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Symmetry changes at the Neél point in an antiferromagnet on a triangular lattice in an external magnetic field

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Abstract. Landau-type theory has been applied to the calculation of symmetry changes at the metamagnetic phase transition in a two-dimensional antiferromagnet on a triangular lattice placed in an external magnetic field parallel or perpendicular to the surface of the system. As the high-temperature phases of the system can be described by non-unitary or unitary magnetic groups, their irreducible corepresentations or representations, respectively, have been applied in this calculation. Two order parameters, magnetic and strain tensor, have been introduced into the thermodynamic potential density due to the fact that the low-temperature phases may be magnetic and distorted. It has been shown that if the magnetic field is perpendicular to the surface of the system, the corepresentations do not induce magnetic phase transitions, which contradicts experimental observations. It means that, in general, a description of magnetic crystals in terms of non-unitary magnetic groups is incorrect.

1. Introduction

A relatively large number of substances are known which, with high accuracy, can be regarded as quasi-two-dimensional antiferromagnets on a triangular lattice (AFMT) [1, 2]. Among them, two vanadium compounds VCl_2 ($T_N = 36$ K), VBr_2 ($T_N = 28.5$ K) [3–7] and the intercalation compound C_6Eu [8, 9], are the most well known. Experimental [9] and theoretical [10] investigations show that the latter substance, which is a metamagnet (the interplane exchange is ferromagnetic), is an easy-plane AFMT.

In this paper we will apply a Landau-type theory (see [11, 12]) to describe symmetry changes and the relevant low-temperature spin structures which occur at the metamagnetic phase transition in a two-dimensional AFMT placed in an external magnetic field parallel or perpendicular to the easy plane of the antiferromagnet.

The symmetry group of the magnetically ordered high-temperature phase of the AFMT is the maximal common subgroup of the unmagnetized AFMT and the magnetic field (Curie principle, see [13]). Two possibilities appear here. We can either describe this high-temperature phase in terms of a non-unitary or a unitary magnetic group, and hence in terms of corepresentations (see [14]) or representations, respectively. A description of a magnetic crystal in terms of a non-unitary group has been given by Cracknell [15] in his calculation of a symmetry change at a spin–flop transition between

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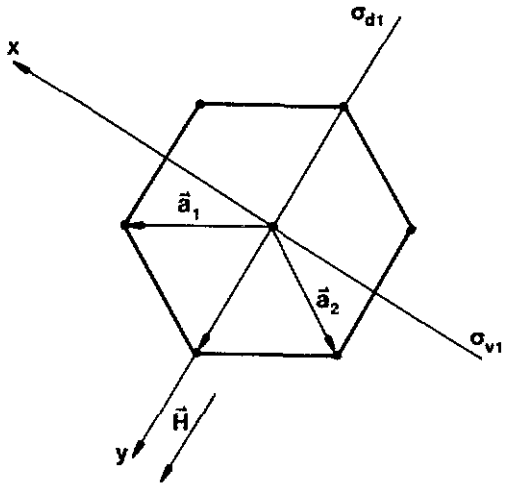

Figure 1. The basis vectors a_1 and a_2, the symmetry elements of the two-dimensional group *cmm'* and the direction of an external magnetic field.

two magnetically ordered phases in MnF_2 crystals. Magnetic crystals have been described in terms of non-unitary groups by Dimmock and Wheeler [16] and by Bradley and Cracknell [14]. On the other hand, Opechowski and Guccione [17] in their classification of magnetic crystals treated the operation of time reversal as a unitary operation. The same standpoint was accepted by Kovalev [18] in his paper on symmetry changes at a continuous phase transition from a paramagnetic phase to magnetically ordered phases. Kociński and Osuch [11] applied both descriptions in their calculations of symmetry changes in $FeCl_2$-type metamagnetic crystals and in rare-earth crystals with space-group symmetry $P6_3/mmc$ (D^4_{6h}) and concluded that they are not equivalent. We will also apply both approaches and compare the results.

Our system will be described on the level of the mean-field approximation. Consequently, the spin structure will be divided into sublattices, with parallel spins within each sublattice. This state can be achieved by a strong ferromagnetic coupling within each sublattice.

2. The phase transitions in a magnetic field parallel to the surface of the system

2.1. The thermodynamic potential density

Without a magnetic field and for temperatures above or at the Neél point the space group of the AFMT is the two-dimensional space group number 17: *p6mm* (see [19]). When the AFMT is placed in an external magnetic field parallel to its surface (see figure 1) we deal with a composite system: a two-dimensional AFMT plus field. According to the Curie principle the symmetry group of the composite system, which is the maximal common subgroup of the symmetry group of the two-dimensional AFMT and of the field symmetry group, is the two-dimensional magnetic group number 21: *cmm'* (see [20]):

$$cmm' = c1m1 + \theta\sigma_{d_1}c1m1 \tag{1}$$

when the field is directed along one of the hexagon diagonals, or the two-dimensional magnetic group number 1; *p2'*:

Table 1. The irreducible representations and corepresentations of the two-dimensional magnetic group cmm' at the point X of the reciprocal lattice space. In labelling the group elements we use symbols of Bradley and Cracknell [14]. The representation matrices for the group elements which contain the time-inversion operator have been multiplied by -1.

	E	θC_{2z}	$\theta\sigma_{d1}$	σ_{v1}	$n_1a_1 + n_2a_2$
A_1	1	−1	−1	1	$(-1)^{n_1+n_2}$
B_2, DA'	1	1	1	1	
A_2	1	−1	1	−1	
B_1, DA''	1	1	−1	−1	

Table 2. The irreducible representations and corepresentation of the two-dimensional magnetic group $p2'$ at the point X of the reciprocal lattice space. The representation matrices for the group elements which contain the time-inversion operator have been multiplied by -1.

	E	θC_{2z}	$n_1a_1 + n_2a_2$
A	1	−1	$(-1)^{n_1+n_2}$
B, DA	1	1	

$$p2' = p1 + \theta C_{2z}p1 \tag{2}$$

when the field is not parallel to one of the diagonals, where $c1m1$ and $p1$ are the two-dimensional space groups number 5 and number 1 (see [19]), and σ_{d1} and C_{2z} are the reflection in the y-axis and the rotation about the point (0,0) by π (see figure 1), respectively.

As the high- and low-temperature phases of the AFMT are magnetic and may be distorted we have to introduce two order parameters: a magnetic order parameter and a strain tensor [21]. The magnetic order parameter $M_s(x_p)$ at the lattice site x_p can be defined by the following equations (see [11]):

$$M_s(x_p) = M(x_p) - M(x_p + x_q) \qquad p = 1, 2, \ldots, z/2 \tag{3}$$

for a collinear spin structure, with constant x_q, and with z denoting the number of sublattices, and

$$[M_s(x_p)]^2 = [M_{x_p}(x_p) - M_{g^{-1}x_p}(g^{-1}x_p)]^2 \qquad g \in G_{M1} \tag{4}$$

for a non-collinear spin structure, where g is an element of the low-temperature symmetry group G_{M1}. By definition the symmetry group of $M_s(x_p)$ determines the symmetry of the low-temperature phase. Depending on whether the groups cmm' and $p2'$ are considered to be unitary or non-unitary magnetic groups, this order parameter transforms according to their irreducible representations or corepresentations at the point X (which is equivalent to the point M of the unmagnetized phase see [19]) of the reciprocal lattice space, respectively. The irreducible representations A_1, A_2, B_1, B_2 of cmm' and A, B of $p2'$, which can be calculated from Kovalev's formula (see [13]), are both Landau and Lifshitz active. They are given in table 1 and table 2, respectively. The application of the appropriate formulas given by Bradley and Cracknell [14] allows us to calculate the irreducible corepresentations DA', DA'' of cmm' and DA of $p2'$, which are collected

in table 1 and table 2, respectively. All of them belong to case (a) (see [14]), and are Landau and Lifshitz active. The corepresentations DA', DA'' and DA are formally identical to the representations B_2, B_1 and B. However, due to different transformation properties, they may induce different phase transitions.

On the other hand the strain tensor transforms according to the symmetrized square $[D_p]^2$ of the polar vector representation D_p of the crystallographic point group $mm2$ and 2, respectively (see [22]). After the reduction of $[D_p]^2$ we obtain the following results:

$$[D_p]^2 = 2A_1 \oplus A_2 \qquad \text{for } mm2 \tag{5}$$

and

$$[D_p]^2 = 3A \qquad \text{for } 2 \tag{6}$$

where, now, A_1 and A are the unit representations, and A_2 is given in the tables of Bradley and Cracknell [14]. Inspecting table 1, we can see that there is no change of the crystallographic point group $mm2$ at the possible phase transitions from the high-temperature group cmm'. Therefore, according to Neumann's principle (see [13]), the strain tensor does not change either. It must be, thus, connected with the unit representation A_1, and excluded from the thermodynamic potential density. In the case of $p2'$ the strain tensor also transforms according to the unit representation A and is excluded from the potential density. From the tables of Birrs [23] we find the strain tensors,

$$\begin{bmatrix} \varepsilon_{11} & 0 \\ 0 & \varepsilon_{22} \end{bmatrix} \qquad \text{and} \qquad \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{bmatrix} \tag{7}$$

in the high- and low-temperature phases for the groups cmm' and $p2'$, respectively. The above matrices are written in the coordinate system (x, y) shown in figure 1. The forms of the tensors, (7), indicate that the lattice distortions in the directions parallel and perpendicular to the magnetic field are different.

The thermodynamic potential density ϕ has the form (see [11])

$$\phi = \phi(M) + \phi(M_s) + \phi(M, M_s)$$

where M is the magnetization vector. It can be shown that the external field term $\phi(M)$ has the symmetry of the high-temperature phase and since it does not depend on the components of M_s it is irrelevant in the determination of the minima of ϕ. The term $\phi(M_s)$ has the customary form of an expansion in terms of the components c_j of the order parameter. The lowest-degree invariant which appears in the term $\phi(M, M_s)$ representing the coupling between M and M_s can be incorporated into the potential density $\phi(M_s)$. Therefore, with accuracy to the sixth-order term, the thermodynamic potential density, which is invariant under the symmetry operations represented by the one-dimensional irreducible representations and corepresentations of cmm' and $p2'$, has the form

$$\phi(M_s) = A(T, H)c^2 + C(T, H)c^4 + D(T, H)c^6 \tag{8}$$

where c transforms under $A_1, A_2, B_1, B_2, DA', DA'', A, B$ or DA, respectively, and

$$\begin{aligned} A(T, H) &= a_T(T - T_t) + a_H(H - H_t) \\ C(T, H) &= c_T(T - T_c) + c_H(H - H_c) \end{aligned} \tag{9}$$

with $a_T c_H \neq a_H c_T$ (see [24]), where T_t, H_t and T_c, H_c are the temperature and the

magnetic field at the critical and tricritical point, respectively. The type of the phase transition described by ϕ depends on the sign of the coefficient $C(T, H)$. For a positive C we can have a continuous transition, while for a negative C we can have a discontinuous transition. The equilibrium value of c is determined on the basis of the potential density (8). The necessary and sufficient conditions can be written out and fulfilled with appropriate values of the phenomenological coefficients A, C and D (see [13]).

2.2. *The symmetry changes and spin structures*

The magnetic order parameter (3) or (4) in the low-temperature phase of the AFMT can be expressed by the formula

$$\boldsymbol{M}_s(\boldsymbol{r}) = c(T, H)\boldsymbol{f}(\boldsymbol{r}) \tag{10}$$

where $\boldsymbol{f}(\boldsymbol{r})$ is an axial-vector basis function of any of the above calculated irreducible representations and corepresentations of cmm' and $p2'$, and $c(T, H)$ is the equilibrium value of c in (8).

The set of two basis functions of each of the one-dimensional corepresentations DA', DA'' of cmm' and DA of $p2'$ consists of the basis function φ_i of the unitary subgroup $c1m1$ or $p1$ (see (1) and (2)), respectively, and of the basis function φ_i'' obtained from the formula: $A\varphi_i = \varphi_i'$, where $i = 1, 2$ for cmm' and $i = 1$ for $p2'$. The functions φ_i can be calculated in the customary way (see [11]) by acting with the projection operators

$$p^i = \tfrac{1}{2}\sum_{R\in m} \Gamma_i(R)T(R) \qquad i = 1, 2, \text{ for } c1m1 \tag{11}$$

and

$$p^1 = T(E) \qquad \text{for } p1$$

where $\Gamma_i(R)$ denotes the value of the irreducible representation Γ_i of $c1m1$ for the symmetry element $R \in c1m1$, on the axial-vector trial function:

$$\boldsymbol{\psi}(\boldsymbol{r}) = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}}$$

where $\boldsymbol{k}_1$ is the wavevector at the point X of the reciprocal lattice space and d_1, d_2 are complex numbers which refer to the axes x, y in figure 1. In turn, the basis functions connected with the two irreducible blocks of a reduced case (a) corepresentation are obtained by applying to the set of the basis functions φ_i, φ_i' the appropriate transformations U and V (see [14]). This procedure leads to the following bases.

$$\boldsymbol{f}_{DA'}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ d_2 + d_2^* \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \boldsymbol{f}^{(-)}_{DA'}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ d_2^* - d_2 \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \text{for } DA'$$

$$\boldsymbol{f}_{DA''}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} -d_1 - d_1^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \boldsymbol{f}^{(-)}_{DA''}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_1 - d_1^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \text{for } DA'' \tag{12}$$

$$\boldsymbol{f}_{DA}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_1 + d_1^* \\ d_2 + d_2^* \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \boldsymbol{f}^{(-)}_{DA}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_1^* - d_1 \\ d_2^* - d_2 \end{bmatrix} e^{i\boldsymbol{k}_1\boldsymbol{r}} \quad \text{for } DA.$$

We observe that the basis functions $\boldsymbol{f}_{DA'}$, $\boldsymbol{f}_{DA''}$ and $\boldsymbol{f}_{DA}$ are real at the lattice sites and, therefore, can be used in the expansion (10) with a real coefficient c. On the contrary,

Table 3. The low-temperature phase symmetry groups induced by the irreducible representations and corepresentations of *cmm'* and *p2'*.

Representation or corepresentation	Symmetry elements	Group symbol
B_2, DA'	$\{E\|a_1-a_2\}, \{E\|a_1+a_2\}, \{\theta\|a_1\}, E, \theta C_{2z}, \theta\sigma_{d1}, \sigma_{v1}$ $t=\frac{1}{2}a_1$	Number 28 $p_c' mg$
B_1, DA''	$\{E\|a_1-a_2\}, \{E\|a_1+a_2\}, \{\theta\|a_1\}, E, \theta C_{2z}, \theta\{\sigma_{d1}\|a_1\}, \{\sigma_{v1}\|a_1\}$ $t=0$	Number 28 $p_c' mg$
B, DA	$\{E\|a_1\}, \{E\|2a_2\}, \{\theta\|a_2\}, E, \theta C_{2z}$ $t=0$	Number 3 $p_b' mg$

the basis functions $f_{DA'}^{(-)}$, $f_{DA''}^{(-)}$ and $f_{DA}^{(-)}$, which stem from the negative sign in the formula (7.3.45) of [14] and which generate corepresentations (these corepresentations are formally identical to the representations A_1, A_2 of *cmm'* and A of *p2'*, respectively) equivalent to DA', DA'' and DA, respectively, are imaginary and, therefore, can only be applied in the expansion of M_s with an imaginary c. Due to the anti-unitariness of θ they lead to the same symmetry groups of M_s and the same spin structures as the functions $f_{DA'}$, $f_{DA''}$ and f_{DA}. For real d_1 and d_2 the functions $f_{DA'}^{(-)}$, $f_{DA'}$, $f_{DA''}^{(-)}$, $f_{DA''}$, $f_{DA}^{(-)}$, f_{DA} become basis functions of the irreducible representations A_1, B_2, A_2, B_1 of *cmm'* and A, B of *p2'*, respectively.

Introducing the functions (12) into (10) and utilizing (3), which connects the order parameter with the sublattice magnetizations, and the assumption that the symmetry of M_s determines the symmetry of the low-temperature phase, we obtain the magnetic moment $M(r)$ at the lattice site $r = n_1a_1 + n_2a_2$ of this phase:

$$M(r) = \frac{c(T,H)}{\sqrt{2}}\left\{\begin{bmatrix}0\\ d_2+d_2^*\end{bmatrix}(-1)^{n_1+n_2}, \begin{bmatrix}-d_1-d_1^*\\ 0\end{bmatrix}(-1)^{n_1+n_2}, \begin{bmatrix}d_1+d_1^*\\ d_2+d_2^*\end{bmatrix}(-1)^{n_1+n_2}\right\} \tag{13}$$

for DA', DA'' and DA, respectively,

$$M(r) = \begin{bmatrix}0\\ 0\\ 0\end{bmatrix} \qquad \text{for } A_1, A_2, A$$

and

$$M(r) = \frac{c(T,H)}{\sqrt{2}}\left\{\begin{bmatrix}-d_1\\ 0\end{bmatrix}(-1)^{n_1+n_2}, \begin{bmatrix}0\\ d_2\end{bmatrix}(-1)^{n_1+n_2}, \begin{bmatrix}d_1\\ d_2\end{bmatrix}(-1)^{n_1+n_2}\right\} \tag{14}$$

for B_1, B_2 and B, respectively. Thus we can conclude that the representations A_1, A_2 of *cmm'* and A of *p2'* do not induce magnetic phase transitions. The corepresentations DA', DA'' and DA generate spin structures which are identical to those obtained for the representations B_2, B_1 and B, respectively.

Acting on $M_s(r)$ with the symmetry operations of the group *cmm'* and *p2'* we determine the low-temperature groups, which we collect in table 3. In order to classify

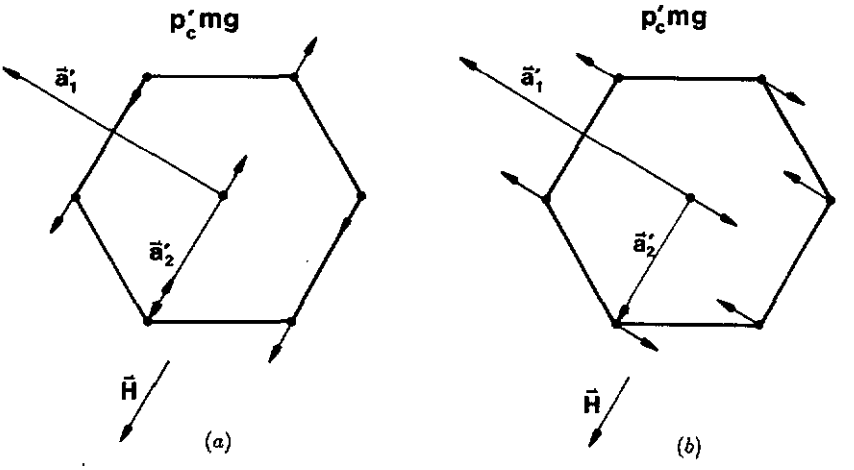

Figure 2. The low-temperature spin structures induced by the irreducible representations B_1 and B_2 and the corepresentations DA' and DA'' of the high-temperature symmetry group cmm'; (*a*) is induced by B_2 and DA', (*b*) is induced by B_1, DA''. Spin arrangements in the low-temperature phases induced by the irreducible representations and corepresentations of $p2'$ are analogous.

these groups with tabulated two-dimensional magnetic groups [20] we have to perform the following operations:

(i) move the origin of the coordinate system (x–y) by the appropriate vector t (see table 3),

(ii) introduce the new elementary translations

$$\boldsymbol{a}_1' = \boldsymbol{a}_1 - \boldsymbol{a}_2 \qquad \boldsymbol{a}_2' = \boldsymbol{a}_1 + \boldsymbol{a}_2 \tag{15}$$

for the groups induced by B_1, B_2, DA' and DA'', and

$$\boldsymbol{a}_1' = \boldsymbol{a}_1 \qquad \boldsymbol{a}_2' = 2\boldsymbol{a}_2 \tag{16}$$

for the groups induced by B and DA.

The results of the application of this procedure are given in table 3. The low-temperature spin structures connected with the calculated groups, which are determined by the formulas (13) and (14), are shown in figure 2.

An experimental verification of which of the calculated spin structures exists in the system is facilitated when the cross-section for elastic magnetic scattering of neutrons is known. The neutron magnetic scattering cross-section has the form (see [25])

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \sim |F(\boldsymbol{\kappa})|^2 \sum_{r,r'} \sum_{\alpha,\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta) M_\alpha^*(\boldsymbol{r}) M_\beta(\boldsymbol{r}') \exp[\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{r} - \boldsymbol{r}')] \tag{17}$$

where $F(\boldsymbol{\kappa})$ denotes the form factor, $\boldsymbol{\kappa}$ is the scattering vector, $\boldsymbol{e} = \boldsymbol{\kappa}/\kappa$, $\alpha, \beta = x, y$, $M_\alpha(\boldsymbol{r})$ and $M_\beta(\boldsymbol{r}')$ are the thermodynamic averages of the spin operator components at the lattice sites $\boldsymbol{r}$ and $\boldsymbol{r}'$, respectively. These spin vectors are determined by (10). Inserting

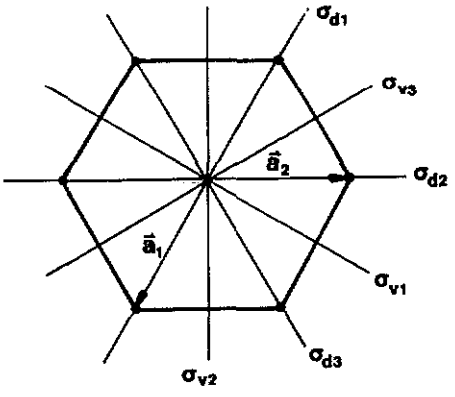

Figure 3. The basis vectors a_1 and a_2 and the symmetry elements of the diperiodic magnetic group $P6m'm'$. The magnetic field is perpendicular to the plane of the figure.

(10), with $f(r)$ determined by (12), into formula (17) and performing the summations, we obtain the magnetic scattering cross-section

$$\frac{d\sigma}{d\Omega} \sim |F(\kappa)|^2 a_2^2 (1 - e_y^2) \sum_K \delta(\kappa - k_1 - K) \tag{18}$$

for the spin structure induced by DA' and a similar formula with a_2, e_y replaced by a_1, e_x, for the structure induced by DA'', and

$$\frac{d\sigma}{d\Omega} \sim |F(\kappa)|^2 [a_1^2 (1 - e_x^2) - 2a_1 a_2 e_x e_y + a_2^2 (1 - e_y^2)] \sum_K \delta(\kappa - k_1 - K) \tag{19}$$

for the structure induced by DA. K is a reciprocal lattice vector, $a_1 = c(d_1 + d_1^*)$ and $a_2 = c(d_2 + d_2^*)$. For real d_1, d_2 the cross-sections (18) and (19) become the magnetic scattering cross-sections for the magnetic structures induced by the representations B_2, B_1 and B, respectively.

3. The phase transitions in a magnetic field perpendicular to the surface of the system

3.1. The thermodynamic potential density

As a magnetic field, which is perpendicular to the surface of the AFMT introduces the third dimension, the AFMT becomes a system with diperiodic symmetry, i.e. a system which has an infinite periodicity in only two dimensions but additionally allows symmetry elements which may affect the non-periodic third dimension. Therefore, the symmetry group of the AFMT is the diperiodic space group number 77: *P6mm* (see [26]). Consequently, the magnetic symmetry group of the composite system, consisting of the two-dimensional AFMT and the magnetic field, which is the maximal common subgroup of *P6mm* and of the symmetry group of the field, is the diperiodic magnetic space group

$$P6 + \theta\sigma_{d1} P6 \tag{20}$$

where $P6$ is the diperiodic space group number 76 (see [26]). Since the diperiodic magnetic space groups have not been classified yet, we shall follow Shubnikov and Belov [20] in their labelling of the two-dimensional magnetic space groups and call the group in (20) $P6m'm'$ (see figure 3).

Table 4. The irreducible, Landau and Lifshitz active representations and corepresentations of the diperiodic magnetic space group $P6m'm'$ at the point M of the reciprocal lattice space and the irreducible representation E_2 of the crystallographic point group $6mm$. In labelling the group elements we use symbols of Bradley and Cracknell [14]. The representation matrices for the group elements which contain the time-inversion operator have been multiplied by -1.

	E	C_6^+	$\theta\sigma_{d1}$	$n_1a_1 + n_2a_2$
B_1, DB	$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&0&-1\\1&0&0\\0&1&0\end{matrix}$	$\begin{matrix}-1&0&0\\0&0&1\\0&1&0\end{matrix}$	$\begin{bmatrix}\exp(in_2\pi) & 0 & 0\\ 0 & \exp[i(n_2-n_1)\pi] & 0\\ 0 & 0 & \exp(in_1\pi)\end{bmatrix}$
B_2	$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&0&-1\\1&0&0\\0&1&0\end{matrix}$	$\begin{matrix}1&0&0\\0&0&-1\\0&-1&0\end{matrix}$	
A_1, DA	$\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	$\begin{matrix}0&0&1\\1&0&0\\0&1&0\end{matrix}$	$\begin{matrix}-1&0&0\\0&0&-1\\0&-1&0\end{matrix}$	
E_2	$\begin{matrix}1&0\\0&1\end{matrix}$	$\begin{matrix}-\frac{1}{2}&-\frac{1}{2}\sqrt{3}\\ \frac{1}{2}\sqrt{3}&-\frac{1}{2}\end{matrix}$	$\begin{matrix}1&0\\0&-1\end{matrix}$	

The magnetic order parameter defined by (3) or (4) transforms according to the irreducible representations or corepresentations of $P6m'm'$ at the point M of the reciprocal lattice space. The irreducible, Landau and Lifshitz active representations A_1, B_1 and B_2 of $P6m'm'$ can be calculated from Kovalev's formula, and are given in table 4. As in the previous case, the irreducible corepresentations DA and DB of $P6m'm'$ can be obtained with the application of the algorithm given by Bradley and Cracknell [14]. The matrices of DB and DA are collected in table 4.

Consulting the tables of Birrs [23], we find the form of the strain tensor

$$\begin{bmatrix}\varepsilon_{11} & 0\\ 0 & \varepsilon_{11}\end{bmatrix}$$

which indicates that the high-temperature phase is not distorted. The symmetrized square $[D_p]^2$ of the polar vector representation of the crystallographic point group $6mm$, according to which this tensor transforms, may be reduced in the following way:

$$[D_p]^2 = A_1 \oplus E_2 \tag{21}$$

where now A_1 is the unit representation of $6mm$ and E_2 is given in table 4. The lattice distortion of the low-temperature phase, therefore, must be connected with the two-dimensional representation E_2.

With accuracy to sixth-order terms, the thermodynamic potential density which contains terms connected with both order parameters and mixed 'interaction' terms and which is invariant under the symmetry operations represented by the matrices of A_1, B_1, B_2, DB, DA and E_2 has the form:

$$\begin{aligned}\phi = \phi_0 &+ \tfrac{1}{2}A(T,H)(c_1^2 + c_2^2 + c_3^2) + \tfrac{1}{4}C_1(T,H)(c_1^2 + c_2^2 + c_3^2)^2\\ &+ \tfrac{1}{4}C_2(T,H)(c_1^4 + c_2^4 + c_3^4) + \tfrac{1}{2}D_1(T,H)(c_1^2c_2^2c_3^2)\\ &+ \tfrac{1}{8}D_2(T,H)(c_1^2 + c_2^2 + c_3^2)^3 + \tfrac{1}{8}D_3(T,H)(c_1^6 + c_2^6 + c_3^6)\end{aligned}$$

Table 5. The low-temperature phase symmetry groups induced by the active representations of $P6m'm'$ and the symmetry groups of the strain tensors. r depends on the phenomenological coefficients in the thermodynamic potential density (22). In the last column we list the non-zero components of the strain tensors.

Rep. or corep./ expansion coefficient	B_2	Group symbol	B_1	Group symbol	Symmetry of strain tensor	Orientation of reference axes	Tensor components
$c_1 \neq 0$ $c_2 = c_3 = 0$ $\gamma_1 \neq 0$ $\gamma_2 = 0$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $\theta\sigma_{d1}, \theta\{\sigma_{v1}\|a_2\}$ $a_1' = -a_1$ $a_2' = a_1 + 2a_2$ $t = \frac{1}{2}a_2$	$P_c'2ma$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $\theta\{\sigma_{d1}\|a_2\}\theta\sigma_{v1}$ $a_1' = -a_1$ $a_2' = +a_1 + 2a_2$ $t = \frac{1}{2}a_2$	$P_c'2ma$	$mm2$	$x\|\|\sigma_{d1}$ $y\|\|\sigma_{v1}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_2 \neq 0$ $c_1 = c_3 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\mp\sqrt{3}/2)$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $\theta\sigma_{d3}, \theta\{\sigma_{v3}\|a_1\}$ $a_1' = a_1 - a_2$ $a_2' = a_1 + a_2$ $t = \frac{1}{2}a_2$	$P_c'2ma$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $\theta\{\sigma_{d3}\|a_1\}, \theta\sigma_{v3}$ $a_1' = a_1 + a_2$ $a_2' = a_2 - a_1$ $t = \frac{1}{2}a_2$	$P_c'2ma$	$mm2$	$x\|\|\sigma_{d3}$ $y\|\|\sigma_{v3}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_3 \neq 0$ $c_1 = c_2 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\pm\sqrt{3}/2)$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $\theta\sigma_{d2}, \theta\{\sigma_{v2}\|a_1\}$ $a_1' = 2a_1 + a_2$ $a_2' = a_2$ $t = \frac{1}{2}a_1$	$P_c'2ma$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $\theta\{\sigma_{d2}\|a_1\}, \theta\sigma_{v2}$ $a_1' = -a_2$ $a_2' = 2a_1 + a_2$ $t = \frac{1}{2}a_1$	$P_c'2ma$	$mm2$	$x\|\|\sigma_{d2}$ $y\|\|\sigma_{v2}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_1 = c_2$ $c_3 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\pm\sqrt{3}/2)$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $\theta\{\sigma_{d2}\|a_2\}, \theta\sigma_{v2}$ $a_1' = 2a_1$ $a_2' = 2a_1 + 2a_2$ $t = \frac{1}{2}a_2$	$C_c'2mm$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $\theta\sigma_{d2}, \theta\{\sigma_{v2}\|a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_1 + 2a_2$ $t = a_1 + \frac{1}{2}a_2$	$C_c'2mm$	$mm2$	$x\|\|\sigma_{d2}$ $y\|\|\sigma_{v2}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_1 = c_3$ $c_2 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\mp\sqrt{3}/2)$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $\theta\sigma_{d3}, \theta\{\sigma_{v3}\|a_1 + a_2\}$ $a_1' = 2a_2$ $a_2' = -2a_1$ $t = \frac{1}{2}(a_1 + a_2)$	$C_c'2mm$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $\theta\{\sigma_{d3}\|a_1 + a_2\}, \theta\sigma_{v3}$ $a_1' = 2a_2$ $a_2' = -2a_1$ $t = \frac{3}{2}a_1 + \frac{1}{2}a_2$	$C_c'2mm$	$mm2$	$x\|\|\sigma_{d3}$ $y\|\|\sigma_{v3}$	$\varepsilon_{11}, \varepsilon_{22}$

$c_2 = c_3$ $c_1 = 0$ $\gamma_1 \neq 0$ $\gamma_2 = 0$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$, $\theta\{\sigma_{d1}\|a_1\}, \theta\sigma_{v1}$ $a_1' = 2a_1 + 2a_2$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1 + a_2$	$C_c'2mm$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$, $\theta\sigma_{d1}, \theta\{\sigma_{v1}\|a_1\}$, $a_1' = 2a_1 + 2a_2$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1$	$C_c'2mm$	$mm2$	$x\|\sigma_{d1}$ $y\|\sigma_{v1}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_1 = -c_2$ $c_3 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\pm\sqrt{3}/2)$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$, $\theta\{\sigma_{d2}\|a_2\}, \theta\sigma_{v2}$ $a_1' = 2a_1$ $a_2' = 2a_1 + 2a_2$ $t = a_1 + \frac{1}{2}a_2$	$C_c'2mm$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$, $\theta\sigma_{d2}, \theta\{\sigma_{v2}\|a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_1 + 2a_2$ $t = \frac{1}{2}a_2$	$C_c'2mm$	$mm2$	$x\|\sigma_{d2}$ $y\|\sigma_{v2}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_1 = -c_3$ $c_2 = 0$ $\gamma_1 = r(\pm 1/2)$ $\gamma_2 = r(\mp\sqrt{3}/2)$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $\theta\sigma_{d3}, \theta\{\sigma_{v3}\|a_1 + a_2\}$ $a_1' = 2a_2$ $a_2' = -2a_1$ $t = \frac{1}{2}a_1 + a_2$	$C_c'2mm$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $\theta\{\sigma_{d3}\|a_1 + a_2\}, \theta\sigma_{v3}$ $a_1' = 2a_2$ $a_2' = -2a_1$ $t = \frac{3}{2}a_1 + \frac{1}{2}a_2$	$C_c'2mm$	$mm2$	$x\|\sigma_{d3}$ $y\|\sigma_{v3}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_2 = -c_3$ $c_1 = 0$ $\gamma_1 \neq 0$ $\gamma_2 = 0$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$, $\theta\{\sigma_{d1}\|a_1\}, \theta\sigma_{v1}$ $a_1' = 2a_1 + 2a_2$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1 + a_2$	$C_c'2mm$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$, $\theta\sigma_{d1}, \theta\{\sigma_{v1}\|a_1\}$, $a_1' = 2a_1 + 2a_2$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1$	$C_c'2mm$	$mm2$	$x\|\sigma_{d1}$ $y\|\sigma_{v1}$	$\varepsilon_{11}, \varepsilon_{22}$
$c_1 \neq \pm c_2$ $c_3 = 0$ $\gamma_1 = \gamma_2$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}a_2$	$P_b'211$	$E, \{\theta\|a_2\}, \{C_{2z}\|a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}a_2$	$P_b'211$	2	$z\|C_{2z}$	$\varepsilon_{11}, \varepsilon_{12}$ $\varepsilon_{21}, \varepsilon_{22}$
$c_1 \neq \pm c_3$ $c_2 = 0$ $\gamma_1 = \gamma_2$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}(a_1 + a_2)$	$P_b'211$	$E, \{\theta\|a_1 + a_2\}, \{C_{2z}\|a_1 + a_2\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}(a_1 + a_2)$	$P_b'211$	2	$z\|C_{2z}$	$\varepsilon_{11}, \varepsilon_{12}$ $\varepsilon_{21}, \varepsilon_{22}$
$c_2 \neq \pm c_3$ $c_1 = 0$ $\gamma_1 = \gamma_2$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1$	$P_b'211$	$E, \{\theta\|a_1\}, \{C_{2z}\|a_1\}$ $a_1' = 2a_1$ $a_2' = 2a_2$ $t = \frac{1}{2}a_1$	$P_b'211$	2	$z\|C_{2z}$	$\varepsilon_{11}, \varepsilon_{12}$ $\varepsilon_{21}, \varepsilon_{22}$

$$+\tfrac{1}{2}A'(T,H)(\gamma_1^2+\gamma_2^2)+\tfrac{1}{3}E(T,H)(\gamma_1^3-3\gamma_1\gamma_2^2)+\tfrac{1}{4}C_3(T,H)(\gamma_1^2+\gamma_2^2)^2$$
$$+\tfrac{1}{5}F(T,H)(\gamma_1^5-2\gamma_1^3\gamma_2^2-3\gamma_1\gamma_2^4)+\tfrac{1}{6}D_4(T,H)(\gamma_1^2+\gamma_2^2)^3$$
$$+G_1(T,H)\left[\left(3c_1^2-\sum_{i=1}^{3}c_i^2\right)\gamma_1+\sqrt{3}(c_2^2-c_3^2)\gamma_2\right]$$
$$+G_2(T,H)\left[\left(3c_1^4-\sum_{i=1}^{3}c_i^4\right)\gamma_1+\sqrt{3}(c_2^4-c_3^4)\gamma_2\right] \tag{22}$$

where (c_1,c_2,c_3) and (γ_1,γ_2) transform under A_1, B_1, B_2, DB or DA and E_2, respectively, and

$$A(T,H)=a_T(T-T_t)+a_H(H-H_t) \qquad C_1(T,H)=c_T(T-T_c)+c_H(H-H_c) \tag{23}$$

with $a_Tc_H \neq a_Hc_T$. The minimization of ϕ is facilitated if we introduce the angular coordinates by the equations:

$$c_1=R\sin\theta\cos\varphi \qquad c_2=R\sin\theta\sin\varphi \qquad c_3=R\cos\theta$$
$$\gamma_1=r\cos\alpha \qquad \gamma_2=r\sin\alpha. \tag{24}$$

The necessary conditions for the minimum of ϕ lead to the sets of values of the coefficients c_1, c_2, c_3, γ_1 and γ_2 which are collected in table 5. The sufficient conditions can also be written out and fulfilled with appropriate values of the phenomenological parameters $A, A', C_1, C_2, C_3, D_1, D_2, D_3, D_4, E, F, G_1$ and G_2.

3.2. The symmetry changes and spin structures

The sets of values of the coefficients c_i which minimize the potential density (22) (see table 5) determine the magnetic order parameter below the critical point

$$\boldsymbol{M}_s(r)=c_1(T,H)\boldsymbol{f}_1(r)+c_2(T,H)\boldsymbol{f}_2(r)+c_3(T,H)\boldsymbol{f}_3(r) \tag{25}$$

where $\boldsymbol{f}_1, \boldsymbol{f}_2, \boldsymbol{f}_3$ are axial-vector basis functions of A_1, B_1, B_2, DA or DB, respectively.

The basis functions of DA and DB, which can be calculated with the method described in the previous section, have the following form

$$\boldsymbol{f}_{DA}^{1}(r)=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\d_3-d_3^*\end{bmatrix}e^{ik_1r} \qquad \boldsymbol{f}_{DA}^{2}(r)=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\d_3-d_3^*\end{bmatrix}e^{ik_2r}$$

$$\boldsymbol{f}_{DA}^{3}(r)=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\d_3-d_3^*\end{bmatrix}e^{ik_3r}$$

$$\boldsymbol{f}_{DA}^{1(-)}(r)=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\-d_3-d_3^*\end{bmatrix}e^{ik_1r} \qquad \boldsymbol{f}_{DA}^{2(-)}(r)=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\-d_3-d_3^*\end{bmatrix}e^{ik_2r}$$

$$f_{DA}^{3(-)}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 0 \\ -d_3 - d_3^* \end{bmatrix} e^{i\boldsymbol{k}_3 \boldsymbol{r}} \tag{26}$$

$$f_{DB}^{2}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_1 - d_1^* + d_2^* \\ d_2 + d_2^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_1 \boldsymbol{r}} \qquad f_{DB}^{2}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_1 - d_1^* - d_2 \\ d_1 - d_1^* + d_2^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_2 \boldsymbol{r}}$$

$$f_{DB}^{3}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} -d_2 - d_2^* \\ d_1 - d_1^* - d_2 \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_3 \boldsymbol{r}}$$

$$f_{DB}^{1(-)}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} -d_1 - d_1^* + d_2^* \\ -d_2 + d_2^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_1 \boldsymbol{r}} \qquad f_{DB}^{2(-)}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} -d_1 - d_1^* + d_2 \\ -d_1 - d_1^* + d_2^* \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_2 \boldsymbol{r}}$$

$$f_{DB}^{3(-)}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\begin{bmatrix} d_2 - d_2^* \\ -d_1 - d_1^* + d_2 \\ 0 \end{bmatrix} e^{i\boldsymbol{k}_3 \boldsymbol{r}}$$

where $\boldsymbol{k}_1 = \frac{1}{2}\boldsymbol{b}_2$ is the wavevector at the point M of the reciprocal lattice space, $\boldsymbol{k}_2 = (\boldsymbol{b}_1 - \boldsymbol{b}_2)$, $\boldsymbol{k}_3 = \frac{1}{2}\boldsymbol{b}_1$ are the wavevectors from the star ${}^*\boldsymbol{k}_1$, and d_1, d_2, d_3 are complex numbers referred to the axes (x, y, z) of the coordinate system determined by the Bravais lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ of the high-temperature phase (see figure 3). For real d_1, d_2, d_3 the functions $f_{DA}^{1,2,3}$, $f_{DB}^{1,2,3}$ and $f_{DB}^{1,2,3(-)}$ become axial-vector basis functions of the representations A_1, B_1 and B_2, respectively.

We notice that the functions $f_{DB}^{1,2,3}$ and $f_{DB}^{1,2,3(-)}$ contain real and complex components and therefore cannot be applied in expansion (25) of the magnetic order parameter, which is a real function. This means that the corepresentation DB does not induce magnetic phase transitions. On the other hand the functions $f_{DA}^{1,2,3}$, which are pure imaginary, can only be used in the expansion of M_s with imaginary parameters c_1, c_2, c_3. These parameters, however, transform according to the corepresentation DA^-, (i.e. the corepresentation generated by the functions $f_{DA}^{1,2,3(-)}$), which is not Landau active. We therefore conclude that the active corepresentations DA, DB of $p6m'm'$ cannot be applied to describe magnetic phase transitions and, consequently, the low-temperature spin structures of the system.

Since the axial-vector basis functions of A_1 vanish (see (26)), this representation cannot generate magnetic phase transitions of the system. Introducing the basis functions of the remaining representations into (25) and using the assumption concerning the symmetry of a possible low-temperature phase (see the previous section), we obtain the magnetic structures shown in figure 4. The symmetry groups of these structures are given in table 5. To identify these groups we have shifted the origin of the coordinate system x–y by the appropriate vector $\boldsymbol{t}$, which we also give in table 5. In the labelling of the low-temperature, diperiodic magnetic space groups we applied the same method which had earlier been proposed by Shubnikov and Belov [20].

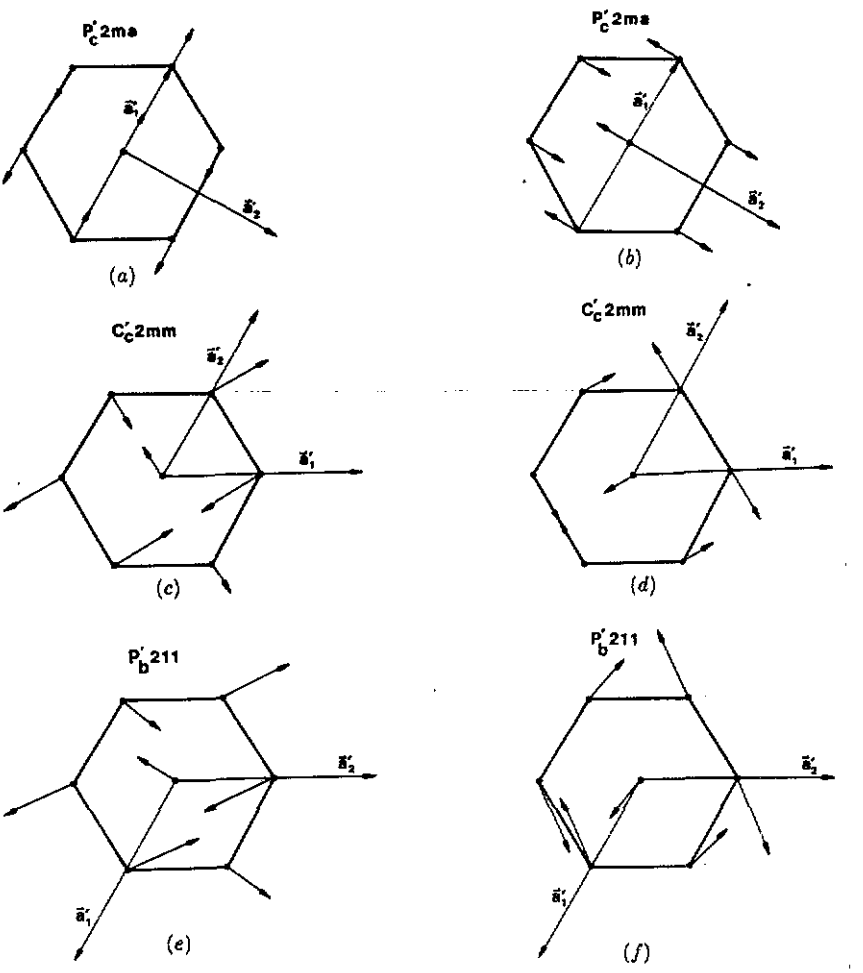

Figure 4. The low-temperature spin structures induced by the irreducible representations B_1 and B_2 of the high-temperature symmetry group $P6m'm'$; (*a*), (*c*), (*e*) are induced by B_2 and (*b*), (*d*), (*f*) by B_1.

Similarly, the equilibrium values of γ_i determine the symmetry groups of the strain tensors connected with the low-temperature phases of the system. The strain tensors, which can be found from the tables of Birrs [23], are collected in table 5. They describe the lattice distortions that accompany the magnetic phase transitions of the system. Among the sets of c_i and γ_i which minimize the potential density (22) there also appear ones that violate Neumann's criterion, i.e. that lead to the low-temperature symmetry groups whose crystallographic classes do not coincide with the symmetry groups of the relevant strain tensors. As they do not have any physical meaning, we have excluded them from table 5.

The neutron magnetic scattering cross-sections for the spin structures determined by the sets of values of c_i collected in table 5 can again be calculated on the grounds of (17). In the Cartesian coordinate system (x, y, z) whose x and z axes are defined by the magnetic moment direction at the origin of the $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$ system (see figures 3 and 4)

and the a_3 vector, respectively, these cross-sections have the following form

$$\frac{d\sigma}{d\Omega} \sim |F(\kappa)|^2 a_i^2 (1 - e_x^2) \sum_K \delta(\kappa - k_i - K)$$

for the solutions with $c_i \neq 0$,

$$\frac{d\sigma}{d\Omega} \sim |F(\kappa)|^2 \Big\{ [a_1^2(1 - e_x^2) + b_1^2(1 - e_y^2)] \Big[\sum_K (\delta(\kappa - k_1 - K) + \delta(\kappa - k_2 - K)) \Big]$$
$$-2a_1 b_1 e_x e_y \Big[\sum_K (\delta(\kappa - k_2 - K) - \delta(\kappa - k_1 - K)) \Big] \Big\} \tag{27}$$

for the solutions with $c_i, c_j \neq 0$, $c_i = \pm c_j$, and

$$\frac{d\sigma}{d\Omega} \sim |F(\kappa)|^2 \Big\{ (1 - e_x^2) \Big[\sum_K (a_1^2 \delta(\kappa - k_1 - K) + a_2^2 \delta(\kappa - k_2 - K)) \Big]$$
$$+ (1 - e_y^2) \Big[\sum_K (b_1^2 \delta(\kappa - k_1 - K) + b_2^2 \delta(\kappa - k_2 - K)) \Big]$$
$$-2e_x e_y \Big[\sum_K (a_2 b_2 \delta(\kappa - k_2 - K) - a_1 b_1 \delta(\kappa - k_1 - K)) \Big] \Big\}$$

for the solutions with c_i, $c_j \neq 0$, $c_i \neq \pm c_j$, where now $a_i = (\sqrt{3}/2\sqrt{2})c_i(-2d_1 + d_2)$, $b_i = (1/2\sqrt{2})c_i(-2d_1 + d_2)$, $i = 1, 2$.

The cross-sections above can facilitate the experimental identification of the various magnetic structures shown in figure 4.

4. Conclusions

We have discussed symmetry changes in a two-dimensional AFMT placed in an external magnetic field. Depending on whether the field is parallel or perpendicular to the surface of the antiferromagnet, the composite system (two-dimensional AFMT plus field) is described by a two-dimensional magnetic group (cmm' or $p2'$) or by a diperiodic magnetic space group ($P6m'm'$). These groups were treated as unitary or non-unitary and their irreducible representations or corepresentations, respectively, were applied in the calculation. The two descriptions of the high-temperature magnetically ordered phases proved to be equivalent when the magnetic field is parallel, and contradictory when it is perpendicular to the surface of the AFMT. In the second case, contrary to the experimental observations (see the Introduction), the corepresentations do not induce magnetic phase transitions. It means that, in this case, the description of the high-temperature phase of the antiferromagnet by the non-unitary group $P6m'm'$ is incorrect. However, when this group is treated as unitary, we obtain a variety of spin arrangements (see figure 4) including experimentally observed antiferromagnetic spin structures.

We thus conclude that, in general, a description of magnetic crystals in terms of non-unitary magnetic groups is incorrect. We also notice that, due to the fact that real corepresentations may have non-real axial-vector basis functions, particular care should be taken while applying corepresentations of magnetic groups to the calculation of symmetry changes at magnetic phase transitions within the framework of Birman's theory (see [13]). The group-theoretical criteria of Birman should, in this case, be supplemented with a condition of reality of basis functions of irreducible co-representations.

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