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SPIN P-SYMMETRY OF MAGNETIC CRYSTALS.

MONOCLINIC AND ORTHORHOMBIC STRUCTURES

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Спиновая P-симметрия магнитных кристаллов. Моноклинные и ромбические структуры

Рассмотрена теория пространственных спиновых групп в приближении P-симметрии и указана общая схема их вывода. Задача вывода всех пространственных спиновых групп поставлена здесь для тех "семейств" спиновых групп, которые связаны с реальными магнитными структурами. Для этого должна быть определена спиновая симметрия экспериментально установленных магнитоупорядоченных кристаллов. Приведены таблицы групп симметрии структур моноклинной и ромбической систем. Спиновые пространственные группы определены на основе существующих нейтронографических данных.

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Spin P-Symmetry of Magnetic Crystals. Monoclinic and Orthorhombic Structures

The theory of spin space groups in P-symmetry approximation is briefly reviewed. The spin space groups of magnetic structures belonging to the monoclinic and orthorhombic systems are given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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The spin space group of P-symmetry $\tilde{\Phi}_S^{(p)}$ is defined /1-6/ as the group of all spin-space transformations (p,ϕ) which leave invariant a spin density function $\vec{S}(\vec{r})$:

$$(p,\phi)\vec{S}(\vec{r}) = p\vec{S}(\phi^{-1}\vec{r}) = \vec{S}(\vec{r}). \qquad (1)$$

Here, ϕ is an element of the space (Fedorov) group $\Phi = TG$, p is an element of the group $\tilde{P} = \infty\infty 1'$ consisting of all three-dimensional rotations and time inversion $1'$.

The group $\tilde{\Phi}_S^{(p)}$ is a subgroup of the direct product of the "load" group $\tilde{P}$ and the "basis" group Φ:

$$\tilde{\Phi}_S^{(p)} \subseteq \tilde{P} \times \Phi \qquad (2)$$

The groups $\tilde{P}$ and Φ act in different spaces. In eq. (1), an element ϕ of Φ acts only on the coordinates $\vec{r}$ of magnetic atoms, while an element p of $\tilde{P}$ acts only on the components of the spin vectors.

A spin space group is a direct product of a spin-only group ρ and a junior (nontrivial) spin space group $\Phi_S^{(p)}$ /2,6/. The groups ρ are as follows:

$$\rho_\ell = 1^{(\infty 2' 2')}, \quad \rho_p = 1^{(2'_\perp)}, \quad \rho_s = 1^{(1)} \qquad (3)$$

for linear, planar and spatial magnetic structures, respectively. According to the general theory of P-symmetry [7-9], a collection of load elements p in the junior group $\Phi_s^{(p)} \to \Phi$ forms a group, which is isomorphic to the factor group Φ/Φ^*. The load elements p of $\tilde{P}$ are paired with basis elements ϕ of Φ by the homomorphism:

$$\Phi \to P \leftrightarrow \Phi/\Phi^*, \qquad (4)$$

where Φ^* is a normal subgroup of Φ and P is a subgroup of $\tilde{P}$. Every nontrivial spin group $\Phi_s^{(p)}$ is isomorphic to basis group Φ.

The scheme (4) is used as the general principle of derivation of all spin groups. The spin point groups

$$G_s^{(p)} \subseteq \tilde{P} \times G, \quad G_s^{(p)} \leftrightarrow G, \qquad (5)$$

where G is a crystallographic point group, are tabulated in [5,11]. Spin translation groups

$$T_s^{(p)} \subseteq \tilde{P} \times T, \quad T_s^{(p)} \leftrightarrow T \lhd \Phi, \qquad (6)$$

where T is a translation group belonging to one of the 14 Bravais classes, are tabulated in [10]. No tables of spin space groups are available. In principle, two categories of spin space groups are known. There are $\Phi_s^{(p)} = TG_s^{(p)}$ and $\Phi_s^{(p)} = T_s^{(p)}G$. For the third category $\Phi_s^{(p)} = T_s^{(p)}G_s^{(p)}$ only the so-called 2-,3-,4-,5-coloured groups of the general P-symmetry are known [4,16].

The number of spin space groups is very large, so we limited a derivation of spin groups to some of the "families" of space groups that are connected with the experimentally determined magnetic structures. For that, the spin symmetry of real magnetic structures have to be known.

In this paper, a description of the symmetry of magnetic structures belonging to the monoclinic and orthorhombic systems is given. Only the case of P-symmetry is considered. The description of more complicated strutures by the use of the theory of W-symmetry [12,13] will be given elsewhere.

The spin space groups were established on the basis of experimental data contained in the "Magnetic Structures Determined by Neutron Diffraction" [14].

The magnetic compounds listed here are collected in Tables 1 and 2 according to the crystallographic systems with an alphabetical order of chemical symbols of the compounds within each system. The Tables are divided into four parts named on page 8. First, the chemical symbol of the magnetic compound is given. Second, the magnetic atoms of the compound are specified (with their positions in the crystal unit cell in Wyckoff notation), as in ref. [15]. Next, the symbol of the spin space group is given.

The notation of spin space groups is based on the international notation of space groups and it is a straightforward generalization of the notation of magnetic space groups. The symbol of a spin space group $\tilde{\Phi}_s^{(p)}$ consists of the symbols denoting the spin-only group, the spin lattice of $\Phi_s^{(p)}$ and the rotations and reflections (with the corresponding non-primitive translations) of $\Phi_s^{(p)}$. The spin lattice is indicated by an international symbol P, C, A, B, I, F of the crystal lattice with a subscript

$(p_1 p_2 p_3)$, where $p_i = p(\vec{a}_i)$ are the loading elements of three translations $\vec{a}_i$ $(i=1,2,3)$ which generate the crystal lattice.

The setting of lattices is chosen as follows:

The primitive lattice P is defined by the primitive vectors $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$. The monoclinic side-centred C by $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$, $\{\vec{a}_1 = \frac{\vec{a}+\vec{b}}{2}, \vec{a}_2 = \frac{\vec{a}-\vec{b}}{2}, \vec{a}_3 = \vec{c}\}$ with the two-fold axis parallel to $\vec{b}$. The orthorhombic centred lattices are defined by

$$A = \{\vec{a}_1 = \vec{a},\ \vec{a}_2 = \frac{\vec{b}+\vec{c}}{2},\ \vec{a}_3 = \frac{\vec{b}-\vec{c}}{2}\},$$

$$B = \{a_1 = \frac{\vec{a}+\vec{c}}{2},\ a_2 = \vec{b},\ a_3 = \frac{\vec{a}-\vec{c}}{2}\},$$

$$C = \{\vec{a}_1 = \frac{\vec{a}+\vec{b}}{2},\ a_2 = \frac{\vec{a}-\vec{b}}{2},\ \vec{a}_3 = \vec{c}\},$$

$$I = \{\vec{a}_1 = \frac{-\vec{a}+\vec{b}+\vec{c}}{2},\ a_2 = \frac{\vec{a}-\vec{b}+\vec{c}}{2},\ c = \frac{\vec{a}+\vec{b}-\vec{c}}{2}\}.$$

In the rotational part of the symbol of the spin space group $\Phi_S^{(p)}$ the spin elements are denoted by $\phi_j^{(pk)}$, where $\phi_j = (R_j / \vec{\tau}(R_j)), p_k = p_k(R_j)$. R_j is a proper or improper rotation, $\vec{\tau}(R_j)$ is the nonprimitive translation associated with R_j, $p_k(R_j)$ is an element of the load group P.

In the fourth column of the Tables, the axial vector $\vec{S}(\vec{r})$ representing the magnetic structure of the compound is given for one position vector $\vec{r}_1$. The position vector $\vec{r}_1$ is chosen from the set of equivalent positions and it is expressed in fractions of the crystal unit cell edges, as in ref. /15/. The components of spin vectors $\vec{S}(\vec{r})$ are given in local system of coordinates xyz, arbitrary oriented to the crystal lattice axes XYZ. For convenience, the axes xyz can be chosen as coinciding with the axes XYZ.

The magnetic structure of the one-lattice model of the crystal (simple crystal) can be generated by the spin space group $\tilde{\Phi}_S^{(p)}$ from the single spin located at $\vec{r}_1$:

$$\{\vec{S}(\vec{r}_i) = (p_i, \phi_i)\vec{S}(\vec{r}_1) \mid (p_i, \phi_i) \in \tilde{\Phi}_S^{(p)}\}. \qquad (7)$$

For many-lattice crystal, the magnetic structure can be generated by the same spin group from the spins $\vec{S}(\vec{r}_1)_I$, $\vec{S}(\vec{r}_1)_{II}$, etc. The common spin space group for different magnetic structures (simple crystals) or for different phases is explicitly denoted by a curly bracket $\{$.

It is important to notice, that the same senior spin space group $\tilde{\Phi}_S^{(p)}$ can be determined by p and by different equivalent junior groups $\Phi_S^{(p)}$. In Table 1 and Table 2, as a representative group $\Phi_S^{(p)}$ the simplest one is chosen.

In the fourth column, the symbols T and T_t denote temperature and transition temperature, respectively; q, real numbers. All numerical data can be found in ref. /14/.

Compound	Positions of magnetic atoms	Spin space group	Spin vectors
		Table 1. MONOCLINIC SYSTEM	
Au_5Mn_2	Mn_I /a /	$p_1 \otimes C_{(111')}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (U,V,W)$
$CoCl_2 \cdot 2H_2O$ $CoCl_2 \cdot 2D_2O$	Co /a /	$p_1 \otimes C_{(1'1'1)}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (0,V,0)$
$CoCl_2 \cdot 6H_2O$	Co /a /	$p_1 \otimes C_{(111')}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (0,0,W)$
$CoFe_2Se_4$	Fe /c /	$p_1 \otimes C_{(111)}\, 2^{(1)}/m^{(1)}$	$S(0,0,\frac{1}{2}) = (U,0,0)$
$CoWO_4$	Co /f /	$p_1 \otimes P_{(1'11)}\, 2^{(1')}/c^{(1')}$	$S(\frac{1}{2},y,\frac{1}{4}) = (U,0,W)$
CrF_2	Cr /a /	$p_1 \otimes P_{(111)}\, 2_1^{(1')}/c^{(1')}$	$S(0,0,0) = (U,0,W)$
$CrFe_2Se_4$	Fe_I /c /	$p_1 \otimes C_{(111)}\, 2^{(1)}/m^{(1)}$	$S(0,0,\frac{1}{2}) = (0,V,W)$
Cr_2NiS_4	Ni /c / Cr /i /	$p_1 \otimes C_{(111')}\, 2^{(1)}/m^{(1)}$	$S(0,0,\frac{1}{2}) = (U,V,W)$ $S(x,0,z) = -q(U,V,W)$
CrS	Cr /d /	$p_1 \otimes C_{(111)}\, 2^{(1)}/c^{(1')}$	$S(\frac{1}{4},\frac{1}{4},\frac{1}{2}) = (U,V,W)$

Table 1, cont.

Cr_3S_4 Cr_3Te_4	Cr_I /c / Cr_{II} /i /	$p_1 \otimes C_{(111)}\, 2^{(1)}/m^{(1)}$	$S(0,0,\frac{1}{2}) = (U_1,V_1,W_1)$ $S(x,0,z) = (U_2,V_2,W_2)$
$CuF_2 \cdot 2H_2O$	Cu /a /	$p_1 \otimes C_{(1'1'1)}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (0,0,W)$
$CuWO_4$	Cu /f /	$p_1 \otimes P_{(1'11)}\, 2^{(1')}/c^{(1')}$	$S(\frac{1}{2},y,\frac{1}{4}) = (U,0,W)$
DyOOH	Dy /e /	$p_1 \otimes P_{(111)}\, 2_1^{(1')}/m^{(1)}$	$S(x,\frac{1}{4},z) = (U,0,W)$
ErOOH	Er /e /	$p_1 \otimes P_{(111)}\, 2_1^{(1)}/m^{(1')}$	$S(x,\frac{1}{4},z) = (0,V,0)$
$FeCr_2Se_4$	Fe /c /	$p_1 \otimes C_{(111')}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (U,0,W)$
$Fe(HCOO) \cdot 2H_2O$	Fe_I /a / Fe_{II} /d /	$p_1 \otimes P_{(111)}\, 2_1^{(1')}/c^{(1')}$	$S(0,0,0) = (U,0,W)$ $S(\frac{1}{2},0,\frac{1}{2}) = -q(U,0,W)$
$FeNbO_4$	Fe /f /	$p_1 \otimes P_{(1'11)}\, 2^{(1')}/c^{(1')}$	$S(\frac{1}{2},y,\frac{1}{4}) = (U,0,W)$
$Fe_3(PO_4)_2 \cdot 4H_2O$	Fe_I /a / Fe_{II} /e /	$p_p \otimes P_{(111)}\, 2_1^{(2y)}/a^{(2y)}$	$S(0,0,0) = (U,V,W)$ $S(x,y,z) = (U,V,W)$
$Fe_3(PO_4)_2 \cdot 8H_2O$	Fe_I /a / Fe_{II} /g /	$p_1 \otimes C_{(111')}\, 2^{(1)}/m^{(1)}$	$S(0,0,0) = (U,0,W)$ $S(0,y,0) = (U,0,W)$
Fe_3Se_4	Fe_I /c / Fe_{II} /g /	$p_1 \otimes C_{(111)}\, 2^{(1)}/m^{(1)}$	$S(0,0,\frac{1}{2}) = (U,0,0)$ $S(x,0,z) = (U,0,0)$

Table 1, cont.

$FeWO_4$	Fe /f /	$p_L \otimes P_{(1'11)}\ 2^{(1')}/c^{(1')}$	$S(\frac{1}{2},y,\frac{1}{4}) = (U,0,W)$
$LiCuCl_3 \cdot 2H_2O$	Cu/e /	$p_L \otimes P_{(111)}\ 2_1^{(1)}/c^{(1')}$	$S(x,y,z) = (U,0,W)$
$Mn(DCOO)_2 \cdot 2H_2O$	Mn_I /a /	$p_L \otimes P_{(111)}\ 2_1^{(1)}/c^{(1)}$	$S(0,0,0) = (0,V,0)$ $T > T_t$
$Mn(DCOO)_2 \cdot 2D_2O$	Mn_{II} /d /	$p_L \otimes P_{(111)}\ 2_1^{(1')}/c^{(1')}$	$\begin{cases} S(0,0,0) = (U,0,W) & T < T_t \\ S(\frac{1}{2},0,\frac{1}{2}) = -q(U,0,W) \end{cases}$
MnF_3	Mn_I /a / Mn_{II} /f /	$p_L \otimes C_{(111)}\ 2^{(1)}/c^{(1')}$	$S(0,0,0) = (U,V,\bar{U})$ $S(x,y,z) = q(U,V,\bar{U})$
$NiCl_2 \cdot 6H_2O$	Ni /a /	$p_L \otimes \overset{+}{I}_{(111')}\ 2^{(1)}/m^{(1)}$	$S(0,0,0) = (U,0,W)$
$NiWO_4$	Ni /f /	$p_L \otimes P_{(1'11)}\ 2^{(1')}/c^{(1')}$	$S(\frac{1}{2},y,\frac{1}{4}) = (U,0,W)$
$\alpha - O_2$	O_2 /a /	$p_L \otimes C_{(1'1'1)}\ 2^{(1)}/m^{(1)}$	$S(0,0,0) = (U,0,W)$

Table 2. ORTHORHOMBIC SYSTEM

AgF	Ag /a /	$p_P \otimes P_{(111)}\ b^{(1)}cc^{(2y)}_{a}a^{(2y)}$	$S(0,0,0) = (0,V,W)$
$BaFe_2O_4$	Fe_I /f / Fe_{II} /f /	$p_L \otimes B_{(1'1'1)}\ m^{(1')}2^{(1)}m^{(1')}$ or $p_L \otimes B_{(1'1'1)}\ 2^{(1')}m^{(1')}m^{(1')}$	$\begin{cases} S(x_1,y_1,z_1) = (0,0,W) \\ S(x_2,y_2,z_2) = (0,0,W) \end{cases}$
$BiMn_2O_5$	Mn_I /f / Mn_{II} /g /	$p_P \otimes P_{(1'1'1)}\ b^{(2y)}a^{(2y)}m^{(1)}$	$\begin{cases} S(0,\frac{1}{2},z) = (U_1,V_1,0) \\ S(x,y,0) = (U_2,V_2,0_2) \end{cases}$
$CaFe_2O_4$	Fe_I /c / Fe_{II} / c /	$p_L \otimes P_{(111)}\ n^{(1)}a^{(1)}m^{(1)}$ or $p_L \otimes P_{(111)}\ n^{(1')}a^{(1)}m^{(1)}$	$\begin{cases} S(x_1,y_1,\frac{1}{4}) = (0,0,W_1) \\ S(x_2,y_2,\frac{1}{4}) = (0,0,W_2) \end{cases}$
$Ca_2Fe_2O_5$	Fe_I/a / Fe_{II} /b /	$p_L \otimes P_{(111)}\ c^{(1')}m^{(1)}n^{(1')}$	$\begin{cases} S(0,0,0) = (0,0,W) \\ S(\frac{1}{2},0,0) = (0,0,W) \end{cases}$
$CaMn_2O_4$	Mn /e /	$p_L \otimes P_{(1'11)}\ b^{(1)}c^{(1')}m^{(1')}$	$S(x,y,z) = (U,0,0)$
$CeZn_2$	Ce /e /	$p_L \otimes I_{(111)}\ m^{(1)}m^{(1)}a^{(1')}$	$S(0,\frac{1}{4},z) = (0,V,0)$
$\alpha - CoSO_4$	Co /a /	$p_L \otimes C_{(1'1'1)}\ m^{(1)}c^{(1')}m^{(1')}$	$S(0,0,0) = (0,V,W)$

Table 2, cont.

β-$CoSO_4$	Co /a /	$p_s \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_y)} m^{(2_z)}$	$S(0,0,0) = (U,V,W)$
$CoCrO_4$	Co /a /	$p_t \otimes C_{(111')}\, m^{(1)} c^{(1')} m^{(1)}$	$S(0,0,0) = (U,0,W)$
$CoSeO_4$	Co /a /	$p_s \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_y)} m^{(2_z)}$	$S(0,0,0) = (U,V,W)$
Co_2SiO_4	Co_I /c / Co_{II} /c /	$p_t \otimes \mathcal{P}_{(111)}\, n^{(1')} m^{(1)} a^{(1')}$	$S(x_1,\frac{1}{4},z_1) = (0,V,0)$ $S(x_2,\frac{1}{4},z_2) = (0,V,0)$
$Co_3V_2O_8$	Co_I /a / Co_{II} /e /	$p_t \otimes A_{(111)}\, b^{(1)} a^{(1)} m^{(1)}$	$S(0,0,0) = (0,0,W)$ $S(\frac{1}{4},y,\frac{1}{4}) = (0,0,W)$
$CrUO_4$	Cr /c / U /c /	$p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} c^{(1')} n^{(1')}$	$S(0,y_1,\frac{1}{4}) = (0,V,0)$ $S(0,y_2,\frac{1}{4}) = (0,V,0)$
$CrTiNdO_3$	Nd /g /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} a^{(2_x')} m^{(1)}$	$S(x,y,0) = (U,V,0)$
$CrVO_4$	Cr /a /	$p_t \otimes C_{(111)}\, m^{(1)} c^{(1')} m^{(1')}$	$S(0,0,0) = (U,V,W)$
$CsCoCl_3 \cdot 2H_2O$	Co /c /	$p_p \otimes \mathcal{P}_{(11'1)}\, c^{(2_x)} c^{(1')} a^{(2_x)}$	$S(0,y,\frac{1}{4}) = (U,0,W)$
$CuCl_2 \cdot 2H_2O$ $CuCl_2 \cdot 2D_2O$	Cu /a /	$p_p \otimes \mathcal{P}_{(111')}\, b^{(2_x)} m^{(1)} n^{(2_x)}$	$S(0,0,0) = (U,0,W)$
$CuSO_4$	Cu /a /	$p_s \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_y)} m^{(2_z)}$	$S(0,0,0) = (U,0,0)$
$CuSeO_4$	Cu /a /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_x')} m^{(1')}$	$S(0,0,0) = (U,V,0)$

Table 2, cont.

$DyAlO_3$	Dy /c /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x')} n^{(2_x)} m^{(1)}$	$S(x,y,\frac{1}{4}) = (U,V,0)$
$DyCoO_3$	Dy /c/	$p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1')} m^{(1)}$	$S(x,y,\frac{1}{4}) = (U,V,0)$
$DyCrO_3$	Dy /c / Cr /b /	$p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1')} m^{(1)}$	$S(x,y,\frac{1}{4}) = (U,V,0)$ $S(\frac{1}{2},0,0) = (0,0,W)$
DyFeO	Fe /b / Dy /c /	$p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$ $p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_x')} m^{(1)}$ or $p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x')} n^{(2_x)} m^{(1)}$	$S(\frac{1}{2},0,0) = (U,0,0)$ $T > T_t$ $S(\frac{1}{2},0,0) = (0,U,0)$ $T < T_t$ $S(x,y,\frac{1}{4}) = (U_1,V_1,0)$
DyNi	Dy /c /	$p_p \otimes \mathcal{P}_{(111)}\, n^{(2_x)} m^{(1)} a^{(2_x)}$	$S(x,\frac{1}{4},z) = (U,0,W)$
Er_3Co	Er_I /c / Er_{II} /d /	$p_s \otimes \mathcal{P}_{(111)}\, n^{(2_x')} m^{(2_y)} a^{(2_x')}$	$S(x_1,\frac{1}{4},z_1) = (0,V_1,0)$ $S(x_2,y_2,z_2) = (U,V,W)$
$ErCrO_3$	Cr /b / Er /c /	$p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$ $p_t \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1')} m^{(1)}$	$S(\frac{1}{2},0,0) = (U,0,0)$ $T > T_t$ $S(\frac{1}{2},0,00) = (U,V,0)$ $T < T_t$ $S(x,y,\frac{1}{4}) = (0,0,W)$
ErGa	Er /c /	$p_p \otimes C_{(111)}\, m^{(1)} c^{(2_x)} m^{(2_x)}$	$S(0,y,\frac{1}{4}) = (U,V,0)$
ErNi	Er /c /	$p_p \otimes \mathcal{P}_{(111)}\, n^{(2_x)} m^{(1)} a^{(2_x)}$	$S(x,\frac{1}{4},z) = (U,0,W)$

Table 2, cont.

$ErVO_3$	V /b/ Er /c/	$p_p \otimes P_{(111)}\, b^{(1')} n^{(2y)} m^{(2y)}$	$S(\frac{1}{2},0,0) = (0,V,0)$ $S(x,y,\frac{1}{4}) = (0,0,W)$
Fe_2GeS_4	Fe_I /a/ Fe_{II} /c/	$p_p \otimes P_{(111)}\, n^{(2x)} m^{(2x')} a^{(1')}$	$S(0,0,0) = (U_1,V_1,0)$ $T > T_t$ $S(x,\frac{1}{4},z) = (U_2,V_2,0)$
		$p_s \otimes P_{(111)}\, n^{(2x')} m^{(2y')} a^{(2x)}$	$S(0,0,0) = (U_3,V_3,W_3)$ $T < T_t$ $S(x,\frac{1}{4},z) = (U_4,0,W_4)$
β-$FeNaO_2$	Fe /a/	$p_p \otimes P_{(111)}\, n^{(1)} a^{(2y)} 2_1^{(2y)}$	$S(x,y,z) = (0,V,W)$
α-FeOOH	Fe /c/	$p_t \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1)}$	$S(x,\frac{1}{4},z) = (0,V,0)$
γ-FeOOH	Fe /c/	$p_t \otimes C_{(111)}\, m^{(1)} c^{(1')} m^{(1')}$	$S(0,y,\frac{1}{4}) = (U,V,0)$
$FeSO_4$	Fe /a/	$p_t \otimes C_{(1'1'1)}\, m^{(1)} c^{(1')} m^{(1')}$	$S(0,0,0) = (0,V,0)$
Fe_2SiO_4	Fe_I /a/	$p_t \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1')}$	$S(0,0,0) = (0,V,0)$ $T > T_t$
	Fe_{II} /c/	$p_s \otimes P_{(111)}\, n^{(2x)} m^{(2y)} a^{(2x)}$	$S(0,0,0) = (U,V,W)$ $T < T_t$ $S(x,\frac{1}{4},z) == (0,V,0)$
$FeUO_4$	Fe /c/ U /c/	$p_t \otimes P_{(111)}\, b^{(1')} c^{(1)} n^{(1')}$	$S(0,y_1,\frac{1}{4}) = (0,V_1,0)$ $T > T_t$ $S(0,y_2,\frac{1}{4}) = (0,V_2,0)$
		$p_p \otimes P_{(111)}\, b^{(2x)} c^{(1)} n^{(2x)}$	$S(0,y_1,\frac{1}{4}) = (U_1,0,W_1)$ $T < T_t$ $S(0,y_2,\frac{1}{4}) = (U_2,0,0)$

Table 2, cont.

$GdCoO_3$	Gd /c/	$p_t \otimes P_{(111)}\, b^{(1)} n^{(1')} m^{(1)}$	$S(x,y,\frac{1}{4}) = (0,V,0)$
$GdFeO_3$	Fe /b/	$p_t \otimes P_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$ $T > T_t$
$GeMnO_3$	Mn_I/c/ Mn_{II}/c/	$p_t \otimes P_{(111)}\, b^{(1)} c^{(1)} a^{(1')}$	$S(x_1,y_1,z_1) = (0,V_1,0)$ $S(x_2,y_2,z_2) = (0,V_2,0)$
HoAl	Ho_I /d/ Ho_{II} /d/	$p_p \otimes P_{(111)}\, b^{(2y)} c^{(2y)} m^{(1)}$	$S(x_1,y_1,\frac{1}{4}) = (U,V,0)$ $S(x_2,y_2,\frac{1}{4}) = (U,V,0)$
$HoCoO_3$	Ho /c/	$p_p \otimes P_{(111)}\, b^{(2y)} n^{(2y')} m^{(1)}$	$S(x,y,\frac{1}{4}) = (U,V,0)$
$HoCrO_3$	Cr /b/	$p_t \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,W)$ $T > T_t$ $S(\frac{1}{2},0,0) = (0,0,W_1)$ $T < T_t$
	Ho /c/	$p_s \otimes P_{(111)}\, b^{(2x)} n^{(2y')} m^{(2x')}$	$S(x,y,\frac{1}{4}) = (U_2,V_2,0)$
$HoFeO_3$	Fe /b/	$p_t \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$ $T > T_{t_1}$ $S(\frac{1}{2},0,0) = (V,V,W)$ $T_{t_2} < T < T_{t_1}$ $S(\frac{1}{2},0,0) = (0,0,W_1)$ $T < T_{t_2}$
	Ho /c/	$p_s \otimes P_{(111)}\, b^{(2x)} n^{(2y')} m^{(2x')}$	$S(x,y,\frac{1}{4}) = (U_2,V_2,0)$
$KFeCl_3$	Fe /c/	$p_t \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1')}$	$S(x,\frac{1}{4},z) = (0,V,0)$

Table 2, cont.

$KFeF_4$	Fe /a /	$p_L \otimes A_{(111)}\, m^{(1')} m^{(1)} a^{(1')}$	$S(0,0,0) = (0,0,W)$
$LaErO_3$	Er /b /	$p_S \otimes P_{(111)}\, b^{(2x)} n^{(2y)} m^{(2x)}$	$S(\frac{1}{2},0,0) = (U,V,W)$
$LaMnO_3$	Mn /a /	$p_P \otimes P_{(111)}\, n^{(2y)} m^{(2y)} a^{(1)}$	$S(0,0,0) = (U,V,0)$
$LiCoPO_4$	Co /c /	$p_L \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1)}$	$S(x,\frac{1}{4},z) = (0,V,0)$
$LiMnPO_4$	Mn /c /	$p_L \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1)}$	$S(x,\frac{1}{4},z) = (U,0,0)$
$LiNiPO_4$	Ni /c /	$p_L \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1)}$	$S(x,\frac{1}{4},z) = (0,0,W)$
$LuCrO_3$	Cr /b /2	$p_L \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,W)$
$LuFeO_3$	Fe /b /	$p_L \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$
Mn_2GeS_4	Mn_I /a / Mn_{II} /c /	$p_L \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1')}$	$S(0,0,0) = (0,V,0)$ $S(x,\frac{1}{4},z) = (0,V,0)$
MnP	Mn /c /	$p_L \otimes P_{(111)}\, b^{(1)} n^{(1)} m^{(1)}$	$S(x,y,\frac{1}{4}) = (0,0,W)$ $T > T_t$
Mn_2N	Mn /d /	$p_P \otimes P_{(111)}\, b^{(2y)} n^{(2y)} a^{(1)}$	$S(x,y,z) = (U,V,0)$
$MnSeO_4$	Mn /a /	$p_L \otimes P_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$	$S(0,0,0) = (U,V,0)$
$MnUO_4$	Mn /b /	$p_L \otimes I_{(1'1'1')}\, m^{(1)} m^{(1)} a^{(1)}$	$S(0,0,\frac{1}{2}) = (0,V,0)$

Table 2, cont.

Mn_2SiO_4	Mn_I /a / Mn_{II} /c /	$p_L \otimes P_{(111)}\, n^{(1')} m^{(1)} a^{(1')}$ $p_P \otimes P_{(111)}\, n^{(2x)} m^{(2x')} a^{(1')}$	$S(0,0,0) = (U_1,0,0)$ $T > T_t$ $S(0,0,0) = (U,0,W)$ $T < T_t$ $S(x,\frac{1}{4},z) = (U_2,0,0)$
$NaCoF_3$	Co / b/	$p_L \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (0,V,0)$
$NaNiF_3$	Ni /b /	$p_P \otimes P_{(111)}\, b^{(2x)} n^{(1)} m^{(2x)}$	$S(\frac{1}{2},0,0) = (U,0,W)$
Na_2NiFeF_3	Ni /c / Fe /d /	$p_L \otimes I_{(111)}\, m^{(1)} m^{(1)} 2^{(1)}$	$S(x,0,z) = (U_1,0,0)$ $S(0,y,z) = (U_2,0,0)$
NdAl	Nd_I /d / Nd_{II} /d /	$p_P \otimes P_{(1'11)}\, b^{(2x)} c^{(2x')} m^{(1)}$	$S(x_1,y_1,\frac{1}{4}) = (U,V,0)$ $S(x_2,y_2,\frac{1}{4}) = (U,V,0)$
$NdCrO_3$	Cr /b / Nd /c /	$p_P \otimes P_{(111)}\, b^{(1')} n^{(2x')} m^{(2x)}$	$S(\frac{1}{2},0,0) = (U,0,0)$ $T > T_t$ $S(\frac{1}{2},0,0) = (V,V,0)$ $T < T_t$ $S(x,y,\frac{1}{4}) = (0,0,W)$
$NdFeO_3$	Fe /b /	$p_L \otimes P_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$
$NdMnO_3$	Mn /b /	$p_L \otimes P_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,V,0)$
$NiCrO_3$	Ni /a /	$p_L \otimes C_{(111)}\, m^{(1)} c^{(1')} m^{(1')}$	$S(0,0,0) = (U,0,0)$
$Ni(IO_3)_2 \cdot 2D_2O$	Ni /a /	$p_S \otimes P_{(111)}\, b^{(2x')} c^{(2y')} a^{(2x)}$	$S(0,0,0) = (U,V,W)$

Table 2, cont.

$NiSO_4$	Ni /a /	$p_l \otimes C_{(1'1'1)}\, m^{(1)} c^{(1')} m^{(1')}$	$S(0,0,0) = (0,V,0)$
$PrCrO_3$	Cr /b / Pr /c /	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$\begin{cases} S(\frac{1}{2},0,0) = (U,0,0) \\ S(x,y,\frac{1}{4}) = (0,0,W) \end{cases}$
$PrFeO_3$	Fe /b / Pr /c /	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$\begin{cases} S(\frac{1}{2},0,0) = (U,0,0) \\ S(x,y,\frac{1}{4}) = (0,0,W) \end{cases}$
$PrMnO_3$	Mn /b /	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$	$S(\frac{1}{2},0,0) = (0,V,0)$
$SmCrO_3$	Cr /b /	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$ $p_l \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0) \quad T > T_t$ $S(\frac{1}{2},0,0) = (0,0,W) \quad T < T_t$
$SmFeO_3$	Fe /b /	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1)} n^{(1')} m^{(1')}$ $p_l \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0) \quad T > T_t$ $S(\frac{1}{2},0,0) = (0,0,W) \quad T < T_t$
$Sr_2Fe_2O_5$	Fe_I /a / Fe_{II} /b /	$p_l \otimes \mathcal{P}_{(111)}\, c^{(1)} m^{(1')} n^{(1')}$	$\begin{cases} S(0,0,0) = (0,0,W) \\ S(\frac{1}{2},0,0) = (0,0,W) \end{cases}$
TbAl	Tb_I/d / Tb_{II} /d /	$p_p \otimes \mathcal{P}_{(1'11)}\, b^{(2_x)} c^{(2_x')} m^{(1)}$	$\begin{cases} S(x_1,y_1,\frac{1}{4}) = (U,V,0) \\ S(x_2,y_2,\frac{1}{4}) = (U,V,0) \end{cases}$
$TbAlO_3$	Tb /c /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x')} n^{(2_x)} m^{(1)}$	$S(x,y,\frac{1}{4}) = (U,V,0)$
$TbCoO_3$	Co /b /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_x)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,V,0)$

Table 2, cont.

$TbCrO_3$	**Cr /b /** **Tb /c /**	$p_s \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_y')} m^{(2_z')}$	$\begin{cases} S(\frac{1}{2},0,0) = (0,0,W) \\ S(x,y,\frac{1}{4}) = (U,V,0) \quad T > T_t \end{cases}$
$TbFeO_3$	**Fe /b /** **Tb /c /**	$p_l \otimes \mathcal{P}_{(111)}\, b^{(1')} n^{(1)} m^{(1')}$ $p_s \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_y')} m^{(2_z')}$ $p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(2_x)} m^{(1)}$	$S(\frac{1}{2},0,0) = (U_1,0,0) \quad T > T_{N_2}$ $S(\frac{1}{2},0,0) = (0,0,W) \quad T < T_{N_2}$ $S(\frac{1}{2},0,0) = (U_2,0,0) \quad T < T_t$ $S(x,y,\frac{1}{4}) = (U_3,V_3,0) \quad T < T_{N_2}$ $S(x,y,\frac{1}{4}) = (U_4,V_4,0) \quad T < T_t$
TbGa	Tb /c /	$p_l \otimes C_{(111)}\, m^{(1)} c^{(1)} m^{(1)}$	$S(0,y,\frac{1}{4}) = (0,0,W)$
$TbVO_3$	V /b / **Tb /c /**	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_y)} n^{(2_y)} m^{(1)}$	$\begin{cases} S(\frac{1}{2},0,0) = (U,0,0) \\ S(x,y,\frac{1}{4}) = (V,V,0) \end{cases}$
TmAl	Tm_I /d / Tm_{II} /d /	$p_p \otimes \mathcal{P}_{(1'11)}\, b^{(2_x')} c^{(2_x)} m^{(1)}$	$\begin{cases} S(x_1,y_1,\frac{1}{4}) = (U,V,0) \\ S(x_2,y_2,\frac{1}{4}) = (U,V,0) \end{cases}$
$TmCrO_3$	Cr /b / Tm /c /	$p_p \otimes \mathcal{P}_{(111)}\, b^{(2_x)} n^{(1)} m^{(2_x)}$	$\begin{cases} S(\frac{1}{2},0,0) = (U,0,W) \quad T > T_t \\ S(\frac{1}{2},0,0) = (U_1,0,0) \quad T < T_t \\ S(x,y,\frac{1}{4}) = (0,0,W_1) \end{cases}$
TmNi	Tm /c /	$p_p \otimes \mathcal{P}_{(111)}\, n^{(2_x)} m^{(2_x)} a^{(1)}$	$S(x,\frac{1}{4},z) = (U,0,W)$

Table 2, cont.

$TmFeO_3$	Fe /b/	$\mathcal{P}_P \otimes \mathcal{P}_{(1111)} b^{(2_2)} n^{(1)} m^{(2_2)}$	$S(\frac{1}{2},0,0) = (U,0,W)$ $T > T_t$
		$\mathcal{P}_2 \otimes \mathcal{P}_{(1111)} b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (0,0,W_1)$ $T < T_t$
TmSi	Tm /c/	$\mathcal{P}_2 \otimes C_{(1111)} m^{(1)} c^{(1')} m^{(1)}$	$S(0,y,\frac{1}{4}) = (U,0,0)$
$YCrO_3$	Cr /b/	$\mathcal{P}_2 \otimes \mathcal{P}_{(1111)} b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$
$YFeO_3$	Fe /b/	$\mathcal{P}_2 \otimes \mathcal{P}_{(1111)} b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,0)$
$YbCrO_3$	Cr /b/	$\mathcal{P}_2 \otimes \mathcal{P}_{(1111)} b^{(1')} n^{(1)} m^{(1')}$	$S(\frac{1}{2},0,0) = (U,0,W)$
$YbFeO_3$	Fe /b/	$\mathcal{P}_2 \otimes \mathcal{P}_{(1111)} b^{(1')} n^{(1)} m^{(1')}$	$\left\{\begin{array}{l} S(\frac{1}{2},0,0) = (U,0,0) \quad T > T_t \\ S(\frac{1}{2},0,0) = (0,0,W) \quad T < T_t \end{array}\right.$

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