

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	$3_{x\bar{y}z}$	$\bar{3}_{xyz}$	$\bar{3}_{x\bar{y}z}$
$3_{\bar{x}yz}$	$3_{x\bar{y}\bar{z}}$	$\bar{3}_{x\bar{y}\bar{z}}$	$\bar{3}_{xyz}$
3_{xyz}^2	$3_{\bar{x}yz}$	$\bar{3}_{x\bar{y}z}$	$\bar{3}_{x\bar{y}\bar{z}}$
$3_{x\bar{y}z}^2$	$3_{x\bar{y}\bar{z}}$	$\bar{3}_{x\bar{y}\bar{z}}$	$\bar{3}_{xyz}$
$2_{\bar{x}y}$	4_z	$\bar{4}_z^2$	m_{xy}
4_z^3	2_{xy}	$m_{\bar{x}y}$	$\bar{4}_z$
$2_{\bar{y}z}$	4_x^3	m_{yz}	$\bar{4}_x$
4_x	2_{yz}	$\bar{4}_x^3$	$m_{\bar{y}z}$
$2_{\bar{x}z}$	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

of the award committee, K. N. Trueblood, Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90024, USA (BITNET address: TRUEBLOOD@UCLACH), or to any of the other

members of the committee: Dr Helen Berman, Dr Philip Coppens, and Dr Michael James.

The deadline for receipt of nominations is 1 December 1989.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

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Solids and surfaces: a chemist's view of bonding in extended surfaces. By ROALD HOFFMANN. Pp. x + 142. Weinheim and New York: VCH Verlag, 1988. Price DM 48.00, £16.25.

This book is a timely addition to the literature of two related and vigorously developing fields of chemical research: solid-state chemistry and the chemistry of well defined solid surfaces. The book focuses on the chemist's view of bonding in extended periodic structures, developing the relationship between geometric structure and electronic structure and asking the question 'where are the bonds in these systems?'

Chemists have contributed a great deal to the advance of our knowledge of both the solid state and the behaviour of molecules at surfaces. They have provided new methods of synthesis of materials, discovered new and fascinating structures and attempted to tailor make materials with desirable physical and chemical properties. The chemist's understanding of bonding in the solid state, and the bonding of molecules at surfaces, is based on concepts developed from investigations of discrete small molecules. This has tended to emphasize the importance of local coordination geometry and localized bonding pictures, which provide qualitative rationalizations of some of the observed properties of solids.

The physics community, with its elegant use of mathematical models, has meanwhile provided a sound framework for understanding some of the quantitative aspects of the properties of solids. The languages that these two communities use to describe the same materials and to explain the same phenomena often appear profoundly different at first sight. This is particularly so when bonding in extended structures is being discussed. How can the chemists, who like to think in terms of localized bonds in the real solid structure or at a solid surface, relate their insights to those of the physicists who are happy with band-structure calculations and diagrams of energy dispersion relations plotted in reciprocal space? Perhaps a guide book is needed which takes the reader on a tour of some of the main attractions of both terrains and provides a dictionary which enables the language of one tribe to be translated into that of the other. Hoffmann's book provides such a guide which specifically sets out to show how the physicist's band picture can be related to the chemist's bond picture.

Hoffmann's book is derived from a number of his papers which have already appeared in the literature and which cover much of the same material. The book is an extended

enthusiastic essay presenting a non-mathematical, interesting and elegant summary of his view of the bonding in solids and on surfaces. The book is profusely illustrated with at least one diagram per page, all of which help to clarify the argument in the text and make the finished book visually appealing.

The approach adopted views the solid as a giant molecule and constructs one-electron 'molecular orbitals' using the linear combination of atomic orbitals familiar to all chemists. Bloch functions, wavevectors and energy bands are introduced in simple one-dimensional examples. Band folding, together with the Peierls distortion and its relationship to the more familiar Jahn-Teller effect, are explained. The complications which arise in two-dimensional and three-dimensional periodic structures are described. Various examples of band structures of one-, two- and three-dimensional solids, calculated using the extended Hückel approach, are included in the discussion and related to band structures that would be predicted by the sort of qualitative reasoning familiar to chemists. The chemist's familiar local bond picture is retrieved from the band structures by the introduction of density-of-states diagrams and crystal-orbital-overlap populations. These are clearly explained, and interesting examples of their use are scattered throughout the book. The approach developed in the text is used to examine a number of two- and three-dimensional structures and to rationalize variations which occur among compounds with related structures, such as the AB_2X_2 compounds with A = rare earth, B = transition metal and X = group 15, 14 or 13.

The bonding of ordered overlayers of CO and various hydrocarbon species on metal surfaces is discussed. The observed trends in chemisorption experiments on well defined surfaces are rationalized in terms of the bonding models developed. A brief investigation of bond-breaking and bond-making processes involved in surface reactions is included, and references to further theoretical work in this area are given.

The book has a useful annotated reference section which directs the reader to many related papers and original contributions which add to our understanding of bonding at surfaces and in the solid state.

This book will appeal to any chemist studying solid-state or surface chemistry who wishes to be able to interpret the band-structure diagrams so often encountered in the literature and who wishes to develop new ways of thinking about bonding in extended structures. The discussions could be understood easily by third-year undergraduates as well as beginning graduate students. The text will be