

Table 3. Bond lengths and angles

Cl-O <sub>1</sub>	1.453 ± 0.009 Å	} weighted mean	1.452 ± 0.005 Å
Cl-O <sub>2</sub>	1.439 ± 0.009		
Cl-O <sub>3</sub>	1.465 ± 0.008		
O <sub>1</sub> -Cl O <sub>3</sub>	108° 9' ± 30'		
O <sub>1</sub> -Cl-O <sub>2</sub>	111° 30' ± 30'		
O <sub>2</sub> -Cl O <sub>3</sub>	110° 30' ± 30'		

again demonstrated the importance of correcting for rotational oscillation.

#### Hydrogen atoms

Lee & Carpenter were unable to find the hydrogen atoms in projection, nor did they find three O<sub>5</sub>...O distances shorter than the others such as might be expected for a hydrogen-bonded H<sub>3</sub>O<sup>+</sup> ion. They suggested either (i) that there is free rotation of the hydrogen atoms about the oxygen atom, or (ii) that the hydrogen atoms were equidistant from pairs of oxygen atoms on the neighbouring perchlorate ions.

In an endeavour to locate the hydrogen atoms a three-dimensional difference synthesis was carried out with  $F_c$  from the final anisotropic parameters. As might be expected from the small value of  $R$ , there were no large peaks or troughs and the positive values within a radius

of 1.5 Å from O<sub>5</sub> were smaller than those in positions which could not be attributed to hydrogen atoms. This evidence indicates the free rotation of the hydroxonium ions, and is consistent with the preliminary results of a neutron-diffraction study (Smith & Levy, 1959).

Computation was carried out on the Leeds University Ferranti Pegasus computer with programmes published in 1960 (Cruikshank, Pilling and in part Bujosa, Lovell & Truter).

I am grateful for the use of the facilities of the Computing Laboratory and to my colleagues for the use of their programmes.

#### References

- CRUICKSHANK, D. W. J. (1956). *Acta Cryst.* **9**, 757.  
 CRUICKSHANK, D. W. J. & PILLING, D. E. and in part  
 BUJOSA, A., LOVELL, F. M. & TRUTER, M. R. (1960).  
 Proceedings of the Glasgow computer conference.  
 LEE, F. S. & CARPENTER, G. B. (1959). *J. Phys. Chem.*  
**63**, 279.  
 SMITH, H. G. & LEVY, H. A. (1959). Abstract for ACA  
 meeting.  
 TRUTER, M. R., CRUICKSHANK, D. W. J. & JEFFREY, G. A.  
 (1960). *Acta Cryst.* **13**, 855.

*Acta Cryst.* (1961). **14**, 319

**Coloured polyhedra.** By G. S. PAWLEY, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England.*

(Received 4 August 1960)

#### Introduction

Klein (1884) gave an account of the subgroups contained in any point-group, but thought it unnecessary to enumerate these subgroups in his book. Recently Wittke & Garrido (1959) tabulated some of these, but restricted their attention to crystallographic point-groups. In this present note the treatment is extended to the icosahedral point-groups, and the general case for the point-groups  $r$ ,  $r2$ ,  $rm$ ,  $\bar{r}$ ,  $\bar{r}m$ ,  $r/m$  and  $r/mmm$  can be obtained by Klein's analysis. The notation here used is the same as that of Wittke & Garrido.

#### Definition of a coloured polyhedron

A 'coloured polyhedron' has its shape governed by a point-group  $G$  but has its faces coloured in a way that obeys a different point-group  $\mathfrak{g}$ .  $\mathfrak{g}$  is a subgroup of  $G$ , and  $\mathfrak{g}'$  is any group for which  $\mathfrak{g}, \mathfrak{g}' = G$ .  $G$  and  $\mathfrak{g}$  have  $M$  and  $m_g$  faces in their general forms respectively, thus the number of colours  $s$  required for the general coloured polyhedron is  $M/m_g$ . All the symmetry operations of  $G$  not included in  $\mathfrak{g}$  do not necessarily form a group, but must change the colour of any face on which they act, and these are called colour symmetry operations.

#### Multicoloured faces

The number of different colours related by  $m_c$  (colour mirror),  $r_c$  (colour  $r$ -fold axis) and  $r_c m_c$  ( $r_c$  in the plane of  $m_c$ ) are clearly 2,  $r$  and  $2r$  respectively. A special form of  $G$  is produced if the face normal lies in a mirror plane

or parallels an  $r$ -fold axis, and this is denoted in the tables by  $m$  or  $r$ . The faces of any special form can be sectioned by lines in such a way that the sections, considered as separate, obey the general point-group symmetry. These lines can be obtained from the edges

Table 1. The number of colours  $n$  present on each face of the special forms of the point group  $5m\bar{3}m$

$\mathfrak{g}$	$m_g$	$s$	5	3	2	$m$	$\mathfrak{g}'$	*
$5m\bar{3}m$	120	1	1	1	1	1	1	
532	60	2	2	2	2	2	$m$	
52	10	12	2,10	6	2,4	2	$3m$	
$\bar{5}$	5	24	2,10	6	4	2	$3m$	
$\bar{5}$	10	12	2,10	6	4	2	$3m$	
$\bar{5}m$	10	12	1,5	3	2	1,2	3	
$\bar{5}m(2)$	20	6	1,5	3	2	1,2	3	
$m\bar{3}(2)$	24	5	5	2,3	1,4	1,2	5	*
23	12	10	10	2,6	2,4	2	$5m$	*
32	6	20	10	2,6	2,4	2	$5m$	*
3	3	40	10	2,6	4	2	$5m$	*
$\bar{3}$	6	20	10	2,6	4	2	$5m$	*
$3m$	6	20	5	1,6	2,4	1,2	5	*
$\bar{3}m(2)$	12	10	5	1,6	2,4	1,2	5	*
222	4	30	10	6	2,4	2	$5m$	*
2	2	60	10	6	2,4	2	$5m\bar{3}m$	*
$mmm(2)$	8	15	5	3,6	1,4	1,2	5	*
$mm(2)$	4	30	5,10	3,6	1,2,4	1,2	532	*
$2/m$	4	30	5,10	3,6	2,4	1,2	532	*
$\bar{m}$	2	60	5,10	3,6	2,4	1,2	532	*
$\bar{1}$	2	60	10	6	4	2	532	*
1	1	120	10	6	4	2	$5m\bar{3}m$	*

\* Denotes a crystallographic subgroup.

Table 2. The number of colours  $n$  present on each face of the special forms of the point group 532

$\mathfrak{g}$	$m_{\mathfrak{g}}$	$s$	5	3	2	$\mathfrak{g}'$ *
532	60	1	1	1	1	1
52	10	6	1,5	3	1,2	3
5	5	12	1,5	3	2	3
23	12	5	5	1,3	1,2	5 *
32	6	10	5	1,3	1,2	5 *
3	3	20	5	1,3	2	5 *
222	4	15	5	3	1,2	5 *
2	2	30	5	3	1,2	52 *
1	1	60	5	3	2	532 *

\* Denotes a crystallographic subgroup.

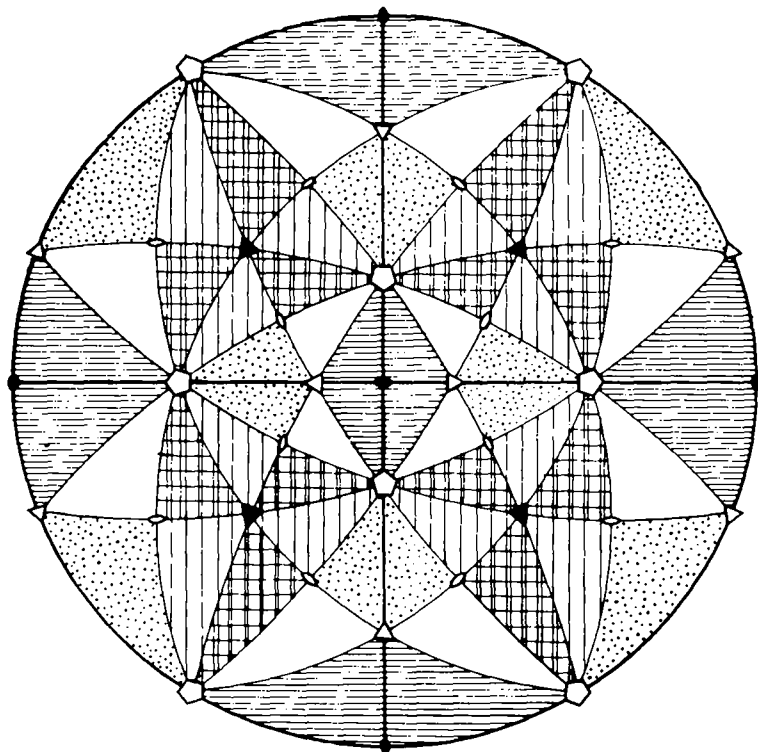


Fig. 1.  $G = 5m3m$ ,  $\mathfrak{g} = m3$ .

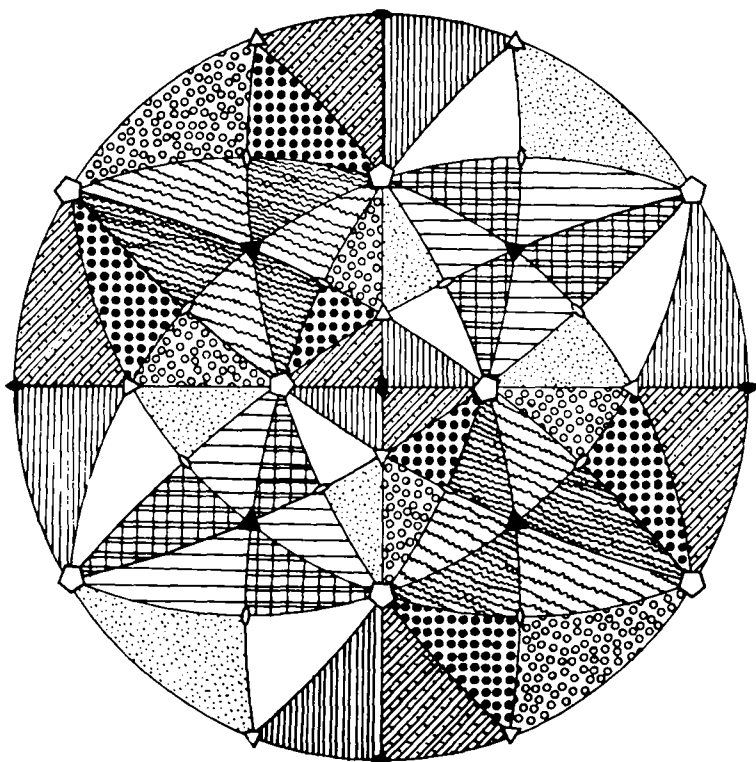


Fig. 2.  $G = 5m3m$ ,  $\mathfrak{g} = 23$ .

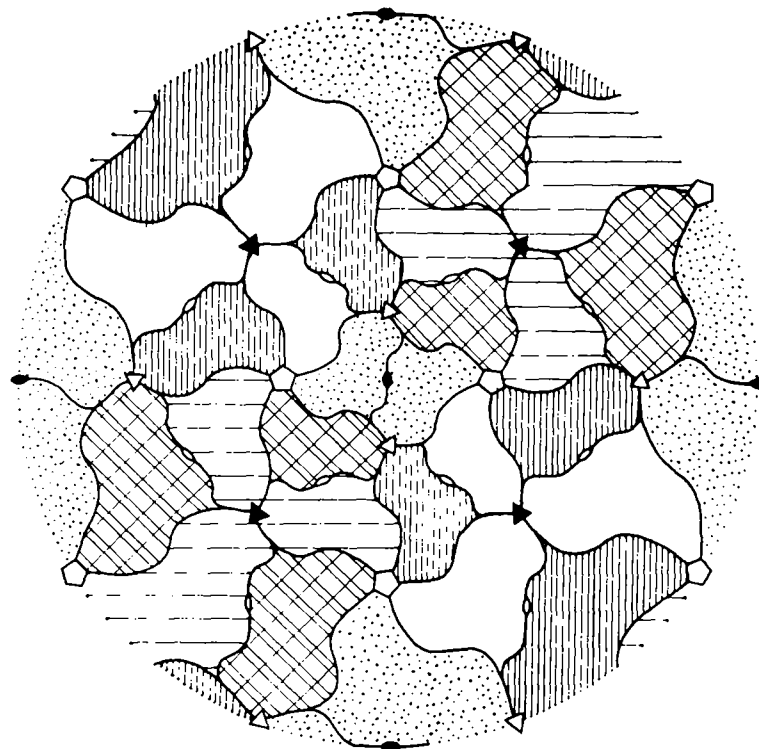


Fig. 3.  $G = 532$ ,  $\mathfrak{g} = 23$ .

between faces of the general form whose normals tend to parallel those of the special form. If the special form face normal lies in an  $m_c$ , or is parallel to an  $r_c$ , or both, then the sections of this face will be in  $n$  different colours, which will be 2,  $r$  and  $2r$  respectively. Wittke & Garrido superimposed all these  $n$  colours on the face, but then this sometimes destroys colour operators. A simple example is given by  $G = m3m$  and  $\mathfrak{g} = 23$  with the special form (110), (or in this notation 2). All the faces then have  $n = 4$  and if these are superimposed the colour mirror planes become true mirrors.

A symmetry operator, say  $r$ , might occur more than once in  $G$  but not all of these need belong to  $\mathfrak{g}$ . Then some faces of the special form produced when the face normals are parallel to the  $r$ -fold axis will be brought into self-coincidence by an  $r_c$ , whereas the other faces will still have  $n = 1$ . When this occurs the two values of  $n$  are tabulated in the same space.

Tables 1 and 2 give  $n$  for the icosahedral point-groups, and a note is made of the cases where  $\mathfrak{g}$  is a crystallographic point-group. The interesting cases, Figs. 1, 2 and 3 have cubic subgroups. Their importance lies in the fact that some viruses which crystallize in the cubic system have the symmetry of the point-group  $5m3m$  or  $532$  about each lattice point (Horne *et al.*, 1959).

I wish to thank Dr N. Joel for his encouragement and Dr W. Cochran for valuable criticism.

#### References

- HORNE, R. W., BRENNER, S., WATERSON, A. P. & WILDY, P. (1959). *J. Mol. Biol.* **1**, 84.  
 KLEIN, F. (1884). *Lectures on the icosahedron and the solutions of equations of the fifth degree*. English translation: Dover Publications Inc., 1956.  
 WITTKKE, O. & GARRIDO, J. (1959). *Bull. Soc. franç. Minér. Crist.* **82**, 223.