# The Spacegroup Manual

Version 1.2.1

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# Contents

# 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 $La_2CuO_4$:

```
'Bmab'                                  : hrmg
10.0605232 10.0605232  24.972729        : a, b, c
 90.0     90.0     90.0                 : bc, ac, ab
 1  1  1                                 : ncell
 .true.                                  : primcell
 3                                       : nspecies
 'La'                                    : spsymb
 1                                       : nwpos
 0.0000    0.0000    0.3608              : wpos
 '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).

`bc`, `ac`, `ab`
Angles in degrees between lattice vectors **b** and **c** ($\alpha$); **a** and **c** ($\beta$); and **a** and **b** ($\gamma$).

`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 | $D_{2h}^{13}$ | 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 | $C_4^1$ | $P4_{11}$ | 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)
```

---

## 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 findprimcell (Source File: findprimcell.f90)

INTERFACE:

```
subroutine findprimcell
```

*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)
```

*INPUT/OUTPUT PARAMETERS:*

```
eps : zero component tolerance (in,real)
v   : input vector (inout,real(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 $(1-\epsilon, 1]$.

REVISION HISTORY:

```
Created January 2003 (JKD)
Removed iv, September 2011 (JKD)
```

---

### 4.5 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)
```

---

### 4.6 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)
```

---

### 4.7 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)
```

---

### 4.8 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)
```