References

BAUDOUR, J. L. & SANQUER, M. (1983). *Acta Cryst.* B39, 75-84.
BÖHM, H. (1978). *Z. Kristallogr.* **148**, 207-211.
DAM, B., JANNER, A., BENNEMA, P., VAN DEN LINDEN, W. H. & RASING, TH. (1983). *Phys. Rev. Lett.* **50**, 849-852.
HEINE, V. (1960). *Group Theory in Quantum Mechanics.* Oxford: Pergamon.
HEINE, V., LYNDEN-BELL, R. M., MCCONNELL, J. D. C. & MCDONALD, I. R. (1984). *Z. Phys. B*, **56**, 229-239.
HEINE, V. & PRICE, S. (1985). *J. Phys. C*, **18**, 5259-5278.
IIZUMI, M., AXE, J. D., SHIRANE, G. & SHIMAOKA, K. (1977). *Phys. Rev. B*, **15**, 4392-4411.
JANNER, A. & JANSSEN, T. (1980). *Acta Cryst.* A36, 399-408.
JANNER, A., RASING, TH., BENNEMA, P. & VAN DEN LINDEN, W. H. (1980). *Phys. Rev. Lett.* **45**, 1700-1702.
KUCHARCZYK, D. & PACIOREK, W. A. (1985). *Acta Cryst.* **A41**, 466-469.
LIFSHITZ, E. M. & PITAEVSKII, L. P. (1980). *Statistical Physics*, 3rd ed., Part 1. Oxford: Pergamon.
MCCONNELL, J. D. C. & HEINE, V. (1984). *Acta Cryst.* **A40**, 473-482.
PACIOREK, W. A. & KUCHARCZYK, D. (1984). Conference abstract. Unpublished. Private communication.
PATER, C. J. DE & VAN DIJK, C. (1978). *Phys. Rev. B*, **18**, 1281-1293.
SIMMONS, E. H. (1987). In preparation.
SIMMONS, E. H. & HEINE, V. (1987). *Acta Cryst.* Submitted.
WOLFF, P. M. DE (1974). *Acta Cryst.* A30, 777-785.
WOLFF, P. M. DE, JANSSEN, T. & JANNER, A. (1981). *Acta Cryst.* A37, 625-636.

Acta Cryst. (1987). A43, 294-304

Crystallography, Geometry and Physics in Higher Dimensions. III. Geometrical Symbols for the 227 Crystallographic Point Groups in Four-Dimensional Space

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Abstract

A geometrical 'WPV' notation for crystallographic point symmetry groups (PSG) in four-dimensional space is proposed. This simple notation generalizes the Hermann-Mauguin notation and makes it possible to retrieve the PSG elements easily. Tables classifying all elements of each PSG for systems 1 to 28 are presented. For higher systems, from 29 up to 33 inclusive, the results of the work are not reported owing to the space required, but they are at the disposal of the reader upon request.

Introduction

The present article is the continuation of two previous papers; we first defined the crystallographic point symmetry operations (PSOs) as elements of crystallographic point symmetry groups (PSGs) in $\mathbb{E}^4$, $\mathbb{E}^5$ and $\mathbb{E}^6$ (Weigel, Veysseyre, Phan, Effantin & Billiet, 1984), then we gave an extensive description of the 384 elements of the crystallographic PSG for the holohedry of the primitive hypercubic crystal system in $\mathbb{E}^4$ (Veysseyre, Weigel, Phan & Effantin, 1984). For some PSGs in $\mathbb{E}^4$ we proposed geometric symbols which were generalizations of Hermann-Mauguin symbols but we did not give a listing of all PSOs of these PSGs (Weigel, Phan & Veysseyre, 1984; Veysseyre, Phan & Weigel, 1985).

By means of a completely different approach, Whittaker (1984) recently published a list of rather complicated symbols for the 227 groups but did not propose any list of PSOs. Furthermore his symbolism is far from the Hermann-Mauguin notation except for some polar groups.

In this paper we propose simple geometric symbols for each of the 227 crystallographic PSGs of $\mathbb{E}^4$; then we give the entire listing of all PSOs, elements of each of 161 crystallographic PSGs among the total of 227. It should be pointed out that for each PSG of $\mathbb{E}^4$ our geometric symbol is a generalization of a Hermann-Mauguin symbol for physical space $\mathbb{E}^3$ and makes it possible to retrieve any symbol of any PSO, an element of the PSG.

We recall that Wondratschek, Bülow & Neubüser (1971) determined the number of crystallographic PSGs of $\mathbb{E}^4$. There are 227 belonging to 33 crystallographic systems which in turn are grouped into 23 families, indicated by a Roman numeral. The 227 PSGs of $\mathbb{E}^4$ are all subgroups of at least one of the four following PSGs: 20-22; 30-13; 31-07 and 33-16: here the first number characterizes the system (*cf.* Table 1, fourth column), the second number the PSG

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Table 1. *Elements and notations of the* 161 *crystallographic PSGs of the families* I *to* XX

The table is divided into subtables, one for each family; if necessary, one subtable is divided into two or three parts for each system belonging to this family. For each crystal system heading, the system name is given and between parentheses the name given by Wondratschek, Bülow & Neubüser (1971). Each family is characterized by a roman numeral (I to XXIII) and each system by an arabic numeral (1 to 28). For each PSG the first column gives its number in the system, the second its order, the third some subgroups, the fourth its elements, which are not elements of the subgroups of the third column, the fifth its WPV notation, the seventh its PSG$^+$ when the PSG itself is a PSG$^-$. In the sixth column the filled circle • indicates polar groups and the symbol ▴ indicates PSGs containing $\bar{1}_4$. In the listing of the elements of each PSG, the following abbreviations are employed:

□: $x, y, x+y, x-y$ ∇: $x-y, x-2y, 2x-y$ ■: $z, t, z+t, z-t$ ▼: $z-t, z-2t, 2z-t$
△: $x, y, x+y$ O: $x, y, x+y, x-y, x-2y, 2x-y$ ▲: $z, t, z+t$ ●: $z, t, z+t, z-t, z-2t, 2z-t$.

Class	Order	Subgroups	PSO				WPV NOTATION		PSG$^+$
			I 01 Hexaclinic*						
01	1		1				1	•	—
02	2	01	$\bar{1}_4$				$\bar{1}_4$	▴	—
			II 02 Right hyperprism based on parallelepiped (*xyz*) [triclinic]*						
01	2		1	m_t			m	•	1
02	2		1			$\bar{1}_{xyz}$	$\bar{1}$	•	1
03	4	01-02	$\bar{1}_4$				$\bar{1}\perp m$	▴	$\bar{1}_4$
			III 03 Di orthogonal parallelograms (*xy*), (*zt*) [diclinic]						
01	2		1		2_{xy}		2	•	—
02	4	01	$\bar{1}_4$		2_{zt}		$2\perp 2$	▴	—
			IV 04 Orthogonal parallelogram (*xy*) rectangle (*zt*) [monoclinic]						
01	4		1	m_z, m_t	2_{zt}		$m, m, 2$	•	2
02	4		1	m_z	2_{xy}	$\bar{1}_{xyz}$	$\frac{2}{m}$	•	2
03	4		1		2_{zt}	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$2, \bar{1}, \bar{1}$		2
04	8	01	$\bar{1}_4$		2_{xy}	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$2\perp 2, m, m$	▴	$2\perp 2$
			V 05 Di orthogonal rectangles (*xy*), (*zt*) *KU*-centred [orthogonal *KU*-centred]						
01	4		1		$2_{xy}, 2_{xz}, 2_{yz}$		$2, 2, 2$	•	—
02	8	01	$\bar{1}_4$		$2_{xt}, 2_{yt}, 2_{zt}$		$(2, 2, 2)\otimes\bar{1}_4$	▴	—
			06 Di orthogonal rectangles (*xy*), (*zt*) [orthogonal]						
01	8		1	m_x, m_y, m_z	$2_{xy}, 2_{xz}, 2_{yz}$	$\bar{1}_{xyz}$	$\frac{2}{m}, \frac{2}{m}, \frac{2}{m}$	•	$2, 2, 2$
02	8		1	m_t	$2_{xy}, 2_{xz}, 2_{yz}$	$\bar{1}_{xyt}, \bar{1}_{xzt}, \bar{1}_{yzt}$	$(2, 2, 2)\perp m$		$2, 2, 2$
03	16	01-02	$\bar{1}_4$		$2_{xt}, 2_{yt}, 2_{zt}$		$m, m, 2\perp 2, m, m$	▴	$(2, 2, 2)\otimes\bar{1}_4$
			VI 07 orthogonal parallelogram (*xy*) square (*zt*) [tetragonal monoclinic]						
01	4		1		$2_{xy}4_{zt}^{\pm 1}, 2_{zt}$		24		—
02	4		1		$4_{zt}^{\pm 1}, 2_{zt}$		4	•	—
03	8	01-02	$\bar{1}_4$		2_{xy}		$2\perp 4$	▴	—
04	8	01		$m_{z\pm t}$		$\bar{1}_{xyz}, \bar{1}_{xyt}$	$24, m, \bar{1}$		24
05	8	02				$4\times\bar{1}_{xy\blacksquare}$	$4, \bar{1}, \bar{1}$		4
06	8	02		$4\times m_{\blacksquare}$			$4, m, m$	•	4
07	16	03-06				$4\times\bar{1}_{xy\blacksquare}$	$2\perp 4, m, m$	▴	$2\perp 4$
			VII 08 Orthogonal parallelogram (*xy*) hexagon (*zt*) *R*(2, 3, 4)-centred [hexagonal monoclinic *R*(2, 3, 4)-centred]						
01	3		1		$3_{zt}^{\pm 1}$		3	•	—
02	6	01	$\bar{1}_4$		$2_{xy}6_{zt}^{\pm 1}$		26	▴	—
03	6	01		$3\times m_{\blacktriangle}$			$3, m$	•	3
04	6	01				$3\times\bar{1}_{xy\blacktriangledown}$	$3, \bar{1}$		3
05	12	02-03				$3\times\bar{1}_{xy\blacktriangledown}$	$26, m, \bar{1}$	▴	26
			09 Orthogonal parallelogram (*xy*) hexagon (*zt*) [hexagonal monoclinic]						
01	6		1		$6_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{zt}$		6	•	—
02	6		1		$2_{xy}3_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{xy}$		$2\perp 3$		—
03	12	01-02	$\bar{1}_4$		$2_{xy}6_{zt}^{\pm 1}$		$2\perp 6$	▴	—
04	12	01		$6\times m_{\text{●}}$			$6, m, m$	•	6
05	12	01				$6\times\bar{1}_{xy\text{●}}$	$6, \bar{1}, \bar{1}$		6
06	12	02		$3\times m_{\blacktriangle}$		$3\times\bar{1}_{xy\blacktriangle}$	$2\perp 3, m$		$2\perp 3$
07	24	03-04				$6\times\bar{1}_{xy\text{●}}$	$2\perp 6, m, m$	▴	$2\perp 6$
			VIII 10 Di diclinic squares (*xy*), (*zt*) [ditetragonal diclinic]*						
01	4		1 $\bar{1}_4$		$4_{xy}^{1}4_{\gamma\delta}^{1}, 4_{xy}^{-1}4_{\gamma\delta}^{-1}$		44*	▴	—
			IX 11 Di diclinic hexagons (*xy*), (*zt*) [dihexagonal diclinic]*						
01	3		1		$3_{xy}^{1}3_{\gamma\delta}^{1}, 3_{xy}^{-1}3_{\gamma\delta}^{-1}$		33*		—
02	6	01	$\bar{1}_4$		$6_{xy}^{1}6_{\gamma\delta}^{1}, 6_{xy}^{-1}6_{\gamma\delta}^{-1}$		66*	▴	—

Table 1 (*cont.*)

Class	Order	Subgroups	PSO				WPV NOTATION		PSG$^+$
			X 12	Orthogonal rectangle (xy) square (zt) KG-centred [tetragonal orthogonal KG-centred]					
01	4		1		$m_x 4_{zt}^{\pm 1}, 2_{zt}$		$\bar{4}$	•	2
02	8	01	$\bar{1}_4$		$m_y 4_{zt}^{\pm 1}, 2_{xy}$		$2\perp\bar{4}$	▎	$2\perp 2$
03	8	01		m_z, m_t	$2_{xz\pm t}$		$\bar{4}, 2, m$	•	2, 2, 2
04	8	01			$2_{yz\pm t}$	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$\bar{4}, 2, \bar{1}$		2, 2, 2
05	16	02–03			$2_{yz\pm t}$	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$2\perp\bar{4}, 2, m$	▎	$(2, 2, 2)\otimes\bar{1}_4$
			13	Orthogonal rectangle (xy) square (zt) [tetragonal orthogonal]					
01	8		1	m_x	$m_x 4_{zt}^{\pm 1}, 4_{zt}^{\pm 1}, 2_{zt}$	$\bar{1}_{xzt}$	$\frac{4}{m}$		4
02	8		1	m_y	$m_x 4_{zt}^{\pm 1}, 2_{xy} 4_{zt}^{\pm 1}, 2_{zt}$	$\bar{1}_{yzt}$	$\frac{24}{m}$		24
03	8		1		$2_{xy} 4_{zt}^{\pm 1}, 2_{xz}, 2_{xt}, 2_{zt}, 2_{yz\pm t}$		24, 2, 2		—
04	8		1		$4_{zt}^{\pm 1}, 2_{zt}, 4\times 2_{x\blacksquare}$		4, 2, 2	•	—
05	16	01–02	$\bar{1}_4$		$m_y 4_{zt}^{\pm 1}, 2_{xy}$		$m, m, 2\perp 4$	▎	$2\perp 4$
06	16	01		$4\times m_{\blacksquare}$	$4\times 2_{x\blacksquare}$		$\frac{4}{m}, \frac{2}{m}, \frac{2}{m}$	•	4, 2, 2
07	16	02		$m_{z\pm t}$	$2_{xz}, 2_{xt}, 2_{yz\pm t}$	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$\frac{24}{m}, 2, 2$		24, 2, 2
08	16	01			$4\times 2_{y\blacksquare}$	$4\times\bar{1}_{xy\blacksquare}$	$\frac{4}{m}, 2, 2$		4, 2, 2
09	16	04	$\bar{1}_4$		$4\times 2_{y\blacksquare}, 2_{xy} 4_{zt}^{\pm 1}, 2_{xy}$		$2\perp 4, 2, 2$	▎	—
10	32	05		$4\times m_{\blacksquare}$	$4\times 2_{x\blacksquare}, 4\times 2_{y\blacksquare}$	$4\times\bar{1}_{xy\blacksquare}$	$m, m, 2\perp 4, m, m$	▎	$2\perp 4, 2, 2$
			XI 14	Orthogonal rectangle (xy) hexagon (zt) $R(2, 3, 4)$-centred [hexagonal orthogonal $R(2, 3, 4)$-centred]					
01	6		1		$m_y 6_{zt}^{\pm 1}, 3_{zt}^{\pm 1}$	$\bar{1}_{yzt}$	$\bar{3}$	•	3
02	6		1	m_x	$m_x 3_{zt}^{\pm 1}, 3_{zt}^{\pm 1}$		$\bar{6}$	•	3
03	6		1		$3_{zt}^{\pm 1}, 3\times 2_{x\blacktriangle}$		3, 2	•	—
04	12	01-02	$\bar{1}_4$		$2_{xy} 6_{zt}^{\pm 1}$		$\frac{26}{m}$	▎	26
05	12	03	$\bar{1}_4$		$2_{xy} 6_{zt}^{\pm 1}, 3\times 2_{y\blacktriangledown}$		26, 2, 2	▎	—
06	12	01		$3\times m_{\blacktriangle}$	$3\times 2_{y\blacktriangledown}$		$\bar{3}, \frac{2}{m}$	•	3, 2
07	12	01-03				$3\times\bar{1}_{xy\blacktriangledown}$	$\bar{3}, 2, \bar{1}$		3, 2
08	12	02-03		$3\times m_{\blacktriangle}$			$\bar{6}, m, 2$	•	3, 2
09	12	02			$3\times 2_{y\blacktriangledown}$	$3\times\bar{1}_{xy\blacktriangledown}$	$\bar{6}, 2, \bar{1}$		3, 2
10	24	04–05		$3\times m_{\blacktriangle}$		$3\times\bar{1}_{xy\blacktriangledown}$	$\frac{26}{m}, 2, 2$	▎	26, 2, 2
			15	Orthogonal rectangle (xy) hexagon (zt) [hexagonal orthogonal]					
01	12		1	m_x	$m_x 6_{zt}^{\pm 1}, m_x 3_{zt}^{\pm 1}, 6_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{zt}$	$\bar{1}_{xzt}$	$\frac{6}{m}$	•	6
02	12		1	m_x, m_y	$m_x 3_{zt}^{\pm 1}, m_y 3_{zt}^{\pm 1}, 2_{xy} 3_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{xy}$		$m, m, 2\perp 3$		$2\perp 3$
03	12		1		$m_x 6_{zt}^{\pm 1}, m_y 6_{zt}^{\pm 1}, 2_{xy} 3_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{xy}$	$\bar{1}_{xzt}, \bar{1}_{yzt}$	$2\perp\bar{3}$		$2\perp 3$
04	12		1		$6_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{zt}, 6\times 2_{y\bullet}$		6, 2, 2	•	—
05	12		1		$2_{xy} 3_{zt}^{\pm 1}, 3_{zt}^{\pm 1}, 2_{xy}, 3\times 2_{x\blacktriangledown}, 3\times 2_{y\blacktriangledown}$		$2\perp 3, 2$		—
06	24	01		$6\times m_{\bullet}$	$6\times 2_{x\bullet}$		$\frac{6}{m}, \frac{2}{m}, \frac{2}{m}$	•	6, 2, 2
07	24	02		$3\times m_{\blacktriangle}$	$3\times 2_{x\blacktriangle}, 3\times 2_{y\blacktriangle}$	$3\times\bar{1}_{xy\blacktriangle}$	$m, m, 2\perp 3, m$		$2\perp 3, 2$
08	24	01-02	$\bar{1}_4$		$2_{xy} 6_{zt}^{\pm 1}, m_y 6_{zt}^{\pm 1}$	$\bar{1}_{yzt}$	$m, m, 2\perp 6$	▎	$2\perp 6$
09	24	01-04				$6\times\bar{1}_{xy\bullet}$	$\frac{6}{m}, 2, 2$		6, 2, 2
10	24	03-05		$3\times m_{\blacktriangle}$		$3\times\bar{1}_{xy\blacktriangle}$	$2\perp\bar{3}, 2, \bar{1}$		$2\perp 3, 2$
11	24	04–05	$\bar{1}_4$		$2_{xy} 6_{zt}^{\pm 1}, 3\times 2_{x\blacktriangle}$		$2\perp 6, 2, 2$	▎	—
12	48	08		$6\times m_{\bullet}$	$6\times 2_{x\bullet}, 6\times 2_{y\bullet}$	$6\times\bar{1}_{xy\bullet}$	$m, m, 2\perp 6, m, m$	▎	$2\perp 6, 2, 2$
			XII 16	Di monoclinic squares (xy), (zt) [ditetragonal monoclinic]					
01	8		1 $\bar{1}_4$		$4_{xy}^{1} 4_{\gamma\delta}^{1}, 4_{xy}^{-1} 4_{\gamma\delta}^{-1}, 2_{xz}, 2_{yt}, 2_{x+yz+t}, 2_{x-yz-t}$		$44^*, 2$	▎	—
			XIII 17	Di monoclinic hexagons (xy), (zt) [dihexagonal monoclinic]					
01	6		1		$3_{xy}^{1}, 3_{\gamma\delta}^{1}, 3_{xy}^{-1} 3_{\gamma\delta}^{-1}, 2_{xz}, 2_{yt}, 2_{x-yz-t}$		$33^*, 2$		—
02	12	01	$\bar{1}_4$		$6_{xy}^{1} 6_{\gamma\delta}^{1}, 6_{xy}^{-1} 6_{\gamma\delta}^{-1}, 2_{x+yz+t}, 2_{2x-y2z-t}, 2_{x-2yz-2t}$		$2, 66^*, 2$	▎	—
			XIV 18	Di orthogonal squares (xy), (zt) $D(1, 4)(2, 3)$-centred [ditetragonal orthogonal $D(1, 4)(2, 3)$-centred]					
01	8		1 $\bar{1}_4$		$4_{xy}^{\pm 1} 4_{zt}^{\pm 1}, 2_{xy}, 2_{zt}$		44	▎	—
02	16	01		m_x, m_y	$m_{x\pm y} 4_{zt}^{\pm 1}$	$\bar{1}_{xzt}, \bar{1}_{yzt}$	$44, m, \bar{1}$	▎	44
03	16		1 $\bar{1}_4$		$4_{xy}^{\pm 1} m_{z\pm t}, m_{x\pm y} 4_{zt}^{\pm 1}, 2_{xy}, 2_{xz}, 2_{xt}, 2_{yz}, 2_{yt}, 2_{zt}$		$\bar{4}\perp\bar{4}$	▎	$(2, 2, 2)\otimes\bar{1}_4$
04	16	01			$2_{xz}, 2_{xt}, 2_{yz}, 2_{yt}, 2_{x\pm yz\pm t}$		2, 44, 2	▎	—
05	32	02-04		m_z, m_t	$4_{xy}^{\pm 1} m_{z\pm t}$	$\bar{1}_{xyz}, \bar{1}_{xyt}$	$m, 44, m$	▎	2, 44, 2

Table 1 (*cont.*)

Class	Order	Subgroups			PSO		WPV NOTATION		PSG$^+$
			19 Di orthogonal squares (xy), (zt) [ditetragonal orthogonal]						
01	16		1 $\bar{1}_4$		$2_{xy}, 2_{zt}, 4^{\pm1}_{xy}, 4^{\pm1}_{xy}2_{zt}, 4\times m_{\square}4^{\pm1}_{zt}$		$4\perp\bar{4}$	▴	$4\perp2$
02	16		1 $\bar{1}_4$		$4^{\pm1}_{xy}, 4^{\pm1}_{zt}, 4^{\pm1}_{xy}4^{\pm1}_{zt}, 4^{\pm1}_{xy}2_{zt}, 2_{xy}4^{\pm1}_{zt}, 2_{xy}, 2_{zt}$		$4\perp4$	▴	—
03	32	02		$4\times m_{\square}$	$4\times m_{\square}4^{\pm1}_{zt}$	$4\times\bar{1}_{\square zt}$	$4\perp4, m, m$	▴	$4\perp4$
04	32	01		$m_{z\pm t}$	$4^{\pm1}_{xy}m_{z\pm t}, 4\times2_{\square z}, 4\times2_{\square t}$	$\bar{1}_{xyz\pm t}$	$4\perp\bar{4}, 2, m$	▴	$2\perp4, 2, 2$
05	32	02			$16\times2_{\square\blacksquare}$		$(4\perp4)\wedge2$	▴	—
06	64	03-05		$4\times m_{\blacksquare}$	$4\times4^{\pm1}_{xy}m_{\blacksquare}$	$4\times\bar{1}_{xy\blacksquare}$	$m, m, 4\perp4, m, m$	▴	$(4\perp4)\wedge2$
			XV 20 Orthogonal square (xy) hexagon (zt) [hexagonal tetragonal]						
01	12		1		$4^{\pm1}_{xy}, 3^{\pm1}_{zt}, 4^{\pm1}_{xy}3^{\pm1}_{zt}, 2_{xy}, 2_{xy}3^{\pm1}_{zt}$		$4\perp3$		—
02	12		1		$2_{xy}, 3^{\pm1}_{zt}, 4^{\pm1}_{xy}2_{zt}, 2_{xy}3^{\pm1}_{zt}, 4^{\pm1}_{xy}6^{\pm1}_{zt}$		46		—
03	12		1		$2_{xy}, 3^{\pm1}_{zt}, 2_{xy}3^{\pm1}_{zt}, 3\times4^{\pm1}_{xy}m_{\blacktriangle}$		$\bar{4}\perp3$		$2\perp3$
04	24	03		$3\times m_{\blacktriangle}$	$4^{\pm1}_{xy}, 4^{\pm1}_{xy}3^{\pm1}_{zt}$	$3\times\bar{1}_{xy\blacktriangle}$	$\bar{4}\perp3, m$		$4\perp3$
05	24	01-02	$\bar{1}_4$		$6^{\pm1}_{zt}, 2_{zt}, 2_{xy}6^{\pm1}_{zt}$		$4\perp6$	▴	—
06	24	01			$4\times m_{\square}6^{\pm1}_{zt}$	$4\times\bar{1}_{\square zt}$	$4\perp\bar{3}$		$4\perp3$
07	24	01			$12\times2_{\square\blacktriangledown}$		$2, 2, 4\perp3$		—
08	24	01		$4\times m_{\square}$	$4\times m_{\square}3^{\pm1}_{zt}$		$m, m, 4\perp3$		$4\perp3$
09	24	02		$3\times m_{\blacktriangle}$	$3\times4^{\pm1}_{xy}m_{\blacktriangle}$	$3\times\bar{1}_{xy\blacktriangle}$	$46, m, \bar{1}$		46
10	24	02		$m_{x\pm y}$	$m_x6^{\pm1}_{zt}, m_y6^{\pm1}_{zt}, m_{x\pm y}3^{\pm1}_{zt}$	$\bar{1}_{xzt}, \bar{1}_{yzt}$	$\bar{1}, m, 46$		46
11	24	02			$3\times2_{x\blacktriangle}, 3\times2_{y\blacktriangle}, 3\times2_{x\pm y\blacktriangledown}$		$46, 2, 2$		—
12	24		1	m_x, m_y	$2_{xy}, 3^{\pm1}_{zt}, 2_{xy}3^{\pm1}_{zt}, m_x3^{\pm1}_{zt}, m_y3^{\pm1}_{zt}, 3\times4^{\pm1}_{xy}m_{\blacktriangledown}, 3\times2_{x\pm y\blacktriangledown}$		$m, 2, \bar{4}\perp3$		$2\perp3, 2$
13	24	03			$m_x6^{\pm1}_{zt}, m_y6^{\pm1}_{zt}, 3\times2_{x\pm y\blacktriangledown}$	$\bar{1}_{xzt}, \bar{1}_{yzt}$	$\bar{4}\perp\bar{3}$		$2\perp3, 2$
14	24	03	$\bar{1}_4$		$6^{\pm1}_{zt}, 2_{zt}, 2_{xy}6^{\pm1}_{zt}, 3\times4^{\pm1}_{xy}m_{\blacktriangledown}$		$\bar{4}\perp6$	▴	$2\perp6$
15	48	05		$6\times m_{\bullet}$	$6\times4^{\pm1}_{xy}m_{\bullet}$	$6\times\bar{1}_{xy\bullet}$	$4\perp6, m, m$	▴	$4\perp6$
16	48	06		$3\times m_{\blacktriangle}$	$3\times4^{\pm1}_{xy}m_{\blacktriangle}, 12\times2_{\square\blacktriangledown}$	$3\times\bar{1}_{xy\blacktriangle}$	$4\perp\bar{3}, \frac{2}{m}$		$2, 2, 4\perp3$
17	48	04-08			$12\times2_{\square\blacktriangle}$		$m, m, 4\perp3, m$		$2, 2, 4\perp3$
18	48	05-08			$4\times m_{\square}6^{\pm1}_{zt}$	$4\times\bar{1}_{\square zt}$	$m; m, 4\perp6$	▴	$4\perp6$
19	48	05-07			$12\times2_{\square\blacktriangle}$		$2, 2, 4\perp6$	▴	—
20	48	09-10			$3\times2_{x\blacktriangledown}, 3\times2_{y\blacktriangledown}, 3\times2_{x\pm y\blacktriangle}$		$\bar{1}, m, 46, m$		$46, 2, 2$
21	48	12-14			$m_x6^{\pm1}_{zt}, m_y6^{\pm1}_{zt}, 3\times2_{x\pm y\blacktriangle}$	$\bar{1}_{xzt}, \bar{1}_{yzt}$	$m, 2, \bar{4}\perp6$	▴	$2\perp6, 2, 2$
22	96	15-18			$24\times2_{\square\bullet}$		$m, m, 4\perp6, m, m$	▴	$2, 2, 4\perp6$
			XVI 21 Di orthogonal hexagons (xy), (zt) $G(2,3)$-centred [dihexagonal orthogonal $G(2,3)$-centred]						
01	6		1		$3^1_{xy}6^{-1}_{zt}, 3^{-1}_{xy}6^1_{zt}, 3^1_{xy}3^1_{zt}, 3^{-1}_{xy}3^{-1}_{zt}, 2_{zt}$		36		—
02	12	01	$\bar{1}_4$		$6^1_{xy}6^1_{zt}, 6^{-1}_{xy}6^{-1}_{zt}, 6^1_{xy}3^{-1}_{zt}, 6^{-1}_{xy}3^1_{zt}, 2_{xy}$		$36\otimes\bar{1}_4$	▴	—
03	12	01			$2_{yz}, 2_{xz\pm t}, 2_{yz+2t}, 2_{x+yt}, 2_{x+y\,2z+t}$		$36, 2, 2$		—
04	24	02-03			$2_{x-yt}, 2_{x-y2z+t}, 2_{2x+yz}, 2_{2x+yz+2t}, 2_{x+2y\,z\pm t}$		$(36, 2, 2)\otimes\bar{1}_4$	▴	—
			22 Di orthogonal hexagons (xy), (zt) RR_2-centred [di hexagonal orthogonal RR_2-centred]						
01	9		1		$3^{\pm1}_{xy}, 3^{\pm1}_{zt}, 3^{\pm1}_{xy}3^{\pm1}_{zt}$		$3\perp3$		—
02	18	01	$\bar{1}_4$		$2_{xy}6^{\pm1}_{zt}, 6^{\pm1}_{xy}2_{zt}, 6^{\pm1}_{xy}6^{\pm1}_{zt}$		$(3\perp3)\otimes\bar{1}_4$	▴	—
03	18	01		$3\times m_{\blacktriangle}$	$3\times3^{\pm1}_{xy}m_{\blacktriangle}$		$3\perp3, m$		$3\perp3$
04	18	01			$3\times6^{\pm1}_{xy}m_{\blacktriangledown}$	$3\times\bar{1}_{xy\blacktriangledown}$	$3\perp\bar{3}$		$3\perp3$
05	18	01			$9\times2_{\triangle\blacktriangle}$		$(3\perp3)\wedge2$		—
06	36	03-04	$\bar{1}_4$		$2_{xy}6^{\pm1}_{zt}, 6^{\pm1}_{xy}2_{zt}, 6^{\pm1}_{xy}6^{\pm1}_{zt}$		$\bar{3}\perp3, m$	▴	$(3\perp3)\otimes\bar{1}_4$
07	36	02-05			$9\times2_{\triangledown\blacktriangledown}$		$(3\perp3, 2)\otimes\bar{1}_4$	▴	—
08	36	03		$3\times m_{\triangle}$	$3\times m_{\triangle}3^{\pm1}_{zt}, 9\times2_{\triangle\blacktriangle}$		$m, 3\perp3, m$		$(3\perp3)\wedge2$
09	36	01		$3\times m_{\blacktriangle}$	$3\times m_{\triangledown}6^{\pm1}_{zt}, 3\times3^{\pm1}_{xy}m_{\blacktriangle}, 9\times2_{\triangledown\blacktriangledown}$	$3\times\bar{1}_{\triangledown zt}$	$\bar{3}\perp3, 2$		$(3\perp3)\wedge2$
10	36	04			$3\times m_{\triangledown}6^{\pm1}_{zt}, 9\times2_{\triangle\blacktriangle}$	$3\times\bar{1}_{\triangledown zt}$	$\bar{3}\perp\bar{3}$		$(3\perp3)\wedge2$
11	72	07-08			$3\times m_{\triangledown}6^{\pm1}_{zt}, 3\times6^{\pm1}_{xy}m_{\blacktriangledown}$	$3\times\bar{1}_{\triangledown zt}, 3\times\bar{1}_{xy\blacktriangledown}$	$(m, 3\perp3, m)\otimes\bar{1}_4$	▴	$(3\perp3, 2)\otimes\bar{1}_4$
			23 Di orthogonal hexagons (xy), (zt) [dihexagonal orthogonal]						
01	18		1		$6^{\pm1}_{xy}, 3^{\pm1}_{zt}, 6^{\pm1}_{xy}3^{\pm1}_{zt}, 3^{\pm1}_{xy}, 2_{xy}, 2_{xy}3^{\pm1}_{zt}, 3^{\pm1}_{xy}3^{\pm1}_{zt}$		$6\perp3$		—
02	36	01	$\bar{1}_4$		$6^{\pm1}_{zt}, 2_{zt}, 2_{xy}6^{\pm1}_{zt}, 6^{\pm1}_{xy}2_{zt}, 3^{\pm1}_{xy}2_{zt}, 3^{\pm1}_{xy}6^{\pm1}_{zt}, 6^{\pm1}_{xy}6^{\pm1}_{zt}$		$6\perp6$	▴	—
03	36	01			$6\times m_{\circ}6^{\pm1}_{zt}$	$6\times\bar{1}_{\circ zt}$	$6\perp\bar{3}$		$6\perp3$
04	36	01		$6\times m_{\circ}$	$6\times m_{\circ}3^{\pm1}_{zt}$		$m, m, 6\perp3$		$6\perp3$
05	36	01			$18\times2_{\circ\blacktriangle}$		$(6\perp3)\wedge2$		—
06	36	01		$3\times m_{\blacktriangledown}$	$3\times6^{\pm1}_{xy}m_{\blacktriangledown}, 3\times3^{\pm1}_{xy}m_{\blacktriangledown}$	$3\times\bar{1}_{xy\blacktriangledown}$	$6\perp3, m$		$6\perp3$
07	72	02-04			$6\times m_{\circ}6^{\pm1}_{zt}$	$6\times\bar{1}_{\circ zt}$	$6\perp6, m, m$	▴	$6\perp6$
08	72	02			$36\times2_{\circ\bullet}$		$(6\perp6)\wedge2$	▴	—
09	72	03		$3\times m_{\blacktriangledown}$	$3\times3^{\pm1}_{xy}m_{\blacktriangledown}, 3\times6^{\pm1}_{xy}m_{\blacktriangledown}, 18\times2_{\circ\blacktriangle}$	$3\times\bar{1}_{xy\blacktriangledown}$	$6\perp\bar{3}, \frac{2}{m}$		$(6\perp3)\wedge2$
10	72	04		$3\times m_{\blacktriangle}$	$3\times6^{\pm1}_{xy}m_{\blacktriangle}, 3\times3^{\pm1}_{xy}m_{\blacktriangle}, 18\times2_{\circ\blacktriangle}$	$3\times\bar{1}_{xy\blacktriangle}$	$m, m, 6\perp3, 2$		$(6\perp3)\wedge2$
11	144	07		$6\times m_{\bullet}$	$6\times6^{\pm1}_{xy}m_{\bullet}, 6\times3^{\pm1}_{xy}m_{\bullet}, 36\times2_{\circ\bullet}$	$6\times\bar{1}_{xy\bullet}$	$m, m, 6\perp6, m, m$	▴	$(6\perp6)\wedge2$
			XVII 24 Right hyperprism based on cube (yzt) KU-centred [cubic orthogonal KU-centred]						
01	12		1		$2_{yz}, 2_{yt}, 2_{zt}, 3^{\pm1}_{y\pm z\,y\pm t}$		$2, 3$	•	—
02	24	01	$\bar{1}_4$		$2_{xy}, 2_{xz}, 2_{xt}$, [26]		$(2, 3)\otimes\bar{1}_4$	▴	—
03	24	01		$m_{y\pm z}, m_{y\pm t}, m_{z\pm t}$	$m_y4^{\pm1}_{zt}, m_z4^{\pm1}_{yt}, m_t4^{\pm1}_{yz}$		$\bar{4}, 3, m$	•	$2, 3$
04	24	01			$m_x4^{\pm1}_{yz}, m_x4^{\pm1}_{yt}, m_x4^{\pm1}_{zt}$	$\bar{1}_{xyz\pm t}, \bar{1}_{xzy\pm t}, \bar{1}_{xty\pm z}$	$\bar{4}, 3, \bar{1}$		$2, 3$
05	48	02-03			$m_x4^{\pm1}_{yz}, m_x4^{\pm1}_{yt}, m_x4^{\pm1}_{zt}$	$\bar{1}_{xyz\pm t}, \bar{1}_{xzy\pm t}, \bar{1}_{xty\pm z}$	$(\bar{4}, 3, m)\otimes\bar{1}_4$	▴	$(2, 3)\otimes\bar{1}_4$

Table 1 (*cont.*)

Class	Order	Subgroups	PSO				WPV NOTATION		PSG$^+$
			25 Right hyperprism based on cube (yzt) [cubic orthogonal]						
01	24		1	m_y, m_z, m_t	$2_{yz}, 2_{yt}, 2_{zt}, 3^{\pm1}_{y\pm z\, y\pm t}, [m6]$	$\bar{1}_{yzt}$	$\frac{2}{m}, \bar{3}$	•	2, 3
02	24		1	m_x	$2_{yz}, 2_{yt}, 2_{zt}, 3^{\pm1}_{y\pm z\, y\pm t}, m_x 3^{\pm1}_{y\pm z\, y\pm t}$	$\bar{1}_{xyz}, \bar{1}_{xyt}, \bar{1}_{xzt}$	$(2,3)\perp m$		2, 3
03	24		1		$4\times 2_{y\blacksquare}, 2_{zt}, 2_{zy\pm t}, 2_{ty\pm z}, 4^{\pm1}_{yz}, 4^{\pm1}_{yt}, 4^{\pm1}_{zt}, 3^{\pm1}_{y\pm z\, y\pm t}$		4, 3, 2	•	—
04	24		1		$2_{yz}, 2_{yt}, 2_{zt}, 2_{xy\pm z}, 2_{xy\pm t}, 2_{xz\pm t}$, $2_{xy}4^{\pm1}_{zt}, 2_{xz}4^{\pm1}_{yt}, 2_{xt}4^{\pm1}_{yz}, 3^{\pm1}_{y\pm z\, y\pm t}$		24, 3, 2		—
05	48	01-02	$\bar{1}_4$		$2_{xy}, 2_{xz}, 2_{xt}, [26]$		$\left(\frac{2}{m}, \bar{3}\right)\perp m$	ı	$(2,3)\otimes\bar{1}_4$
06	48	03-04	$\bar{1}_4$		$2_{xy}, 2_{xz}, 2_{xt}, [26]$		$(4,3,2)\otimes\bar{1}_4$	ı	—
07	48	01-03		$m_{y\pm z}, m_{y\pm t}, m_{z\pm t}$	$m_y 4^{\pm1}_{zt}, m_z 4^{\pm1}_{yt}, m_t 4^{\pm1}_{yz}$		$\frac{4}{m}, \bar{3}, \frac{2}{m}$	•	4, 3, 2
08	48	01-04			$m_x 4^{\pm1}_{yz}, m_x 4^{\pm1}_{yt}, m_x 4^{\pm1}_{zt}$	$\bar{1}_{xyz\pm t}, \bar{1}_{xzy\pm t}, \bar{1}_{xty\pm z}$	$\frac{24}{m}, \bar{3}, \bar{1}$		24, 3, 2
09	48	02-04		$m_{y\pm z}, m_{y\pm t}, m_{z\pm t}$	$m_y 4^{\pm1}_{zt}, m_z 4^{\pm1}_{yt}, m_t 4^{\pm1}_{yz}$		$(\bar{4}, 3, m)\perp m$		24, 3, 2
10	48	02-03			$m_x 4^{\pm1}_{yz}, m_x 4^{\pm1}_{yt}, m_x 4^{\pm1}_{zt}$	$\bar{1}_{xyz\pm t}, \bar{1}_{xzy\pm t}, \bar{1}_{xty\pm z}$	$(4,3,2)\perp m$		4, 3, 2
11	96	06-07-10					$\left(\frac{4}{m}, \bar{3}, \frac{2}{m}\right)\perp m$	ı	$(4,3,2)\otimes\bar{1}_4$
			$[26] = 2_{xy-z-t}6^{\pm1}_{y+z\, y+t}, 2_{xy+z+t}6^{\pm1}_{y-z\, y-t}, 2_{xy-z+t}6^{\pm1}_{y+z\, y-t}, 2_{xy+z-t}6^{\pm1}_{y-z\, y+t}$						
			$[m6] = m_{y-z-t}6^{\pm1}_{y+z\, y+t}, m_{y+z+t}6^{\pm1}_{y-z\, y-t}, m_{y-z+t}6^{\pm1}_{y+z\, y-t}, m_{y+z-t}6^{\pm1}_{y-z\, y+t}$						
			XVIII 26 Di isosquares (xz) (yt) [monoclinic octagonal]						
01	8		1 $\bar{1}_4$		$8^1_{AB}8^3_{CD}, 8^3_{AB}8^1_{CD}, 8^{-1}_{AB}8^{-3}_{CD}, 8^{-3}_{AB}8^{-1}_{CD}, 4^1_{AB}4^{-1}_{CD}, 4^{-1}_{AB}4^1_{CD}$		88	ı	—
02	16	01			$2_{x-y\, z+t}, 2_{x+y\, z-t}, 2_{x+t\, y+z}, 2_{x-t\, z-y}, 2_{zy+t}, 2_{xy-t}, 2_{yx+z}, 2_{tx-z}$		$88\wedge 2$	ı	—
			$A = t+(\sqrt{2}/2)(x-z)$ $B = -y+(\sqrt{2}/2)(x+z)$ $C = t-(\sqrt{2}/2)(x-z)$ $D = y+(\sqrt{2}/2)(x+z)$						
			XIX 27 Di particular monoclinic isorhombus (xy), (zt) [decagonal]						
01	5		1		$5^1_{AB}5^{-2}_{CD}, 5^{-1}_{AB}5^2_{CD}, 5^2_{AB}5^1_{CD}, 5^{-2}_{AB}5^{-1}_{CD}$		55		—
02	10	01	$\bar{1}_4$		$10^3_{AB}10^{-1}_{CD}, 10^{-1}_{AB}10^{-3}_{CD}, 10^1_{AB}10^{-3}_{CD}, 10^{-3}_{AB}10^1_{CD}$		1010	ı	—
03	10	01			$2_{x-ty-z}, 2_{x+2y+2tz-t}, 2_{2x+z+2t\, y-t}$, $2_{2x+2z+tx-y}, 2_{2x+y+2t\, x-z}$		$55\wedge 2$		—
04	20	02-03			$2_{xz+t}, 2_{yx+z}, 2_{zy+t}, 2_{tx+y}, 2_{x+t\, y+z}$		$1010\wedge 2$	ı	—
			$A = \frac{1}{2}y+z+t-\beta(x-z)$ $B = +\gamma y+\delta(x+y+z)$ $C = \frac{1}{2}y+z+t-\alpha(x-z)$ $D = -\gamma(x+y+z)+\delta y$						
			$\alpha = \cos 4\pi/5$ $\gamma = \sin 4\pi/5$ $\beta = \cos 2\pi/5$ $\delta = \sin 2\pi/5$						
			XX 28 Di isohexagons (xz), (yt) monoclinic [dodecagonal]						
01	12		1 $\bar{1}_4$		$12^1_{AB}12^5_{CD}, 12^{-1}_{AB}12^{-5}_{CD}, 12^5_{AB}12^1_{CD}, 12^{-5}_{AB}12^{-1}_{CD}$, $6^1_{xz}6^{-1}_{ty}, 6^{-1}_{xz}6^1_{ty}, 3^1_{xz}3^{-1}_{ty}, 3^{-1}_{xz}3^1_{ty}, 4^1_{xy}4^1_{zt}, 4^{-1}_{xy}4^{-1}_{zt}$		1212	ı	—
02	24	01			$2_{x+z\, y-t}, 2_{x-z\, y+t}, 2_{z+t\, x-y-t}, 2_{t-z\, x+y+z}, 2_{x+t\, y+z}, 2_{x-t\, y-z}$, $2_{x+y\, x+z-t}, 2_{x-y\, x+z+t}, 2_{x\, y+2t}, 2_{y\, 2x+z}, 2_{z\, 2y+t}, 2_{t\, 2x+z}$		$1212\wedge 2$	ı	—
			$A = \frac{1}{2}y+t-(\sqrt{3}/2)x$ $B = -\frac{1}{2}x-(\sqrt{3}/2)y-z$ $C = (\sqrt{3}/2)x+\frac{1}{2}y+t$ $D = -\frac{1}{2}x+(\sqrt{3}/2)y-z$						

of the highest symmetry in the system (*cf.* Table 1, first column).

I. Names of the crystal systems

In Table 1 we indicate between parentheses in the fourth column the name given to each of the 23 crystal families by Wondratschek, Bülow & Neubüser (1971); for instance, family XV is called hexagonal tetragonal.

For each family we propose a name much more relevant to the geometry of the crystal cell. For instance, let (x, y, z, t) denote a vector basis for the cell of family XV; the matrix of the quadratic form is

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & b & b/2 \\ 0 & 0 & b/2 & b \end{pmatrix},$$

*i.e.**

$$x^2 = y^2 = a$$
$$z^2 = t^2 = b$$
$$zt = b/2$$
$$xy = yz = xz = xt = yt = 0.$$

Therefore we call it orthogonal square (xy) hexagon (zt).

II. Geometric symbols and list of elements for each PSG

Table 1 gives a list of all elements belonging to each point group: rotations $(2, 43, \ldots)$, mirrors (m), inversions $(\bar{1})$, rotation-reflections $(m3 = \bar{6}, \ldots)$. In addition some subgroups are indicated in most cases (third column) and in the case of a PSG$^-$ the corresponding

* xy indicates the scalar product of the vectors x and y.

PSG^+ is indicated* (seventh column). The second column gives the order of the PSG.

The study of these elements leads us to propose a generalized geometric symbol suitable for the Hermann-Mauguin notation for the PSG in $\mathbb{E}^3$. It will be noticed that the same symbol, except for additional commas, is assigned to both a PSG in $\mathbb{E}^3$ and the polar group (Weigel & Veysseyre, 1982) it generates in $\mathbb{E}^4$. These 32 polar groups in $\mathbb{E}^4$ are identified by a filled circle • in column 6 of Table 1; for instance IV 04-02 is denoted by $\frac{2}{m}$. In the same column, PSGs containing $\bar{1}_4$ (total *homothetie* -1 in $\mathbb{E}^4$) are identified with the symbol ▲. These PSGs are the leaders of Friedel–Laue classes.

For the symbols in $\mathbb{E}^4$ commas are of major importance; for instance, they make a clear distinction between the cyclic group 26 of order 6 generated by the double rotation $2_{xy}6^1_{zt}$ (08-02) and the group 6,2,2 of order 12 (15-04) where double rotations 26 do not exist, but where we find $k\frac{2\pi}{6}$ and π rotations that do not exist in 26.

We made as much effort as possible to comply with the conventions of Hermann–Mauguin notation in $\mathbb{E}^3$ to the full extent of its capabilities. For instance, in our notation 46,m,$\bar{1}$ (20-09), m and $\bar{1}$ stand beside the 6: this means that there exist three mirror hyperplanes (m) and three inversion axes ($\bar{1}$). On the other hand, in our notation $\bar{1}$,m,46 (20-10), since m and $\bar{1}$ stand beside the 4 then there exist two mirror hyperplanes and two inversion axes.

Consider the group 20-02 (12 elements): it is generated by the rotation $4^{+1}_{xy}6^{+1}_{zt}$. Therefore we denote it by the symbol 46. Consider now the group 14-07 (12 elements): it is built up with the group $\bar{3}$ (or 14-01), three rotations 2 and three inversions $\bar{1}$. Therefore we denote it by the symbol $\bar{3}$,2,$\bar{1}$.

At this point three new symbols need to be defined:

(a) *Symbol* $\perp$. Some PSGs may be generated by two rotations of equal or different angles in two supplementary orthogonal planes of $\mathbb{E}^4$. Such is the case for PSG 03-02 denoted by $2\perp2$, or PSG 20-01 denoted by $4\perp3$. The PSG 09-03 denoted by $2\perp6$ is generated by a rotation 2_{xy} *and* a rotation 6^1_{zt}. Its 12 elements are then

$$1, \bar{1}_4, 2_{xy}, 6^{\pm1}_{zt}, 3^{\pm1}_{zt}, 2_{xy}6^{\pm1}_{zt}, 2_{xy}3^{\pm1}_{zt}, 2_{zt}.$$

We note that $2\perp6$ contains the cyclic group 26.

The second PSG of the system 06 is denoted by $(2,2,2)\perp m$ since the mirror is the hyperplane containing the three planes of rotation 2. This PSG contains eight elements:

$$1, 2_{xy}, 2_{yz}, 2_{xz}, m_t, \bar{1}_{xyt}, \bar{1}_{yzt}, \bar{1}_{xzt}$$

since the product of rotation 2_{xy} and reflection m_t leads to inversion $\bar{1}_{xyt}$ around the inversion axis z.

(b) *Symbol* $\otimes$. This represents the direct product, in its mathematical meaning of two subgroups (see Appendix 1). For instance, PSG 21-02 denoted by $36\otimes\bar{1}_4$ is the direct product of the two subgroups 36 and $\bar{1}_4$.

(c) *Symbol* $\wedge$. This indicates a semi-direct product (see Appendix 1) in the case where this mathematical symbol proves itself simpler and more concrete than the pure geometrical symbol. For instance, PSG 19-05 is denoted by $(4\perp4)\wedge\bar{2}$. In the same way PSG 30-11 is denoted by $(6\perp6)\wedge\bar{4}$.

A full list of PSOs has been established for the PSGs of systems 29, 30, 31, 32 and 33; owing to the space required this is not reported in this paper.* For this reason Table 2 only indicates the PSGs together with their geometric symbols (column 4), some subgroups (column 3) and, in the case of a PSG^-, the corresponding PSG^+ (column 6). PSGs containing $\bar{1}_4$ are identified with the symbol ▲ in the fifth column.

III. Degenerate PSOs, PSGs and crystal systems

1. *Degenerate PSOs*

Definition (Weigel, Veysseyre, Phan, Effantin & Billiet, 1984): A PSO is degenerate if its characteristic polynomial has multiple roots. It is fully degenerate either if it has only one root of order n in a space of dimension n or if it has a pair, in the form $[\exp(i\theta), \exp(-i\theta)]$, of complex roots each of order m, in a space of dimension $2m$. In any other circumstances, the PSO is only partly degenerate.

Examples

	Fully degenerate PSOs	Partly degenerate PSOs
$\mathbb{E}^1$	—	
$\mathbb{E}^2$	1, 2	
$\mathbb{E}^3$	1, $\bar{1}$	m, 2
$\mathbb{E}^4$	1, $\bar{1}_4$, 4^14^1, 3^13^1, 6^16^1	$\bar{1}$, m, 2, 3, 4, 6
$\mathbb{E}^5$	1, $\bar{1}_5$	4^14^1, 3^13^1
$\mathbb{E}^6$	1, $\bar{1}_6$, $4^14^14^1$, $3^13^13^1$, $6^16^16^1$	3^13^1

In $\mathbb{E}^4$, 4^14^1 and 4^14^{-1} are fully degenerate, 8^18^3 and 12^112^5 are not degenerate. If it was a PSO, 8^18^{-1} should be degenerate.

*Remember that the PSG^+ related to a PSG is defined as its subgroup containing all the rotations or $PSOs^+$ (Weigel, Veysseyre, Phan, Effantin & Billiet, 1984).

* A full list of PSOs for the PSGs of systems 29, 30, 31, 32 and 33 have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP43869 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Notations of the* 66 *crystallographic PSGs of the families* XX *to* XXIII

This table contains three subtables corresponding to the families XXI, XXII, XXIII and to five systems; in this table we have suppressed the column giving the elements of each PSG; the other columns are unchanged.

Class	Order	Subgroups	WPV notation		PSG$^+$
XXI 29	Di isohexagons (xy), (zt) orthogonal RR_2-centred [di isohexagonal RR_2-centred]				
01	18		$36, 3\perp3$		—
02	36	01	$(36, 3\perp3)\otimes\bar{1}_4$	▲	—
03	36	01	$(36, 3\perp3)\wedge2$		—
04	36		$(3\perp3)\wedge\bar{4}$		$(3\perp3)\wedge2$
05	72	02-03	$[(36, 3\perp3)\wedge2]\otimes\bar{1}_4$	▲	—
06	72	04	$[(3\perp3)\wedge\bar{4}]\otimes\bar{1}_4$	▲	$[(3\perp3)\wedge2]\otimes\bar{1}_4$
07	72	03-04	$\bar{4}(m, 3\perp3, m)\bar{4}$		$(36, 3\perp3)\wedge2$
08	72	03	$\bar{4}(\bar{3}\perp\bar{3})\bar{4}$		$(36, 3\perp3)\wedge2$
09	144	05-06-07	$[\bar{4}(m, 3\perp3, m)\bar{4}]\otimes\bar{1}_4$	▲	$[(36, 3\perp3)\wedge2]\otimes\bar{1}_4$
30	Di isohexagons (xy), (zt) orthogonal [di isohexagonal orthogonal]				
01	12		$66^*, 44^*$	▲	—
02	24		$1212, 44^*$	▲	—
03	24		$1212, 36$	▲	—
04	24	01	$(66^*, 44^*)\wedge2$	▲	—
05	36	01	$1212, 3\perp3$	▲	—
06	48	02-03	$36, 1212, 44^*$	▲	—
07	72		$1212, 6\perp6$	▲	—
08	72		$1212, 3\perp3, 36$	▲	—
09	72	05	$1212, 3\perp3, 1212$	▲	—
10	144	07-08-09	$1212, 6\perp6, 1212$	▲	—
11	144		$(6\perp6)\wedge\bar{4}$	▲	$(6\perp6)\wedge2$
12	144	09	$(m, 3\perp3, m)1212$	▲	$1212, 3\perp3, 1212$
13	288	10-11-12	$(m, m, 6\perp6, m, m)1212$	▲	$1212, 6\perp6, 1212$
XXII 31	Particular rhombotope $\cos\alpha = -\frac{1}{4}$[icosahedral]				
01	20		$55, \bar{4}$		$2, 55, 2$
02	40		$\bar{4}, 1010, \bar{4}$	▲	$2, 1010, 2$
03	60		$(2, 3)55$		—
04	120	03	$(\bar{4}, 3, m)55$		$(2, 3)55$
05	120	03	$(\bar{4}, 3, \bar{1})55$		$(2, 3)55$
06	120	03	$(2, 3)1010$	▲	—
07	240	04-05-06	$(\bar{4}, 3, m)1010$	▲	$(2, 3)1010$
XXIII 32	**Hypercubic**				
01	8		$44^*, 44^*, 44^*$	▲	—
02	16		$88, 88$	▲	—
03	16	01	$44^*, 88, 44^*$	▲	—
04	16	01	$44^*, 44, 44^*$	▲	—
05	24	01	$44^*, 3$	▲	—
06	32	02-04	$44^*, 88, 88, 44^*$	▲	—
07	32	02	$88, 44, 88$	▲	—
08	32	02	$88, 4\perp4$	▲	—
09	32		$44^*(\bar{4}\perp\bar{4})44^*$	▲	$2, 44, 2$
10	32	04	$44, 44$	▲	—
11	48	03-05	$88, 3$	▲	—
12	64	06-07-08-10	$88, 4\perp4, 88$	▲	—
13	64	07	$88, \bar{4}\perp\bar{4}, 88$	▲	$88, 44, 88$
14	64	10	$44(m, 44, m)44$	▲	$44, 44$
15	64		$\bar{4}(4\perp4)\bar{4}$	▲	$(4\perp4)\wedge2$
16	96	10	$(2, 3)44$	▲	—
17	128	12-13-14-15	$(88, 4\perp4, 88)\wedge m$	▲	$88, 4\perp4, 88$
18	192	16	$\left(\frac{2}{m}, \bar{3}\right)44$	▲	$(2, 3)44$
19	192	16	$(\bar{4}, 3, m)44$	▲	$(2, 3)44$
20	192	11-12-16	$(4, 3, 2)88$	▲	—
21	384	20	$\left(\frac{4}{m}, \bar{3}, \frac{2}{m}\right)88$	▲	$(4, 3, 2)88$

Table 2 (*cont.*)

Class	Order	Subgroups	WPV notation		PSG⁺
	33 Hypercubic *z*-centred				
1	24		1212, 1212	▲	—
2	24		1212, 88	▲	—
3	24		66*, 44*, 66*	▲	—
4	48	01–02	$(1212, 88)\wedge 2$	▲	—
5	48	03	1212, 44, 1212	▲	—
6	48	03	88, 66*	▲	—
7	72	01–03	1212, 3, 1212	▲	—
8	96	01	1212, 1212, 1212	▲	—
9	96	05–06	1212, 88, 66*	▲	—
10	96	05	$1212, 4\perp 4$	▲	—
11	144	04–07	(2, 3)88	▲	—
12	192	04–08	$1212, 4\perp 4, 1212$	▲	—
13	288	08	(2, 3)1212	▲	—
14	576	13	$(\bar{4}, 3, m)1212$	▲	(2, 3)1212
15	576	13	(4, 3, 2)1212	▲	—
16	1152	14–15	$\left(\frac{4}{m}, \bar{3}, \frac{2}{m}\right)1212$	▲	(4, 3, 2)1212

2. *Fully degenerate PSGs*

Definition: A PSG is fully degenerate whenever any of its PSOs is fully degenerate.

Examples

$\mathbb{E}^1$: none $\quad$ $\mathbb{E}^4$: $1, \bar{1}_4, 44^\star, 33^\star, 66^\star$

$\mathbb{E}^2$: $1, 2$ $\quad$ $\mathbb{E}^5$: $1, \bar{1}_5$

$\mathbb{E}^3$: $1, \bar{1}$ $\quad$ $\mathbb{E}^6$: $1, \bar{1}_6, 444^\star, 333^\star, 666^\star$

In $\mathbb{E}^4$ we mark with a star * the symbols of fully degenerate PSGs (excluding 1 and $\bar{1}_4$). It can be noticed that $44^\star,2$ is not fully degenerate since it contains 2_{xy} which is not a fully degenerate PSO in $\mathbb{E}^4$. In such a case the star only applies to part of the symbol.

3. *Fully degenerate crystal systems*

Definition: A crystal system is called degenerate if any PSG belonging to it is fully degenerate.

Examples

$\mathbb{E}^1$: none

$\mathbb{E}^2$: oblique (or parallelogram)

$\mathbb{E}^3$: triclinic

$\mathbb{E}^4$: hexaclinic: 1 and $\bar{1}_4$

di diclinic squares: $44^\star$

di diclinic hexagons: $33^\star$ and $66^\star$

Property: A fully degenerate crystal system has no edge or face of its Bravais-type cells whose direction can be defined uniquely.

Nevertheless, by adding a convention we can define a classical lattice. First, let us examine two examples of fully degenerate crystal systems:

(*a*) *Oblique in* $\mathbb{E}^2$. There is an infinite number of possibilities for determining the Bravais-type cells associated with the parallelogram of the crystal lattice shown in Fig. 1. But the parallelogram drawn with the continuous line is the conventional Bravais-type cell: as a matter of fact, among all possible parallelograms it differs in that its angles are closest to right angles.

(*b*) *Crystal system* 10: *di diclinic squares in* $\mathbb{E}^4$. The matrix associated with the quadratic form of the system 10 is

$$\begin{pmatrix} a & 0 & c & d \\ 0 & a & -d & c \\ c & -d & b & 0 \\ d & c & 0 & b \end{pmatrix}.$$

One can note that

$$x^2 = y^2 = a \qquad xz = yt = c$$
$$z^2 = t^2 = b \qquad xt = -yz = d$$
$$xy = zt = 0.$$

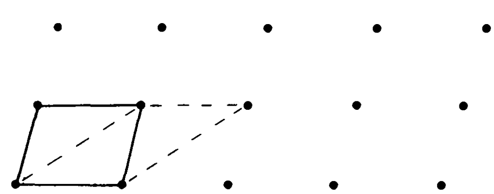

Fig. 1. An example of the Bravais type of cell associated with the parallelogram of the crystal lattice.

We call this system di diclinic squares (xy), (zt), since the two planes xy and zt of the two squares are not orthogonal and their four angles depend on two angular parameters c and d. More generally we can find an infinite number of pairs of diclinic squares for defining the Bravais cell of a crystal in $\mathbb{E}^4$ and belonging to this crystal system 10 (see Appendix 2). The elements of the PSG 10-01, 44* are 1, $\bar{1}_4$ and two rotations $4^1_{xy}4^1_{\gamma\delta}$, $4^{-1}_{xy}4^{-1}_{\gamma\delta}$, with

$$\gamma = [a(ab - c^2 - d^2)]^{-1/2}(-cx + dy + az),$$
$$\delta = [a(ab - c^2 - d^2)]^{-1/2}(-dx - cy + at),$$

the basis $(xa^{-1/2}, ya^{-1/2}, \gamma, \delta)$ being orthonormal. We cannot denote these elements by $4^1_{xy}4^1_{zt}$ since the planes xy and zt are not orthogonal. Furthermore the vectors γ and δ are not elements of the crystal translation group and so we cannot choose them to define the Bravais-type cells of this system 10.

On the contrary the system 16, called di monoclinic squares, is neither a fully nor a partly degenerate system and the squares belong to well defined planes because the PSG 44*,2 of this system contains the rotations 2_{xy} and 2_{zt} in the well defined planes xy and zt. The matrix of the quadratic form is

$$\begin{pmatrix} a & 0 & c & 0 \\ 0 & a & 0 & c \\ c & 0 & b & 0 \\ 0 & c & 0 & b \end{pmatrix}$$

in (x, y, z, t) and

$$\begin{pmatrix} \begin{matrix} a & c \\ c & b \end{matrix} & 0 \\ 0 & \begin{matrix} a & c \\ c & b \end{matrix} \end{pmatrix}$$

in (x, z, y, t). In the basis (x, z, y, t) we have then found two equal orthogonal parallelograms. So another possible name for the crystal system 16 is di iso orthogonal parallelograms (xz), (yt).

IV. Cyclic groups

Any PSG denoted by only one symbol is cyclic, except 44 (*i.e.* 18-01). For instance $\bar{3}$ is the cyclic group of order 6 generated by $m_y 6^1_{zt}$.

Consider now the PSG 28-01 denoted by 1212. It is a cyclic group of order 12 generated by $g = 12^1_{AB}12^5_{CD}$. Its successive powers are $g^2 = 6^1_{AB}6^{-1}_{CD}$, $g^3 = 4^1_{AB}4^1_{CD}$, $g^4 = 3^1_{AB}3^{-1}_{CD}$, $g^5 = 12^5_{AB}12^1_{CD}$, $g^6 = \bar{1}_4$, $g^7 = 12^{-5}_{AB}12^{-1}_{CD}, \ldots$.

We notice that only powers of first, fifth, seventh and eleventh order yield double rotations in two perfectly characterized orthogonal planes. All remaining powers yield fully degenerate double rotations. Considering the six PSOs g^2, g^3, g^4, g^8, g^9 and g^{10}, one can easily show that the couples of planes (AB, CD) and $(xz, y't')$* consist of two particular couples among the family of orthogonal couples of planes adequate for these fully degenerate rotations. Therefore it can be proved, for instance, that $g^2 = 6^1_{AB}6^{-1}_{CD} = 6^1_{xz}6^{-1}_{t'y'}$.

44 is the only non-cyclic group denoted by only one symbol. Its only elements are: $4^{\pm 1}_{xy}4^{\pm 1}_{zt}$, 2_{xy}, 2_{zt}, $\bar{1}_4$ and 1. It is the direct product of 44* and 2.

On the other hand multi-symbol PSGs may be cyclic, such as, for instance, $2\perp 3$ and $4\perp 3$; these two PSGs could be denoted by 23 and 43 (since 2 and 3 on the one hand, and 4 and 3 on the other hand are prime) but such notation would be confusing with PSG 23 in $\mathbb{E}^3$.

However, 46 and $4\perp 6$ are different: 46 is cyclic and $4\perp 6$ includes both 46 and the rotation 2_{zt}.

Concluding remarks

Among the various examples of the crystallographic PSGs of four-dimensional space, special consideration should be given to the point groups for structured magnetic configurations on one hand and to point groups for the incommensurate phases with one only internal dimension on the other hand.

From this point of view, it is of major interest to rely on unified geometric symbols taking into account the 227 PSGs in $\mathbb{E}^4$ and consistent with both approaches, the former leading to magnetic symbols (Bradley & Cracknell, 1972) and the latter leading to the symbols for 'incommensurate groups' in $\mathbb{E}^4$ (de Wolff, Janssen & Janner, 1981); incommensurate groups are groups of $\mathbb{E}^4$ which describe incommensurate phases of physical space in their superspace $\mathbb{E}^4$.

The purpose of this article was to emphasize the 'WPV' symbols. In a further paper, we shall give the correspondence between our symbols and the magnetic symbols on one hand and the symbols for incommensurate phases on the other hand.

In addition we shall devote a further article to extensively detailing the geometry of the parallelotopes related to the 33 crystal system cell types and of some polytopes inscribed in these types of cells.

APPENDIX 1

The group G is said to be the *direct product* of the two subgroups H and K and we write $G = H \otimes K$ if the following three properties are true:

(1) For any element h_i of H and for any element k_j of K we have $h_i * k_j = k_j * h_i$ where $*$ is the symbol of the group operation.

(2) Any element of G can be written $g = h_i * k_j$ where h_i belongs to H and k_j to K.

* $y' = 2bx + 3ay + 4bz$, $t' = 2bx - ay - 2at$ with $a = x^2 = y^2 = z^2 = t^2$; $b = xt = -yz$.

(3) Only the element identity of G is common to H and K.

Hence it follows that H and K are normal subgroups of G and the factorization of any element of G is unique.

The group G is said to be the *semi-direct product* of the two subgroups H and K and we write $G = H \wedge K$ if the following three properties are verified:

(1) For any element k_i of K we have

$$k_i * H = H * k_i.$$

(2), (3) The properties (2) and (3) above are unchanged.

Hence it follows that H is a normal subgroup of G and the factorization of any element of G is unique. (Altmann, 1963*a*, *b*).

Remark: the direct product of two subgroups is commutative but the semi-direct product is not commutative.

APPENDIX 2

Bravais cell types of degenerate crystal system 10

As mentioned in the text (§ III) it is possible to find an infinite number of pairs of diclinic squares for defining the Bravais cell of a crystal in $\mathbb{E}^4$ belonging to the crystal system 10.

A plane in $\mathbb{E}^4$ is defined by two independent vectors so that we can write

$$V_1 = A_1x + B_1y + C_1z + D_1t$$
$$V_1' = A_1'x + B_1'y + C_1'z + D_1't$$

for the first plane and

$$V_2 = A_2x + B_2y + C_2z + D_2t$$
$$V_2' = A_2'x + B_2'y + C_2'z + D_2't$$

for the second one.

From these relations and the results of § III, we obtain

$$\begin{aligned} V_1 . V_1' &= (A_1x + B_1y + C_1z + D_1t) \\ &\quad \times (A_1'x + B_1'y + C_1'z + D_1't) \\ &= (A_1A_1' + B_1B_1')a + (C_1C_1' + D_1D_1')b \\ &\quad + c(A_1'C_1 + B_1'D_1 + A_1C_1' + B_1D_1') \\ &\quad + d(A_1'D_1 - B_1'C_1 + A_1D_1' - B_1C_1'), \end{aligned}$$

$$\begin{aligned} V_1^2 &= (A_1^2 + B_1^2)a + (C_1^2 + D_1^2)d \\ &\quad + 2[c(A_1C_1 + B_1D_1) + d(A_1D_1 - B_1C_1)], \end{aligned}$$

$$\begin{aligned} V_1'^2 &= (A_1'^2 + B_1'^2)a + (C_1'^2 + D_1'^2)d \\ &\quad + 2[c(A_1'C_1' + B_1'D_1') + d(A_1'D_1' - B_1'C_1')], \end{aligned}$$

and similar relations for $V_2 . V_2'$, V_2^2, $V_2'^2$.

The condition $V_1 V_1' = 0$ must be true for all possible values of a, b, c and d, and as a result

$$A_1A_1' + B_1B_1' = 0$$
$$A_1'C_1 + B_1'D_1 + A_1C_1' + B_1D_1' = 0$$
$$C_1C_1' + D_1D_1' = 0$$
$$A_1'D_1 - B_1'C_1 + A_1D_1' - B_1C_1' = 0,$$

from which it follows that

$$A_1' = k_1B_1 \qquad C_1' = k_1D_1$$
$$B_1' = -k_1A_1 \qquad D_1' = -k_1C_1$$

where k_1 is a real non-zero number. Then the condition $V_1^2 = V_2^2$ implies $k_1^2 = 1$. The same relation holds, of course, for the vectors V_2 and V_2'.

The pair of planes which contain squares is now defined by the vectors

$$V_1 = A_1x + B_1y + C_1z + D_1t$$
$$V_1' = k_1(B_1x - A_1y + D_1z - C_1t)$$

and

$$V_2 = A_2x + B_2y + C_2z + D_2t$$
$$V_2' = k_2(B_2x - A_2y + D_2z - C_2t)$$

where $k_1^2 = 1$ and $k_2^2 = 1$.

We next determine the numbers k_1 and k_2. After an easy calculation, we obtain

$$V_1'V_2' = k_1k_2V_1V_2$$
$$k_2V_1'V_2 = -k_1V_1V_2'.$$

The properties $V_1V_2 = V_1'V_2'$ and $V_1V_2' = -V_1'V_2$ of the matrix associated with the quadratic form of the system 10 require the conditions

$$k_1k_2 = 1 \qquad \text{and} \qquad k_2 = k_1;$$

that is, $k_1 = k_2 = 1$ or $k_1 = k_2 = -1$.

As pointed out above, we conclude that there exists an infinite number of pairs of diclinic squares belonging to the crystal system 10 which are in the planes

$$V_1 = A_1x + B_1y + C_1z + D_1t$$
$$V_1' = k(B_1x - A_1y + D_1z - C_1t)$$
$$V_2 = A_2x + B_2y + C_2z + D_2t$$
$$V_2' = k(B_2x - A_2y + D_2z - C_2t),$$

with the condition $k = 1$ or $k = -1$.

If we choose all the coefficients A, B, C, D as integers the vectors V_1, V_1', V_2 and V_2' belong to the space group of system 10, and so define the infinite number of possible Bravais cells of this degenerate crystal system.

References

ALTMANN, S. L. (1963*a*). *Philos. Trans. R. Soc. London Ser. A*, **255**, 216–240.

ALTMANN, S. L. (1963*b*). *Rev. Mod. Phys.* **35**, 641-645.
BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids.* Oxford: Clarendon Press.
VEYSSEYRE, R., PHAN, T. & WEIGEL, D. (1985). *C.R. Acad. Sci.* **300**, 51-54.
VEYSSEYRE, R., WEIGEL, D., PHAN, T. & EFFANTIN, J. M. (1984). *Acta Cryst.* **A40**, 331-337.
WEIGEL, D., PHAN, T. & VEYSSEYRE, R. (1984). *C.R. Acad. Sci.* **298**, 825-828.
WEIGEL, D. & VEYSSEYRE, R. (1982). *C.R. Acad. Sci.* **295**, 317-322.
WEIGEL, D., VEYSSEYRE, R., PHAN, T., EFFANTIN, J. M. & BILLIET, Y. (1984). *Acta Cryst.* **A40**, 323-330.
WHITTAKER, E. J. W. (1984). *Acta Cryst.* **A40**, 404-410.
WOLFF, P. M. DE, JANSSEN, T. & JANNER, A. (1981). *Acta Cryst.* **A37**, 625-636.
WONDRATSCHEK, H., BÜLOW, R. & NEUBÜSER, J. (1971). *Acta Cryst.* **A27**, 523-535.

Acta Cryst. (1987). **A43**, 304-316

Extinction in the Framework of Transfer Equations for General-Type Crystals

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Abstract

An improvement of the classical theory of extinction in mosaic crystals is made by starting from the energy transfer equations valid for a general-type crystal according to Zachariasen's [*Acta Cryst.* (1967), **23**, 558-564] classification. Within the assumption that only the integrated intensity of the diffraction peak is needed, the equations are first simplified and then solved. The result obtained for the extinction factor is similar to that of Becker & Coppens [*Acta Cryst.* (1974), **A30**, 129-147], but two new parameters appear if the crystal is not of type I. One of them, determining the peculiarity of the transfer equations, gives differences in the extinction factor not greater than 8%. The other, representing the ratio of the kinematical cross-section strengths along the diffracted and incident beams, gives differences up to 50%. For crystals of ellipsoidal shape, empirical formulae appropriate for structure refinement programs are proposed.

1. Introduction

In this paper we re-analyse the problem of secondary extinction in the framework of classical transfer theory. The transfer equations for secondary extinction in finite crystals were first written by Hamilton (1957) and were based on the mosaic model of Darwin (1922) for the ideal imperfect crystal. Zachariasen (1967) has used similar equations to describe extinction in real crystals, so henceforth we will call these equations Hamilton-Zachariasen (HZ) equations. Zachariasen stated that any real crystal is situated between two limiting types, distinguished by the nature of the peak width: type I if the width is given exclusively by the mosaic and type II if the width is given by the crystallite size only. Correspondingly, the secondary extinction follows the same classification. So far as primary extinction in small mosaic blocks is concerned, a description by the same transfer equations has been considered good enough under the assumption that this extinction is weak. The unified theory of Zachariasen has been very much criticized both for some mathematical errors and for its physical basis. On the same basis, Becker & Coppens (1974*a*) (BC) have re-analysed the HZ equations. The solution which they provided has become very popular both for its convenient parametrization for least-squares-refinement programs and for its resistance to numerous experimental tests (see *e.g.* Hutton, Nelmes & Scheel, 1981).

The limitations on the classical theory of extinction in real crystals were clarified by the new dynamical statistical theory of Kato (1976*a*, *b*, 1979, 1980). Starting from the dynamical equations for a distorted crystal and assuming a homogeneous and isotropic distribution of the defects, Kato derived a system of energy transfer equations valid for extinction only if the coherence distance t_c is smaller than the extinction distance $\Lambda = (n\lambda|F|)^{-1}$. Here λ is the wavelength, F the structure factor and n the density of unit cells. The energy transfer equations of Kato are similar to but not identical with the HZ equations. The differences discussed in detail by Kato (1976*b*, 1979) are in the form and physical interpretation of the coupling constants. Analysing the equivalence between the two kinds of energy transfer equations, Becker (1977) concludes that the range of validity found by Kato

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