POSSIBLE NONCOLLINEAR MAGNETIC STRUCTURES ON $CaMnO_3$ AND $LaMnO_3$

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ABSTRACT

POSSIBLE NONCOLLINEAR MAGNETIC STRUCTURES ON $CAMNO_3$ AND $LAMNO_3$. $CaMnO_3$ and $LaMnO_3$ ceramics crystallize in the orthorhombic P*nma* and monoclinic P112$_1$/*a* space group, respectively. It has been reported that the ceramics order collinear antiferromagnetically below T=140K and 130K, respectively. The manganese magnetic atoms in $CaMnO_3$ are located in the 4(b) site, while those in $LaMnO_3$ are in 2(c) and 2(d). As the manganese atoms are neither located in the rotation axis or the mirror plane of the crystallographic symmetry, the noncollinear arrangements should not be excluded. This paper reports the derivation of the possible magnetic structures of $CaMnO_3$ and $LaMnO_3$. The derivation is based on the magnetic(Shubnikov) space group and the group theory. The result is that all of the possible models allow for three moment components in the noncollinear arrangements. The possible magnetic structures for $CaMnO_3$ are noncollinear antiferromagnetic, noncollinear ferromagnetic in the *a*-direction, noncollinear ferromagnetic in the *b*-direction, noncollinear ferromagnetic in the *c*-direction. The possible magnetic structures for $LaMnO_3$ are noncollinear ferromagnetic in the *c*-direction and in the *ab*-plane.

Key words : $CaMnO_3$, $LaMnO_3$, magnetic, structure, noncollinear, shubnikov, group theory

ABSTRAK

STRUKTUR MAGNETIK NONKOLINIER YANG MUNGKIN MUNCUL PADA $CaMnO_3$ AND $LaMnO_3$. $CaMnO_3$ and $LaMnO_3$ masing-masing mengkristal pada grup ruang P*nma* dan monoklinik P112$_1$/*a*. Telah dilaporkan bahwa momen magnetik keramik tersebut tersusun secara kolinier antiferomagnet masing-masing dibawah suhu 140 K dan 130 K. Atom mangan magnetik dalam $CaMnO_3$ terletak pada kedudukan simetri 4(b), sementara dalam $LaMnO_3$ pada kedudukan 2(c) dan 2(d). Karena atom mangan tersebut tidak terletak pada sumbu rotasi ataupun bidang cermin dari simetri kristalnya, susunan nonkolinear harus dipertimbangkan. Makalah ini melaporkan penurunan struktur magnetik yang mungkin muncul pada $CaMnO_3$ and $LaMnO_3$. Penurunannya dilakukan dengan menggunakan analisis grup ruang magnetik (*Shubnikov*) dan teori grup. Hasilnya adalah bahwa semua model yang mungkin mempunyai 3 komponen momen dengan susunan nonkolinear. Struktur magnetik yang mungkin muncul untuk $CaMnO_3$ adalah nonkolinier antiferomagnetik, nonkolinier feromagnetik pada arah sumbu-*a*, nonkolinier feromagnetik pada arah sumbu-*b*, nonkolinier feromagnetik pada arah sumbu-*c*. Struktur magnetik yang mungkin untuk $LaMnO_3$ adalah nonkolinier feromagnetik pada arah sumbu-*c* dan bidang *ab*.

Kata kunci : $CaMnO_3$, $LaMnO_3$, magnetik, struktur, nonkolinier, *shubnikov*, teori grup

INTRODUCTION

The manganese perovskite provide an ideal physical system for the elucidation of a variety of fundamental physical questions related with the magnetic, electronic and structural properties of condensed matter in a strongly-correlated electronic system. The most important topic to emerge from studies of manganites physics is the competition between localising and delocalising effects in close connection with lattice, spin and charge degrees of freedom.

The low temperature of magnetic structure of $CaMnO_3$ has been reported as G-type (+-+-) antiferromagnetic along the *z*-axis [1]. As manganese magnetic atoms are not in the symmetry positions, one might suspect that there might be non-zero components also along the *x*- and *y*-axis. For $LaMnO_3$, four distinct crystallographic phases have been identified, depending on the sample preparation [2], i.e., those crystallize in the orthorhombic P*nma*, orthorhombic P*nma* with smaller splitting, monoclinic P1121/*a* and rombohedral R3*c* space groups closely related to perovskite structure. The first has the stoichiometric composition $LaMnO_3$, while the rest are progresively richer in oxygen (and thus Mn^{4+}). No evidence of ordering of Mn^{3+} and Mn^{4+} was reported in the monoclinic phase.

The work details a derivation of possible magnetic configuration on the orthorhombic $CaMnO_3$

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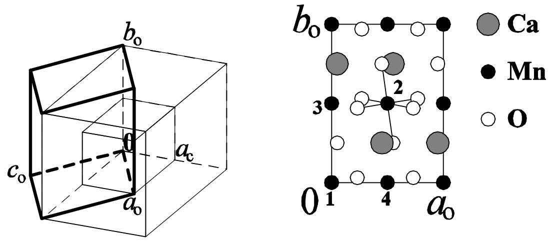
and the monoclinic $LaMnO_3$. The monoclinic phase of $LaMnO_3$ has been chosen due to new evidence [3].

$CaMnO_3$ CERAMICS

Crystallographic Structure



(a). Schematic (b). Projected

Figure 1. (a) Schematic unit cell (thicker lines) and (b) crystallographic structure projected onto a-b plane. In (a), the relation of the CaMnO3 unit cell to the cubic perovskite unit cell, with the lattice parameter ac, is shown. The CaMnO3 lattice parameters are ao, bo, co with the value of 2ac+ ; 2 ac+ ; 2ac- . In (b), the atom positions and the unit cell are drawn to scale, while the atomic radii are not.

The derivation of the possible magnetic structures starts from the crystallographic symmetry of the magnetic atoms. $CaMnO_3$ crystallizes [1] in the orthorhombic P*nma* space group with the equivalent positions at (*x*, *y*, *z*), (½-*x*, ½+*y*, ½+*z*), (*x*, ½-*y*, *z*), (½-*x*, -*y*, ½+*z*) and the corresponding atoms related through the inversion symmetry. The magnetic atoms of interest are Mn atoms at 4(b) site symmetry with the positions at (0, 0, ½), (½, ½, 0), (0, ½, ½), and (½, 0, 0) for Mn atom number 1, 2, 3 and 4, respectively. Figure 1 shows the schematic unit cell and the crystallographic structure of $CaMnO_3$ projected onto *a*-*b* plane.

Table 1 details the crystallographic symmetry notations [4, 5]. The location of each symmetry element in a unit cell is listed in Table 2. Table 2 details the atom permutation of the 4(b) site symmetry due to the symmetry application in P*nma* (D_{2h}^{16}). The symmetry elements in the first column are applied to the manganese atoms with in sequence 1, 2, 3 and 4. Clearly, there are only 2 symmetry elements, i.e.; h_1 and h_{25}, which leave the atom sequences unchanged. As the coordinate permutation also unchanged for both symmetry elements, the character of them are 12, each, i.e.; The character of the group is $\chi^{(q=0)}(h_1) = \chi^{(q=0)}(h_{25}) = 12$ and 0, otherwise. The character is of importance for the group theory to be discussed further.

Magnetic (Shubnikov) Space Group Analysis

For P*nma* space group, one can choose the symmetry element 1, m_1, m_2 and m_3 as generators to represent all crystallographic symmetries listed in Table 1. There is no need to consider the translation

Table 1. Crystallographic symmetry notations.

Kovalev [4]	IT [5]	IT [5]	Remark
h_1	(*x*,*y*,*z*)	1	Identity
h_2	(*x*,-*y*,-*z*)	4_1^2	180^0 rotation along *a*
h_3	(-*x*,*y*,-*z*)	4_2^2	180^0 rotation along *b*
h_4	(-*x*,-*y*,*z*)	4_3^2	180^0 rotation along *c*
h_{25}	(-*x*,-*y*,-*z*)	-1	Inverse
h_{26}	(-*x*,*y*,*z*)	m_1	Reflection ⊥ *a*
h_{27}	(*x*,-*y*,*z*)	m_2	Reflection ⊥ *b*
h_{28}	(*x*,*y*,-*z*)	m_3	Reflection ⊥ *c*

Table 2. Atom permutation of the 4(b) site symmetry due to the symmetry application in Pnma (D_{2h}^{16}).

Element	Mn atom number			
h_1|0 0 0	1	2	3	4
h_2|½ ½ ½	2	1(-100)	4	3(-100)
h_3|0 ½ 0	3	4(1-10)	1(0-10)	2(100)
h_4|½ 0 ½	4(00-1)	3(01-1)	2(010)	1
h_{25}|0 0 0	1(001)	2	3(001)	4
h_{26}|½ ½ ½	2(00-1)	1(0-10)	4(0-1-1)	3
h_{27}|0 ½ 0	3(001)	4(101)	1	2(100)
h_{28}|½ 0 ½	4	3(-100)	2	1(-100)

vectors rising from the glide, the screw or the symmetry element position as the magnetic wave propagation vector is zero. Numbers in the parenthesis listed in Table 2 can then be ignored. One notes that as the magnetic moment is an axial vector, the application of the mirror symmetry would result a direction reversal as compared to that of the polar vector.

To provide an exhaustive list of possible magnetic structures, one can apply the time-reversal symmetry on the generators, as well as the crystallographic symmetries. Applying the time-reversal symmetry reverses the direction of the magnetic moment, which is basically the axial vector.

Table 3 shows μ_1, μ_2, and μ_4 configurations but not μ_3. In order to realize μ_3, one can use Eq. (1) and the coordinate effect due to the symmetry operation m_1 or m_1' shown in Table 4. Eq. (1) relates μ_3 to μ_4, which means that one can obtain μ_3 from μ_4. One must take into account that the symmetry m_1 reverses the direction of the *y*- and *z*-components. The symmetry m_1' reverses the direction of the *x*-component. One could equally use Eq. (2) and (3) to realize μ_3 in the magnetic configuration. For example, if one uses Eq. (2), μ_3 can be obtained in relation with μ_1. The corresponding symmetries are m_2 and m_2'. The former reverses the direction of the x- and z-components, while the latter reverses the direction of the y-components.

Using the result shown in Table 3, one proceeds further neglecting the configurations with zero moments. For example, the configuration with generator $m_1 m_2 m_3$, results not only the configuration listed in Table 3, but also results the configuration with all possible moments

Table 3. Possible moment configurations with prime in generators indicating the time reversal symmetry

Generators	Resulted Moment	Remark
$m_1\, m_2\, m_3$	$\mu_{1x} = \mu_{2x} = -\mu_{4x} = \mu_{1x}$ $\mu_{1y} = -\mu_{2y} = -\mu_{4y} = \mu_{1y}$ $\mu_{1z} = -\mu_{2z} = \mu_{4z} = \mu_{1z}$	Anti ferro
$m_1\, m_2\, m_3'$	$\mu_{1x} = \mu_{2x} = -\mu_{4x} = -\mu_{1x}$ $\mu_{1y} = -\mu_{2y} = -\mu_{4y} = -\mu_{1y}$ $\mu_{1z} = -\mu_{2z} = \mu_{4z} = -\mu_{1z}$	Zero moment
$m_1\, m_2'\, m_3'$	$\mu_{1x} = \mu_{2x} = \mu_{4x} = \mu_{1x}$ $\mu_{1y} = -\mu_{2y} = \mu_{4y} = \mu_{1y}$ $\mu_{1z} = -\mu_{2z} = -\mu_{4z} = \mu_{1z}$	Ferro Along *a*-axis
$m_1'\, m_2'\, m_3'$	$\mu_{1x} = -\mu_{2x} = -\mu_{4x} = -\mu_{1x}$ $\mu_{1y} = \mu_{2y} = -\mu_{4y} = -\mu_{1y}$ $\mu_{1z} = \mu_{2z} = \mu_{4z} = -\mu_{1z}$	Zero moment
$m_1'\, m_2\, m_3'$	$\mu_{1x} = -\mu_{2x} = \mu_{4x} = \mu_{1x}$ $\mu_{1y} = \mu_{2y} = \mu_{4y} = \mu_{1y}$ $\mu_{1z} = \mu_{2z} = -\mu_{4z} = \mu_{1z}$	Ferro Along *b*-axis
$m_1'\, m_2'\, m_3$	$\mu_{1x} = -\mu_{2x} = -\mu_{4x} = \mu_{1x}$ $\mu_{1y} = \mu_{2y} = -\mu_{4y} = \mu_{1y}$ $\mu_{1z} = \mu_{2z} = \mu_{4z} = \mu_{1z}$	Ferro Along *c*-axis
$m_1\, m_2'\, m_3$	$\mu_{1x} = \mu_{2x} = \mu_{4x} = -\mu_{1x}$ $\mu_{1y} = -\mu_{2y} = \mu_{4y} = -\mu_{1y}$ $\mu_{1z} = -\mu_{2z} = -\mu_{4z} = -\mu_{1z}$	Zero moment
$m_1'\, m_2\, m_3$	$\mu_{1x} = -\mu_{2x} = \mu_{4x} = -\mu_{1x}$ $\mu_{1y} = \mu_{2y} = \mu_{4y} = -\mu_{1y}$ $\mu_{1z} = \mu_{2z} = -\mu_{4z} = -\mu_{1z}$	Zero moment

in the left side of the configuration equation. With 4 atoms and 3 Cartesian components, there are 12 rows of the equations with 3 rows have already been listed in Table 3. Since there are 4 configurations with non zero moments, one needs to write down 48 rows of equations altogether.

To write concisely, one can separate the matrices belonging to the atom effect and the coordinate effect. As m_1 symmetry element interchanges atom 1 to 2 (and 3 to 4), one can write the matrix $P(m_1)$ belonging to m_1 as:

$$P(m_1) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \text{............................} \quad (1)$$

As m_2 symmetry element interchanges atom 1 to 3 (and 2 to 4), one can write the matrix $P(m_2)$ belonging to m_2 as:

$$P(m_2) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \text{............................} \quad (2)$$

As m_3 symmetry element interchanges atom 1 to 4 (and 2 to 3), one can write the matrix $P(m_3)$ belonging to m_3 as:

$$P(m_3) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \text{..............................} \quad (3)$$

Eqs. (1), (2), and (3) remain the same, independent of whether the time reversal symmetry is applied or not. One notes that these equations summarized the last three rows listed in Table 2.

Table 4 details the coordinate effects due to the generators listed in Table 3. The effect on the identity symmetry is also listed to provide a reference. The time reversal symmetry is indicated by the prime following the mirror symmetry, with the effect of reversing the direction of the previously mirrored moments.

Table 4. Coordinate effects due to generators listed in Table 3.

No	Structure	Coordinate Effect
1	Anti Ferro	1: (u, v, w) m_1: $(u, -v, -w)$ m_2: $(-u, v, -w)$ m_3: $(-u, -v, w)$
2	Ferro Along *a*-axis	1: (u, v, w) m_1: $(u, -v, -w)$ m_2': $(u, -v, w)$ m_3': $(u, v, -w)$
3	Ferro Along *b*-axis	1: (u, v, w) m_1': $(-u, v, w)$ m_2: $(-u, v, -w)$ m_3': $(u, v, -w)$
4	Ferro Along *c*-axis	1: (u, v, w) m_1': $(-u, v, w)$ m_2': $(u, -v, w)$ m_3: $(-u, -v, w)$

Figure 2 illustrates possible magnetic structures of CaMnO$_3$ based on the magnetic (*Shubnikov*) space group analysis. Similar structures are also obtained from the group theory as explained in the next section.

Group Theory

In order to apply group theory to generate all possible magnetic structures, one must have the irreducible representations associated with the site symmetry in the crystallographic space group. One could derive the irreducible representations or simply get them from the table listed elsewhere [4].

In order to obtain the irreducible representation, one can choose to use the table listed elsewhere [4]. With the knowledge that the space group is P*nma* with the magnetic propagation vector q=0, the procedure is as follow:

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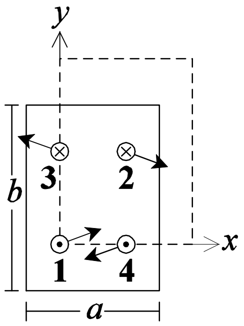
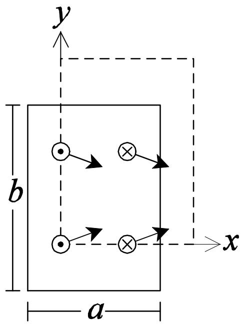
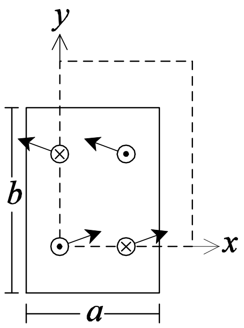


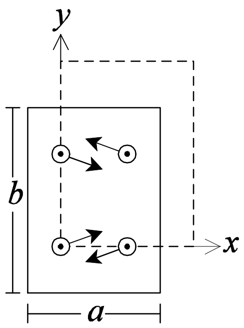
(a). P n m a



(b). P n m' a'



(a). P n' m a'



(b). P n' m' a

Figure 2. Possible magnetic structures of $CaMnO_3$ based on the magnetic (Shubnikov) space group analysis. Similar structures are also obtained from the group theory as explained in the next section. In (a), numbers indicate the sequence number of the magnetic atoms with the z-component of ½, 0, ½, 0, respectively.

1. The space group D_{2h}^{16}, which is equivalent to P*nma*, with the space group number 62, is listed on page 78. For q=0, identified as k_{19}, the corresponding notation is k19-32. This indicates that the corresponding Loaded Irreducible Representations (LIR's) are listed in Table T32.
2. Based on LIR index from C system listed on page 387, it is known that Table T32 is on page 231.
3. The content of Table T32 is shown in Table 3.
4. Table 3 shows that there are 8 1-D real irreducible representations.

Table 5. Irreducible representations for D2h16 with the magnetic propagation vector q=0, with components in h1 and 1 are all 1's.

T32	h_2	h_3	h_4	h_{25}	h_{26}	h_{27}	h_{28}
τ_2	1	1	1	-1	-1	-1	-1
τ_3	1	-1	-1	1	1	-1	-1
τ_5	-1	1	-1	1	-1	1	-1
τ_7	-1	-1	1	1	-1	-1	1
$\tau_4=\tau_3\times\tau_2$							
$\tau_6=\tau_5\times\tau_2$							
$\tau_8=\tau_7\times\tau_2$							

The multiplicity of each irreducible representation in the full representation is:

$$a^{(\nu)} = \frac{1}{g}\sum_j g_j \chi_j^{(\nu)} \chi_j \quad \ldots\ldots (4)$$

$$a^{(1)} = a^{(3)} = a^{(5)} = a^{(7)} = \frac{1}{8}(1\cdot 12 + 1\cdot 12) = 3 \quad \ldots. (5)$$

$$a^{(2)} = a^{(4)} = a^{(6)} = a^{(8)} = \frac{1}{8}(1\cdot 12 - 1\cdot 12) = 0 \quad \ldots. (6)$$

The full (reducible) representation can then be expressed in terms of the irreducible representations, i.e.;

$$\Gamma = 3\left(\Gamma^{(1)} + \Gamma^{(3)} + \Gamma^{(5)} + \Gamma^{(7)}\right) \quad \ldots\ldots (7)$$

The projection operator for particular **q** is

$$P_{rc}^{(\nu)} = \frac{n^{(\nu)}}{g}\sum_S \left(\tau_{rc}^{(\nu)}(S)\right)^* O(S) \quad \ldots\ldots (8)$$

The application of the projection operator, which should be consistent with the multiplicity calculation, results:

$$\begin{aligned}
4P^{(1)}\mu_{1x} &= \mu_{1x} + \mu_{2x} - \mu_{3x} - \mu_{4x}\\
4P^{(1)}\mu_{1y} &= \mu_{1y} - \mu_{2y} + \mu_{3y} - \mu_{4y} \quad \ldots\ldots (9)\\
4P^{(1)}\mu_{1z} &= \mu_{1z} - \mu_{2z} - \mu_{3z} + \mu_{4z}
\end{aligned}$$

$$\begin{aligned}
4P^{(3)}\mu_{1x} &= \mu_{1x} + \mu_{2x} + \mu_{3x} + \mu_{4x}\\
4P^{(3)}\mu_{1y} &= \mu_{1y} - \mu_{2y} - \mu_{3y} + \mu_{4y} \quad \ldots\ldots (10)\\
4P^{(3)}\mu_{1z} &= \mu_{1z} - \mu_{2z} + \mu_{3z} - \mu_{4z}
\end{aligned}$$

$$\begin{aligned}
4P^{(5)}\mu_{1x} &= \mu_{1x} - \mu_{2x} - \mu_{3x} + \mu_{4x}\\
4P^{(5)}\mu_{1y} &= \mu_{1y} + \mu_{2y} + \mu_{3y} + \mu_{4y} \quad \ldots\ldots (11)\\
4P^{(5)}\mu_{1z} &= \mu_{1z} + \mu_{2z} - \mu_{3z} - \mu_{4z}
\end{aligned}$$

$$\begin{aligned}
4P^{(7)}\mu_{1x} &= \mu_{1x} - \mu_{2x} + \mu_{3x} - \mu_{4x}\\
4P^{(7)}\mu_{1y} &= \mu_{1y} + \mu_{2y} - \mu_{3y} - \mu_{4y} \quad \ldots\ldots (12)\\
4P^{(7)}\mu_{1z} &= \mu_{1z} + \mu_{2z} + \mu_{3z} + \mu_{4z}
\end{aligned}$$

Table 6 shows the magnetic structure basis resulted from the projection operator application with the manganese sequence according to manganese atoms shown in Figure 1. One observes that, based on the projection operation, the irreducible representations number 2, 4, 6, and 8, project to zero moments. This is consistent with the multiplicity calculation. The irreducible representations number 1, 3, 5 and 7 exist in the representation and based on the multiplicity calculation, each must have the multiplicity of 3.

Table 6. Magnetic structure basis with the manganese sequence according to manganese atoms shown in Figure 1.

	Mn_1	Mn_2	Mn_3	Mn_4	Remark	
1	100	100	-100	-100	C_x	Anti
	010	0-10	010	0-10	G_y	Ferro
	001	00-1	00-1	001	A_z	
3	100	100	100	100	F_x	Ferro
	010	0-10	0-10	010	A_y	Along
	001	00-1	001	00-1	G_z	*a*-axis
5	100	-100	-100	100	A_x	Ferro
	010	010	010	010	F_y	Along
	001	001	00-1	00-1	C_z	*b*-axis
7	100	-100	100	-100	G_x	Ferro
	010	010	0-10	0-10	C_y	Along
	001	001	001	001	F_z	*c*-axis

$LaMnO_3$ CERAMICS

Crystallographic Structure

$LaMnO_3$ crystallizes [2] in several crystallographic structures depending on the sample preparations. In this work, the author chose $LaMnO_3$ crystallizing in the monoclinic $P112_1/a$ space group, No. 14[5] with the equivalent positions at 4e site symmetry: (x, y, z), (½-x, -y, ½+z) and the corresponding atoms related through the inversion symmetry. The magnetic atoms of interest are Mn atoms at 2c(½, 0, 0) and 2d(½,½, 0) site symmetry. All manganese atoms are then similar to those of $CaMnO_3$, i.e.; at (0, 0, ½), (½, ½, 0), (0, ½, ½), and (½, 0, 0) for Mn atom number 1, 2, 3 and 4, respectively. An important difference is that the symmetry only relates manganese atom number 1 and 4 (similarly 2 and 3). The existing generator is only m_3, while the others are broken. The schematic unit cell and the crystallographic structure of $LaMnO_3$ projected onto a-b plane are similar to those of $CaMnO_3$, but with a slight distortion.

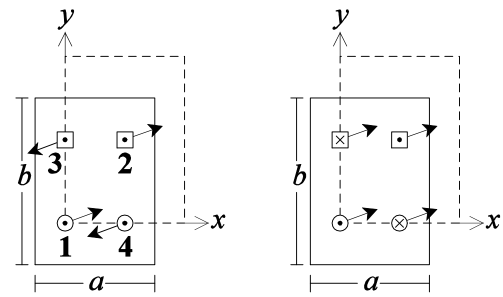
Table 7. Atom permutation of the 2(c) site symmetry due to the symmetry application in $P112_1/a$ (C_{2h}^5).

Element	Mn atom number	
h_1|0 0 0	1	4
h_4|½ 0 ½	4(00-1)	1
h_{25}|0 0 0	1(001)	4
h_{28}|½ 0 ½	4	1(-100)

Table 7 details the atom permutation of in the 2(c) site symmetry due to the symmetry application in $P112_1/a$. The symmetry elements in the first column are applied to the manganese atoms with in sequence 1, 2, 3 and 4. Clearly, there are only 2 symmetry elements, i.e.; h_1 and h_{25}, which leave the atom sequences unchanged. As the coordinate permutation also unchanged for both symmetry elements, the character of them are 6, each, i.e.; $\chi^{(q=0)}(h_1) = \chi^{(q=0)}(h_{25}) = 6$ and 0, otherwise. The character is of importance for the group theory to be discussed further.

Magnetic (Shubnikov) Space Group Analysis

The derivation of the possible magnetic structures for $LaMnO_3$ is greatly simplified by the fact that the crystallographic structure is closely related to that of $CaMnO_3$ and the symmetry breaking which leave atoms 1, 4 uncoupled with 2, 3. Figure 3 details the possible magnetic structure of LaMnO3, with a caution that there is no coupling between atom 1, 4 with 2, 3. The existing coupling allowed by the crystallographic symmetry only relates atom 1 with atom 4 (similarly, atom 2 with atom 3). This situation is carefully depicted in Figure 3 such that the coupling only exists between atoms indicated by similar legend (either open-circle of open-square).



(a). a (b). a'

Figure 3. Possible magnetic structures of $LaMnO_3$ based on the magnetic (Shubnikov) space group analysis. Similar structures are also obtained from the group theory as explained in the next section. The coupling only exists between atoms indicated by similar legend (either open-circle of open-square).

Group Theory

Procedures to obtain the irreducible representations are as follow:

1. The space group C_{2h}^5, which is equivalent to $P2_1/b$, with the space group number 14, is listed on page 56. For q=0, identified as k_7, the corresponding notation is $k7$, $k13$-4. This indicates that the corresponding Loaded Irreducible Representations (LIR's) are listed in Table T4.

Table 8. Irreducible representations for D2h16 with the magnetic propagation vector q=0, with components in h1 and 1 are all 1's.

T4	h_1	h_4	h_{25}	h_{28}
τ_1	1	1	1	1
τ_2	1	1	-1	-1
τ_3	1	-1	1	-1
τ_4	1	-1	-1	1

Table 9. Magnetic structure basis with the manganese sequence according to manganese atoms shown in Figure 1. Similar basis apply for Mn4 and Mn1, respectively

	Mn_2	Mn_3	Remark
1	100	-100	Ferromagnetic in c-direction
	010	0-10	
	001	001	
3	100	100	Ferromagnetic in ab-plane

2. Based on LIR index of simple groups (C system) listed on page 387, it is known that Table T4 is on page 229.
3. The content of Table T4 is shown in Table 8, which is in agreement as that of Basirep [6].
4. Table 8 shows that there are 4 1-D real irreducible representations.

CONCLUSION

The possible magnetic structures for $CaMnO_3$ crystallizing in the P*nma* space group are noncollinear antiferromagnetic, noncollinear ferromagnetic in the *a*-direction, noncollinear ferromagnetic in the *b*-direction, noncollinear ferromagnetic in the *c*-direction. The possible magnetic structures for $LaMnO_3$ crystallizing in the $P112_1/a$ space group are noncollinear ferromagnetic in the *c*-direction and in the *ab*-plane. All noncollinear configurations exist due to the fact that the magnetic atoms are not located in any crystallographic symmetry elements.

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