4.7. Symmetry dictionary (symCIF)

BY I. D. BROWN

This is version 1.0.1 of the symmetry CIF dictionary (symCIF), which gives a more complete description of symmetry than was included in the original core CIF dictionary. A detailed commentary on the philosophy behind the dictionary and its use may be found in Chapter 3.8.

SPACE_GROUP

Contains all the data items that refer to the space group as a whole, such as its name, Laue group *etc.* It may be looped, for example in a list of space groups and their properties. Space-group types are identified by their number as listed in *International Tables for Crystallography* Volume A, or by their Schoenflies symbol. Specific settings of the space groups can be identified by their Hall symbol, by specifying their symmetry operations or generators, or by giving the transformation that relates the specific setting to the reference setting based on *International Tables* Volume A and stored in this dictionary. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but several different Hermann–Mauguin symbols may refer to the same space-group type. A Hermann–Mauguin symbol contains information on the choice of the basis, but not on the choice of origin.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Mandatory category.

Category key(s): **`_space_group.id`**

Example 1 – description of the C2/c space group, No. 15 in International Tables for Crystallography Volume A.

```
_space_group.id                    1
_space_group.name_H-M_ref          'C 2/c'
_space_group.name_Schoenflies      C2h.6
_space_group.IT_number             15
_space_group.name_Hall             '-C 2yc'
_space_group.Bravais_type          mS
_space_group.Laue_class            2/m
_space_group.crystal_system        monoclinic
_space_group.centring_type         C
_space_group.Patterson_name_H-M    'C 2/m'
```

`_space_group.Bravais_type` (*char*)

The symbol denoting the lattice type (Bravais type) to which the translational subgroup (vector lattice) of the space group belongs. It consists of a lower-case letter indicating the crystal system followed by an upper-case letter indicating the lattice centring. The setting-independent symbol *mS* replaces the setting-dependent symbols *mB* and *mC*, and the setting-independent symbol *oS* replaces the setting-dependent symbols *oA*, *oB* and *oC*.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed., p. 15. Dordrecht: Kluwer Academic Publishers.

The data value must be one of the following:

```
aP
mP mS
oP oS oI oF
tP tI
hP hR
cP cI cF
```

Example: '`aP`' (triclinic (anorthic) primitive lattice). **`[space_group]`**

`_space_group.IT_coordinate_system_code` (*char*)

A qualifier taken from the enumeration list identifying which setting in *International Tables for Crystallography* Volume A (2002) (*IT*) is used. See *IT* Table 4.3.2.1, Section 2.2.16, Table 2.2.16.1, Section 2.2.16.1 and Fig. 2.2.6.4. This item is not computer-interpretable and cannot be used to define the coordinate system. Use **`_space_group.transform_*`** instead.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

The data value must be one of the following:

`b1`	monoclinic unique axis *b*, cell choice 1, **abc**
`b2`	monoclinic unique axis *b*, cell choice 2, **abc**
`b3`	monoclinic unique axis *b*, cell choice 3, **abc**
`-b1`	monoclinic unique axis *b*, cell choice 1, **$\bar{c}$ba**
`-b2`	monoclinic unique axis *b*, cell choice 2, **$\bar{c}$ba**
`-b3`	monoclinic unique axis *b*, cell choice 3, **$\bar{c}$ba**
`c1`	monoclinic unique axis *c*, cell choice 1, **abc**
`c2`	monoclinic unique axis *c*, cell choice 2, **abc**
`c3`	monoclinic unique axis *c*, cell choice 3, **abc**
`-c1`	monoclinic unique axis *c*, cell choice 1, **ba$\bar{c}$**
`-c2`	monoclinic unique axis *c*, cell choice 2, **ba$\bar{c}$**
`-c3`	monoclinic unique axis *c*, cell choice 3, **ba$\bar{c}$**
`a1`	monoclinic unique axis *a*, cell choice 1, **abc**
`a2`	monoclinic unique axis *a*, cell choice 2, **abc**
`a3`	monoclinic unique axis *a*, cell choice 3, **abc**
`-a1`	monoclinic unique axis *a*, cell choice 1, **$\bar{a}$cb**
`-a2`	monoclinic unique axis *a*, cell choice 2, **$\bar{a}$cb**
`-a3`	monoclinic unique axis *a*, cell choice 3, **$\bar{a}$cb**
`abc`	orthorhombic
`ba-c`	orthorhombic
`cab`	orthorhombic
`-cba`	orthorhombic
`bca`	orthorhombic
`a-cb`	orthorhombic
`1abc`	orthorhombic origin choice 1
`1ba-c`	orthorhombic origin choice 1
`1cab`	orthorhombic origin choice 1
`1-cba`	orthorhombic origin choice 1
`1bca`	orthorhombic origin choice 1
`1a-cb`	orthorhombic origin choice 1
`2abc`	orthorhombic origin choice 2
`2ba-c`	orthorhombic origin choice 2
`2cab`	orthorhombic origin choice 2
`2-cba`	orthorhombic origin choice 2
`2bca`	orthorhombic origin choice 2
`2a-cb`	orthorhombic origin choice 2
`1`	tetragonal or cubic origin choice 1
`2`	tetragonal or cubic origin choice 2
`h`	trigonal using hexagonal axes
`r`	trigonal using rhombohedral axes

`[space_group]`

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_space_group.IT_number (*numb*)

_symmetry_Int_Tables_number (*cif_core.dic 1.0*)

The number as assigned in *International Tables for Crystallography* Volume A, specifying the proper affine class (*i.e.* the orientation-preserving affine class) of space groups (crystallographic space-group type) to which the space group belongs. This number defines the space-group type but not the coordinate system in which it is expressed.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

The permitted range is (1, 230). **[space_group]**

_space_group.Laue_class (*char*)

The Hermann–Mauguin symbol of the geometric crystal class of the point group of the space group where a centre of inversion is added if not already present.

The data value must be one of the following:

```
-1
2/m   mmm
4/m   4/mmm
-3   -3m
6/m   6/mmm
m-3   m-3m
```
[space_group]

_space_group.Patterson_name_H-M (*char*)

The Hermann–Mauguin symbol of the type of that centrosymmetric symmorphic space group to which the Patterson function belongs; see Table 2.2.5.1 in *International Tables for Crystallography* Volume A (2002). A space separates each symbol referring to different axes. Underscores may replace the spaces, but this use is discouraged. Subscripts should appear without special symbols. Bars should be given as negative signs before the number to which they apply.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed., Table 2.2.5.1. Dordrecht: Kluwer Academic Publishers.

Examples: 'P -1', 'P 2/m', 'C 2/m', 'P m m m', 'C m m m', 'I m m m', 'F m m m', 'P 4/m', 'I 4/m', 'P 4/m m m', 'I 4/m m m', 'P -3', 'R -3', 'P -3 m 1', 'R -3 m', 'P -3 1 m', 'P 6/m', 'P 6/m m m', 'P m -3', 'I m -3', 'F m -3', 'P m -3 m', 'I m -3 m', 'F m -3 m'. **[space_group]**

_space_group.centring_type (*char*)

Symbol for the lattice centring. This symbol may be dependent on the coordinate system chosen.

The data value must be one of the following:

P	primitive no centring
A	*A*-face centred (0, 1/2, 1/2)
B	*B*-face centred (1/2, 0, 1/2)
C	*C*-face centred (1/2, 1/2, 0)
F	all faces centred (0, 1/2, 1/2), (1/2, 0, 1/2), (1/2, 1/2, 0)
I	body centred (1/2, 1/2, 1/2)
R	rhombohedral obverse centred (2/3, 1/3, 1/3), (1/3, 2/3, 2/3)
Rrev	rhombohedral reverse centred (1/3, 2/3, 1/3), (2/3, 1/3, 2/3)
H	hexagonal centred (2/3, 1/3, 0), (1/3, 2/3, 0)

[space_group]

_space_group.crystal_system (*char*)

_symmetry_cell_setting (*cif_core.dic 1.0*)

The name of the system of geometric crystal classes of space groups (crystal system) to which the space group belongs. Note that crystals with the *hR* lattice type belong to the trigonal system.

The data value must be one of the following:

```
triclinic
monoclinic
orthorhombic
tetragonal
trigonal
hexagonal
cubic
```
[space_group]

*_space_group.id (*char*)

This is an identifier needed if **_space_group**.* items are looped.

The following item(s) have an equivalent role in their respective categories:

_space_group_symop.sg_id,

_space_group_Wyckoff.sg_id. **[space_group]**

_space_group.name_H-M_alt (*char*)

_symmetry_space_group_name_H-M (*cif_core.dic 1.0*)

_space_group.name_H-M_alt allows for an alternative Hermann–Mauguin symbol to be given. The way in which this item is used is determined by the user and should be described in the item **_space_group.name_H-M_alt_description**. It may, for example, be used to give one of the extended Hermann–Mauguin symbols given in Table 4.3.2.1 of *International Tables for Crystallography* Volume A (2002) or a full Hermann–Mauguin symbol for an unconventional setting. Each component of the space-group name is separated by a space or an underscore character. The use of a space is strongly recommended. The underscore is only retained because it was used in older CIFs. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely, but a given space-group type may be described by more than one Hermann–Mauguin symbol. The space-group type is best described using **_space_group.IT_number** or **_space_group.name_Schoenflies**. The Hermann–Mauguin symbol may contain information on the choice of basis but does not contain information on the choice of origin. To define the setting uniquely, use **_space_group.name_Hall**, list the symmetry operations or generators, or give the transformation that relates the setting to the reference setting defined in this dictionary under **_space_group.reference_setting**.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Related items: **_space_group.name_H-M_ref** (alternate), **_space_group.name_H-M_full** (alternate) .

Example:

```
; loop_
  _space_group.name_H-M_alt
  _space_group.name_H-M_alt_description
  'C m c m(b n n)'
  'Extended Hermann-Mauguin symbol'
  'C 2/c 2/m 21/m'
  'Full unconventional Hermann-Mauguin symbol'
  'A m a m'
  'Hermann-Mauguin symbol corresponding to setting used'
;  (Three examples for space group No. 63.)
```
[space_group]

_space_group.name_H-M_alt_description (*char*)

A free-text description of the code appearing in **_space_group.name_H-M_alt**.

[space_group]

_space_group.name_H-M_full (*char*)

symmetry.space_group_name_H-M (*cif_mm.dic 1.0.0*)

The full international Hermann–Mauguin space-group symbol as defined in Section 2.2.3 and given as the second item of the second line of each of the space-group tables of Part 7 of *International Tables for Crystallography* Volume A (2002). Each component of the space-group name is separated by a space or an underscore character. The use of a space is strongly recommended. The underscore is only retained because it was used in old CIFs. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but a given

space-group type may be described by more than one Hermann–Mauguin symbol. The space-group type is best described using **_space_group.IT_number** or **_space_group.name_Schoenflies**. The full international Hermann–Mauguin symbol contains information about the choice of basis for monoclinic and orthorhombic space groups but does not give information about the choice of origin. To define the setting uniquely use **_space_group.name_Hall**, list the symmetry operations or generators, or give the transformation relating the setting used to the reference setting defined in this dictionary under **_space_group.reference_setting**.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Related items: **_space_group.name_H-M_ref** (alternate), **_space_group.name_H-M_alt** (alternate) .

Example: '`P 21/n 21/m 21/a`' (full symbol for *Pnma*). **[space_group]**

_space_group.name_H-M_ref (*char*)

The short international Hermann–Mauguin space-group symbol as defined in Section 2.2.3 and given as the first item of each space-group table in Part 7 of *International Tables for Crystallography* Volume A (2002). Each component of the space-group name is separated by a space or an underscore character. The use of a space is strongly recommended. The underscore is only retained because it was used in old CIFs. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The short international Hermann–Mauguin symbol determines the space-group type uniquely. However, the space-group type is better described using **_space_group.IT_number** or **_space_group.name_Schoenflies**. The short international Hermann–Mauguin symbol contains no information on the choice of basis or origin. To define the setting uniquely use **_space_group.name_Hall**, list the symmetry operations or generators, or give the transformation that relates the setting to the reference setting defined in this dictionary under **_space_group.reference_setting**. **_space_group.name_H-M_alt** may be used to give the Hermann–Mauguin symbol corresponding to the setting used. In the enumeration list below, each possible value is identified by space-group number and Schoenflies symbol.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Related items: **_space_group.name_H-M_full** (alternate), **_space_group.name_H-M_alt** (alternate).

The data value must be one of the following:

'P 1'	1 C_1^1	'P -1'	2 C_i^1
'P 2'	3 C_2^1	'P 21'	4 C_2^2
'C 2'	5 C_2^3	'P m'	6 C_s^1
'P c'	7 C_s^2	'C m'	8 C_s^3
'C c'	9 C_s^4	'P 2/m'	10 C_{2h}^1
'P 21/m'	11 C_{2h}^2	'C 2/m'	12 C_{2h}^3
'P 2/c'	13 C_{2h}^4	'P 21/c'	14 C_{2h}^5
'C 2/c'	15 C_{2h}^6	'P 2 2 2'	16 D_2^1
'P 2 2 21'	17 D_2^2	'P 21 21 2'	18 D_2^3
'P 21 21 21'	19 D_2^4	'C 2 2 21'	20 D_2^5
'C 2 2 2'	21 D_2^6	'F 2 2 2'	22 D_2^7
'I 2 2 2'	23 D_2^8	'I 21 21 21'	24 D_2^9
'P m m 2'	25 C_{2v}^1	'P m c 21'	26 C_{2v}^2
'P c c 2'	27 C_{2v}^3	'P m a 2'	28 C_{2v}^4
'P c a 21'	29 C_{2v}^5	'P n c 2'	30 C_{2v}^6
'P m n 21'	31 C_{2v}^7	'P b a 2'	32 C_{2v}^8
'P n a 21'	33 C_{2v}^9	'P n n 2'	34 C_{2v}^{10}
'C m m 2'	35 C_{2v}^{11}	'C m c 21'	36 C_{2v}^{12}
'C c c 2'	37 C_{2v}^{13}	'A m m 2'	38 C_{2v}^{14}
'A e m 2'	39 C_{2v}^{15}	'A m a 2'	40 C_{2v}^{16}
'A e a 2'	41 C_{2v}^{17}	'F m m 2'	42 C_{2v}^{18}
'F d d 2'	43 C_{2v}^{19}	'I m m 2'	44 C_{2v}^{20}
'I b a 2'	45 C_{2v}^{21}	'I m a 2'	46 C_{2v}^{22}
'P m m m'	47 D_{2h}^1	'P n n n'	48 D_{2h}^2
'P c c m'	49 D_{2h}^3	'P b a n'	50 D_{2h}^4
'P m m a'	51 D_{2h}^5	'P n n a'	52 D_{2h}^6
'P m n a'	53 D_{2h}^7	'P c c a'	54 D_{2h}^8
'P b a m'	55 D_{2h}^9	'P c c n'	56 D_{2h}^{10}
'P b c m'	57 D_{2h}^{11}	'P n n m'	58 D_{2h}^{12}
'P m m n'	59 D_{2h}^{13}	'P b c n'	60 D_{2h}^{14}
'P b c a'	61 D_{2h}^{15}	'P n m a'	62 D_{2h}^{16}
'C m c m'	63 D_{2h}^{17}	'C m c e'	64 D_{2h}^{18}
'C m m m'	65 D_{2h}^{19}	'C c c m'	66 D_{2h}^{20}
'C m m e'	67 D_{2h}^{21}	'C c c e'	68 D_{2h}^{22}
'F m m m'	69 D_{2h}^{23}	'F d d d'	70 D_{2h}^{24}
'I m m m'	71 D_{2h}^{25}	'I b a m'	72 D_{2h}^{26}
'I b c a'	73 D_{2h}^{27}	'I m m a'	74 D_{2h}^{28}
'P 4'	75 C_4^1	'P 41'	76 C_4^2
'P 42'	77 C_4^3	'P 43'	78 C_4^4
'I 4'	79 C_4^5	'I 41'	80 C_4^6
'P -4'	81 S_4^1	'I -4'	82 S_4^2
'P 4/m'	83 C_{4h}^1	'P 42/m'	84 C_{4h}^2
'P 4/n'	85 C_{4h}^3	'P 42/n'	86 C_{4h}^4
'I 4/m'	87 C_{4h}^5	'I 41/a'	88 C_{4h}^6
'P 4 2 2'	89 D_4^1	'P 4 21 2'	90 D_4^2
'P 41 2 2'	91 D_4^3	'P 41 21 2'	92 D_4^4
'P 42 2 2'	93 D_4^5	'P 42 21 2'	94 D_4^6
'P 43 2 2'	95 D_4^7	'P 43 21 2'	96 D_4^8
'I 4 2 2'	97 D_4^9	'I 41 2 2'	98 D_4^{10}
'P 4 m m'	99 C_{4v}^1	'P 4 b m'	100 C_{4v}^2
'P 42 c m'	101 C_{4v}^3	'P 42 n m'	102 C_{4v}^4
'P 4 c c'	103 C_{4v}^5	'P 4 n c'	104 C_{4v}^6
'P 42 m c'	105 C_{4v}^7	'P 42 b c'	106 C_{4v}^8
'I 4 m m'	107 C_{4v}^9	'I 4 c m'	108 C_{4v}^{10}
'I 41 m d'	109 C_{4v}^{11}	'I 41 c d'	110 C_{4v}^{12}
'P -4 2 m'	111 D_{2d}^1	'P -4 2 c'	112 D_{2d}^2
'P -4 21 m'	113 D_{2d}^3	'P -4 21 c'	114 D_{2d}^4
'P -4 m 2'	115 D_{2d}^5	'P -4 c 2'	116 D_{2d}^6
'P -4 b 2'	117 D_{2d}^7	'P -4 n 2'	118 D_{2d}^8
'I -4 m 2'	119 D_{2d}^9	'I -4 c 2'	120 D_{2d}^{10}
'I -4 2 m'	121 D_{2d}^{11}	'I -4 2 d'	122 D_{2d}^{12}
'P 4/m m m'	123 D_{4h}^1	'P 4/m c c'	124 D_{4h}^2
'P 4/n b m'	125 D_{4h}^3	'P 4/n n c'	126 D_{4h}^4
'P 4/m b m'	127 D_{4h}^5	'P 4/m n c'	128 D_{4h}^6
'P 4/n m m'	129 D_{4h}^7	'P 4/n c c'	130 D_{4h}^8
'P 42/m m c'	131 D_{4h}^9	'P 42/m c m'	132 D_{4h}^{10}
'P 42/n b c'	133 D_{4h}^{11}	'P 42/n n m'	134 D_{4h}^{12}
'P 42/m b c'	135 D_{4h}^{13}	'P 42/m n m'	136 D_{4h}^{14}
'P 42/n m c'	137 D_{4h}^{15}	'P 42/n c m'	138 D_{4h}^{16}
'I 4/m m m'	139 D_{4h}^{17}	'I 4/m c m'	140 D_{4h}^{18}
'I 41/a m d'	141 D_{4h}^{19}	'I 41/a c d'	142 D_{4h}^{20}
'P 3'	143 C_3^1	'P 31'	144 C_3^2
'P 32'	145 C_3^3	'R 3'	146 C_3^4
'P -3'	147 C_{3i}^1	'R -3'	148 C_{3i}^2
'P 3 1 2'	149 D_3^1	'P 3 2 1'	150 D_3^2
'P 31 1 2'	151 D_3^3	'P 31 2 1'	152 D_3^4

'P 32 1 2'	153	D_3^5	'P 32 2 1'	154	D_3^6
'R 3 2'	155	D_3^7	'P 3 m 1'	156	C_{3v}^1
'P 3 1 m'	157	C_{3v}^2	'P 3 c 1'	158	C_{3v}^3
'P 3 1 c'	159	C_{3v}^4	'R 3 m'	160	C_{3v}^5
'R 3 c'	161	C_{3v}^6	'P -3 1 m'	162	D_{3d}^1
'P -3 1 c'	163	D_{3d}^2	'P -3 m 1'	164	D_{3d}^3
'P -3 c 1'	165	D_{3d}^4	'R -3 m'	166	D_{3d}^5
'R -3 c'	167	D_{3d}^6	'P 6'	168	C_6^1
'P 61'	169	C_6^2	'P 65'	170	C_6^3
'P 62'	171	C_6^4	'P 64'	172	C_6^5
'P 63'	173	C_6^6	'P -6'	174	C_{3h}^1
'P 6/m '	175	C_{6h}^1	'P 63/m'	176	C_{6h}^2
'P 6 2 2'	177	D_6^1	'P 61 2 2'	178	D_6^2
'P 65 2 2'	179	D_6^3	'P 62 2 2'	180	D_6^4
'P 64 2 2'	181	D_6^5	'P 63 2 2'	182	D_6^6
'P 6 m m'	183	C_{6v}^1	'P 6 c c'	184	C_{6v}^2
'P 63 c m'	185	C_{6v}^3	'P 63 m c'	186	C_{6v}^4
'P -6 m 2'	187	D_{3h}^1	'P -6 c 2'	188	D_{3h}^2
'P -6 2 m'	189	D_{3h}^3	'P -6 2 c'	190	D_{3h}^4
'P 6/m m m'	191	D_{6h}^1	'P 6/m c c'	192	D_{6h}^2
'P 63/m c m'	193	D_{6h}^3	'P 63/m m c'	194	D_{6h}^4
'P 2 3'	195	T^1	'F 2 3'	196	T^2
'I 2 3'	197	T^3	'P 21 3'	198	T^4
'I 21 3'	199	T^5	'P m -3'	200	T_h^1
'P n -3'	201	T_h^2	'F m -3'	202	T_h^3
'F d -3'	203	T_h^4	'I m -3'	204	T_h^5
'P a -3'	205	T_h^6	'I a -3'	206	T_h^7
'P 4 3 2'	207	O^1	'P 42 3 2'	208	O^2
'F 4 3 2'	209	O^3	'F 41 3 2'	210	O^4
'I 4 3 2'	211	O^5	'P 43 3 2'	212	O^6
'P 41 3 2'	213	O^7	'I 41 3 2'	214	O^8
'P -4 3 m'	215	T_d^1	'F -4 3 m'	216	T_d^2
'I -4 3 m'	217	T_d^3	'P -4 3 n'	218	T_d^4
'F -4 3 c'	219	T_d^5	'I -4 3 d'	220	T_d^6
'P m -3 m'	221	O_h^1	'P n -3 n'	222	O_h^2
'P m -3 n'	223	O_h^3	'P n -3 m'	224	O_h^4
'F m -3 m'	225	O_h^5	'F m -3 c'	226	O_h^6
'F d -3 m'	227	O_h^7	'F d -3 c'	228	O_h^8
'I m -3 m'	229	O_h^9	'I a -3 d'	230	O_h^{10}

Examples: '`P 21/c`', '`P m n a`', '`P -1`', '`F m -3 m`', '`P 63/m m m`'.
[space_group]

_space_group.name_Hall (*char*)

_symmetry_space_group_name_Hall(*cif_core.dic 1.0*)

Space-group symbol defined by Hall. **_space_group.name_Hall** uniquely defines the space group and its reference to a particular coordinate system. Each component of the space-group name is separated by a space or an underscore character. The use of a space is strongly recommended. The underscore is only retained because it was used in old CIFs. It should not be used in new CIFs.

References: Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525; erratum (1981), A**37**, 921. *International Tables for Crystallography* (2001). Volume B, *Reciprocal space*, edited by U. Shmueli, 2nd ed., Appendix 1.4.2. Dordrecht: Kluwer Academic Publishers.

Examples: '`P 2c -2ac`' (equivalent to $Pca2_1$), '`-I 4bd 2ab 3`' (equivalent to $Ia3d$).
[space_group]

_space_group.name_Schoenflies (*char*)

The Schoenflies symbol as listed in *International Tables for Crystallography* Volume A denoting the proper affine class (*i.e.* orientation-preserving affine class) of space groups (space-group type) to which the space group belongs. This symbol defines the space-group type independently of the coordinate system in which the space group is expressed. The symbol is given with a period, '.', separating the Schoenflies point group and the superscript.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

The data value must be one of the following:

C1.1	Ci.1	C2.1	C2.2	C2.3	Cs.1	Cs.2
Cs.3	Cs.4	C2h.1	C2h.2	C2h.3	C2h.4	C2h.5
C2h.6	D2.1	D2.2	D2.3	D2.4	D2.5	D2.6
D2.7	D2.8	D2.9	C2v.1	C2v.2	C2v.3	C2v.4
C2v.5	C2v.6	C2v.7	C2v.8	C2v.9	C2v.10	C2v.11
C2v.12	C2v.13	C2v.14	C2v.15	C2v.16	C2v.17	C2v.18
C2v.19	C2v.20	C2v.21	C2v.22	D2h.1	D2h.2	D2h.3
D2h.4	D2h.5	D2h.6	D2h.7	D2h.8	D2h.9	D2h.10
D2h.11	D2h.12	D2h.13	D2h.14	D2h.15	D2h.16	D2h.17
D2h.18	D2h.19	D2h.20	D2h.21	D2h.22	D2h.23	D2h.24
D2h.25	D2h.26	D2h.27	D2h.28	C4.1	C4.2	C4.3
C4.4	C4.5	C4.6	S4.1	S4.2	C4h.1	C4h.2
C4h.3	C4h.4	C4h.5	C4h.6	D4.1	D4.2	D4.3
D4.4	D4.5	D4.6	D4.7	D4.8	D4.9	D4.10
C4v.1	C4v.2	C4v.3	C4v.4	C4v.5	C4v.6	C4v.7
C4v.8	C4v.9	C4v.10	C4v.11	C4v.12	D2d.1	D2d.2
D2d.3	D2d.4	D2d.5	D2d.6	D2d.7	D2d.8	D2d.9
D2d.10	D2d.11	D2d.12	D4h.1	D4h.2	D4h.3	D4h.4
D4h.5	D4h.6	D4h.7	D4h.8	D4h.9	D4h.10	D4h.11
D4h.12	D4h.13	D4h.14	D4h.15	D4h.16	D4h.17	D4h.18
D4h.19	D4h.20	C3.1	C3.2	C3.3	C3.4	C3i.1
C3i.2	D3.1	D3.2	D3.3	D3.4	D3.5	D3.6
D3.7	C3v.1	C3v.2	C3v.3	C3v.4	C3v.5	C3v.6
D3d.1	D3d.2	D3d.3	D3d.4	D3d.5	D3d.6	C6.1
C6.2	C6.3	C6.4	C6.5	C6.6	C3h.1	C6h.1
C6h.2	D6.1	D6.2	D6.3	D6.4	D6.5	D6.6
C6v.1	C6v.2	C6v.3	C6v.4	D3h.1	D3h.2	D3h.3
D3h.4	D6h.1	D6h.2	D6h.3	D6h.4	T.1	T.2
T.3	T.4	T.5	Th.1	Th.2	Th.3	Th.4
Th.5	Th.6	Th.7	O.1	O.2	O.3	O.4
O.5	O.6	O.7	O.8	Td.1	Td.2	Td.3
Td.4	Td.5	Td.6	Oh.1	Oh.2	Oh.3	Oh.4
Oh.5	Oh.6	Oh.7	Oh.8	Oh.9	Oh.10	

Example: '`C2h.5`' (Schoenflies symbol for space group No. 14). **[space_group]**

_space_group.point_group_H-M (*char*)

The Hermann–Mauguin symbol denoting the geometric crystal class of space groups to which the space group belongs, and the geometric crystal class of point groups to which the point group of the space group belongs.

Examples: '`-4`', '`4/m`'. **[space_group]**

_space_group.reference_setting (*char*)

The reference setting of a given space group is the setting chosen by the International Union of Crystallography as a unique setting to which other settings can be referred using the transformation matrix column pair given in **_space_group.transform_Pp_abc** and **_space_group.transform_Qq_xyz**. The settings are given in the enumeration list in the form '**_space_group.IT_number: _space_group.name_Hall**'. The space-group number defines the space-group type and the Hall symbol specifies the symmetry generators referred to the reference coordinate system. The 230 reference settings chosen are identical to the settings listed in *International Tables for Crystallography* Volume A (2002). For the space groups where more than one setting is given in *International Tables*, the following choices have been made. For monoclinic space groups: unique axis *b* and cell choice 1. For space groups with two origins: origin choice 2 (origin at inversion centre, indicated by adding :2 to the Hermann–Mauguin symbol in

the enumeration list). For rhombohedral space groups: hexagonal axes (indicated by adding :h to the Hermann–Mauguin symbol in the enumeration list). Based on the symmetry table of R. W. Grosse-Kunstleve, ETH, Zurich. The enumeration list may be extracted from the dictionary and stored as a separate CIF that can be referred to as required.

In the enumeration list below, each reference setting is identified by Schoenflies symbol and by the Hermann–Mauguin symbol, augmented by :2 or :h suffixes as described above.

References: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers. Grosse-Kunstleve, R. W. (2001). *Xtal System of Crystallographic Programs, System Documentation*. http://xtal.crystal.uwa.edu.au/man/xtal3.7-228.html (or follow links to Docs→Space-Group Symbols from http://xtal.sourceforge.net).

The data value must be one of the following:

'001:P 1'	C_1^1	$P\,1$
'002:-P 1'	C_i^1	$P\,\bar{1}$
'003:P 2y'	C_2^1	$P\,1\,2\,1$
'004:P 2yb'	C_2^2	$P\,1\,2_1\,1$
'005:C 2y'	C_2^3	$C\,1\,2\,1$
'006:P -2y'	C_s^1	$P\,1\,m\,1$
'007:P -2yc'	C_s^2	$P\,1\,c\,1$
'008:C -2y'	C_s^3	$C\,1\,m\,1$
'009:C -2yc'	C_s^4	$C\,1\,c\,1$
'010:-P 2y'	C_{2h}^1	$P\,1\,2/m\,1$
'011:-P 2yb'	C_{2h}^2	$P\,1\,2_1/m\,1$
'012:-C 2y'	C_{2h}^3	$C\,1\,2/m\,1$
'013:-P 2yc'	C_{2h}^4	$P\,1\,2/c\,1$
'014:-P 2ybc'	C_{2h}^5	$P\,1\,2_1/c\,1$
'015:-C 2yc'	C_{2h}^6	$C\,1\,2/c\,1$
'016:P 2 2'	D_2^1	$P\,2\,2\,2$
'017:P 2c 2'	D_2^2	$P\,2\,2\,2_1$
'018:P 2 2ab'	D_2^3	$P\,2_1\,2_1\,2$
'019:P 2ac 2ab'	D_2^4	$P\,2_1\,2_1\,2_1$
'020:C 2c 2'	D_2^5	$C\,2\,2\,2_1$
'021:C 2 2'	D_2^6	$C\,2\,2\,2$
'022:F 2 2'	D_2^7	$F\,2\,2\,2$
'023:I 2 2'	D_2^8	$I\,2\,2\,2$
'024:I 2b 2c'	D_2^9	$I\,2_1\,2_1\,2_1$
'025:P 2 -2'	C_{2v}^1	$P\,m\,m\,2$
'026:P 2c -2'	C_{2v}^2	$P\,m\,c\,2_1$
'027:P 2 -2c'	C_{2v}^3	$P\,c\,c\,2$
'028:P 2 -2a'	C_{2v}^4	$P\,m\,a\,2$
'029:P 2c -2ac'	C_{2v}^5	$P\,c\,a\,2_1$
'030:P 2 -2bc'	C_{2v}^6	$P\,n\,c\,2$
'031:P 2ac -2'	C_{2v}^7	$P\,m\,n\,2_1$
'032:P 2 -2ab'	C_{2v}^8	$P\,b\,a\,2$
'033:P 2c -2n'	C_{2v}^9	$P\,n\,a\,2_1$
'034:P 2 -2n'	C_{2v}^{10}	$P\,n\,n\,2$
'035:C 2 -2'	C_{2v}^{11}	$C\,m\,m\,2$
'036:C 2c -2'	C_{2v}^{12}	$C\,m\,c\,2_1$
'037:C 2 -2c'	C_{2v}^{13}	$C\,c\,c\,2$
'038:A 2 -2'	C_{2v}^{14}	$A\,m\,m\,2$
'039:A 2 -2b'	C_{2v}^{15}	$A\,e\,m\,2$
'040:A 2 -2a'	C_{2v}^{16}	$A\,m\,a\,2$
'041:A 2 -2ab'	C_{2v}^{17}	$A\,e\,a\,2$
'042:F 2 -2'	C_{2v}^{18}	$F\,m\,m\,2$
'043:F 2 -2d'	C_{2v}^{19}	$F\,d\,d\,2$
'044:I 2 -2'	C_{2v}^{20}	$I\,m\,m\,2$
'045:I 2 -2c'	C_{2v}^{21}	$I\,b\,a\,2$
'046:I 2 -2a'	C_{2v}^{22}	$I\,m\,a\,2$
'047:-P 2 2'	D_{2h}^1	$P\,m\,m\,m$
'048:-P 2ab 2bc'	D_{2h}^2	$P\,n\,n\,n$:2
'049:-P 2 2c'	D_{2h}^3	$P\,c\,c\,m$
'050:-P 2ab 2b'	D_{2h}^4	$P\,b\,a\,n$:2
'051:-P 2a 2a'	D_{2h}^5	$P\,m\,m\,a$
'052:-P 2a 2bc'	D_{2h}^6	$P\,n\,n\,a$
'053:-P 2ac 2'	D_{2h}^7	$P\,m\,n\,a$
'054:-P 2a 2ac'	D_{2h}^8	$P\,c\,c\,a$
'055:-P 2 2ab'	D_{2h}^9	$P\,b\,a\,m$
'056:-P 2ab 2ac'	D_{2h}^{10}	$P\,c\,c\,n$
'057:-P 2c 2b'	D_{2h}^{11}	$P\,b\,c\,m$
'058:-P 2 2n'	D_{2h}^{12}	$P\,n\,n\,m$
'059:-P 2ab 2a'	D_{2h}^{13}	$P\,m\,m\,n$:2
'060:-P 2n 2ab'	D_{2h}^{14}	$P\,b\,c\,n$
'061:-P 2ac 2ab'	D_{2h}^{15}	$P\,b\,c\,a$
'062:-P 2ac 2n'	D_{2h}^{16}	$P\,n\,m\,a$
'063:-C 2c 2'	D_{2h}^{17}	$C\,m\,c\,m$
'064:-C 2ac 2'	D_{2h}^{18}	$C\,m\,c\,e$
'065:-C 2 2'	D_{2h}^{19}	$C\,m\,m\,m$
'066:-C 2 2c'	D_{2h}^{20}	$C\,c\,c\,m$
'067:-C 2a 2'	D_{2h}^{21}	$C\,m\,m\,e$
'068:-C 2a 2ac'	D_{2h}^{22}	$C\,c\,c\,e$:2
'069:-F 2 2'	D_{2h}^{23}	$F\,m\,m\,m$
'070:-F 2uv 2vw'	D_{2h}^{24}	$F\,d\,d\,d$:2
'071:-I 2 2'	D_{2h}^{25}	$I\,m\,m\,m$
'072:-I 2 2c'	D_{2h}^{26}	$I\,b\,a\,m$
'073:-I 2b 2c'	D_{2h}^{27}	$I\,b\,c\,a$
'074:-I 2b 2'	D_{2h}^{28}	$I\,m\,m\,a$
'075:P 4'	C_4^1	$P\,4$
'076:P 4w'	C_4^2	$P\,4_1$
'077:P 4c'	C_4^3	$P\,4_2$
'078:P 4cw'	C_4^4	$P\,4_3$
'079:I 4'	C_4^5	$I\,4$
'080:I 4bw'	C_4^6	$I\,4_1$
'081:P -4'	S_4^1	$P\,\bar{4}$
'082:I -4'	S_4^2	$I\,\bar{4}$
'083:-P 4'	C_{4h}^1	$P\,4/m$
'084:-P 4c'	C_{4h}^2	$P\,4_2/m$
'085:-P 4a'	C_{4h}^3	$P\,4/n$:2
'086:-P 4bc'	C_{4h}^4	$P\,4_2/n$:2
'087:-I 4'	C_{4h}^5	$I\,4/m$
'088:-I 4ad'	C_{4h}^6	$I\,4_1/a$:2
'089:P 4 2'	D_4^1	$P\,4\,2\,2$
'090:P 4ab 2ab'	D_4^2	$P\,4\,2_1\,2$
'091:P 4w 2c'	D_4^3	$P\,4_1\,2\,2$
'092:P 4abw 2nw'	D_4^4	$P\,4_1\,2_1\,2$
'093:P 4c 2'	D_4^5	$P\,4_2\,2\,2$
'094:P 4n 2n'	D_4^6	$P\,4_2\,2_1\,2$
'095:P 4cw 2c'	D_4^7	$P\,4_3\,2\,2$
'096:P 4nw 2abw'	D_4^8	$P\,4_3\,2_1\,2$
'097:I 4 2'	D_4^9	$I\,4\,2\,2$
'098:I 4bw 2bw'	D_4^{10}	$I\,4_1\,2\,2$
'099:P 4 -2'	C_{4v}^1	$P\,4\,m\,m$
'100:P 4 -2ab'	C_{4v}^2	$P\,4\,b\,m$
'101:P 4c -2c'	C_{4v}^3	$P\,4_2\,c\,m$
'102:P 4n -2n'	C_{4v}^4	$P\,4_2\,n\,m$
'103:P 4 -2c'	C_{4v}^5	$P\,4\,c\,c$
'104:P 4 -2n'	C_{4v}^6	$P\,4\,n\,c$
'105:P 4c -2'	C_{4v}^7	$P\,4_2\,m\,c$

'106:P 4c -2ab'	C_{4v}^{8}	$P\,4_2\,b\,c$
'107:I 4 -2'	C_{4v}^{9}	$I\,4\,m\,m$
'108:I 4 -2c'	C_{4v}^{10}	$I\,4\,c\,m$
'109:I 4bw -2'	C_{4v}^{11}	$I\,4_1\,m\,d$
'110:I 4bw -2c'	C_{4v}^{12}	$I\,4_1\,c\,d$
'111:P -4 2'	D_{2d}^{1}	$P\,\bar{4}\,2\,m$
'112:P -4 2c'	D_{2d}^{2}	$P\,\bar{4}\,2\,c$
'113:P -4 2ab'	D_{2d}^{3}	$P\,\bar{4}\,2_1\,m$
'114:P -4 2n'	D_{2d}^{4}	$P\,\bar{4}\,2_1\,c$
'115:P -4 -2'	D_{2d}^{5}	$P\,\bar{4}\,m\,2$
'116:P -4 -2c'	D_{2d}^{6}	$P\,\bar{4}\,c\,2$
'117:P -4 -2ab'	D_{2d}^{7}	$P\,\bar{4}\,b\,2$
'118:P -4 -2n'	D_{2d}^{8}	$P\,\bar{4}\,n\,2$
'119:I -4 -2'	D_{2d}^{9}	$I\,\bar{4}\,m\,2$
'120:I -4 -2c'	D_{2d}^{10}	$I\,\bar{4}\,c\,2$
'121:I -4 2'	D_{2d}^{11}	$I\,\bar{4}\,2\,m$
'122:I -4 2bw'	D_{2d}^{12}	$I\,\bar{4}\,2\,d$
'123:-P 4 2'	D_{4h}^{1}	$P\,4/m\,m\,m$
'124:-P 4 2c'	D_{4h}^{2}	$P\,4/m\,c\,c$
'125:-P 4a 2b'	D_{4h}^{3}	$P\,4/n\,b\,m$:2
'126:-P 4a 2bc'	D_{4h}^{4}	$P\,4/n\,n\,c$:2
'127:-P 4 2ab'	D_{4h}^{5}	$P\,4/m\,b\,m$
'128:-P 4 2n'	D_{4h}^{6}	$P\,4/m\,n\,c$
'129:-P 4a 2a'	D_{4h}^{7}	$P\,4/n\,m\,m$:2
'130:-P 4a 2ac'	D_{4h}^{8}	$P\,4/n\,c\,c$:2
'131:-P 4c 2'	D_{4h}^{9}	$P\,4_2/m\,m\,c$
'132:-P 4c 2c'	D_{4h}^{10}	$P\,4_2/m\,c\,m$
'133:-P 4ac 2b'	D_{4h}^{11}	$P\,4_2/n\,b\,c$:2
'134:-P 4ac 2bc'	D_{4h}^{12}	$P\,4_2/n\,n\,m$:2
'135:-P 4c 2ab'	D_{4h}^{13}	$P\,4_2/m\,b\,c$
'136:-P 4n 2n'	D_{4h}^{14}	$P\,4_2/m\,n\,m$
'137:-P 4ac 2a'	D_{4h}^{15}	$P\,4_2/n\,m\,c$:2
'138:-P 4ac 2ac'	D_{4h}^{16}	$P\,4_2/n\,c\,m$:2
'139:-I 4 2'	D_{4h}^{17}	$I\,4/m\,m\,m$
'140:-I 4 2c'	D_{4h}^{18}	$I\,4/m\,c\,m$
'141:-I 4bd 2'	D_{4h}^{19}	$I\,4_1/a\,m\,d$:2
'142:-I 4bd 2c'	D_{4h}^{20}	$I\,4_1/a\,c\,d$:2
'143:P 3'	C_{3}^{1}	$P\,3$
'144:P 31'	C_{3}^{2}	$P\,3_1$
'145:P 32'	C_{3}^{3}	$P\,3_2$
'146:R 3'	C_{3}^{4}	$R\,3$:h
'147:-P 3'	C_{3i}^{1}	$P\,\bar{3}$
'148:-R 3'	C_{3i}^{2}	$R\,\bar{3}$:h
'149:P 3 2'	D_{3}^{1}	$P\,3\,1\,2$
'150:P 3 2"'	D_{3}^{2}	$P\,3\,2\,1$
'151:P 31 2 (0 0 4)'	D_{3}^{3}	$P\,3_1\,1\,2$
'152:P 31 2"'	D_{3}^{4}	$P\,3_1\,2\,1$
'153:P 32 2 (0 0 2)'	D_{3}^{5}	$P\,3_2\,1\,2$
'154:P 32 2"'	D_{3}^{6}	$P\,3_2\,2\,1$
'155:R 3 2"'	D_{3}^{7}	$R\,3\,2$:h
'156:P 3 -2"'	C_{3v}^{1}	$P\,3\,m\,1$
'157:P 3 -2'	C_{3v}^{2}	$P\,3\,1\,m$
'158:P 3 -2"c'	C_{3v}^{3}	$P\,3\,c\,1$
'159:P 3 -2c'	C_{3v}^{4}	$P\,3\,1\,c$
'160:R 3 -2"'	C_{3v}^{5}	$R\,3\,m$:h
'161:R 3 -2"c'	C_{3v}^{6}	$R\,3\,c$:h
'162:-P 3 2'	D_{3d}^{1}	$P\,\bar{3}\,1\,m$
'163:-P 3 2c'	D_{3d}^{2}	$P\,\bar{3}\,1\,c$
'164:-P 3 2"'	D_{3d}^{3}	$P\,\bar{3}\,m\,1$
'165:-P 3 2"c'	D_{3d}^{4}	$P\,\bar{3}\,c\,1$
'166:-R 3 2"'	D_{3d}^{5}	$R\,\bar{3}\,m$:h
'167:-R 3 2"c'	D_{3d}^{6}	$R\,\bar{3}\,c$:h
'168:P 6'	C_{6}^{1}	$P\,6$
'169:P 61'	C_{6}^{2}	$P\,6_1$
'170:P 65'	C_{6}^{3}	$P\,6_5$
'171:P 62'	C_{6}^{4}	$P\,6_2$
'172:P 64'	C_{6}^{5}	$P\,6_4$
'173:P 6c'	C_{6}^{6}	$P\,6_3$
'174:P -6'	C_{3h}^{1}	$P\,\bar{6}$
'175:-P 6'	C_{6h}^{1}	$P\,6/m$
'176:-P 6c'	C_{6h}^{2}	$P\,6_3/m$
'177:P 6 2'	D_{6}^{1}	$P\,6\,2\,2$
'178:P 61 2 (0 0 5)'	D_{6}^{2}	$P\,6_1\,2\,2$
'179:P 65 2 (0 0 1)'	D_{6}^{3}	$P\,6_5\,2\,2$
'180:P 62 2 (0 0 4)'	D_{6}^{4}	$P\,6_2\,2\,2$
'181:P 64 2 (0 0 2)'	D_{6}^{5}	$P\,6_4\,2\,2$
'182:P 6c 2c'	D_{6}^{6}	$P\,6_3\,2\,2$
'183:P 6 -2'	C_{6v}^{1}	$P\,6\,m\,m$
'184:P 6 -2c'	C_{6v}^{2}	$P\,6\,c\,c$
'185:P 6c -2'	C_{6v}^{3}	$P\,6_3\,c\,m$
'186:P 6c -2c'	C_{6v}^{4}	$P\,6_3\,m\,c$
'187:P -6 2'	D_{3h}^{1}	$P\,\bar{6}\,m\,2$
'188:P -6c 2'	D_{3h}^{2}	$P\,\bar{6}\,c\,2$
'189:P -6 -2'	D_{3h}^{3}	$P\,\bar{6}\,2\,m$
'190:P -6c -2c'	D_{3h}^{4}	$P\,\bar{6}\,2\,c$
'191:-P 6 2'	D_{6h}^{1}	$P\,6/m\,m\,m$
'192:-P 6 2c'	D_{6h}^{2}	$P\,6/m\,c\,c$
'193:-P 6c 2'	D_{6h}^{3}	$P\,6_3/m\,c\,m$
'194:-P 6c 2c'	D_{6h}^{4}	$P\,6_3/m\,m\,c$
'195:P 2 2 3'	T^{1}	$P\,2\,3$
'196:F 2 2 3'	T^{2}	$F\,2\,3$
'197:I 2 2 3'	T^{3}	$I\,2\,3$
'198:P 2ac 2ab 3'	T^{4}	$P\,2_1\,3$
'199:I 2b 2c 3'	T^{5}	$I\,2_1\,3$
'200:-P 2 2 3'	T_{h}^{1}	$P\,m\,\bar{3}$
'201:-P 2ab 2bc 3'	T_{h}^{2}	$P\,n\,\bar{3}$:2
'202:-F 2 2 3'	T_{h}^{3}	$F\,m\,\bar{3}$
'203:-F 2uv 2vw 3'	T_{h}^{4}	$F\,d\,\bar{3}$:2
'204:-I 2 2 3'	T_{h}^{5}	$I\,m\,\bar{3}$
'205:-P 2ac 2ab 3'	T_{h}^{6}	$P\,a\,\bar{3}$
'206:-I 2b 2c 3'	T_{h}^{7}	$I\,a\,\bar{3}$
'207:P 4 2 3'	O^{1}	$P\,4\,3\,2$
'208:P 4n 2 3'	O^{2}	$P\,4_2\,3\,2$
'209:F 4 2 3'	O^{3}	$F\,4\,3\,2$
'210:F 4d 2 3'	O^{4}	$F\,4_1\,3\,2$
'211:I 4 2 3'	O^{5}	$I\,4\,3\,2$
'212:P 4acd 2ab 3'	O^{6}	$P\,4_3\,3\,2$
'213:P 4bd 2ab 3'	O^{7}	$P\,4_1\,3\,2$
'214:I 4bd 2c 3'	O^{8}	$I\,4_1\,3\,2$
'215:P -4 2 3'	T_{d}^{1}	$P\,\bar{4}\,3\,m$
'216:F -4 2 3'	T_{d}^{2}	$F\,\bar{4}\,3\,m$
'217:I -4 2 3'	T_{d}^{3}	$I\,\bar{4}\,3\,m$
'218:P -4n 2 3'	T_{d}^{4}	$P\,\bar{4}\,3\,n$
'219:F -4a 2 3'	T_{d}^{5}	$F\,\bar{4}\,3\,c$
'220:I -4bd 2c 3'	T_{d}^{6}	$I\,\bar{4}\,3\,d$
'221:-P 4 2 3'	O_{h}^{1}	$P\,m\,\bar{3}\,m$

'222:-P 4a 2bc 3'	O_h^2	$P\,n\,\bar{3}\,n$:2
'223:-P 4n 2 3'	O_h^3	$P\,m\,\bar{3}\,n$
'224:-P 4bc 2bc 3'	O_h^4	$P\,n\,\bar{3}\,m$:2
'225:-F 4 2 3'	O_h^5	$F\,m\,\bar{3}\,m$
'226:-F 4a 2 3'	O_h^6	$F\,m\,\bar{3}\,c$
'227:-F 4vw 2vw 3'	O_h^7	$F\,d\,\bar{3}\,m$:2
'228:-F 4ud 2vw 3'	O_h^8	$F\,d\,\bar{3}\,c$:2
'229:-I 4 2 3'	O_h^9	$I\,m\,\bar{3}\,m$
'230:-I 4bd 2c 3'	O_h^{10}	$I\,a\,\bar{3}\,d$

[space_group]

_space_group.transform_Pp_abc

This item specifies the transformation $(P,\mathbf{p})$ of the basis vectors from the setting used in the CIF (a,b,c) to the reference setting given in **_space_group.reference_setting** (a',b',c'). The value is given in Jones–Faithful notation corresponding to the rotational matrix P combined with the origin shift vector $\mathbf{p}$ in the expression

$$(a',b',c') = (a,b,c)P + \mathbf{p}.$$

P is a post-multiplication matrix of a row (a,b,c) of column vectors. It is related to the inverse transformation $(Q,\mathbf{q})$ by

$$P = Q^{-1},$$
$$\mathbf{p} = Pq = -(Q^{-1})\mathbf{q}.$$

These transformations are applied as follows: atomic coordinates $(x',y',z') = Q(x,y,z) + \mathbf{q}$, Miller indices $(h',k',l') = (h,k,l)P$, symmetry operations $W' = (Q,\mathbf{q})W(P,\mathbf{p})$, basis vectors $(a',b',c') = (a,b,c)P + \mathbf{p}$.

This item is given as a character string involving the characters *a*, *b* and *c* with commas separating the expressions for the a', b' and c' vectors. The numeric values may be given as integers, fractions or real numbers. Multiplication is implicit, division must be explicit. White space within the string is optional.

Examples: '`-b+c, a+c, -a+b+c`' (*R*3:r to *R*3:h), '`a-1/4, b-1/4, c-1/4`' (*Pnnn*:1 to *Pnnn*:2), '`b-1/2, c-1/2, a-1/2`' (*Bbab*:1 to *Ccca*:2). **[space_group]**

_space_group.transform_Qq_xyz

This item specifies the transformation $(Q,\mathbf{q})$ of the atomic coordinates from the setting used in the CIF [(x,y,z) referred to the basis vectors (a,b,c)] to the reference setting given in **_space_group.reference_setting** [(x',y',z') referred to the basis vectors (a',b',c')]. The value given in Jones–Faithful notation corresponds to the rotational matrix Q combined with the origin shift vector $\mathbf{q}$ in the expression

$$(x',y',z') = Q(x,y,z) + \mathbf{q}.$$

Q is a pre-multiplication matrix of the column vector (x,y,z). It is related to the inverse transformation $(P,\mathbf{p})$ by

$$P = Q^{-1},$$
$$\mathbf{p} = P\mathbf{q} = -(Q^{-1})\mathbf{q},$$

where the P and Q transformations are applied as follows: atomic coordinates $(x',y',z') = Q(x,y,z) + \mathbf{q}$, Miller indices $(h',k',l') = (h,k,l)P$, symmetry operations $W' = (Q,\mathbf{q})W(P,\mathbf{p})$, basis vectors $(a',b',c') = (a,b,c)P + \mathbf{p}$.

This item is given as a character string involving the characters *x*, *y* and *z* with commas separating the expressions for the x', y' and z' components. The numeric values may be given as integers, fractions or real numbers. Multiplication is implicit, division must be explicit. White space within the string is optional.

Examples: '`-x/3+2y/3-z/3, -2x/3+y/3+z/3, x/3+y/3+z/3`' (*R*3:r to *R*3:h), '`x+1/4,y+1/4,z+1/4`' (*Pnnn*:1 to *Pnnn*:2), '`z+1/2,x+1/2,y+1/2`' (*Bbab*:1 to *Ccca*:2). **[space_group]**

SPACE_GROUP_SYMOP

Contains information about the symmetry operations of the space group.

Category key(s): **_space_group_symop.id**

Example 1 – the symmetry operations for the space group $P2_1/c$.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
_space_group_symop.operation_description
  1    x,y,z              'identity mapping'
  2    -x,-y,-z           'inversion'
  3    -x,1/2+y,1/2-z
          '2-fold screw rotation with axis in (0,y,1/4)'
  4    x,1/2-y,1/2+z
          'c glide reflection through the plane (x,1/4,y)'
```

_space_group_symop.generator_xyz (*char*)

A parsable string giving one of the symmetry generators of the space group in algebraic form. If W is a matrix representation of the rotational part of the generator defined by the positions and signs of *x*, *y* and *z*, and $\mathbf{w}$ is a column of translations defined by the fractions, an equivalent position $\boldsymbol{x}'$ is generated from a given position $\boldsymbol{x}$ by

$$\boldsymbol{x}' = W\boldsymbol{x} + \mathbf{w}.$$

When a list of symmetry generators is given, it is assumed that the complete list of symmetry operations of the space group (including the identity operation) can be generated through repeated multiplication of the generators, that is, $(W_3,\mathbf{w}_3)$ is an operation of the space group if $(W_2,\mathbf{w}_2)$ and $(W_1,\mathbf{w}_1)$ [where $(W_1,\mathbf{w}_1)$ is applied first] are either operations or generators and

$$W_3 = W_2 \times W_1,$$
$$\mathbf{w}_3 = W_2 \times \mathbf{w}_1 + \mathbf{w}_2.$$

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Related item: **_space_group_symop.operation_xyz** (alternate). Where no value is given, the assumed value is '`x,y,z`'.

Example: '`x,1/2-y,1/2+z`' (*c* glide reflection through the plane (*x*, 1/4, *z*) chosen as one of the generators of the space group). **[space_group_symop]**

*_space_group_symop.id (*char*)

_symmetry_equiv_pos_site_id (*cif_core.dic 1.0*)
_symmetry_equiv.id (*cif_mm.dic 1.0*)

An arbitrary identifier that uniquely labels each symmetry operation in the list.

[space_group_symop]

_space_group_symop.operation_description (*char*)

An optional text description of a particular symmetry operation of the space group.

[space_group_symop]

_space_group_symop.operation_xyz (*char*)

_symmetry_equiv_pos_as_xyz (*cif_core.dic 1.0*)

A parsable string giving one of the symmetry operations of the space group in algebraic form. If W is a matrix representation of the rotational part of the symmetry operation defined by the positions and signs of *x*, *y* and *z*, and $\mathbf{w}$ is a column of translations defined by the fractions, an equivalent position $\boldsymbol{x}'$ is generated from a given position $\boldsymbol{x}$ by

$$\boldsymbol{x}' = W\boldsymbol{x} + \mathbf{w}.$$

When a list of symmetry operations is given, it is assumed that the list contains all the operations of the space group (including the identity operation) as given by the representatives of the general position in *International Tables for Crystallography* Volume A.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Related item: **_space_group_symop.generator_xyz** (alternate). Where no value is given, the assumed value is 'x,y,z'.

Example: 'x,1/2-y,1/2+z' (*c* glide reflection through the plane (*x*, 1/4, *z*)).

[space_group_symop]

_space_group_symop.sg_id (*numb*)

A child of **_space_group.id** allowing the symmetry operation to be identified with a particular space group.

[space_group_symop]

SPACE_GROUP_WYCKOFF

Contains information about Wyckoff positions of a space group. Only one site can be given for each special position but the remainder can be generated by applying the symmetry operations stored in **_space_group_symop.operation_xyz**.

Category key(s): **_space_group_Wyckoff.id**

Example 1 – this example is taken from the space group $Fd\bar{3}c$ (No. 228, origin choice 2). For brevity only a selection of special positions are listed. The coordinates of only one site per special position can be given in this item, but the coordinates of the other sites can be generated using the symmetry operations given in the SPACE_GROUP_SYMOP category.

```
loop_
_space_group_Wyckoff.id
_space_group_Wyckoff.multiplicity
_space_group_Wyckoff.letter
_space_group_Wyckoff.site_symmetry
_space_group_Wyckoff.coord_xyz
    1  192   h   1      x,y,z
    2   96   g   ..2    1/4,y,-y
    3   96   f   2..    x,1/8,1/8
    4   32   b   .32    1/4,1/4,1/4
```

_space_group_Wyckoff.coords_xyz (*char*)

Coordinates of one site of a Wyckoff position expressed in terms of its fractional coordinates (*x*, *y*, *z*) in the unit cell. To generate the coordinates of all sites of this Wyckoff position, it is necessary to multiply these coordinates by the symmetry operations stored in **_space_group_symop.operation_xyz**.

Where no value is given, the assumed value is 'x,y,z'.

Example: 'x,1/2,0' (coordinates of Wyckoff site with 2.. symmetry).

[space_group_Wyckoff]

*_space_group_Wyckoff.id (*char*)

An arbitrary identifier that is unique to a particular Wyckoff position.

[space_group_Wyckoff]

_space_group_Wyckoff.letter (*char*)

The Wyckoff letter associated with this position, as given in *International Tables for Crystallography* Volume A. The enumeration value \a corresponds to the Greek letter 'α' used in *International Tables*.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

The data value must be one of the following:

a b c d e f g h i j k l m n o p q r s t u v w x y z \a

[space_group_Wyckoff]

_space_group_Wyckoff.multiplicity (*numb*)

The multiplicity of this Wyckoff position as given in *International Tables* Volume A. It is the number of equivalent sites per conventional unit cell.

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

The permitted range is $[1, \infty)$.

[space_group_Wyckoff]

_space_group_Wyckoff.sg_id (*char*)

A child of **_space_group.id** allowing the Wyckoff position to be identified with a particular space group.

[space_group_Wyckoff]

_space_group_Wyckoff.site_symmetry (*char*)

The subgroup of the space group that leaves the point fixed. It is isomorphic to a subgroup of the point group of the space group. The site-symmetry symbol indicates the symmetry in the symmetry direction determined by the Hermann–Mauguin symbol of the space group (see *International Tables for Crystallography* Volume A, Section 2.2.12).

Reference: *International Tables for Crystallography* (2002). Volume A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

Examples: '2.22' (position 2*b* in space group No. 94, $P4_22_12$), '42.2' (position 6*b* in space group No. 222, $Pn\bar{3}n$), '2..' (Site symmetry for the Wyckoff position 96*f* in space group No. 228, $Fd\bar{3}c$. The site-symmetry group is isomorphic to the point group 2 with the twofold axis along one of the 100 directions.).

[space_group_Wyckoff]