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Morphology of the Heesch Magnetic Groups and Associated Magnetic Aspects

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The structures of the 122 magnetic point groups (Heesch groups) and their relation to the structures of the 32 associated magnetic aspect groups, underlying point groups and invariant subgroups are studied and enumerated in a physically meaningful scheme. It is shown that in many instances the number of classes of a given group is simply related to the number of classes of an associated group, and these relations are given.

The concept of generalization of the crystallographic point and space groups through inclusion of an operation which reverses the value of a two-valued quantity was originally introduced by Heesch (1930). This concept has turned out to be a very useful one in the study of magnetic crystal structures (Donnay, Corliss, Donnay, Elliott & Hastings, 1958). There result, from the generalization of the 32 ordinary crystallographic point groups through the introduction of a change-of-color (black–white) operation and its identification with time reversal, 122 magnetic groups (Donnay & Donnay, 1959; Donnay, 1967) which have been called the Heesch groups (Riedel & Spence, 1960; Spence & van Dalen, 1968).

The group A, obtained from a given Heesch group H by replacing all improper rotations by the corresponding proper rotations, and by replacing all time-reversing proper and improper rotations by the corresponding improper rotations was introduced by Donnay & Donnay (1959) and was called the (magnetic) aspect group by Spence & van Dalen (1968). The importance of the magnetic aspect group derives from the fact that it is uniquely determinable by n.m.r. experiments.

The underlying point group G is obtained from H by replacing all time-reversing elements of H by the corresponding non-time-reversing elements. The invariant subgroup S is that group which is obtained by deleting all time-reversing elements from H. In the case that H is one of the 32 grey or one of the 58 black-white Heesch groups, S is an invariant subgroup of H of index 2. In the case that H is one of the 32 colorless Heesch groups, the invariant subgroup S is equal to H itself.

The above definitions are summarized in Table 1. Throughout, time reversal will be denoted by single prime and improper rotations by a bar affixed to the appropriate symbols.

Table 1. *Relation between the elements of the Heesch group H, aspect group A, underlying point group G, and invariant subgroup S*

Operation in H	H	A	G	S
n-fold rotation	n	n	n	n
n-fold time-reversal rotation	n'	$\bar{n}$	n	omit
n-fold improper rotation	$\bar{n}$	n	$\bar{n}$	$\bar{n}$
n-fold improper time-reversal rotation	$\bar{n}'$	$\bar{n}$	$\bar{n}$	omit

Any group A, G, or S can be shown to be one of the ordinary 32 crystallographic point groups which can be classified as follows:

Type I: This type is comprised of the 11 pure rotation groups 1,2, 3, 4, 6, 222, 32, 422, 622, 23, and 432 and will be designated by R.

Type II: These are the 11 groups obtained as the direct product group of a Type I group with the inversion group $\bar{1}$, viz., $\bar{1}$, $2/m$, $\bar{3}$, $4/m$, $6/m$, mmm, $\bar{3}m$, $4/mmm$, $6/mmm$, $m3$, and $m3m$. These groups are thus $R\times\bar{1}=R+\bar{R}=R+\bar{1}R$ and have R as an invariant subgroup of index 2. Here the symbol $\bar{1}$ denotes the inversion operation and $\bar{1}R=\bar{R}$ is the coset of R obtained by multiplying each element of R by the inversion. The number of classes of the group $R+\bar{R}$ is equal to twice the number of classes of R. Type II is the only type which contains the inversion $\bar{1}$ as a group element.

Type III: The remaining ten crystallographic point groups, *viz.* $mm2$, $3m$, $4mm$, $6mm$, m, $\bar{6}$, $\bar{4}2m$, $\bar{6}m2$, $\bar{4}$, and $\bar{4}3m$ have the structure $R+\bar{K}$ where R is a pure rotation group and $\bar{K}$ is a set of improper rotations such that no element of the set of corresponding proper rotations K is in R, and R is an invariant subgroup of $R+\bar{K}$. Thus $R+\bar{K}=R+\bar{r}R=R+r\bar{R}$, where $\bar{r}$ is a coset representative of the coset $\bar{K}$ and r is the corresponding proper rotation. It can be shown (Lomont, 1959) that the pure rotation group $R+K$ is isomorphic to $R+\bar{K}$. Therefore, the number of classes of $R+\bar{K}$ is equal to the number of classes of $R+K$. Both R and $\bar{K}$ (or K) consist of complete classes. However, the number of classes of $R+\bar{K}$ is not necessarily equal to twice the number of classes of R unless both R and $R+\bar{K}$ are Abelian. Furthermore, the number of classes of the pure rotation group R, when taken by itself, is not, in general, equal to the number of classes of the invariant subgroup R of G $=R+\bar{K}$ when R is part of G.

In accordance with the above discussion the three types of crystallographic point group will be designated as: R (Type I); $R+\bar{R}=R+\bar{1}R$ (Type II); and $R+\bar{K}=R+r\bar{R}$ (Type III).

32 Colorless Heesch groups

Here three cases arise as follows:

(*a*) $H=G=S=R$ $\quad A=R$
(*b*) $H=G=S=R+\bar{R}$ $\quad A=R$
(*c*) $H=G=S=R+\bar{K}$ $\quad A=R+K$

Thus, G and S may be either Type I, II, or III, but the aspect group is always Type I. For the number of classes n one has

$n_H=n_G=n_S=n_A$ for (*a*) and (*c*), S does not contain $\bar{1}$
$n_H=n_G=n_S=2n_A$ for (*b*), S contains $\bar{1}$.

It is easy to prove that all the above statements are also valid for the corresponding double groups.

32 Grey Heesch groups

The grey groups contain time reversal $1'$ as an element and therefore their aspect group must contain the inversion $\bar{1}$ as an element, *i.e.*, A is Type II. Three cases can be distinguished according as S is Type I, II, or III, as follows:

(*a*) $H=G+G'=R+R'$
$S=R \quad A=R+\bar{R}$

(*b*) $H=G+G'=(R+\bar{R})+(R+\bar{R})'$
$S=R+\bar{R} \quad A=R+\bar{R}$

(*c*) $H=G+G'=(R+\bar{K})+(R+\bar{K})'$
$S=R+\bar{K} \quad A=(R+\bar{K})+(\overline{R+\bar{K}})$.

From this it can be seen that one has for the classes:

$n_H=2n_G=2n_S=n_A$ for (*a*) and (*c*), S does not contain $\bar{1}$
$n_H=2n_G=2n_S=2n_A$ for (*b*), S contains $\bar{1}$.

These considerations are also valid for the double groups.

21 Black–white Heesch groups with type II aspect groups

Since the time-reversing elements of H go to improper rotations in the formation of the aspect group, black-white groups cannot have Type I aspect groups. In this section we consider the black–white Heesch groups that have Type II aspect groups, and the Type III aspect groups will be discussed in the section following.

If A is of Type II, then H contains $\bar{1}'$ and hence H cannot contain $\bar{1}$ since H is black–white. Therefore G contains $\bar{1}$ and is of Type II; and S does not contain $\bar{1}$, so S is either of Type I or of Type III. We thus have two cases as follows:

(*a*) S is of Type I:
$H=R+\bar{R}'$ $\quad G=R+\bar{R}$ $\quad S=R$ $\quad A=R+\bar{R}=G$.

For the second case, let R_s be a Type I invariant subgroup of the pure rotation group R, $R=R_s+rR_s$ where r is a coset representative of the coset rR_s. Then

(*b*) S is of Type III:
$H=(R_s+r\bar{R}_s)+(\bar{R}_s+rR_s)'$
$G=R_s+r\bar{R}_s+\bar{R}_s+rR_s=R+\bar{R}$
$S=R_s+r\bar{R}_s$
$A=R+\bar{R}=G$.

From this it follows for both (*a*) and (*b*) that

$$n_H=n_G=2n_S=n_A$$

with the same relations also valid for the double groups.

All eleven Type I and all ten Type III point groups appear as S in this category because every R can be used as the group S to generate a distinct Heesch group, case (*a*), and every $R+\bar{K}$ can be used as the group S to generate a distinct Heesch group, case (*b*). There are, therefore, 21 black-white Heesch groups with Type II aspect groups.

37 Black–white Heesch groups with type III aspect groups

When A is of Type III, A does not contain $\bar{1}$, therefore H does not contain $\bar{1}'$. Hence S may contain $\bar{1}$ but need not necessarily. If S contains $\bar{1}$ (Type II), then H

contains $\bar{1}$, and if S does not contain $\bar{1}$ (Type I or Type III), then H does not contain $\bar{1}$. With this it is possible to distinguish four cases:

(*a*) $H=R+rR'$	$G=R+rR$ (Type I)
$S=R$ (Type I)	$A=R+r\bar{R}=R+\bar{K}$
(*b*) $H=R+r\bar{R}'$	$G=R+r\bar{R}=R+\bar{K}$ (Type II)
$S=R$ (Type I)	$A=R+r\bar{R}=R+\bar{K}=G$
(*c*) $H=(R+\bar{R})+r(R+\bar{R})'$	$G=(R+rR)+(\bar{R}+r\bar{R})$ (Type II)
$S=R+\bar{R}$ (Type II)	$A=R+r\bar{R}=R+\bar{K}$
(*d*) $H=R_s+\bar{K}_s+r(R_s+\bar{K}_s)'$	$G=R_s+\bar{K}_s+r(R_s+\bar{K}_s)$ (Type III)
$S=R_s+\bar{K}_s$ (Type III)	$A=R+r\bar{R}=R+\bar{K}$

where $R=R_s+K_s$, $r\bar{R}=\bar{K}=r(\bar{R}_s+\bar{K}_s)$.

From the above, one can determine that for both the single and the double groups

$n_H=n_G=n_A=n_{R+\bar{K}}$ and $n_S=n_R$ for (*a*), (*b*) and (*d*), S does not contain $\bar{1}$,

$n_H=n_G=2n_A=2n_{R+\bar{K}}$ and $n_S=2n_R$ for (*c*), S contains $\bar{1}$.

There exists, however, no simple general proportionality between $n_{R+\bar{K}}$ and n_R unless both R and $R+\bar{K}$ are Abelian in which case necessarily $2n_R=n_{R+\bar{K}}$. This is the case for the single and double groups $R+\bar{K}=m$, $\bar{4}$, and $\bar{6}$, and for the single group $R+\bar{K}=mm2$. The number of classes $n_{R+\bar{K}}=n_{R+K}$ and n_R are given in Table 2 for all ten $R+\bar{K}$. All possibilities of our enumeration scheme are now exhausted, and they are summarized in Table 3.

Table 2. *The number of classes in the groups $R+\bar{K}$ and R*

			Single groups		Double groups	
$R+\bar{K}$	$R+K$	R	$n_{R+\bar{K}}$	n_R	$n_{R+\bar{K}}$	n_R
m	2	1	2	1	4	2
$\bar{4}$	4	2	4	2	8	4
$\bar{6}$	6	3	6	3	12	6
$mm2$	222	2	4	2	5	4
$4mm$	422	4	5	4	7	8
$\bar{4}2m$	422	222	5	4	7	5
$3m$	32	3	3	3	6	6
$\bar{4}3m$	432	23	5	4	8	7
$6mm$	622	6	6	6	9	12
$\bar{6}m2$	622	32	6	3	9	6

Table 3. *Classification of the groups G, S, and A into types* I, II, *and* III

Group:	G	S	A	H	Number of H
Type:	I	I	I	colorless	11
	II	II	I	colorless	11
	III	III	I	colorless	10
	I	I	II	grey	11
	II	II	II	grey	11
	III	III	II	grey	10
	II	I	II	black–white	11
	II	III	II	black–white	10
	I	I	III	black–white	10
	II	I	III	black–white	10
	II	II	III	black–white	10
	III	III	III	black–white	7

Discussion

In general, the classes of a group are the same in number as the sets of like operations around physically equivalent axes. When it is found that the number of classes of one of the groups considered is equal to the number of classes of a related group, the two groups have an equal number of sets of like operations around equivalent axes, whereas a doubling of classes implies that the number of sets of equivalent axes is doubled (or halved) when one forms one group from the other according to the pattern of Table 1. Our analysis shows that in the case of the Heesch groups with Type III aspect groups, the number of sets of equivalent axes of the invariant subgroup S is, in general, neither unchanged, nor halved, nor doubled when compared to the number of equivalent axes of the related groups, whereas in the other instances it is.

The theory of group representations for unitary groups shows that the number of classes of a group is equal to its number of nonequivalent irreducible representations. Therefore, all relations we have stated concerning the number of classes of G, S, A, and H are also true for the number of nonequivalent irreducible representations of G, S, A, and H.

The nonequivalent irreducible representations of H are identical with the nonequivalent irreducible representations of G when H is colorless (since $H=G$), and also when H is black–white since in that case H

Table 4. *Errata, Spence & van Dalen* (1968), *Table* 1

Heesch group no.	Incorrect	Corrected
5	$1'$	$\bar{1}'$
18	$mm'2'$	$2'm'm$
19	$22'2'$	$2'2'2$
20	$mm'm'$	$m'm'm$
40	$4'2'2$	$4'22'$
43	$\bar{4}2'm$	$\bar{4}'m2'$
44	$4/mmm'$	$4'/mmm'$
57	$4/mmm$	$4/m'm'm'$
59	$4'/m'mm$	$4'/m'm'm$
81	$6/m$	$6'/m'$
85	$6/m$	$6/m'$
86	$6/m$	$6'/m$
91	$\bar{6}2m$	$\bar{6}m2$
92	$\bar{6}'m2'$	$\bar{6}'2'm$
94	$6mm$	$6'm'm$
95	$6'/mmm'$	$6'/m'm'm$
97	$6mm$	$6m'm'$
100	$6'/mm'm'$	$6/m'm'm'$
101	$6'/mmm$	$6/m'mm$
102	$6'/mm'm'$	$6'/mm'm$
111	$m3$	$m'3$
115	$\bar{4}m3$	$\bar{4}'3m'$
116	432	$4'32'$
117	$m3m$	$m3m'$
121	$m3m$	$m'3m'$
122	$m3m$	$m'3m$

and G have identical multiplication tables when considered in the abstract and thus are isomorphic. When H is grey, it is equal to the direct product group $G \times 1'$ and hence it has two representations for each representation of G which are readily generated by the direct product procedure. If, however, the time-reversing elements of the grey and black–white Heesch groups are interpreted as antiunitary operators, then the number of nonequivalent irreducible corepresentations of H (Wigner, 1959) is no longer necessarily equal to the number, or twice the number, of nonequivalent irreducible representations of G. Rather, the number of nonequivalent irreducible co-representations of H is less than or equal to the number of classes of S, and it is less than the number of classes of S by the number of pairs of nonequivalent irreducible representations of S which 'stick together'. For the grey groups, the pairs of nonequivalent irreducible representations of S which stick together are those with complex characters, but this is not generally true for the black–white groups (Dimmock & Wheeler, 1962).

Errata

We give in Table 4 a listing of errata we have located in Table 1 of Spence & van Dalen (1968).

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Indétermination sur les Dimensions de la Maille magnétique dans l'Étude par Diffraction neutronique sur Poudres de Corps cubiques ou uniaxes

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An ambiguity arises in the study by powder neutron diffraction of compounds where the magnetic atoms lie on a uniaxial or cubic Bravais lattice, when the magnetic lines are indexed $\{\frac{h}{2}kl\}$ or $\{\frac{h}{2}\frac{k}{2}l\}$. Many multiaxial configurations, all having the same isotropic coupling energy, are compatible with a given set of lines. For a simple cubic lattice it is shown that every multiaxial configuration is indistinguishable, using powder intensities, from a particular uniaxial one, and that both have the same dipolar energy.

Introduction

On sait (Shirane, 1959) que, dans un composé à structure magnétique colinéaire où les atomes sont aux noeuds d'un réseau de Bravais cubique ou uniaxe, la diffraction neutronique sur poudres ne permet pas de déterminer complètement la direction des moments. Par ailleurs, dans certains cas: MnO (Li, 1955; Keffer & O'Sullivan, 1957; Roth, 1958), βMnS (Keffer, 1962). $MnTe_2$ (Hastings, Corliss, Blume & Pasternak, 1970), des alliages fer–manganèse (Kouvel & Kasper, 1963; Umebayashi & Ishikawa, 1966), il apparait une indétermination entre des structures colinéaires et des structures multiaxiales, mais il n'y a pas d'ambiguïté sur les dimensions de la maille magnétique.

Nous étudions ici un type d'indétermination analogue mais qui porte sur les directions des moments et en même temps sur les dimensions de la maille. Soit, par exemple, un réseau de Bravais quadratique ou hexagonal pour lequel les indices des raies magnétiques d'un diagramme de poudre, rapportés à la maille chimique, sont de la forme $\{\frac{h}{2}kl\}$. On peut interpréter ceci en faisant l'hypothèse d'une structure magnétique colinéaire de vecteur de propagation $\mathbf{k}$ $[\frac{1}{2},0,0]$, la maille étant doublée dans la direction $\mathbf{x}$ par exemple. Mais une hypothèse plus générale consiste à considérer que l'on peut observer la superposition de réflexions $\frac{h}{2}kl$ et $h\frac{k}{2}l$, la maille magnétique pouvant être doublée dans les deux directions équivalentes $\mathbf{x}$ et $\mathbf{y}$. Le même problème se pose évidemment pour un réseau cubique ou rhomboédrique avec une indexation de type $\{\frac{h}{2}kl\}$ ou $\{\frac{h}{2}\frac{k}{2}l\}$.

Nous avons déjà considéré ce cas pour le composé cubique DyCu (Wintenberger, Chamard-Bois, Belak-