

## A Table of the Colored Crystallographic and Icosahedral Point Groups, Including Their Chirality and Diamorphism

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(Received 10 March 1975; accepted 1 July 1975)

All the colored crystallographic and icosahedral point groups that obey the van der Waerden and Burckhardt definition are tabulated here, using a symbolism based on a suggestion of Shubnikov and Koptsik. Each asymmetric domain of the object has a single color – or scalar quality. The symbol of each colored point group  $G(H'|H)$  contains  $G$ , the geometrical point group of the object; its subgroup  $H'$  that is the point group of each of the object's monochromatic domains; and  $H$ , the invariant subgroup of  $G$  that is the intersection of all the conjugate subgroups  $H'$ . If  $H'$  and  $H$  are the same, the symbol  $G(H'|H)$  is changed to  $G(H)$ . If  $H$  is chiral, so is the colored point group. If  $G$  is not chiral, but  $H$  is, the chirality is only chromatic. These phenomena are listed in the table. If more color permutations are possible than occur in the operations of a colored point group, different arrangements of the same colors on the same geometrical object are fundamentally different: these are called diamorphs of each other; their number is listed. 'Color', as used here, symbolizes any scalar property that can vary from one asymmetric domain to another.

### Introduction

The definition of a colored point group used here is based on that in the classic paper of van der Waerden & Burckhardt (1961). Let the point group of  $n$  classical geometrical symmetry operations of a finite object be symbolized by  $G$ . This object will have a colored symmetry point group  $GP$ , if each of the  $n$  asymmetric domains of which it is composed has a single color, and if these are distributed in such a way that a group of color permutations  $p_i$  can be combined with the classic group of operations  $g_i$  of  $G$  to form a group of operations  $g_i p_i$ , each of which restores the object to a condition indistinguishable from its original state. The group of  $n$  operations  $g_i p_i$ ,  $i=1, \dots, n$  is the colored symmetry point group  $GP$  of the object.

Suppose there are  $s$  different colors ( $s \leq n$ ) present on the object's subunits. For a color permutation  $p_i$  to be possible, there must be the same number of units of each color. Also, since a geometrical symmetry operation  $g_i$  replaces all the subunits of a certain color by those of another, each set of subunits of any one color must have the same geometrical structure. Each such set of like-colored asymmetrical subunits has a geometrical point group  $H'$  which must be a subgroup of  $G$  ( $H' \subset G$ ). Its order is  $n/s$ , of course.\* The  $s$  different subgroups  $H'$  of  $G$  are geometrically conjugate to one another, and their intersection  $H$  is an invariant subgroup of  $G$  ( $H \triangleleft G$ ) of index  $t$ .  $H$  is the set of operations

of  $G$  which requires no permutation of the colors, *i.e.* which combines with the non-permutation ( $-$ ) of the colors. The  $t$  members of the factor group ( $G/H$ ) are  $H$  and its cosets, each of which combines with a particular color permutation; consequently, the color permutation group (or subgroup)  $P$ , that combines with  $G$  to form  $PG$ , also has the order  $t$ . If  $t=n$ ,  $H=1$ , and  $P$  is isomorphic with  $G$  ( $P \leftrightarrow G$ ). Otherwise,  $G$  is homomorphic onto  $P$  ( $G \rightarrow P$ ), and  $n/t$  geometrical operations  $g_i$  correspond to a particular color permutation  $p_j$ .

Following a suggestion of Shubnikov & Koptsik (1974), in their book *Symmetry in Science and Art*, the colored point group of an object will be symbolized in these tables by  $G(H'|H)$  or, if  $H'$  and  $H$  are the same, by  $G(H)$ . (Incidentally, Chapter 10 of this book contains an excellent outline of group theory.) In these tables  $G$ ,  $H'$ , and  $H$  will be written in the standard abbreviated Hermann–Mauguin notation, and no attempt will be made to make the positions in the symbols for  $G$ ,  $H'$ , and  $H$  correspond with one another. I find that this attempt – made by several authors, including Shubnikov & Koptsik – leads to a great deal of confusion.

### Structure of the Table

The Table of Colored Point Groups is divided into sections, as follows:

I. Triclinic, II. Monoclinic, III. Orthorhombic, IV. Hypotetragonal, V. Hypotrigonal, VI. Hypohexagonal, VII. Holotetragonal, VIII. Holotrigonal, IX. Holohexagonal, X. Hypocubic, XI. Holocubic, XII. Icosahedral.

\* Two subgroups  $H'$  belonging to differently colored domains may possess some, or all, of their symmetry elements in common; they must nevertheless be counted separately, one to each color.

The nomenclature used here was suggested by J. D. H. Donnay, for which I thank him.

Each section of the Table consists of columns with the following headings:

$G$  is the classic point group on which the colored point groups in each class are based. The international abbreviated Hermann-Mauguin notation is used.

$H'$  is the subgroup of  $G$  that is the point group of each set of asymmetric subunits of the object that all have the same color, *i.e.*, the symmetry of a monochromatic domain of the polychromatic object. Its order is  $m'$ .

$s$  is the number of different colors in the colored object with the point group  $GP$ . It is obtained by dividing  $n$ , the order of  $G$ , by  $m'$ , the order of  $H'$ . (If  $H'=1$ ,  $s=n$ .)

$H$  is the invariant subgroup of  $G$  that consists of the geometrical elements common to all the different conjugate subgroups  $H'$  of the object. In sections I through VI  $H$  is always the same as  $H'$ , and this column is absent. In sections VII through XII there is

an entry in this column if  $H$  is different from  $H'$ , but only three dots ... appear if  $H=H'$ .

$t$  is the number obtained by dividing  $n$ , the order of  $G$ , by  $m$ , the order of  $H$ ; it is the number of different permutations of colors needed to make up the group  $P$ . If  $H=H'$ ,  $t$  is the same as the number of colors  $s$ , and is replaced by three dots ... This column is absent for sections I through VI, since  $s=t$  throughout this part of the Table.

$F$  is the abstract group isomorphic with the factor group  $(G/H)$  [or  $(G/H')$  if  $H=H'$ ].  $F$  is isomorphic with the color permutation group  $P$  used by the object. If  $H=H'=1$ , the abstract structure of  $G$  is  $F$ .  $P$  may

Table of the colored crystallographic and icosahedral point groups

I. Triclinic						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
1	1	1	$C_1$	1	$G$	1
$\bar{1}$	$\bar{1}$	1	$C_1$	1	$N$	$\bar{1}$
	1	2	$C_2$	1	$C$	$\bar{1}$ (1)
II. Monoclinic						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
2	2	1	$C_1$	1	$G$	2
	1	2	$C_2$	1	$G$	2 (1)
$m$	$m$	1	$C_1$	1	$N$	$m$
	1	2	$C_2$	1	$C$	$m$ (1)
$2/m$	$2/m$	1	$C_1$	1	$N$	$2/m$
	2	2	$C_2$	1	$C$	$2/m$ (2)
	$m$	2	$C_2$	1	$N$	$2/m$ ( $m$ )
	$\bar{1}$	2	$C_2$	1	$N$	$2/m$ ( $\bar{1}$ )
	1	4	$D_2$	6	$C$	$2/m$ (1)
III. Orthorhombic						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
222	222	1	$C_1$	1	$G$	222
	2	2	$C_2$	1	$G$	222 (2)
	1	4	$D_2$	6	$G$	222 (1)
	$mm2$	$mm2$	1	$C_1$	1	$N$
$mm2$	2	2	$C_2$	1	$C$	$mm2$ (2)
	$m$	2	$C_2$	1	$N$	$mm2$ ( $m$ )
	1	4	$D_2$	6	$C$	$mm2$ (1)
$mmm$	$mmm$	1	$C_1$	1	$N$	$mmm$
	222	2	$C_2$	1	$C$	$mmm$ (222)
	$mm2$	2	$C_2$	1	$N$	$mmm$ ( $mm2$ )
	$2/m$	2	$C_2$	1	$N$	$mmm$ ( $2/m$ )
	2	4	$D_2$	6	$C$	$mmm$ (2)
	$m$	4	$D_2$	6	$N$	$mmm$ ( $m$ )
	$\bar{1}$	4	$D_2$	6	$N$	$mmm$ ( $\bar{1}$ )
	1	8	$D_2 \times C_2$	5040	$C$	$mmm$ (1)

Table (cont.)

IV. Hypotetragonal						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
4	4	1	$C_2$	1	$G$	4
	2	2	$C_2$	1	$G$	4 (2)
	1	4	$C_4$	6	$G$	4 (1)
$\bar{4}$	$\bar{4}$	1	$C_1$	1	$N$	$\bar{4}$
	2	2	$C_2$	1	$C$	$\bar{4}$ (2)
	1	4	$C_4$	6	$C$	$\bar{4}$ (1)
$4/m$	$4/m$	1	$C_1$	1	$N$	$4/m$
	4	2	$C_2$	1	$C$	$4/m$ (4)
	$\bar{4}$	2	$C_2$	1	$N$	$4/m$ ( $\bar{4}$ )
	$2/m$	2	$C_2$	1	$N$	$4/m$ ( $2/m$ )
	2	4	$D_2$	6	$C$	$4/m$ (2)
	$m$	4	$C_4$	6	$N$	$4/m$ ( $m$ )
	$\bar{1}$	4	$C_4$	6	$N$	$4/m$ ( $\bar{1}$ )
	1	8	$C_4 \times C_2$	5040	$C$	$4/m$ (1)
V. Hypotrigonal						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
3	3	1	$C_1$	1	$G$	3
	1	3	$C_3$	2	$G$	3 (1)
$\bar{3}$	$\bar{3}$	1	$C_1$	1	$N$	$\bar{3}$
	3	2	$C_2$	1	$C$	$\bar{3}$ (3)
	$\bar{1}$	3	$C_3$	2	$N$	$\bar{3}$ ( $\bar{1}$ )
	1	6	$C_6$	120	$C$	$\bar{3}$ (1)
VI. Hypohexagonal						
$G$	$H'$	$s$	$F$	$d$	Chir-ality	Symbol
6	6	1	$C_1$	1	$G$	6
	3	2	$C_2$	1	$G$	6 (3)
	2	3	$C_3$	2	$G$	6 (2)
	1	6	$C_6$	120	$G$	6 (1)
$\bar{6}$	$\bar{6}$	1	$C_1$	1	$N$	$\bar{6}$
	3	2	$C_2$	1	$C$	$\bar{6}$ (3)
	$m$	3	$C_3$	2	$N$	$\bar{6}$ ( $m$ )
	1	6	$C_6$	120	$C$	$\bar{6}$ (1)
$6/m$	$6/m$	1	$C_1$	1	$N$	$6/m$
	6	2	$C_2$	1	$C$	$6/m$ (6)
	$\bar{6}$	2	$C_2$	1	$N$	$6/m$ ( $\bar{6}$ )
	$\bar{3}$	2	$C_2$	1	$N$	$6/m$ ( $\bar{3}$ )
	$2/m$	3	$C_3$	2	$N$	$6/m$ ( $2/m$ )
	3	4	$D_2$	6	$C$	$6/m$ (3)
	2	6	$C_6$	120	$C$	$6/m$ (2)
	$m$	6	$C_6$	120	$N$	$6/m$ ( $m$ )
	$\bar{1}$	6	$C_6$	120	$N$	$6/m$ ( $\bar{1}$ )
	1	12	$C_6 \times C_2$	11!	$C$	$6/m$ (1)

be a subgroup of the full group of  $s!$  permutations possible for the  $s$  colors present on the object. ( $Y$  is the symbol for the abstract group isomorphic with 532.)

$d$  is the number  $s!/t$ . It is the number of different arrangements of the same colors that will produce the same colored point group. Each such arrangement is a

Table (cont.)

VII. Holotetragonal								
$G$	$H'$	$s$	$H$	$t$	$F$	$d$	Chirality	Symbol
422	422	1	...	...	$C_1$	1	$G$	422
	222	2	...	...	$C_2$	1	$G$	422 (222)
	4	2	...	...	$C_2$	1	$G$	422 (4)
	2	4	...	...	$D_2$	6	$G$	422 (2)
	2*	4	1	8	$D_4$	3	$G$	422 (2 1)
	1	8	...	...	$D_4$	7!	$G$	422 (1)
4mm	4mm	1	...	...	$C_1$	1	$N$	4mm
	mm2	2	...	...	$C_2$	1	$N$	4mm(mm2)
	4	2	...	...	$C_2$	1	$C$	4mm(4)
	2	4	...	...	$D_2$	6	$C$	4mm(2)
	$m$	4	1	8	$D_4$	3	$C$	4mm( $m$  1)
	1	8	...	...	$D_4$	7!	$C$	4mm(1)
$\bar{4}2m$	$\bar{4}2m$	1	...	...	$C_1$	1	$N$	$\bar{4}2m$
	222	2	...	...	$C_2$	1	$C$	$\bar{4}2m(222)$
	mm2	2	...	...	$C_2$	1	$N$	$\bar{4}2m(mm2)$
	$\bar{4}$	2	...	...	$C_2$	1	$N$	$\bar{4}2m(4)$
	2	4	...	...	$D_2$	6	$C$	$\bar{4}2m(2)$
	2*	4	1	8	$D_4$	3	$C$	$\bar{4}2m(2 1)$
	$m$	4	1	8	$D_4$	3	$C$	$\bar{4}2m(m 1)$
	1	8	...	...	$D_4$	7!	$C$	$\bar{4}2m(1)$
	4/mmm	4/mmm	1	...	...	$C_1$	1	$N$
422		2	...	...	$C_2$	1	$C$	4/mmm(422)
4mm		2	...	...	$C_2$	1	$N$	4/mmm(4mm)
$\bar{4}2m$		2	...	...	$C_2$	1	$N$	4/mmm( $\bar{4}2m$ )
4/m		2	...	...	$C_2$	1	$N$	4/mmm(4/m)
mmm		2	...	...	$C_2$	1	$N$	4/mmm(mmm)
4		4	...	...	$D_2$	6	$C$	4/mmm(4)
$\bar{4}$		4	...	...	$D_2$	6	$N$	4/mmm( $\bar{4}$ )
222		4	...	...	$D_2$	6	$C$	4/mmm(222)
mm2		4	...	...	$D_2$	6	$N$	4/mmm(mm2)
2/m		4	...	...	$D_2$	6	$N$	4/mmm(2/m)
mm2*		4	$m$	8	$D_4$	3	$N$	4/mmm(mm2 m)
2*/ $m^*$		4	$\bar{1}$	8	$D_4$	3	$N$	4/mmm(2/m  $\bar{1}$ )
$m$		8	...	...	$D_4$	7!	$N$	4/mmm( $m$ )
$\bar{1}$		8	...	...	$D_4$	7!	$N$	4/mmm( $\bar{1}$ )
2		8	...	...	$D_2 \times C_2$	7!	$C$	4/mmm(2)
$m^*$		8	1	16	$D_4 \times C_2$	7!/2	$C$	4/mmm( $m$  1)
2*	8	1	16	$D_4 \times C_2$	7!/2	$C$	4/mmm(2 1)	
1	16	...	...	$D_4 \times C_2$	15!	$C$	4/mmm(1)	
VIII. Holotrigonal								
$G$	$H'$	$s$	$H$	$t$	$F$	$d$	Chirality	Symbol
32	32	1	...	...	$C_1$	1	$G$	32
	3	2	...	...	$C_2$	1	$G$	32 (3)
	2	3	1	6	$D_3$	1	$G$	32 (2 1)
	1	6	...	...	$D_3$	120	$G$	32 (1)
3m	3m	1	...	...	$C_1$	1	$N$	3m
	3	2	...	...	$C_2$	1	$C$	3m(3)
	$m$	3	1	6	$D_3$	1	$C$	3m( $m$  1)
	1	6	...	...	$D_3$	120	$C$	3m(1)
$\bar{3}m$	$\bar{3}m$	1	...	...	$C_1$	1	$N$	$\bar{3}m$
	$\bar{3}$	2	...	...	$C_2$	1	$N$	$\bar{3}m(\bar{3})$
	32	2	...	...	$C_2$	1	$C$	$\bar{3}m(32)$
	3m	2	...	...	$C_2$	1	$N$	$\bar{3}m(3m)$
	2/m	3	$\bar{1}$	6	$D_3$	1	$N$	$\bar{3}m(2/m \bar{1})$
	3	4	...	...	$D_2$	6	$C$	$\bar{3}m(3)$
	$\bar{1}$	6	...	...	$D_3$	120	$N$	$\bar{3}m(\bar{1})$
	2	6	1	12	$D_6$	60	$C$	$\bar{3}m(2 1)$
	$m$	6	1	12	$D_6$	60	$C$	$\bar{3}m(m 1)$
1	12	...	...	$D_6$	11!	$C$	$\bar{3}m(1)$	

diamorph. A pair of mirror images is counted here as a single arrangement.

Chirality: If  $H$  contains rotation-inversions, no chirality is possible; this is symbolized  $N$  (for 'None'). If  $G$  contains only pure rotations, geometrical chirality (or enantiomorphism) is present; this is noted  $G$  (for 'Geometric'). If  $G$  contains rotation-inversions, but  $H$  does not, then the object exists in right- and left-handed forms, but only with respect to color arrangement; this chromatic chirality (or enantiochroism) is noted  $C$  (for 'Chromatic').

Symbol: This is  $G(H'|H)$ , or, if  $H=H'$ ,  $G(H)$ . This symbol contains sufficient information to specify completely the colored symmetry of the object as defined above.

#### Notes

(a) An asterisk superscript on a symmetry element in  $H'$  indicates that this symmetry element is not associated with a principal axial direction. Thus, take the entry  $2^*$  under  $H'$  for  $G=422$ ; this means that this twofold axis is not the one included within the fourfold

Table (cont.)

IX.	Holoheaxagonal						Chirality	Symbol		
	$G$	$H'$	$s$	$H$	$t$	$F$			$d$	
622	622	622	1	...	...	$C_1$	1	$G$	622	
		6	2	...	...	$C_2$	1	$G$	622 (6)	
		32	2	...	...	$C_2$	1	$G$	622 (32)	
		222	3	2	6	$D_3$	1	$G$	622 (222 2)	
		3	4	...	...	$D_2$	6	$G$	622 (3)	
		2	6	...	...	$D_3$	120	$G$	622 (2)	
		2*	6	1	12	$D_6$	60	$G$	622 (2 1)	
		1	12	...	...	$D_6$	60	$G$	622 (1)	
	6mm	6mm	6mm	1	...	...	$C_1$	1	$N$	6mm
			6	2	...	...	$C_2$	1	$C$	6mm(6)
		3m	2	...	...	$C_2$	1	$N$	6mm(3m)	
		mm2	3	2	6	$D_3$	1	$C$	6mm(mm2 2)	
		3	4	...	...	$D_2$	6	$C$	6mm(3)	
		2	6	...	...	$D_3$	20	$C$	6mm(2)	
		m	6	1	12	$D_6$	160	$C$	6mm(m 1)	
		1	12	...	...	$D_6$	11!	$C$	6mm(1)	
$\bar{6}m2$	$\bar{6}m2$	$\bar{6}m2$	1	...	...	$C_1$	1	$N$	$\bar{6}m2$	
		$\bar{6}$	2	...	...	$C_2$	1	$N$	$\bar{6}m2(6)$	
		3m	2	...	...	$C_2$	1	$N$	$\bar{6}m2(3m)$	
		32	2	...	...	$C_2$	1	$C$	$\bar{6}m2(32)$	
		mm2	3	m	6	$D_3$	1	$N$	$\bar{6}m2(mm2 m)$	
		3	4	...	...	$D_2$	6	$C$	$\bar{6}m2(3)$	
		m	6	...	...	$D_3$	120	$N$	$\bar{6}m2(m)$	
		m*	6	1	12	$D_6$	60	$C$	$\bar{6}m2(m 1)$	
		2	6	1	12	$D_6$	60	$C$	$\bar{6}m2(2 1)$	
		1	12	...	...	$D_6$	11!	$C$	$\bar{6}m2(1)$	
6/mmm	6/mmm	6/mmm	1	...	...	$C_1$	1	$N$	6/mmm	
		622	2	...	...	$C_2$	1	$C$	6/mmm(622)	
		6mm	2	...	...	$C_2$	1	$N$	6/mmm(6mm)	
		$\bar{6}m2$	2	...	...	$C_2$	1	$N$	6/mmm( $\bar{6}m2$ )	
		6/m	2	...	...	$C_2$	1	$N$	6/mmm(6/m)	
		3m	2	...	...	$C_2$	1	$N$	6/mmm(3m)	
		mmm	3	2/m	6	$D_3$	1	$N$	6/mmm(mmm 2/m)	
		6	4	...	...	$D_2$	6	$C$	6/mmm(6)	
		$\bar{6}$	4	...	...	$D_2$	6	$N$	6/mmm( $\bar{6}$ )	
		32	4	...	...	$D_2$	6	$C$	6/mmm(32)	
		3m	4	...	...	$D_2$	6	$N$	6/mmm(3m)	
		3	4	...	...	$D_2$	6	$N$	6/mmm(3)	
		2/m	6	...	...	$D_3$	120	$N$	6/mmm(2/m)	
		2* m*	6	1	12	$D_6$	60	$N$	6/mmm(2/m 1)	
		222	6	2	12	$D_6$	60	$C$	6/mmm(222 2)	
		m*m*2	6	2	12	$D_6$	60	$C$	6/mmm(mm2 2)	
		mm*2*	6	m	12	$D_6$	60	$N$	6/mmm(mm2 m)	
		3	8	...	...	$D_2 \times C_2$	7!	$C$	6/mmm(3)	
		2	12	...	...	$D_6$	11!	$C$	6/mmm(2)	
		m	12	...	...	$D_6$	11!	$N$	6/mmm(m)	
		1	12	...	...	$D_6$	11!	$N$	6/mmm(1)	
		2*	12	1	24	$D_6 \times C_2$	11!/2	$C$	6/mmm(2 1)	
		m*	12	1	24	$D_6 \times C_2$	11!/2	$C$	6/mmm(m 1)	
	1	24	...	...	$D_6 \times C_2$	23!	$C$	6/mmm(1)		

axis. The asterisk does not appear in the symbol  $G(H'|H)=422(2|1)$ , since no ambiguity is possible in this case. If ambiguity is possible, asterisks appear in the symbol  $G(H'|H)$ , e.g.,  $m3m(2|1)$  and  $m3m(2^*|1)$  are different. Thus, in cases where ambiguities can occur, asterisks are used to remove them.

(b) If  $G$ ,  $H'$ , and  $H$  are all the same, the point group is just the classical geometric one, i.e., a one-colored point group. In this case, the usual international symbol is used as the colored symmetry symbol.

*Example*

An example may be helpful at this point. Let the object be a regular octahedron with opposite triangular faces colored alike. Then  $G=m3m$ ,  $H'=\bar{3}m$ ,  $H=\bar{1}$  and the symbol is  $m3m(3m|\bar{1})$ . (See Section XI of the Table.) The order of  $G$  is 48, of  $H'$  is 12, and of  $H$  is 2. Thus, there are  $\frac{4 \cdot 8}{2} = 4$  colors present, and  $\frac{4 \cdot 8}{2} = 24$  permutations are required. The total number of possible permutations of four colors is  $4! = 24$ , so that  $P$  is the complete permutation group, which has the abstract structure  $O$ . The subgroup  $H=\bar{1}$ , together with its 23 cosets, make up the factor group  $(m3m/\bar{1})$ ; each of its elements is a pair of geometrical operations connected to one of the 24 permutations of the four colors present. Since  $H=\bar{1}$ , each asymmetric domain and its enantiomorph occur with the same color, and the object is equal to its mirror image; there is thus no chirality present. Since  $4! = 24$  and  $P$  has the order 24, there is only one diamorph possible.

Shubnikov & Koptsik (1974) present tables (on pages 266–267, 287–290, and 381–384) listing all of the colored crystallographic point groups  $G(H'|H)$  and  $G(H)$  given in the Table here. They omit from their tables, however, the colored icosahedral point groups. They do not note the number of diamorphs, nor the types of chirality present.

Shubnikov & Koptsik (1974) use a notation different from the one used in the Table presented here. They

include a great deal of relevant information in each of their symbols; for instance: my  $m3m(4m2|222)$  appears in their tables thus:

$$\left( \frac{4^{(2,2)}}{m^{(2)}} \bar{3}^{(6)} \frac{2^{(2)}}{m^{(2,2)}} \right)^{(6)} |\bar{4}^{(2,2)} 1m^{(2,2)}|211.$$

In my symbol, all the same information is implied: the order of  $m3m$  is 48, and that of  $\bar{4}m2$  is 8; this gives  $\frac{4 \cdot 8}{8} = 6$  as the number of colors. The subgroup  $H$  is 222, of order 4;  $\frac{4 \cdot 8}{4} = 12$  is, therefore, the order of  $P$ , the permutation group.  $P$  must be isomorphic with  $F$ , and  $F$  must be either  $C_6 \times C_2$ ,  $D_6$ , or  $T$ , the only crystallographically possible ones of order 12. If it is necessary to know the exact form of  $F$ , expand  $m3m$  into cosets of its subgroup 222. It turns out that, of the twelve cosets, only two consist of elements of order 6, and these are inverses of each other. Consequently,  $F = D_6$ , since  $T$  contains no elements of order 6, and  $C_6 \times C_2$  contains four different elements of order 6. Each permutation in  $P$  corresponds to  $\frac{4 \cdot 8}{12} = 4$  different operations of  $G$ . Since  $G$  contains improper rotations, while  $H$  does not, this colored point group has chromatic chirality. The full permutation group of six colors contains  $6! = 720$  members, while  $P$  is of order 12; hence, there are 60 diamorphs. The color permutation  $p_i$  associated with each geometrical operation  $g_i$  is easily written down by inspection of a model, or a diagram, of an object with the colored point group  $m3m(4m2|222)$ .

Wittke & Garrido (1959) have listed all but one of the combinations of  $G$  and  $H'$  possible for the crystallographic point groups. (They apparently overlooked the combination of  $m3m$  with  $mm2$  where the 2 of  $mm2$  is  $\parallel$  to 4 of  $m3m$  and the  $m$ 's are diagonal.) They assigned a number  $s$  of colors, just as other authors have done, by dividing the order of  $G$  by that of  $H'$ . However, differently from other workers, they fixed one of the possible subgroups  $H'$  in a single posi-

Table (cont.)

X.	Hypocubic							Chirality	Symbol
	$G$	$H'$	$s$	$H$	$t$	$F$	$d$		
23	23	1	...	...	$C_1$	1	$G$	23	
	222	3	...	...	$C_3$	2	$G$	23 (222)	
	3	4	1	12	$T$	2	$G$	23 (3 1)	
	2	6	1	12	$T$	60	$G$	23 (2 1)	
	1	12	...	...	$T$	11!	$G$	23 (1)	
$m3$	$m3$	1	...	...	$C_1$	1	$N$	$m3$	
	23	2	...	...	$C_2$	1	$C$	$m3(23)$	
	$mmm$	3	...	...	$C_3$	2	$N$	$m3(mmm)$	
	$\bar{3}$	4	$\bar{1}$	12	$T$	2	$N$	$m3(\bar{3} \bar{1})$	
	222	6	...	...	$C_6$	120	$C$	$m3(222)$	
	$mm2$	6	1	24	$T \times C_2$	30	$C$	$m3(mm2 1)$	
	$2/m$	6	$\bar{1}$	12	$T$	60	$N$	$m3(2/m \bar{1})$	
	3	8	1	24	$T \times C_2$	1680	$C$	$m3(3 1)$	
	$\bar{1}$	12	...	...	$T$	11!	$N$	$m3(\bar{1})$	
	2	12	1	24	$T \times C_2$	11!/2	$C$	$m3(2 1)$	
	$m$	12	1	24	$T \times C_2$	11!/2	$C$	$m3(m 1)$	
	1	24	...	...	$T \times C_2$	23!	$C$	$m3(1)$	

tion and distributed the  $s$  colors so that *all* the colors are unaffected by the operations of this  $H'$ . [Each asymmetric unit, *i.e.*, general face ( $hkl$ ), has a single color in this scheme, just as in mine.] This procedure results in a color distribution that does not obey my rules of colored symmetry, unless  $H'=H$  is an invariant subgroup of  $G$ .

Shubnikov & Koptsik (1974) have rationalized the Wittke–Garrido colored point groups with  $H' \neq H$ ,

by defining colored symmetry operations that permute colors in more than one way at the same time. For instance: the operation of a  $4^{(\pm 4)}$  axis (Shubnikov–Koptsik notation) permutes the four colors  $a, b, c, d$  by the operator  $4(abcd)$  in the region above the plane normal to the fourfold color axis, and by the operator  $4(adcb)$  below this plane. Such operators are clumsy to use, and inconvenient in many other ways. Physical objects colored according to Wittke–Garrido

Table (cont.)

XI.		Holocubic							
$G$	$H'$	$s$	$H$	$t$	$F$	$d$	Chirality	Symbol	
432	432	1	...	...	$C_1$	1	$G$	432	
	23	2	...	...	$C_2$	1	$G$	432 (23)	
	422	3	222	6	$D_3$	1	$G$	432 (422 222)	
	32	4	1	24	$O$	1	$G$	432 (32 1)	
	222	6	...	...	$D_3$	120	$G$	432 (222)	
	$2^*2^*2$	6	1	24	$O$	30	$G$	432 (222 1)	
	4	6	1	24	$O$	30	$G$	432 (4 1)	
	3	8	1	24	$O$	1680	$G$	432 (3 1)	
	2	12	1	24	$O$	11!/2	$G$	432 (2 1)	
	$2^*$	12	1	24	$O$	11!/2	$G$	432 ( $2^*$  1)	
	1	24	...	...	$O$	23!	$G$	432 (1)	
	$\bar{4}3m$	$\bar{4}3m$	1	...	...	$C_1$	1	$N$	$\bar{4}3m$
		23	2	...	...	$C_2$	1	$C$	$\bar{4}3m(23)$
$\bar{4}m2$		3	222	6	$D_3$	1	$C$	$\bar{4}3m(\bar{4}m2 222)$	
$3m$		4	1	24	$O$	1	$C$	$\bar{4}3m(3m 1)$	
222		6	...	...	$D_3$	120	$C$	$\bar{4}3m(222)$	
$mm2$		6	1	24	$O$	30	$C$	$\bar{4}3m(mm2 1)$	
$\bar{4}$		6	1	24	$O$	30	$C$	$\bar{4}3m(\bar{4} 1)$	
3		8	1	24	$O$	1680	$C$	$\bar{4}3m(3 1)$	
2		12	1	24	$O$	11!/2	$C$	$\bar{4}3m(2 1)$	
$m$		12	1	24	$O$	11!/2	$C$	$\bar{4}3m(m 1)$	
1		24	...	...	$O$	23!	$C$	$\bar{4}3m(1)$	
$m\bar{3}m$		$m\bar{3}m$	1	...	...	$C_1$	1	$N$	$m\bar{3}m$
		432	2	...	...	$C_2$	1	$C$	$m\bar{3}m(432)$
	$\bar{4}3m$	2	...	...	$C_2$	1	$N$	$m\bar{3}m(\bar{4}3m)$	
	$m\bar{3}$	2	...	...	$C_2$	1	$N$	$m\bar{3}m(m\bar{3})$	
	$4/m\bar{m}m$	3	$m\bar{m}m$	6	$D_3$	1	$N$	$m\bar{3}m(4/m\bar{m}m m\bar{m}m)$	
	23	4	...	...	$D_2$	6	$C$	$m\bar{3}m(23)$	
	$\bar{3}m$	4	$\bar{1}$	24	$O$	1	$N$	$m\bar{3}m(\bar{3}m \bar{1})$	
	422	6	222	12	$D_6$	60	$C$	$m\bar{3}m(422 222)$	
	$\bar{4}m^*2$	6	222	12	$D_6$	60	$C$	$m\bar{3}m(\bar{4}m^*2 222)$	
	$4/m$	6	$\bar{1}$	24	$O$	30	$N$	$m\bar{3}m(4/m \bar{1})$	
	$\bar{4}m2^*$	6	1	48	$O \times C_2$	15	$C$	$m\bar{3}m(\bar{4}m2^* 1)$	
	$4mm$	6	1	48	$O \times C_2$	15	$C$	$m\bar{3}m(4mm 1)$	
	$m\bar{m}m$	6	...	...	$D_3$	120	$N$	$m\bar{3}m(m\bar{m}m)$	
	$m^*m^*m$	6	$\bar{1}$	24	$O$	30	$N$	$m\bar{3}m(m\bar{m}m \bar{1})$	
	$3m$	8	1	48	$O \times C_2$	840	$C$	$m\bar{3}m(3m 1)$	
	32	8	1	48	$O \times C_2$	840	$C$	$m\bar{3}m(32 1)$	
	$\bar{3}$	8	$\bar{1}$	24	$O$	1680	$N$	$m\bar{3}m(\bar{3} \bar{1})$	
	4	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(4 1)$	
	$\bar{4}$	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(\bar{4} 1)$	
	222	12	...	...	$D_6$	11!	$C$	$m\bar{3}m(222)$	
	$22^*2^*$	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(222 1)$	
	$mm2$	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(mm2 1)$	
	$m^*m^*2$	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(m^*m^*2 1)$	
	$mm^*2^*$	12	1	48	$O \times C_2$	11!/4	$C$	$m\bar{3}m(mm^*2^* 1)$	
	$2/m$	12	$\bar{1}$	24	$O$	11!/2	$N$	$m\bar{3}m(2/m \bar{1})$	
	$2^*/m^*$	12	$\bar{1}$	24	$O$	11!/2	$N$	$m\bar{3}m(2^*/m^* \bar{1})$	
	3	16	1	48	$O \times C_2$	15!/3	$C$	$m\bar{3}m(3 1)$	
	2	24	1	48	$O \times C_2$	23!/2	$C$	$m\bar{3}m(2 1)$	
	$2^*$	24	1	48	$O \times C_2$	23!/2	$C$	$m\bar{3}m(2^* 1)$	
	$m$	24	1	48	$O \times C_2$	23!/2	$C$	$m\bar{3}m(m 1)$	
	$m^*$	24	1	48	$O \times C_2$	23!/2	$C$	$m\bar{3}m(m^* 1)$	
	$\bar{1}$	24	...	...	$O$	23!	$N$	$m\bar{3}m(\bar{1})$	
1	48	...	...	$O \times C_2$	47!	$C$	$m\bar{3}m(1)$		

Table (cont.)

XII.	<i>G</i>	<i>H'</i>	<i>s</i>	<i>H</i>	Icosahedral			<i>d</i>	Chirality	Symbol
					<i>t</i>	<i>F</i>				
	532	532	1	...	...	$C_1$	1	<i>G</i>	532	
		23	5	1	60	<i>Y</i>	2	<i>G</i>	532 (23 1)	
		52	6	1	60	<i>Y</i>	12	<i>G</i>	532 (52 1)	
		32	10	1	60	<i>Y</i>	9!/6	<i>G</i>	532 (32 1)	
		5	12	1	60	<i>Y</i>	11!/5	<i>G</i>	532 (5 1)	
		222	15	1	60	<i>Y</i>	14!/4	<i>G</i>	532 (222 1)	
		3	20	1	60	<i>Y</i>	19!/3	<i>G</i>	532 (3 1)	
		2	30	1	60	<i>Y</i>	29!/2	<i>G</i>	532 (2 1)	
		1	60	...	...	<i>Y</i>	59!	<i>G</i>	532 (1)	
	$\bar{5}3m$	$\bar{5}3m$	1	...	...	$C_1$	1	<i>N</i>	$\bar{5}3m$	
		532	2	...	...	$C_2$	1	<i>C</i>	$\bar{5}3m(532)$	
		$m\bar{3}$	5	$\bar{1}$	60	<i>Y</i>	2	<i>N</i>	$\bar{5}3m(m\bar{3} \bar{1})$	
		$\bar{5}m$	6	$\bar{1}$	60	<i>Y</i>	12	<i>N</i>	$\bar{5}3m(\bar{5}m \bar{1})$	
		23	10	1	120	$Y \times C_2$	9!/12	<i>C</i>	$\bar{5}3m(23 1)$	
		$\bar{3}m$	10	$\bar{1}$	60	<i>Y</i>	9!/6	<i>N</i>	$\bar{5}3m(\bar{3}m \bar{1})$	
		$\bar{3}$	12	$\bar{1}$	60	<i>Y</i>	11!/5	<i>N</i>	$\bar{5}3m(\bar{3} \bar{1})$	
		52	12	1	120	$Y \times C_2$	11!/10	<i>C</i>	$\bar{5}3m(52 1)$	
		$5m$	12	1	120	$Y \times C_2$	11!/10	<i>C</i>	$\bar{5}3m(5m 1)$	
		$mmm$	15	$\bar{1}$	60	<i>Y</i>	14!/4	<i>N</i>	$\bar{5}3m(mmm \bar{1})$	
		$\bar{3}$	20	$\bar{1}$	60	<i>Y</i>	19!/3	<i>N</i>	$\bar{5}3m(\bar{3} \bar{1})$	
		32	20	1	120	$Y \times C_2$	19!/6	<i>C</i>	$\bar{5}3m(32 1)$	
		$3m$	20	1	120	$Y \times C_2$	19!/6	<i>C</i>	$\bar{5}3m(3m 1)$	
		5	24	1	120	$Y \times C_2$	23!/5	<i>C</i>	$\bar{5}3m(5 1)$	
		222	30	1	120	$Y \times C_2$	29!/4	<i>C</i>	$\bar{5}3m(222 1)$	
		$mm\bar{2}$	30	1	120	$Y \times C_2$	29!/4	<i>C</i>	$\bar{5}3m(mm\bar{2} 1)$	
		$2/m$	30	$\bar{1}$	60	<i>Y</i>	29!/2	<i>N</i>	$\bar{5}3m(2/m \bar{1})$	
		3	40	1	120	$Y \times C_2$	39!/3	<i>C</i>	$\bar{5}3m(3 1)$	
		2	60	1	120	$Y \times C_2$	59!/2	<i>C</i>	$\bar{5}3m(2 1)$	
		$m$	60	1	120	$Y \times C_2$	59!/2	<i>C</i>	$\bar{5}3m(m 1)$	
		$\bar{1}$	60	...	...	<i>Y</i>	59!	<i>N</i>	$\bar{5}3m(\bar{1})$	
		1	120	...	...	$Y \times C_2$	119!	<i>C</i>	$\bar{5}3m(1)$	

point groups with  $H' \neq H$  provide some asymmetric subunits with neighbors of the same color, while others have only differently colored neighbors. Thus, such a group does not treat an object's subunits consistently, if  $H' \neq H$ . The Wittke-Garrido colored point groups are listed in the book, *Symmetry in Science and Art*, by Shubnikov & Koptsik (1974); they will not be considered further here.

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*Acta Cryst.* (1976). A **32**, 139

## An Example of the Use of Quartet and Triplet Structure Invariants when Enantiomorph Discrimination is Difficult

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(Received 17 June 1975; accepted 23 June 1975)

Problems relating to enantiomorph discrimination in the structure determination of the alborixin antibiotic ( $C_{48}O_{14}H_{84}, K^+$ ) are studied. To select the starting set, quartet structure invariants are used to define two orthogonal classes of reflexions, and a variation of the tangent formula refinement using the phases of the triplet invariants is described.

### Introduction

Since the use and automation of multiresolution methods, of which *MULTAN* (Germain, Main & Woolfson,

1970) is the best example, problems rarely occur in crystal structure determination, even if the number of heavy atoms in the asymmetric unit is rather large (50 to 80 for instance). The few failures of *MULTAN*