南方科技大学
SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

findspingroup.com: an online program for identifying the Spin Space Group symmetry of magnetic materials

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Outline

南方科技大学
SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

- Brief introduction on spin point/space group
- Four index nomenclature and International notations
- Online program
- Generating SSG elements

Spin point group

Spin point group: $G_{SPG} = G_{NSS} \times G_{SO}$

G_{NSS}: nontrivial spin group

G_{SO}: spin only group

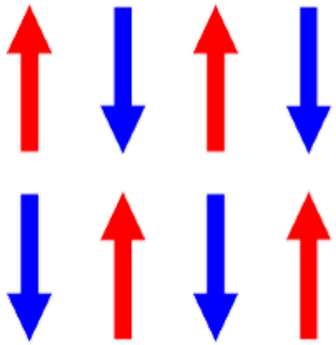
$$G_{NSS} = {}^{g_{s_1}}g_1\ {}^{g_{s_2}}g_2\ {}^{g_{s_3}}g_3$$

$${}^{g_{s_i}}g_i : \{U_m(\phi), TU_m(\phi) \| C_n(\theta), IC_n(\theta)\}$$

Spin rotation Lattice rotation

Collinear:

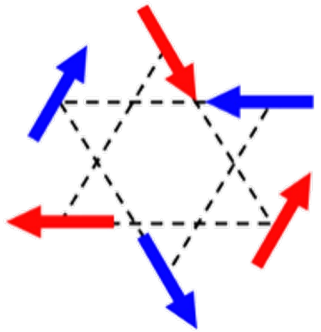
$G_{SO} = Z_2^K \ltimes SO(2)$



90

Coplanar:

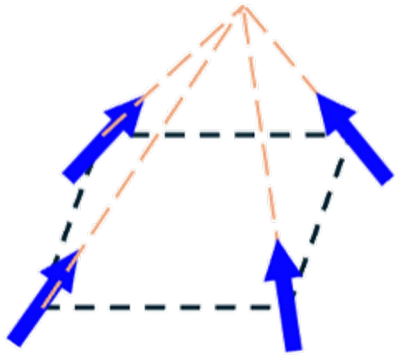
$G_{SO} = Z_2^K$



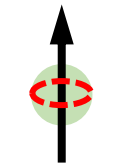
253

Noncoplanar:

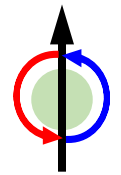
$G_{SO} = E$



598



$SO(2) = \{E, U_Z(\phi)\} = {}^{\infty}1$



$Z_2^K = \{E, TU_n(\pi)\} = {}^{m}1$

D. B. Litvin, Acta Crystallogr. A **33**, 279 (1977)

P. Liu, Q. Liu*, et al. Phys. Rev. X 12, 021016 (2022)

Spin space group

Spin space group: $G_{SSG} = G_{NSS} \times G_{SO}$

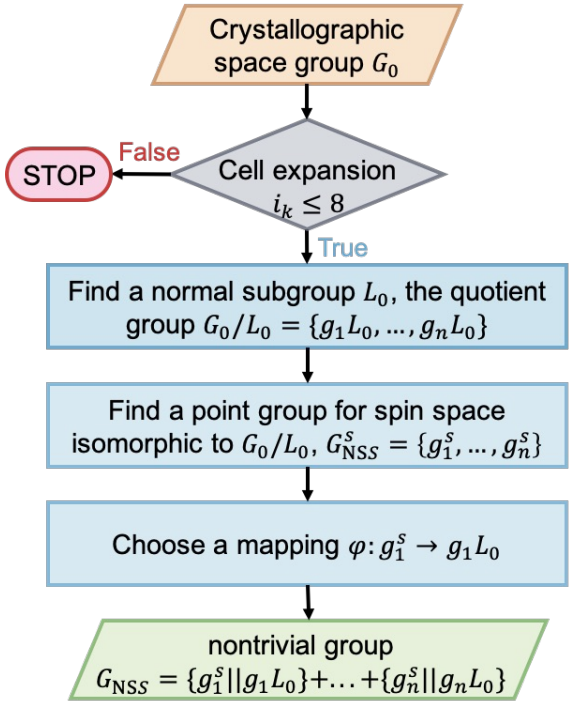
G_{NSS}: nontrivial spin group

G_{SO}: spin only group

$$G_{NSS} = {}^{g_{s_1}}g_1 \, {}^{g_{s_2}}g_2 \, {}^{g_{s_3}}g_3$$

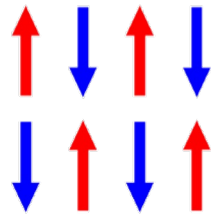
$${}^{g_{s_i}}g_i : \{U_m(\phi), TU_m(\phi) \| C_n(\theta), IC_n(\theta) | \tau\}$$

Spin rotation Lattice rotation

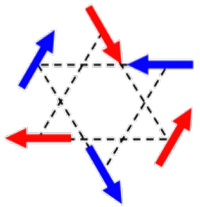


Crystal system	Collinear only	Coplanar	Noncoplanar only	Total
Triclinic (2)	5	55	0	60
Monoclinic (13)	78	3540	0	3618
Orthorhombic (59)	503	53734	0	54237
Tetragonal (68)	502	31185	0	31687
Trigonal (25)	83	2331	62	2476
Hexagonal (27)	137	7149	111	7397
Cubic (36)	113	840	184	1137
Total (230)	1421	98834	357	100612

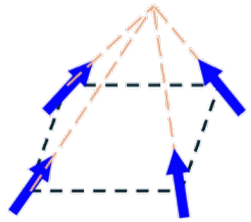
Collinear
(1421)
$G_{SO} = Z_2^K \ltimes SO(2)$



Coplanar
(16383)
$G_{SO} = Z_2^K$



Noncoplanar
(100612)
$G_{SO} = E$



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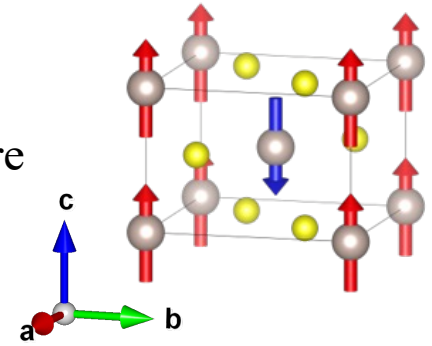
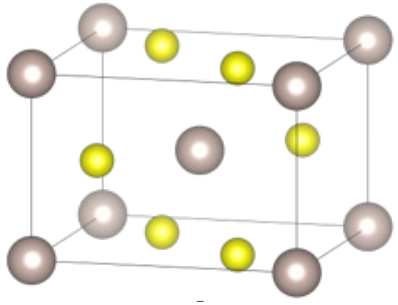
- Online program
- Generating SSG elements

Nomenclature (four-index & International Notation)

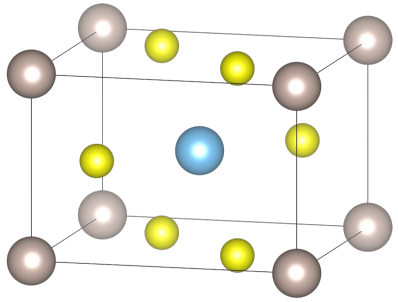
four-index nomenclature $(L_0.G_0.i_k.m)$ $i_t = |P(G_0)|/|P(L_0)|, i_k = |T(G_0)|/|T(L_0)|, x: index$

structure

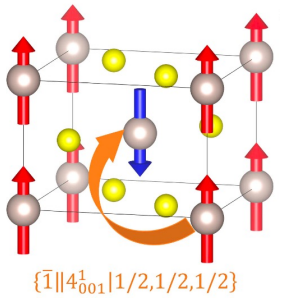




$G_0 = P4_2/mnm$
(136)



$L_0 = Cmmm$
(65)



$G^s = -1$
$i_t = 2, i_k = 1$

Group 65.136.1.1

International notation (G_0 basis)

Space group $G = Bg_1g_2g_3$

t-type SSG: $i_k = 1 \Longrightarrow G_{NSS} = B^{g_{s1}}g_1{}^{g_{s2}}g_2{}^{g_{s3}}g_3$

SSG	G^s	International notations
65.136.1.1**	-1	$P^{-1}4_2/{}^1m^{-1}n^1m$
65.136.1.2	2	$P^{2_{001}}4_2/{}^1m^{2_{001}}n^1m$
65.136.1.3	m	$P^{m_{001}}4_2/{}^1m^{m_{001}}n^1m$

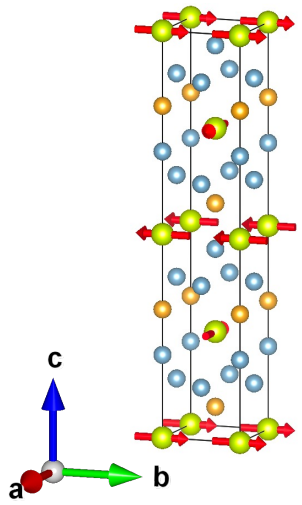
Spin-only group
collinear: $G^l_{SO} = Z_2^K \otimes SO(2) = {}^{\infty m}1$
coplanar: $G^p_{SO} = Z_2^K = {}^m1$
noncoplanar: $G^n_{SO} = 1$ (omitted)

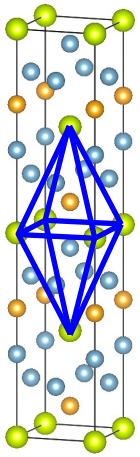
$$P^{-1}4_2/{}^1m^{-1}n^1m^{\infty m}1$$

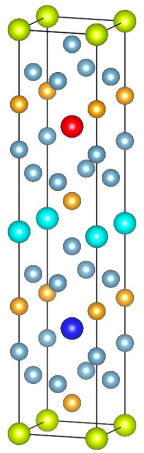
Nomenclature (four-index & International Notation)

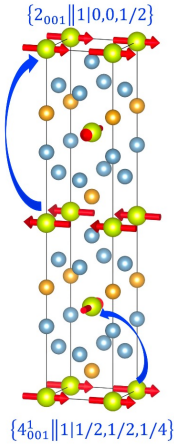
four-index nomenclature ($L_0.G_0.i_k.m$) $i_t = |P(G_0)|/|P(L_0)|, i_k = |T(G_0)|/|T(L_0)|, m: index$

structure









Group **99**.**107**.**4**.1

$G_0 = I4mm$ (**107**)

$L_0 = P4mm$ (**99**)

$G^s = 4$, $i_t = 1, i_k = 4$

International notation (L_0 basis)

Space group $G = B g_1 g_2 g_3$

k-type SSG: $i_t = 1 \Longrightarrow G_{NSS} = B^1 g_1{}^1 g_2{}^1 g_3{}^{g_{s_1}\tau_1 g_{s_2}\tau_2 g_{s_3}\tau_3}$

SSG	G^s	International notations
99.107.4.1	4	$P^1 4^1 m^1 m^{4^1_{001}}(1/2\ 1/2\ 1/4)$
99.107.4.2	-4	$P^1 4^1 m^1 m^{-4^3_{001}}(1/2\ 1/2\ 1/4)$

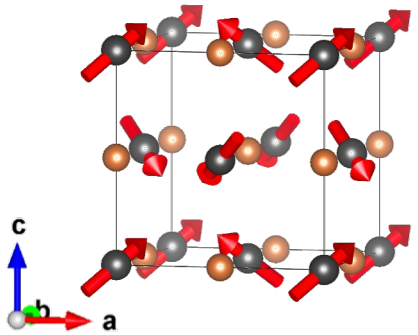
Spin-only group
collinear: $G^l_{SO} = Z_2^K \otimes SO(2) = {}^{\infty m}1$
coplanar: $G^p_{SO} = Z_2^K = {}^m1$
noncoplanar: $G^n_{SO} = 1$ (omitted)

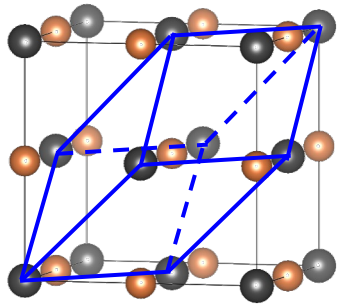
$$P^1 4^1 m^1 m^{4^1_{001}}(1/2\ 1/2\ 1/4)^{m}\mathbf{1}$$

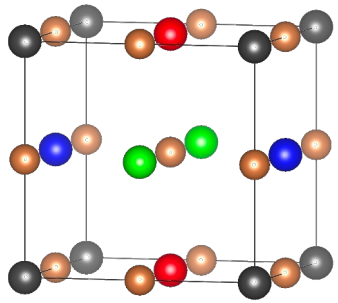
Nomenclature (four-index & International Notation)

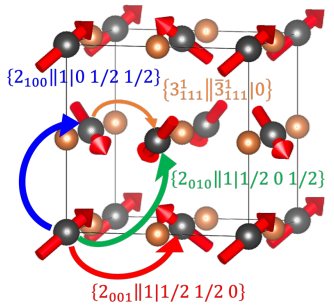
four-index nomenclature $(L_0.G_0.i_k.m)$ $i_t = |P(G_0)|/|P(L_0)|, i_k = |T(G_0)|/|T(L_0)|, m: index$

structure









Group 47.225.4.2

$G_0 = Fm\bar{3}m$ (225)

$L_0 = Pmmm$ (47)

$G^s = -43m$

$i_t = 6, i_k = 4$

International notation (G_0 basis)

Space group $G = Bg_1g_2g_3t_at_bt_cb_1b_2b_3$

g-type SSG: $G_{NSS} = B^{g_{s_1}}g_1{}^{g_{s_2}}g_2{}^{g_{s_3}}g_3|(g_{s_4}, g_{s_5}, g_{s_6}; g_{s_7}, g_{s_8}, g_{s_9})$

Bravais lattice	b_1	b_2	b_3
P			
F	{1|1/2 1/2 0}	{1|1/2 0 1/2}	{1|0 1/2 1/2}
I	{1|1/2 1/2 1/2}		
A	{1|0 1/2 1/2}		
C	{1|1/2 1/2 0}		
R	{1|2/3 1/3 1/3}	{1|1/3 2/3 2/3}	

Spin-only group

coplanar: $G_{SO}^p = Z_2^K = {}^m1$

noncoplanar: $G_{SO}^n = 1$ (omitted)

$F^1m^{3^1_{111}}\bar{3}^{m_{01\bar{1}}}m|(1,1,1; 2_{001}, 2_{010}, 2_{100})$

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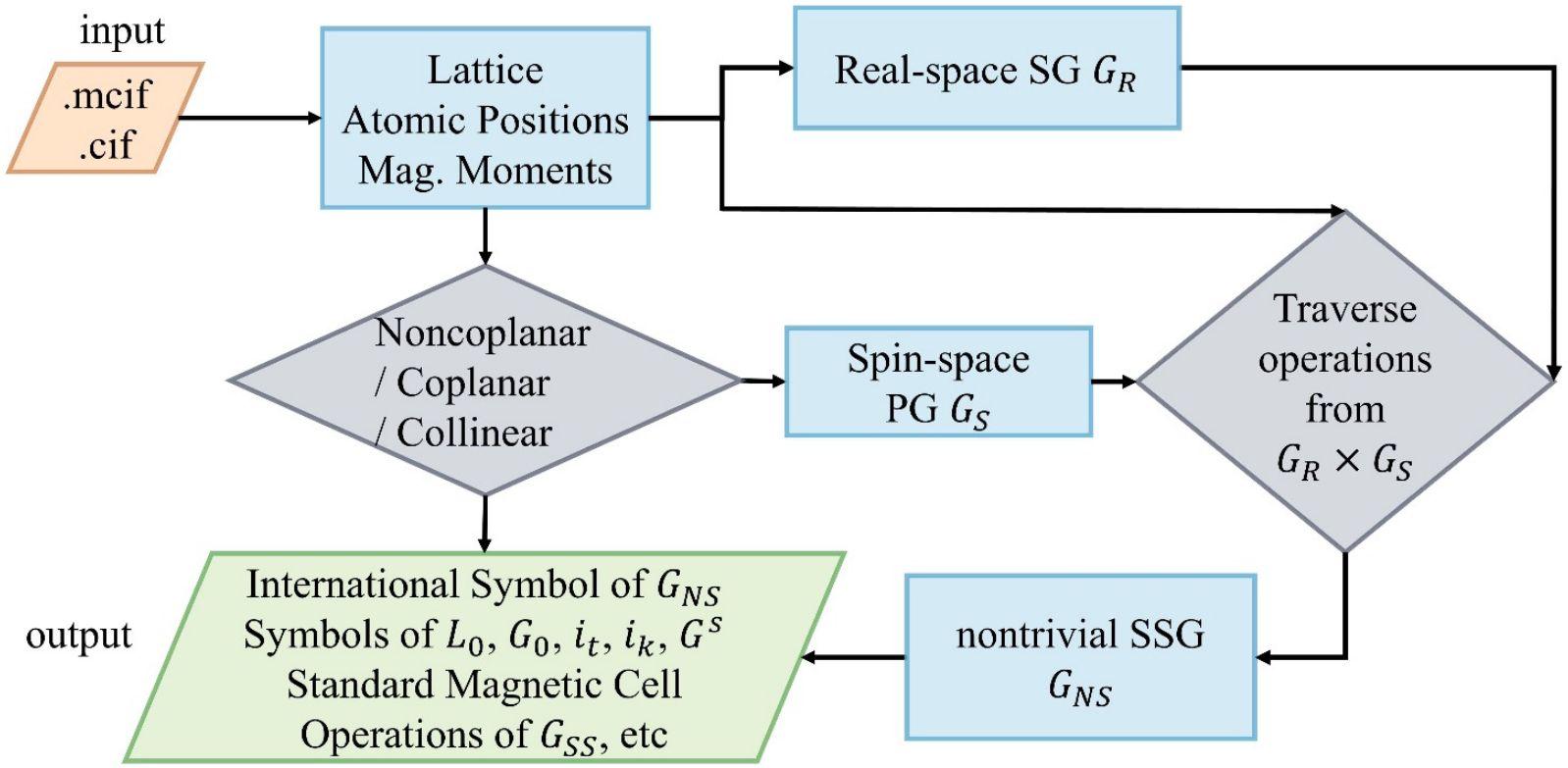
Identification of spin space group

Interactive online program: findspingroup.com



Step 1: find G_R and G_S describing lattice and magnetic geometry, respectively
Step 2: find operations in $G_R \times G_S$ that leaves the magnetic structure invariant
Step 3: find the G_{SO} and G_{NS}, then output

Identification of spin space group

Interactive online program: findspingroup.com

Identify Spin Space Group

All experimentally determined magnetic structures available in the MAGNDATA database have been identified and provided *here*.

Report bug

Identify Spin Space Group (version-0.34)

Input tolerance

0.001

For .cif data

Select a material file:

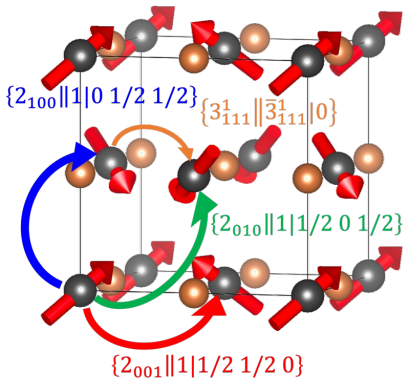
.cif, .mcif or .txt 浏览文件

Or customize material structure by clicking 'Submit' without upload a file.

Submit

Click the 'submit' to get the detail data. You can submit without uploading a file.

1. input mcif / cif



3.7 NpBi

Modify Parameters

Atomic tolerance:

0.02

How close that two atoms will be considered as one atom.

Moment tolerance

0.02

Moment eigen_tolerance

0.000004

Bigger value bigger PG

2. tolerance in finding SSG

Lattice:

6.370000 6.370000 6.370000 90.000000 90.000000 90.000000

Form:a b c α β γ

Types of atoms:

4*Bi 4*Np

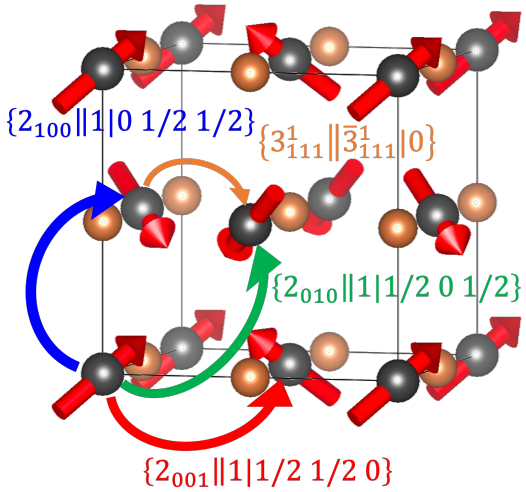
Align in order corresponding to the structure below .

Material Structure : (x y z Occupancy Mx My Mz)

```
0.500000 0.500000 0.500000 1.000000 0.000000 0.000000 0.000000
0.500000 0.000000 0.000000 1.000000 0.000000 0.000000 0.000000
0.000000 0.500000 0.000000 1.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.500000 1.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 1.000000 1.400000 1.400000 1.400000
0.000000 0.500000 0.500000 1.000000 1.400000 -1.400000 -1.400000
0.500000 0.000000 0.500000 1.000000 -1.400000 1.400000 -1.400000
0.500000 0.500000 0.000000 1.000000 -1.400000 -1.400000 1.400000
```

3. Position and magnetic moments of each atom in the unit cell. (in lattice coordinates)

Identification of spin space group



$F^1m^{3^1_{111}}\bar{3}^{m_{011}}m|(1,1,1;2_{001},2_{010},2_{100})$

G0-std Unit Magnetic Cell:

a	b	c	alpha	beta	gamma
6.37	6.37	6.37	90.0	90.0	90.0

Fractional Coordinates & Moments (in G0-std Unit Magnetic Cell)

No.	Atom	Site	Moment (in lattice)
1	Np	[0.0, 0.0, 0.0]	[1.4, 1.4, 1.4]
2	Np	[0.0, 0.5, 0.5]	[1.4, -1.4, -1.4]
3	Np	[0.5, 0.0, 0.5]	[-1.4, 1.4, -1.4]
4	Np	[0.5, 0.5, 0.0]	[-1.4, -1.4, 1.4]
5	Bi	[0.5, 0.0, 0.0]	[0.0, 0.0, 0.0]
6	Bi	[0.5, 0.5, 0.5]	[0.0, 0.0, 0.0]
7	Bi	[0.0, 0.0, 0.5]	[0.0, 0.0, 0.0]
8	Bi	[0.0, 0.5, 0.0]	[0.0, 0.0, 0.0]

Magnetic cell in G_0 basis

G_0 basis: t, g-type ; L_0 basis: k-type

Interactive online program: findspingroup.com

File Name	Spin Space Group	G0 Symbol	L0 Symbol	it	ik
$3.7/NpBi$	$F^1m^{3^1_{111}}-3^{m_{1-10}}m\|(1,1,1;2_{001},2_{010},2_{100})$	$Fm-3m(225)$	$Pmmm(47)$	6	4

$$G_{SS} = G_{NS} \times G_{SO}$$

Magnetic Phase

Space Group	Magnetic Space Group	Spin Part PG	Configuration	Magnetic Phase
$Fm-3m(225)$	$Pn-3m'(224.113)$ $Type\ III$	Td $-43m$	$Noncoplanar$	AFM

Spin Splitting

Little Cogroup at General Position		Spin Splitting	
without SOC	with SOC	without SOC	with SOC
$^{222}1$	1	No	Yes

Anomalous Hall effect

Effective Magnetic Point Group	Anomalous Hall Effect	
	without SOC	with SOC
$m-3m'$	No	No

All group elements are also given in list.

In progress: Symmetry-restricted Tensors …

All known magnetic structures in MAGNDATA

findspingroup.com

Identify Spin Space Group

All experimentally determined magnetic structures available in the MAGNDATA database have been identified and provided *here*.

Report bug

1978 commensurate magnetic materials (now)

SSGs of magnetic structures provided in the MAGNDATA database

No.	ID	Chemical formula	SG	MSG	four-index G_{NS}	G^s		International notation G_{NS}	G_{SO}
1	1.172	$NiTa_2O_6$	136	41.217	40.28.2.1	-1		$A^1m^1a^12^{-1}(0\ 1/2\ 0)$	${}^{\infty m}1$
2	1.583	$La_{1.5}Ca_{0.5}CoO_4$	35	7.28	40.28.2.1	-1		$A^1m^1a^12^{-1}(0\ 1/2\ 0)$	${}^{\infty m}1$
3	2.16	Ce_2PdGe_3	131	6.20	38.38.1.1	1		$A^1m^1m^12$	${}^{m}1$
4	1.740	$CeAuSb_2$	129	39.201	38.25.2.1	-1		$A^1m^1m^12^{-1}(0\ 1/2\ 0)$	${}^{\infty m}1$
5	0.26	TmAgGe	189	38.191	6.38.1.3	m		$A^1m^{m_{001}}m^{m_{001}}2$	${}^{m}1$
6	0.138	$BiCrO_3$	15	15.85	15.15.1.1	1		$C^12/^1c$	${}^{\infty m}1$
7	0.139	$BiCrO_3$	15	2.4	15.15.1.1	1		$C^12/^1c$	${}^{\infty m}1$
8	0.297	$NaCrGe_2O_6$	15	15.89	15.15.1.1	1		$C^12/^1c$	${}^{\infty m}1$
9	0.428	$BaMn_2Si_2O_7$	15	15.85	15.15.1.1	1		$C^12/^1c$	${}^{\infty m}1$
10	1.0.50	$CoGeO_3$	15	15.89	15.15.1.1	1		$C^12/^1c$	${}^{m}1$

Link towards MAGNDATA

four-index nomenclature of nontrivial SSG G_{NS}

SSGs in International Notations
nontrivial SSG G_{NS}
spin-only group G_{SO}

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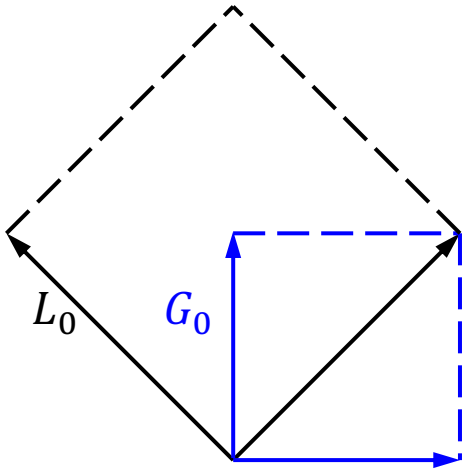
t-type SSG 65.136.1.1

1. Generate SSG from HM-notation

65.136.1.1** -1 $P^{-1}4_2/^1m^{-1}n^1m$ $M_{191} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

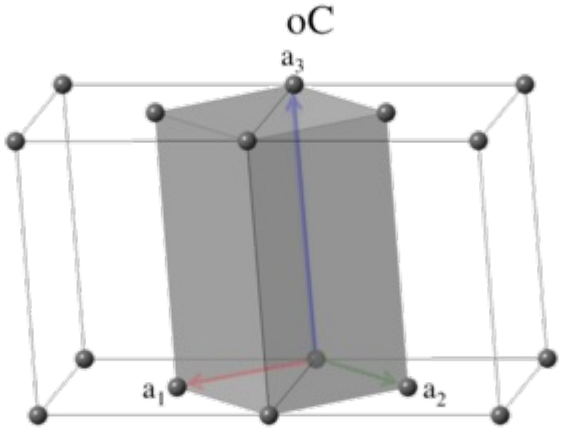
65 Cmmm 136 $P4_2/mnm$



G^S	G_0 (in G_0 basis, τ_1= (1/2, 1/2, 1/2))
1	$\{1\|0\}, \{2_{110}\|0\}, \{2_{1-10}\|0\}, \{2_{001}\|0\}, \{-1\|0\}, \{m_{110}\|0\}, \{m_{1-10}\|0\}, \{m_{001}\|0\}$
-1	$\{4^1_{001}\|\tau_1\}, \{4^3_{001}\|\tau_1\}, \{2_{100}\|\tau_1\}, \{2_{010}\|\tau_1\}, \{-4^1_{001}\|\tau_1\}, \{-4^3_{001}\|\tau_1\}, \{m_{100}\|\tau_1\}, \{m_{010}\|\tau_1\}$

G^S	G_0 (in L_0 basis, τ_2= (1/2, 0, 1/2))
1	$\{1\|0\}, \{2_{010}\|0\}, \{2_{100}\|0\}, \{2_{001}\|0\}, \{-1\|0\}, \{m_{010}\|0\}, \{m_{100}\|0\}, \{m_{001}\|0\}$
-1	$\{4^1_{001}\|\tau_2\}, \{4^3_{001}\|\tau_2\}, \{2_{110}\|\tau_2\}, \{2_{1-10}\|\tau_2\}, \{-4^1_{001}\|\tau_2\}, \{-4^3_{001}\|\tau_2\}, \{m_{110}\|\tau_2\}, \{m_{1-10}\|\tau_2\}$

body	basis	H-M notation
G_0	G_0	$P^{-1}4_2/^1m^{-1}n^1m$



t-type SSG 47.221.1.2

1. Generate SSG from HM-notation

47.221.1.2 3m $P^{1}m^{3^{1}_{001}}\text{-}3^{m_{010}}m$

$$M_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

47 Pmmm 221 Pm-3m

Table S13

221	Pm-3m	$\{m_{100}\|0\}$	$\{-3^{1}_{111}\|0\}$	$\{m_{110}\|0\}$

G^S	G_0
1	$1, 2_{100}, 2_{010}, 2_{001}, -1, m_{100}, m_{010}, m_{001}$
3^1_{001}	$3^1_{111}, 3^1_{1-11}, 3^1_{1-1-1}, 3^1_{11-1}, -3^1_{111}, -3^1_{1-11}, -3^1_{1-1-1}, -3^1_{11-1}$
3^2_{001}	$3^2_{111}, 3^2_{1-11}, 3^2_{1-1-1}, 3^2_{11-1}, -3^2_{111}, -3^2_{1-11}, -3^2_{1-1-1}, -3^2_{11-1}$
m_{010}	$2_{110}, 2_{1-10}, 4^1_{001}, 4^3_{001}, m_{110}, m_{1-10}, -4^1_{001}, -4^3_{001}$
$m_{\pi/6}$	$2_{011}, 2_{01-1}, 4^1_{100}, 4^3_{100}, m_{011}, m_{01-1}, -4^1_{100}, -4^3_{100}$
$m_{5\pi/6}$	$2_{101}, 2_{10-1}, 4^1_{010}, 4^3_{010}, m_{101}, m_{10-1}, -4^1_{010}, -4^3_{010}$

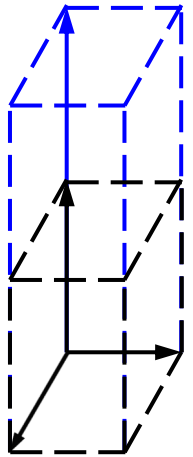
body	basis	H-M notation
G_0	G_0	$P^{1}m^{3^{1}_{001}}\text{-}3^{m_{010}}m$

k-type SSG

1. Generate SSG from HM-notation

99.107.4.1 4 $P^{1}4^{1}m^{1}m^{4^{1}_{001}}(1/2\ 1/2\ 1/4)$ $M_{250}=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&2&0\end{bmatrix}$

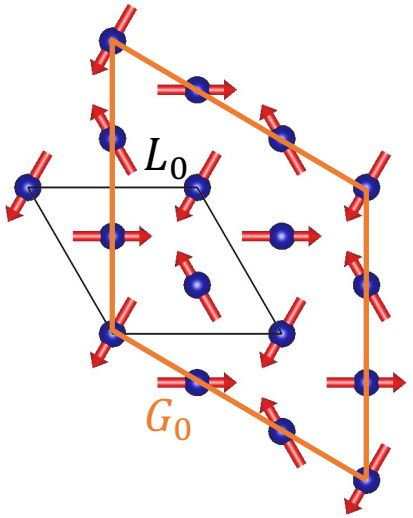
99 P4mm 107 I4mm



$L_0\ basis$: $I4mm/P4mm = \{1||1|0\} + \{4^{1}_{001}\|1|1/2\ 1/2\ 1/4\} + \{2_{001}\|1|0\ 0\ 1/2\} + \{4^{3}_{001}\|1|1/2\ 1/2\ 3/4\}$

body	basis	H-M notation
L_0	L_0	$P^{1}4^{1}m^{1}m^{4^{1}_{001}}(1/2\ 1/2\ 1/4)$

174.174.3.1 3 $P^{1}\text{-}6^{3^{1}_{001}}(2/3\ 1/3\ 0)$ $M_{478}=\begin{bmatrix}1&1&0&0\\-1&2&0&0\\0&0&1&0\end{bmatrix}$



$L_0\ basis$: $P-6/P-6 = \{1||1|0\} + \{3^{1}_{001}\|1|2/3\ 1/3\ 0\} + \{3^{2}_{001}\|1|1/3\ 2/3\ 0\}$

$G_0\ basis$: $P-6/P-6 = \{1||1|0\} + \{3^{1}_{001}\|1|1\ 0\ 0\} + \{3^{2}_{001}\|1|1\ 1\ 0\}$

g-type SSG 4.182.4.2

4.182.4.2 -43m $P3^2_{-11-1}6_3{}^{m_{110}}2^{m_{011}}2|(2_{001}, 2_{100}, 1)$ Matrix form: (**P**,p)= $\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & -1 & 1/4 \\ 0 & 1/2 & 0 & 0 \end{pmatrix}$

G^S	G_R
1	$\{1\|0\}, \{2_{001}\|0\ 0\ 1/2\}$
3^1_{-11-1}	$\{3^1_{001}\|0\}, \{6^5_{001}\|0\ 0\ 1/2\}$
3^2_{-11-1}	$\{3^2_{001}\|0\}, \{6^1_{001}\|0\ 0\ 1/2\}$
m_{-101}	$\{2_{110}\|0\}, \{2_{1-10}\|0\ 0\ 1/2\}$
m_{110}	$\{2_{100}\|0\}, \{2_{120}\|0\ 0\ 1/2\}$
m_{011}	$\{2_{010}\|0\}, \{2_{210}\|0\ 0\ 1/2\}$

body	basis	H-M notation
G_0	G_0	$P3^1_{-11-1}6_3{}^{m_{110}}2^{m_{011}}2\|(2_{001}, 2_{100}, 1)$

Spin translation group

G_T^S	G_T
1	$\{1\|2\ 2\ 1\}$
2_{001}	$\{1\|1\ 0\ 0\}$
2_{100}	$\{1\|0\ 1\ 0\}$
2_{010}	$\{1\|1\ 1\ 0\}$