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Magnetic Symmetry Groups and Their Representation by Stereographic Projections

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Using the theory of representation analysis [Bertaut, E. F. (1968). *Acta Cryst.* **A24**, 217–231] and with the aid of some newly introduced symmetry symbols we present the stereographic projections for all the magnetic symmetry groups. These groups are useful in studying the properties of magnetically ordered crystals.

Introduction

The aim of the present paper is to use the information contained in several related papers (Bertaut, 1968; Boyle, 1969; Krishnamurti & Gopalakrishnamurti, 1969) to construct and present the stereographic projections of all the magnetic point groups. The stereograms for all these groups have been given by Koptsick (1966) in a rather inconvenient and unattractive fashion using red and black colours. We show here by introducing some new symmetry symbols, which are really extensions of the well known ordinary point-group symmetry symbols, that the construction of the stereographic projections for all the magnetic symmetry groups becomes relatively simple. Furthermore the method emphasizes the idea of antisymmetry in a very instructive manner. In the next section we shall briefly introduce the idea of antisymmetry and outline the method used by Bertaut (1968), Boyle (1969) and Krishnamurti & Gopalakrishnamurti (1969) to construct the magnetic symmetry groups.

Antisymmetry and representation theory

In recent years neutron diffraction studies have revealed that all macroscopic properties of magnetic crystals should be characterized by one of the magnetic groups or Shubnikov groups (Shubnikov, 1951; Shubnikov &

Belov, 1964; Tavger & Zaitsev, 1956; Opechowski & Guccione, 1965). This is because the 32 ordinary crystallographic point groups merely describe the possible point symmetry of the mean charge-density function $\rho(\mathbf{r})$ of the crystal in the equilibrium state. In magnetic crystals however, besides $\rho(\mathbf{r})$ there may also be present a non-vanishing time-averaged distribution of current density $J(\mathbf{r})$ and spin density $S(\mathbf{r})$, or in other words a total magnetic moment density $\mu(\mathbf{r}) = J(\mathbf{r}) + S(\mathbf{r})$. Now the symmetry of $\mu(\mathbf{r})$ is characterized by a special symmetry transformation which involves the reversal of the vector direction (Tavger & Zaitsev, 1956; Dimmock & Wheeler, 1962*a,b*; Wigner, 1959). This specific operation of vector reversal, which is not present in the ordinary crystallographic point groups, is incorporated in magnetic groups by means of a new antisymmetry operator R which simply reverses the sign of magnetic moment at each point in space but does not act on the space coordinates. Shubnikov (1951) introduced the idea of antisymmetry by studying the symmetry groups of the polyhedra with coloured faces and derived 122 coloured groups. These groups have now been shown to be isomorphic with the magnetic groups and are therefore appropriate for describing ordered magnetic crystals. The Shubnikov antisymmetry operator may be thought of as a colour-changing operator (*i.e.* changing black \leftrightarrow white) if the lattice points are thought of as having two possible

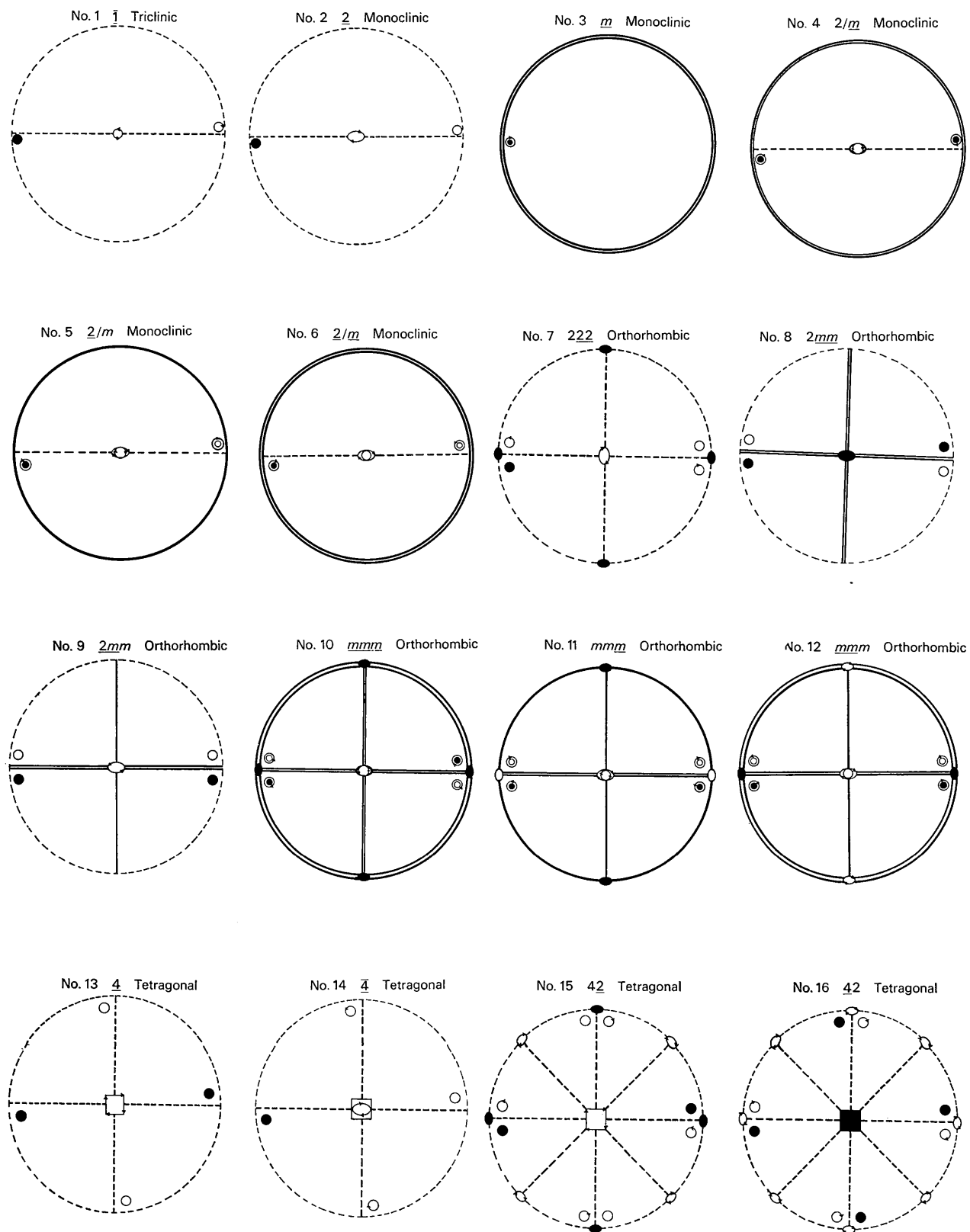


Fig. 1. Stereograms of the 58 type III magnetic point groups as given by Boyle (1969). The symmetry symbols are explained in Table 1. The headings for each stereogram are: Number [as given in Table 1, Boyle (1969)]. Magnetic point-group symbol. (International notation). Crystal system.

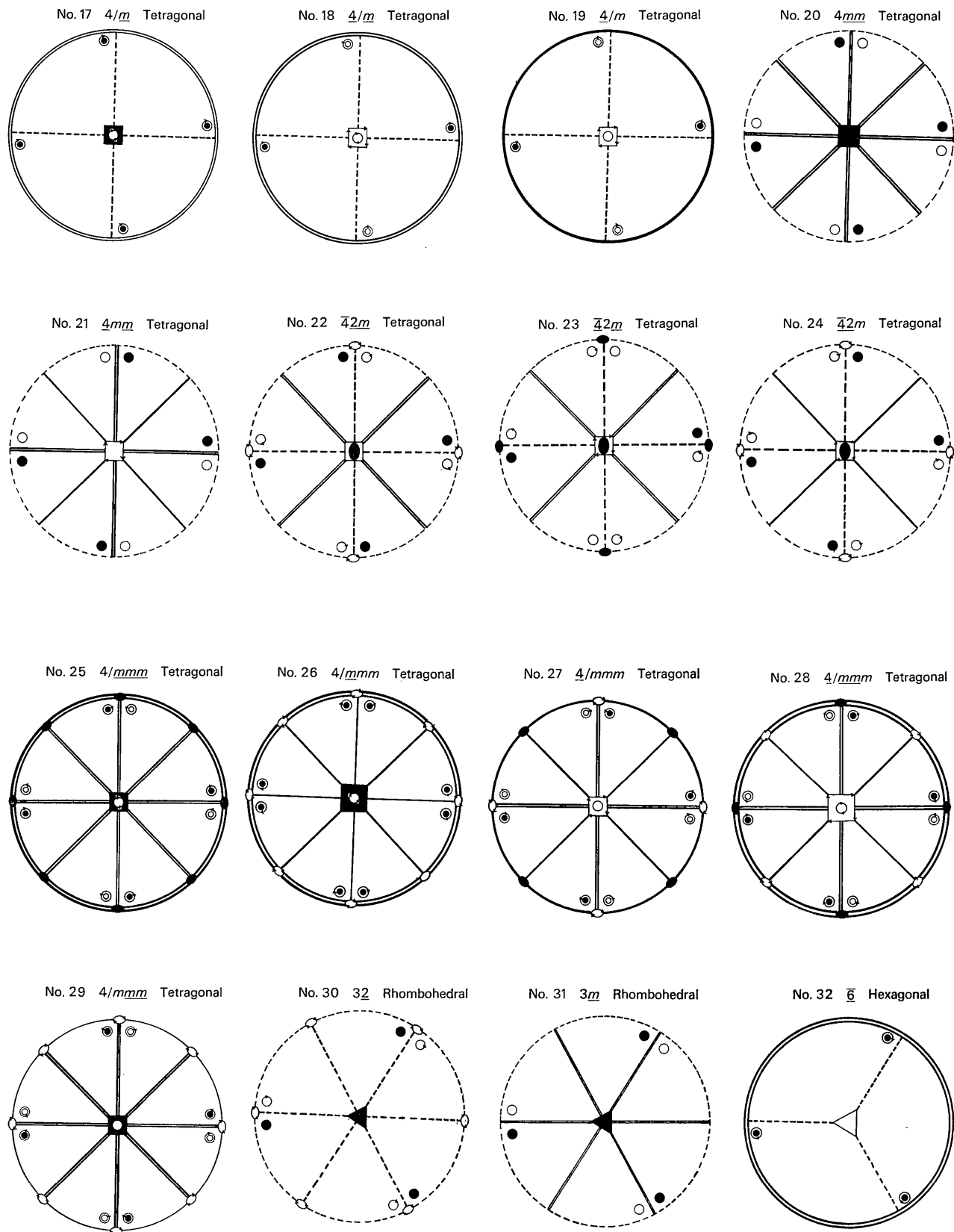


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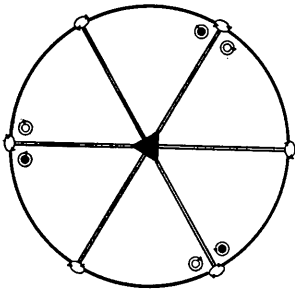
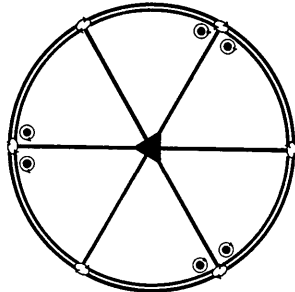
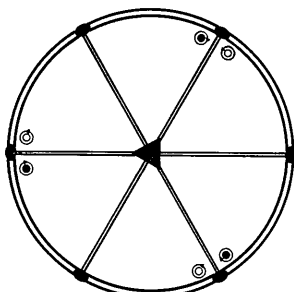
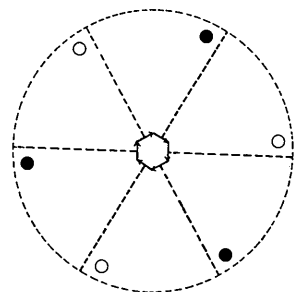
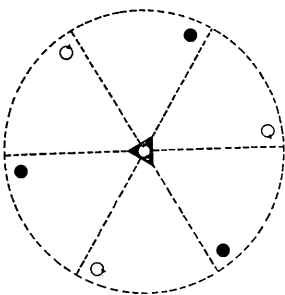
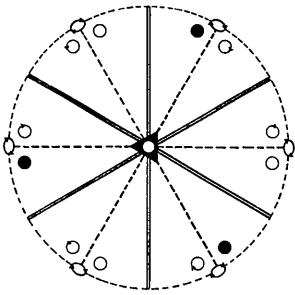
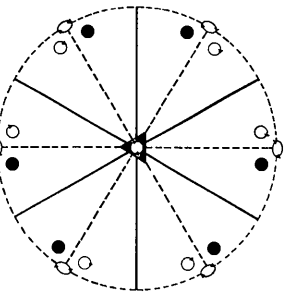
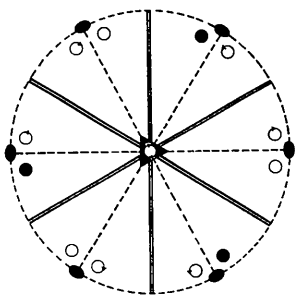
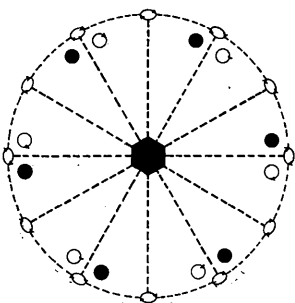
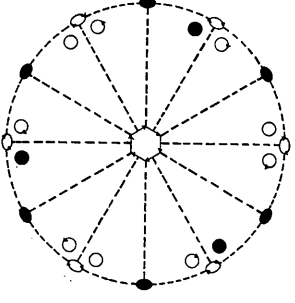
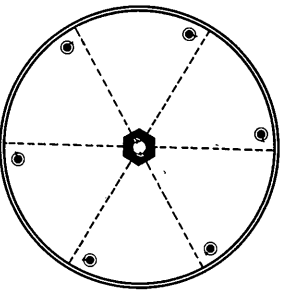
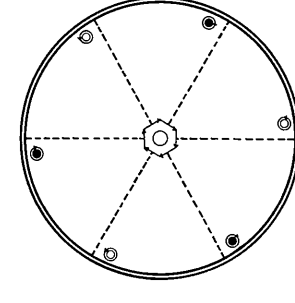
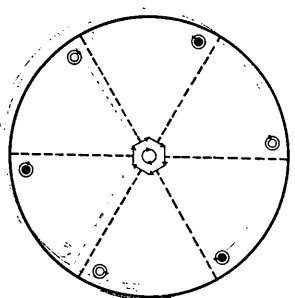
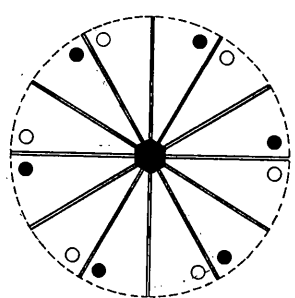
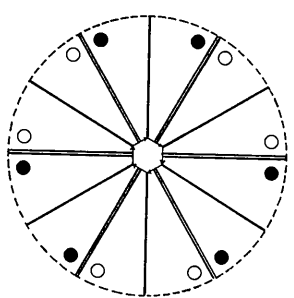
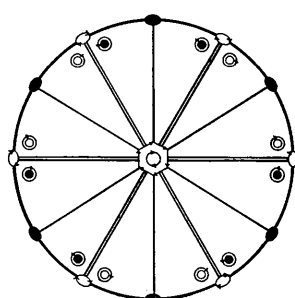
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Fig.1 (cont.)

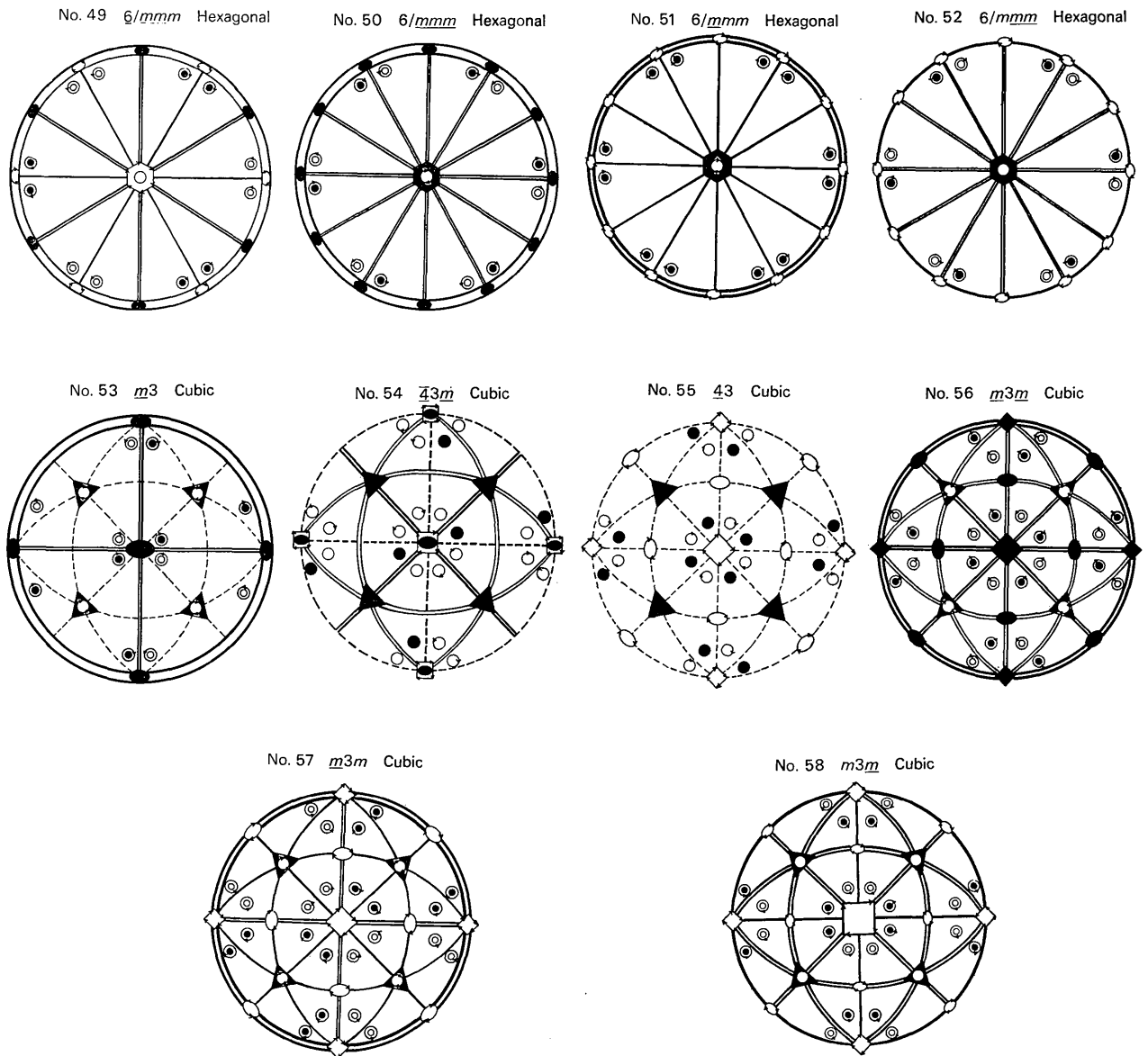


Fig.1 (cont.)

colours (black and white). The colour changing operation is thus completely analogous to the operation R which reverses the sign of the magnetic moment (or current direction) at each site. By adjoining R to the ordinary point groups in an appropriate way we get the so-called magnetic groups or Shubnikov colour groups (Shubnikov, 1951; Tavger & Zaitsev, 1956; Hamermesh, 1962). These number 122 in all and are usually classified into 3 types as uncoloured (32), grey (32) and black and white (58). The classification has been described more fully by Boyle (1969) and we shall use his notations.

In terms of representation theory (Bertaut, 1968) the magnetic groups are derived quite easily by analysing the character tables for the 32 ordinary point


















groups. As the method has been given in several papers we shall consider it very briefly here. We use the character tables of Koster, Dimmock, Wheeler & Statz (1963) as these are now being very widely used by solid-state physicists. The method of construction can be summarized as follows:

(i) The totally symmetric representation Γ_1 or Γ_1^+ is considered as being synonymous with the ordinary point group. This therefore gives us the 32 type I groups.

(ii) The remaining real one-dimensional representations are used to construct the type III magnetic groups.

(iii) If Γ_i is a real one-dimensional representation, a magnetic group is constructed by taking all those

Table 1. Symbols used in drawing the stereograms of the magnetic point groups

Symbol	Description
	Inversion
	Anti-inversion
	Rotation-diad
	Antirotation-diad
	Rotation-triad
	Rotation-tetrad
	Antirotation-tetrad
	Rotation-hexad
	Antirotation-hexad
	Reflexion
	Antireflexion
	General point (neglecting spin) above plane of paper
	General point (neglecting spin) below plane of paper
	General point with spin up above plane of paper
	General point with spin down above plane of paper
	General point with spin up below plane of paper
	General point with spin down below plane of paper

elements with character $+1$ to be in the unitary subgroup and all those elements with character -1 to be in the antiunitary subgroup and therefore to be associated with the antiunitary operator R .

(iv) The complex one-dimensional representations and the degenerate representations are of no relevance in this context.

The results have been given by Boyle (1969) and we shall use his Table 1 in labelling the stereograms of the magnetic groups. The graphical symbols used in drawing these projections are summarized in Table 1. The symbols are self explanatory and are simple extensions of the standard notations. As can be readily seen the character tables are a useful aid in drawing these stereograms since all symmetry elements with character

-1 are represented with the corresponding symbols of anti-operation. The three-dimensional stereograms of all the type III magnetic groups as tabulated by Boyle (1969) are given in Fig. 1.

The point groups treated here can obviously be extended to the space groups such that equivalent general-position and symmetry diagrams for all the 1651 magnetic space groups could be drawn to conform with the conventional *International Tables for X-ray Crystallography* (1952). However, it would be a very arduous task here to draw the symmetry diagrams for all the magnetic space groups and we make no attempt to do this.

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