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SHORT COMMUNICATIONS

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The coset and double coset decomposition of the 32 crystallographic point groups. By V. JANOVEC and E. DVORAKOVA, *Institute of Physics, Czechoslovak Academy of Sciences, POB 24, Na Slovance 2, 18040 Prague 8, Czechoslovakia* and T. R. WIKE* and D. B. LITVIN, *Department of Physics, The Pennsylvania State University, The Berks Campus, PO Box 7009, Reading, PA 19610-6009, USA*

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Abstract

The coset and double coset decompositions of the 32 crystallographic point groups with respect to each of their subgroups are tabulated.

I. Introduction

The mathematical concept of the coset decomposition of a group with respect to one of its subgroups has wide applications in crystallography and solid-state physics. The points of any crystallographic orbit are in a one-to-one correspondence with the cosets of the coset decomposition of the crystallographic group with respect to the site symmetry group of one of its points (Wondratschek, 1983). Coset decompositions have been applied in the analysis of domains of ferroic crystals using coset decompositions of point groups (Aizu, 1970; Janovec, 1972) and of space groups (Aizu, 1974; Janovec, 1972, 1976). This concept has also been used in the derivation of twin laws for (pseudo-)merohedry (Flack, 1987).

The mathematical concept of the double coset decomposition of a group is less well known and has been used in applications to a lesser extent than the coset decomposition [see Ruch & Klein (1987) and references therein]. 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).

In § II we briefly review the definitions of coset and double coset decompositions. Tables of the coset and double coset decompositions of the 32 crystallographic point groups with respect to each of their subgroups are given in § III.

II. 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

$$G = H + g_2H + g_3H + \dots + g_nH$$

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 , $i = 1, 2, \dots, n$, is called a left coset of G with respect to H , and the elements g_i , $i = 1, 2, \dots, n$, of G are called the left coset representatives of the left coset decomposition of G with respect to H .

The subset of elements of G in each coset of the left coset decomposition of G with respect to H is unique, but the coset representatives are not unique. A coset representative g_i can be replaced by the element g_ih , where h is an arbitrary element of the subgroup H .

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

$$G = H + Hg_2^{\text{dc}}H + Hg_3^{\text{dc}}H + \dots + Hg_m^{\text{dc}}H$$

where $Hg_j^{\text{dc}}H$ denotes the subset of *distinct* elements of G

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Table 1. *The coset and double coset decomposition of $G = m\bar{3}m$ with respect to $H = m_z m_x 2_y$*

Each row contains the elements of a single coset. Sets of cosets constituting a single double coset are separated, in general, by a horizontal dashed line, but members of pairs of complementary double cosets are separated by a horizontal dotted line.

1	2_y	m_x	m_z
2_x	2_z	$\bar{1}$	m_y
3_{xyz}^2	$3_{xy\bar{z}}$	$\bar{3}_{xyz}$	$\bar{3}_{xy\bar{z}}$
$3_{\bar{x}yz}$	$3_{x\bar{y}z}$	$\bar{3}_{\bar{x}yz}$	$\bar{3}_{x\bar{y}z}$
3_{xyz}^2	$3_{\bar{x}yz}$	$\bar{3}_{xy\bar{z}}$	$\bar{3}_{\bar{x}yz}$
$3_{x\bar{y}z}^2$	$3_{x\bar{y}z}$	$\bar{3}_{x\bar{y}z}$	$\bar{3}_{x\bar{y}z}$
$2_{\bar{x}y}$	4_z	$\bar{4}_z^2$	m_{xy}
4_z^3	2_{xy}	$m_{\bar{x}y}$	$\bar{4}_z$
2_{yz}	4_x^3	m_{yz}	$\bar{4}_x$
4_x	2_{yz}	$\bar{4}_x^3$	m_{yz}
2_{xz}	2_{xz}	$\bar{4}_y$	$\bar{4}_y^3$
4_y^3	4_y	m_{xz}	m_{xz}

obtained by multiplying each element of the coset $g_j^{dc}H$ from the left by every element of the subgroup H (Hall, 1959).^{*} Each subset of elements $Hg_j^{dc}H$, $j = 1, 2, \dots, m$, is called a double coset of G with respect to H , and the elements g_j^{dc} , $j = 1, 2, \dots, m$, are called the double coset representatives of the double coset decomposition of G with respect to H . By their definition, each double coset consists of a specific number of cosets of the coset decomposition of G with respect to H .

The subset of elements of G in each double coset of the double coset decomposition of G with respect to H is unique, but the double coset representatives are not unique. The double coset representative g_j^{dc} can be replaced by $h'g_j^{dc}h$ where h and h' are arbitrary elements of the subgroup H .

The elements of the two double cosets $Hg_j^{dc}H$ and $H(g_j^{dc})^{-1}H$ are either identical or disjoint. If identical, the double coset $Hg_j^{dc}H$ is called an *ambivalent* double coset and the inverse of each element is contained in the double

^{*} This definition of a double coset decomposition of a group G with respect to a subgroup H , which we use in this paper, is the special case of the more general definition of a double coset decomposition of a group G with respect to two subgroups H and H' (Hasselbarth, Ruch, Klein & Seligman, 1980) when $H' = H$.

coset. If disjoint, the two double cosets are called *complementary* double cosets, and the inverse of each element in one of a pair of complementary double cosets is found in the other double coset.

III. Tables of coset and double coset decompositions

Tables of the coset and double coset decomposition of the 32 crystallographic point groups with respect to one of each set of conjugate subgroups were given by Janovec & Dvorakova (1974). These tables are extended here and retabulated in International (Hermann-Mauguin) notation to include all subgroups of the 32 crystallographic point groups. In Table 1 we give an example of these tables,^{*} the coset and double coset decomposition of the point group $G = m\bar{3}m$ with respect to the subgroup $H = m_z m_x 2_y$. Each row contains the elements of a single coset. In general, double cosets are separated by horizontal dashed lines but the members of a pair of complementary double cosets are separated by a horizontal dotted line.

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^{*} The complete tables have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52108 (485 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. A computer program on disk for IBM compatible personal computers entitled *The 32 Crystallographic Point Groups* is also available through the Executive Secretary. This program calculates the notation, elements, subgroups, centralizers, normalizers, normal subgroups, and coset and double coset decompositions of the 32 crystallographic point groups.

Notes and News

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Nominations sought for the Patterson Award for 1990

One of the four major triennial awards of the American Crystallographic Association, named after a major figure in structural crystallography and in the ACA, Arthur Lindo Patterson, will be awarded at the ACA New Orleans meeting in April 1990. The award is to 'recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the

methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information'. The purpose of the award is not only to recognize achievement, but also to inspire further effort and research, and shall be given without regard to nationality, ACA membership or age.

Nominations should include a concise statement summarizing the work to be recognized by the award, including references. They should be sent to the Chair