Table 3. *Observed and calculated structure factors*

In order to obtain F_o and F_c on the absolute scale, the values in the Table must be divided by 10

hk0	$\|F_o\|$	F_c	hk0	$\|F_o\|$	F_c	hhl	$\|F_o\|$	$\|F_o\|$	$\alpha/2\pi$
200	838	787	730	331	346-	001	868	896	0.000
400	697	716	830	105	103	002	321	331	0.000
600	568	551	930	156	166-	003	276	278	0.500
800	162	158	440	586	557	004	577	603	0.500
10,0,0	216	234	540	120	117-	005	454	468	0.500
12,0,0	48	66	640	418	412	006	219	178	0.500
110	595	637-	840	246	253	111	1100	1079	0.286
210	415	372	940	144	152-	112	508	470	0.436
310	667	573-	10,4,0	150	158	113	373	365	0.112
410	270	260-	12,4,0	81	70	114	385	391	0.034
510	682	681-	550	472	469-	115	303	286	0.757
610	234	245	650	108	98	221	796	775	0.811
710	303	311-	750	144	138-	222	310	283	0.783
910	171	178-	850	81	91	223	358	330	0.580
11,1,0	99	111-	950	129	134-	224	409	404	0.527
220	1280	1253	10,5,0	75	70	225	355	360	0.265
320	123	104	11,5,0	111	108-	331	733	741	0.506
420	598	591	660	352	351	332	267	261	0.416
520	63	49	760	153	158-	333	201	188	0.060
620	373	355	860	141	152	334	427	418	0.004
720	102	108-	10,6,0	123	133	335	294	293	0.009
820	361	381	11,6,0	72	75-	441	406	417	0.845
10,2,0	114	114	770	207	201-	442	295	285	0.907
11,2,0	54	61-	870	90	80	443	255	264	0.642
12,2,0	99	94	970	111	116-	444	249	232	0.569
330	967	905-	880	156	172	551	439	461	0.280
430	261	255	980	66	82-	554	258	250	0.021
530	246	246-	990	99	94-	661	234	218	0.818

equal to the difference $|U_{11}(\mathrm{Cl}) - U_{11}(\mathrm{I})|$, which should be zero for the ion to be a rigid body.

As the z coordinates of iodine and chlorine show no significant difference, the ICl_2^- ion is linear within experimental error. The I–Cl bond length, 2·55 e.s.d. 0·02 Å, is much larger than the value reported by Mooney, 2·34 Å. It is also much larger than the sum of the covalent radii, 2·32 Å. This is compatible with a bonding scheme in which delocalized molecular orbitals are formed by a linear combination of p-orbitals of the halogen atoms (Havinga & Wiebenga, 1959).

It is remarkable that the N–C distance obtained from the least-squares refinement, 1·47 e.s.d. 0·03 Å, is close to the usually accepted value, 1·48 Å, although the carbon atoms look rather blurred in the Fourier syntheses.

We are grateful to Prof. E. H. Wiebenga for suggesting the structure refinement and for reading the manuscript. We wish to thank Dr J. S. Rollett for executing the anisotropic least-squares refinements and Mr H. Schurer for operating Zebra.

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Diffraction symbols.

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In reporting the results of a crystallographic investigation a problem of symbolism arises: how to represent, in as compact a form as possible, all the information that has been obtained by X-ray diffraction concerning the symmetry of a crystalline species.

Two solutions have been proposed: one by Donnay & Harker (1940), the other by Buerger (1942). Both are presented in *International Tables for X-ray Crystallography* (1952). The former has been reprinted as an Appendix to *Crystal Data* (1954, 1963).

Donnay & Harker have introduced the concept of *aspect* (either as 'morphological aspect' or as 'diffraction aspect'). An *aspect* is a statement of a set of criteria that govern the systematic absences in one or several space groups, in any given crystal system. Examples: In the orthorhombic system $P{*}{*}{*}$ stands for *Pmmm*, *P*222, *Pmm*2, *P*2*mm*, *Pm*2*m*. In the tetragonal system $I4_1{*}{*}$ stands for $I4_1$ and $I4_122$.

Buerger's *diffraction symbol* is more informative. It gives the Laue class symbol, followed by the aspect symbol. The above examples become: $mmmP{-}{-}{-}$, which stands for the same space groups as $P{*}{*}{*}$; $4/mI4_1{-}{-}$ and $4/mmmI4_1{-}{-}$, which stand respectively for $I4_1$ and $I4_122$.

Both notations are based on the fact that only those elements of symmetry that involve a translation component (glide planes and screw axes) can be symbolized. Other elements of symmetry (mirrors, rotation axes, inversion axes) are replaced by asterisks (in the aspect symbol) or by hyphens (in the diffraction symbol).† The asterisk, in some cases, stands for the absence of symmetry element, as in the tetragonal aspect $Pn{*}{*}$, which stands for *P*4/*nmm* and *P*4/*n*.

Neither solution is completely satisfactory. The aspect symbolism has the following drawbacks:

(1) Any aspect that corresponds to a single space group is unnecessary; the space-group symbol itself should be used. Example: $P222_1$ instead of $P{*}{*}2_1$.
(2) Some aspect symbols are identical with space-group symbols. Example: Two space groups, *C*2/*c* and *Cc*, are represented by the aspect symbol *Cc*, which gives no indication of its being an aspect rather than a space-group symbol.

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† Asterisks and hyphens have been changed to dots in *International Tables*.

Table 1. *Space groups not uniquely determined by diffraction criteria*

(1)

Laue class $\bar{1}$

	$\bar{1}$	1
$\bar{1}P*$	$P\bar{1}$	P1

(2)

Laue class 2/*m*

	2/m	2	m
P*/*	P2/m	P2	Pm
$P2_1/*$	$P2_1/m$	$P2_1$	
P*/c	P2/c		Pc
P*/a	P2/a		Pa
P*/n	P2/n		Pn
C*/*	C2/m	C2	Cm
A*/*	A2/m	A2	Am
I*/*	I2/m	I2	Im
C*/c	C2/c		Cc
A*/a	A2/a		Aa
I*/a	I2/a		Ia

(3)

Laue class *mmm*

	mmm	222	2mm	m2m	mm2
P***	Pmmm	P222	P2mm	Pm2m	Pmm2
P**a	Pmma		P2ma	Pm2a	
P**b	Pmmb		P2mb	Pm2b	
P*c*	Pmcm		P2cm		Pmc2
P*a*	Pmam		P2am		Pma2
Pb**	Pbmm			Pb2m	Pbm2
Pc**	Pcmm			Pc2m	Pcm2
Pn**	Pnmm			Pn2m	Pnm2
P*n*	Pmnm		P2nm		Pmn2
P**n	Pmmn		P2mn	Pm2n	
P*aa	Pmaa		P2aa		
Pb*b	Pbmb			Pb2b	
Pcc*	Pccm				Pcc2
P*ab	Pmab		P2ab		
P*ca	Pmca		P2ca		
Pb*a	Pbma			Pb2a	
Pc*b	Pcmb			Pc2b	
Pbc*	Pbcm				Pbc2
Pca*	Pcam				Pca2
P*cb	Pmcb		P2cb		
Pc*a	Pcma			Pc2a	
Pba*	Pbam				Pba2
P*an	Pman		P2an		
P*na	Pmna		P2na		
Pn*b	Pnmb			Pn2b	
Pb*n	Pbmn			Pb2n	
Pcn*	Pcnm				Pcn2
Pnc*	Pncm				Pnc2
P*cn	Pmcn		P2cn		
P*nb	Pmnb		P2nb		
Pc*n	Pcmn			Pc2n	
Pn*a	Pnma			Pn2a	
Pbn*	Pbnm				Pbn2
Pna*	Pnam				Pna2
P*nn	Pmnn		P2nn		
Pn*n	Pnmn			Pn2n	
Pnn*	Pnnm				Pnn2
A***	Ammm	A222	A2mm	Am2m	Amm2
B***	Bmmm	B222	B2mm	Bm2m	Bmm2
C***	Cmmm	C222	C2mm	Cm2m	Cmm2
A*a*	Amam		A2am		Ama2
A**a	Amma		A2ma	Am2a	
B**b	Bmmb		B2mb	Bm2b	
Bb**	Bbmm			Bb2m	Bbm2
Cc**	Ccmm			Cc2m	Ccm2
C*c*	Cmcm		C2cm		Cmc2
Ab**	Abmm			Ab2m	Abm2
B*a*	Bmam		B2am		Bma2
C**a	Cmma		C2ma	Cm2a	
B*ab	Bmab		B2ab		
C*ca	Cmca		C2ca		
Cc*a	Ccma			Cc2a	
Ab*a	Abma			Ab2a	
Aba*	Abam				Aba2
Bba*	Bbam				Bba2
A*aa	Amaa		A2aa		
Bb*b	Bbmb			Bb2b	
Ccc*	Cccm				Ccc2
I***	Immm	I222 $I2_12_12_1$	I2mm	Im2m	Imm2
Ib**	Ibmm			Ib2m	Ibm2
I*a*	Imam		I2am		Ima2
I**a	Imma		I2ma	Im2a	
I*aa	Imaa		I2aa		
Ib*a	Ibma			Ib2a	
Iba*	Ibam				Iba2
F***	Fmmm	F222	F2mm	Fm2m	Fmm2

(4)

Laue class 4/*mmm*

	4/mmm	422	4mm	$\bar{4}2m$	$\bar{4}m2$
P4/***	P4/mmm	P422	P4mm	$P\bar{4}2m$	$P\bar{4}m2$
$P4_{1,3}22$		$P4_122$ $P4_322$			
$P42_1*$		$P42_12$		$P\bar{4}2_1m$	
$P4_{1,3}2_12$		$P4_12_12$ $P4_32_12$			
P4/**c	P4/mmc		P4mc	$P\bar{4}2c$	
P4/*b*	P4/mbm		P4bm		$P\bar{4}b2$
P4/*bc	P4/mbc		P4bc		
P4/*c*	P4/mcm		P4cm		$P\bar{4}c2$
P4/*cc	P4/mcc		P4cc		
P4/*n*	P4/mnm		P4nm		$P\bar{4}n2$
P4/*nc	P4/mnc		P4nc		
I4/***	I4/mmm	I422	I4mm	$I\bar{4}2m$	$I\bar{4}m2$
I4/*c*	I4/mcm		I4cm		$I\bar{4}c2$
I4*d			I4md	$I\bar{4}2d$	

(5)

Laue class 4/*m*

	4/m	4	$\bar{4}$
P4/*	P4/m	P4	$P\bar{4}$
$P4_2/*$	$P4_2/m$	$P4_2$	
$P4_{1,3}$		$P4_1$ $P4_3$	
I4/*	I4/m	I4	$I\bar{4}$

Table 1 (*cont.*)

(6)

Laue class $6/mmm$

	$6/mmm$	622	$6mm$	$\bar{6}m2$	$\bar{6}2m$
$P6/***$	$P6/mmm$	$P622$	$P6mm$	$P\bar{6}m2$	$P\bar{6}2m$
$P6_{2,4}22$		$P6_2 22$ $P6_4 22$			
$P6_{1,5}22$		$P6_1 22$ $P6_5 22$			
$P6/*c*$	$P6/mcm$		$P6cm$	$P\bar{6}c2$	
$P6/**c$	$P6/mmc$		$P6mc$		$P\bar{6}2c$
$P6/*cc$	$P6/mcc$		$P6cc$		

(7)

Laue class $6/m$

	$6/m$	6	$\bar{6}$
$P6/*$	$P6/m$	$P6$	$P\bar{6}$
$P6_3/*$	$P6_3/m$	$P6_3$	
$P6_{2,4}$	$P6_2$ $P6_4$		
$P6_{1,5}$	$P6_1$ $P6_5$		

(8)

Laue class $\bar{3}m$

	$\bar{3}m$	32	$3m$
$P3*1$	$P\bar{3}m1$	$P321$	$P3m1$
$P31*$	$P\bar{3}1m$	$P312$	$P31m$
$P3_{1,2}21$		$P3_1 21$ $P3_2 21$	
$P3_{1,2}12$		$P3_1 12$ $P3_2 12$	
$\bar{3}mP*c1$	$P\bar{3}c1$		$P3c1$
$\bar{3}mP*1c$	$P\bar{3}1c$		$P31c$
$R**$	$R\bar{3}m$	$R32$	$R3m$
$R*c$	$R\bar{3}c$		$R3c$

(9)

Laue class $\bar{3}$

	$\bar{3}$	3
$\bar{3}P*$	$P\bar{3}$	$P3$
$P3_{1,2}$		$P3_1$ $P3_2$
$R*$	$R\bar{3}$	$R3$

(10)

Laue class $m\bar{3}m$

	$m\bar{3}m$	432	$\bar{4}3m$
$P*3*$	$Pm3m$	$P432$	$P\bar{4}3m$
$P4_{1,3}32$		$P4_1 32$ $P4_3 32$	
$P*3n$	$Pm3n$		$P\bar{4}3n$
$I*3*$	$Im3m$	$I432$	$I\bar{4}3m$
$F*3*$	$Fm3m$	$F432$	$F\bar{4}3m$
$F*3c$	$Fm3c$		$F\bar{4}3c$

(11)

Laue class $m\bar{3}$

	$m\bar{3}$	23
$P*3$	$Pm3$	$P23$
$I*3$	$Im3$	$I23$ $I2_1 3$
$F*3$	$Fm3$	$F23$

(3) A pair of enantiomorphous holoaxial groups, such as $P4_1 32$ and $P4_3 32$ is represented by a symbol, $P4_1**$, in which the right screw axis stands for either a right or a left screw axis.

(4) In the aspect symbols 6_2 stands for 3_1 and 3_2 as well as for 6_4.

(5) Except in the trimetric systems, the aspect symbol does not convey the full information, as it leaves out the Laue class.

The diffraction symbols are open to the same objections as the aspect symbols, except that they do give explicit information on the Laue class. They are unnecessarily lengthened in the low symmetry systems, where each system contains only one Laue class.

We wish to propose a modified symbolism based on the following principles:

(1) No diffraction symbol is necessary when the observed diffraction criteria uniquely define one space group. In this case the space-group symbol should be used.

(2) When the observed criteria allow several space groups in one Laue class, the diffraction symbol should not be confused with a space-group symbol; it should imply the Laue class and clearly indicate the various possible space groups.

(3) Since the Laue class can be obtained by X-ray diffraction, aspect symbols that correspond to a crystal system can be dispensed with. For example the aspect symbol $I4_1**$, which was used to designate space groups $I4_1 22$ and $I4_1$, is superfluous because once the Laue class is known the space group itself is uniquely determined.

The desired results can be achieved by first writing an asterisk for each possible symmetry element that can occur in the space-group symbol (as written in *International Tables*) and then replacing by the appropriate glide-plane or screw-axis symbols those asterisks whose meaning is indicated by the space-group criteria. Example: $P*/*$, for monoclinic $P2/m$, Pm, or $P2$; $C*/c$ for $C2/c$ or Cc. In addition it may be necessary to specify a symmetry axis in order to differentiate between crystal systems: 4 (to stand for 4 or $\bar{4}$) in the tetragonal system, 6 (to stand for 6 or $\bar{6}$) or 3 (to stand for 3 or $\bar{3}$) in the hexagonal system (if the lattice is not rhombohedral), 3 in second position in cubic symbols. Example: $P***$ is retained as an orthorhombic aspect, but is replaced by $P4/***$ or $P4/*$ in the tetragonal system, by $P*3*$ or $P*3$ in the cubic system. Wherever the space-group symbol would be ambiguous, the Buerger diffraction symbol is retained. There are four such cases: $\bar{1}P*$, $\bar{3}P*$, $\bar{3}mP*c1$, and $\bar{3}mP*1c$.

We present (Table 1) the list of all the new symbols that will be needed to represent the choice of space groups corresponding to every set of absence criteria in each Laue class. The use of these symbols, instead of the previous ones, is recommended whenever the absence criteria do not uniquely determine the space group, and until such time as the latter would become known from other properties, such as morphology, piezoelectricity, pyroelectricity, optical activity, intensity statistics, or a structure determination.

Note that, in the monoclinic and orthorhombic systems, all possible orientations are foreseen. They are collected in braces. All the symbols given may be needed when the cell edges are labelled according to metric considerations (for instance, monoclinic: $c<a$; orthorhombic: $c<a<b$).

In Laue class $\bar{3}m$ aspect $P3{*}{*}$ has been split into $P3{*}1$ and $P31{*}$; and aspect $P3_{1,2}21$ and $P3_{1,2}12$. In each case the distinction can be made on upper level photographs (Bokii & Porai-Koshits, 1952).

We wish to thank Dr Gabrielle Donnay for a critical reading of the manuscript.

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Book Reviews

Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, University College, Cathays Park, Cardiff, Great Britain). As far as practicable books will be reviewed in a country different from that of publication.

Electron Microscopy and Strength of Crystals.

Edited by GARETH THOMAS and JACK WASHBURN. New York: Interscience, 1963. Pp. xi + 1022. Price £11.

All the old favourites are here: Amelinckx and Delavignette on dislocations in layer structures; Keh and Weissmann on b.c.c. metals; Marcinkowski on superlattices; Nicholson on the nucleation of precipitates; Price on hexagonal crystals; Segall on fatigued metals; Thomas on precipitation hardening alloys; Swann on dislocation arrangements in f.c.c. metals; Washburn on MgO; Whelan on defects produced by quenching and irradiation. These articles contain little that is new, but serve as an introduction for a research student to the various important aspects of transmission electron microscopy.

English metallurgists should read with particular interest the two loosely related papers from Stuttgart by Mader and by Seeger, Mader & Kronmüller. These bring together a range of ideas and references which will prove as valuable as Seeger's famous Lake Placid (1957) article. There are also particularly interesting articles by Friedel and Saada; the former condensing what seems to be slightly *more* than his book into forty pages.

It is remarkable how *little* impact electron microscopy has made on the theories of the strength of crystals. Most of the theories proposed at this conference have no basis in thin foil observations. Few people have indeed troubled to make the sort of detailed correlation between microstructure and mechanical properties which is required for further advance. Exceptions which spring to mind are Ashby's attempt to correlate flow-stress and particle spacing in internally oxidized alloys, and so to confirm Orowan's theory of strength, and, of course, the slip-line-stress-strain curve studies of the Stuttgart School. These serve to show what can be done.

This collection of papers gives us the by now familiar story of how powerfully transmission microscopy can provide quantitative information on a wide range of metallurgical investigations; information, that is, on a micron or hundred-Ångström scale. What the collection only hints at is the still obscure and fascinating question of the cooperative and dynamic behaviour of many dislocations in a straining crystal.

The book can be said to be a timely summary of a specialized field, and if it were not so highly priced, it would be a useful addition to every microscopist's library.

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