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1 Routine/Function Prologues

1.0.1 r3frac (Source File: r3frac.f90)

INTERFACE:

```
subroutine r3frac(eps,v,iv)
```

INPUT/OUTPUT PARAMETERS:

```
eps : zero component tolerance (in,real)
v   : input vector (inout,real(3))
iv  : integer parts of v (out,integer(3))
```

DESCRIPTION:

Finds the fractional part of each component of a real 3-vector using the function $\mathrm{frac}\,(x) = x - \lfloor x \rfloor$. A component is taken to be zero if it lies within the intervals $[0, \epsilon)$ or $(1 - \epsilon, 1]$. The integer components of `v` are returned in the variable `iv`.

REVISION HISTORY:

```
Created January 2003 (JKD)
```

1.1 Fortran: Module Interface modmain (Source File: modspacegroup.f90)

Contains all the global variables required by the spacegroup code.

REVISION HISTORY:

```
Created October 2006 (JKD)
```

2 Introduction

Spacegroup is a utility which produces crystal geometry for use with the EXCITING code, from the space group defined by its Hermann-Mauguin symbol and lattice vector lengths and angles. Spacegroup recognises all 230 space groups in various coordinate settings giving a total of 530 possible symbols, which are tabulated below. The code also provides output compatible with the XCrysDen or V_Sim packages for visualisation of the crystal structure.

3 Usage

Only one input file, `spacegroup.in`, is required. The structure of this file is illustrated by the following example for the high T_c superconductor La_2CuO_4:

```
'Bmab'                                : hrmg
10.0605232 10.0605232  24.972729      : a, b, c
 90.0     90.0     90.0               : ab, ac, bc
 1  1  1                              : ncell
 .true.                               : primcell
 3                                    : nspecies
```

```
'La' 'La.in'                          : spsymb, spfname
1                                     : nwpos
0.0000    0.0000    0.3608            : wpos
'Cu' 'Cu.in'
1
0.0000    0.0000    0.0000
'O' 'O.in'
2
0.2500    0.2500    0.0000
0.0000    0.0000    0.1820
```

The input parameters are defined as follows:

`hrmg`
The Hermann-Mauguin symbol of a space group listed in the table below (case-sensitive)

`a`, `b`, `c`
Lattice vector lengths in Bohr (i.e. atomic units, **NOT** Ångstroms)

`ab`, `ac`, `bc`
Angles in degrees between lattice vectors **a** and **b**; **a** and **c**; and **b** and **c**, respectively

`ncell`
The number of unit cells required in each direction

`primcell`
Set to `.true.` if the primitive unit cell should be found

`nspecies`
Number of atomic species

`spsymb`, `spfname`
The species symbol and the species filename required by EXCITING

`nwpos`
The number of Wyckoff positional coordinates

`wpos`
Wyckoff positional coordinates in fractions of the lattice vectors

Note that `nwpos` and `wpos` are repeated as many times as there are species. After creating the input file, the `spacegroup` command is run and the files `GEOMETRY.OUT` and `crystal.xsf` should be produced. The `GEOMETRY.OUT` file can simply be appended to an `exciting.in` file. If XCrysDen is available, then use the command

```
xcrysden --xsf crystal.xsf
```

to render the unit cell.

4 Table of space group symbols

We acknowledge Ralf W. Grosse-Kunstleve (`http://cci.lbl.gov/sginfo/`) for the following table which associates space group numbers, Schönflies symbols, Hermann-Mauguin symbols, and Hall symbols.

Number	Schoenflies	Hermann-Mauguin	Hall
1	C_1^1	P1	P 1
2	C_i^1	P-1	-P 1
3:b	C_2^1	P2:b = P121	P 2y
3:c	C_2^1	P2:c = P112	P 2
3:a	C_2^1	P2:a = P211	P 2x
4:b	C_2^2	P21:b = P1211	P 2yb
4:c	C_2^2	P21:c = P1121	P 2c
4:a	C_2^2	P21:a = P2111	P 2xa
5:b1	C_2^3	C2:b1 = C121	C 2y
5:b2	C_2^3	C2:b2 = A121	A 2y
5:b3	C_2^3	C2:b3 = I121	I 2y
5:c1	C_2^3	C2:c1 = A112	A 2
5:c2	C_2^3	C2:c2 = B112 = B2	B 2
5:c3	C_2^3	C2:c3 = I112	I 2
5:a1	C_2^3	C2:a1 = B211	B 2x
5:a2	C_2^3	C2:a2 = C211	C 2x
5:a3	C_2^3	C2:a3 = I211	I 2x
6:b	C_s^1	Pm:b = P1m1	P -2y
6:c	C_s^1	Pm:c = P11m	P -2
6:a	C_s^1	Pm:a = Pm11	P -2x
7:b1	C_s^2	Pc:b1 = P1c1	P -2yc
7:b2	C_s^2	Pc:b2 = P1n1	P -2yac
7:b3	C_s^2	Pc:b3 = P1a1	P -2ya
7:c1	C_s^2	Pc:c1 = P11a	P -2a
7:c2	C_s^2	Pc:c2 = P11n	P -2ab
7:c3	C_s^2	Pc:c3 = P11b = Pb	P -2b
7:a1	C_s^2	Pc:a1 = Pb11	P -2xb
7:a2	C_s^2	Pc:a2 = Pn11	P -2xbc
7:a3	C_s^2	Pc:a3 = Pc11	P -2xc
8:b1	C_s^3	Cm:b1 = C1m1	C -2y
8:b2	C_s^3	Cm:b2 = A1m1	A -2y
8:b3	C_s^3	Cm:b3 = I1m1	I -2y
8:c1	C_s^3	Cm:c1 = A11m	A -2
8:c2	C_s^3	Cm:c2 = B11m = Bm	B -2
8:c3	C_s^3	Cm:c3 = I11m	I -2
8:a1	C_s^3	Cm:a1 = Bm11	B -2x
8:a2	C_s^3	Cm:a2 = Cm11	C -2x
8:a3	C_s^3	Cm:a3 = Im11	I -2x
9:b1	C_s^4	Cc:b1 = C1c1	C -2yc
9:b2	C_s^4	Cc:b2 = A1n1	A -2yac
9:b3	C_s^4	Cc:b3 = I1a1	I -2ya
9:-b1	C_s^4	Cc:-b1 = A1a1	A -2ya
9:-b2	C_s^4	Cc:-b2 = C1n1	C -2ybc
9:-b3	C_s^4	Cc:-b3 = I1c1	I -2yc
9:c1	C_s^4	Cc:c1 = A11a	A -2a
9:c2	C_s^4	Cc:c2 = B11n	B -2bc
9:c3	C_s^4	Cc:c3 = I11b	I -2b
9:-c1	C_s^4	Cc:-c1 = B11b = Bb	B -2b
9:-c2	C_s^4	Cc:-c2 = A11n	A -2ac
9:-c3	C_s^4	Cc:-c3 = I11a	I -2a

Number	Schoenflies	Hermann-Mauguin	Hall
9:a1	C_s^4	Cc:a1 = Bb11	B -2xb
9:a2	C_s^4	Cc:a2 = Cn11	C -2xbc
9:a3	C_s^4	Cc:a3 = Ic11	I -2xc
9:-a1	C_s^4	Cc:-a1 = Cc11	C -2xc
9:-a2	C_s^4	Cc:-a2 = Bn11	B -2xbc
9:-a3	C_s^4	Cc:-a3 = Ib11	I -2xb
10:b	C_{2h}^1	P2/m:b = P12/m1	-P 2y
10:c	C_{2h}^1	P2/m:c = P112/m	-P 2
10:a	C_{2h}^1	P2/m:a = P2/m11	-P 2x
11:b	C_{2h}^2	P21/m:b = P121/m1	-P 2yb
11:c	C_{2h}^2	P21/m:c = P1121/m	-P 2c
11:a	C_{2h}^2	P21/m:a = P21/m11	-P 2xa
12:b1	C_{2h}^3	C2/m:b1 = C12/m1	-C 2y
12:b2	C_{2h}^3	C2/m:b2 = A12/m1	-A 2y
12:b3	C_{2h}^3	C2/m:b3 = I12/m1	-I 2y
12:c1	C_{2h}^3	C2/m:c1 = A112/m	-A 2
12:c2	C_{2h}^3	C2/m:c2 = B112/m = B2/m	-B 2
12:c3	C_{2h}^3	C2/m:c3 = I112/m	-I 2
12:a1	C_{2h}^3	C2/m:a1 = B2/m11	-B 2x
12:a2	C_{2h}^3	C2/m:a2 = C2/m11	-C 2x
12:a3	C_{2h}^3	C2/m:a3 = I2/m11	-I 2x
13:b1	C_{2h}^4	P2/c:b1 = P12/c1	-P 2yc
13:b2	C_{2h}^4	P2/c:b2 = P12/n1	-P 2yac
13:b3	C_{2h}^4	P2/c:b3 = P12/a1	-P 2ya
13:c1	C_{2h}^4	P2/c:c1 = P112/a	-P 2a
13:c2	C_{2h}^4	P2/c:c2 = P112/n	-P 2ab
13:c3	C_{2h}^4	P2/c:c3 = P112/b = P2/b	-P 2b
13:a1	C_{2h}^4	P2/c:a1 = P2/b11	-P 2xb
13:a2	C_{2h}^4	P2/c:a2 = P2/n11	-P 2xbc
13:a3	C_{2h}^4	P2/c:a3 = P2/c11	-P 2xc
14:b1	C_{2h}^5	P21/c:b1 = P121/c1	-P 2ybc
14:b2	C_{2h}^5	P21/c:b2 = P121/n1	-P 2yn
14:b3	C_{2h}^5	P21/c:b3 = P121/a1	-P 2yab
14:c1	C_{2h}^5	P21/c:c1 = P1121/a	-P 2ac
14:c2	C_{2h}^5	P21/c:c2 = P1121/n	-P 2n
14:c3	C_{2h}^5	P21/c:c3 = P1121/b = P21/b	-P 2bc
14:a1	C_{2h}^5	P21/c:a1 = P21/b11	-P 2xab
14:a2	C_{2h}^5	P21/c:a2 = P21/n11	-P 2xn
14:a3	C_{2h}^5	P21/c:a3 = P21/c11	-P 2xac
15:b1	C_{2h}^6	C2/c:b1 = C12/c1	-C 2yc
15:b2	C_{2h}^6	C2/c:b2 = A12/n1	-A 2yac
15:b3	C_{2h}^6	C2/c:b3 = I12/a1	-I 2ya
15:-b1	C_{2h}^6	C2/c:-b1 = A12/a1	-A 2ya
15:-b2	C_{2h}^6	C2/c:-b2 = C12/n1	-C 2ybc
15:-b3	C_{2h}^6	C2/c:-b3 = I12/c1	-I 2yc
15:c1	C_{2h}^6	C2/c:c1 = A112/a	-A 2a
15:c2	C_{2h}^6	C2/c:c2 = B112/n	-B 2bc
15:c3	C_{2h}^6	C2/c:c3 = I112/b	-I 2b
15:-c1	C_{2h}^6	C2/c:-c1 = B112/b = B2/b	-B 2b
15:-c2	C_{2h}^6	C2/c:-c2 = A112/n	-A 2ac

Number	Schoenflies	Hermann-Mauguin	Hall
15:-c3	C_{2h}^6	C2/c:-c3 = I112/a	-I 2a
15:a1	C_{2h}^6	C2/c:a1 = B2/b11	-B 2xb
15:a2	C_{2h}^6	C2/c:a2 = C2/n11	-C 2xbc
15:a3	C_{2h}^6	C2/c:a3 = I2/c11	-I 2xc
15:-a1	C_{2h}^6	C2/c:-a1 = C2/c11	-C 2xc
15:-a2	C_{2h}^6	C2/c:-a2 = B2/n11	-B 2xbc
15:-a3	C_{2h}^6	C2/c:-a3 = I2/b11	-I 2xb
16	D_2^1	P222	P 2 2
17	D_2^2	P2221	P 2c 2
17:cab	D_2^2	P2122	P 2a 2a
17:bca	D_2^2	P2212	P 2 2b
18	D_2^3	P21212	P 2 2ab
18:cab	D_2^3	P22121	P 2bc 2
18:bca	D_2^3	P21221	P 2ac 2ac
19	D_2^4	P212121	P 2ac 2ab
20	D_2^5	C2221	C 2c 2
20:cab	D_2^5	A2122	A 2a 2a
20:bca	D_2^5	B2212	B 2 2b
21	D_2^6	C222	C 2 2
21:cab	D_2^6	A222	A 2 2
21:bca	D_2^6	B222	B 2 2
22	D_2^7	F222	F 2 2
23	D_2^8	I222	I 2 2
24	D_2^9	I212121	I 2b 2c
25	C_{2v}^1	Pmm2	P 2 -2
25:cab	C_{2v}^1	P2mm	P -2 2
25:bca	C_{2v}^1	Pm2m	P -2 -2
26	C_{2v}^2	Pmc21	P 2c -2
26:ba-c	C_{2v}^2	Pcm21	P 2c -2c
26:cab	C_{2v}^2	P21ma	P -2a 2a
26:-cba	C_{2v}^2	P21am	P -2 2a
26:bca	C_{2v}^2	Pb21m	P -2 -2b
26:a-cb	C_{2v}^2	Pm21b	P -2b -2
27	C_{2v}^3	Pcc2	P 2 -2c
27:cab	C_{2v}^3	P2aa	P -2a 2
27:bca	C_{2v}^3	Pb2b	P -2b -2b
28	C_{2v}^4	Pma2	P 2 -2a
28:ba-c	C_{2v}^4	Pbm2	P 2 -2b
28:cab	C_{2v}^4	P2mb	P -2b 2
28:-cba	C_{2v}^4	P2cm	P -2c 2
28:bca	C_{2v}^4	Pc2m	P -2c -2c
28:a-cb	C_{2v}^4	Pm2a	P -2a -2a
29	C_{2v}^5	Pca21	P 2c -2ac
29:ba-c	C_{2v}^5	Pbc21	P 2c -2b
29:cab	C_{2v}^5	P21ab	P -2b 2a
29:-cba	C_{2v}^5	P21ca	P -2ac 2a
29:bca	C_{2v}^5	Pc21b	P -2bc -2c
29:a-cb	C_{2v}^5	Pb21a	P -2a -2ab
30	C_{2v}^6	Pnc2	P 2 -2bc
30:ba-c	C_{2v}^6	Pcn2	P 2 -2ac

Number	Schoenflies	Hermann-Mauguin	Hall
30:cab	C_{2v}^{6}	P2na	P -2ac 2
30:-cba	C_{2v}^{6}	P2an	P -2ab 2
30:bca	C_{2v}^{6}	Pb2n	P -2ab -2ab
30:a-cb	C_{2v}^{6}	Pn2b	P -2bc -2bc
31	C_{2v}^{7}	Pmn21	P 2ac -2
31:ba-c	C_{2v}^{7}	Pnm21	P 2bc -2bc
31:cab	C_{2v}^{7}	P21mn	P -2ab 2ab
31:-cba	C_{2v}^{7}	P21nm	P -2 2ac
31:bca	C_{2v}^{7}	Pn21m	P -2 -2bc
31:a-cb	C_{2v}^{7}	Pm21n	P -2ab -2
32	C_{2v}^{8}	Pba2	P 2 -2ab
32:cab	C_{2v}^{8}	P2cb	P -2bc 2
32:bca	C_{2v}^{8}	Pc2a	P -2ac -2ac
33	C_{2v}^{9}	Pna21	P 2c -2n
33:ba-c	C_{2v}^{9}	Pbn21	P 2c -2ab
33:cab	C_{2v}^{9}	P21nb	P -2bc 2a
33:-cba	C_{2v}^{9}	P21cn	P -2n 2a
33:bca	C_{2v}^{9}	Pc21n	P -2n -2ac
33:a-cb	C_{2v}^{9}	Pn21a	P -2ac -2n
34	C_{2v}^{10}	Pnn2	P 2 -2n
34:cab	C_{2v}^{10}	P2nn	P -2n 2
34:bca	C_{2v}^{10}	Pn2n	P -2n -2n
35	C_{2v}^{11}	Cmm2	C 2 -2
35:cab	C_{2v}^{11}	A2mm	A -2 2
35:bca	C_{2v}^{11}	Bm2m	B -2 -2
36	C_{2v}^{12}	Cmc21	C 2c -2
36:ba-c	C_{2v}^{12}	Ccm21	C 2c -2c
36:cab	C_{2v}^{12}	A21ma	A -2a 2a
36:-cba	C_{2v}^{12}	A21am	A -2 2a
36:bca	C_{2v}^{12}	Bb21m	B -2 -2b
36:a-cb	C_{2v}^{12}	Bm21b	B -2b -2
37	C_{2v}^{13}	Ccc2	C 2 -2c
37:cab	C_{2v}^{13}	A2aa	A -2a 2
37:bca	C_{2v}^{13}	Bb2b	B -2b -2b
38	C_{2v}^{14}	Amm2	A 2 -2
38:ba-c	C_{2v}^{14}	Bmm2	B 2 -2
38:cab	C_{2v}^{14}	B2mm	B -2 2
38:-cba	C_{2v}^{14}	C2mm	C -2 2
38:bca	C_{2v}^{14}	Cm2m	C -2 -2
38:a-cb	C_{2v}^{14}	Am2m	A -2 -2
39	C_{2v}^{15}	Abm2	A 2 -2c
39:ba-c	C_{2v}^{15}	Bma2	B 2 -2c
39:cab	C_{2v}^{15}	B2cm	B -2c 2
39:-cba	C_{2v}^{15}	C2mb	C -2b 2
39:bca	C_{2v}^{15}	Cm2a	C -2b -2b
39:a-cb	C_{2v}^{15}	Ac2m	A -2c -2c
40	C_{2v}^{16}	Ama2	A 2 -2a
40:ba-c	C_{2v}^{16}	Bbm2	B 2 -2b
40:cab	C_{2v}^{16}	B2mb	B -2b 2
40:-cba	C_{2v}^{16}	C2cm	C -2c 2

Number	Schoenflies	Hermann-Mauguin	Hall
40:bca	C_{2v}^{16}	Cc2m	C -2c -2c
40:a-cb	C_{2v}^{16}	Am2a	A -2a -2a
41	C_{2v}^{17}	Aba2	A 2 -2ac
41:ba-c	C_{2v}^{17}	Bba2	B 2 -2bc
41:cab	C_{2v}^{17}	B2cb	B -2bc 2
41:-cba	C_{2v}^{17}	C2cb	C -2bc 2
41:bca	C_{2v}^{17}	Cc2a	C -2bc -2bc
41:a-cb	C_{2v}^{17}	Ac2a	A -2ac -2ac
42	C_{2v}^{18}	Fmm2	F 2 -2
42:cab	C_{2v}^{18}	F2mm	F -2 2
42:bca	C_{2v}^{18}	Fm2m	F -2 -2
43	C_{2v}^{19}	Fdd2	F 2 -2d
43:cab	C_{2v}^{19}	F2dd	F -2d 2
43:bca	C_{2v}^{19}	Fd2d	F -2d -2d
44	C_{2v}^{20}	Imm2	I 2 -2
44:cab	C_{2v}^{20}	I2mm	I -2 2
44:bca	C_{2v}^{20}	Im2m	I -2 -2
45	C_{2v}^{21}	Iba2	I 2 -2c
45:cab	C_{2v}^{21}	I2cb	I -2a 2
45:bca	C_{2v}^{21}	Ic2a	I -2b -2b
46	C_{2v}^{22}	Ima2	I 2 -2a
46:ba-c	C_{2v}^{22}	Ibm2	I 2 -2b
46:cab	C_{2v}^{22}	I2mb	I -2b 2
46:-cba	C_{2v}^{22}	I2cm	I -2c 2
46:bca	C_{2v}^{22}	Ic2m	I -2c -2c
46:a-cb	C_{2v}^{22}	Im2a	I -2a -2a
47	D_{2h}^{1}	Pmmm	-P 2 2
48:1	D_{2h}^{2}	Pnnn:1	P 2 2 -1n
48:2	D_{2h}^{2}	Pnnn:2	-P 2ab 2bc
49	D_{2h}^{3}	Pccm	-P 2 2c
49:cab	D_{2h}^{3}	Pmaa	-P 2a 2
49:bca	D_{2h}^{3}	Pbmb	-P 2b 2b
50:1	D_{2h}^{4}	Pban:1	P 2 2 -1ab
50:2	D_{2h}^{4}	Pban:2	-P 2ab 2b
50:1cab	D_{2h}^{4}	Pncb:1	P 2 2 -1bc
50:2cab	D_{2h}^{4}	Pncb:2	-P 2b 2bc
50:1bca	D_{2h}^{4}	Pcna:1	P 2 2 -1ac
50:2bca	D_{2h}^{4}	Pcna:2	-P 2a 2c
51	D_{2h}^{5}	Pmma	-P 2a 2a
51:ba-c	D_{2h}^{5}	Pmmb	-P 2b 2
51:cab	D_{2h}^{5}	Pbmm	-P 2 2b
51:-cba	D_{2h}^{5}	Pcmm	-P 2c 2c
51:bca	D_{2h}^{5}	Pmcm	-P 2c 2
51:a-cb	D_{2h}^{5}	Pmam	-P 2 2a
52	D_{2h}^{6}	Pnna	-P 2a 2bc
52:ba-c	D_{2h}^{6}	Pnnb	-P 2b 2n
52:cab	D_{2h}^{6}	Pbnn	-P 2n 2b
52:-cba	D_{2h}^{6}	Pcnn	-P 2ab 2c
52:bca	D_{2h}^{6}	Pncn	-P 2ab 2n
52:a-cb	D_{2h}^{6}	Pnan	-P 2n 2bc

Number	Schoenflies	Hermann-Mauguin	Hall
53	D_{2h}^{7}	Pmna	-P 2ac 2
53:ba-c	D_{2h}^{7}	Pnmb	-P 2bc 2bc
53:cab	D_{2h}^{7}	Pbmn	-P 2ab 2ab
53:-cba	D_{2h}^{7}	Pcnm	-P 2 2ac
53:bca	D_{2h}^{7}	Pncm	-P 2 2bc
53:a-cb	D_{2h}^{7}	Pman	-P 2ab 2
54	D_{2h}^{8}	Pcca	-P 2a 2ac
54:ba-c	D_{2h}^{8}	Pccb	-P 2b 2c
54:cab	D_{2h}^{8}	Pbaa	-P 2a 2b
54:-cba	D_{2h}^{8}	Pcaa	-P 2ac 2c
54:bca	D_{2h}^{8}	Pbcb	-P 2bc 2b
54:a-cb	D_{2h}^{8}	Pbab	-P 2b 2ab
55	D_{2h}^{9}	Pbam	-P 2 2ab
55:cab	D_{2h}^{9}	Pmcb	-P 2bc 2
55:bca	D_{2h}^{9}	Pcma	-P 2ac 2ac
56	D_{2h}^{10}	Pccn	-P 2ab 2ac
56:cab	D_{2h}^{10}	Pnaa	-P 2ac 2bc
56:bca	D_{2h}^{10}	Pbnb	-P 2bc 2ab
57	D_{2h}^{11}	Pbcm	-P 2c 2b
57:ba-c	D_{2h}^{11}	Pcam	-P 2c 2ac
57:cab	D_{2h}^{11}	Pmca	-P 2ac 2a
57:-cba	D_{2h}^{11}	Pmab	-P 2b 2a
57:bca	D_{2h}^{11}	Pbma	-P 2a 2ab
57:a-cb	D_{2h}^{11}	Pcmb	-P 2bc 2c
58	D_{2h}^{12}	Pnnm	-P 2 2n
58:cab	D_{2h}^{12}	Pmnn	-P 2n 2
58:bca	D_{2h}^{12}	Pnmn	-P 2n 2n
59:1	D_{2h}^{13}	Pmmn:1	P 2 2ab -1ab
59:2	D_{2h}^{13}	Pmmn:2	-P 2ab 2a
59:1cab	D_{2h}^{13}	Pnmm:1	P 2bc 2 -1bc
59:2cab	D_{2h}^{13}	Pnmm:2	-P 2c 2bc
59:1bca	D_{2h}^{13}	Pmnm:1	P 2ac 2ac -1ac
59:2bca	D_{2h}^{13}	Pmnm:2	-P 2c 2a
60	D_{2h}^{14}	Pbcn	-P 2n 2ab
60:ba-c	D_{2h}^{14}	Pcan	-P 2n 2c
60:cab	D_{2h}^{14}	Pnca	-P 2a 2n
60:-cba	D_{2h}^{14}	Pnab	-P 2bc 2n
60:bca	D_{2h}^{14}	Pbna	-P 2ac 2b
60:a-cb	D_{2h}^{14}	Pcnb	-P 2b 2ac
61	D_{2h}^{15}	Pbca	-P 2ac 2ab
61:ba-c	D_{2h}^{15}	Pcab	-P 2bc 2ac
62	D_{2h}^{16}	Pnma	-P 2ac 2n
62:ba-c	D_{2h}^{16}	Pmnb	-P 2bc 2a
62:cab	D_{2h}^{16}	Pbnm	-P 2c 2ab
62:-cba	D_{2h}^{16}	Pcmn	-P 2n 2ac
62:bca	D_{2h}^{16}	Pmcn	-P 2n 2a
62:a-cb	D_{2h}^{16}	Pnam	-P 2c 2n
63	D_{2h}^{17}	Cmcm	-C 2c 2
63:ba-c	D_{2h}^{17}	Ccmm	-C 2c 2c
63:cab	D_{2h}^{17}	Amma	-A 2a 2a

Number	Schoenflies	Hermann-Mauguin	Hall
63:-cba	D_{2h}^{17}	Amam	-A 2 2a
63:bca	D_{2h}^{17}	Bbmm	-B 2 2b
63:a-cb	D_{2h}^{17}	Bmmb	-B 2b 2
64	D_{2h}^{18}	Cmca	-C 2bc 2
64:ba-c	D_{2h}^{18}	Ccmb	-C 2bc 2bc
64:cab	D_{2h}^{18}	Abma	-A 2ac 2ac
64:-cba	D_{2h}^{18}	Acam	-A 2 2ac
64:bca	D_{2h}^{18}	Bbcm	-B 2 2bc
64:a-cb	D_{2h}^{18}	Bmab	-B 2bc 2
65	D_{2h}^{19}	Cmmm	-C 2 2
65:cab	D_{2h}^{19}	Ammm	-A 2 2
65:bca	D_{2h}^{19}	Bmmm	-B 2 2
66	D_{2h}^{20}	Cccm	-C 2 2c
66:cab	D_{2h}^{20}	Amaa	-A 2a 2
66:bca	D_{2h}^{20}	Bbmb	-B 2b 2b
67	D_{2h}^{21}	Cmma	-C 2b 2
67:ba-c	D_{2h}^{21}	Cmmb	-C 2b 2b
67:cab	D_{2h}^{21}	Abmm	-A 2c 2c
67:-cba	D_{2h}^{21}	Acmm	-A 2 2c
67:bca	D_{2h}^{21}	Bmcm	-B 2 2c
67:a-cb	D_{2h}^{21}	Bmam	-B 2c 2
68:1	D_{2h}^{22}	Ccca:1	C 2 2 -1bc
68:2	D_{2h}^{22}	Ccca:2	-C 2b 2bc
68:1ba-c	D_{2h}^{22}	Cccb:1	C 2 2 -1bc
68:2ba-c	D_{2h}^{22}	Cccb:2	-C 2b 2c
68:1cab	D_{2h}^{22}	Abaa:1	A 2 2 -1ac
68:2cab	D_{2h}^{22}	Abaa:2	-A 2a 2c
68:1-cba	D_{2h}^{22}	Acaa:1	A 2 2 -1ac
68:2-cba	D_{2h}^{22}	Acaa:2	-A 2ac 2c
68:1bca	D_{2h}^{22}	Bbcb:1	B 2 2 -1bc
68:2bca	D_{2h}^{22}	Bbcb:2	-B 2bc 2b
68:1a-cb	D_{2h}^{22}	Bbab:1	B 2 2 -1bc
68:2a-cb	D_{2h}^{22}	Bbab:2	-B 2b 2bc
69	D_{2h}^{23}	Fmmm	-F 2 2
70:1	D_{2h}^{24}	Fddd:1	F 2 2 -1d
70:2	D_{2h}^{24}	Fddd:2	-F 2uv 2vw
71	D_{2h}^{25}	Immm	-I 2 2
72	D_{2h}^{26}	Ibam	-I 2 2c
72:cab	D_{2h}^{26}	Imcb	-I 2a 2
72:bca	D_{2h}^{26}	Icma	-I 2b 2b
73	D_{2h}^{27}	Ibca	-I 2b 2c
73:ba-c	D_{2h}^{27}	Icab	-I 2a 2b
74	D_{2h}^{28}	Imma	-I 2b 2
74:ba-c	D_{2h}^{28}	Immb	-I 2a 2a
74:cab	D_{2h}^{28}	Ibmm	-I 2c 2c
74:-cba	D_{2h}^{28}	Icmm	-I 2 2b
74:bca	D_{2h}^{28}	Imcm	-I 2 2a
74:a-cb	D_{2h}^{28}	Imam	-I 2c 2
75	C_4^1	P4	P 4
76	C_4^2	P41	P 4w

Number	Schoenflies	Hermann-Mauguin	Hall
77	C_4^3	P42	P 4c
78	C_4^4	P43	P 4cw
79	C_4^5	I4	I 4
80	C_4^6	I41	I 4bw
81	S_4^1	P-4	P -4
82	S_4^2	I-4	I -4
83	C_{4h}^1	P4/m	-P 4
84	C_{4h}^2	P42/m	-P 4c
85:1	C_{4h}^3	P4/n:1	P 4ab -1ab
85:2	C_{4h}^3	P4/n:2	-P 4a
86:1	C_{4h}^4	P42/n:1	P 4n -1n
86:2	C_{4h}^4	P42/n:2	-P 4bc
87	C_{4h}^5	I4/m	-I 4
88:1	C_{4h}^6	I41/a:1	I 4bw -1bw
88:2	C_{4h}^6	I41/a:2	-I 4ad
89	D_4^1	P422	P 4 2
90	D_4^2	P4212	P 4ab 2ab
91	D_4^3	P4122	P 4w 2c
92	D_4^4	P41212	P 4abw 2nw
93	D_4^5	P4222	P 4c 2
94	D_4^6	P42212	P 4n 2n
95	D_4^7	P4322	P 4cw 2c
96	D_4^8	P43212	P 4nw 2abw
97	D_4^9	I422	I 4 2
98	D_4^{10}	I4122	I 4bw 2bw
99	C_{4v}^1	P4mm	P 4 -2
100	C_{4v}^2	P4bm	P 4 -2ab
101	C_{4v}^3	P42cm	P 4c -2c
102	C_{4v}^4	P42nm	P 4n -2n
103	C_{4v}^5	P4cc	P 4 -2c
104	C_{4v}^6	P4nc	P 4 -2n
105	C_{4v}^7	P42mc	P 4c -2
106	C_{4v}^8	P42bc	P 4c -2ab
107	C_{4v}^9	I4mm	I 4 -2
108	C_{4v}^{10}	I4cm	I 4 -2c
109	C_{4v}^{11}	I41md	I 4bw -2
110	C_{4v}^{12}	I41cd	I 4bw -2c
111	D_{2d}^1	P-42m	P -4 2
112	D_{2d}^2	P-42c	P -4 2c
113	D_{2d}^3	P-421m	P -4 2ab
114	D_{2d}^4	P-421c	P -4 2n
115	D_{2d}^5	P-4m2	P -4 -2
116	D_{2d}^6	P-4c2	P -4 -2c
117	D_{2d}^7	P-4b2	P -4 -2ab
118	D_{2d}^8	P-4n2	P -4 -2n
119	D_{2d}^9	I-4m2	I -4 -2
120	D_{2d}^{10}	I-4c2	I -4 -2c
121	D_{2d}^{11}	I-42m	I -4 2
122	D_{2d}^{12}	I-42d	I -4 2bw
123	D_{4h}^1	P4/mmm	-P 4 2

Number	Schoenflies	Hermann-Mauguin	Hall
124	D_{4h}^{2}	P4/mcc	-P 4 2c
125:1	D_{4h}^{3}	P4/nbm:1	P 4 2 -1ab
125:2	D_{4h}^{3}	P4/nbm:2	-P 4a 2b
126:1	D_{4h}^{4}	P4/nnc:1	P 4 2 -1n
126:2	D_{4h}^{4}	P4/nnc:2	-P 4a 2bc
127	D_{4h}^{5}	P4/mbm	-P 4 2ab
128	D_{4h}^{6}	P4/mnc	-P 4 2n
129:1	D_{4h}^{7}	P4/nmm:1	P 4ab 2ab -1ab
129:2	D_{4h}^{7}	P4/nmm:2	-P 4a 2a
130:1	D_{4h}^{8}	P4/ncc:1	P 4ab 2n -1ab
130:2	D_{4h}^{8}	P4/ncc:2	-P 4a 2ac
131	D_{4h}^{9}	P42/mmc	-P 4c 2
132	D_{4h}^{10}	P42/mcm	-P 4c 2c
133:1	D_{4h}^{11}	P42/nbc:1	P 4n 2c -1n
133:2	D_{4h}^{11}	P42/nbc:2	-P 4ac 2b
134:1	D_{4h}^{12}	P42/nnm:1	P 4n 2 -1n
134:2	D_{4h}^{12}	P42/nnm:2	-P 4ac 2bc
135	D_{4h}^{13}	P42/mbc	-P 4c 2ab
136	D_{4h}^{14}	P42/mnm	-P 4n 2n
137:1	D_{4h}^{15}	P42/nmc:1	P 4n 2n -1n
137:2	D_{4h}^{15}	P42/nmc:2	-P 4ac 2a
138:1	D_{4h}^{16}	P42/ncm:1	P 4n 2ab -1n
138:2	D_{4h}^{16}	P42/ncm:2	-P 4ac 2ac
139	D_{4h}^{17}	I4/mmm	-I 4 2
140	D_{4h}^{18}	I4/mcm	-I 4 2c
141:1	D_{4h}^{19}	I41/amd:1	I 4bw 2bw -1bw
141:2	D_{4h}^{19}	I41/amd:2	-I 4bd 2
142:1	D_{4h}^{20}	I41/acd:1	I 4bw 2aw -1bw
142:2	D_{4h}^{20}	I41/acd:2	-I 4bd 2c
143	C_{3}^{1}	P3	P 3
144	C_{3}^{2}	P31	P 31
145	C_{3}^{3}	P32	P 32
146:H	C_{3}^{4}	R3:H	R 3
146:R	C_{3}^{4}	R3:R	P 3*
147	C_{3i}^{1}	P-3	-P 3
148:H	C_{3i}^{2}	R-3:H	-R 3
148:R	C_{3i}^{2}	R-3:R	-P 3*
149	D_{3}^{1}	P312	P 3 2
150	D_{3}^{2}	P321	P 3 2″
151	D_{3}^{3}	P3112	P 31 2c (0 0 1)
152	D_{3}^{4}	P3121	P 31 2″
153	D_{3}^{5}	P3212	P 32 2c (0 0 -1)
154	D_{3}^{6}	P3221	P 32 2″
155:H	D_{3}^{7}	R32:H	R 3 2″
155:R	D_{3}^{7}	R32:R	P 3* 2
156	C_{3v}^{1}	P3m1	P 3 -2″
157	C_{3v}^{2}	P31m	P 3 -2
158	C_{3v}^{3}	P3c1	P 3 -2″c
159	C_{3v}^{4}	P31c	P 3 -2c
160:H	C_{3v}^{5}	R3m:H	R 3 -2″

Number	Schoenflies	Hermann-Mauguin	Hall
160:R	C_{3v}^5	R3m:R	P 3* -2
161:H	C_{3v}^6	R3c:H	R 3 -2″c
161:R	C_{3v}^6	R3c:R	P 3* -2n
162	D_{3d}^1	P-31m	-P 3 2
163	D_{3d}^2	P-31c	-P 3 2c
164	D_{3d}^3	P-3m1	-P 3 2″
165	D_{3d}^4	P-3c1	-P 3 2″c
166:H	D_{3d}^5	R-3m:H	-R 3 2″
166:R	D_{3d}^5	R-3m:R	-P 3* 2
167:H	D_{3d}^6	R-3c:H	-R 3 2″c
167:R	D_{3d}^6	R-3c:R	-P 3* 2n
168	C_6^1	P6	P 6
169	C_6^2	P61	P 61
170	C_6^3	P65	P 65
171	C_6^4	P62	P 62
172	C_6^5	P64	P 64
173	C_6^6	P63	P 6c
174	C_{3h}^1	P-6	P -6
175	C_{6h}^1	P6/m	-P 6
176	C_{6h}^2	P63/m	-P 6c
177	D_6^1	P622	P 6 2
178	D_6^2	P6122	P 61 2 (0 0 -1)
179	D_6^3	P6522	P 65 2 (0 0 1)
180	D_6^4	P6222	P 62 2c (0 0 1)
181	D_6^5	P6422	P 64 2c (0 0 -1)
182	D_6^6	P6322	P 6c 2c
183	C_{6v}^1	P6mm	P 6 -2
184	C_{6v}^2	P6cc	P 6 -2c
185	C_{6v}^3	P63cm	P 6c -2
186	C_{6v}^4	P63mc	P 6c -2c
187	D_{3h}^1	P-6m2	P -6 2
188	D_{3h}^2	P-6c2	P -6c 2
189	D_{3h}^3	P-62m	P -6 -2
190	D_{3h}^4	P-62c	P -6c -2c
191	D_{6h}^1	P6/mmm	-P 6 2
192	D_{6h}^2	P6/mcc	-P 6 2c
193	D_{6h}^3	P63/mcm	-P 6c 2
194	D_{6h}^4	P63/mmc	-P 6c 2c
195	T^1	P23	P 2 2 3
196	T^2	F23	F 2 2 3
197	T^3	I23	I 2 2 3
198	T^4	P213	P 2ac 2ab 3
199	T^5	I213	I 2b 2c 3
200	T_h^1	Pm-3	-P 2 2 3
201:1	T_h^2	Pn-3:1	P 2 2 3 -1n
201:2	T_h^2	Pn-3:2	-P 2ab 2bc 3
202	T_h^3	Fm-3	-F 2 2 3
203:1	T_h^4	Fd-3:1	F 2 2 3 -1d
203:2	T_h^4	Fd-3:2	-F 2uv 2vw 3
204	T_h^5	Im-3	-I 2 2 3

Number	Schoenflies	Hermann-Mauguin	Hall
205	T_h^6	Pa-3	-P 2ac 2ab 3
206	T_h^7	Ia-3	-I 2b 2c 3
207	O^1	P432	P 4 2 3
208	O^2	P4232	P 4n 2 3
209	O^3	F432	F 4 2 3
210	O^4	F4132	F 4d 2 3
211	O^5	I432	I 4 2 3
212	O^6	P4332	P 4acd 2ab 3
213	O^7	P4132	P 4bd 2ab 3
214	O^8	I4132	I 4bd 2c 3
215	T_d^1	P-43m	P -4 2 3
216	T_d^2	F-43m	F -4 2 3
217	T_d^3	I-43m	I -4 2 3
218	T_d^4	P-43n	P -4n 2 3
219	T_d^5	F-43c	F -4c 2 3
220	T_d^6	I-43d	I -4bd 2c 3
221	O_h^1	Pm-3m	-P 4 2 3
222:1	O_h^2	Pn-3n:1	P 4 2 3 -1n
222:2	O_h^2	Pn-3n:2	-P 4a 2bc 3
223	O_h^3	Pm-3n	-P 4n 2 3
224:1	O_h^4	Pn-3m:1	P 4n 2 3 -1n
224:2	O_h^4	Pn-3m:2	-P 4bc 2bc 3
225	O_h^5	Fm-3m	-F 4 2 3
226	O_h^6	Fm-3c	-F 4c 2 3
227:1	O_h^7	Fd-3m:1	F 4d 2 3 -1d
227:2	O_h^7	Fd-3m:2	-F 4vw 2vw 3
228:1	O_h^8	Fd-3c:1	F 4d 2 3 -1cd
228:2	O_h^8	Fd-3c:2	-F 4cvw 2vw 3
229	O_h^9	Im-3m	-I 4 2 3
230	O_h^{10}	Ia-3d	-I 4bd 2c 3

4.0.1 r3dot (Source File: r3dot.f90)

INTERFACE:

```
real(8) function r3dot(x,y)
```

INPUT/OUTPUT PARAMETERS:

```
x : input vector 1 (in,real(3))
y : input vector 2 (in,real(3))
```

DESCRIPTION:

Returns the dot-product of two real 3-vectors.

REVISION HISTORY:

```
Created January 2003 (JKD)
```

4.0.2 r3cross (Source File: r3cross.f90)

INTERFACE:

```
subroutine r3cross(x,y,z)
```

INPUT/OUTPUT PARAMETERS:

```
x : input vector 1 (in,real(3))
y : input vector 2 (in,real(3))
z : output cross-product (out,real(3))
```

DESCRIPTION:

Returns the cross product of two real 3-vectors.

REVISION HISTORY:

```
Created September 2002 (JKD)
```

4.0.3 findprim (Source File: findprim.f90)

INTERFACE:

```
subroutine findprim
```

USES:

```
use modinput
use modspacegroup
```

DESCRIPTION:

This routine finds the smallest primitive cell which produces the same crystal structure as the conventional cell. This is done by searching through all the vectors which connect atomic positions and finding those which leave the crystal structure invariant. Of these, the three shortest which produce a non-zero unit cell volume are chosen.

REVISION HISTORY:

```
Created April 2007 (JKD)
```

4.0.4 sgsymb (Source File: sgsymb.f90)

INTERFACE:

```
subroutine sgsymb(hrmg,num,schn,hall)
```

INPUT/OUTPUT PARAMETERS:

```
hrmg : Hermann-Mauguin symbol (in,character(20))
num  : space group number (out,character(20))
schn : Schoenflies symbol (out,character(20))
hall : Hall symbol (out,character(20))
```

DESCRIPTION:

Returns the space group number, Schoenflies and Hall symbols given the Hermann-Mauguin symbol. The routine is case-sensitive. With acknowledgements to Ralf W. Grosse-Kunstleve and the tables available at `http://cci.lbl.gov/sginfo/`.

REVISION HISTORY:

```
Created October 2006 (JKD)
```

4.0.5 r3minv (Source File: r3minv.f90)

INTERFACE:

```
subroutine r3minv(a,b)
```

INPUT/OUTPUT PARAMETERS:

```
a : input matrix (in,real(3,3))
b : output matrix (in,real(3,3))
```

DESCRIPTION:

Computes the inverse of a real 3×3 matrix.

REVISION HISTORY:

```
Created April 2003 (JKD)
```

4.0.6 r3mv (Source File: r3mv.f90)

INTERFACE:

```
subroutine r3mv(a,x,y)
```

INPUT/OUTPUT PARAMETERS:

```
a : input matrix (in,real(3,3))
x : input vector (in,real(3))
y : output vector (out,real(3))
```

DESCRIPTION:

Multiplies a real 3×3 matrix with a vector.

REVISION HISTORY:

```
Created January 2003 (JKD)
```

4.0.7 r3mm (Source File: r3mm.f90)

INTERFACE:

```
subroutine r3mm(a,b,c)
```

INPUT/OUTPUT PARAMETERS:

```
a : input matrix 1 (in,real(3,3))
b : input matrix 2 (in,real(3,3))
c : output matrix (out,real(3,3))
```

DESCRIPTION:

Multiplies two real 3×3 matrices.

REVISION HISTORY:

```
Created April 2003 (JKD)
```

4.1 Fortran: Module Interface modmain (Source File: modmain.f90)

Contains all the global variables required by the spacegroup code.

REVISION HISTORY:

```
Created October 2006 (JKD)
```

4.1.1 r3taxi (Source File: r3taxi.f90)

INTERFACE:

```
real(8) function r3taxi(x,y)
```

INPUT/OUTPUT PARAMETERS:

```
x : input vector 1 (in,real(3))
y : input vector 2 (in,real(3))
```

DESCRIPTION:

Returns the taxi-cab distance between two real 3-vectors: $d = |x_1 - y_1| + |x_2 - y_2| + |x_3 - y_3|$.

REVISION HISTORY:

```
Created March 2006 (JKD)
```