Symmetry Properties of Wave Functions in Magnetic Crystals*†

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The symmetry properties of wave functions in magnetic crystals are discussed in terms of the irreducible representations of magnetic space groups. The specific effects of the magnetic ordering on the crystal eigenstates are found to be of three types: (1) There is a lifting of some eigenfunction degeneracies because the crystal symmetry is reduced in the magnetic state. (2) New Brillouin zone surfaces are introduced if there is a reduction in translational symmetry. (3) The symmetry of the energy band in K space may be reduced. The rutile structure is considered as a specific example, and the space groups of MnF_2 and MnO_2 in their magnetic and nonmagnetic states are obtained. A magnetic structure of MnO_2 where the Mn^{2+} spins point toward the nearest-neighbor oxygens is assumed. The space groups considered are $P4_2/mnm$ (D_{4h}^{14}), $Pnnm$ (D_{2h}^{12}), $I\bar{4}2d$ (D_{2d}^{12}), $P4_2/mnm\ 1'$, $P4_2'/mnm'$, and $I_c\bar{4}2d$. The theory is applied to spin-wave states, and it is found that the structure of the spin-wave energy bands throughout the Brillouin zone may be obtained.

I. INTRODUCTION

THE problem of determining the eigenstates of a crystal is greatly simplified by the classification of these states according to the irreducible representations of the crystal space group. Such a classification results not only in the selection of the possible state function symmetries and degeneracies but also in the determination of the selection rules governing transitions between these states. The use of group theory in this way first introduced by Bouckaert, Smoluchowski, and Wigner.[1] Since their work many contributions have added to our understanding of the effect of the crystal symmetry on its wave functions.[2] Most important to the present work is the employment of time-reversal symmetry by Herring,[3] who presented a procedure by which the additional eigenfunction degeneracies, due to the invariance of the crystal potential under the reversal of time, could be determined.

Let us consider a crystal which below some temperature T_n, called the *Néel* point temperature, exhibits a magnetic structure. That is, it becomes either ferro-, antiferro-, or ferrimagnetic. It is the purpose of this paper to discuss the symmetry properties and degeneracies of the wave functions of these crystals in their magnetic state. It is also of interest to determine specifically what role the magnetic ordering has in the selection of these symmetries. The eigenstates of the magnetic lattice are determined partly by the symmetry of the nonmagnetic lattice, that is by the space group of the crystal above T_n, and partly by magnetic ordering which occurs when the crystal temperature is lowered through T_n. It is convenient to think of the magnetic ordering as producing a perturbation on the eigenstates of the paramagnetic lattice, even though this perturbation may not be small. The group theoretical results, of course, do not depend on its magnitude. Above T_n the crystal is invariant under a group H of unitary spatial operators, which is what one considers as the space group of the crystal. In the paramagnetic state the crystal potential is also invariant under the time-reversal operator $\boldsymbol{\theta}$, and products of $\boldsymbol{\theta}$ with the numbers of H, since we assume that in this state the crystal possesses a vanishing time-averaged–magnetic-moment density. The full space group of the paramagnetic crystal is then G, where $G=H+H\cdot\boldsymbol{\theta}$. Below T_n the crystal will no longer be invariant under all the operations of G. The reduction in symmetry comes about through the magnetic ordering of the lattice (introduction of a nonvanishing time-averaged–magnetic-moment density) and possible magnetostriction. For example, $\boldsymbol{\theta}$ does not leave the magnetic crystal unchanged. It, however, will now be invariant under a group $\mathcal{H}$ of unitary operators which turn not only the lattice but also the magnetic moment density into itself. In addition, if there exists some spatial operator $\mathbf{v}_0$ which takes the crystal into itself but reverses the sign of the magnetic moment density, then the magnetic crystal will be invariant under the operation $\mathbf{a}_0=\mathbf{v}_0\cdot\boldsymbol{\theta}$. Thus its full magnetic space group will be $\mathcal{G}=\mathcal{H}+\mathcal{H}\cdot\mathbf{a}_0$.[4] Since the time reversal operator $\boldsymbol{\theta}$ is

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[1] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58 (1936). This was the first time the irreducible representations of space groups were used to classify crystal state functions. The first application of group theory to crystal lattices was given by H. Bethe, Ann. Physik **3**, 133 (1929). He was, however, concerned only with point-group representations. The mathematics of space-group representations was obtained by F. Seitz, Z. Krist. **88**, 433 (1934); **90**, 289 (1935); **91**, 336 (1935); **94**, 100 (1936); Ann. Math. **37**, 17 (1936).

[2] We do not attempt a complete reference list since several review articles exist which contain these references. See, for example, G. F. Koster, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 173. D. F. Johnston, *Reports on Progress in Physics* (The Physical Society, London, 1960), Vol. 23, p. 66. A. V. Sokolov and V. P. Shirokovski, Uspekhi Fiz. Nauk **71**, 485 (1960) [translation: Soviet Phys.-Uspekhi **3**, 551 (1961)].

[3] C. Herring, Phys. Rev. **32**, 361 (1937).

[4] The symmetry of magnetic crystals has been discussed by several authors. See for example: L. Landau and E. Lifshitz, *Electrodynamics of Continuous Media* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1960), p. 116. B. A. Tavger and V. M. Zaitsev, J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 564

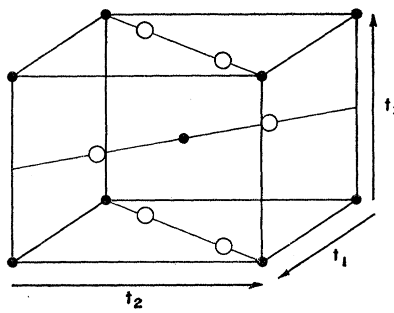

FIG. 1. The nonmagnetic unit cell of MnF_2, CoF_2, FeF_2, NiF_2, and MnO_2 showing the positions of the ion sites. The fourfold axis is in the direction $\mathbf{t}_3$. ●, magnetic ion; ○, nonmagnetic ion.

antiunitary, and thus $\mathbf{a}_0$ is antiunitary, the groups G and $\mathcal{G}$ contain both unitary and antiunitary operators. These groups will be called nonunitary. The groups H and $\mathcal{H}$ are unitary. From the above discussion it is seen that H and $\mathcal{H}$ form the invariant unitary subgroups of G and $\mathcal{G}$, respectively. Further, $\mathcal{G}$ and $\mathcal{H}$ are subgroups of G and H, respectively. The subgroup relations between these four groups which characterize the crystal in its magnetic and nonmagnetic states are expressed in the following diagram.

	Non-unitary		Unitary
Nonmagnetic	G	$\rightarrow$	H
	$\downarrow$		$\downarrow$
Magnetic	$\mathcal{G}$	$\rightarrow$	$\mathcal{H}$

The symmetry properties of the eigenstates of the paramagnetic crystal are determined by finding the irreducible representations of the groups of the wave vector $H_{\mathbf{k}}$ for the points and lines of symmetry of the first Brillouin zone of the nonmagnetic lattice for the appropriate space group H. The additional degeneracies of the corresponding representations of $G_{\mathbf{k}}$ may be obtained by the procedure developed by Herring.[3] Similarly, the symmetry properties of the eigenstates of the crystal in its magnetic state are determined by finding the irreducible representations of the groups of the wave vector $\mathcal{H}_{\mathbf{k}}$ for the points and lines of symmetry of the first Brillouin zone of the magnetic lattice for the appropriate unitary space group $\mathcal{H}$. The additional degeneracies of the corresponding representations of $\mathcal{G}_{\mathbf{k}}$ may be obtained by the procedure previously developed.[5] This procedure is outlined in Sec. II.

The effect of the magnetic ordering is now seen by forming the compatibility tables between the representations of $H_{\mathbf{k}}$ and $\mathcal{H}_{\mathbf{k}}$ for corresponding points in the nonmagnetic and magnetic Brillouin zones. When the magnetic and nonmagnetic unit cells of the crystal are the same, that is, when the translation symmetry is unchanged by the magnetic ordering, the Brillouin zones for the two lattices are the same. In this case $\mathcal{H}_{\mathbf{k}}$ will be a subgroup of $H_{\mathbf{k}}$ and $\mathcal{G}_{\mathbf{k}}$ will be a subgroup of $G_{\mathbf{k}}$ for corresponding points. The compatibility tables are thus formed in a straightforward manner. However, when the magnetic unit cell is some multiple of the nonmagnetic unit cell the Brillouin zones for the two lattices will not be the same. In this case the Brillouin zone of the magnetic lattice will be contained within that of the nonmagnetic lattice such that for points common to both, with the exception of those which are on the surface of the magnetic zone, but not on the surface of the nonmagnetic zone, the subgroup relations will hold. The representations for points within or on the nonmagnetic Brillouin zone, but outside the magnetic Brillouin zone, may be found from the relations $\mathcal{H}_{\mathbf{k}+\mathbf{K}_q}=\mathcal{H}_{\mathbf{k}}$ and $\mathcal{G}_{\mathbf{k}+\mathbf{K}_q}=\mathcal{G}_{\mathbf{k}}$, where $\mathbf{K}_q$ is a primitive translation of the magnetic reciprocal lattice. For these points also the compatibility tables may be immediately formed. The only points for which a difficulty occurs are those which lie on the surface of the magnetic Brillouin zone where this surface does not coincide with that of the nonmagnetic zone. If the group $\mathcal{H}_{\mathbf{k}}$ contains operators $\mathbf{u}=\{\boldsymbol{\sigma}|\boldsymbol{\tau}\}$ where, in the usual space group notation, $\boldsymbol{\sigma}$ is a point operator and $\boldsymbol{\tau}$ is a translation operator, such that $\boldsymbol{\sigma}\mathbf{k}=\mathbf{k}+\mathbf{K}_q$ where $\mathbf{K}_q\neq 0$, then $\mathcal{H}_{\mathbf{k}}$ and $\mathcal{G}_{\mathbf{k}}$ will not be subgroups of $H_{\mathbf{k}}$ and $G_{\mathbf{k}}$, respectively, since $H_{\mathbf{k}}$ and $G_{\mathbf{k}}$ may contain no such operators, $\mathbf{k}$ not being on the surface of the nonmagnetic Brillouin zone. These points will be clarified in Sec. III where we consider an example of this. However, even in these cases one may obtain information concerning the effects of the magnetic sublattice on the energy surfaces by a comparison of the representations of $\mathcal{H}_{\mathbf{k}}$ and $H_{\mathbf{k}}$.

It might be mentioned here that the group theoretical results determine how the introduction of the magnetic sublattice splits the energy bands of the nonmagnetic crystal. It does not indicate how or to what extent the bands may be shifted. Furthermore, in the above case when the magnetic and nonmagnetic lattices are dissimilar, additional discontinuities in the energy surfaces (band gaps) will be introduced. This occurs at the magnetic zone boundary, and it is clear that at this boundary the energy bands of the magnetic and nonmagnetic materials will be quite different.

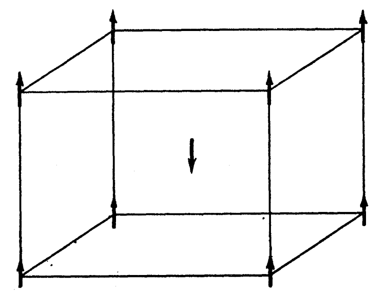

FIG. 2. The magnetic unit cell of MnF_2, CoF_2, and FeF_2 showing the spin orientation of the magnetic ions. The fourfold axis is in the corection of the spin vectors. The nonmagnetic ions are not shown.

(1956) [translation: Soviet Physics—JETP 3, 430 (1956)]. Y. LeCorre, J. phys. radium 19, 750 (1958). A more complete list of references is contained in the reference of footnote 5.

[5] J. O. Dimmock and R. G. Wheeler, J. Phys. Chem. Solids (to be published).

II. DETERMINATION OF THE EXTRA "TIME-REVERSAL" DEGENERACIES[5]

Consider that the unitary group of the wave vector $\mathcal{H}_\mathbf{k}$ consists of a set of spatial operators $\mathbf{u}$. The corresponding nonunitary group $\mathcal{G}_\mathbf{k}$ will contain in addition to the unitary operators of $\mathcal{H}_\mathbf{k}$ an equal number of antiunitary operators $\mathbf{a}$. Let us choose one of these and write $\mathbf{a}_0=\mathbf{v}_0\cdot\boldsymbol{\theta}=\{\boldsymbol{\rho}_0|\boldsymbol{\tau}_0\}\cdot\boldsymbol{\theta}$, where $\boldsymbol{\rho}_0$ is a point operator and $\boldsymbol{\tau}_0$ is a translation operator. Recall that $\mathbf{u}=\{\boldsymbol{\sigma}|\boldsymbol{\tau}\}$. Since $\boldsymbol{\theta}\cdot\mathbf{k}=-\mathbf{k}$ we have

$$\boldsymbol{\sigma}\mathbf{k}=\mathbf{k}+\mathbf{K}_q \quad \text{and} \quad \boldsymbol{\rho}_0\mathbf{k}=-\mathbf{k}+\mathbf{K}_{q'}, \tag{1}$$

where $\mathbf{K}_q$ and $\mathbf{K}_{q'}$ are primitive translations of the reciprocal lattice in question.

Wigner[6] showed how one could obtain the irreducible representations of a group containing both unitary and antiunitary operators from those of the invariant subgroup of pure unitary operators. As a result of his analysis it is seen that the representations of $\mathcal{G}_\mathbf{k}$ are obtained from those of $\mathcal{H}_\mathbf{k}$ in one of three ways. In case (a) the representation $\mathbf{D}^{(i)}$ of $\mathcal{G}_\mathbf{k}$ corresponds to a single representation $\boldsymbol{\Delta}^{(i)}$ of $\mathcal{H}_\mathbf{k}$ and has the same dimension; hence, in this case no new degeneracy is introduced. In case (b), $\mathbf{D}^{(i)}$ again corresponds to a single representation $\boldsymbol{\Delta}^{(i)}$ but has twice its degeneracy; hence, in this case the degeneracy of $\boldsymbol{\Delta}^{(i)}$ is doubled. In case (c), $\mathbf{D}^{(i)}$ corresponds to two different representations of $\mathcal{H}_k$, $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$, and $\boldsymbol{\Delta}^{(i)}(\mathbf{v}_0^{-1}\mathbf{u}\mathbf{v}_0)^*=\boldsymbol{\Delta}^{(j)}(\mathbf{u})$ such that, in this case, the introduction of the antiunitary operators, $\mathbf{a}$, causes $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$ and $\boldsymbol{\Delta}^{(j)}(\mathbf{u})$ to become degenerate. In summary, the following three cases are distinguished.

Case (a). No new degeneracy is introduced.

Case (b). The degeneracy of $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$ is doubled.

Case (c). The representation $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$ is degenerate with the representation $\boldsymbol{\Delta}^{(j)}(\mathbf{u})=\boldsymbol{\Delta}^{(i)}(\mathbf{v}_0^{-1}\mathbf{u}\mathbf{v}_0)^*$ where $i\neq j$.

The criterion by which we decide to which of the above three cases $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$ belongs is

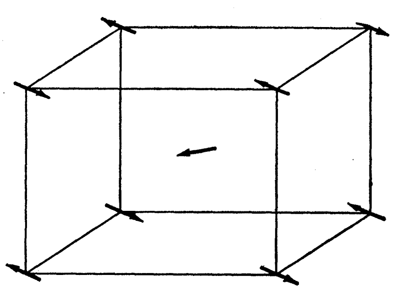

FIG. 3. The orientation of the magnetic ion spins in the older structure of MnO_2. The spins were chosen to point toward the oxygen sites.

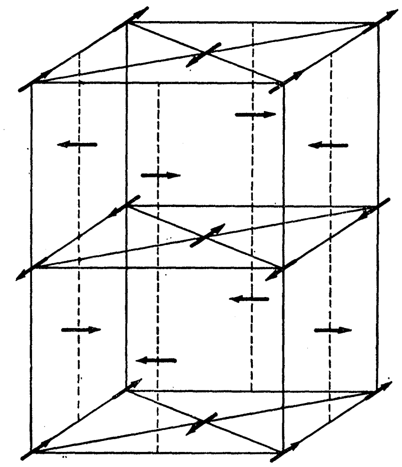

FIG. 4. The magnetic unit cell of the earlier structure of MnO_2. This figure is rotated 45° with respect to the other figures in the paper. The fourfold axis is again vertical, but vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ are along the horizontal face diagonals.

$$\begin{aligned}\sum_{\boldsymbol{\sigma}} \chi\{\boldsymbol{\Delta}^{(i)}[\mathbf{v}_0^{-1}(\boldsymbol{\sigma}|\boldsymbol{\tau})\mathbf{v}_0(\boldsymbol{\sigma}|\boldsymbol{\tau})]\} &= +\omega\chi\{\boldsymbol{\Delta}^{(i)}(\mathbf{v}_0^2)\}M/n_i, \text{ case (a)}\\ &= -\omega\chi\{\boldsymbol{\Delta}^{(i)}(\mathbf{v}_0^2)\}M/n_i, \text{ case (b)}\\ &= 0, \qquad \text{case (c).}\end{aligned} \tag{2}$$

The sum is to be taken over the distinct point operators $\boldsymbol{\sigma}$ in $\mathcal{H}_\mathbf{k}$ and consists of M terms. To each $\boldsymbol{\sigma}$ we associate only one $\boldsymbol{\tau}$. The dimension of $\boldsymbol{\Delta}^{(i)}(\mathbf{u})$ is n_i, and χ denotes the character of the representation. For single-group representations $\omega=+1$, and for double-group representations $\omega=-1$.[7] It is almost always true that $\mathbf{a}_0$ can be so chosen that

$$\mathbf{v}_0^2=\{E|\mathbf{R}_n\} \quad \text{or} \quad \{\bar{E}|\mathbf{R}_n\}, \tag{3}$$

where E is the identity point operator and $\bar{E}$ is equal to E, except that it changes the sign of the spin function ($\bar{E}=\omega E$), and $\mathbf{R}_n$ is a primitive translation of the lattice. If this is the case, then Eq. (2) takes on a simplified form,

$$\begin{aligned}\sum_{\boldsymbol{\sigma}} \chi\{\boldsymbol{\Delta}^{(i)}[\mathbf{v}_0(\boldsymbol{\sigma}|\boldsymbol{\tau})\mathbf{v}_0(\boldsymbol{\sigma}|\boldsymbol{\tau})]\} &= +\omega M, \text{ case (a)}\\ &= -\omega M, \text{ case (b)}\\ &= 0, \qquad \text{case (c).}\end{aligned} \tag{4}$$

In the examples considered in the next section, Eq. (3) is valid such that the simplification Eq. (4) may always be used. The preceding analysis applies equally well to the nonmagnetic groups $G_\mathbf{k}$ and $H_\mathbf{k}$ for which Eq. (3) is always true and Eq. (4) is identical with Herring's result.[3] It is worth mentioning at this point that the group $\mathcal{G}_\mathbf{k}$ may coincide with $\mathcal{H}_\mathbf{k}$ for some values of $\mathbf{k}$. This results in no increased degeneracy even though we are considering a magnetic space group with antiunitary operators. This occurs when no operator $\mathbf{a}_0$ can be found such that $\boldsymbol{\rho}_0\mathbf{k}=-\mathbf{k}+\mathbf{K}_{q'}$.

[6] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), Chap. 26.

[7] R. J. Elliott, Phys. Rev. **96**, 280 (1954).

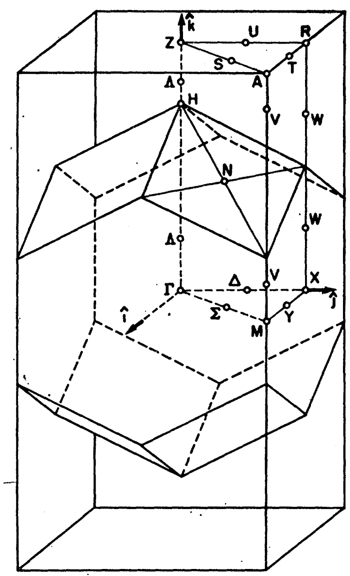

FIG. 5. The Brillouin zones for the simple tetragonal and body-centered tetragonal lattices, with the points and lines of symmetry indicated. The tetragonal prism is the Brillouin zone for the simple lattice defined by the primitive translations $\mathbf{t}_1=a\hat{\imath}$, $\mathbf{t}_2=a\hat{\jmath}$, and $\mathbf{t}_3=c\hat{k}$. The figure enclosed within the prism is the Brillouin zone for the body-centered tetragonal lattice defined by the primitive translations $\mathbf{t}_1+\mathbf{t}_3$, $\mathbf{t}_2-\mathbf{t}_3$, and $\mathbf{t}_1-\mathbf{t}_2$, provided $a>\sqrt{2}c$. For the structures under consideration this requirement is satisfied. The rhombus-shaped plane of which N is the center is the perpendicular bisector of the line ΓA. The point N lies on this line.

III. IRREDUCIBLE REPRESENTATIONS OF MAGNETIC SPACE GROUPS: THE RUTILE STRUCTURE

In this section the remarks of Secs. I and II are illustrated by the consideration of some specific groups. The nonmagnetic space group chosen is that of the rutile (TiO_2) structure. The magnetic materials MnF_2, FeF_2, CoF_2, NiF_2, and MnO_2 all have this structure in their paramagnetic states. The nonmagnetic space groups G and H of these compounds are, respectively, $P4_2/mnm\ 1'$ and $P4_2/mnm$. The notation is that of Belov, Neronova, and Smirnova[8] for the Shubnikov groups and is based on the international short form notation. The $1'$ in the symbol for the group G indicates that the time reversal operator is a member of this group. Figure 1 shows the unit cell of the rutile structure. The magnetic space groups $\mathcal{G}$ and $\mathcal{H}$ for MnF_2, FeF_2, and CoF_2 are $P4_2'/mnm'$ and $Pnnm$,[9] respectively. The nonmagnetic and magnetic unit cells for these compounds are the same. The spins of the magnetic ions are directed along the fourfold axis of the crystal[10] as shown in Fig. 2. For NiF_2 the chemical and magnetic unit cells are also the same. Since the analysis in this case would proceed in the same way as that of the previous case, we shall not be concerned with this compound.[11] The magnetic structure of MnO_2 which we will be considering in this section was originally suggested by Erickson[12] as a result of some early neutron diffraction experiments. However, some recent unpublished neutron diffraction work, also by Erickson, has been interpreted by Yoshimori[13] in terms of a screw-type structure. Nevertheless, we will be using the earlier structure since it is an interesting example of a case where the magnetic and nonmagnetic cells are different. Figure 3 shows the orientation of the magnetic moments, and the magnetic unit cell is shown in Fig. 4. The magnetic space groups $\mathcal{G}$ and $\mathcal{H}$ of the earlier structure of MnO_2 are $I_c\bar{4}2d$ and $I\bar{4}2d$, respectively. Notice that this structure has four magnetic sublattices, whereas the other structure considered has only two.

In the following three subsections the irreducible representations of the groups of the wave vector, for the lines and points of symmetry of the appropriate Brillouin zones, are obtained for the three space groups $P4_2/mnm$, $Pnnm$, and $I\bar{4}2d$. Since we are concerned with a comparison, through the compatibility relations, of the representations of these groups for corresponding points in K space, the operators are defined in the same way for each group. The point of intersection for all the rotation axes, and hence the inversion point, is taken to be one of the magnetic ion sites.

A. Space Group $P4_2/mnm$

This is the space group of the rutile structure shown in Fig. 1. The primitive translations of the tetragonal lattice are $\mathbf{t}_1=a\hat{\imath}$, $\mathbf{t}_2=a\hat{\jmath}$, and $\mathbf{t}_3=c\hat{k}$, where $\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$ are unit vectors in the x, y, and z directions, respectively. The nonprimitive translation is taken to be $\boldsymbol{\tau}=\frac{1}{2}(\mathbf{t}_1+\mathbf{t}_2+\mathbf{t}_3)$. The reciprocal lattice vectors $\mathbf{b}_i$ defined by the equation $\mathbf{b}_i\cdot\mathbf{t}_j=2\pi\delta_{ij}$ are $\mathbf{b}_1=(2\pi/a)\hat{\imath}$, $\mathbf{b}_2=(2\pi/a)\hat{\jmath}$, and $\mathbf{b}_3=(2\pi/c)\hat{k}$. The operators of the space group $P4_2/mnm$ are defined as follows:

$\{E|\mathbf{0}\}$, the identity operator;
$\{C_4|\boldsymbol{\tau}\}$, a counterclockwise rotation about the z axis through 90°, followed by the translation $\boldsymbol{\tau}$;
$\{C_4^{-1}|\boldsymbol{\tau}\}$, a clockwise rotation about the z axis through 90°, followed by the translation $\boldsymbol{\tau}$;
$\{C_2|\mathbf{0}\}$, a counterclockwise rotation about the z axis through 180°;
$\{C_{2a}|\mathbf{0}\}$, $\{C_{2b}|\mathbf{0}\}$, counterclockwise rotations through 180° about the axes $\mathbf{a}=\hat{\imath}+\hat{\jmath}$ and $\mathbf{b}=\hat{\imath}-\hat{\jmath}$, respectively;
$\{C_{2x}|\boldsymbol{\tau}\}$, $\{C_{2y}|\boldsymbol{\tau}\}$, counterclockwise rotations through 180° about the x axis (y axis) followed by the translation $\boldsymbol{\tau}$;
$\{I|\mathbf{0}\}$, the inversion operator;
$\{S_4|\boldsymbol{\tau}\}=\{C_4^{-1}|\boldsymbol{\tau}\}\cdot\{I|\mathbf{0}\}$;
$\{S_4^{-1}|\boldsymbol{\tau}\}=\{C_4|\boldsymbol{\tau}\}\cdot\{I|\mathbf{0}\}$;
$\{\sigma_h|\mathbf{0}\}=\{C_2|\mathbf{0}\}\cdot\{I|\mathbf{0}\}$, reflection in the xy plane;
$\{\sigma_{da}|\mathbf{0}\}=\{C_{2a}|\mathbf{0}\}\cdot\{I|\mathbf{0}\}$;
$\{\sigma_{db}|\mathbf{0}\}=\{C_{2b}|\mathbf{0}\}\cdot\{I|\mathbf{0}\}$;
$\{\sigma_{vx}|\boldsymbol{\tau}\}=\{C_{2x}|\boldsymbol{\tau}\}\cdot\{I|\mathbf{0}\}$;
$\{\sigma_{vy}|\boldsymbol{\tau}\}=\{C_{2y}|\boldsymbol{\tau}\}\cdot\{I|\mathbf{0}\}$.

[8] N. V. Belov, N. N. Neronova, and T. S. Smirnova, Kristallografiya 2, 315 (1957) [translation: Soviet Phys.—Cryst. 2, 311 (1957)].
[9] Y. LeCorre, J. phys. radium 19, 750 (1958).
[10] R. A. Erickson, Phys. Rev. 90, 779 (1953).
[11] The magnetic structure of NiF_2 has been recently obtained by R. A. Alikhanov, Soviet Phys.—JETP 37 (10), 814 (1960). See also R. A. Erickson, Phys. Rev. 90, 779 (1953).
[12] R. A. Erickson, Phys. Rev. 85, 365 (1952).
[13] A. Yoshimori, J. Phys. Soc. (Japan) 14, 807 (1959).

TABLE I. Character table for the point $\Gamma(0,0,0)$ of the group $P4_2/mnm$.

	Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
$\{E\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	2	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	-2	-2	-2	-2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	1	1	-1	-1	0	1	1	-1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	1	1	-1	-1	0	1	1	-1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	1	1	1	1	-2	1	1	1	1	-2	0	0	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\},\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	1	-1	1	-1	0	1	-1	1	-1	0	0	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{0}\}$	1	-1	-1	1	0	1	-1	-1	1	0	0	0	0	0
$\{I\|\mathbf{0}\}$	1	1	1	1	2	-1	-1	-1	-1	-2	2	2	-2	-2
$\{\bar{I}\|\mathbf{0}\}$	1	1	1	1	2	-1	-1	-1	-1	-2	-2	-2	2	2
$\{S_4,S_4^{-1}\|\boldsymbol{\tau}\}$	1	1	-1	-1	0	-1	-1	1	1	0	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$\{\bar{S}_4,\bar{S}_4^{-1}\|\boldsymbol{\tau}\}$	1	1	-1	-1	0	-1	-1	1	1	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	1	1	-2	-1	-1	-1	-1	2	0	0	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	1	-1	1	-1	0	-1	1	-1	1	0	0	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	-1	-1	1	0	-1	1	1	-1	0	0	0	0	0
Time inv.	a	a	a	a	a	a	a	a	a	a	a	a	a	a

TABLE II. Character table for the point $\Lambda(0,0,\gamma)$ of the group $P4_2/mnm$.[a]

	Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_6	Λ_7
$\{E\|\mathbf{0}\}$	1	1	1	1	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	-2	-2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	ω	ω	$-\omega$	$-\omega$	0	$\omega\sqrt{2}$	$-\omega\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	ω	ω	$-\omega$	$-\omega$	0	$-\omega\sqrt{2}$	$\omega\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	1	1	1	1	-2	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	-1	-1	1	0	0	0
Time inv.	a	a	a	a	a	a	a

[a] $\omega=\exp(\frac{1}{2}ic\gamma)$, $0<\gamma<\pi/c$.

TABLE III. Character table for the point $\Delta(0,\beta,0)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	-2
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-\omega$	ω	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	-1	-1	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0
$P4_2/mnm$ time inv.	a	a	a	a	a

[a] $\omega=\exp(\frac{1}{2}ia\beta)$, $0<\beta<\pi/a$.

TABLE IV. Character table for the points $\Sigma(\alpha,\alpha,0)$ and $S(\alpha,\alpha,\pi/c)$ for the group $P4_2/mnm$.[a]

	Σ_1 S_1	Σ_2 S_2	Σ_3 S_3	Σ_4 S_4	Σ_5 S_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	-2
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\}$	1	-1	1	-1	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	-1	-1	0
$\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	-1	-1	1	0
Time inv.	a	a	a	a	a

[a] $0<\alpha<\pi/a$.

Also, we have products of the above with the members $\{E|\mathbf{R}_n\}$ and $\{\bar{E}|\mathbf{R}_n\}$ of the translation group, where $\mathbf{R}_n=n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3$ (n_1, n_2, and n_3 integers). The space group $P4_2/mnm\,1'$ has, in addition to the above operators, their products with the time reversal operator $\boldsymbol{\theta}$.

Figure 5 shows the Brillouin zones for the simple and body-centered tetragonal lattices with the points and lines of symmetry indicated. The enclosing tetragonal prism is the appropriate Brillouin zone for the nonmagnetic space groups $P4_2/mnm$ and $P4_2/mnm\,1'$ and

TABLE V. Character table for the points $Z(0,0,\pi/c)$ and $A(\pi/a,\pi/a,\pi/c)$ for the group $P4_2/mnm$.

	Z_1 A_1	Z_2 A_2	Z_3 A_3	Z_4 A_4	Z_5 A_5
$\{E\|\mathbf{0}\}$	2	2	2	2	4
$\{\bar{E}\|\mathbf{0}\}$	2	2	2	2	-4
$\{E\|\mathbf{t}_3\}$	-2	-2	-2	-2	-4
$\{\bar{E}\|\mathbf{t}_3\}$	-2	-2	-2	-2	4
$\{C_4,C_4^{-1}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	2	2	-2	-2	0
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	-2	-2	2	2	0
$\{C_{2x},\bar{C}_{2x},C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{t}_3\}$	0	0	2	-2	0
$\{C_{2b},\bar{C}_{2b}\|\mathbf{0}\},\{C_{2a},\bar{C}_{2a}\|\mathbf{t}_3\}$	0	0	-2	2	0
$\{I\|\mathbf{0}\},\{I\|\mathbf{t}_3\}$	0	0	0	0	0
$\{\bar{I}\|\mathbf{0}\},\{\bar{I}\|\mathbf{t}_3\}$	0	0	0	0	0
$\{S_4,S_4^{-1}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{\bar{S}_4,\bar{S}_4^{-1}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\},\{\sigma_h,\bar{\sigma}_h\|\mathbf{t}_3\}$	0	0	0	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx},\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	2	-2	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{t}_3\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{t}_3\}$	-2	2	0	0	0
Time inv.	a	a	a	a	a

TABLE VI. Character table for the point $M(\pi/a,\pi/a,0)$ of the group $P4_2/mnm$.

	M_1^+	M_2^+	M_3^+	M_4^+	M_5^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^-	M_6^+	M_7^+	M_6^-	M_7^-
$\{E\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	2	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	1	1	1	1	2	-2	-2	-2	-2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	i	$-i$	i	$-i$	0	$i\sqrt{2}$	$-i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	i	$-i$	i	$-i$	0	$-i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$	$i\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{0}\}$	1	1	1	1	-2	1	1	1	1	-2	0	0	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\},\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	i	$-i$	$-i$	i	0	i	$-i$	$-i$	i	0	0	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{0}\}$	1	1	-1	-1	0	1	1	-1	-1	0	0	0	0	0
$\{I\|\mathbf{0}\}$	1	1	1	1	2	-1	-1	-1	-1	-2	2	2	-2	-2
$\{\bar{I}\|\mathbf{0}\}$	1	1	1	1	2	-1	-1	-1	-1	-2	-2	-2	2	2
$\{S_4,S_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	$-i$	i	$-i$	i	0	$i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$i\sqrt{2}$
$\{\bar{S}_4,\bar{S}_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	$-i$	i	$-i$	i	0	$-i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	1	1	-2	-1	-1	-1	-1	2	0	0	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	i	$-i$	$-i$	i	0	$-i$	i	i	$-i$	0	0	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|\mathbf{0}\},\{\sigma_{db},\bar{\sigma}_{db}\|\mathbf{0}\}$	1	1	-1	-1	0	-1	-1	1	1	0	0	0	0	0
Time inv.	c —	c	c —	c	a	c —	c	c —	c	a	c —	c	c —	c

TABLE VII. Character table for the point $R(0,\pi/a,\pi/c)$ for the groups $P4_2/mnm$ and $Pnnm$.

	R_1^+	R_1^-	R_2^+	R_3^+	R_4^+	R_5^+	R_2^-	R_3^-	R_4^-	R_5^-
$\{E\|\mathbf{0}\}$	2	2	1	1	1	1	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	2	2	-1	-1	-1	-1	-1	-1	-1	-1
$\{E\|\mathbf{t}_3\}$	-2	-2	-1	-1	-1	-1	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_3\}$	-2	-2	1	1	1	1	1	1	1	1
$\{C_2\|\mathbf{0}\},\{\bar{C}_2\|\mathbf{t}_3\}$	0	0	i	$-i$	i	$-i$	i	$-i$	i	$-i$
$\{\bar{C}_2\|\mathbf{0}\},\{C_2\|\mathbf{t}_3\}$	0	0	$-i$	i	$-i$	i	$-i$	i	$-i$	i
$\{C_{2x}\|\boldsymbol{\tau}\},\{\bar{C}_{2x}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	i	$-i$	$-i$	i	i	$-i$	$-i$	i
$\{\bar{C}_{2x}\|\boldsymbol{\tau}\},\{C_{2x}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	$-i$	i	i	$-i$	$-i$	i	i	$-i$
$\{C_{2y}\|\boldsymbol{\tau}\},\{\bar{C}_{2y}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	1	1	-1	-1	1	1	-1	-1
$\{\bar{C}_{2y}\|\boldsymbol{\tau}\},\{C_{2y}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	-1	-1	1	1	-1	-1	1	1
$\{I\|\mathbf{0}\}$	2	-2	1	1	1	1	-1	-1	-1	-1
$\{\bar{I}\|\mathbf{0}\}$	2	-2	-1	-1	-1	-1	1	1	1	1
$\{I\|\mathbf{t}_3\}$	-2	2	-1	-1	-1	-1	1	1	1	1
$\{\bar{I}\|\mathbf{t}_3\}$	-2	2	1	1	1	1	-1	-1	-1	-1
$\{\sigma_h\|\mathbf{0}\},\{\bar{\sigma}_h\|\mathbf{t}_3\}$	0	0	i	$-i$	i	$-i$	$-i$	i	$-i$	i
$\{\bar{\sigma}_h\|\mathbf{0}\},\{\sigma_h\|\mathbf{t}_3\}$	0	0	$-i$	i	$-i$	i	i	$-i$	i	$-i$
$\{\sigma_{vx}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	i	$-i$	$-i$	i	$-i$	i	i	$-i$
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vx}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	$-i$	i	i	$-i$	i	$-i$	$-i$	i
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	1	1	-1	-1	-1	-1	1	1
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	-1	-1	1	1	1	1	-1	-1
$P4_2/mnm$ time inv.	a	a	c —	c	c —	c	c —	c	c —	c

TABLE VIII. Character table for the point $X(0,\pi/a,0)$ of the groups $P4_2/mnm$ and $Pnnm$.

	X_1	X_2	X_3	X_4
$\{E\|\mathbf{0}\}$	2	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	2	2	-2	-2
$\{E\|\mathbf{t}_2\}$	-2	-2	-2	-2
$\{\bar{E}\|\mathbf{t}_2\}$	-2	-2	2	2
$\{C_2\|\mathbf{0}\},\{\bar{C}_2\|\mathbf{t}_2\}$	0	0	$2i$	$-2i$
$\{\bar{C}_2\|\mathbf{0}\},\{C_2\|\mathbf{t}_2\}$	0	0	$-2i$	$2i$
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_2\}$	0	0	0	0
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_2\}$	0	0	0	0
$\{I\|\mathbf{0}\},\{I\|\mathbf{t}_2\}$	0	0	0	0
$\{\bar{I}\|\mathbf{0}\},\{\bar{I}\|\mathbf{t}_2\}$	0	0	0	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	2	-2	0	0
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{t}_2\}$	-2	2	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_2\}$	0	0	0	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau},\ \boldsymbol{\tau}+\mathbf{t}_2\}$	0	0	0	0
Time inv.	a	a	c —	c

for the magnetic space groups $Pnnm$ and $P4_2'/mnm'$. The Brillouin zone for the $I\bar{4}2d$ and $I_c\bar{4}2d$ magnetic space groups is that of a body-centered tetragonal lattice and is shown in its proper relative position contained within the prism. We will discuss this in more detail when considering the group $I\bar{4}2d$. In Tables I through XIII we give the characters of the groups of

TABLE IX. Character table for the point $Y(\alpha,\pi/a,0)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	Y_1	Y_2	Y_3	Y_4	Y_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	-2
$\{\sigma_h,\bar{\sigma}_h\|\mathbf{0}\}$	1	1	-1	-1	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-\omega$	ω	0
$P4_2/mnm$, time inv.	c —	c	c —	c	b

[a] $\omega=\exp(\frac{1}{2}i\alpha a)$, $0<\alpha<\pi/a$.

TABLE X. Character table for the point $V(\pi/a,\pi/a,\gamma)$ for the group $P4_2/mnm$.[a]

	V_1	V_2	V_3	V_4	V_5	V_6	V_7
$\{E\|0\}$	1	1	1	1	2	2	2
$\{\bar{E}\|0\}$	1	1	1	1	2	-2	-2
$\{C_4,C_4^{-1}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$i\omega$	$-i\omega$	0	$i\omega\sqrt{2}$	$-i\omega\sqrt{2}$
$\{\bar{C}_4,\bar{C}_4^{-1}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$i\omega$	$-i\omega$	0	$-i\omega\sqrt{2}$	$i\omega\sqrt{2}$
$\{C_2,\bar{C}_2\|0\}$	1	1	1	1	-2	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$-i\omega$	$i\omega$	0	0	0
$\{\sigma_{da},\bar{\sigma}_{da}\|0\},\{\sigma_{db},\bar{\sigma}_{db}\|0\}$	1	1	-1	-1	0	0	0
Time inv.	c —	c	c —	c	a	c —	c

[a] $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XI. Character table for the point $W(0,\pi/a,\gamma)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	W_1	W_2	W_3	W_4	W_5
$\{E\|0\}$	2	1	1	1	1
$\{\bar{E}\|0\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_2\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_2\}$	-2	1	1	1	1
$\{C_2\|0\},\{\bar{C}_2\|\mathbf{t}_2\}$	0	i	$-i$	i	$-i$
$\{\bar{C}_2\|0\},\{C_2\|\mathbf{t}_2\}$	0	$-i$	i	$-i$	i
$\{\sigma_{vx}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}+\mathbf{t}_2\}$	0	ω	$-\omega$	$-\omega$	ω
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vx}\|\boldsymbol{\tau}+\mathbf{t}_2\}$	0	$-\omega$	ω	ω	$-\omega$
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}+\mathbf{t}_2\}$	0	$-i\omega$	$-i\omega$	$i\omega$	$i\omega$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\boldsymbol{\tau}+\mathbf{t}_2\}$	0	$i\omega$	$i\omega$	$-i\omega$	$-i\omega$
$P4_2/mnm$ time inv.	a	c —	c	c —	c

[a] $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XII. Character table for the point $U(0,\beta,\pi/c)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	U_1	U_2	U_3	U_4	U_5
$\{E\|0\}$	2	1	1	1	1
$\{\bar{E}\|0\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_3\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_3\}$	-2	1	1	1	1
$\{\sigma_h\|0\},\{\bar{\sigma}_h\|\mathbf{t}_3\}$	0	i	$-i$	i	$-i$
$\{\bar{\sigma}_h\|0\},\{\sigma_h\|\mathbf{t}_3\}$	0	$-i$	i	$-i$	i
$\{\sigma_{vx}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	ω	$-\omega$	$-\omega$	ω
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}\},\{\sigma_{vx}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$-\omega$	ω	ω	$-\omega$
$\{C_{2y}\|\boldsymbol{\tau}\},\{\bar{C}_{2y}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$-i\omega$	$-i\omega$	$i\omega$	$i\omega$
$\{\bar{C}_{2y}\|\boldsymbol{\tau}\},\{C_{2y}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$i\omega$	$i\omega$	$-i\omega$	$-i\omega$
$P4_2/mnm$ time inv.	a	c —	c	c —	c

[a] $\omega=\exp(\frac{1}{2}i\beta a)$, $0<\beta<\pi/a$.

TABLE XIII. Character table for the point $T(\alpha,\pi/a,\pi/c)$ of the groups $P4_2/mnm$ and $Pnnm$.[a]

	T_1	T_2	T_3	T_4	T_5
$\{E\|0\}$	2	1	1	1	1
$\{\bar{E}\|0\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_3\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_3\}$	-2	1	1	1	1
$\{\sigma_h\|0\},\{\bar{\sigma}_h\|\mathbf{t}_3\}$	0	i	$-i$	i	$-i$
$\{\bar{\sigma}_h\|0\},\{\sigma_h\|\mathbf{t}_3\}$	0	$-i$	i	$-i$	i
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	ω	ω	$-\omega$	$-\omega$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$-\omega$	$-\omega$	ω	ω
$\{C_{2x}\|\boldsymbol{\tau}\},\{\bar{C}_{2x}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$i\omega$	$-i\omega$	$-i\omega$	$i\omega$
$\{\bar{C}_{2x}\|\boldsymbol{\tau}\},\{C_{2x}\|\boldsymbol{\tau}+\mathbf{t}_3\}$	0	$-i\omega$	$i\omega$	$i\omega$	$-i\omega$
$P4_2/mnm$ time inv.	a	c —	c	c —	c

[a] $\omega=\exp(\frac{1}{2}i\alpha a)$, $0<\alpha<\pi/a$.

the wave vector for the space group $P4_2/mnm$. For a point defined by the vector $\mathbf{k}$ the representation of the operator $\{E|\mathbf{R}_n\}$ is given by[14]

$$\Delta^{(i)}\{E|\mathbf{R}_n\}=\exp(i\mathbf{k}\cdot\mathbf{R}_n)\Delta^{(i)}\{E|0\},$$

whence it is not necessary to include the characters of these operators in the tables but only give the coordinates of the point considered. The symbol (α,β,γ) indicates that $\mathbf{k}=\alpha\hat{\imath}+\beta\hat{\jmath}+\gamma\hat{k}$. Table XIV gives the compatibility relations for the irreducible representations.

B. Space Group *Pnnm*

This is the unitary space group of the compounds MnF_2, FeF_2, and CoF_2 below their respective Néel points. The unit cell, primitive translations, reciprocal lattice vectors, and Brillouin zone are the same as for the space group $P4_2/mnm$. The operators of the space group $Pnnm$ are as follows:

$$\{E|0\},\quad \{C_2|0\},\quad \{C_{2x}|\boldsymbol{\tau}\},\quad \{C_{2y}|\boldsymbol{\tau}\},$$
$$\{I|0\},\quad \{\sigma_h|0\},\quad \{\sigma_{vx}|\boldsymbol{\tau}\},\quad \{\sigma_{vy}|\boldsymbol{\tau}\},$$

with the operators defined as in the group $P4_2/mnm$, and products of the above with $\{E|\mathbf{R}_n\}$ and $\{\bar{E}|\mathbf{R}_n\}$, where again $\mathbf{R}_n=n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3$. The nonunitary magnetic space group of these compounds, $P4_2'/mnm'$, contains in addition to the elements of $Pnnm$ the following,

$$\{C_4|\boldsymbol{\tau}\}\cdot\theta,\quad \{C_4^{-1}|\boldsymbol{\tau}\}\cdot\theta,\quad \{C_{2a}|0\}\cdot\theta,\quad \{C_{2b}|0\}\cdot\theta,$$
$$\{S_4|\boldsymbol{\tau}\}\cdot\theta,\quad \{S_4^{-1}|\boldsymbol{\tau}\}\cdot\theta,\quad \{\sigma_{da}|0\}\cdot\theta,\quad \{\sigma_{db}|0\}\cdot\theta,$$

and their products with $\{E|\mathbf{R}_n\}$ and $\{\bar{E}|\mathbf{R}_n\}$. The subgroup diagram (see Sec. I) for this structure is

	Nonunitary		Unitary
Nonmagnetic	$P4_2/mnm\ 1'$	$\rightarrow$	$P4_2/mnm$
	$\downarrow$		$\downarrow$
Magnetic	$P4_2'/mnm'$	$\rightarrow$	$Pnnm$

In Tables XV through XX we give the characters of the groups of the wave vector for the space group $Pnnm$ for the points Γ, Λ, Σ, S, Z, A, M, and V. The additional degeneracies of the corresponding repre-

[14] G. F. Koster, reference 2.

TABLE XIV. Compatibility tables for the group $P4_2/mnm$.

Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_2	Λ_1	Λ_4	Λ_3	Λ_5	Λ_6	Λ_7	Λ_6	Λ_7
Σ_1	Σ_2	Σ_2	Σ_1	$\Sigma_3+\Sigma_4$	Σ_3	Σ_4	Σ_4	Σ_3	$\Sigma_1+\Sigma_2$	Σ_5	Σ_5	Σ_5	Σ_5
Δ_1	Δ_2	Δ_1	Δ_2	$\Delta_3+\Delta_4$	Δ_3	Δ_4	Δ_3	Δ_4	$\Delta_1+\Delta_2$	Δ_5	Δ_5	Δ_5	Δ_5

M_1^+	M_2^+	M_3^+	M_4^+	M_5^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^-	M_6^+	M_7^+	M_6^-	M_7^-
V_1	V_2	V_3	V_4	V_5	V_3	V_4	V_1	V_2	V_5	V_6	V_7	V_6	V_7
Y_1	Y_2	Y_2	Y_1	Y_3+Y_4	Y_3	Y_4	Y_4	Y_3	Y_1+Y_2	Y_5	Y_5	Y_5	Y_5
Σ_1	Σ_1	Σ_2	Σ_2	$\Sigma_3+\Sigma_4$	Σ_3	Σ_3	Σ_4	Σ_4	$\Sigma_1+\Sigma_2$	Σ_5	Σ_5	Σ_5	Σ_5

Z_1	Z_2	Z_3	Z_4	Z_5
S_1+S_4	S_2+S_3	S_1+S_3	S_2+S_4	$2S_5$
$\Lambda_1+\Lambda_4$	$\Lambda_2+\Lambda_3$	Λ_5	Λ_5	$\Lambda_6+\Lambda_7$
U_1	U_1	U_1	U_1	$U_2+U_3+U_4+U_5$

A_1	A_2	A_3	A_4	A_5
S_1+S_4	S_2+S_3	S_1+S_3	S_2+S_4	$2S_5$
V_1+V_2	V_3+V_4	V_5	V_5	V_6+V_7
T_1	T_1	T_1	T_1	$T_2+T_3+T_4+T_5$

R_1^+	R_1^-	R_2^+	R_3^+	R_4^+	R_5^+	R_2^-	R_3^-	R_4^-	R_5^-
U_1	U_1	U_2	U_3	U_4	U_5	U_3	U_2	U_5	U_4
W_1	W_1	W_2	W_3	W_4	W_5	W_4	W_5	W_2	W_3
T_1	T_1	T_2	T_3	T_4	T_5	T_5	T_4	T_3	T_2

X_1	X_2	X_3	X_4
W_1	W_1	W_2+W_4	W_3+W_5
Y_1+Y_2	Y_3+Y_4	Y_5	Y_5
$\Delta_1+\Delta_2$	$\Delta_3+\Delta_4$	Δ_5	Δ_5

TABLE XV. Character table for the point $\Gamma(0,0,0)$ of the group $Pnnm$.[a]

	Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^+	Γ_5^-
$\{E\|0\}$	1	1	1	1	1	1	1	1	2	2
$\{\bar{E}\|0\}$	1	1	1	1	1	1	1	1	−2	−2
$\{C_2,\bar{C}_2\|0\}$	1	1	−1	−1	1	1	−1	−1	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\}$	1	−1	1	−1	1	−1	1	−1	0	0
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	1	−1	−1	1	1	−1	−1	1	0	0
$\{I\|0\}$	1	1	1	1	−1	−1	−1	−1	2	−2
$\{\bar{I}\|0\}$	1	1	1	1	−1	−1	−1	−1	−2	2
$\{\sigma_h,\bar{\sigma}_h\|0\}$	1	1	−1	−1	−1	−1	1	1	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	1	−1	1	−1	−1	1	−1	1	0	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	1	−1	−1	1	−1	1	1	−1	0	0
Time inv.	a	a	c —	c	a	a	c —	c	a	a

[a] $v_0=\{C_{2a}|0\}$.

TABLE XVI. Character table for the point $\Lambda(0,0,\gamma)$ of the group $Pnnm$.[a]

	Λ_1	Λ_2	Λ_3	Λ_4	Λ_5
$\{E\|0\}$	1	1	1	1	2
$\{\bar{E}\|0\}$	1	1	1	1	−2
$\{C_2,\bar{C}_2\|0\}$	1	1	−1	−1	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	ω	$-\omega$	ω	$-\omega$	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-\omega$	ω	0
Time inv.	a	a	c —	c	a

[a] $v_0=\{C_{2a}|0\}$, $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XVII. Character table for the points $\Sigma(\alpha,\alpha,0)$ and $S(\alpha,\alpha,\pi/c)$ of the group $Pnnm$.[a]

	Σ_1 S_1	Σ_2 S_2	Σ_3 S_3	Σ_4 S_4
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	1	1	−1	−1
$\{\sigma_h\|0\}$	1	−1	i	$-i$
$\{\bar{\sigma}_h\|0\}$	1	−1	$-i$	i
Time inv.	a	a	a	a

[a] $v_0=\{C_{2b}|0\}$, $0<\alpha<\pi/a$.

sentations of $P4_2'/mnm'$ are indicated in the row labeled time inv. In each table the operator $\mathbf{v}_0$ is indicated (see Sec. II). For the remaining points in the zone the groups of the wave vector are the same as those of the group $P4_2/mnm$, and thus we may use the same character tables. However, no additional degeneracy arises in these representations since no operator $\mathbf{a}_0$ exists in $P4_2'/mnm'$ such that $\boldsymbol{\varrho}_0\mathbf{k}=-\mathbf{k}+\mathbf{K}_q$, and the groups $H_{\mathbf{k}}$, $\mathcal{G}_{\mathbf{k}}$, and $\mathcal{H}_{\mathbf{k}}$ are identical for the values of $\mathbf{k}$ associated with these points. In Table XXI we give the compatibility tables between the representations of $Pnnm$ for the points Γ, Z, A, and M. The tables for the points R and X are obviously the same as those of $P4_2/mnm$.

In Table XXII we give the compatibility relations for the irreducible representations of the groups of the wave vector between the groups $P4_2/mnm$ and $Pnnm$ for the corresponding points in the Brillouin zone. Those tables where the groups of the wave vector are the same are omitted. These also serve as the compatibility tables between the groups $P4_2/mnm\,1'$ and $P4_2'/mnm'$ when the time reversal invariance is considered. For the points R, X, W, Y, T, U, and Δ it is clear that the introduction of the magnetic sublattice simply lifts the degeneracy introduced by the fact that the nonmagnetic lattice is invariant under time reversal.

TABLE XVIII. Character table for the points $Z(0,0,\pi/c)$ and $A(\pi/a,\pi/a,\pi/c)$ of the group $Pnnm$.[a]

	Z_1 A_1	Z_2 A_2	Z_3 A_3	Z_4 A_4
$\{E\|0\}$	2	2	2	2
$\{\bar{E}\|0\}$	2	2	-2	-2
$\{E\|\mathbf{t}_3\}$	-2	-2	-2	-2
$\{\bar{E}\|\mathbf{t}_3\}$	-2	-2	2	2
$\{C_2,\bar{C}_2\|0\}$	2	-2	0	0
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	-2	2	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0
$\{I\|0\},\{I\|\mathbf{t}_3\}$	0	0	0	0
$\{\bar{I}\|0\},\{\bar{I}\|\mathbf{t}_3\}$	0	0	0	0
$\{\sigma_h\|0\},\{\bar{\sigma}_h\|\mathbf{t}_3\}$	0	0	$2i$	$-2i$
$\{\bar{\sigma}_h\|0\},\{\sigma_h\|\mathbf{t}_3\}$	0	0	$-2i$	$2i$
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_3\}$	0	0	0	0
Time inv.	a	a	a	a

[a] $\mathbf{v}_0=\{C_{2a}\|0\}$.

C. Space Group $I\bar{4}2d$

The unit cell for this group is shown in Fig. 4 with the spin directions of the magnetic ions given. It is a body-centered tetragonal structure with the following primitive translations: $\mathbf{t}_1+\mathbf{t}_3$, $\mathbf{t}_2-\mathbf{t}_3$, and $\mathbf{t}_1-\mathbf{t}_2$. The reciprocal lattice vectors $\mathbf{b}_i$ are

$$\mathbf{b}_1=(\pi/a)(\hat{\imath}+\hat{\jmath})+(\pi/c)\hat{k},$$
$$\mathbf{b}_2=(\pi/a)(\hat{\imath}+\hat{\jmath})-(\pi/c)\hat{k},$$
$$\mathbf{b}_3=(\pi/a)(\hat{\imath}-\hat{\jmath})-(\pi/c)\hat{k},$$

TABLE XIX. Character table for the point $M(\pi/a,\pi/a,0)$ of the group $Pnnm$.[a]

	M_1^+	M_2^+	M_3^+	M_4^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^+	M_5^-
$\{E\|0\}$	1	1	1	1	1	1	1	1	2	2
$\{\bar{E}\|0\}$	1	1	1	1	1	1	1	1	-2	-2
$\{C_2,\bar{C}_2\|0\}$	1	1	-1	-1	1	1	-1	-1	0	0
$\{C_{2x},\bar{C}_{2x}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	i	$-i$	i	$-i$	0	0
$\{C_{2y},\bar{C}_{2y}\|\boldsymbol{\tau}\}$	i	$-i$	$-i$	i	i	$-i$	$-i$	i	0	0
$\{I\|0\}$	1	1	1	1	-1	-1	-1	-1	2	-2
$\{\bar{I}\|0\}$	1	1	1	1	-1	-1	-1	-1	-2	2
$\{\sigma_h,\bar{\sigma}_h\|0\}$	1	1	-1	-1	-1	-1	1	1	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	$-i$	i	$-i$	i	0	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	i	$-i$	$-i$	i	$-i$	i	i	$-i$	0	0
Time inv.	c —	c	a	a	c —	c	a	a	a	a

[a] $\mathbf{v}_0=\{C_{2a}\|0\}$.

TABLE XX. Character table for the point $V(\pi/a,\pi/a,\gamma)$ of the group $Pnnm$.[a]

	V_1	V_2	V_3	V_4	V_5
$\{E\|0\}$	1	1	1	1	2
$\{\bar{E}\|0\}$	1	1	1	1	-2
$\{C_2,\bar{C}_2\|0\}$	1	1	-1	-1	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$i\omega$	$-i\omega$	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$-i\omega$	$i\omega$	0
Time inv.	c —	c	a	a	a

[a] $\mathbf{v}_0=\{C_{2b}\|0\}$, $0<\gamma<\pi/c$.

and the Brillouin zone is shown in Fig. 5 enclosed within the Brillouin zone of the simple tetragonal lattice with the basis vectors $\mathbf{t}_1$, $\mathbf{t}_2$, and $\mathbf{t}_3$. As mentioned above, the magnetic sublattice, in those cases where its introduction increases the size of the unit cell (decreases the size of the Brillouin zone), creates new discontinuities in the energy-band surfaces. In the present case these new discontinuities occur on the eight rhombus-shaped faces of the magnetic Brillouin zone.

TABLE XXI. Compatibility tables for the group *Pnnm*.

Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^+	Γ_5^-
Λ_1	Λ_2	Λ_3	Λ_4	Λ_2	Λ_1	Λ_4	Λ_3	Λ_5	Λ_5
Δ_1	Δ_2	Δ_3	Δ_4	Δ_4	Δ_3	Δ_2	Δ_1	Δ_5	Δ_5
Σ_1	Σ_1	Σ_2	Σ_2	Σ_2	Σ_2	Σ_1	Σ_1	$\Sigma_3+\Sigma_4$	$\Sigma_3+\Sigma_4$

M_1^+	M_2^+	M_3^+	M_4^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^+	M_5^-
V_1	V_2	V_3	V_4	V_2	V_1	V_4	V_3	V_5	V_5
Y_1	Y_2	Y_3	Y_4	Y_3	Y_4	Y_1	Y_2	Y_5	Y_5
Σ_1	Σ_1	Σ_2	Σ_2	Σ_2	Σ_2	Σ_1	Σ_1	$\Sigma_3+\Sigma_4$	$\Sigma_3+\Sigma_4$

Z_1	Z_2	Z_3	Z_4
$\Lambda_1+\Lambda_2$	$\Lambda_3+\Lambda_4$	Λ_5	Λ_5
S_1+S_2	S_1+S_2	$2S_3$	$2S_4$
U_1	U_1	U_2+U_4	U_3+U_5

A_1	A_2	A_3	A_4
V_1+V_2	V_3+V_4	V_5	V_5
S_1+S_2	S_1+S_2	$2S_3$	$2S_4$
T_1	T_1	T_2+T_4	T_3+T_5

TABLE XXII. Compatibility tables between the groups $P4_2/mnm$ and *Pnnm* for corresponding points.

Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
Γ_1^+	Γ_2^+	Γ_1^+	Γ_2^+	$\Gamma_3^++\Gamma_4^+$	Γ_1^-	Γ_2^-	Γ_1^-	Γ_2^-	$\Gamma_3^-+\Gamma_4^-$	Γ_5^+	Γ_5^+	Γ_5^-	Γ_5^-

M_1^+	M_2^+	M_3^+	M_4^+	M_5^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^-	M_6^+	M_7^+	M_6^-	M_7^-
M_1^+	M_2^+	M_2^+	M_1^+	$M_3^++M_4^+$	M_1^-	M_2^-	M_2^-	M_1^-	$M_3^-+M_4^-$	M_5^+	M_5^+	M_5^-	M_5^-

Z_1	Z_2	Z_3	Z_4	Z_5
Z_1	Z_1	Z_2	Z_2	Z_3+Z_4

A_1	A_2	A_3	A_4	A_5
A_1	A_1	A_2	A_2	A_3+A_4

Σ_1	Σ_2	Σ_3	Σ_4	Σ_5
Σ_1	Σ_1	Σ_2	Σ_2	$\Sigma_3+\Sigma_4$

S_1	S_2	S_3	S_4	S_5
S_1	S_1	S_2	S_2	S_3+S_4

Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_6	Λ_7
Λ_1	Λ_2	Λ_1	Λ_2	$\Lambda_3+\Lambda_4$	Λ_5	Λ_5

V_1	V_2	V_3	V_4	V_5	V_6	V_7
V_1	V_2	V_2	V_1	V_3+V_4	V_5	V_5

TABLE XXIII. Character table for the points $\Gamma(0,0,0)$ and $A(\pi/a,\pi/a,\pi/c)$ of the group $I\bar{4}2d$.[a]

	Γ_1 A_1	Γ_2 A_2	Γ_3 A_3	Γ_4 A_4	Γ_5 A_5	Γ_6 A_6	Γ_7 A_7
$\{E\|\mathbf{0}\}$	1	1	1	1	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	−2	−2
$\{S_4\|\boldsymbol{\tau}-\mathbf{t}_3\},\{S_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	$\sqrt{2}$	$-\sqrt{2}$
$\{\bar{S}_4\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\bar{S}_4^{-1}\|\boldsymbol{\tau}\}$	1	1	−1	−1	0	$-\sqrt{2}$	$\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	1	1	1	1	−2	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	1	−1	1	−1	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{t}_3\}$	1	−1	−1	1	0	0	0
Time inv.	*a*	*a*	*a*	*a*	*a*	*a*	*a*

[a] $\mathbf{v}_0=\{E|\mathbf{t}_3\}$.

TABLE XXIV. Character table for the point $\Lambda(0,0,\gamma)$ of the group $I\bar{4}2d$.[a]

	Λ_1	Λ_2	Λ_3	Λ_4	Λ_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	−2
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	ω^2	ω^2	$-\omega^2$	$-\omega^2$	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	ω^*	$-\omega^*$	ω^*	$-\omega^*$	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-\omega$	ω	0
Time inv.	*a*	*a*	*c*	*c*	*a*

[a] $\mathbf{v}_0=\{C_{2b}|\mathbf{0}\}$, $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XXV. Character table for the point $\Delta(0,\beta,0)$ of the group $I\bar{4}2d$.[a]

	Δ_1	Δ_2	Δ_3	Δ_4
$\{E\|\mathbf{0}\}$	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	1	1	−1	−1
$\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	ω	$-\omega$	$i\omega$	$-i\omega$
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	ω	$-\omega$	$-i\omega$	$i\omega$
Time inv.	*a*	*a*	*a*	*a*

[a] $\mathbf{v}_0=\{C_2|\mathbf{0}\}$, $\omega=\exp(\frac{1}{2}i\beta a)$, $0<\beta<\pi/a$.

The space group $I\bar{4}2d$ consists of the following elements,

$$\{E|\mathbf{0}\},\quad \{S_4|\boldsymbol{\tau}-\mathbf{t}_3\},\quad \{S_4^{-1}|\boldsymbol{\tau}\},\quad \{C_2|\mathbf{t}_3\},$$
$$\{C_{2a}|\mathbf{0}\},\quad \{C_{2b}|\mathbf{t}_3\},\quad \{\sigma_{vx}|\boldsymbol{\tau}-\mathbf{t}_3\},\quad \{\sigma_{vy}|\boldsymbol{\tau}\}.$$

Also we have products of the above with the members $\{E|\mathbf{R}_n'\}$ and $\{\bar{E}|\mathbf{R}_n'\}$ of the translation group where $\mathbf{R}_n'=n_1(\mathbf{t}_1+\mathbf{t}_3)+n_2(\mathbf{t}_2-\mathbf{t}_3)+n_3(\mathbf{t}_1-\mathbf{t}_2)$, (with n_1, n_2, and n_3 integers). In addition to the operators of $I\bar{4}2d$, the group $I_c\bar{4}2d$ contains their products with the antitranslation $\{E|\mathbf{t}_3\}\cdot\boldsymbol{\theta}$.

TABLE XXVI. Character table for the point $\Sigma(\alpha,\alpha,0)$ and $S(\alpha,\alpha,\pi/c)$ of the group $I\bar{4}2d$.[a]

	Σ_1 S_1	Σ_2 S_2	Σ_3 S_3	Σ_4 S_4
$\{E\|\mathbf{0}\}$	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	1	1	-1	-1
$\{C_{2a}\|\mathbf{0}\}$	1	-1	i	$-i$
$\{\bar{C}_{2a}\|\mathbf{0}\}$	1	-1	$-i$	i
Time inv.	a	a	a	a

[a] $\mathbf{v}_0=\{C_2|\mathbf{0}\}$.

TABLE XXVII. Character table for the points $M(\pi/a,\pi/a,0)$ and $Z(0,0,\pi/c)$ of the group $I\bar{4}2d$.[a]

	M_1 Z_1	M_2 Z_2	M_3 Z_3	M_4 Z_4	M_5 Z_5	M_6 Z_6	M_7 Z_7
$\{E\|\mathbf{0}\}$	1	1	1	1	2	2	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	2	-2	-2
$\{S_4\|\boldsymbol{\tau}-\mathbf{t}_3\},\{S_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	$i\sqrt{2}$	$-i\sqrt{2}$
$\{\bar{S}_4\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\bar{S}_4^{-1}\|\boldsymbol{\tau}\}$	i	$-i$	i	$-i$	0	$-i\sqrt{2}$	$i\sqrt{2}$
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	1	1	1	1	-2	0	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	i	$-i$	$-i$	i	0	0	0
$\{C_{2a},\bar{C}_{2a}\|\mathbf{0}\},\{C_{2b},\bar{C}_{2b}\|\mathbf{t}_3\}$	1	1	-1	-1	0	0	0
Time inv.	c —	c	c —	c	a	c —	c

[a] $\mathbf{v}_0=\{E|\mathbf{t}_3\}$.

TABLE XXVIII. Character table for the point $X(0,\pi/a,0)$ of the group $I\bar{4}2d$.[a]

	X_1	X_2	X_3	X_4	X_5
$\{E\|\mathbf{0}\}$	2	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_2-\mathbf{t}_3\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_2-\mathbf{t}_3\}$	-2	1	1	1	1
$\{C_2\|\mathbf{t}_3\},\{\bar{C}_2\|\mathbf{t}_2\}$	0	i	$-i$	i	$-i$
$\{\bar{C}_2\|\mathbf{t}_3\},\{C_2\|\mathbf{t}_2\}$	0	$-i$	i	$-i$	i
$\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_2\}$	0	1	1	-1	-1
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_2\}$	0	-1	-1	1	1
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3-\mathbf{t}_2\}$	0	$-i$	i	i	$-i$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\boldsymbol{\tau}+\mathbf{t}_3-\mathbf{t}_2\}$	0	i	$-i$	$-i$	i
Time inv.	a	c —	c	c —	c

[a] $\mathbf{v}_0=\{E|\mathbf{t}_3\}$.

TABLE XXIX. Character table for the point $R(0,\pi/a,\pi/c)$ of the group $I\bar{4}2d$.[a]

	R_1	R_2	R_3	R_4	R_5
$\{E\|\mathbf{0}\}$	2	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_1+\mathbf{t}_3\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_1+\mathbf{t}_3\}$	-2	1	1	1	1
$\{C_2\|\mathbf{t}_3\},\{\bar{C}_2\|\mathbf{t}_1\}$	0	i	$-i$	i	$-i$
$\{\bar{C}_2\|\mathbf{t}_3\},\{C_2\|\mathbf{t}_1\}$	0	$-i$	i	$-i$	i
$\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}+\mathbf{t}_1\}$	0	i	$-i$	$-i$	i
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\sigma_{vx}\|\boldsymbol{\tau}+\mathbf{t}_1\}$	0	$-i$	i	i	$-i$
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}+\mathbf{t}_1-\mathbf{t}_3\}$	0	1	1	-1	-1
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\boldsymbol{\tau}+\mathbf{t}_1-\mathbf{t}_3\}$	0	-1	-1	1	1
Time inv.	a	c —	c	c —	c

[a] $\mathbf{v}_0=\{E|\mathbf{t}_3\}$.

TABLE XXX. Character table for the point $V(\pi/a,\pi/a,\gamma)$ of the group $I\bar{4}2d$.[a]

	V_1	V_2	V_3	V_4	V_5
$\{E\|\mathbf{0}\}$	1	1	1	1	2
$\{\bar{E}\|\mathbf{0}\}$	1	1	1	1	-2
$\{C_2,\bar{C}_2\|\mathbf{t}_3\}$	ω^2	ω^2	$-\omega^2$	$-\omega^2$	0
$\{\sigma_{vx},\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	$i\omega^*$	$-i\omega^*$	$i\omega^*$	$-i\omega^*$	0
$\{\sigma_{vy},\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	$i\omega$	$-i\omega$	$-i\omega$	$i\omega$	0
Time inv.	c —	c	a	a	a

[a] $\mathbf{v}_0=\{C_{2b}|\mathbf{0}\}$, $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XXXI. Character table for the point $Y(\alpha,\pi/a,0)$ of the group $I\bar{4}2d$.[a]

	Y_1	Y_2	Y_3	Y_4
$\{E\|\mathbf{0}\}$	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	1	1	-1	-1
$\{\sigma_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$i\omega$	$-i\omega$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	ω	$-\omega$	$-i\omega$	$i\omega$
Time inv.	c —	c	c —	c

[a] $\mathbf{v}_0=\{C_2|\mathbf{0}\}$, $\omega=\exp(\frac{1}{2}i\alpha a)$, $0<\alpha<\pi/a$.

TABLE XXXII. Character table for the point $U(0,\beta,\pi/c)$ of the group $I\bar{4}2d$,[a]

	U_1	U_2	U_3	U_4
$\{E\|\mathbf{0}\}$	1	1	1	1
$\{\bar{E}\|\mathbf{0}\}$	1	1	-1	-1
$\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	$i\omega$	$-i\omega$	ω	$-\omega$
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\}$	$i\omega$	$-i\omega$	$-\omega$	ω
Time inv.	c —	c	c —	c

[a] $\mathbf{v}_0=\{C_2|\mathbf{0}\}$, $\omega=\exp(\frac{1}{2}i\beta a)$, $0<\beta<\pi/a$.

TABLE XXXIII. Character table for the point $W(0,\pi/a,\gamma)$ of the group $I\bar{4}2d$.[a]

	W_1	W_2	W_3	W_4	W_5
$\{E\|0\}$	2	1	1	1	1
$\{\bar{E}\|0\}$	2	-1	-1	-1	-1
$\{E\|\mathbf{t}_1+\mathbf{t}_2\}$	-2	-1	-1	-1	-1
$\{\bar{E}\|\mathbf{t}_1+\mathbf{t}_2\}$	-2	1	1	1	1
$\{C_2\|\mathbf{t}_3\},\{\bar{C}_2\|\mathbf{t}_3+\mathbf{t}_1+\mathbf{t}_2\}$	0	$i\omega^2$	$-i\omega^2$	$i\omega^2$	$-i\omega^2$
$\{\bar{C}_2\|\mathbf{t}_3\},\{C_2\|\mathbf{t}_3+\mathbf{t}_1+\mathbf{t}_2\}$	0	$-i\omega^2$	$i\omega^2$	$-i\omega^2$	$i\omega^2$
$\{\sigma_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\bar{\sigma}_{vx}\|-\boldsymbol{\tau}\}$	0	ω^*	ω^*	$-\omega^*$	$-\omega^*$
$\{\bar{\sigma}_{vx}\|\boldsymbol{\tau}-\mathbf{t}_3\},\{\sigma_{vx}\|-\boldsymbol{\tau}\}$	0	$-\omega^*$	$-\omega^*$	ω^*	ω^*
$\{\sigma_{vy}\|\boldsymbol{\tau}\},\{\bar{\sigma}_{vy}\|\mathbf{t}_3-\boldsymbol{\tau}\}$	0	$-i\omega$	$i\omega$	$i\omega$	$-i\omega$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\},\{\sigma_{vy}\|\mathbf{t}_3-\boldsymbol{\tau}\}$	0	$i\omega$	$-i\omega$	$-i\omega$	$i\omega$
No time inv.					

[a] $\omega=\exp(\frac{1}{2}i\gamma c)$, $0<\gamma<\pi/c$.

TABLE XXXIV. Character table for the point $T(\alpha,\pi/a,\pi/c)$ of the group $I\bar{4}2d$.[a]

	T_1	T_2	T_3	T_4
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	1	1	-1	-1
$\{\sigma_{vy}\|\boldsymbol{\tau}\}$	$-i\omega$	$i\omega$	ω	$-\omega$
$\{\bar{\sigma}_{vy}\|\boldsymbol{\tau}\}$	$-i\omega$	$i\omega$	$-\omega$	ω
Time inv.	a	a	a	a

[a] $\mathbf{v}_0=\{C_2\|0\}$, $\omega=\exp(\frac{1}{2}i\alpha a)$, $0<\alpha<\pi/a$.

The subgroup diagram for this structure is

	Nonunitary		Unitary
Nonmagnetic	$P4_2/mnm\,1'$	$\rightarrow$	$P4_2/mnm$
	$\downarrow$		$\downarrow$
Magnetic	$I_c\bar{4}2d$	$\rightarrow$	$I\bar{4}2d$

In Tables XXIII through XXXV we give the characters for the irreducible representations of the groups of the wave vector for the points of symmetry of the magnetic and nonmagnetic zones. Table XXXVII gives the compatibility relations between these representations, and Table XXXVIII gives the compatibility relations between the representations of $I\bar{4}2d$ and $P4_2/mnm$.

TABLE XXXV. Character table for the point $N(\pi/2a,\pi/2a,\pi/2c)$ of the group $I\bar{4}2d$.[a]

	N_1	N_2	N_3	N_4
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	1	1	-1	-1
$\{C_{2b}\|\mathbf{t}_3\}$	1	-1	i	$-i$
$\{\bar{C}_{2b}\|\mathbf{t}_3\}$	1	-1	$-i$	i
Time inv.	c —	c	a	a

[a] $\mathbf{v}_0=\{E\|\mathbf{t}_3\}$.

TABLE XXXVI. Character table for the point $N(\pi/2a,\pi/2a,\pi/2c)$ of the group $P4_2/mnm$.

	N_1	N_2	N_3	N_4
$\{E\|0\}$	1	1	1	1
$\{\bar{E}\|0\}$	1	1	-1	-1
$\{\sigma_{db}\|0\}$	1	-1	i	$-i$
$\{\bar{\sigma}_{db}\|0\}$	1	-1	$-i$	i
Time inv.	a	a	c —	c

The reciprocal lattice point N is of special interest because it lies on a rhombus-shaped face of the magnetic Brillouin zone. Recall that for this point we may not expect $\mathcal{G}_\mathbf{k}$ and $\mathcal{H}_\mathbf{k}$ to be subgroups of $G_\mathbf{k}$ and $H_\mathbf{k}$, respectively. The characters for the representations of $\mathcal{H}_\mathbf{k}$ are given in Table XXXV with the additional degeneracies of $\mathcal{G}_\mathbf{k}$ indicated in the usual way. The character table for $H_\mathbf{k}$ is given in Table XXXVI. From these tables we see that the introduction of the magnetic lattice has *increased* the degeneracy of the single-group representations while lifting the degeneracy of the double-group representations.

IV. DISCUSSION

In Secs. I and II we have described the procedure by which one uses the magnetic symmetry of a crystal to determine the symmetry properties of its eigenstates. The qualitative changes in the band structure due to the introduction of the magnetic ordering at the Néel

TABLE XXXVII. Compatibility tables for the group $I\bar{4}2d$.

Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7
Λ_1	Λ_2	Λ_1	Λ_2	$\Lambda_3+\Lambda_4$	Λ_5	Λ_5
Δ_1	Δ_2	Δ_1	Δ_2	$\Delta_1+\Delta_2$	$\Delta_3+\Delta_4$	$\Delta_3+\Delta_4$
Σ_1	Σ_2	Σ_2	Σ_1	$\Sigma_1+\Sigma_2$	$\Sigma_3+\Sigma_4$	$\Sigma_3+\Sigma_4$

M_1	M_2	M_3	M_4	M_5	M_6	M_7
V_1	V_2	V_2	V_1	V_3+V_4	V_5	V_5
Y_1	Y_2	Y_2	Y_1	Y_1+Y_2	Y_3+Y_4	Y_3+Y_4
Σ_1	Σ_1	Σ_2	Σ_2	$\Sigma_1+\Sigma_2$	$\Sigma_3+\Sigma_4$	$\Sigma_3+\Sigma_4$

A_1	A_2	A_3	A_4	A_5	A_6	A_7
V_3	V_4	V_3	V_4	V_1+V_2	V_5	V_5
T_1	T_2	T_1	T_2	T_1+T_2	T_3+T_4	T_3+T_4
S_1	S_2	S_2	S_1	S_1+S_2	S_3+S_4	S_3+S_4

Z_1	Z_2	Z_3	Z_4	Z_5	Z_6	Z_7
Λ_4	Λ_3	Λ_3	Λ_4	$\Lambda_1+\Lambda_2$	Λ_5	Λ_5
U_1	U_2	U_2	U_1	U_1+U_2	U_3+U_4	U_3+U_4
S_1	S_1	S_2	S_2	S_1+S_2	S_3+S_4	S_3+S_4

X_1	X_2	X_3	X_4	X_5
W_1	W_2	W_3	W_4	W_5
Y_1+Y_2	Y_4	Y_3	Y_3	Y_4
$\Delta_1+\Delta_2$	Δ_4	Δ_4	Δ_3	Δ_3

R_1	R_2	R_3	R_4	R_5
W_1	W_5	W_2	W_3	W_4
U_1+U_2	U_3	U_4	U_4	U_3
T_1+T_2	T_3	T_3	T_4	T_4

TABLE XXXVIII. Compatibility tables between the groups $P4_2/mnm$ and $I\bar{4}2d$ for corresponding points.

Γ_1^+	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-	Γ_6^+	Γ_7^+	Γ_6^-	Γ_7^-
Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_4	Γ_3	Γ_2	Γ_1	Γ_5	Γ_6	Γ_7	Γ_7	Γ_6

M_1^+	M_2^+	M_3^+	M_4^+	M_5^+	M_1^-	M_2^-	M_3^-	M_4^-	M_5^-	M_6^+	M_7^+	M_6^-	M_7^-
M_1	M_2	M_3	M_4	M_5	M_2	M_1	M_4	M_3	M_5	M_6	M_7	M_7	M_6

Z_1	Z_2	Z_3	Z_4	Z_5
Z_5	Z_5	Z_1+Z_2	Z_3+Z_4	Z_6+Z_7

A_1	A_2	A_3	A_4	A_5
A_5	A_5	A_1+A_4	A_2+A_3	A_6+A_7

R_1^+	R_1^-	R_2^+	R_3^+	R_4^+	R_5^+	R_2^-	R_3^-	R_4^-	R_5^-
R_1	R_1	R_3	R_2	R_5	R_4	R_5	R_4	R_3	R_2

X_1	X_2	X_3	X_4
X_1	X_1	X_2+X_4	X_3+X_5

Y_1	Y_2	Y_3	Y_4	Y_5
Y_1	Y_2	Y_2	Y_1	Y_3+Y_4

Σ_1	Σ_2	Σ_3	Σ_4	Σ_5
Σ_1	Σ_2	Σ_1	Σ_2	$\Sigma_3+\Sigma_4$

S_1	S_2	S_3	S_4	S_5
S_1	S_2	S_1	S_2	S_3+S_4

Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_6	Λ_7
Λ_1	Λ_2	Λ_1	Λ_2	$\Lambda_3+\Lambda_4$	Λ_5	Λ_5

Δ_1	Δ_2	Δ_3	Δ_4	Δ_5
Δ_1	Δ_2	Δ_1	Δ_2	$\Delta_3+\Delta_4$

V_1	V_2	V_3	V_4	V_5	V_6	V_7
V_1	V_2	V_2	V_1	V_3+V_4	V_5	V_5

T_1	T_2	T_3	T_4	T_5
T_1+T_2	T_3	T_3	T_4	T_4

U_1	U_2	U_3	U_4	U_5
U_1+U_2	U_4	U_3	U_3	U_4

W_1	W_2	W_3	W_4	W_5
W_1	W_2	W_5	W_4	W_3

point were found to be of two distinct types. The first is simply the lifting of certain degeneracies due to the general reduction of symmetry, while the second is the introduction of new surfaces of band discontinuity. In addition to these band structure changes, examples of which were considered in Sec. III, the following obvious result may be mentioned. If the group G of the nonmagnetic lattice contains an operator which takes a given wave vector $\mathbf{k}_1$ into another wave vector $\mathbf{k}_2$, then it is generally recognized that for every energy state at $\mathbf{k}_1$, $E^{(i)}(\mathbf{k}_1)$, there must be an energy state at $\mathbf{k}_2$, $E^{(j)}(\mathbf{k}_2)$ such that $E^{(i)}(\mathbf{k}_1)=E^{(j)}(\mathbf{k}_2)$. In particular, since $\boldsymbol{\theta}$ is a member of G and $\boldsymbol{\theta}\cdot\mathbf{k}=-\mathbf{k}$, $E^{(i)}(\mathbf{k})=E^{(j)}(-\mathbf{k})$. This is a general property of energy bands in nonmagnetic crystals and does not depend on the spatial symmetry of the lattice. Since the magnetic group $\mathcal{G}$ is a group of lower order than G we see that the magnetic ordering *may* reduce the band symmetry in $\mathbf{k}$ space. For example, in those magnetic crystals lacking inversion symmetry, whose magnetic space group $\mathcal{G}$ contains $\boldsymbol{\theta}$ only in combination with rotation operators, the energy bands will not satisfy the relation $E^{(i)}(\mathbf{k})=E^{(j)}(-\mathbf{k})$ for all values of $\mathbf{k}$. However, in neither of the two cases considered does any symmetry reduction occur, as can be seen by an examination of the operators of each group. A reduction in symmetry will, however, occur in NiF_2 for example.

In a previous work[5] we considered the irreducible representations of magnetic point groups. These would be useful in obtaining the symmetry properties of localized states in magnetic crystals, as impurity or single ion states in the tight-binding approximation. Magnetic space groups as considered here are useful, on the other hand, in describing nonlocalized states. Such states would arise in any single-particle or band approximations which might be attempted. More immediately interesting, however, is the application of these magnetic groups to the question of spin waves and their interactions. Since there is much literature on spin waves, we mention only their transformation properties, as these are important in our present work.[15] If the crystal under consideration has a sublattice whose direction of magnetization is ξ, then a spin wave traveling through this sublattice with wave vector $\mathbf{k}$ will transform in the group of the wave vector $\mathbf{k}$ as $S_\zeta - iS_\eta$, where ξ, ζ, and η form a right-handed co-

[15] See for example, J. Van Kranendonk and J. H. Van Vleck, Revs. Modern Phys. **30**, 1 (1958).

ordinate system ($\boldsymbol{\xi}=\boldsymbol{\zeta}\times\boldsymbol{\eta}$), and S_ζ and S_η transform as pseudovectors in the direction $\boldsymbol{\zeta}$ and $\boldsymbol{\eta}$, respectively. That is, the spin wave transforms as a unit of angular momentum directed along $-\boldsymbol{\xi}$. If the substance in question possesses more than one magnetic sublattice, a wave confined to one will not be an eigenstate of the spin wave Hamiltonian, since in general there is a coupling between sublattices. However, the transformation properties may be obtained by considering isolated waves, and in fact the selection of eigenstates and the determination of degeneracies results from an application of the group theory.[16]

Let us consider our two examples. In the MnF_2 structure at $\mathbf{k}=0$ the spin waves will transform as S_x-iS_y and S_x+iS_y. These functions belong to the representations Γ_3^+ and Γ_4^+ of the group *Pnnm* (see Table XV) which become degenerate in the group $P4_2'/mnm'$. Thus in MnF_2 at $\mathbf{k}=0$ we expect the spin-wave spectra to be doubly degenerate in the absence of external fields. This has also been predicted by direct calculation[17] and indeed has been observed.[18] In the MnO_2 structure at $\mathbf{k}=0$ the spin waves will transform as $S_z\pm iS_{x-y}$ and $S_z\pm iS_{x+y}$. These functions belong to the representations Γ_2, Γ_3, and Γ_5 of the group $I\bar{4}2d$ (see Table XXIII). Since in this case there is no additional degeneracy in $I_c\bar{4}2d$, we expect the spin wave spectra in this structure to be split into three levels, two nondegenerate and one doubly degenerate, in the absence of external fields. A similar argument predicts two nondegenerate spin wave states at $\mathbf{k}=0$ in NiF_2 as has been obtained by direct calculation.[19] This analysis can, of course, be carried out for any point in the Brillouin zone such that by using the transformation properties of spin waves and the character tables one may obtain the spin-wave band structure throughout the zone.

Note added in proof. It has come to the attention of the authors that the nonmagnetic space group $P4_2/mnm$ has also been considered by K. Olbrychski [Bull. acad. polon. sci. **9**, 537 (1961)]. However, he has omitted the points Z, A, and M on the zone surface as well as the time reversal degeneracies.

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[16] Basis functions for the representations contained in this work have been obtained, and are included in the thesis submitted to Yale University in partial fulfillment of the requirements for the Ph.D. degree, by J. O. Dimmock. The transformation properties of the spin-wave states for all points in the Brillouin zone are contained in these tables.

[17] F. Keffer and C. Kittel, Phys. Rev. **85**, 329 (1952).

[18] F. M. Johnson and A. H. Nethercot, Jr., Phys. Rev. **114**, 705 (1959). See also R. C. Ohlmann and M. Tinkham, *ibid.* **123**, 425 (1961).

[19] T. Moriya, Phys. Rev. **117**, 635 (1960).