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Coset and double-coset decompositions of the magnetic point groups[1]

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The coset and double-coset decompositions of the 420 subgroups of $m_z\bar{3}_{xyz}m_{xy}1'$ (O_h1') and the 236 subgroups of $6_z/m_zm_xm_11'$ ($D_{6h}1'$) with respect to each of their subgroups are calculated along with additional mathematical properties of these groups.

1. Introduction

Coset decompositions have been applied in the analysis of domains of ferroic crystals using coset decompositions of non-magnetic point groups (Aizu, 1970; Janovec, 1972) and of space groups (Aizu, 1974; Janovec, 1976). The double-coset decomposition has been used in a tensorial classification of domain pairs in the case where each domain is characterized by a unique form of a physical property tensor (Janovec, 1972) and in the case where more than a single domain is characterized by a specific form of a physical property tensor (Litvin & Wike, 1989). The coset and double-coset decomposition of the 32 non-magnetic crystallographic point groups have been given, along with additional mathematical properties of the non-magnetic crystallographic point groups, by Janovec *et al.* (1989). This served as the basis for the calculation by Schlessman & Litvin (1995) of non-magnetic *twin laws* for the analysis of the physical properties of pairs of non-magnetic domains in ferroic crystals.

In §2, we briefly review the definitions of coset and double-coset decompositions. In §3, we give the list of properties, in addition to the coset and double-coset decompositions, of magnetic point groups which have been tabulated. An example of a coset and double-coset decomposition of a magnetic point group is given and the tabulations of the subgroups of magnetic point groups are compared to the listings of Ascher & Janner (1965).

2. Coset and double-coset decompositions

For a given group G and subgroup H, one writes the left coset decomposition of G with respect to H symbolically as

$$G = H + g_2H + g_3H + \ldots + g_nH,$$

where g_iH denotes the subset of elements of G obtained by multiplying each element of the subgroup H from the left by the element g_i of G (Hall, 1959). Each subset of elements g_iH, $i = 1, 2, \ldots, n$, is called a left coset of G with respect to H, and the elements g_i, $i = 1, 2, \ldots, n$, of G are called left coset representatives of the left coset decomposition of G with respect to H. While an analogous, and possibly distinct, right coset decomposition of G with respect to H can be defined, it is the left coset decomposition that is applicable in the symmetry analysis of ferroic materials (Aizu, 1970; Janovec, 1972).

For a given group G and subgroup H, one writes the double-coset decomposition of G with respect to H symbolically as

$$G = H + Hg_2^{\rm dc}H + Hg_3^{\rm dc}H + \ldots + Hg_m^{\rm dc}H,$$

where $Hg_j^{\rm dc}H$ denotes the subset of *distinct* elements of G obtained by multiplying each element of the coset $g_j^{\rm dc}H$ by every element of the subgroup H (Hall, 1959). Each subset of elements $Hg_j^{\rm dc}H$, $j = 1, 2, \ldots, m$, is called a double coset of G with respect to H, and the elements $g_j^{\rm dc}$, $j = 1, 2, \ldots, m$, are called double coset representatives of the double-coset decomposition of G with respect to H. Each double coset consists of a specific number of cosets of the coset decomposition of G with respect to H. The elements of the two double cosets $Hg_j^{\rm dc}H$ and $H(g_j^{\rm dc})^{-1}H$ are either identical or disjoint. If identical, the double coset $Hg_j^{\rm dc}H$ is called an *ambivalent* double coset and, if disjoint, the two double cosets are called *complementary* double cosets (Janovec, 1972). The double-coset decomposition of magnetic point groups serves as a basis for the calculation of magnetic *twin laws* (Schlessman & Litvin, 2001) for the analysis of the physical properties of pairs of magnetic domains in ferroic crystals.

3. Properties

The magnetic point groups referred to in this paper are the 420 subgroups of $m_z\bar{3}_{xyz}m_{xy}1'$ (O_h1') and the 236 subgroups of $6_z/m_zm_xm_11'$ ($D_{6h}1'$). This is performed instead of considering only one group of each of the 122 types of magnetic point groups to allow consideration of groups of the same type but of different orientations. The following properties of these magnetic groups have been tabulated:[2]

Elements
Products of elements
Conjugation of elements
Subgroups
Normal subgroups
Conjugate subgroups
Centralizers of subsets and subgroups
Normalizers of subsets and subgroups
Coset and double-coset decompositions

As an example, we give in Table 1 the coset and double-coset decompositions of $G = m_z'\bar{3}_{xyz}'m_{xy}$ with respect to $H = m_z'm_x'2_y$. Each

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[2] A computer program entitled *Properties of the Magnetic Point Groups* is available from the IUCr electronic archives (Reference: DR0009). Services for accessing these data are described at the back of the journal.

Table 1
The coset and double-coset decomposition of $G = m'_z\bar{3}'_{xyz}m_{xy}$ with respect to $H = m'_z m'_x 2_y$.

1	2_y	m'_x	m'_z
2_x	2_z	$\bar{1}'$	m'_y
3^2_{xyz}	$3_{xy\bar{z}}$	$\bar{3}'_{x\bar{y}z}$	$\bar{3}'_{\bar{x}yz}$
$3_{\bar{x}yz}$	$3_{x\bar{y}z}$	$\bar{3}'_{xy\bar{z}}$	$\bar{3}^{5\prime}_{xyz}$
3_{xyz}	$3^2_{\bar{x}yz}$	$\bar{3}^{5\prime}_{xy\bar{z}}$	$\bar{3}^{5\prime}_{x\bar{y}z}$
$3^2_{xy\bar{z}}$	$3^2_{x\bar{y}z}$	$\bar{3}'_{xyz}$	$\bar{3}^{5\prime}_{\bar{x}yz}$
m_{xy}	$\bar{4}^3_z$	$2'_{\bar{x}y}$	$4'_z$
$m_{\bar{x}y}$	$\bar{4}_z$	$2'_{xy}$	$4^{3\prime}_z$
$m_{\bar{y}z}$	$\bar{4}^3_x$	$2'_{yz}$	$4'_x$
m_{yz}	$\bar{4}_x$	$2'_{\bar{y}z}$	$4^{3\prime}_x$
$\bar{4}_y$	$\bar{4}^3_y$	$2'_{xz}$	$2'_{\bar{x}z}$
m_{xz}	$m_{\bar{x}z}$	$4'_y$	$4^{3\prime}_y$

row contains the elements of a single coset. Sets of cosets that constitute a single double coset are set within brackets. The third and fourth double cosets from the top of Table 1 are complementary while the remainder are ambivalent.

Of the remaining properties of the magnetic point groups, we shall discuss only *subgroups*: We have compared our computer-generated tables of subgroups to *hand-made* tables of the number of subgroups (Ascher & Janner, 1965; Janner, 1998). For the magnetic point groups $4_z/m_z m_x m_{xy}1'$ and $m_z\bar{3}_{xyz}1'$, we find 158 and 92 subgroups, respectively, while Ascher & Janner (1965) list the number of these subgroups as 146 and 88. In the former case, we find 6, and not 2, subgroups of each of the types $mm21'$, $m'mm$, and $m'm'm$. In the latter case, we find 4, and not 0, subgroups of the type $\bar{3}1'$.

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