |       |        |       |

#### 59 Orthorhombic Space Groups

|         |          |            |            |          |         |
|---------|----------|------------|------------|----------|---------|
| P 2 2 2 | P 2 2 21 | P 21 21 2  | P 21 21 21 | C 2 2 21 | C 2 2 2 |
| F 2 2 2 | I 2 2 2  | I 21 21 21 | P M M 2    | P M C 21 | P C C 2 |

|         |          |          |          |         |          |
|---------|----------|----------|----------|---------|----------|
| P M A 2 | P C A 21 | P N C 2  | P M N 21 | P B A 2 | P N A 21 |
| P N N 2 | C M M 2  | C M C 21 | C C C 2  | A M M 2 | A B M 2  |
| A M A 2 | A B A 2  | F M M 2  | F D D 2  | I M M 2 | I B A 2  |
| I M A 2 | P M M M  | P N N N  | P C C M  | P B A N | P M M A  |
| P N N A | P M N A  | P C C A  | P B A M  | P C C N | P B C M  |
| P N N M | P M M N  | P B C N  | P B C A  | P N M A | C M C M  |
| C M C A | C M M M  | C C C M  | C M M A  | C C C A | F M M M  |
| F D D D | I M M M  | I B A M  | I B C A  | I M M A |          |

## 68 Tetragonal Space Groups

|            |            |            |            |            |            |
|------------|------------|------------|------------|------------|------------|
| P 4        | P 41       | P 42       | P 43       | I 4        | I 41       |
| P -4       | I -4       | P 4/M      | P 42/M     | P 4/N      | P 42/N     |
| I 4/M      | I 41/A     | P 4 2 2    | P 4 21 2   | P 41 2 2   | P 41 21 2  |
| P 42 2 2   | P 42 21 2  | P 43 2 2   | P 43 21 2  | I 4 2 2    | I 41 2 2   |
| P 4 M M    | P 4 B M    | P 42 C M   | P 42 N M   | P 4 C C    | P 4 N C    |
| P 42 M C   | P 42 B C   | I 4 M M    | I 4 C M    | I 41 M D   | I 41 C D   |
| P -4 2 M   | P -4 2 C   | P -4 21 M  | P -4 21 C  | P -4 M 2   | P -4 C 2   |
| P -4 B 2   | P -4N2     | I -4 M 2   | I -4 C 2   | I -42 M    | I -42 D    |
| P 4/M M M  | P 4/M C C  | P 4/N B M  | P 4/N N C  | P 4/M B M  | P 4/M N C  |
| P 4/N M M  | P 4/N C C  | P 42/M M C | P 42/M C M | P 42/N B C | P 42/N N M |
| P 42/M B C | P 42/M N M | P 42/N M C | P 42/N C M | I 4/M M M  | I 4/M C M  |
| I 41/A M D | I 41/A C D |            |            |            |            |

## 25 Trigonal Space Groups

|         |          |          |          |          |          |
|---------|----------|----------|----------|----------|----------|
| P 3     | P 3 1    | P 32     | R3       | P -3     | R -3     |
| P 3 1 2 | P 3 2 1  | P 31 1 2 | P 31 2 1 | P 32 1 2 | P 32 2 1 |
| R 32    | P 3 M 1  | P 3 1 M  | P 3 C 1  | P 3 1 C  | R 3 M    |
| R 3C    | P -3 1 M | P -3 1 C | P -3 M 1 | P -3 C 1 | R -3 M   |
| R -3 C  |          |          |          |          |          |

## 27 Hexagonal Space Groups

|           |            |            |          |          |           |
|-----------|------------|------------|----------|----------|-----------|
| P 6       | P 61       | P 65       | P 62     | P 64     | P 63      |
| P -6      | P 6/M      | P 63/M     | P 62 2   | P 61 2 2 | P 65 2 2  |
| P 62 2 2  | P 64 2 2   | P 63 2 2   | P 6 M M  | P 6 C C  | P 63 C M  |
| P 63 M C  | P -6 M 2   | P -6 C 2   | P -6 2 M | P -62 C  | P 6/M M M |
| P 6/M C C | P 63/M C M | P 63/M M C |          |          |           |

## 36 Cubic Space Groups

|       |       |       |        |        |       |
|-------|-------|-------|--------|--------|-------|
| P 2 3 | F 2 3 | I 2 3 | P 21 3 | I 21 3 | P M 3 |
|-------|-------|-------|--------|--------|-------|

|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
| P N 3    | F M 3    | F D 3    | I M 3    | P A 3    | I A 3    |
| P 4 3 2  | P 42 3 2 | F 4 3 2  | F 41 3 2 | I 4 3 2  | P 43 3 2 |
| P 41 3 2 | I 41 3 2 | P -4 3 M | F -4 3 M | I -4 3 M | P -4 3 N |
| F -4 3 C | I -4 3 D | P M 3 M  | P N 3 N  | P M 3 N  | P N 3 M  |
| F M 3 M  | F M 3 C  | F D 3 M  | F D 3 C  | I M 3 M  | I A 3 D  |

### A.4.2 Nonstandard Notations

Here are the notations for the alternate settings of the monoclinic and orthorhombic space groups. Also presented are the notations for tetragonal space groups that have been rotated by 45 degrees resulting in a unit cell of doubled volume and of a different Bravais type.

In an monoclinic or orthorhombic space group, the Hermann-Maguin symbols are identical for the various settings if none of the three axes possess special symmetry properties. In this case the three axes are distinguished only by length and the symbol is the same for all settings.

The column headings below indicate the orientations of the alternative settings relative to the standard setting. For instance, **cab** is a setting with axes and coordinates cyclically permuted from the standard setting. This is equivalent to a rotation of 120 degrees about an axis in a  $\langle 111 \rangle$  direction relative to the Cartesian axes. The setting **a-cb** is rotated by 90 degrees about the A axis. Thus the B and C axes are swapped and the y and z coordinates in the standard setting map onto the z and -y coordinates of the alternate setting. In ATOMS, when an alternative setting is specified in **atoms.inp**, the axes and coordinates are multiplied by the appropriate permutation matrix onto the standard setting. The positions in the unit cell are expanded according to the Hermann-Maguin symbol for the standard setting. The contents of the unit cell are then permuted back to the specified setting.

#### Symbols for Monoclinic Groups of Various Settings

| standard<br>abc |               | bca   |  | standard<br>abc |               | bca   |
|-----------------|---------------|-------|--|-----------------|---------------|-------|
| P 2             | both settings |       |  | P 21            | both settings |       |
| B 2             | or            | C 2   |  | P M             | both settings |       |
| P B             | or            | P C   |  | B M             | or            | C M   |
| B B             | or            | C C   |  | P 2/M           | both settings |       |
| P 21/M          | both settings |       |  | B 2/M           | or            | C 2/M |
| P 2/B           | or            | P 2/C |  | P 21/B          | or            | P 2/C |
| B 2/B           | or            | C 2/C |  |                 |               |       |

#### Symbols for Orthorhombic Groups of Various Settings

| standard<br>abc | cab          | bca | a-cb | ba-c | -cab |
|-----------------|--------------|-----|------|------|------|
| P 2 2 2         | each setting |     |      |      |      |



P 2 2 21    P 21 2 2    P 2 21 2    P 2 21 2    P 2 2 21    P 21 2 2  
 P 21 21 2    P 2 21 21    P 21 2 21    P 21 2 21    P 21 21 2    P 2 21 21  
 P 21 21 21    each setting  
 C 2 2 21    A 21 2 2    B 2 21 2    B 2 21 2    C 2 2 21    A 21 2 2  
 C 2 2 2    A 2 2 2    B 2 2 2    B 2 2 2    C 2 2 2    A 2 2 2  
 F 2 2 2    each setting  
 I 2 2 2    each setting  
 I 21 21 21    each setting  
 P M M 2    P 2 M M    P M 2 M    P M 2 M    P M M 2    P 2 M M  
 P M C 21    P 21 M A    P B 21 M    P M 21 B    P C M 21    P 21 A M  
 P C C 2    P 2 A A    P B 2 B    P B 2 B    P C C 2    P 2 A A  
 P M A 2    P 2 M B    P C 2 M    P M 2 A    P B M 2    P 2 C M  
 P C A 21    P 21 A B    P C 21 B    P B 21 A    P B C 21    P 21 C A  
 P N C 2    P 2 N A    P B 2 N    P N 2 B    P C N 2    P 2 A N  
 P M N 21    P 21 M N    P N 21 M    P M 21 N    P N M 21    P 2 N M  
 P B A 2    P 2 C B    P C 2 A    P C 2 A    P B A 2    P 2 C B  
 P N A 21    P 21 N B    P C 21 N    P N 21 A    P B N 21    P 2 C N  
 P N N 2    P 2 N N    P N 2 N    P N 2 N    P N N 2    P 2 N N  
 C M M 2    A 2 M M    B M 2 M    B M 2 M    C M M 2    A 2 M M  
 C M C 21    A 21 M A    B B 21 M    B M 21 B    C C M 21    A 21 A M  
 C C C 2    A 2 C A    B B 2 C    B B 2 B    C C C 2    A 2 A A  
 A M M 2    B 2 M M    C M 2 M    A M 2 M    B M M 2    C 2 M M  
 A B M 2    B 2 C M    C M 2 A    A C 2 M    B M A 2    C 2 M B  
 A M A 2    B 2 M B    C C 2 M    A M 2 A    B B M 2    C 2 C M  
 A B A 2    B 2 C B    C C 2 A    A C 2 A    B B A 2    C 2 C B  
 F M M 2    F 2 M M    F M 2 M    F M 2 M    F M M 2    F 2 M M  
 F D D 2    F 2 D D    F D 2 D    F D 2 D    F D D 2    F 2 D D  
 I M M 2    I 2 M M    I M 2 M    I M 2 M    I M M 2    I 2 M M  
 I B A 2    I 2 C B    I C 2 A    I C 2 A    I B A 2    I 2 C B  
 I M A 2    I 2 M B    I C 2 M    I M 2 A    I B M 2    I 2 C M  
 P M M M    each setting  
 P N N N    each setting  
 P C C M    P M A A    P B M B    P B M B    P C C M    P M A A  
 P B A N    P N C B    P C N A    P C N A    P B A N    P N C B  
 P M M A    P B M M    P M C M    P M A M    P M M B    P C M M  
 P N N A    P B N N    P N C N    P N A N    P N N B    P C N N  
 P M N A    P B M N    P N C M    P M A N    P N M B    P C N M  
 P C C A    P B A A    P B C B    P B A B    P C C B    P C A A  
 P B A M    P M C B    P C M A    P C M A    P B A M    P M C B  
 P C C N    P N A A    P B N B    P B N B    P C C N    P N A A  
 P B C M    P M C A    P B M A    P C M B    P C A M    P M A B  
 P N N M    P M N N    P N M N    P N M N    P N N M    P M N N  
 P M M N    P N M M    P M N M    P M N M    P M M N    P N M M  
 P B C N    P N C A    P B N A    P C N B    P C A N    P N A B  
 P B C A    P B C A    P B C A    P C A B    P C A B    P C A B  
 P N M A    P B N M    P M C N    P N A M    P M N B    P C M N  
 C M C M    A M M A    B B M M    B M M B    C C M M    A M A M

|         |              |         |         |         |         |
|---------|--------------|---------|---------|---------|---------|
| C M C A | A B M A      | B B C M | B M A B | C C M B | A C A M |
| C M M M | A M M M      | B M M M | B M M M | C M M M | A M M M |
| C C C M | A M A A      | B B M B | B B M B | C C C M | A M A A |
| C M M A | A B M M      | B M C M | B M A M | C M M B | A C M M |
| C C C A | A B A A      | B B C B | B B A B | C C C B | A C A A |
| F M M M | each setting |         |         |         |         |
| F D D D | each setting |         |         |         |         |
| I M M M | each setting |         |         |         |         |
| I B A M | I M C B      | I C M A | I C M A | I B A M | I M C B |
| I B C A | I B C A      | I B C A | I C A B | I C A B | I C A B |
| I M M A | I B M M      | I M C M | I M A M | I M M B | I C M M |

Symbols for Tetragonal Groups of Various Orientations

| standard<br>abc | (a+b)(b-a)c  |  | standard<br>abc | (a+b)(b-a)c  |
|-----------------|--------------|--|-----------------|--------------|
| P 4             | or C 4       |  | P 41            | or C 41      |
| P 42            | or C 42      |  | P 43            | or C 43      |
| I 4             | or F 4       |  | I 41            | or F 41      |
| P -4            | or C -4      |  | I -4            | or F -4      |
| P 4/M           | or C 4/M     |  | P 42/M          | or C 42/M    |
| P 4/N           | or C 4/A     |  | P 42/M          | or C 42/A    |
| I 4/M           | or F 4/M     |  | I 41/A          | or F 41/D    |
| P 4 2 2         | or C 4 2 2   |  | P 4 2 21        | or C 4 2 21  |
| P 41 2 2        | or C 41 2 2  |  | P 41 2 21       | or C 41 2 21 |
| P 42 2 2        | or C 42 2 2  |  | P 42 2 21       | or C 42 2 21 |
| P 43 2 2        | or C 43 2 2  |  | P 43 2 21       | or C 43 2 21 |
| I 4 2 2         | or F 4 2 2   |  | I 41 2 2        | or F 41 2 2  |
| P 4 M M         | or C 4 M M   |  | P 4 B M         | or C 4 M B   |
| P 42 C M        | or C 42 M C  |  | P 42 N M        | or C 42 M N  |
| P 4 C C         | or C 4 C C   |  | P 4 N C         | or C 4 C N   |
| P 42 M C        | or C 42 C M  |  | P 42 B C        | or C 42 C B  |
| I 4 M M         | or F 4 M M   |  | I 4 C M         | or F 4 M C   |
| I 41 M D        | or F 41 D M  |  | I 41 C D        | or F 41 D C  |
| P -4 2 M        | or C -4 M 2  |  | P -4 2 C        | or C -4 C 2  |
| P -4 21 M       | or C -4 M 21 |  | P -4 21 C       | or C -4 C 21 |
| P -4 M 2        | or C -4 2 M  |  | P -4 C 2        | or C -4 2 C  |
| P -4 B 2        | or C -4 2 B  |  | P -4 N 2        | or C -4 2 N  |
| I -4 M 2        | or F -4 2 M  |  | I -4 C 2        | or F -4 2 C  |
| I -4 2 M        | or F -4 M 2  |  | I -4 2 D        | or F -4 D 2  |
| P 4/M M M       | or C 4/M M M |  | P 4/M C C       | or C 4/M C C |
| P 4/N B M       | or C 4/A M B |  | P 4/N N C       | or C 4/A C N |
| P 4/M B M       | or C 4/M M B |  | P 4/M N C       | or C 4/M C N |
| P 4/N M M       | or C 4/A M M |  | P 4/N C C       | or C 4/A C C |

|            |               |            |    |            |
|------------|---------------|------------|----|------------|
| P 42/M M C | or C 42/M C M | P 42/M C M | or | C 42/M M C |
| P 42/N B C | or C 42/A C B | P 42/N N M | or | C 42/A M N |
| P 42/M B C | or C 42/M C B | P 42/M N M | or | C 42/M M N |
| P 42/N M C | or C 42/A C M | P 42/N C M | or | C 42/A M C |
| I 4/M M M  | or F 4/M M M  | I 4/M C M  | or | F 4/M M C  |
| I 41/A M D | or F 41/D D M | I 41/A C D | or | F 41/D D C |

## A.5 The Schoenflies Notation

### 2 Triclinic and 13 Monoclinic Space Groups

|            |            |            |            |            |            |
|------------|------------|------------|------------|------------|------------|
| $C_1^1$    | $C_I^1$    | $C_2^1$    | $C_2^2$    | $C_2^3$    | $C_S^1$    |
| $C_S^2$    | $C_S^3$    | $C_S^4$    | $C_{2H}^1$ | $C_{2H}^2$ | $C_{2H}^3$ |
| $C_{2H}^4$ | $C_{2H}^5$ | $C_{2H}^6$ |            |            |            |

### 59 orthorhombic space groups

|               |               |               |               |               |               |
|---------------|---------------|---------------|---------------|---------------|---------------|
| $D_2^1$       | $D_2^2$       | $D_2^3$       | $D_2^4$       | $D_2^5$       | $D_2^6$       |
| $D_2^7$       | $D_2^8$       | $D_2^9$       | $C_{2V}^1$    | $C_{2V}^2$    | $C_{2V}^3$    |
| $C_{2V}^4$    | $C_{2V}^5$    | $C_{2V}^6$    | $C_{2V}^7$    | $C_{2V}^8$    | $C_{2V}^9$    |
| $C_{2V}^{10}$ | $C_{2V}^{11}$ | $C_{2V}^{12}$ | $C_{2V}^{13}$ | $C_{2V}^{14}$ | $C_{2V}^{15}$ |
| $C_{2V}^{16}$ | $C_{2V}^{17}$ | $C_{2V}^{18}$ | $C_{2V}^{19}$ | $C_{2V}^{20}$ | $C_{2V}^{21}$ |
| $C_{2V}^{22}$ | $D_{2H}^1$    | $D_{2H}^2$    | $D_{2H}^3$    | $D_{2H}^4$    | $D_{2H}^5$    |
| $D_{2H}^6$    | $D_{2H}^7$    | $D_{2H}^8$    | $D_{2H}^9$    | $D_{2H}^{10}$ | $D_{2H}^{11}$ |
| $D_{2H}^{12}$ | $D_{2H}^{13}$ | $D_{2H}^{14}$ | $D_{2H}^{15}$ | $D_{2H}^{16}$ | $D_{2H}^{17}$ |
| $D_{2H}^{18}$ | $D_{2H}^{19}$ | $D_{2H}^{20}$ | $D_{2H}^{21}$ | $D_{2H}^{22}$ | $D_{2H}^{23}$ |
| $D_{2H}^{24}$ | $D_{2H}^{25}$ | $D_{2H}^{26}$ | $D_{2H}^{27}$ | $D_{2H}^{28}$ |               |

### 68 Tetragonal space groups

|               |               |               |               |               |               |
|---------------|---------------|---------------|---------------|---------------|---------------|
| $C_4^1$       | $C_4^2$       | $C_4^3$       | $C_4^4$       | $C_4^5$       | $C_4^6$       |
| $S_4^1$       | $S_4^2$       | $C_{4H}^1$    | $C_{4H}^2$    | $C_{4H}^3$    | $C_{4H}^4$    |
| $C_{4H}^5$    | $C_{4H}^6$    | $D_4^1$       | $D_4^2$       | $D_4^3$       | $D_4^4$       |
| $D_4^5$       | $D_4^6$       | $D_4^7$       | $D_4^8$       | $D_4^9$       | $D_4^{10}$    |
| $C_{4V}^1$    | $C_{4V}^2$    | $C_{4V}^3$    | $C_{4V}^4$    | $C_{4V}^5$    | $C_{4V}^6$    |
| $C_{4V}^7$    | $C_{4V}^8$    | $C_{4V}^9$    | $C_{4V}^{10}$ | $C_{4V}^{11}$ | $C_{4V}^{12}$ |
| $D_{2D}^1$    | $D_{2D}^2$    | $D_{2D}^3$    | $D_{2D}^4$    | $D_{2D}^5$    | $D_{2D}^6$    |
| $D_{2D}^7$    | $D_{2D}^8$    | $D_{2D}^9$    | $D_{2D}^{10}$ | $D_{2D}^{11}$ | $D_{2D}^{12}$ |
| $D_{4H}^1$    | $D_{4H}^2$    | $D_{4H}^3$    | $D_{4H}^4$    | $D_{4H}^5$    | $D_{4H}^6$    |
| $D_{4H}^7$    | $D_{4H}^8$    | $D_{4H}^9$    | $D_{4H}^{10}$ | $D_{4H}^{11}$ | $D_{4H}^{12}$ |
| $D_{4H}^{13}$ | $D_{4H}^{14}$ | $D_{4H}^{15}$ | $D_{4H}^{16}$ | $D_{4H}^{17}$ | $D_{4H}^{18}$ |
| $D_{4H}^{19}$ | $D_{4H}^{20}$ |               |               |               |               |

### 25 Trigonal space groups

|            |            |            |            |            |            |
|------------|------------|------------|------------|------------|------------|
| $C_3^1$    | $C_3^2$    | $C_3^3$    | $C_3^4$    | $C_{3I}^1$ | $C_{3I}^2$ |
| $D_3^1$    | $D_3^2$    | $D_3^3$    | $D_3^4$    | $D_3^5$    | $D_3^6$    |
| $D_3^7$    | $C_{3V}^1$ | $C_{3V}^2$ | $C_{3V}^3$ | $C_{3V}^4$ | $C_{3V}^5$ |
| $C_{3V}^6$ | $D_{3D}^1$ | $D_{3D}^2$ | $D_{3D}^3$ | $D_{3D}^4$ | $D_{3D}^5$ |
| $D_{3D}^6$ |            |            |            |            |            |

## 27 Hexagonal space groups

|            |            |            |            |            |            |
|------------|------------|------------|------------|------------|------------|
| $C_6^1$    | $C_6^2$    | $C_6^3$    | $C_6^4$    | $C_6^5$    | $C_6^6$    |
| $C_{3H}^1$ | $C_{6H}^1$ | $C_{6H}^2$ | $D_6^1$    | $D_6^2$    | $D_6^3$    |
| $D_6^4$    | $D_6^5$    | $D_6^6$    | $C_{6V}^1$ | $C_{6V}^2$ | $C_{6V}^3$ |
| $C_{6V}^4$ | $D_{3H}^1$ | $D_{3H}^2$ | $D_{3H}^3$ | $D_{3H}^4$ | $D_{6H}^1$ |
| $D_{6H}^2$ | $D_{6H}^3$ | $D_{6H}^4$ |            |            |            |

## 36 Cubic space groups

|         |         |         |         |         |            |
|---------|---------|---------|---------|---------|------------|
| $T^1$   | $T^2$   | $T^3$   | $T^4$   | $T^5$   | $T_H^1$    |
| $T_H^2$ | $T_H^3$ | $T_H^4$ | $T_H^5$ | $T_H^6$ | $T_H^7$    |
| $O^1$   | $O^2$   | $O^3$   | $O^4$   | $O^5$   | $O^6$      |
| $O^7$   | $O^8$   | $T_D^1$ | $T_D^2$ | $T_D^3$ | $T_D^4$    |
| $T_D^5$ | $T_D^6$ | $O_H^1$ | $O_H^2$ | $O_H^3$ | $O_H^4$    |
| $O_H^5$ | $O_H^6$ | $O_H^7$ | $O_H^8$ | $O_H^9$ | $O_H^{10}$ |

## Appendix B 40 Example Input Files

The next several pages have numerous examples of `atoms.inp` files that produce the correct output. In these examples you might find a material of interest or its isomorph and you will certainly get clues for making ATOMS work the way you want. By far the most useful resource for the crystallographic data needed for these input files is the *Crystal Structures* series by R.W.G. Wyckoff.

These examples and many others are available on the Internet. The World wide Web URL for a big list of input files is <http://krazy.phys.washington.edu/html/atoms.html>.

### B.1 Pure Elements

These are examples of `atoms.inp` files for several pure elements.

The following elements commonly crystallize in the bcc structure:

Li, Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Ta, W, Eu

The following elements commonly crystallize in the fcc structure:

Al, Ca, Ni, Cu, Sr, Rh, Pd, Ag, Ir, Pt, Au, Pb, Ce, Yb, Th

The following elements commonly crystallize in the hcp structure:

Be, Mg, Sc, Ti, Co, Zn, Y, Zr, Tc, Ru, Cd, Hf, Re, Os, Tl, Gd, Tb, Dy, Ho, Er, Tm, Lu

The following elements commonly crystallize in the diamond structure:

C, Si, Ge, alpha-Sn

Included in this section are these examples of disordered pure elements:

Ga, In, S, white-Sn, As

```

title Cr  metal  bcc a=2.88
space bcc      ! shorthand for I M 3 M
rmax=6.0  a=2.88
atom
!  At.type   x   y   z
   Cr       0.0 0.0 0.0
-----

title Cu  metal  fcc a=3.61
space fcc      ! shorthand for F M 3 M
rmax=6.0  a=3.61
out=feff.inp ! index=true
atom
!  At.type   x   y   z
   Cu       0.0 0.0 0.0
-----

title Ti  metal  hcp a=2.950 c=4.8646
space hcp      ! shorthand for P 63/M M C

```

```

rmax=6.0  a=2.95  c=4.6846
out=feff.inp  ! index=true
atom
!  At.type    x        y        z
   ti        0.33333  0.66667  0.25
-----

title  alpha-tin  diamond structure
a = 6.485  space diamond  ! shorthand for I D 3 M
atom
!  At.type    x        y        z
   sn        0.125  0.125  0.125
-----

title  Gallium, orthorhombic
space D_2h^18          ! same as C m c a
a=4.5107  b=7.6448  c=4.5167
atom
  Ga  0.0  0.1525  0.0785
-----

title Indium, tetragonal
space  I 4/m m m
% note that case is unimportant
a=3.2446  C=4.9367
atom
!  At.type    x    y    z    tag
   In        0.0  0.0  0.0
-----

title Rhombic Sulfur
!  Wyckoff "Crystal Structures" vol.1 pp 33-34
!  correct with this origin
!  see the spinel input for an example of the SHIFT keyword
space  F D D D
rmax=10.0  a=10.467  b=12.870  c=24.493
core = S3
atom
! At.type    x        y        z        tag
   S        0.8554  0.9526  0.9516  S1
   S        0.7844  0.0301  0.0763  S2
   S        0.7069  0.9795  0.0040  S3
   S        0.7862  0.9073  0.1290  S4

```

```

-----
title  white tin
Space  D_4H^19          ! same as I 41/a m d
rmax = 7.00
a      = 5.8197      c = 3.175
atom
! At.type   x      y      z
   Sn       0.0    0.25  -0.125
-----

```

```

-----
title  rhombohedral arsenic
space  R -3 m
a = 4.123  alpha = 54.16667
atom
   As     0.226  0.226  0.226
-----

```

## B.2 Common Lattice Types

These are examples of `atoms.inp` files for the following common lattice types:

- zincblende
- sodium chloride
- cesium chloride
- spinel
- perovskite
- wurtzite
- ilmenite

```

-----
title  zinc sulfide (zincblende) structure
space  zns              ! shorthand for F -4 3 M
a 3.615 rmax 8.0  core = Zn
atom
   Zn  0.0  0.0  0.0
   S   0.25 0.25 0.25
-----

```

```

-----
title  FeO, sodium chloride structure
space  salt             ! shorthand for F M 3 M
rmax=6.0  a=3.3108      core=Fe
atom
! At.type   x      y      z      cent.
   Fe       0.0    0.0    0.0
   O        0.5    0.5    0.5
-----

```

```

-----
title  CsCl Cesium Chloride structure
space = cscl      ! shorthand for P M 3 M
a = 4.11  core = Cs  rmax = 8.22
atom
  Cs    0.0    0.0    0.0
  Cl    0.5    0.5    0.5
-----

```

```

-----
title  Cubic Spinel Structure, MgAl2O4
Space  f d 3 m
rmax=7  a=8.0800  !from Wyckoff
shift = -0.125 -0.125 -0.125
core = Mg
atom
! At.type  x      y      z      cent.
  Mg      0.0      0.0      0.0
  Al      0.625    0.625    0.625
  O       0.387    0.387    0.387
! u=0.387 in Wyckoff, shift coords
! by (-1/8,-1/8,-1/8)
-----

```

```

-----
title  cubic EuTiO3, perovskite structure
rmax=7.0  a=3.90  Space P M 3 M  core = Ti
atom
! At.type  x      y      z      cent.
  Eu      0.0      0.0      0.0
  Ti      0.5      0.5      0.5
  O       0.0      0.5      0.5
-----

```

```

-----
title  ZnS hexagonal wurtzite structure
space = P 63 m c  ! same as c_6v^4
a=3.81  c=6.23  ! gamma set to 120 by ATOM
core = S
atom
  Zn    0.33333  0.66666  0.0
  S     0.33333  0.66666  0.375
-----

```



```

title  alpha-Fe2O3, ilmenite structure
Space  C_3I^2          ! same as R -3
rmax = 7.00      core = Fe      a      = 5.538      alpha = 54.6833333
atom
! At.type      x          y          z
  Fe          .358      .358      .358
  Ti          .142      .142      .142
  O           .555      -.04      .235

```

---

### B.3 Binary and Ternary Compounds

Here are various examples of crystal structures containing two or three atomic species. Included here are:

- Aluminum Oxide
- Aluminum Boride
- alpha-Iron Oxide
- alpha-Lead Oxide
- Boron Nitride (graphitic)
- Boron Nitride (hexatic)
- Calcium Carbide
- Fluorite (PrO<sub>2</sub>)
- Cadmium Chloride
- Tenorite (Copper Monoxide)
- Cinnebar (HgS)
- Potassium Nitrofluorite (K<sub>2</sub>NiF<sub>4</sub>)
- Hausmannite (Mn<sub>3</sub>O<sub>4</sub>)
- Cassiterite (MnO<sub>2</sub>)
- Cubic Bixbyite (Yttria, Y<sub>2</sub>O<sub>3</sub>)
- Ferroelectric Distorted Perovskite (PbTiO<sub>3</sub>)
- Antiferroelectric Distorted Perovskite (PbZrO<sub>3</sub>)
- Platinum Silicide (PtSi)

```

title  Al2O3
Space  R -3 C          ! same as D_3D^6
a=4.7628  c=13.0032  gamma=120      core = Al
rmax=7
atom
! At.type  x          y          z          cent.
  Al       0.0        0.0        0.352
  O        0.306      0.0        0.25

```

---

```

title AlB2, hexagonal aluminum boride structure
space P -3 M 1
rmax=7.0 a=3.009 c=3.262 gamma=120 core = Al
atom
  Al 0.0 0.0 0.0
  B 0.33333 0.66667 0.5
-----

```

```

title alpha-Fe2O3
Space D_3d^6 ! same as R -3 C
rmax = 7.00 core = iron
a = 5.4135 alpha = 55.2833333
atom
! At.type x y z tag
  Fe .355 .355 .355 iron
  O .550 -.050 .25 oxy
-----

```

```

title alpha Lead Oxide (PbO2)
space p b c n
rmax=6.0 a=4.947 b=5.951 c=5.497 core = Pb
atom
  Pb 0.0 0.178 0.25
  O 0.276 0.410 0.425
-----

```

```

title BN primary structure
space p 63/m m c
a 2.504 c 6.661 rmax 8.0 core B
atom
  B 0.333333 0.666667 0.25
  N 0.333333 0.666667 0.75
-----

```

```

title BN hexagonal structure
space hcp
a 2.504 c 10.01 rmax 8.0 core B
atom
  B 0.0 0.0 0.0
  N 0.0 0.0 0.333333
-----

```

```
title CaC2, calcium carbide structure
rmax=7.0 Space D_4h^17
a=3.87 c=6.37 core Ca
atom
! At.type x y z tag
Ca 0.0 0.0 0.0
C 0.0 0.0 0.406
```

---

```
title PrO2 Fluorite structure
space f m 3 m
a=4.9 edge=k rmax=10 core = Pr
atom
Pr 0.0 0.0 0.0
O 0.25 0.25 0.25
```

---

```
title Cadmium Chloride structure (hexagonal)
space R -3 M
a=3.854 c=17.457 gamma=120
rmax=6.0 core = Cd
atom
Cd 0.0 0.0 0.0
Cl 0.0 0.0 0.25
```

---

```
title monoclinic CuO (tenorite structure)
space c 2/c ! same as C_2h^6
a=4.653 b=3.410 c=5.108 beta=99.4833 core = Cu
atom
Cu 0.25 0.25 0.0
O 0.0 0.584 0.25
```

---

```
title HgS, cinnebar, trigonal
a=4.146 c=9.497 gamma=120 core = Hg
space = P 31 2 1
atom
Hg 0.720 0.0 0.333333
S 0.485 0.0 0.833333
```

---

```

title K2 Ni F4 structure
space I 4/m m m
a=3.8      c=13.2      core = nick.
atom
!
      tag
K      0.0      0.0      0.36      pot.
Ni     0.0      0.0      0.0       nick.
O      0.0      0.5      0.0       01
O      0.0      0.0      0.18      02

```

---

```

title Mn3O4, hausmannite structure
a 5.75      c 9.42      core Mn2
rmax=7.0    Space i 41/a m d
atom
! At.type  x      y      z      tag
Mn      0.0      0.75     0.125     Mn1
Mn      0.0      0.0      0.5       Mn2
O       0.0      0.25     0.375

```

---

```

title MnO2, cassiterite structure
a 4.396      c 2.871      core Mn
rmax=6.0    Space P 42/M N M
atom
! At.type  x      y      z      tag
Mn      0.0      0.0      0.0
O       .3      .3      0.0

```

---

```

title sodium chromate, Na2CrO4
space c m c m
a 5.861      b 9.259      c 7.138
rmax 7      core Na2
atom
Na      0.0      0.20     0.25      Na1
Na      0.0      0.50     0.0       Na2
Cr      0.0      0.85     0.25
O       0.28     0.45     0.25      01
O       0.0      0.25     0.57      02

```

---

```

title Y2O3, cubic bixbyite structure

```

```

rmax=7.0   Space   I A 3
a=10.604   core = Y2
atom
! At.type  x          y          z          tag
   Y       0.25       0.25       0.25       Y1
   Y      -0.0314     0.0        0.25       Y2
   O       0.389     0.150     0.377

```

---

```

title PbTiO3, distorted perovskite
Space   P 4 m m
a=3.885   c=4.139
rmax=7    core = Ti
atom
! At.type  x          y          z          tag
   Pb      0.0        0.0        0.0
   Ti      0.5        0.5        0.5377
   O       0.5        0.5        0.1118   axial
   O       0.0        0.5        0.6174   planar

```

---

```

title PbZrO3 distorted perovskite
a = 5.88   b = 11.78   c = 8.22   core = Pb1
rmax=5.0   Space   p b a m
atom
! At.type  x          y          z          Tag
   Pb      0.7064     0.1266     0.0        Pb1
   Pb      0.7064     0.1266     0.5        Pb2
   Zr      0.2423     0.125      0.25
   O       0.271      0.156      0.0        O1
   O       0.288      0.096      0.5        O2
   O       0.032     0.2608     0.283     O3
   O       0.0        0.5        0.206     O4
   O       0.0        0.0        0.248     O5

```

---

```

title Platinum Silicide, PtSi
title P b m n in Wyckoff, just for the sake of confusion
a = 5.595   b = 3.603   c = 5.932   core = Pt
rmax=5.2   Space   p n m a
atom
! At.type  x          y          z          Tag
   Pt      0.010     0.250     0.195

```

```
Si      0.195   0.250   0.590
```

---

## B.4 High Temperature Superconductors.

Here are several examples of `atoms.inp` files for various High Tc superconductors. The crystallographic literature on this class of materials is quite large and there are significant structural differences even between similar materials. Two recommended resources for crystal information are *Copper Oxide Superconductors* by Poole, Datta, and Farach, Wiley-Interscience, New York (1988) and *Physical Properties of High Temperature Superconductors II*, ed. by Ginsberg, World Scientific (1990).

```
title YBCO: Y Ba2 Cu3 O7 (1-2-3 structure)
space P M M M
rmax=5.2          a 3.823   b 3.886 c 11.681
dwarf on   core = Cu1
atom
! At.type   x       y       z       tag
  Y         0.5     0.5     0.5
  Ba        0.5     0.5     0.184
  Cu         0       0       0       Cu1
  Cu         0       0       0.356   Cu2
  O          0       0.5     0       O1
  O          0       0       0.158   O2
  O          0       0.5     0.379   O3
  O         0.5     0       0.377   O4
```

---

```
title Bi2 Sr2 Ca Cu2 O8 (2-2-1-2 structure)
space F m m m
a=5.411   b=5.418   c=30.89   core = Cu
atom
  Bi        0.0     0.0     0.20
  Sr        0.0     0.5     0.11
  Ca        0.0     0.5     0.0
  Cu        0.0     0.0     0.05
  O         0.25    0.25    0.05   O1
  O         0.0     0.5     0.20   O2
  O         0.0     0.0     0.13   O3
```

---

```
title Pb2 Y Sr2 Cu3 O8 (2-1-2-3 structure)
space P 4/m m m
a=3.813   c=15.76   core = Cu1
atom
  Pb        0.5     0.5     0.39
  Sr        0.0     0.0     0.22
  Y         0.0     0.0     0.0
```

|    |     |     |      |     |
|----|-----|-----|------|-----|
| Cu | 0.5 | 0.5 | 0.11 | Cu1 |
| Cu | 0.0 | 0.0 | 0.5  | Cu2 |
| O  | 0.0 | 0.5 | 0.10 | O1  |
| O  | 0.5 | 0.5 | 0.25 | O2  |
| O  | 0.0 | 0.0 | 0.38 | O3  |

---

```

title tetragonal Tl2 Ba2 Cu O6, (2-2-0-1 structure)
space I 4/m m m
a = 3.866 c = 23.239 rmax = 6.0 core = Cu
atom
  Tl      0.5  0.5  0.20265
  Ba      0.0  0.0  0.08301
  Cu      0.5  0.5  0.0
  O       0.0  0.5  0.0          O1
  O       0.5  0.5  0.1168      O2
  O       0.5  0.5  0.2889      O3

```

---

```

title Y Ba2 Cu4 O8 (1-2-4 structure)
space C m m m
a=3.8415 b=3.8707 c=27.240 core = Cu1
atom
! Type      x      y      z      tag
  Y      0.5  0.5  0.0
  Ba      0.5  0.5  0.1356
  Cu      0.0  0.0  0.2127  Cu1
  Cu      0.0  0.0  0.0614  Cu2
  O       0.0  0.0  0.1454  O1
  O       0.5  0.0  0.0524  O2
  O       0.0  0.5  0.0528  O3
  O       0.0  0.5  0.2181  O4

```

## Short Contents

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