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HEXAGONAL PEROVSKITES.

II. Praphase, Structural and Magnetic Phase Transition

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INTRODUCTION

The symmetry analysis of hexagonal perovskites $ReMnO_3$ (Re: Er, Ho, Lu, Sc, Tm, Y) made on the basis of the paramagnetic group $C_{6v}^3 \cdot 1$ [1] has shown that the simultaneous appearance of S_{xy} and S_z -components should be described by two irreducible representations of space group (IRS) C_{6v}^3 of the star $\{\vec{k}_{11}\}$ (notation according to the Tables [2]) which for the magnetic-structure model proposed by experimentalists [3-7] are not attendant [8] and belong to different exchange multiplets [9].

A detailed analysis of the structure C_{6v}^3 of compounds $ReMnO_3$ allowed us in part 1 of this work to propose the existence of the praphase D_{6h}^4 which is an initial phase for the structure phase transition $D_{6h}^4 \rightarrow C_{6v}^3$ with wave vector $k \neq 0$ and for the magnetic transition.

Based on the symmetry group of praphase D_{6h}^4 , we have shown in part 2 that the magnetic structure observed in $ReMnO_3$ is described by two stars: the component along the z-axis is described by the star $\vec{k} = 0, \{\vec{k}_{16}\}$, while the component in the basis plane, like the structure phase transition, is described by the star $\{\vec{k}_{13}\}$. The magnetic moments in the basis plane appear because of the displacement of Mn atoms in the transition $D_{6h}^4 \rightarrow C_{6v}^3$. Thus, supposing the praphase to exist in the compounds $ReMnO_3$ we could more exactly define the structure of hexagonal perovskites preceding the magnetic transition and describe the reason for which such a complicated magnetic structure is realized. In the course of analysis of the structure and magnetic phase transitions we have formulated several criteria which may be checked experimentally.

1. THE CHOICE OF PRAPHASE; STRUCTURE TRANSITION

From the results obtained in experimental investigations [3-7] it is found that near the point of magnetic transition these compounds form the structure of perovskites with the hexagonal symmetry of the group C_{6v}^3 . Atoms of Re are in positions (2a) and (4b), atoms of Mn in position (6c); oxygen atoms O_I , in (2a); O_{II} , in (4b); O_{III} ,in (6c); O_{IV},in (6c), where:

(2a): $1(0,0, z)$; $2(0, 0, z + \frac{1}{2})$

$$(4b): \quad 1(\tfrac{1}{3}, \tfrac{2}{3}, z); \; 2(\tfrac{2}{3}, \tfrac{1}{3}, z); \; 3(\tfrac{1}{3}, \tfrac{2}{3}, \tfrac{1}{2}+z); \; 4(\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{2}+z), \quad (1.1)$$

$$(6c): \quad 1(x,0,z); \; 2(0,x,z); \; 3(\bar{x}\bar{x},z); \; 4(\bar{x},0,\tfrac{1}{2}+z); \; 5(0,\bar{x},\tfrac{1}{2}+z); \; 6(x,x,\tfrac{1}{2}+z).$$

Running parameters are not determined exactly, but for the atom of Mn in all compounds of the family it is indicated that x is almost equal to 1/3. For the case of $LuMnO_3$ it is approximately found that [3,4]:

$$Lu_I \;(4b): \quad z = 0.27, \quad Lu_{II} \;(2a): \quad z = 0.23,$$

$$Mn \;\;(6c): \quad x = \tfrac{1}{3}, \quad z = 0,$$

$$O_I \;\;(2a): \quad z \simeq \tfrac{1}{2}; \quad O_{II} \;(4b): \quad z \simeq 0,$$

$$(1.2)$$

$$O_{III} \;(6c): \quad x \simeq \tfrac{1}{6}, \quad z \simeq \tfrac{1}{6},$$

$$O_{IV} \;(6c): \quad x \simeq \tfrac{2}{3}, \quad z \simeq \tfrac{1}{3}.$$

These structure experimental data on the position of atoms in $LuMnO_3$ allow an idealized version of the structure of this compound. For this purpose we put z for atoms Lu_I (2a) and Lu_{II} (4b) to equal 0.25. Parameters x and z for atoms Mn and O will be chosen as defined in ref.[3] but taken to have exact values instead of approximate ones. The idealized structure, we shall call the praphase, is shown in Fig.1.

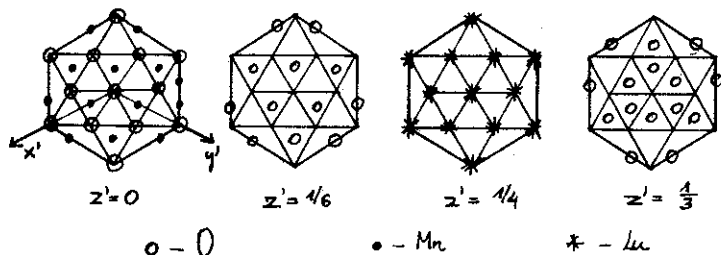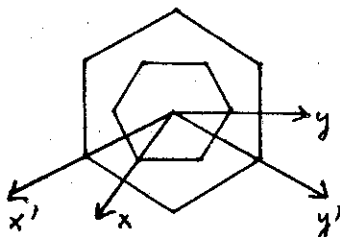Fig.1. The idealized structure of the $LuMnO_3$ in the coordinate system connected with a primitive cell of the C_{6v}^3 group. The next four layers with $z'=1/2$, $z' = 2/3$, $z'=3/4$, $z'=5/6$ are turned with respect to first four layers by 60°.

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Fig.2. The imbedding of elementary cells of praphase G and phase C_{6v}^3 for the idealized structure of hexagonal perovskites.

$$z' = z - \frac{1}{4}$$

Let us now define the group of symmetry of the praphase of LuMnO$_3$. We assume that the structure C_{6v}^3 is a result of a phase transition of the type of displacement from the praphase whose symmetry is described by the group G. In this case we consider that the crystal atom displacements are small ($u_i \ll a$, where a is a lattice parameter). Hence it follows that the group G should be a supergroup of group C_{6v}^3.

In considering all supergroups G of group C_{6v}^3 we can very reduce the list of supergroups if we establish the channel of transition[10-13] from the praphase to phase C_{6v}^3. In other words, we should first define the lattice type of the praphase, the star of the wave vector and the set of its arms describing the transition $G \rightarrow C_{6v}^3$.

From Fig.1 it is seen that the idealized structure LuMnO$_3$ has the hexagonal lattice Γ_h of axis x, y which make the angle 30^0 with x', y', respectively, of lattice Γ_h of structure C_{6v}^3. The imbedding of elementary cells of praphase G and phase C_{6v}^3 is drawn in Fig.2.

From tables of possible changes of the transition symmetry of crystals in phase transitions (see[10,12]and[14])we find that such an imbedding of elementary cells of highly and low symmetric phases is achieved in the transition along the arms $\vec{k}_1 = 1/3(\vec{b}_1 + \vec{b}_2)$ and $\vec{k}_2 = -\vec{k}_1$ of the star $\{k_{13}\}$ of lattice Γ_h (channel 4 according to tables).

To define the group of symmetry G of the praphase, we utilize tables of subgroups with $\vec{k} \neq 0$ of space groups[14]. These tables, for each space group of the hexagonal system, contain all subgroups with increasing cell ($\vec{k} \neq 0$); for each transition channel there is given the corresponding list of subgroups. The group C_{6v}^3 is a subgroup of the praphase symmetry group G and should be contained in the channel 4 of lattice Γ_h. From tables[14] it follows that only the group D_{6h}^4 has the subgroup C_{6v}^3 in channel 4.

So, the praphase in compounds ReMnO$_3$ has symmetry D_{6h}^4. Atoms of Re take the position (2a); atoms of Mn. (2c); atoms

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of O_I ,(2b); and O_{II}(4f) with $z=1/12$. The atoms coordinates are:

Re (2a): $1(0, 0, 0)$; $2(0, 0, \frac{1}{2})$

Mn (2c): $1(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$; $2(\frac{2}{3}, \frac{1}{3}, \frac{3}{4})$

O_I (2b): $1(0, 0, \frac{1}{4})$; $2(0, 0, \frac{3}{4})$ $\qquad\qquad$ (1.3)

O_{II} (4f): $\Lambda(\frac{1}{3}, \frac{2}{3}, z)$; $2(\frac{2}{3}, \frac{1}{3}, z)$; $3(\frac{2}{3}, \frac{1}{3}, \frac{1}{2}+z)$; $4(\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z)$;

$\qquad z = \frac{1}{12}$.

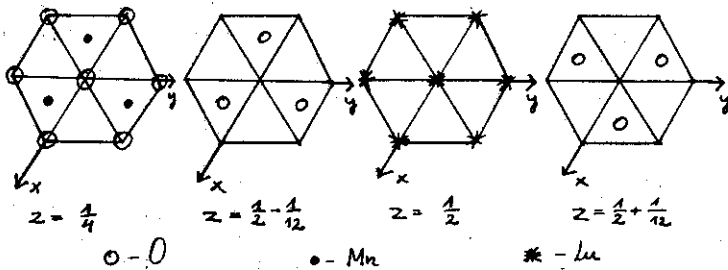The elementary cell of the praphase with positions (1.3) is shown in Fig.3.

Fig.3. D_{6h}^{4} elementary cell with positions of atoms: Re $-*$, Mn $-\bullet$, O $- \circ$. The remaining 4 layers $z=3/4$, $z=0$, $z=1/12$, $z=-1/12$ are turned with respect to the drawn ones at $60°$.

Comparing Figs.1 and 3 we see that the symmetry and coordinates of atoms in the praphase D_{6h}^{4} , are defined correctly. The praphase D_{6h}^{4} was observed at high temperature for $YMnO_3$ [16]. Supposing the praphase to exist in $ReMnO_3$ we can obtain an information on the structure in the C_{6v}^{3} phase much larger than from the analysis of experimental data [3-7]. We determine now possible displacements of atoms in $ReMnO_3$ in the transition $D_{6h}^{4} \rightarrow C_{6v}^{3}$ with the star $\{\vec{k}_{13}\}$.Using standard formulae [11,12] we evaluate the mechanical representation and modes of displacement of atoms. The mechanical representation has the form:

2a: $d_m^{\vec{k}_{13}} = \tau_3 \oplus \tau_4 \oplus \tau_5 \oplus \tau_6$

2b: $d_m^{\vec{k}_{13}} = \tau_2 \oplus \tau_4 \oplus 2\tau_5$

2c: $d_m^{\vec{k}_{13}} = \tau_1 \oplus \tau_3 \oplus \tau_5 \oplus \tau_6$, $\qquad\qquad$ (1.4)

4f: $d_m^{\vec{k}_{13}} = \tau_1 \oplus \tau_2 \oplus \tau_3 \oplus \tau_4 \oplus 2\tau_5 \oplus 2\tau_6$.

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The modes of displacements of atoms are listed in Table 1.

To find the displacements of atoms in the transition $D_{6h}^4 \rightarrow C_{6v}^3$ we should define the representation of this transition. For this purpose we shall determine the restriction of group D_{6h}^4 on subgroup C_{6v}^3. From Kovalev [2] we write out all elements of the zero block of group D_{6h}^4 :

$$(h_1|0),\ (h_2|\tau),\ (h_3|0),\ (h_4|\tau),\ (h_5|0),\ (h_6|\tau),$$

$$(h_7|0),\ (h_8|\tau),\ (h_9|0),\ (h_{10}|\tau),\ (h_{11}|0),\ (h_{12}|\tau), \qquad (1.5)$$

$$(h_{13}|0),\ (h_{14}|\tau),\ (h_{15}|0),\ (h_{16}|\tau),\ (h_{17}|0),\ (h_{18}|\tau),$$

$$(h_{19}|0),\ (h_{20}|\tau),\ (h_{21}|0),\ (h_{22}|\tau),\ (h_{23}|0),\ (h_{24}|\tau),$$

and of group C_{6v}^3 :

$$(h_1|0),\ (h_2|\tau),\ (h_3|0),\ (h_4|\tau),\ (h_5|0),\ (h_6|\tau),$$

$$(h_{19}|\tau),\ (h_{20}|0),\ (h_{21}|\tau),\ (h_{22}|0),\ (h_{23}|\tau),\ (h_{24}|0). \qquad (1.6)$$

Table 1

The modes of displacements of atoms in ReMnO$_3$ transition $D_{6h}^4 \rightarrow C_{6v}^3$ with the star $\{\vec{k}_{13}\}$ $\lambda \cdot \epsilon = e^{i\frac{2\pi}{3}}$

Represen- tation	Arm	Position (2a)					
		0 cell		$+\vec{a}_1, +\vec{a}_2, -(\vec{a}_1+\vec{a}_2)$		$-\vec{a}_1, -\vec{a}_2, +(\vec{a}_1+\vec{a}_2)$	
		1	2	1	2	1	2
T_3	K_1	001	001	00ε	$00\bar{\varepsilon}$	$00\varepsilon^2$	$00\bar{\varepsilon}^2$
	K_2	001	$00\bar{1}$	$00\varepsilon^2$	$00\bar{\varepsilon}^2$	00ε	$00\bar{\varepsilon}$
T_4	K_1	001	001	00ε	00ε	$00\varepsilon^2$	$00\varepsilon^2$
	K_2	$00\bar{1}$	$00\bar{1}$	$00\bar{\varepsilon}^2$	$00\bar{\varepsilon}^2$	$00\bar{\varepsilon}$	$00\bar{\varepsilon}$
T_5	K_1	$\bar{\varepsilon}^2\bar{\varepsilon}0$	$\bar{\varepsilon}^2\varepsilon0$	$\bar{1}\varepsilon^20$	$\bar{1}\varepsilon^20$	$\bar{\varepsilon}10$	$\bar{\varepsilon}10$
	K_2	$\varepsilon\bar{\varepsilon}0$	$\varepsilon\bar{\varepsilon}0$	$\varepsilon\bar{1}0$	$\varepsilon\bar{1}0$	$1\bar{\varepsilon}^20$	$1\bar{\varepsilon}^20$
	K_1	$\varepsilon^2\bar{1}0$	$\varepsilon^2\bar{1}0$	$1\bar{\varepsilon}0$	$1\bar{\varepsilon}0$	$\varepsilon\bar{\varepsilon}^20$	$\varepsilon\bar{\varepsilon}^20$
	K_2	$\bar{\varepsilon}^210$	ε^210	$\bar{\varepsilon}\varepsilon^20$	$\bar{\varepsilon}\varepsilon^20$	$\bar{1}\varepsilon0$	$\bar{1}\varepsilon0$
T_6	K_1	$\bar{\varepsilon}^2\varepsilon0$	$\varepsilon^2\bar{\varepsilon}0$	$\bar{1}\varepsilon^20$	$1\bar{\varepsilon}^20$	$\bar{\varepsilon}10$	$\varepsilon\bar{1}0$
	K_2	$\varepsilon^2\bar{\varepsilon}0$	$\varepsilon^2\varepsilon0$	$\varepsilon\bar{1}0$	$\bar{\varepsilon}10$	$1\bar{\varepsilon}^20$	$\bar{1}\varepsilon^20$
	K_1	$\bar{\varepsilon}^2\bar{1}0$	$\bar{\varepsilon}^210$	$1\bar{\varepsilon}0$	$\bar{1}\varepsilon0$	$\varepsilon\bar{\varepsilon}^20$	$\bar{\varepsilon}\varepsilon^20$
	K_2	$\bar{\varepsilon}^210$	$\varepsilon^2\bar{1}0$	$\bar{\varepsilon}\varepsilon^20$	$\varepsilon\bar{\varepsilon}^20$	$\bar{1}\varepsilon0$	$1\bar{\varepsilon}0$

Representation	Arm	Position (2b)					
		0 cell		$+\bar{\alpha}_1,+\bar{\alpha}_2,-(\bar{\alpha}_1+\bar{\alpha}_2)$		$-\bar{\alpha}_1,-\bar{\alpha}_2,+(\alpha_1+\alpha_2)$	
		1	2	1	2	1	2
τ_2	K_1	001	$00\bar{1}$	00ε	$00\bar{\varepsilon}$	$00\varepsilon^2$	$00\bar{\varepsilon}^2$
	K_2	001	$00\bar{1}$	$00\bar{\varepsilon}^2$	$00\bar{\varepsilon}^2$	00ε	$00\bar{\varepsilon}$
τ_4	K_1	001	001	00ε	00ε	$00\varepsilon^2$	$00\varepsilon^2$
	K_2	$00\bar{1}$	$00\bar{1}$	$00\bar{\varepsilon}^2$	$00\bar{\varepsilon}^2$	$00\bar{\varepsilon}$	$00\bar{\varepsilon}$
τ_5	K_{11}	$\bar{\varepsilon}^2\varepsilon 0$	000	$\bar{1}\varepsilon 0$	000	$\bar{\varepsilon}10$	000
	K_2	000	$\varepsilon^2\bar{\varepsilon}0$	000	$\varepsilon\bar{1}0$	000	$1\bar{\varepsilon}0$
	K_1	000	$\varepsilon^2\bar{1}0$	000	$1\bar{\varepsilon}0$	000	$\varepsilon\bar{\varepsilon}^20$
	K_2	$\hat{\varepsilon}^210$	000	$\bar{\varepsilon}\varepsilon^20$	000	$\bar{1}\varepsilon 0$	000
τ_5'	K_1	000	$\bar{1}\varepsilon^20$	000	$\bar{\varepsilon}10$	$\bar{\varepsilon}^2\varepsilon 0$	000
	K_2	$1\bar{\varepsilon}^20$	000	$\varepsilon^2\bar{\varepsilon}0$	000	$\varepsilon\bar{1}0$	000
	K_1	$1\bar{\varepsilon}0$	000	$\varepsilon\bar{1}0$	000	$\varepsilon^2\bar{1}0$	000
	K_2	000	$\bar{1}\varepsilon 0$	000	$\bar{\varepsilon}^210$	000	$\bar{\varepsilon}10$

Representation	Arm	Position (2c)					
		0 cell		$+\vec{a}_1,+\vec{a}_2,-(\vec{a}_1+\vec{a}_2)$		$-\vec{a}_1,-\vec{a}_2,+(\vec{a}_1+\vec{a}_2)$	
		1	2	1	2	1	2
τ_1	K_1	$1\bar{\varepsilon}0$	$\bar{\varepsilon}10$	$\varepsilon\bar{\varepsilon}^20$	$\bar{\varepsilon}^2\varepsilon 0$	$\varepsilon^2\bar{1}0$	$\bar{1}\varepsilon^20$
	K_2	$\varepsilon^2\bar{\varepsilon}0$	$\bar{\varepsilon}\varepsilon^20$	$\varepsilon\bar{1}0$	$\bar{1}\varepsilon 0$	$1\bar{\varepsilon}0$	$\bar{\varepsilon}^210$
τ_3	K_1	$1\bar{\varepsilon}0$	$\varepsilon\bar{1}0$	$\varepsilon\bar{\varepsilon}^20$	$\varepsilon^2\bar{\varepsilon}0$	$\varepsilon^2\bar{1}0$	$1\bar{\varepsilon}^20$
	K_2	$\bar{\varepsilon}^2\varepsilon 0$	$\bar{\varepsilon}\varepsilon^20$	$\bar{\varepsilon}10$	$\bar{1}\varepsilon 0$	$\bar{1}\varepsilon^20$	$\bar{\varepsilon}^2\bar{1}0$
τ_5	K_1	000	$1\bar{\varepsilon}0$	000	$\varepsilon\bar{\varepsilon}^20$	000	$\varepsilon^2\bar{1}0$
	K_2	$\bar{\varepsilon}\varepsilon^20$	000	$\bar{1}\varepsilon 0$	000	$\bar{\varepsilon}\bar{1}0$	000
	K_1	$\bar{\varepsilon}^2\varepsilon 0$	000	$\bar{1}\varepsilon^20$	000	$\bar{\varepsilon}10$	000
	K_2	000	$1\bar{\varepsilon}^20$	000	$\varepsilon^2\bar{\varepsilon}0$	000	$\varepsilon\bar{1}0$
τ_6	K_1	001	000	00ε	000	$00\varepsilon^2$	000
	K_2	000	$00\bar{\varepsilon}$	000	$00\bar{1}$	000	$00\bar{\varepsilon}^2$
	K_1	000	$00\bar{\varepsilon}$	000	$00\bar{\varepsilon}^2$	000	$00\bar{1}$
	K_2	$00\bar{\varepsilon}^2$	000	$00\bar{\varepsilon}$	000	$00\bar{1}$	000

Representation	Arm	Position ($4\tfrac{1}{}$) O cell			
		1	2	3	4
T_1	K_1	$1\bar{\varepsilon}0$	$\bar{\varepsilon}10$	$\bar{\varepsilon}10$	$1\bar{\varepsilon}0$
	K_2	$\varepsilon^2\bar{\varepsilon}0$	$\bar{\varepsilon}\varepsilon^20$	$\bar{\varepsilon}\varepsilon^20$	$\varepsilon^2\bar{\varepsilon}0$
T_2	K_1	$1\bar{\varepsilon}0$	$\bar{\varepsilon}10$	$\varepsilon\bar{1}0$	$\bar{1}\varepsilon0$
	K_2	$\varepsilon^2\bar{\varepsilon}0$	$\bar{\varepsilon}\varepsilon^20$	$\varepsilon\bar{\varepsilon}^20$	$\bar{\varepsilon}^2\varepsilon0$
T_3	K_1	$1\bar{\varepsilon}0$	$\varepsilon\bar{1}0$	$\varepsilon\bar{1}0$	$1\bar{\varepsilon}0$
	K_2	$\bar{\varepsilon}^2\varepsilon0$	$\bar{\varepsilon}\varepsilon^20$	$\bar{\varepsilon}\varepsilon^20$	$\bar{\varepsilon}^2\varepsilon0$
T_4	K_1	$1\bar{\varepsilon}0$	$\varepsilon\bar{1}0$	$\bar{\varepsilon}10$	$\bar{1}\varepsilon0$
	K_2	$\bar{\varepsilon}^2\varepsilon0$	$\bar{\varepsilon}\varepsilon^20$	$\varepsilon\bar{\varepsilon}^20$	$\varepsilon^2\bar{\varepsilon}0$
T_5	K_1	001	000	000	$00\bar{1}$
	K_2	000	$00\bar{\varepsilon}$	00ε	000
	K_1	000	$00\bar{\varepsilon}$	$00\varepsilon^2$	000
T_6	K_1	001	000	000	001
	K_2	000	$00\bar{\varepsilon}$	$00\bar{\varepsilon}$	000
	K_1	000	$00\bar{\varepsilon}$	$00\bar{\varepsilon}$	000
	K_2	$00\varepsilon^2$	000	000	$00\varepsilon^2$
T_5'	K_1	000	$1\bar{\varepsilon}0$	$1\bar{\varepsilon}0$	000
	K_2	$\bar{\varepsilon}\varepsilon^20$	000	000	$\bar{\varepsilon}\varepsilon^20$
	K_1	$\bar{\varepsilon}^2\varepsilon0$	000	000	$\bar{\varepsilon}^2\varepsilon0$
	K_2	000	$1\bar{\varepsilon}0$	$1\bar{\varepsilon}0$	000
T_6'	K_1	000	$1\bar{\varepsilon}0$	$\bar{1}\varepsilon0$	000
	K_2	$\bar{\varepsilon}\varepsilon^20$	000	000	$\varepsilon\bar{\varepsilon}^20$
	K_1	$\bar{\varepsilon}^2\varepsilon0$	000	000	$\varepsilon^2\bar{\varepsilon}0$
	K_2	000	$1\bar{\varepsilon}^20$	$\bar{1}\varepsilon^20$	000

Considering that the coordinate system of D_{6h}^4 is turned, with respect to the coordinate system of C_{6v}^3, at angle 30° around the z-axis (see <u>Fig.2</u>), we rewrite the elements of group C_{6v}^3 in the coordinate system of D_{6h}^4:

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$$(h_1 \,|0), \ (h_2 \,|\tau), \ (h_3 \,|0), \ (h_4 \,|\tau), \ (h_5 \,|0), \ (h_6 \,|\tau),$$

$$\text{(1.7)}$$

$$(h_{24} \,|\tau), \ (h_{19} \,|0), \ (h_{20} \,|\tau), \ (h_{21} \,|0), \ (h_{22} \,|\tau), \ (h_{23} \,|0).$$

Comparing (1.7) and (1.5) we see that the set of elements (1.7) is just the searched restriction of D_{6h}^4 on the subgroup C_{6v}^3 in the transition over arms $\vec{k}_1$, $\vec{k}_2$ of the star $\{\vec{k}_{13}\}$ of the lattice Γ_h. Now for each IRS from (1.4) we check whether the representation of this restriction has in the expansion into irreducible representations the identity representation or not (the Birman criterion). It is to be noted that the considered representations should be the representation of space group G induced from irreducible representation of the group $G_{\vec{k}}$ of the wave vector $\vec{k}_1$ of the star $\{\vec{k}_{13}\}$, $(\vec{k}_1 = \frac{1}{3}(\vec{b}_1 + \vec{b}_2))$. Calculations show that the Birman criterion is satisfied only by two IRS – τ_1 and τ_4 of the group D_{6h}^4. The second arm of the star $\{\vec{k}_{13}\}$ was chosen to be the vector $\vec{k}_2 = \vec{h}_{13}\vec{k}_1 = -\vec{k}_1$.

The next step in searching of atom displacements in the transition $D_{6h}^4 \rightarrow C_{6v}^3$ is to determine the coefficients of mixing of modes (basis functions) of the representations τ_1 and τ_4. These coefficients which are structure parameters are defined from the condition of invariance of the density function $\delta\rho$ under the group C_{6v}^3:

$$\delta\rho = c_1^1\phi_1^1 + c_2^1\phi_2^1 + c_1^4\phi_1^4 + c_2^4\phi_2^4 ,\qquad \text{(1.8)}$$

where $\phi_{1,2}^1$ and $\phi_{1,2}^4$ are basis functions of representations τ_1 and τ_4 respectively. Acting by generators of the group $C_{6v}^3((h_2\,|\tau)$, $(h_{24}\,|0))$ on the function $\delta\rho$ (1.8) (which is in practice realized by the action of the corresponding to the generators matrices in the given representation on the "vector" of the structure parameter) and putting $g_i\delta\rho = \delta\rho$, we find the coefficients of mixing of modes of representations τ_1 and τ_4 which describe the displacement of atoms in the transition $D_{6h}^4 \rightarrow C_{6v}^3$: $\tau_1(c_1c_1)$ and $\tau_4(c_4\bar{c}_4)$. The searched displacements of atoms in ReMnO$_3$ are presented in Table 2 and drawn in Fig.4 (for the elementary cell of D_{6h}^4 phase). It should be noted that the obtained displacements in the transition $D_{6h}^4 \rightarrow C_{6v}^3$ make experimental data more precise, namely: atoms of Re taking one set of equivalent positions (2a) in the praphase are separated into two sets (2a) and (4b), and the running parameters z_a and z_b should have opposite signs, and z_a should be twice z_b. (z_a and z_b are reckoned from the idealized position $z' = 1/4$). The oxygen atoms, taking in the praphase positions (2b), are also separated in the low symmetry phase into the positions (2a) and (4b) with the same relation of z_a and z_b, as for Re,

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Table 2

The displacements of atoms in $ReMnO_3$ in the transition $D_{6h}^4 \rightarrow C_{6v}^3$ as a result of mixing of modes $r_1(c_1 c_1)$ and $r_4(c_4 \bar{c}_4)$

Positions	Representation and type of mixing	0 cell		$+\vec{a}_1, +\vec{a}_2, -(\vec{a}_1+\vec{a}_2)$		$-\vec{a}_1, -\vec{a}_2, +(\vec{a}_1+\vec{a}_2)$	
		1	2	1	2	1	2
(2a)	$\tau_4^-(c_4\bar{c}_4)$	002	002	00$\bar{1}$	00$\bar{1}$	00$\bar{1}$	00$\bar{1}$
(2b)	$\tau_4^-(c_4\bar{c}_4)$	002	002	00$\bar{1}$	00$\bar{1}$	00$\bar{1}$	00$\bar{1}$
(2c)	$\tau_1^-(c_1c_1)$	$\bar{1}$20	$\bar{2}$10	210	120	$\bar{1}$10	1$\bar{1}$0
(4f)	$\tau_1^-(c_1c_1)$	$\bar{1}$20	$\bar{2}$10	$\bar{2}$10	$\bar{1}$20		
	$\tau_4^-(c_4\bar{c}_4)$	$\bar{1}$20	210	$\bar{2}$10	120		
Positions		1	2	3	4		
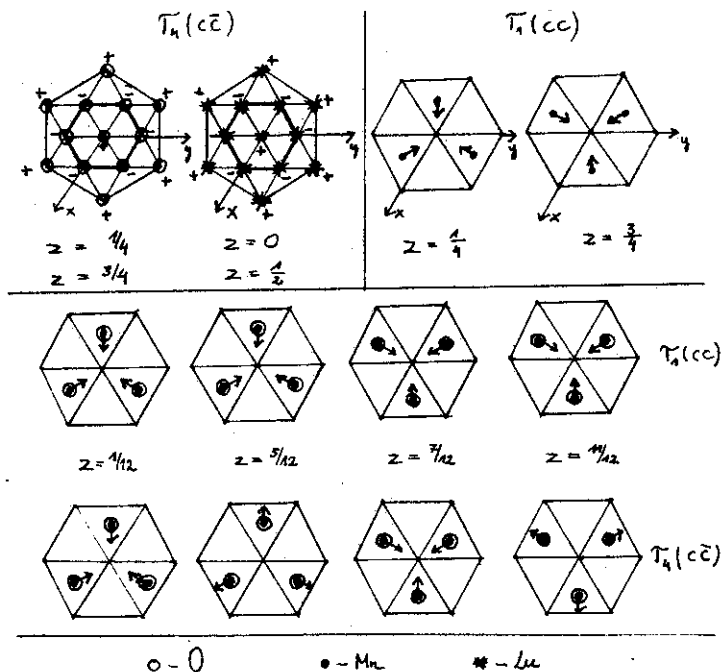
Fig.4. Displacements of atoms in $ReMnO_3$ at the phase transition from D_{6h}^4 to C_{6v}^3 structure.

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but reckoned from the idealized position $z'=0$. The oxygen atoms, taking in the praphase position (4f) are divided into two sets (6c), one set with the running parameter $z'=1/3$, the second with the running parameter $z'=1/6$ exactly (these atoms are displaced only in the xy-plane). The running parameter x for one set (6c) differs in sign from the corresponding parameter for the other set (6c) (calculated with respect to the position $x'=1/3$) in the transition over r_4 and coincides in sign in the transition over r_1. The Mn atoms are also displaced only in the xy-plane.

We find that the phase transition into the phase C_{6v}^3 is described by the star $\{\vec{k}_{13}\}$ and two IRS r_1 and r_4 of the group D_{6h}^4. This result is due to the statement of the problem; namely, we have given the group of symmetry of the asymmetric phase and looked for IRS which may participate in such a transition. If we solve the problem of determination of all possible phases with a given change of the initial elementary cell, then it can be shown that the representation r_1 describes the transition into a phase with symmetry D_{6h}^3 and the representation r_4 into phase C_{6v}^3. The group C_{6v}^3 is a subgroup of D_{6h}^3. Therefore, in analysing the phase transition $D_{6h}^4 \rightarrow$ $\rightarrow C_{6v}^3$ we shall call the representation r_4 relevant and the representation r_1 attendant /8/.

It is interesting to note that in considering the mixing modes of only one, relevant representation r_4 the Mn atoms are not displaced from initial positions and the magnitude of displacements of atoms of O_{II} (4f) is the same for layers $z=\dfrac{1}{12},\dfrac{5}{12},\dfrac{7}{12},\dfrac{11}{12}$. Modes of the attendant representation r_1 describe displacements of Mn atoms and may diminish the magnitude of displacements of atoms of O_{II} (4b) in layers $z=11/12$ and $z=5/12$.

Let us demonstrate that the displacements of atoms of Re and O, which are described by the relevant IRS r_4 are necessarily accompanied by the displacements of Mn atoms. For this we construct the thermodynamical potential Φ from basis functions a_1, a_2 of the representation r_1 and b_1, b_2 of the representation r_4. Matrices of the reducible representation $r_1 \oplus r_4$ have the form:

$$g_1, g_3, g_5, g_{20}, g_{22}, g_{24} = \left(\begin{array}{cc|cc} 1 & 0 & & \\ 0 & 1 & & \\ \hline & & 1 & 0 \\ & & 0 & 1 \end{array} \right),$$

$$g_7, g_9, g_{11}, g_{14}, g_{16}, g_{18} = \left(\begin{array}{cc|cc} 1 & 0 & & \\ 0 & 1 & & \\ \hline & & -1 & 0 \\ & & 0 & -1 \end{array} \right),$$

$$g_2, g_4, g_6, g_{19}, g_{21}, g_{23} = \left(\begin{array}{cc|cc} 0 & 1 & & \\ 1 & 0 & & \\ \hline & & 0 & -1 \\ & & -1 & 0 \end{array}\right) ,$$

$$g_8, g_{10}, g_{12}, g_{13}, g_{15}, g_{17} = \left(\begin{array}{cc|cc} 0 & 1 & & \\ 1 & 0 & & \\ \hline & & 0 & 1 \\ & & 1 & 0 \end{array}\right) , \qquad (1.9)$$

$$t_1, t_2 = \left(\begin{array}{cc|cc} \epsilon & 0 & & \\ 0 & \epsilon^2 & & \\ \hline & & \epsilon & 0 \\ & & 0 & \epsilon^2 \end{array}\right) ,$$

$$t_1 + t_2, \ -t_1, -t_2 = \left(\begin{array}{cc|cc} \epsilon^2 & 0 & & \\ 0 & \epsilon & & \\ \hline & & \epsilon^2 & 0 \\ & & 0 & \epsilon \end{array}\right) .$$

To construct Φ we find the complete rational basis of invariants (CRBI). Following ref./15/ we construct the normal series:

$$G^4_{12} \overset{h_{13}}{\Longrightarrow} G^3_6 \overset{h_7}{\Longrightarrow} G^2_3 \overset{t_1}{\Longrightarrow} G^1_1 \Longrightarrow 1. \qquad (1.10)$$

The numbers below denote the number of elements in the subgroup G^i (i – is the index number). The elements above arrows are representatives of the group expansion in the normal series, for instance, $G^4 \overset{h_{13}}{\Longrightarrow} G^3$ means $G^4 = G^3 + h_{13} G^3$. The CRBI has the form:

$$I_1 = a_1 a_2, \quad I_2 = b_1 b_2, \quad I_3 = a_1^3 + a_2^3, \quad I_4 = a_1 b_1^2 + a_2 b_2^2 ,$$

$$I_5 = b_1^6 + b_2^6, \quad I_6 = a_1^2 b_2^2 + a_2^2 b_1^2, \quad I_7 = b_1^4 a_2 + b_2^4 a_1 , \qquad (1.11)$$

$$I_8 = a_1^3 b_2^6 + a_2^3 b_1^6, \quad I_9 = a_1^2 b_2^4 + a_2^2 b_1^4, \quad I_{10} = a_1^2 b_1^8 + a_2^2 b_2^8 .$$

The thermodynamical potential Φ up to the fourth order in order parameters a_i and b_i is as follows:

$$\Phi = r_1 a_1 a_2 + r_2 b_1 b_2 + v_1 (a_1^3 + a_2^3) + v_2 (a_1 b_1^2 + a_2 b_2^2) +$$

$$+ u_1 a_1^2 a_2^2 + u_2 b_1^2 b_2^2 + u_3 a_1 a_2 b_1 b_2 + u_4 (a_1^2 b_2^2 + a_2^2 b_1^2) . \qquad (1.12)$$

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The obtained relation differs in quadratic terms from the conventional form of Φ. Therefore we introduce the change of variables:

$$a'_1 = a_1 + a_2 \;;\quad b'_1 = b_1 + b_2 \;;$$

$$a'_2 = i(a_1 - a_2)\;;\quad b'_2 = i(b_1 - b_2)\;. \tag{1.13}$$

In new variables (1.12) becomes (primes are omitted for simplicity):

$$\Phi = r_1(a_1^2 + a_2^2) + r_2(b_1^2 + b_2^2) + v_1(a_1^3 - 3a_1 a_2^2) +$$

$$+ v_2[a_1(b_1^2 - b_2^2) - 2a_2 b_1 b_2] + u_1(a_1^2 + a_2^2)^2 + u_2(b_1^2 + b_2^2) + \tag{1.14}$$

$$+ u_3(a_1^2 + a_2^2)(b_1^2 + b_2^2) + u_4(a_1^2 - a_2^2)(b_1^2 - b_2^2)\;.$$

Now let us write the equations of state:

$$\Phi_{a_1} \equiv \frac{\partial \Phi}{\partial a_1} = 0;\quad \Phi_{b_1} \equiv \frac{\partial \Phi}{\partial b_1} = 0\;;$$

$$\Phi_{a_1} = 2r_1 a_1 + v_1(3a_1^2 - 3a_2^2) + v_2(b_1^2 - b_2^2) +$$

$$+ 4u_1 a_1(a_1^2 + a_2^2) + 2u_3 a_1(b_1^2 + b_2^2) +$$

$$+ 2u_4 a_1(b_1^2 - b_2^2) = 0\;,$$

$$\Phi_{a_2} = 2r_1 a_2 + v_1(-6a_1 a_2) + v_2(-2b_1 b_2) +$$

$$+ 4u_1 a_2(a_1^2 + a_2^2) + 2u_3 a_2(b_1^2 + b_2^2) +$$

$$- 2u_4 a_2(b_1^2 - b_2^2) = 0\;,$$

$$\Phi_{b_1} = 2r_2 b_1 + v_2(2a_1 b_1 - 2a_2 b_2) + 4u_2 b_1(b_1^2 + b_2^2) +$$

$$+ 2u_3 b_1(a_1^2 + a_2^2) + 2u_4 b_1(a_1^2 - a_2^2) = 0\;, \tag{1.15}$$

$$\Phi_{b_2} = 2r_2 b_2 + v_2(-2b_2 a_1 - 2a_2 b_1) + 4u_2 b_2(b_1^2 + b_2^2) +$$

$$+ 2u_3 b_2(a_1^2 + a_2^2) - 2u_4 b_2(a_1^2 - a_2^2) = 0\;.$$

Consider the type of the solution $r_1(00)$, $r_4(c\bar{c})$ (it means that $a_1 = a_2 = 0$; $b_1 = -b_2 = c$) corresponding to the displacement of atoms of Re and O provided that Mn atoms are not displaced. Then eqs. (1.15) take the form:

$$\Phi_{a_1}: \quad 0 = 0,$$

$$\Phi_{a_2}: \quad 2v_2 c^2 = 0,$$

$$\Phi_{b_1}: \quad 2r_2 c + 8u_2 c^3 = 0,$$

$$\Phi_{b_2}: \quad 2r_2 c + 8u_2 c^3 = 0. \tag{1.16}$$

Considering that the interaction $v_2 \neq 0$ from the second of eqs. (1.16) we observe that c should be zero. This means that the displacements of atoms of Re and O are necessarily accompanied by the displacements of Mn atoms. The experimentally observed displacements of atoms of Lu[1] are "large", of an order of 0.02 (relative to 0.25). This allows us to consider the Lu displacements to be the main order parameter in agreement with that the representation r_4 describing these displacements is relevant. The magnitude of attendant displacements is defined by the parameter of interaction v_2 and should be smaller than that of Lu displacements. This smallness is, obviously, the reason for which the coordinates of Mn atoms in the structure C_{6v}^3 have not been defined exactly in works[3-7], and for LuMnO$_3$ no displacements of Mn atoms are observed.

2. DESCRIPTION OF THE MAGNETIC STRUCTURE IN THE PRAPHASE SYMMETRY GROUP

The Mn magnetic atoms take position (2c). The magnetic representation with star $\{\vec{k}_{13}\}$ has the form:

$$d_M^{\{\vec{k}_{13}\}} = r_2 \oplus r_4 \oplus r_5 \oplus r_6, \tag{2.1}$$

where r_2, r_4 are one-dimensional IRS of the group $G_{\vec{k}}$ of the wave vector $\vec{k}_1 = 1/3(\vec{b}_1 + \vec{b}_2)$ of the star $\{\vec{k}_{13}\}$ and r_5, r_6 are two-dimensional ones. The magnetic modes calculated by the standard formulae[11,12] are listed in Table 3.

Table 3

The magnetic modes calculated for the star $\{\vec{k}_{13}\}$
of the group D_{6h}^4 (position 2c)

Representation	Arm	0 cell		$+\vec{\alpha}_1, +\vec{\alpha}_2, -(\vec{\alpha}_1+\vec{\alpha}_2)$		$-\vec{\alpha}_1, -\vec{\alpha}_2, +(\vec{\alpha}_1+\vec{\alpha}_2)$	
		1	2	1	2	1	2
τ_2	K_1	$1\bar{E}0$	$\bar{E}10$	$\varepsilon\bar{\varepsilon}^2 0$	$\bar{\varepsilon}^2\varepsilon 0$	$\varepsilon^2\bar{1}0$	$\bar{1}\varepsilon^2 0$
	K_2	$\bar{\varepsilon}^2\varepsilon 0$	$\varepsilon\bar{\varepsilon}^2 0$	$\bar{\varepsilon}10$	$1\bar{E}0$	$\bar{1}\varepsilon^2 0$	$\varepsilon^2\bar{1}0$
τ_4	K_1	$1\bar{E}0$	$\varepsilon\bar{1}0$	$\varepsilon\bar{\varepsilon}^2 0$	$\varepsilon^2\bar{E}0$	$\varepsilon^2\bar{1}0$	$1\bar{\varepsilon}^2 0$
	K_2	$\varepsilon^2\bar{E}0$	$\varepsilon\bar{\varepsilon}^2 0$	$\varepsilon\bar{1}0$	$1\bar{E}0$	$1\bar{\varepsilon}^2 0$	$\varepsilon^2\bar{1}0$
τ_5	K_1	001	00ε	00ε	000	$00\varepsilon^2$	000
	K_2	000	00ε	000	001	000	$00\varepsilon^2$
	K_1	000	$00\bar{\varepsilon}$	000	$00\bar{\varepsilon}^2$	000	$00\bar{1}$
	K_2	$00\bar{\varepsilon}^2$	000	$00\bar{\varepsilon}$	000	$00\bar{1}$	000
τ_6	K_{11}	000	$1\bar{E}0$	000	$\varepsilon\bar{\varepsilon}^2 0$	000	$\varepsilon^2\bar{1}0$
	K_2	$\varepsilon\bar{\varepsilon}^2 0$	000	$1\bar{E}0$	000	$\varepsilon^2\bar{1}0$	000
	K_1	$\bar{\varepsilon}^2\varepsilon 0$	000	$\bar{1}\varepsilon^2 0$	000	$\bar{E}10$	000
	K_2	000	$\bar{1}\bar{\varepsilon}0$	000	$\bar{\varepsilon}^2\varepsilon 0$	000	$\bar{\varepsilon}10$

Let us now define all possible types of the magnetic ordering of Mn atoms whose crystal symmetry will be C_{6v}^3 or the supergroup of C_{6v}^3 in the considered transition channel. There is only one group of this type – D_{6h}^3 (Table [14]). For this we should write out all Shubnikov sungroups of the initial paramagnetic group $D_{6h}^4 \cdot 1'$ with the crystal symmetry D_{6h}^3 or C_{6v}^3. Then the corresponding magnetic structures will be defined by the conditions of invariance of spin density function with respect to generators of the chosen subgroups:

$$g_i \vec{S}(\vec{r}) = \vec{S}(\vec{r}) . \tag{2.2}$$

The spin density function can, in turn, be represented as a superposition of basis functions (magnetic modes) of IRS entering into the magnetic representation (2.1). Then the condition (2.2) is reduced to the action of matrices corresponsing to generators of the chosen subgroup in the given representation on the column of mixing coefficients of basis functions:

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$$d^{\nu}(g_i)\begin{pmatrix} c_1 \\ \vdots \\ \\ \vdots \\ c_k \end{pmatrix} = \begin{pmatrix} c_1 \\ \vdots \\ \\ \vdots \\ c_k \end{pmatrix} . \tag{2.3}$$

It should be noted that here one should use the representation of the Shubnikov group induced by the irreducible representation of group $G_{\vec{k}}$ for arms participating in the transition.

Table 4

The types of spin ordering in the plane xy as a result of possible types of mixing of magnetic modes

Representation and type of mixing	0 cell		$+\vec{a}_1$, $+\vec{a}_2$, $-(\vec{a}_1+\vec{a}_2)$		$-\vec{a}_1$, $-\vec{a}_2$, $+(\vec{a}_1+\vec{a}_2)$	
	1	2	1	2	1	2
$T_2\,(C_2 C_2)$	100	010	010	100	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$
$T_2\,(C_2 \bar{C}_2)$	$\bar{1}\bar{2}0$	$\bar{2}\bar{1}0$	210	120	$\bar{1}10$	$1\bar{1}0$
$T_4\,(C_4 \bar{C}_4)$	100	$0\bar{1}0$	010	$\bar{1}00$	$\bar{1}\bar{1}0$	110
$T_4\,(C_4 C_4)$	$\bar{1}\bar{2}0$	210	210	$\bar{1}\bar{2}0$	$\bar{1}10$	$\bar{1}10$
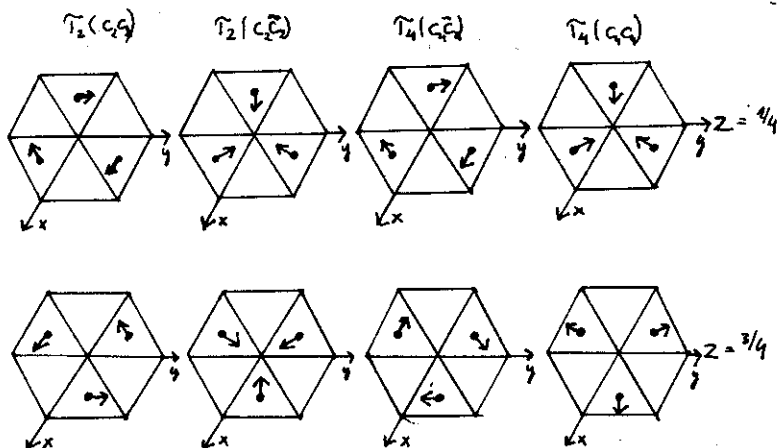
Fig.5. Types of the spin ordering in the xy plane as a result of admissible mixing of magnetic modes.

Matrices of elements $g_i \cdot 1'$ differ in sign from matrices of elements g_i. From (2.3) we obtain a system of equations for determining the coefficients of mixing of magnetic modes. Thus, for each Shubnikov subgroup of group $D_{6h}^4 \cdot 1'$ we find the way of mixing of magnetic modes and the corresponding number of IRS which allows us to draw the magnetic structure. The calculation shows that the representations r_5 and r_6 from (2.1) describe magnetic structures whose crystal symmetry does not coincide with C_{6v}^3 and D_{6h}^3. Therefore one should consider only representations r_2 and r_4 induced for 2 arms of the star $\{\vec{k}_{13}\}$. From the explicit form of matrices of these representations and (2.3) we find that in both the cases there are possible two types of mixing of modes $(c_i c_i)$ and $(c_i \bar{c}_i)$. This gives 4 types of the spin ordering in the plane xy (Table 4, fig.5).

It is easy to see that they coincide with variants of the triangular structure observed experimentally [1]. To obtain the component of magnetic moments along the z-axis (weak ferromagnetism propsed in [4,6]), we should calculate the magnetic modes with the wave vector $\vec{k} = 0$ (star $\{\vec{k}_{16}\}$). The magnetic representation $d_M^{\{\vec{k}_{16}\}}$ is decomposed into IRS as follows:

$$d_M^{\{\vec{k}_{16}\}} = r_3 + r_6 + r_9 + r_{12} .$$ (2.4)

The magnetic modes for representations r_3 and r_6 are given in Table 5.

Table 5

The magnetic modes for representations r_3 and r_6 of the group D_{6h}^4 with the star $\{\vec{k}_{16}\}$

Representation	Position (2c)	
	1	2
r_3	001	001
r_6	001	00$\bar{1}$

As a more detailed calculation shows, the magnetic modes of representations r_9 and r_{12} have no z-components we are interested in, and therefore, we will not consider them. Including these results into the model of the magnetic structure 1), 2), 3), 4) considered earlier we obtain eight variants of the magnetic structures:

1. $\tau_4(c_4c_4)\tau_3(c')$,   5. $\tau_4(c_4c_4)\tau_6(c)$,

2. $\tau_2(c_2c_2)\tau_3(c')$,   6. $\tau_2(c_2c_2)\tau_6(c)$,   (2.5)

3. $\tau_2(c_2\bar{c}_2)\tau_6(c)$,   7. $\tau_2(c_2\bar{c}_2)\tau_3(c')$,

4. $\tau_4(c_4\bar{c}_4)\tau_6(c)$,   8. $\tau_4(c_4\bar{c}_4)\tau_3(c')$.

They exactly correspond to the models proposed in [1]. It is clear that all the eight variants differ in the magnetic symmetry which is defined as the intersection of the magnetic group of the component of the magnetic moment along the z-axis and the magnetic group corresponding to ordering in the xy plane. As the calculation shows, the magnetic symmetry of possible models of ordering in the xy plane is represented as follows (see Table 6). The magnetic symmetry of the z-component corresponding to the representation τ_3 is described by the magnetic group $P6_3c'm'$ and that one corresponding to the representation τ_6 by the magnetic group $P6_3cm'$. Hence it follows that the crystal symmetry $C_{6v}(P6_3cm)$ is defined only by the variants: $\tau_2(c_2\bar{c}_2)\tau_3(c')$ and $\tau_4(c_4c_4)\tau_6(c)$. Therefore, the experimental data testify to the crystal symmetry

Table 6

The magnetic symmetry of possible models of ordering of the magnitude moments in the xy plane

Models of magnetic structures in the xy-plane	The elements of the group												The magnetic group
	1	2	3	4	5	6	19	20	21	22	23	24	
$\bar{T}_2(c_2c_2)$		▨		▨		▨	▨			▨		▨	$P6_3'c'm$
$\bar{T}_2(c_2\bar{c}_2)$							▨	▨	▨	▨	▨	▨	$P6_3c'm'$
$\bar{T}_4(c_4c_4)$		▨		▨		▨	▨		▨		▨		$P6_3'cm'$
$\bar{T}_4(c_4\bar{c}_4)$													$P6_3cm$

☐ → g_i ▨ → $g_i \cdot 1'$

C_{6v}^3 in the magnetic-ordered state, we should discuss only these variants. From Table 6 it is also seen that the crystal symmetry proposed by Koehler [4,6] for magnetic structures $r_2(c_2c_2) + r_4(c_4c_4)$ and $r_2(c_2\bar{c}_2) + r_4(c_4\bar{c}_4)$, whose spins are deviated from x or y directions is not described by group C_{6v}^3. The crystal symmetry of the structure $r_2(c_2c_2) + r_4(c_4c_4)$ is described by group C_6. (The crystal symmetry of the magnetic structure is understood as a symmetry of the group obtained from the magnetic group by neglecting time inversion). Therefore, a correct choice of the initial state in describing the magnetic structures forbids some variants.

A proper choice of the initial phase allows also the separation of the reflexes that contain information on the S_z - component. Indeed, as the S_z -component is described by the star $\vec{k}=0$ of group D_{6h}^4, its definition requires to analyse the magnetic contribution to nuclear reflexes of the structure D_{6h}^4. The S_{xy}-components contribute to the remaining reflexes.

Now we shall construct the thermodynamical potential for describing the phase transition corresponding to the variant $r_4(c_4c_4)r_6(c)$. For simplicity we consider variables corresponding to displacements of the Mn atoms only (parameter (a_1,a_2) corresponding to the representation r_1) and magnetic variables: parameter (c) corresponding to the representation r_6 and parameter (b_1,b_2) corresponding to r_4). To obtain CRBI we should construct five-dimensional matrices $r_6 \oplus r_1 \oplus r_4$ for elements of the group $D_{6h}^4 \cdot 1'$. Then separating all different matrices we construct the normal series, and following ref. [15] construct the CRBI

$$I_1 = c^2, \quad I_2 = a_1 a_2, \quad I_3 = b_1 b_2, \quad I_4 = a_1^3 + a_2^3,$$

$$I_5 = a_1 b_1^2 + a_2 b_2^2, \quad I_6 = b_1^6 + b_2^6, \quad I_7 = a_1^2 b_2^2 + a_2^2 b_1^2,$$

$$I_8 = b_1^4 a_2 + b_2^4 a_1, \quad I_9 = a_1^3 b_2^6 + a_2^3 b_1^6,$$

$$I_{10} = a_1^4 b_2^4 + a_2^4 b_1^4, \quad I_{11} = b_1^8 a_2^2 + b_2^8 a_1^2. \tag{2.6}$$

Changing variables so that the invariants I_2 and I_3 take the usual form: $I_2 = a_1^2 + a_2^2$ and $I_3 = b_1^2 + b_2^2$, we may write the thermodynamical potential in the form:

$$\Phi = r_1 c^2 + r_2 (a_1^2 + a_2^2) + r_3 (b_1^2 + b_2^2) + v_1 (a_1^3 - 3a_1 a_2^2) +$$

$$+ v_2 [a_1 (b_1^2 - b_2^2) - 2a_2 (b_1 b_2)] +$$

$$+ u_1 c^4 + u_2(a_1^2 + a_2^2)^2 + u_3(b_1^2 + b_2^2)^2 + u_4 c^2(a_1^2 + a_2^2) +$$

$$+ u_5 c^2(b_1^2 + b_2^2) + u_6(a_1^2 + a_2^2)(b_1^2 + b_2^2) + u_7(a_1^2 - a_2^2)(b_1^2 - b_2^2) .$$

$$(2.7)$$

The equations of state are as follows:

$$\frac{\partial \Phi}{\partial c}: \quad 2r_1 c + 4u_1 c^3 + 2u_4 c(a_1^2 + a_2^2) + 2u_5 c(b_1^2 + b_2^2) = 0 ,$$

$$\frac{\partial \Phi}{\partial a_1}: \quad 2r_2 a_1 + v_1(3a_1^2 - 3a_2^2) + v_2(b_1^2 - b_2^2) + 4u_2 a_1(a_1^2 + a_2^2) +$$

$$+ 2u_4 c^2 a_1 + 2u_6 a_1(b_1^2 + b_2^2) + 2u_7 a_1(b_1^2 - b_2^2) = 0 , \qquad (2.8)$$

$$\frac{\partial \Phi}{\partial a_2}: \quad 2r_2 a_2 + v_1(-6a_1 a_2) + v_2(-2b_1 b_2) + 4u_2 a_2(a_1^2 + a_2^2) +$$

$$+ 2u_4 c^2 a_2 + 2u_6 a_2(b_1^2 + b_2^2) - 2u_7 a_2(b_1^2 - b_2^2) = 0 ,$$

$$\frac{\partial \Phi}{\partial b_1}: \quad 2r_3 b_1 + v_2(2a_1 b_1 - 2a_2 b_2) + 4u_3 b_1(b_1^2 + b_2^2) +$$

$$+ 2u_5 b_1 c^2 + 2u_6 b_1(a_1^2 + a_2^2) + 2u_7 b_1(a_1^2 - a_2^2) = 0 ,$$

$$\frac{\partial \Phi}{\partial b_2}: \quad 2r_3 b_2 + v_2(-2a_1 b_2 - 2a_2 b_1) + 4u_3 b_2(b_1^2 + b_2^2) +$$

$$+ 2u_5 b_2 c^2 + 2u_6 b_2(a_1^2 + a_2^2) - 2u_7 b_2(a_1^2 - a_2^2) = 0 .$$

Consider the solution corresponding to the appearance of the magnetic structure $r_6(c)$ and $r_4(c_4 c_4)$ provided the Mn atoms do not shift, that means $r_1(0\,0)$: $c \neq 0$, $b_1 = b_2 = c_4$, $a_1 = a_2 = 0$. The equation of state take then on the form:

$$\frac{\partial \Phi}{\partial c}: \quad 2r_1 c + 4u_1 c^3 + 4u_5 c c_4 = 0 ,$$

$$\frac{\partial \Phi}{\partial a_1}: \quad 0 = 0 ,$$

$$\frac{\partial \Phi}{\partial a_2}: \quad 2v_2 c_4^2 = 0 ,$$

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$$\frac{\partial \Phi}{\partial b_1}: \quad 2r_8 c_4 + 8u_8 c_4^3 + 2u_5 c_4 c^2 = 0,$$

$$\frac{\partial \Phi}{\partial b_2}: \quad 2r_8 c_4 + 8u_8 c_4^3 + 2u_5 c_4 c^2 = 0. \tag{2.9}$$

From these equations it is seen that in case when the Mn atoms do not shift, the components of magnetic moments in the xy plane are zero. Therefore it may be assumed that in the considered compounds $ReMnO_3$ the displacements of Mn atoms are the main condition for appearing magnetic components in the xy plane.

A detailed thermodynamical analysis of phase transitions in $ReMnO_3$ will be published elsewhere.

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