MARADUDIN, A. A., MONTROLL, E. W. & WEISS, G. H. (1963). *Solid State Physics*, Suppl. 3, edited by SEITZ and TURNBULL, p. 231. New York: Academic Press.
NICKLOW, R. M. & YOUNG, R. A. (1964). Tech. Rept. No. 3, ONR Contract No. NOnr 991(00) and 991(06); NR-017-623, with Georgia Institute of Technology.
NILSSON, N. (1957). *Ark. Fys.* **12**, 247.
RENNINGER, M. (1952). *Acta Cryst.* **5**, 711.
RENNINGER, M. (1966). *Advanc. X-Ray Anal.* **10**, 42.
SCHWARTZ, L. H. (1964). *Acta Cryst.* **17**, 1614.
WALKER, C. B. & CHIPMAN, D. R. (1969). *Acta Cryst.* A **25**, in the press.
WALLER, I. (1925). Uppsala Dissertation, pp. 1–58.
WALLER, I. (1928). *Z. Phys.* **51**, 213.
WARREN, B. E. (1953). *Acta Cryst.* **6**, 803.
YOUNG, R. A. (1961). Tech. Rept. No. 2, ONR Contract No. NOnr 991(00) and 991(06); NR-017-623, with Georgia Institute of Technology.
ZACHARIASEN, W. H. (1945). *Theory of X-Ray Diffraction in Crystals.* New York: John Wiley.

Acta Cryst. (1969). A **25**, 329

Magnetic Symmetry Groups

BY T. S. G. KRISHNAMURTY AND P. GOPALAKRISHNAMURTY
Andhra University, Waltair, S. India

(*Received* 20 *April* 1968 *and in revised form* 17 *September* 1968)

It is shown that the real one-dimensional irreducible representations of a crystallographic point group induce the magnetic symmetry groups associated with the point group and also give the number of independent non-vanishing constants required to describe any magnetic property for the induced magnetic symmetry groups.

1. Introduction

The crystallographic point groups describe the spatial symmetry operations like rotations and rotation-reflexions by which a crystal is brought into coincidence with itself. By the application of an ordinary symmetry operation on an arrangement of atoms in a point group, although the geometrical structure may be brought into coincidence with itself, it may be that the orientations of some or all of the atomic magnetic moments (spins) are reversed. In such a case a further reversal of the affected spins must follow the usual symmetry operation in order to bring the geometrical structure, together with the spins, into complete coincidence with itself. The time reversal operation, $\mathscr{R}$, has been introduced in this context to account for the reversal of the spins. The need for generalization of the concept of symmetry operations was realized long ago by Shubnikov (1951), Landau & Lifshitz (1960) and several others to explain the magnetic properties of crystals. The introduction of the new symmetry operation $\mathscr{R}$ increases the number of the point groups from 32 to 122. These 122 point groups can be classified broadly into two categories. They are (i) the 32 grey groups containing $\mathscr{R}$ explicitly and (ii) the 90 magnetic symmetry groups. The 32 conventional crystallographic point groups together with the 58 bicoloured magnetic point groups constitute the 90 magnetic symmetry groups. The magnetic symmetry groups have been derived in a variety of ways by Shubnikov (1951), Tavger & Zaitsev (1956), Hamermesh (1962), Tinkham (1964) and Bhagavantam & Pantulu (1964). Recently Koptsik (1966) also discussed the magnetic symmetry groups in connexion with the description of magnetic structures of crystals on the basis of Landau's theory of the second order phase transitions. In this paper it is proposed to derive the magnetic symmetry groups by a more elegant method, based on the representation theory of groups. The method presented here emphasizes the significance of the physical constants occurring in the alternating representations of the conventional point groups, and this is explained in § 4.

2. Description of the method

The magnetic symmetry groups have been constructed (Hamermesh, 1962) by selecting possible subgroups of index 2 from the 32 point groups. A subgroup H of index 2 of a group G is necessarily a self-conjugate subgroup of G. Then G can be written as $G = H + A_iH$, where A_i is any element that belongs to $G - H$. The co-sets H and A_iH form the factor group G/H. Constructing the set $M_{(G)H}$ of elements associated with the group G defined by the relation $M_{(G)H} = H + \mathscr{R}A_iH$, it can be seen that $M_{(G)H}$ forms a group, which is called the magnetic group of G with respect to H. Thus in the construction of the magnetic groups of G, one has $A_i^2H = H$ so that the characters of A_iH in the factor group G/H are ± 1. Hence the representations of A_iH in the factor group are real and one-dimensional. Given a subgroup H of index 2 of G, there corresponds uniquely to it a real one-dimensional irreducible representation of the factor group G/H in which the elements H and A_iH respectively have the characters $+1$ and -1. But the irreducible representations of the factor group G/H induce the irreducible representations of G. There will be as many non-total symmetric real one-dimensional irreducible representations (alternating representations) in G as the number of possible subgroups of index 2 of G. In fact, a one to one correspondence exists (Indenbom, 1959; Niggli, 1959; Bertaut, 1968) between the various subgroups of index 2 of a group G and the alternating representations of G, as explained below. If all the elements which are represented by the character $+1$ in an alternating representation Γ_H of G are taken, they form a subgroup H of index 2 of G corresponding to the alternating representation Γ_H. Therefore from the alternating representations Γ_H of G, one can build up the magnetic groups $M_{(G)H}$ associated with G. The symmetry operation A_i is of even order (Hamermesh, 1962) and the one-dimensional irreducible representations of G with imaginary characters need not be considered so far as the derivation of the magnetic groups of G is concerned, since $A_i^2=E$ (identity).

If the group G is taken as one of the 32 crystallographic point groups, then each one of the real one-dimensional irreducible representations of G induces a magnetic symmetry group corresponding to G. In particular the total symmetric irreducible representation of G induces a magnetic symmetry group of G, wherein all the spins will be left invariant by all the spatial symmetry operations. These groups, 32 in number, are called the single coloured or colourless groups (Bhagavantam, 1966) and are indistinguishable from the 32 crystallographic point groups. Each one of the alternating representations of G induces a double coloured magnetic symmetry group, also known as a magnetic variant of G (Bhagavantam & Pantulu, 1964). If some of the subgroups H of index 2 of a group G are to be regarded as indistinguishable from physical considerations, the corresponding alternating representations Γ_H of G should be regarded as magnetically equivalent (or simply referred to as equivalent hereafter) and the induced magnetic variants of G should be regarded as identical. Adopting the procedure described here, the distinct magnetic variants of the 32 crystallographic point groups have been derived in the following section.

3. Enumeration of the magnetic variants

The distinct magnetic variants induced by the non-equivalent alternating representations of the 32 point groups have been enumerated and described below in terms of the inducing irreducible representations which are given in brackets against the point groups. On account of the possibility of obtaining identical induced magnetic variants of a point group G, the inducing irreducible representations of G may be specified by any one of the equivalent alternating representations. Tisza's (1933) notation* for the description of the real one-dimensional irreducible representations of the 32 point groups is adopted from the text book of Herzberg (1945):

$\bar{1}(A_u)$; $m(A'')$; $2(B)$; $2/m(B_u, A_u, B_g)$; $2mm(B_1, A_2)$; $222(B_3)$; $mmm(B_{1u}, A_u, B_{1g})$; $4(B)$; $\bar{4}(B)$; $4/m(B_u, A_u, B_g)$; $4mm(A_2, B_1)$; $\bar{4}2m(B_1, B_2, A_2)$; $422(A_2, B_1)$; $4/mmm(B_{2u}, A_{2u}, A_{2g}, A_{1u}, B_{1g})$; $\bar{3}(B_u)$; $3m(A_2)$; $32(A_2)$; $\bar{3}m(A_{2g}, A_{2u}, A_{1u})$; $\bar{6}(A'')$; $6(B)$; $6/m(A_u, B_u, B_g)$; $\bar{6}m2(A_2^1, A_2'', A_1'')$; $6mm(A_2, B_1)$; $622(A_2, B_1)$; $6/mmm(A_{2u}, A_{2g}, A_{1u}, B_{1u}, B_{1g})$; $m3(A_u)$; $\bar{4}3m(A_2)$; $432(A_2)$ and $m3m(A_{1u}, A_{2g}, A_{2u})$.

In this way, the 58 magnetic variants of the 32 point groups are obtained. In the above list the point groups 1, 3 and 23 have been omitted as they do not give rise to any magnetic variants. As there can be at most 8 real one-dimensional irreducible representations in some of the 32 point groups, the maximum number of magnetic variants that can correspond to such point groups can only be 7. But on account of the equivalence (Bertaut, 1968) among the induced magnetic variants, this maximum number has not been realized here even in those point groups that contain 8 real one-dimensional irreducible representations.

4. Magnetic constants of the magnetic variants

The advantage of this method can be appreciated best in computing, in a very elegant way, the number of constants required to specify a magnetic property for the magnetic variants of the point groups. The usual method of enumerating the number of non-vanishing independent constants necessary to describe a physical (or magnetic) property of a crystal consists in obtaining that number coming under the total symmetric irreducible representation of the point group G of order N of the crystal from the following established formula (Bhagavantam & Venkatarayudu, 1962):

$$n_i = 1/N \sum_p h_p \chi'_p(R) \chi_i(R)\,, \tag{1}$$

where $\chi'_p(R)$ is the character derived for the physical property, h_p is the number of elements in the conjugate class p of G and $\chi_i(R)$ is the character of the symmetry element R in the ith irreducible representation of G. In equation (1), n_i represents the number of physical constants appearing against the representation i of G.

It will now be shown that the method of computing the number of independent constants required to describe a magnetic property for a magnetic variant corresponding to a point group G is the same as that of determining that number against that alternating re-

* The standard notation employed in molecular spectroscopy for the irreducible representations of the 32 point groups is adhered to: thus A or B always denote one-dimensional irreducible representations. Suffixes g or u distinguish representations which are even or odd with respect to inversion, while a single or a double prime is used to distinguish those which are even or odd with respect to a plane of symmetry.

presentation of G which induces the magnetic variant. The basic idea in the above statement will now be explained through an illustration. Consider the point group $2mm$. The character table of the point group is given below.

$2mm$	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

It has been mentioned in the previous section that the irreducible representations B_1 and A_2 of the point group $2mm$ induce the magnetic variants $\underline{2}m\underline{m}$ and $2\underline{mm}$ respectively. Take the magnetic variant $2\underline{mm}$; the number of constants needed to describe a magnetic property for the magnetic variant $2\underline{mm}$ can be obtained from (1) by taking $\chi_i(R)=1$ for all R, which is characteristic of the total symmetric irreducible representation of the magnetic variant. Since the order of a magnetic variant and the orders of its various conjugate classes associated with a point group G will be the same as the corresponding orders of G, and a complementary symmetry operation introduced by Zheludev (1960) reverses the character of a physical property (Indenbom, 1960), it follows that the number of constants $n_{(m\,.\,v)T}$ in respect of a magnetic property coming under the total symmetric irreducible representation (T) of the magnetic variant $(m\,.\,v)$ $2\underline{mm}$, for which $h_p=1$ for all p and $N=4$, is, from (1), given by:

$$\begin{aligned} n_{(m\,.\,v)T} &= \tfrac{1}{4}\sum_p \chi_p'(R) \\ &= \tfrac{1}{4}[\chi'(E)+\chi'(C_2)+\chi'(\underline{\sigma_v})+\chi'(\underline{\sigma_v'})]^* \\ &= \tfrac{1}{4}[\chi'(E)+\chi'(C_2)-\chi'(\sigma_v)-\chi'(\sigma_v')]\,. \end{aligned} \quad (2)$$

But 1, 1, -1 and -1 are respectively the characters of the symmetry operations E, C_2, σ_v and σ_v' pertaining to the irreducible representation A_2, which induces the magnetic variant $2\underline{mm}$, of the point group $2mm$. Therefore the value of $n_{(m\,.\,v)T}$ given by (2) can be expressed as:

$$\begin{aligned} n_{(m\,.\,v)T} &= \tfrac{1}{4}[\chi'(E)\times 1+\chi'(C_2)\times 1+\chi'(\sigma_v)\times(-1) \\ &\quad +\chi'(\sigma_v')\times(-1)] \\ &= \tfrac{1}{4}[\sum_p \chi_p'(R)\chi_{(A_2)}(R)] \\ &= \frac{1}{N}\sum_p h_p\chi_p'(R)\chi_{(A_2)}(R)\,. \end{aligned} \quad (3)$$

It is easy to recognize from (3) and (1) that $n_{(m\,.\,v)T}=n_{(A_2)}$, where $n_{(A_2)}$ represents the number of non-vanishing independent magnetic constants coming under the irreducible representation A_2 of the point group $2mm$. This is a general result which can in the same way be easily established in respect of any other magnetic variant of any other group. The converse of the above result may also be inferred from the one-to-one correspondence between the magnetic variants of a point group G and the alternating representations of G. Hence it may be said that the number of constants required for the description of a magnetic property in respect of a magnetic variant of a G can be directly obtained from that alternating representation of G which induces the magnetic variant. In other words, a physical significance for the number of constants of a magnetic property appearing against the alternating representations of the 32 point groups now emerges when the magnetic variants of a point group G are regarded as being induced by the alternating representations of G. A similar interpretation can be extended to other physical properties.

* The complementary symmetry operations $\mathcal{R}\sigma_v$ and $\mathcal{R}\sigma_v'$ contained in the magnetic variant $2\underline{mm}$ are denoted by $\underline{\sigma_v}$ and $\underline{\sigma_v'}$.

5. Summary

In the present paper, it is shown that the real one-dimensional irreducible representations of a point group induce the magnetic symmetry groups associated with the point group and also give the number of constants needed to describe any magnetic property for the magnetic symmetry groups. Work on the derivation of magnetic space groups will be dealt with in a separate communication.

The authors wish to express their grateful thanks to Professor T. Venkatarayudu for the stimulating discussions which they had with him on the problem. The authors' thanks are also due to the referee for his valuable suggestions in the presentation of the paper.

References

BERTAUT, E. F. (1968). *Acta Cryst.* A**24**, 217.

BHAGAVANTAM, S. & VENKATARAYUDU, T. (1962). *Theory of Groups and its Application to Physical Problems*, p.76. Waltair (India): Andhra Univ.

BHAGAVANTAM, S. & PANTULU, P. V. (1964). *Proc. Ind. Acad. Sci.* **59**A, 1.

BHAGAVANTAM, S. (1966). *Crystal Symmetry and Physical Properties*, p.55. London: Academic Press.

HAMERMESH, M. (1962). *Group Theory*, p.65. Reading (Mass.): Addison-Wesley.

HERZBERG, G. (1945). *Infrared and Raman Spectra of Polyatomic Molecules* pps.105–123. Princeton: Van Nostrand Company.

INDENBOM, V. L. (1959). *Soviet Phys. Cryst.* **4**, 578.

INDENBOM, V. L. (1960). *Soviet Phys. Cryst.* **5**, 493.

KOPTSIK, V. A. (1966). *Shubnikovskie Gruppy.* Moscow: Univ. Press.

LANDAU, L. D. & LIFSHITZ, E. M. (1960). *Electrodynamics of Continuous Media.* Oxford: Pergamon Press.

NIGGLI, A. (1959). *Z. Kristallogr.* **111**, 288.

SHUBNIKOV, A. V. (1951). *Symmetry and Antisymmetry of Finite Figures.* Moscow: Acad. Sci. USSR.

TAVGER, B. A. & ZAITSEV, V. M. (1956). *Soviet Phys. JETP.* **3**, 430.

TINKHAM, M. (1964). *Group Theory and Quantum Mechanics*, p.299. New York: McGraw-Hill.

TISZA, L. (1933). *Z. Phys.* **82**, 48.

ZHELUDEV, I. S. (1960). *Soviet Phys.-Cryst.* **5**, 328.