

## References

- AGRANOVICH, V. M. (1957). *Optika i Spectrosk. (USSR)*, **2**, 738.
- BELJAEV, L. M. & PEREKALINA, Z. B. (1966). *Acta Cryst.* **21**, A 249.
- BEURSKENS-KERSSEN, G., KROON, J., ENDEMAN, H. J., VAN LAAR, J. & BIJVOET, J. M. (1963). In *Crystallography and Crystal Perfection*, p. 225. Ed. G.N.Ramachandran. New York and London: Academic Press.
- BIJVOET, J. M. (1960). *Acta Cryst.* **13**, 1100.
- BIJVOET, J. M. (1963). In *Crystallography and Crystal Perfection*, p. 236. Ed. G.N.Ramachandran. New York and London: Academic Press.
- BROWN, C. J. & SADANAGA, R. (1965). *Acta Cryst.* **18**, 158.
- CHANDRASEKHAR, S. (1952). *Proc. Indian Acad. Sci. A*, **35**, 531.
- CHANDRASEKHAR, S. (1953a). *Proc. Indian Acad. Sci. A*, **37**, 458.
- CHANDRASEKHAR, S. (1953b). *Proc. Indian Acad. Sci. A*, **37**, 697.
- CHANDRASEKHAR, S. (1961). *Proc. Roy. Soc. A*, **259**, 531.
- CHANDRASEKHAR, S. (1963). In *Crystallography and Crystal Perfection*, p. 236. Ed. G.N.Ramachandran. New York and London: Academic Press.
- KIZEL, V. A., KRASILOV, YU. I. & SHAMRAEV, V. N. (1964). *Optics and Spectrosc. (USSR)*, **17**, 470.
- KIZEL, V. A., KRASILOV, YU. I. & SHAMRAEV, V. N. (1965). *Optics and Spectrosc. (USSR)*, **18**, 62.
- POINSOT, G. & MATHIEU, J. P. (1955). *Ann. Phys.* **10**, 481.
- RAMACHANDRAN, G. N. (1951). *Proc. Indian Acad. Sci. A*, **33**, 309.
- RAMACHANDRAN, G. N. & CHANDRASEKHAR, K. S. (1957). *Acta Cryst.* **10**, 671.
- RAMACHANDRAN, G. N. (1963). In *Crystallography and Crystal Perfection*, p. 236. Ed. G.N.Ramachandran. New York and London: Academic Press.
- ZACHARIASEN, W. H. & PLETINGER, H. A. (1959). *Acta Cryst.* **12**, 526.

*Acta Cryst.* (1967). **23**, 913

## Geometrical Symbols for All Crystallographic Symmetry Groups up to Three Dimensions

By J. BOHM AND K. DORNBERGER-SCHIFF

*Deutsche Akademie der Wissenschaften zu Berlin, II. Physikalisch-Technisches Institut  
and Institut für Strukturforchung, Berlin-Adlershof, Germany (DDR)*

(Received 20 March 1967)

A complete list of the individual symmetry groups belonging to all sets of such groups up to three dimensions is given, each set being characterized by symbols as agreed upon by the Commission on *International Tables* and each symmetry group by a symbol closely connected with the international space group symbols. Each set is characterized by the reducibility of the matrices of the transformations of space corresponding to the symmetry operations.

As pointed out elsewhere (Bohm & Dornberger-Schiff, 1966) the different kinds of symmetry group – not only the purely geometrical groups but also those including antisymmetry and other generalized symmetry – may be described and symbolized as geometrical symmetry groups. It is of advantage to have easily understandable symbols for the different sets of symmetry groups – differing *e.g.* in their dimensions of extension or periodicity – and also for the individual symmetry groups of these sets.

In the following a complete list of the symmetry groups of all sets up to three dimensions is given. In Tables 1 and 2 symbols for these sets are used (symbols  $\mathcal{G}$ ) as agreed upon by the Commission on *International Tables* and originally proposed by Niggli (1966). For comparison, symbols for the sets proposed some time ago by one of the present authors (Bohm, 1963) are given (symbols  $G$ ).

Because we included the possibility that one or more dimensions have a non-geometrical meaning, subsets

of symmetry groups are of importance in which some of the directions (although all with or all without periodicity) are not exchanged by the transformations of the groups. This is indicated in the symbol of the subset by enumerating separately the dimensions which do not exchange (see below).

The matrices representing the symmetry groups of such a set are at least reducible in a characteristic way indicated in the line below the  $G$ -symbols. Matrices with 4 or 3 rows respectively are used in which the last column gives the translational components.

All symbols for the symmetry groups are deduced from the (full) international space group symbols in the following way: The symbols for the symmetry elements retain their well-known meaning. Symmetry elements referred to directions of missing periodicity are enclosed in round brackets. If two or more such directions of missing periodicity exist, and if exchange of these directions is possible within the particular set, the corresponding symmetry symbols are enclosed in

Table 1. *The three-dimen*

Symbol after Niggli		$\mathcal{G}_3$	$\mathcal{G}_2^2$	$\mathcal{G}_2^1$	$\mathcal{G}_3$				
Symbol after Bohm		$G_3$	$G_{32}$	$G_{31}$	$G_{30}$				
Form of matrices		$\left( \begin{array}{ccc c} + & + & + & + \\ + & + & + & + \\ + & + & + & + \\ \hline 0 & 0 & 0 & 1 \end{array} \right)$	$\left( \begin{array}{ccc c} + & + & 0 & + \\ + & + & 0 & + \\ \hline 0 & 0 & + & 0 \\ 0 & 0 & 0 & 1 \end{array} \right)$	$\left( \begin{array}{ccc c} + & 0 & 0 & + \\ \hline 0 & + & + & 0 \\ 0 & + & + & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right)$	$\left( \begin{array}{ccc c} + & + & + & 0 \\ + & + & + & 0 \\ + & + & + & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right)$				
Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
<i>P</i> 1	1	<i>P</i> 111	1	<i>P</i> 11(1)	1	<i>P</i> (11)1	1	(111)	1
<i>P</i> $\bar{1}$	2	<i>P</i> $\bar{1}$ 11	2	<i>P</i> $\bar{1}$ 1(1)	2	<i>P</i> ( $\bar{1}$ 1)1	2	( $\bar{1}$ 11)	$\bar{1}$
<i>P</i> <i>m</i>	3	<i>P</i> 1 <i>m</i> 1	3	<i>P</i> 1 <i>m</i> (1)	3	<i>P</i> (1 <i>m</i> )1	3	(1 <i>m</i> 1)	<i>m</i>
			4	<i>P</i> 11( <i>m</i> )	4	<i>P</i> (11) <i>m</i>			
<i>P</i> <i>c</i>	4	<i>P</i> 1 <i>c</i> 1	5	<i>P</i> 1 <i>a</i> (1)	5	<i>P</i> (1 <i>c</i> )1			
			6	<i>P</i> 11( <i>b</i> )					
<i>C</i> <i>m</i>	5	<i>C</i> 1 <i>m</i> 1	7	<i>C</i> 1 <i>m</i> (1)					
<i>C</i> <i>c</i>	6	<i>C</i> 1 <i>c</i> 1							
<i>P</i> 2	7	<i>P</i> 121	8	<i>P</i> 12(1)	6	<i>P</i> (12)1	4	(121)	2
			9	<i>P</i> 11(2)	7	<i>P</i> (11)2			
<i>P</i> 2 <sub>1</sub>	8	<i>P</i> 12 <sub>1</sub> 1	10	<i>P</i> 12 <sub>1</sub> (1)	8	<i>P</i> (11)2 <sub>1</sub>			
<i>C</i> 2	9	<i>C</i> 121	11	<i>C</i> 12(1)					
<i>P</i> $\frac{2}{m}$	10	<i>P</i> 1 $\frac{2}{m}$ 1	12	<i>P</i> 1 $\frac{2}{m}$ (1)	9	<i>P</i> (1 $\frac{2}{m}$ )1	5	(1 $\frac{2}{m}$ 1)	$\frac{2}{m}$
			13	<i>P</i> 11( $\frac{2}{m}$ )	10	<i>P</i> (11) $\frac{2}{m}$			
<i>P</i> $\frac{2_1}{m}$	11	<i>P</i> 1 $\frac{2_1}{m}$ 1	14	<i>P</i> 1 $\frac{2_1}{m}$ (1)	11	<i>P</i> (11) $\frac{2_1}{m}$			
<i>C</i> $\frac{2}{m}$	12	<i>C</i> 1 $\frac{2}{m}$ 1	15	<i>C</i> 1 $\frac{2}{m}$ (1)					
<i>P</i> $\frac{2}{c}$	13	<i>P</i> 1 $\frac{2}{c}$ 1	16	<i>P</i> 1 $\frac{2}{a}$ (1)	12	<i>P</i> (1 $\frac{2}{c}$ )1			
			17	<i>P</i> 11( $\frac{2}{b}$ )					

sional symmetry groups

$\mathcal{G}_{21}$ $G_{320} = G_{310}$		$\mathcal{G}_{21}$		$\mathcal{G}_{111}$		$\mathcal{G}_{1^{11}}$		$\mathcal{G}_{11^1}$ $G_{321}$		$\mathcal{G}_{111}$ $G_{3210}$	
$\begin{pmatrix} + & + & 0 &   & 0 \\ + & + & 0 &   & 0 \\ 0 & 0 & + &   & 0 \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & + & 0 &   & 0 \\ + & + & 0 &   & 0 \\ 0 & 0 & + &   & 0 \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 & 0 &   & + \\ 0 & + & 0 &   & + \\ 0 & 0 & + &   & + \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 & 0 &   & + \\ 0 & + & 0 &   & + \\ 0 & 0 & + &   & 0 \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 & 0 &   & + \\ 0 & + & 0 &   & 0 \\ 0 & 0 & + &   & 0 \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 & 0 &   & 0 \\ 0 & + & 0 &   & 0 \\ 0 & 0 & + &   & 0 \\ 0 & 0 & 0 &   & 1 \end{pmatrix}$	
No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
1	(11)(1)	1	$P1 1$	1	$P1 1 1$	1	$P1 1(1)$	1	$P(1)(1)1$	1	(1)(1)(1)
2	( $\bar{1}\bar{1}$ )( $\bar{1}$ )	2	$P\bar{1}\bar{1} \bar{1}$	2	$P\bar{1} \bar{1} \bar{1}$	2	$P\bar{1} \bar{1}(1)$	2	$P(\bar{1})(\bar{1})\bar{1}$	2	( $\bar{1}$ )( $\bar{1}$ )( $\bar{1}$ )
3	(1 <i>m</i> )(1)	3	$P1 m 1$	3	$P1 m 1$	3	$P1 m(1)$	3	$P(1)(m)1$	3	(1)( <i>m</i> )(1)
4	(11)( <i>m</i> )	4	$P11 m$	4	$P1 1 m$	4	$P1 1(m)$	4	$P(1)(1)m$	4	(1)(1)( <i>m</i> )
		5	$Pm 1 1$	5	$Pm 1 1$	5	$Pm 1(1)$	5	$P(m)(1)1$	5	( <i>m</i> )(1)(1)
		5	$P1c 1$	6	$P1 c 1$	6	$P1 a(1)$	6	$P(1)(c)1$		
		6	$P11 b$	7	$P1 1 c$	7	$P1 1(b)$	7	$P(c)(1)1$		
		8	$Pc 1 1$	8	$Pc 1 1$	8	$Pb 1(1)$				
		7	$C1m 1$								
		8	$C1c 1$								
5	(12)(1)	9	$P12 1$	9	$P1 2 1$	9	$P1 2(1)$	8	$P(1)(2)1$	6	(1)(2)(1)
6	(11)(2)	10	$P11 2$	10	$P1 1 2$	10	$P1 1(2)$	9	$P(1)(1)2$	7	(1)(1)(2)
				11	$P2 1 1$	11	$P2 1(1)$	10	$P(2)(1)1$	8	(2)(1)(1)
		11	$P12_1 1$	12	$P1 2_1 1$	12	$P1 2_1(1)$				
		12	$P11 2_1$	13	$P1 1 2_1$			11	$P(1)(1)2_1$		
		13	$C12 1$	14	$P2_1 1 1$	13	$P2_1 1(1)$				
7	$(1 \frac{2}{m})(1)$	14	$P1 \frac{2}{m}   1$	15	$P1 \left  \frac{2}{m} \right  1$	14	$P1 \left  \frac{2}{m} (1) \right.$	12	$P(1) \left( \frac{2}{m} \right) 1$	9	$(1) \left( \frac{2}{m} \right) (1)$
8	$(11) \left( \frac{2}{m} \right)$	15	$P11 \left  \frac{2}{m} \right.$	16	$P1 1  \frac{2}{m}$	15	$P1 1 \left( \frac{2}{m} \right)$	13	$P(1)(1) \frac{2}{m}$	10	$(1)(1) \left( \frac{2}{m} \right)$
				17	$P \frac{2}{m}  1 1$	16	$P \frac{2}{m}  1(1)$	14	$P \left( \frac{2}{m} \right) (1)1$	11	$\left( \frac{2}{m} \right) (1)(1)$
		16	$P1 \frac{2_1}{m}   1$	18	$P1 \left  \frac{2_1}{m} \right  1$	17	$P1 \left  \frac{2_1}{m} (1) \right.$				
		17	$P11 \left  \frac{2_1}{m} \right.$	19	$P1 1  \frac{2_1}{m}$			15	$P(1)(1) \frac{2_1}{m}$		
				20	$P \frac{2_1}{m}  1 1$	18	$P \frac{2_1}{m}  1(1)$				
		18	$C1 \frac{2}{m}   1$								
		19	$P1 \frac{2}{c}   1$	21	$P1 \left  \frac{2}{c} \right  1$	19	$P1 \left  \frac{2}{c} (1) \right.$	16	$P(1) \left( \frac{2}{c} \right) 1$		
		20	$P11 \left  \frac{2}{b} \right.$	22	$P1 1  \frac{2}{b}$	20	$P1 1 \left( \frac{2}{b} \right)$				
		21	$P \frac{2}{c}  1 1$	23	$P \frac{2}{c}  1 1$	21	$P \frac{2}{b}  1(1)$	17	$P \left( \frac{2}{c} \right) (1)1$		

## 916 GEOMETRICAL SYMBOLS FOR ALL CRYSTALLOGRAPHIC SYMMETRY GROUPS

Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
$P \frac{2_1}{c}$	14	$P1 \frac{2_1}{c} 1$	18	$P1 \frac{2_1}{a} (1)$					
$C \frac{2}{c}$	15	$C1 \frac{2}{c} 1$							
<i>Pmm</i>	16	<i>Pmm</i> 2	19	<i>Pmm</i> (2)	13	<i>P</i> ( <i>mm</i> )2	6	( <i>mm</i> 2)	<i>mm</i> 2
			20	<i>P</i> 2 <i>m</i> ( <i>m</i> )	14	<i>P</i> (2 <i>m</i> ) <i>m</i>			
<i>Pmc</i>	17	<i>Pmc</i> 2 <sub>1</sub>			15	<i>P</i> ( <i>mc</i> )2 <sub>1</sub>			
			21	<i>P</i> 2 <sub>1</sub> <i>m</i> ( <i>a</i> )					
			22	<i>P</i> 2 <sub>1</sub> <i>a</i> ( <i>m</i> )					
<i>Pcc</i>	18	<i>Pcc</i> 2			16	<i>P</i> ( <i>cc</i> )2			
			23	<i>P</i> 2 <i>a</i> ( <i>a</i> )					
<i>Pma</i>	19	<i>Pma</i> 2	24	<i>Pma</i> (2)					
			25	<i>P</i> 2 <i>m</i> ( <i>b</i> )	17	<i>P</i> (2 <i>c</i> ) <i>m</i>			
<i>Pca</i>	20	<i>Pca</i> 2 <sub>1</sub>							
			26	<i>P</i> 2 <sub>1</sub> <i>a</i> ( <i>b</i> )					
<i>Pnc</i>	21	<i>Pnc</i> 2							
			27	<i>P</i> 2 <i>a</i> ( <i>n</i> )					
<i>Pmn</i>	22	<i>Pmn</i> 2 <sub>1</sub>							
			28	<i>P</i> 2 <sub>1</sub> <i>m</i> ( <i>n</i> )					
<i>Pba</i>	23	<i>Pba</i> 2	29	<i>Pba</i> (2)					
<i>Pna</i>	24	<i>Pna</i> 2 <sub>1</sub>							
<i>Pnn</i>	25	<i>Pnn</i> 2							
<i>Cmm</i>	26	<i>Cmm</i> 2	30	<i>Cmm</i> (2)					
			31	<i>C</i> 2 <i>m</i> ( <i>m</i> )					
<i>Cmc</i>	27	<i>Cmc</i> 2 <sub>1</sub>							
<i>Ccc</i>	28	<i>Ccc</i> 2							
<i>Amm</i>	29	<i>Amm</i> 2							
<i>Abm</i>	30	<i>Abm</i> 2	32	<i>Cm</i> 2( <i>a</i> )					



Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
<i>Ama</i>	31	<i>Ama</i> 2							
<i>Aba</i>	32	<i>Aba</i> 2							
<i>Fmm</i>	33	<i>Fmm</i> 2							
<i>Fdd</i>	34	<i>Fdd</i> 2							
<i>Imm</i>	35	<i>Imm</i> 2							
<i>Iba</i>	36	<i>Iba</i> 2							
<i>Ima</i>	37	<i>Ima</i> 2							
<i>P222</i>	38	<i>P222</i>	33	<i>P22</i> (2)	18	<i>P</i> (22)2	7	(222)	222
<i>P222</i> <sub>1</sub>	39	<i>P222</i> <sub>1</sub>	34	<i>P</i> <sub>2</sub> 2(2)	19	<i>P</i> (22) <sub>2</sub> 1			
<i>P2</i> <sub>1</sub> 2 <sub>1</sub> 2	40	<i>P</i> <sub>2</sub> 2 <sub>1</sub> 2	35	<i>P</i> <sub>2</sub> 2 <sub>1</sub> (2)					
<i>P</i> <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub>	41	<i>P</i> <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub>							
<i>C222</i> <sub>1</sub>	42	<i>C222</i> <sub>1</sub>							
<i>C222</i>	43	<i>C222</i>	36	<i>C22</i> (2)					
<i>F222</i>	44	<i>F222</i>							
<i>I222</i>	45	<i>I222</i>							
<i>I</i> <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub>	46	<i>I</i> <sub>2</sub> 2 <sub>1</sub> 2 <sub>1</sub>							
<i>Pmmm</i>	47	<i>P</i> $\frac{2}{m}$ $\frac{2}{m}$ $\frac{2}{m}$	37	<i>P</i> $\frac{2}{m}$ $\frac{2}{m}$ $\left(\frac{2}{m}\right)$	20	<i>P</i> $\left(\frac{2}{m}$ $\frac{2}{m}\right)$ $\frac{2}{m}$	8	$\left(\frac{2}{m}$ $\frac{2}{m}$ $\frac{2}{m}\right)$	<i>mmm</i>
<i>Pnnn</i>	48	<i>P</i> $\frac{2}{n}$ $\frac{2}{n}$ $\frac{2}{n}$							
<i>Pccm</i>	49	<i>P</i> $\frac{2}{c}$ $\frac{2}{c}$ $\frac{2}{m}$			21	<i>P</i> $\left(\frac{2}{c}$ $\frac{2}{c}\right)$ $\frac{2}{m}$			
			38	<i>P</i> $\frac{2}{m}$ $\frac{2}{a}$ $\left(\frac{2}{a}\right)$					
<i>Pban</i>	50	<i>P</i> $\frac{2}{b}$ $\frac{2}{a}$ $\frac{2}{n}$	39	<i>P</i> $\frac{2}{b}$ $\frac{2}{a}$ $\left(\frac{2}{n}\right)$					
<i>Pmma</i>	51	<i>P</i> $\frac{2_1}{m}$ $\frac{2}{m}$ $\frac{2}{a}$	40	<i>P</i> $\frac{2_1}{m}$ $\frac{2}{m}$ $\left(\frac{2}{a}\right)$					
					22	<i>P</i> $\left(\frac{2}{m}$ $\frac{2}{c}\right)$ $\frac{2_1}{m}$			

Table 1 (cont.)

No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
		49	$C2c m$								
		50	$C2c a$								
<hr/>											
11	$(22)(2)$	51	$P22 2$	54	$P2 2 2$	33	$P2 2(2)$	26	$P(2)(2)2$	15	$(2)(2)(2)$
		52	$P22 2_1$	55	$P2 2 2_1$			27	$P(2)(2)2_1$		
		53	$P2_12 2$	56	$P2_1 2 2$	34	$P2_1 2(2)$				
				57	$P2 2_1 2$	35	$P2 2_1(2)$				
		54	$P2_12_1 2$	58	$P2_1 2_1 2$	36	$P2_1 2_1(2)$				
		55	$P22_1 2_1$	59	$P2 2_1 2_1$						
				60	$P2_1 2 2_1$						
		56	$P2_12_1 2_1$	61	$P2_1 2_1 2_1$						
		57	$C22 2_1$								
		58	$C22 2$								
<hr/>											
12	$\left(\frac{2}{m} \frac{2}{m}\right) \left(\frac{2}{m}\right)$	59	$P \frac{2}{m} \frac{2}{m} \left  \frac{2}{m} \right.$	62	$P \frac{2}{m} \left  \frac{2}{m} \right  \frac{2}{m}$	37	$P \frac{2}{m} \left  \frac{2}{m} \left(\frac{2}{m}\right) \right.$	28	$P \left(\frac{2}{m}\right) \left(\frac{2}{m}\right) \frac{2}{m}$	16	$\left(\frac{2}{m}\right) \left(\frac{2}{m}\right) \left(\frac{2}{m}\right)$
		60	$P \frac{2}{c} \frac{2}{c} \left  \frac{2}{m} \right.$	63	$P \frac{2}{c} \left  \frac{2}{c} \right  \frac{2}{m}$			29	$P \left(\frac{2}{c}\right) \left(\frac{2}{c}\right) \frac{2}{m}$		
		61	$P \frac{2}{m} \frac{2}{a} \left  \frac{2}{a} \right.$	64	$P \frac{2}{m} \left  \frac{2}{a} \right  \frac{2}{a}$	38	$P \frac{2}{m} \left  \frac{2}{a} \left(\frac{2}{a}\right) \right.$				
				65	$P \frac{2}{b} \left  \frac{2}{m} \right  \frac{2}{b}$	39	$P \frac{2}{b} \left  \frac{2}{m} \left(\frac{2}{b}\right) \right.$				
		62	$P \frac{2}{b} \frac{2}{a} \left  \frac{2}{n} \right.$								
		63	$P \frac{2_1}{m} \frac{2}{m} \left  \frac{2}{a} \right.$	66	$P \frac{2_1}{m} \left  \frac{2}{m} \right  \frac{2}{a}$	40	$P \frac{2_1}{m} \left  \frac{2}{m} \left(\frac{2}{a}\right) \right.$				
				67	$P \frac{2}{m} \left  \frac{2_1}{m} \right  \frac{2}{b}$	41	$P \frac{2}{m} \left  \frac{2_1}{m} \left(\frac{2}{b}\right) \right.$				
		64	$P \frac{2_1}{m} \frac{2}{a} \left  \frac{2}{m} \right.$	68	$P \frac{2_1}{m} \left  \frac{2}{a} \right  \frac{2}{m}$	42	$P \frac{2_1}{m} \left  \frac{2}{a} \left(\frac{2}{m}\right) \right.$				
		65	$P \frac{2}{m} \frac{2}{c} \left  \frac{2_1}{m} \right.$	69	$P \frac{2}{m} \left  \frac{2}{c} \right  \frac{2_1}{m}$			30	$P \left(\frac{2}{m}\right) \left(\frac{2}{c}\right) \frac{2_1}{m}$		

Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
			41	$P \frac{2}{b} \frac{2_1}{m} \left( \frac{2}{m} \right)$					
<i>Pnna</i>	52	$P \frac{2}{n} \frac{2_1}{n} \frac{2}{a}$							
<i>Pmna</i>	53	$P \frac{2}{m} \frac{2}{n} \frac{2_1}{a}$							
			42	$P \frac{2_1}{b} \frac{2}{m} \left( \frac{2}{n} \right)$					
<i>Pcca</i>	54	$P \frac{2_1}{c} \frac{2}{c} \frac{2}{a}$							
			43	$P \frac{2}{b} \frac{2_1}{a} \left( \frac{2}{a} \right)$					
<i>Pbam</i>	55	$P \frac{2_1}{b} \frac{2_1}{a} \frac{2}{m}$	44	$P \frac{2_1}{b} \frac{2_1}{a} \left( \frac{2}{m} \right)$					
<i>Pccn</i>	56	$P \frac{2_1}{c} \frac{2_1}{c} \frac{2}{n}$							
<i>Pbcm</i>	57	$P \frac{2}{b} \frac{2_1}{c} \frac{2_1}{m}$							
			45	$P \frac{2_1}{m} \frac{2_1}{a} \left( \frac{2}{b} \right)$					
<i>Pnmm</i>	58	$P \frac{2_1}{n} \frac{2_1}{n} \frac{2}{m}$							
<i>Pmmn</i>	59	$P \frac{2_1}{m} \frac{2_1}{m} \frac{2}{n}$	46	$P \frac{2_1}{m} \frac{2_1}{m} \left( \frac{2}{n} \right)$					





Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
<i>Pbcn</i>	60	$P \frac{2_1}{b} \frac{2}{c} \frac{2_1}{n}$							
<i>Pbca</i>	61	$P \frac{2_1}{b} \frac{2_1}{c} \frac{2_1}{a}$							
<i>Pnma</i>	62	$P \frac{2_1}{n} \frac{2_1}{m} \frac{2_1}{a}$							
<i>Cmcm</i>	63	$C \frac{2}{m} \frac{2}{c} \frac{2_1}{m}$							
<i>Cmca</i>	64	$C \frac{2}{m} \frac{2}{c} \frac{2_1}{a}$							
<i>Cmmm</i>	65	$C \frac{2}{m} \frac{2}{m} \frac{2}{m}$	47	$C \frac{2}{m} \frac{2}{m} \left( \frac{2}{m} \right)$					
<i>Cccm</i>	66	$C \frac{2}{c} \frac{2}{c} \frac{2}{m}$							
<i>Cmma</i>	67	$C \frac{2}{m} \frac{2}{m} \frac{2}{a}$	48	$C \frac{2}{m} \frac{2}{m} \left( \frac{2}{a} \right)$					
<i>Ccca</i>	68	$C \frac{2}{c} \frac{2}{c} \frac{2}{a}$							
<i>Fmmm</i>	69	$F \frac{2}{m} \frac{2}{m} \frac{2}{m}$							
<i>Fddd</i>	70	$F \frac{2}{d} \frac{2}{d} \frac{2}{d}$							
<i>Immm</i>	71	$I \frac{2}{m} \frac{2}{m} \frac{2}{m}$							
<i>Ibam</i>	72	$I \frac{2}{b} \frac{2}{a} \frac{2}{m}$							
<i>Ibca</i>	73	$I \frac{2_1}{b} \frac{2_1}{c} \frac{2_1}{a}$							
<i>Imma</i>	74	$I \frac{2_1}{m} \frac{2_1}{m} \frac{2_1}{a}$							
<i>P<math>\bar{4}</math></i>	75	<i>P<math>\bar{4}</math>11</i>	49	<i>P<math>\bar{4}</math>11</i>	23	<i>P<math>\bar{4}</math>(11)</i>	9	<i>(<math>\bar{4}</math>11)</i>	$\bar{4}$
<i>I<math>\bar{4}</math></i>	76	<i>I<math>\bar{4}</math>11</i>							
<i>P<math>\bar{4}</math>2m</i>	77	<i>P<math>\bar{4}</math>2m</i>	50	<i>P<math>\bar{4}</math>2m</i>	24	<i>P<math>\bar{4}</math>(2m)</i>	10	<i>(<math>\bar{4}</math>2m)</i>	$\bar{4}2m$
<i>P<math>\bar{4}</math>2c</i>	78	<i>P<math>\bar{4}</math>2c</i>			25	<i>P<math>\bar{4}</math>(2c)</i>			
<i>P<math>\bar{4}</math>2<sub>1</sub>m</i>	79	<i>P<math>\bar{4}</math>2<sub>1</sub>m</i>	51	<i>P<math>\bar{4}</math>2<sub>1</sub>m</i>					

Table 1 (cont.)

No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
		77	$P \frac{2_1}{b} \frac{2}{c} \left  \frac{2_1}{n} \right.$						
		78	$P \frac{2}{c} \frac{2_1}{a} \left  \frac{2_1}{n} \right.$						
		79	$P \frac{2_1}{b} \frac{2_1}{c} \left  \frac{2_1}{a} \right.$	87	$P \frac{2_1}{b} \left  \frac{2_1}{c} \right. \left  \frac{2_1}{a} \right.$				
		80	$P \frac{2_1}{c} \frac{2_1}{m} \left  \frac{2_1}{n} \right.$						
		81	$P \frac{2_1}{m} \frac{2_1}{c} \left  \frac{2_1}{n} \right.$						
		82	$C \frac{2}{m} \frac{2}{c} \left  \frac{2_1}{m} \right.$						
		83	$C \frac{2}{m} \frac{2}{c} \left  \frac{2_1}{a} \right.$						
		84	$C \frac{2}{m} \frac{2}{m} \left  \frac{2}{m} \right.$						
		85	$C \frac{2}{c} \frac{2}{c} \left  \frac{2}{m} \right.$						
		86	$C \frac{2}{m} \frac{2}{m} \left  \frac{2}{a} \right.$						
		87	$C \frac{2}{c} \frac{2}{c} \left  \frac{2}{a} \right.$						

---

13  $(\bar{4})(11)$                       88  $P\bar{4}|11$

---

14  $(\bar{4})(2m)$                       89  $P\bar{4}|2m$   
     90  $P\bar{4}|2c$   
     91  $P\bar{4}|2_1m$

Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
$P\bar{4}_2c$	80	$P\bar{4}_2c$							
$C\bar{4}2m$	81	$C\bar{4}2m$	52	$P(\bar{4})m2$					
$C\bar{4}2c$	82	$C\bar{4}2c$							
$C\bar{4}2b$	83	$C\bar{4}2b$	53	$P(\bar{4})b2$					
$C\bar{4}2n$	84	$C\bar{4}2n$							
$F\bar{4}2m$	85	$F\bar{4}2m$							
$F\bar{4}2c$	86	$F\bar{4}2c$							
$I\bar{4}2m$	87	$I\bar{4}2m$							
$I\bar{4}2d$	88	$I\bar{4}2d$							
$P4$	89	$P411$	54	$P(4)11$	26	$P4(11)$	11	(411)	4
$P4_1$	90	$P4_111$			27	$P4_1(11)$			
$P4_2$	91	$P4_211$			28	$P4_2(11)$			
$P4_3$	92	$P4_311$			29	$P4_3(11)$			
$I4$	93	$I411$							
$I4_1$	94	$I4_111$							
$P \frac{4}{m}$	95	$P \frac{4}{m} 11$	55	$P \left( \frac{4}{m} \right) 11$	30	$P \frac{4}{m} (11)$	12	$\left( \frac{4}{m} 11 \right)$	$\frac{4}{m}$
$P \frac{4_2}{m}$	96	$P \frac{4_2}{m} 11$			31	$P \frac{4_2}{m} (11)$			
$P \frac{4}{n}$	97	$P \frac{4}{n} 11$	56	$P \left( \frac{4}{n} \right) 11$					
$P \frac{4_2}{n}$	98	$P \frac{4_2}{n} 11$							
$I \frac{4}{m}$	99	$I \frac{4}{m} 11$							
$I \frac{4_1}{a}$	100	$I \frac{4_1^a}{a} 11$							
$P4mm$	101	$P4mm$	57	$P(4)mm$	32	$P4(mm)$	13	(4mm)	4mm
$P4bm$	102	$P4bm$	58	$P(4)bm$					
$P4_2cm$	103	$P4_2cm$			33	$P4_2(cm)$			
$P4_2nm$	104	$P4_2nm$							
$P4cc$	105	$P4cc$			34	$P4(cc)$			
$P4nc$	106	$P4nc$							
$P4_2mc$	107	$P4_2mc$							

Table 1 (cont.)

No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
		92	$P\bar{4} 2_1c$								
		93	$P\bar{4} m2$								
		94	$P\bar{4} c2$								
		95	$P\bar{4} b2$								
<hr/>											
15	$(4)(11)$	96	$P4 11$								
		97	$P4_1 11$								
		98	$P4_2 11$								
		99	$P4_3 11$								
<hr/>											
16	$\left(\frac{4}{m}\right)(11)$	100	$P\frac{4}{m} 11$								
		101	$P\frac{4_2}{m} 11$								
		102	$P\frac{4}{n} 11$								
<hr/>											
17	$(4)(mm)$	103	$P4 mm$								
		104	$P4 bm$								
		105	$P4_2 cm$								
		106	$P4 cc$								
		107	$P4_2 mc$								

Table 1 (cont.)

Short space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
$P4_2bc$	108	$P4_2bc$							
$I4mm$	109	$I4mm$							
$I4cm$	110	$I4cm$							
$I4_1md$	111	$I4_1md$							
$I4_1cd$	112	$I4_1cd$							
$P42$	113	$P422$	59	$P(4)22$	35	$P4(22)$	14	(422)	422
$P42_1$	114	$P42_12$	60	$P(4)2_12$					
$P4_12$	115	$P4_122$			36	$P4_1(22)$			
$P4_12_1$	116	$P4_12_12$							
$P4_22$	117	$P4_222$			37	$P4_2(22)$			
$P4_22_1$	118	$P4_22_12$							
$P4_32$	119	$P4_322$			38	$P4_3(22)$			
$P4_32_1$	120	$P4_32_12$							
$I42$	121	$I422$							
$I4_12$	122	$I4_122$							
$P \frac{4}{m} mm$	123	$P \frac{4}{m} \frac{2}{m} \frac{2}{m}$	61	$P \left( \frac{4}{m} \right) \frac{2}{m} \frac{2}{m}$	39	$P \frac{4}{m} \left( \frac{2}{m} \frac{2}{m} \right)$	15	$\left( \frac{4}{m} \frac{2}{m} \frac{2}{m} \right) \frac{4}{m} mm$	
$P \frac{4}{m} cc$	124	$P \frac{4}{m} \frac{2}{c} \frac{2}{c}$			40	$P \frac{4}{m} \left( \frac{2}{c} \frac{2}{c} \right)$			
$P \frac{4}{n} bm$	125	$P \frac{4}{n} \frac{2}{b} \frac{2}{m}$	62	$P \left( \frac{4}{n} \right) \frac{2}{b} \frac{2}{m}$					
$P \frac{4}{n} nc$	126	$P \frac{4}{n} \frac{2}{n} \frac{2}{c}$							
$P \frac{4}{m} bm$	127	$P \frac{4}{m} \frac{2_1}{b} \frac{2}{m}$	63	$P \left( \frac{4}{m} \right) \frac{2_1}{b} \frac{2}{m}$					
$P \frac{4}{m} nc$	128	$P \frac{4}{m} \frac{2_1}{n} \frac{2}{c}$							
$P \frac{4}{n} mm$	129	$P \frac{4}{n} \frac{2_1}{m} \frac{2}{m}$	64	$P \left( \frac{4}{n} \right) \frac{2_1}{m} \frac{2}{m}$					
$P \frac{4}{n} cc$	130	$P \frac{4}{n} \frac{2_1}{c} \frac{2}{c}$							
$P \frac{4_2}{m} mc$	131	$P \frac{4_2}{m} \frac{2}{m} \frac{2}{c}$			41	$P \frac{4_2}{m} \left( \frac{2}{m} \frac{2}{c} \right)$			
$P \frac{4_2}{m} cm$	132	$P \frac{4_2}{m} \frac{2}{c} \frac{2}{m}$							
$P \frac{4_2}{n} bc$	133	$P \frac{4_2}{n} \frac{2}{b} \frac{2}{c}$							
$P \frac{4_2}{n} nm$	134	$P \frac{4_2}{n} \frac{2}{n} \frac{2}{m}$							

Table 1 (cont.)

No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
18	(4)(22)	108	$P4 22$						
		109	$P4 2_12$						
		110	$P4_1 22$						
		111	$P4_2 22$						
		112	$P4_3 22$						
19	$\left(\frac{4}{m}\right)\left(\frac{2}{m} \frac{2}{m}\right)$	113	$P \frac{4}{m} \left  \frac{2}{m} \frac{2}{m} \right.$						
		114	$P \frac{4}{m} \left  \frac{2}{c} \frac{2}{c} \right.$						
		115	$P \frac{4}{n} \left  \frac{2}{b} \frac{2}{m} \right.$						
		116	$P \frac{4}{m} \left  \frac{2_1}{b} \frac{2}{m} \right.$						
		117	$P \frac{4}{n} \left  \frac{2_1}{m} \frac{2}{m} \right.$						
		118	$P \frac{4_2}{m} \left  \frac{2}{m} \frac{2}{c} \right.$						
		119	$P \frac{4_2}{m} \left  \frac{2}{c} \frac{2}{m} \right.$						

Table 1 (cont.)

Short Space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
$P \frac{4_2}{m} bc$	135	$P \frac{4_2}{m} \frac{2_1}{b} \frac{2}{c}$							
$P \frac{4_2}{m} nm$	136	$P \frac{4_2}{m} \frac{2_1}{n} \frac{2}{m}$							
$P \frac{4_2}{n} mc$	137	$P \frac{4_2}{n} \frac{2_1}{m} \frac{2}{c}$							
$P \frac{4_2}{n} cm$	138	$P \frac{4_2}{n} \frac{2_1}{c} \frac{2}{m}$							
$I \frac{4}{m} mm$	139	$I \frac{4}{m} \frac{2}{m} \frac{2}{m}$							
$I \frac{4}{m} cm$	140	$I \frac{4}{m} \frac{2}{c} \frac{2}{m}$							
$I \frac{4_1}{a} md$	141	$I \frac{4_1}{a} \frac{2}{m} \frac{2}{d}$							
$I \frac{4_1}{a} cd$	142	$I \frac{4_1}{a} \frac{2}{c} \frac{2}{d}$							
$P3$	143	$P311$	65	$P(3)11$	42	$P3(11)$	16	$(311)$	3
$P3_1$	144	$P3_111$			43	$P3_1(11)$			
$P3_2$	145	$P3_211$			44	$P3_2(11)$			
$R3$	146	$R311$							
$P\bar{3}$	147	$P\bar{3}11$	66	$P(\bar{3})11$	45	$P\bar{3}(11)$	17	$(\bar{3}11)$	$\bar{3}$
$R\bar{3}$	148	$R\bar{3}11$							
$P3m1$	149	$P3m1$	67	$P(3)m1$	46	$P3(m1)$	18	$(3m1)$	$3m$
$P31m$	150	$P31m$	68	$P(3)1m$					
$P3c1$	151	$P3c1$			47	$P3(c1)$			
$P31c$	152	$P31c$							
$R3m$	153	$R3m1$							
$R3c$	154	$R3c1$							
$P321$	155	$P321$	69	$P(3)21$	48	$P3(21)$	19	$(321)$	32
$P312$	156	$P312$	70	$P(3)12$					
$P3_121$	157	$P3_121$			49	$P3_1(21)$			
$P3_112$	158	$P3_112$							
$P3_221$	159	$P3_221$			50	$P3_2(21)$			
$P3_212$	160	$P3_212$							
$R32$	161	$R32$							
$P\bar{3}m1$	162	$P\bar{3}m1$	71	$P(\bar{3})m1$	51	$P\bar{3}(m1)$	20	$(\bar{3}m1)$	$\bar{3}m$
$P\bar{3}c1$	163	$P\bar{3}c1$			52	$P\bar{3}(c1)$			
$P\bar{3}1m$	164	$P\bar{3}1m$	72	$P(\bar{3})1m$					





Table 1 (cont.)

Short Space group	No.	Full symbol	No.	Symbol	No.	Symbol	No.	Symbol	Short symbol
$P\bar{3}1c$	165	$P\bar{3}1c$							
$R\bar{3}2m$	166	$R\bar{3}2m$							
$R\bar{3}2c$	167	$R\bar{3}2c$							
$P\bar{6}$	168	$P\bar{6}11$	73	$P(\bar{6})11$	53	$P\bar{6}(11)$	21	$(\bar{6}11)$	$\bar{6}$
$P\bar{6}m2$	169	$P\bar{6}m2$	74	$P(\bar{6})m2$	54	$P\bar{6}(m2)$	22	$(\bar{6}m2)$	$\bar{6}m2$
$P\bar{6}c2$	170	$P\bar{6}c2$			55	$P\bar{6}(c2)$			
$P\bar{6}2m$	171	$P\bar{6}2m$	75	$P(\bar{6})2m$					
$P\bar{6}2c$	172	$P\bar{6}2c$							
$P6$	173	$P611$	76	$P(6)11$	56	$P6(11)$	23	$(611)$	6
$P6_1$	174	$P6_111$			57	$P6_1(11)$			
$P6_5$	175	$P6_511$			58	$P6_5(11)$			
$P6_2$	176	$P6_211$			59	$P6_2(11)$			
$P6_4$	177	$P6_411$			60	$P6_4(11)$			
$P6_3$	178	$P6_311$			61	$P6_3(11)$			
$P\frac{6}{m}$	179	$P\frac{6}{m}11$	77	$P\left(\frac{6}{m}\right)11$	62	$P\frac{6}{m}(11)$	24	$\left(\frac{6}{m}11\right)$	$\frac{6}{m}$
$P\frac{6_3}{m}$	180	$P\frac{6_3}{m}11$			63	$P\frac{6_3}{m}(11)$			
$P6mm$	181	$P6mm$	78	$P(6)mm$	64	$P6(mm)$	25	$(6mm)$	$6mm$
$P6cc$	182	$P6cc$			65	$P6(cc)$			
$P6_3cm$	183	$P6_3cm$			66	$P6_3(cm)$			
$P6_3mc$	184	$P6_3mc$							
$P62$	185	$P622$	79	$P(6)22$	67	$P6(22)$	26	$(622)$	622
$P6_12$	186	$P6_122$			68	$P6_1(22)$			
$P6_52$	187	$P6_522$			69	$P6_5(22)$			
$P6_22$	188	$P6_222$			70	$P6_2(22)$			
$P6_42$	189	$P6_422$			71	$P6_4(22)$			
$P6_32$	190	$P6_322$			72	$P6_3(22)$			
$P\frac{6}{m}mm$	191	$P\frac{6}{m}\frac{2}{m}\frac{2}{m}$	80	$P\left(\frac{6}{m}\right)\frac{2}{m}\frac{2}{m}$	73	$P\frac{6}{m}\left(\frac{2}{m}\frac{2}{m}\right)$	27	$\left(\frac{6}{m}\frac{2}{m}\frac{2}{m}\right)$	$\frac{6}{m}mm$
$P\frac{6}{m}cc$	192	$P\frac{6}{m}\frac{2}{c}\frac{2}{c}$			74	$P\frac{6}{m}\left(\frac{2}{c}\frac{2}{c}\right)$			
$P\frac{6_3}{m}cm$	193	$P\frac{6_3}{m}\frac{2}{c}\frac{2}{m}$			75	$P\frac{6}{m}\left(\frac{2}{c}\frac{2}{m}\right)$			
$P\frac{6_3}{m}mc$	194	$P\frac{6_3}{m}\frac{2}{m}\frac{2}{c}$							
	+26	cubic space groups					+5	cubic crystal classes	
	230						32		

Table 1 (cont.)

No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
		137	$P\bar{3} 1c$						
25	$(\bar{6}) 11$	138	$P\bar{6} 11$						
26	$(\bar{6}) m2$	139	$P\bar{6} m2$						
		140	$P\bar{6} c2$						
		141	$P\bar{6} 2m$						
		142	$P\bar{6} 2c$						
27	$(6) 11$	143	$P6 11$						
		144	$P6_1 11$						
		145	$P6_5 11$						
		146	$P6_2 11$						
		147	$P6_4 11$						
		148	$P6_3 11$						
28	$\left(\frac{6}{m}\right) 11$	149	$P \frac{6}{m}   11$						
		150	$P \frac{6_3}{m}   11$						
29	$(6) mm$	151	$P6 mm$						
		152	$P6 cc$						
		153	$P6_3 cm$						
		154	$P6_3 mc$						
30	$(6) 22$	155	$P6 22$						
		156	$P6_1 22$						
		157	$P6_5 22$						
		158	$P6_2 22$						
		159	$P6_4 22$						
		160	$P6_3 22$						
31	$\left(\frac{6}{m}\right) \frac{2}{m} \frac{2}{m}$	161	$P \frac{6}{m} \left  \frac{2}{m} \frac{2}{m} \right.$						
		162	$P \frac{6}{m} \left  \frac{2}{c} \frac{2}{c} \right.$						
		163	$P \frac{6}{m} \left  \frac{2}{c} \frac{2}{m} \right.$						
		164	$P \frac{6_3}{m} \left  \frac{2}{m} \frac{2}{c} \right.$						

Table 2. *The two-dimensional symmetry groups*

Symbol after Niggli	$\mathcal{G}_2$		$\mathcal{G}_1^1$		$\mathcal{G}_2$		$\mathcal{G}_{11}$		$\mathcal{G}_{11}$	
Symbol after Bohm	$G_2$		$G_{21}$		$G_{20}$		$G_{210}$			
Form of matrices	$\begin{pmatrix} + & + &   & + \\ + & + &   & + \\ \hline 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 &   & + \\ 0 & + &   & 0 \\ \hline 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & + &   & 0 \\ + & + &   & 0 \\ \hline 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 &   & 0 \\ 0 & + &   & 0 \\ \hline 0 & 0 &   & 1 \end{pmatrix}$		$\begin{pmatrix} + & 0 &   & + \\ 0 & + &   & + \\ \hline 0 & 0 &   & 1 \end{pmatrix}$	
Symbol of the corresponding three-dimensional space group	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol	No.	Symbol
<i>P1</i>	1	<i>p</i> [1]11	1	<i>p</i> [1](1)1	1	[1](11)	1	[1](1)(1)	1	<i>p</i> (1)1 1
<i>Pm</i>	2	<i>p</i> [1] <i>m</i> 1	2	<i>p</i> [1]( <i>m</i> )1	2	[1]( <i>m</i> 1)	2	[1]( <i>m</i> )(1)	2	<i>p</i> [1] <i>m</i>  1
			3	<i>p</i> [1](1) <i>m</i>			3	[1](1)( <i>m</i> )	3	<i>p</i> [1]1  <i>m</i>
<i>Pc</i>	3	<i>p</i> [1] <i>c</i> 1	4	<i>p</i> [1]( <i>c</i> )1					4	<i>p</i> [1] <i>c</i>  1
									5	<i>p</i> [1]1  <i>c</i>
<i>Cm</i>	4	<i>a</i> *[1] <i>m</i> 1								
<i>P2</i>	5	<i>p</i> [2]11	5	<i>p</i> [2](1)1	3	[2](11)	4	[2](1)(1)	6	<i>p</i> [2]1 1
<i>Pmm</i>	6	<i>p</i> [2] <i>mm</i>	6	<i>p</i> [2]( <i>m</i> ) <i>m</i>	4	[2]( <i>mm</i> )	5	[2]( <i>m</i> )( <i>m</i> )	7	<i>p</i> [2] <i>m</i>   <i>m</i>
<i>Pma</i>	7	<i>p</i> [2] <i>ma</i> †	7	<i>p</i> [2]( <i>c</i> ) <i>m</i>					8	<i>p</i> [2] <i>m</i>   <i>a</i> †
									9	<i>p</i> [2] <i>c</i>   <i>m</i>
<i>Pba</i>	8	<i>p</i> [2] <i>cb</i>							10	<i>p</i> [2] <i>c</i>   <i>b</i>
<i>Cmm</i>	9	<i>a</i> *[2] <i>mm</i>								
<i>P4</i>	10	<i>p</i> [4]11			5	[4](11)				
<i>P4mm</i>	11	<i>p</i> [4] <i>mm</i>			6	[4]( <i>mm</i> )				
<i>P4bm</i>	12	<i>p</i> [4] <i>bm</i>								
<i>P3</i>	13	<i>p</i> [3]11			7	[3](11)				
<i>P3m1</i>	14	<i>p</i> [3] <i>m</i> 1			8	[3]( <i>m</i> 1)				
<i>P31m</i>	15	<i>p</i> [3]1 <i>m</i>								
<i>P6</i>	16	<i>p</i> [6]11			9	[6](11)				
<i>P6mm</i>	17	<i>p</i> [6] <i>mm</i>			10	[6]( <i>mm</i> )				

\* *a* means a face-centred lattice.† *a* means a glide-mirror-plane.

one pair of brackets; if such an exchange is not permitted within the set, then separate pairs of brackets are used.

Capital letters are used to indicate the Bravais lattice of objects extending in three dimensions, small letters to indicate the Bravais lattice of two-dimensional objects.

For the symmetry groups with two-dimensional space of transformation (two-dimensional objects) a third place in the symbol is needed not referring to either of the two directions. The place is indicated by square brackets and put in the first position of the symbol. In this way the symbols for the two-dimensional groups correspond closely to the well-known (three-dimensional) space group symbols, as indicated in the first column of Table 2.

Symbols '1' are used to fill places where there are no other symmetry elements.

Sets of symmetry groups with two (or more) non-exchangeable directions with periodicity have not, so far, been listed. They are included in Tables 1 and 2. In their symbols vertical lines separate the symmetry elements corresponding to such non-exchangeable directions. The numbers of the corresponding symmetry groups are: 124  $\mathcal{G}_{21}$ ; 87  $\mathcal{G}_{11}^1$ ; 48  $\mathcal{G}_1^1$ ; and 10  $\mathcal{G}_{11}$ . The numbers of the symmetry groups for the other sets have been known for some time.

In the first column of the Tables the corresponding (three-dimensional, short) space group symbol is listed. Different orientations have to be considered in the various sets, and for each orientation a separate line is used.

For a one-dimensional space of transformation only two sets of symmetry groups exist, with two groups each:

the space groups  $p1$  and  $pm$  for  $\mathcal{G}_1(G_1)$ , and the point groups  $(1)$  and  $(m)$  for  $\mathcal{G}_1(G_{10})$ .

The symbols for symmetry groups proposed here seem to us to have the following advantages: They are sufficiently similar to the international space group symbols to be easily understood and visualized, and the tables of equivalent positions *etc.* given in *Inter-*

*national Tables* can be used almost as they stand for the corresponding symmetry groups of all sets.

#### References

- BOHM, J. (1963). *Neuer. Jb. Miner. Abh.* **100**, 113.  
 BOHM, J. & DORNBERGER-SCHIFF, K. (1966). *Acta Cryst.* **21**, 1004.  
*International Tables for X-ray Crystallography* (1952). Vol. I. Birmingham: Kynoch Press.  
 NIGGLI, A. (1966). Private communication by H. WONDRA-TSCHEK.

*Acta Cryst.* (1967). **23**, 933

## A Scattering Curve for a Rotating Methane Molecule

BY A. WHITAKER

*Department of Physics, Brunel University, Woodlands Avenue, London, W.3, England*

(Received 23 March 1967)

Various scattering factor curves have been calculated for a rotating methane molecule in an attempt to elucidate the effect of slightly different interatomic distances and angular terms. It is concluded that the effect of using slightly different interatomic distances is obscured by effects caused by different methods of obtaining the wave functions, while in the case of methane and, presumably, ammonium the effect of the angular terms is small.

Davis & Whitaker (1966) reported figures for a scattering curve for a spherically symmetrical ammonium group. The scattering curves were calculated for the Hartree self-consistent wave functions of Bernal & Massey (1954) and the analytical wave functions with exchange of Bernal (1953). The values of the scattering factors from these wave functions differed by up to 10% although both wave functions were calculated for the same nitrogen-hydrogen distance of 0.972 Å. This value is somewhat lower than the average value obtained in practice: 1.033 Å (*International Tables for X-ray Crystallography*, 1962, p. 270).

In an attempt to estimate the effect of small differences of interatomic distances on the scattering curves, these have been calculated for a rotating methane molecule.

There are two wave functions for methane comparable with those for ammonium, namely; the Hartree self-consistent wave functions of Buckingham, Massey & Tibbs (1941), calculated assuming a carbon-hydrogen distance of 1.056 Å and the analytical wave functions including exchange of Bernal (1953), calculated assuming a carbon-hydrogen distance of 1.043 Å.

The scattering curve based on the wave functions of Buckingham, Massey & Tibbs (1941) has already been reported (Banyard & March, 1956). However, it has been recalculated for ease in comparison with the other scattering curves; the ammonium wave functions of Bernal & Massey (1954) were calculated by the same method. Bernal (1953) used the same technique for the wave functions of both ammonium and methane. Thus

it was thought that comparison of the various curves for ammonium and methane may give an indication as to the effect of slight differences of interatomic distances on the scattering curves. Incidentally, the interatomic distances for methane for which the wave functions were calculated are all considerably less than the average experimental value 1.091 Å (*International Tables for X-ray Crystallography*, 1962, p. 276).

In addition to these wave functions the Hartree-Fock self-consistent wave functions have also been calculated (Mills, 1958) assuming an interatomic distance of 1.056 Å and, in addition, Mills (1961) estimated the effect of the tetrahedral symmetry of the molecule on the radial density distribution (angular terms). The scattering curves for both these models have been calculated to estimate the effect of including the angular terms.

The electron density distributions of these wave functions are given in Fig. 1; as expected, the effect of using a smaller interatomic distance causes the electron cloud to be contracted; exchange has a similar although smaller effect, while the effect of the angular terms is to make the electron cloud slightly more diffuse. The last conclusion was also obtained by Banyard & March (1961), but it appears that their conclusions were based on the incorrect angular terms given by Mills (1958). These have now been corrected (Mills, 1961).

However, in the case of ammonium, the use of analytical wave functions gives a contracted electron cloud compared with Hartree wave functions even