

# THE SPACEGROUP MANUAL

VERSION 1.1.4

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## 1 Introduction

**Spacegroup** is a utility which produces crystal geometry for use with the Elk 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.

## 2 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  $\text{La}_2\text{CuO}_4$ :

```
'Bmab'
10.0605232 10.0605232 24.972729
90.0      90.0      90.0
1 1 1
.true.
3
'La'
1
0.0000      0.0000      0.3608
'Cu'
1
0.0000      0.0000      0.0000
'O'
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**

The atomic species symbol

**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 **elk.in** file. If XCrysDen is available, then use the command

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

to render the unit cell.

### 3 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	$D_{2h}^{13}$	Pmmm:1	P 2 2ab -1ab
59:2	$D_{2h}^{13}$	Pmmm:2	-P 2ab 2a
59:1cab	$D_{2h}^{13}$	Pmmm:1	P 2bc 2 -1bc
59:2cab	$D_{2h}^{13}$	Pmmm:2	-P 2c 2bc
59:1bca	$D_{2h}^{13}$	Pmmm:1	P 2ac 2ac -1ac
59:2bca	$D_{2h}^{13}$	Pmmm: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 Routine/Function Prologues

### 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)

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### 4.2 *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)

---

### 4.3 *findprim* (Source File: *findprim.f90*)

INTERFACE:

```
subroutine findprim
```

*USES:*

```
use modmain
```

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)

---



#### 4.4 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  $\text{frac}(x) = x - \lfloor x \rfloor$ . 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)

---

#### 4.5 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)

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#### 4.6 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  $3 \times 3$  matrix with a vector.

**REVISION HISTORY:**

Created January 2003 (JKD)

---

#### 4.7 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)

---

#### 4.8 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  $3 \times 3$  matrix.

**REVISION HISTORY:**

Created April 2003 (JKD)

---

## 4.9 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  $3 \times 3$  matrices.

### REVISION HISTORY:

Created April 2003 (JKD)