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Application of the irreducible part of the Brillouin zone to band-structure calculations in ferromagnetic crystals

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Abstract. The irreducible part of the Brillouin zone (IBZ) constructed for a non-magnetic crystal phase is commonly used in band-structure calculations. The IBZ changes its shape and volume in a ferromagnetic crystal phase. We shall show how the IBZ constructed for a non-magnetic crystal phase can be utilized for a ferromagnetic crystal phase in band-structure calculations. Applying magnetic space group theory, we shall justify the last statement.

1. Introduction

In energy band calculations the so-called irreducible part of the Brillouin zone (IBZ) is used. To construct the IBZ in a non-magnetic crystal phase we consider k-vectors in a general position [1–4]. We are dealing with a classical space group G under which the Hamiltonian $\hat{\mathcal{H}}$ is invariant. Formally this means that the commutator $[G, \hat{\mathcal{H}}]$ equals zero. We then find for the energy eigenvalues [1–4]

$$E_n(\boldsymbol{k}) = E_n(\boldsymbol{k}_i) \qquad i = 1, \ldots, N \tag{1.1}$$

where n is the quantum number labelling eigenvalues and where the vectors $\boldsymbol{k}_i$ belong to the N-arm star of a k-vector in a general position [1–4]. The index n will be omitted from here on in the text. The reason for using the IBZ instead of the entire Brillouin zone (BZ) is expressed by the equality [1–4]:

$$\sum_{\boldsymbol{k}\in \mathrm{BZ}} E(\boldsymbol{k}) = |F| \sum_{\boldsymbol{k}\in \mathrm{IBZ}} E(\boldsymbol{k}) \tag{1.2}$$

where $|F|$ is the order of the point group F, which determines the crystal class connected with space group G. The IBZ is of much smaller size than the BZ, hence applying equation (1.2) in band calculations results in an increase of the exactness of these calculations. In these calculations we use a grid of points in momentum space. With the same number of points in the grid we achieve a higher exactness of calculations for the IBZ than for the BZ. Certainly, by enlarging the number of points in the grid we can cope with a larger momentum space, but that is either hardly possible due to computer-in-use limitations or causes a large increase in computer time consumption. In the standard computer programs for band-structure calculations, the IBZ is usually utilized.

The question arises: Is equation (1.2) applicable to magnetic crystals, when we are dealing with the magnetic groups? To answer this question we shall discuss paramagnetic

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and ferromagnetic crystal phases separately. In section 2 we shall show that for the paramagnetic crystal phase equation (1.2) remains valid without any change. Two approaches were proposed to maintain the notion for the IBZ for a ferromagnetic phase. In the first approach, introduced by Singh *et al* [5] on the basis of papers by Falicov and Ruvalds [6] and Cracknell [1, 2] and then used among others by Brooks and Kelly [7] and Fritsche *et al* [8], equation (1.2) is maintained while altering the meaning of the factor $|F|$ and of the IBZ. The factor $|F|$ now denotes the order of type III magnetic point group [7, 8]. The IBZ is modified as compared to that for the non-magnetic case. The modified IBZ (MIBZ) is larger than the non-magnetic, unmodified IBZ, so using it may lower the exactness of the calculations as well. For example, in the case of an iron crystal for magnetization parallel to the [110] direction we find that the volume of the MIBZ is six times larger than that of the IBZ [8]. The second approach was suggested without proof by Kondorskii [9] for the case of a ferromagnetic domain of an iron crystal with the magnetization parallel to the [100] direction or the [110] direction, and keeps the unmodified, non-magnetic IBZ for a ferromagnetic crystal phase with an appropriate change of formula (1.2). Kondorskii's approach saves us the time we had to spend on changing our programs generating the grid of k-vectors for the IBZ into programs generating the grid for the MIBZ. In section 3 we shall present a detailed group-theoretical justification of Kondorskii's suggestion. As a basis we shall use two papers by Cracknell [1, 2] in which the role of magnetic symmetry in energy band calculations was investigated.

A clarification of the situation seems to be needed since the unmodified IBZ together with formula (1.2) were applied to ferromagnetic crystal phases in several papers [10–12].

At the same time the arguments of magnetic group theory have been applied to the Green function (GF) method used in a ferromagnetic crystal phase by Hörmandinger and Weinberger [13]. The reduction of the amount of numerical work has been achieved by use of the MIBZ. The MIBZ in their calculation can be replaced with the IBZ for a non-magnetic crystal phase according to the formula (3.15) of this paper.

2. The IBZ of a paramagnetic crystal

In the one-electron theory the behaviour of an electron in a paramagnetic crystal without an external magnetic field is determined by the Pauli Hamiltonian. To describe a paramagnetic crystal symmetry we use a type II magnetic group G_M (the so-called grey group):

$$G_M = G + \theta G \tag{2.1}$$

where G is a classical space group and θ is the time-reversal operator [1–4, 14, 15].

The question is: Does the use of grey groups in the spinor space (we are dealing with electrons with spin) change formula (1.1). The Pauli Hamiltonian $\hat{\mathcal{H}}$ is invariant under the operations of the group $G_0 = G \otimes \mathrm{SU}(2)$ and under the time-reversal operator θ [15],

$$[G_0, \hat{\mathcal{H}}] = 0. \tag{2.2}$$

The symmetry elements of the group $G \otimes \mathrm{SU}(2)$ are

$$\pm u(R)T(g) \qquad g = \{R|\tau_R + t_n\} \in G \tag{2.3}$$

where τ_R is a fractional translation connected with a rotational element R, t_n is an integral translation and the matrices u constitute the group SU(2). In the one-electron theory the

operator $\theta = \sigma_2 K$, where σ_2 is the Pauli matrix and K is the complex conjugation operator [15]. The action of $\theta T(g)$ on spinor wavefunctions is determined by

$$\theta g \Psi_{k,\uparrow} = \Psi_{-k_i,\downarrow} \qquad \theta g \Psi_{k,\downarrow} = \Psi_{-k_i,\uparrow} \qquad g = \{R|\tau_R\},\ k_i = Rk \tag{2.4}$$

where the arrows $\downarrow$ and $\uparrow$ indicate wavefunctions for spin 'down' and 'up' respectively. From equations (2.1) and (2.4) we obtain the equalities:

$$\begin{aligned} E_\uparrow(k) &= E_\uparrow(k_i) \qquad E_\uparrow(k) = E_\downarrow(-k_i) \\ E_\downarrow(k) &= E_\downarrow(k_i) \qquad E_\downarrow(k) = E_\uparrow(-k_i) \end{aligned} \qquad i = 1, \ldots, N. \tag{2.5}$$

Considering the fact that in the paramagnetic phase the energies for spin 'up' and 'down' are equal, $E_\uparrow(k) = E_\downarrow(k) = E(k)$, and under the condition that a group G from equation (2.1) contains the space-inversion element, using equations (2.5), for each k-vector, we again obtain $E(k) = E(k_i)$, $i = 1, \ldots, N$, i.e. equation (1.1). When the space-inversion operation does not belong to the group G then the order of the star of k in a general position for the grey group $G + \theta G$ is doubled compared to that of G. The IBZ for the group $G + \theta G$ decreases by a factor 2 compared to the IBZ constructed for the classical space group G in equation (2.1). Owing to the equations (2.5) we can utilize the IBZ for the non-magnetic group G also in this case. Hence the IBZ constructed for a classical space group G can be used for the magnetic grey group G_M from equation (2.1). Consequently equation (1.2) holds for a paramagnetic crystal.

3. The IBZ of a ferromagnetic crystal

We consider a single ferromagnetic domain [1,2] with the magnetization vector M_β. Its symmetry is described by a type III magnetic group $G_M[\beta]$

$$G_M[\beta] = H + \theta(G - H) \tag{3.1}$$

where β specifies the magnetization vector and where H is the unitary halving subgroup of the space group G. The group $G_M[\beta]$ is a subgroup of the group $G + \theta G$.

As we have stated in section 1 the definition of the IBZ is connected with the star of the wave vector k in a general position. Conforming with the definition of the magnetic little group [1–3, 16] the star of the k-vector in a general position consists of the vectors [3, 16]

$${}^*k = (k_1, k_2, \ldots, k_{N-1}, k_N,\ k_{N+1}, \ldots, k_{2N}) \tag{3.2a}$$

where N is the order of the star of k_1 for the unitary subgroup of the magnetic group in equation (3.1). The vectors from k_1 to k_N are

$$\{k_1, \ldots, k_N\} = uk \not\equiv k + q \tag{3.2b}$$

where u is a unitary element, and the vectors from k_{N+1} to k_{2N} are

$$\{k_{N+1}, \ldots, k_{2N}\} = ak \not\equiv k + q \tag{3.2c}$$

where a is an anti-unitary element of the magnetic group, and where q is an integral reciprocal lattice vector. The number of vectors in the star of the k-vector in a general

Table 1. Magnetic point groups for magnetization directions: [001], [010], [100]. Notation of the symmetry elements after Bradley and Cracknell [3].

Unitary elements				Anti-unitary elements $\times\theta^{-1}$			
Magnetic group G_M[001]							
E	I	C_{4z}^{+}	S_{4z}^{-}	σ_{db}	C_{2a}	C_{2b}	σ_y
C_{2z}	C_{4z}^{-}	S_{4z}^{+}	σ_z	C_{2y}	C_{2x}	σ_x	σ_{da}
Magnetic group G_M[010]							
E	I	C_{4y}^{+}	S_{4y}^{-}	σ_{dc}	C_{2e}	C_{2x}	σ_z
C_{2y}	C_{4y}^{-}	S_{4y}^{+}	σ_y	C_{2z}	C_{2x}	C_{2c}	σ_{de}
Magnetic group G_M[100]							
E	C_{2x}	C_{4x}^{-}	S_{4x}^{-}	C_{2y}	C_{2f}	σ_y	σ_{df}
I	C_{4x}^{+}	σ_x	S_{4x}^{+}	C_{2z}	C_{2d}	σ_z	σ_{dd}

position for a ferromagnetic phase is equal either to the order of the point group connected with the unitary subgroup H in equation (3.1) or to the order of the magnetic point group connected with the magnetic group $G_M[\beta]$ in equation (3.1).

As an example we consider the star of a k-vector in a general position for a ferromagnetic domain of an iron crystal with magnetization parallel to the [100] direction. In the notation of Bradley and Cracknell [3] the magnetic point group for such a case is $4mm'm$ and is given in table 1. For the vector

$$k = \nu_1 g_1 + \nu_2 g_2 + \nu_3 g_3 \qquad 0 < \nu_1, \nu_2, \nu_3 < 1 \tag{3.3}$$

where g_i $(i = 1, 2, 3)$ are integral reciprocal lattice vectors, we obtain the following star vectors:

$$^*k = \begin{cases} Ek = k, Ik = -k, C_{2x}k, C_{4x}^{-}k, C_{4x}^{+}k, \sigma_x k, S_{4x}^{-}k, S_{4x}^{+}k, \\ \theta C_{2y}k, \theta C_{2z}k, \theta C_{2f}k, \theta C_{2d}k, \theta\sigma_y k, \theta\sigma_z k, \theta\sigma_{df}k, \theta\sigma_{dd}k. \end{cases} \tag{3.4}$$

We recall that the BZ consists of as many IBZ as there are vectors in the star of a k-vector in a general position. For the star in equation (3.4) the MIBZ contains three IBZ, i.e. IBZ_1, IBZ_2, IBZ_3 (see figure 1). Vectors $k = (k_x, k_y, k_z)$ in a general position situated within those IBZ are confined by the following boundaries:

$$IBZ_1 \begin{cases} 0 \leqslant k_z \leqslant 1/2 & & \\ k_z \leqslant k_y \leqslant 1/2 & \text{then} & k_z \leqslant k_x \leqslant k_y \\ 1/2 \leqslant k_y \leqslant 1 - k_z & \text{then} & k_z \leqslant k_x \leqslant -k_y + 1 \end{cases} \tag{3.5a}$$

$$IBZ_2 \begin{cases} 0 \leqslant k_x \leqslant 1/2 & & \\ k_x \leqslant k_y \leqslant 1/2 & \text{then} & k_x \leqslant k_z \leqslant k_y \\ 1/2 \leqslant k_y \leqslant 1 - k_x & \text{then} & k_x \leqslant k_z \leqslant -k_y + 1 \end{cases} \tag{3.5b}$$

$$IBZ_3 \begin{cases} 0 \leqslant k_x \leqslant 1/2 & & \\ k_x \leqslant k_z \leqslant 1/2 & \text{then} & k_x \leqslant k_y \leqslant k_z \\ 1/2 \leqslant k_z \leqslant 1 - k_x & \text{then} & k_x \leqslant k_y \leqslant -k_z + 1. \end{cases} \tag{3.5c}$$

In general the MIBZ consists of m original IBZ, where the number m is equal to $|F|/|F_M|$. For the reasons specified in section 1 utilization of the original IBZ is preferable in numerical

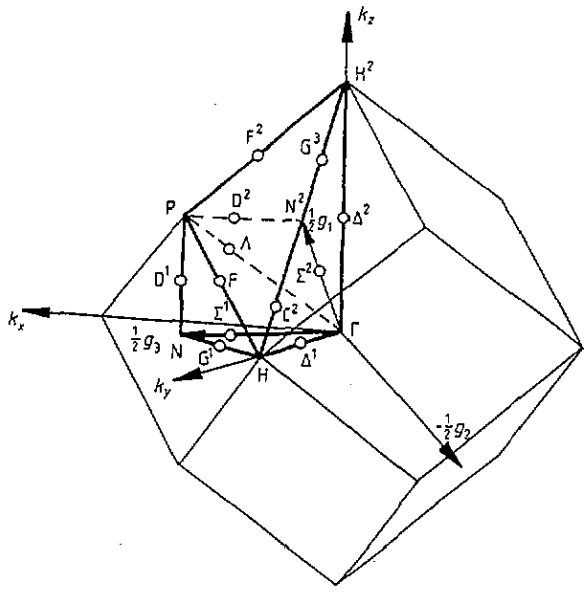

Figure 1. The IBZ in O_h class. The thick line determines the irreducible part of the Brillouin zone for a ferromagnetic crystal phase when magnetization is parallel to [100] (Cracknell [2]). Note that the edges of the IBZ_1 defined in equation (3.5*a*) are determined by the points $\Gamma\ \Delta^1\ H\ G^1\ N\ \Sigma^1\ D^1\ P\ F\ \Lambda$, the edges of the IBZ_2 defined in equation (3.5*b*) are determined by the points $\Gamma\ \Delta^1\ H\ F\ P\ D^2\ N^2\ \Sigma^2\ \Lambda$, and the edges of the IBZ_3 defined in equation (3.5*c*) are determined by the points $\Gamma\ \Lambda\ P\ D^2\ N^2\ \Sigma^2\ \Delta^2\ H^2\ G^3\ F^2$.

calculations. For the case specified in our example we may write:

$$\sum_{k\in BZ} E([100],k) = |F_M| \sum_{k\in MIBZ_1} E([100],k)$$

$$= |F_M|\left(\sum_{k_1\in IBZ_1} E([100],k_1) + \sum_{k_2\in IBZ_2} E([100],k_2) + \sum_{k_3\in IBZ_3} E([100],k_3)\right) \quad (3.6)$$

where the first equality was utilized for example by Fritsche [8] and Kondorskii's idea [9] concerning the last two terms of the second equality is expressed by:

$$\begin{aligned} E([100],k_2 \in IBZ_2) &= E([001],k_1 \in IBZ_1) \\ E([100],k_3 \in IBZ_3) &= E([010],k_1 \in IBZ_1) \end{aligned} \quad (3.7)$$

where the IBZ_i, $i = 1, 2, 3$, are defined by equations (3.5) (see figure 1). The directions [001], [010] and [100] of magnetization are physically equivalent. To the physical equivalence corresponds the equivalence of the respective magnetic groups. This may be verified by applying Burckhardt's theorem [17].

We shall show that equations (3.7) can be generalized to the form

$$E(M_1, k \in IBZ_\alpha) = E(M_\alpha, k \in IBZ_1) \qquad \alpha = 2, \ldots, p \quad (3.8)$$

where each IBZ_α, $\alpha = 2, \ldots, p$, is equal to the original irreducible part of the BZ for the non-magnetic case (see figure 1). In the above example IBZ_1 is defined by (3.5*a*) and IBZ_α is

IBZ$_2$ or IBZ$_3$, from equations (3.5*b*) and (3.5*c*), respectively. The vectors k_i, $i = 1, 2, 3$, on both sides of equation (3.7), belong to the stars of the two magnetic groups of the respective equivalent magnetizations involved. Let the number of physically equivalent directions of magnetization be p. The magnetizations M_α, $\alpha = 2, \ldots, p$, are physically equivalent to the magnetization M_1. Each of the IBZ$_\alpha$ being a part of the MIBZ can be attached to one of the equivalent magnetizations M_α, $\alpha = 1, \ldots, p$. The actual assignment is conditioned by the element g in equation (3.9) below. We observe that if equivalent groups correspond to the magnetizations M_1 and M_α, $\alpha = 2, \ldots, p$, then these magnetizations are on the same orbit [3]. That means that there is such an element g which transforms the vector M_1 into M_α,

$$gM_1 = M_\alpha \qquad g \neq E, I \tag{3.9}$$

where the space inversion I is excluded since the magnetic groups of $\mp M_1$ are the same.

The operation of an element g belonging to a magnetic group $G_M[\beta]$ on a wavefunction is defined by

$$g\Psi(M, k) = \Psi(g^{-1}M, gk) \qquad \text{for any } g \in G_M[\beta]. \tag{3.10}$$

Since the element g commutes with the Pauli Hamiltonian $\hat{\mathcal{H}}$, we have

$$g\hat{\mathcal{H}}\Psi(M_\alpha, k_1) = E(M_\alpha, k_1)g\Psi(M_\alpha, k_1) \tag{3.11}$$

and

$$\hat{\mathcal{H}}\Psi(M_1, gk_1) = E(M_1, k_1)\Psi(M_1, gk_1) \tag{3.12}$$

Hence

$$E(M_\alpha, k_1) = E(M_1, gk_1). \tag{3.13}$$

We require that the element g which according to equation (3.9) changes M_1 into M_α at the same time changes the vector k_1 belonging to the IBZ$_1$ (see figure 1) into the vector $k_q = gk_1$ belonging to the IBZ$_q$, with IBZ$_1$ and IBZ$_q$ being parts of the same MIBZ. With the help of the magnetic groups determined in [1, 2] it can be verified that for ferromagnetic crystals belonging to the cubic or hexagonal crystalline systems two cases can occur:

(a) The element g belongs to a magnetic group $G_M[\beta]$ except for $G_M[\alpha]$ or $G_M[1]$.

(b) The element g belongs to $G + \theta G - \bigcup_{\alpha=1}^{p} G_M[\alpha]$ and is equal to the product $g_\alpha g_\beta$ where g_α and g_β belong to $G_M[\alpha]$ and $G_M[\beta]$ respectively, $G + \theta G$ denotes the grey group of the paramagnetic phase of the considered ferromagnetic domain and p denotes the number of equivalent directions of magnetization.

Case (a). We begin with the observation that g cannot change k_1 into $k_q = gk_1$, being another vector of the same magnetic star, since then $gM_1 = M_\alpha$, contrary to equation (3.9). This means that the vectors k_1 and k_q may both be situated within the MIBZ (see figure 1). We also deduce that k_q cannot be situated in IBZ$_1$. This follows from the fact that $g \in G + \theta G$. Hence the vector gk_1 lies inside one of the remaining non-magnetic IBZ. If that IBZ belongs to the original MIBZ, our goal is achieved. However, the IBZ can belong to another MIBZ (in our example one from the remaining 15 MIBZ). If the element g moves the vector k_1 outside the original MIBZ the gk_1 is in the same star with some vector k_r in the original MIBZ although outside the IBZ$_1$. We therefore have the equality

$$E(M_1, gk_1) = E(M_1, k_r). \tag{3.14}$$

Hence equation (3.13) is equivalent to the condition (3.8).

Case (b). The element g is the product of two elements $g_a g_b$, each belonging to a different magnetic group. Since, owing to $[g_a, \hat{\mathcal{H}}] = 0$ and $[g_b, \hat{\mathcal{H}}] = 0$, we have $[g_a g_b, \hat{\mathcal{H}}] = 0$ the results (3.10)–(3.13) remain valid. Since the preceding argument for case (a) applies also in this case, the last conclusion from case (a) holds.

Consequently, owing to equation (3.8) we may derive a general formula:

$$\sum_{k \in \mathrm{BZ}} E(M_1, k) = |F_{\mathrm{M}}| \sum_{\alpha=1}^{p(M)} \sum_{k \in \mathrm{IBZ}_1} E(M_\alpha, k) \tag{3.15}$$

where $|F_{\mathrm{M}}|$ is the order of the magnetic point group connected with the space group G_{M}[1], $p(M)$ is the number of equivalent directions for M_1, and IBZ_1 is the originally chosen irreducible part of the BZ constructed for the non-magnetic crystal phase; the energy $E(M_\alpha, k)$ is connected with a spin state quantized along the M_α axis. For that IBZ_1 we usually have the standard band-structure computer programs.

4. Conclusions

We have presented a general proof that the irreducible part of the Brillouin zone (IBZ), constructed for a non-magnetic crystal phase, can be applied for a ferromagnetic crystal phase with an appropriate change of equation (1.2), thus justifying Kondorskii's suggestion. Hence the application of the newly derived formula (3.15) does not require the construction of new programs generating the k-vector grid of MIBZ for each magnetization vector separately. Thus it may save a lot of preliminary labour. The application of formula (3.15) can be useful for energy band calculations in ferromagnetic crystal phases.

Table 2. The action of symmetry elements on high-symmetry points. In the first column are given the names of the high-symmetry k-vectors whose components are given in the brackets situated inside of or on the border of IBZ_1 (equation (3.5a)) or inside IBZ_2 (equation (3.5b)). In the second column are given the rotational elements of G_{M}[010]. In the third column are given the rotational elements of G_{M}[100]. In the fourth column are given the coordinates of the k-vectors obtained as a result of application of operations from columns 2 or 3 on k-vectors in column 1. In the fifth column are given the names of k-vectors from column 4, with the assignment of the respective IBZ. Notation of symmetry elements after Bradley and Cracknell [3].

1	2	3	4	5
Σ^1	$C_{2y}, \theta C_{2x}$		$(-\alpha, \alpha, 0)$	
$(\alpha, \alpha, 0)$	$\sigma_y, \theta\sigma_x$		$(\alpha, -\alpha, 0)$	
	$I, \theta\sigma_z$		$(-\alpha, -\alpha, 0)$	
	$C_{4y}^-, \theta C_{2e}$		$(0, \alpha, \alpha)$	$\Sigma^2 \begin{cases} \in \mathrm{IBZ}_2 \\ \in \mathrm{IBZ}_3 \end{cases}$
$\Delta^1 \in \mathrm{IBZ}_1$		$C_{4x}^+, S_{4x}^+, \theta C_{2f}$	$(0, 0, \alpha)$	
$\in \mathrm{IBZ}_2$		$\theta\sigma_{dd}$		$\Delta^2 \in \mathrm{IBZ}_3$
$(0, \alpha, 0)$				
G^1	$C_{4y}^-, \theta C_{2e}$		$(0, \frac{1}{2} + \alpha, \frac{1}{2} - \alpha)$	$G^2 \in \mathrm{IBZ}_2$
$(\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, 0)$				

Appendix

Keeping in mind the results from section 3 we shall show how the argument for both cases (a) and (b) works in a particular case of an iron crystal with magnetization parallel to the [100] direction. This case has been considered as an example throughout section 3. We have to justify equations (3.7). For this we need the symmetry elements g_a and g_b fulfilling the conditions:

$$g_a^{-1}[001] = [100] \tag{A1}$$

$$g_b^{-1}[010] = [100] \tag{A2}$$

and at the same time

$$g_a k_1 = k_2 \tag{A3}$$

$$g_b k_1 = k_3 \tag{A4}$$

where k_i, $i = 1, 2, 3$, are vectors in a general position situated inside IBZ$_i$, $i = 1, 2, 3$, respectively, defined by equations (3.5) (figure 1). If the element g_a is θC_{2e} and belongs to $G_{[010]}$ (see table 1) and the element $g_b = \theta C_{2f}\theta C_{2e}$ (which is the product of elements from $G_{[100]}$ and $G_{[010]}$), then applying the recipe from section 3 we prove that equations (3.7) are correct from the point of view of magnetic symmetry. To reduce the labour involved in the above procedure of finding the appropriate symmetry elements of the type (A1)–(A4) it is useful to construct a table analogous to table 2. There we determine the symmetry elements of the type (A3)–(A4), however acting on the high symmetry points of the BZ. That is much easier than doing it for vectors in a general position from the very beginning. That allows us to narrow down the set of symmetry elements that are most likely to work properly for vector k in a general position.

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