Wahrscheinlichkeit für den kubischen Weiterbau einer hexagonalen Stapelfolge an. $(1-\beta)$ bezeichnet die Wahrscheinlichkeit für den hexagonalen Weiterbau einer kubischen Stapelfolge. Dadurch konnten die Fehlordnungsparameter für die jeweiligen Kristallbereiche ermittelt und daraus die Hexagonalität (Anteil der hexagonalen Packungselemente) entnommen werden: $\sigma=(1-\beta)/(1+\alpha-\beta)$. Bei der Anfertigung der Drehkristallaufnahmen wurde darauf geachtet, dass der Röntgenstrahl nicht gleichzeitig mehrere Kristallgebiete unterschiedlicher Doppelbrechung erfasste; es wurden deshalb möglichst breite einheitlich doppelbrechende Kristallgebiete zur Untersuchung herangezogen. Teilweise, besonders zur Anfertigung der Abtastaufnahmen, wurde der Röntgenstrahl auf eine Breite bis zu 2 $\mu$m ausgeblendet.

### Versuchsergebnisse

Die Abtastaufnahmen in Gebieten konstanter Doppelbrechung zeigten in keinem Fall eine Änderung der Struktur, während bei Änderung der Doppelbrechung auch eine Änderung der Struktur aus den Aufnahmen zu erkennen war.

Tabelle 1 zeigt die quantitativen Ergebnisse der Untersuchungen, die in der Abbildung auch noch graphisch dargestellt sind. Wie aus der Fig. 1 erkenntlich ist, besteht eine Proportionalität zwischen der Doppelbrechung $\Delta n$ und der Hexagonalität $\sigma$ mit dem Doppelbrechungswert der Wurtzitstruktur als Proportionalitätskonstante: $\Delta n=\sigma\cdot\Delta n_{\text{Wurt.}}$

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## Ordering scheme for general positions in *International Tables.*

By E. F. BERTAUT *Laboratoire d'Electrostatique et de Physique du Métal, CNRS, Chemin des Martyrs, Grenoble, France* and H. WONDRATSCHEK, *Institut für Kristallographie der Universität, 75 Karlsruhe* 1, *Kaiserstr.* 12, *Germany*

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A logical scheme is proposed for the ordering of general positions in *International Tables for X-ray Crystallography.*

It is the authors' opinion that some questions debated at meetings of the Commission on *International Tables* should be brought to the attention of a broader audience.

The general positions in the *International Tables for X-ray Crystallography* (1969) (I.T.) can be taken as shorthand notation for the matrices $(\alpha/\tau_\alpha)$ ($\alpha$ = rotation or rotatory inversion, $\tau_\alpha$ = translation component) describing the transformation $r=xyz$ to $r'=x'y'z'$ by

$$r'=(\alpha/\tau_\alpha)r\,. \tag{1}$$

The listing of general positions in I.T. seems to offer more typographical than mathematical convenience. There are many ways of ordering the general positions. One of them takes advantage of the property (well known to mathematicians) that a space group $N_k$ in three dimensions is a soluble group, *i.e.* that there is a chain

$$N_0\subset N_1\subset N_2\ \ldots\ \subset N_k \tag{2}$$

such that $N_i$ is an invariant subgroup of $N_{i+1}$ for $i=0, \ldots, k-1$ and that $N_{i+1}/N_i$ is a cyclic group. According to this proposal generators $a_i$ for the space group $N_k$ are chosen in such a way that $N_i a_{i+1}$ is a generating coset of the cyclic group $N_{i+1}/N_i$. The advantage of such a generation of the space groups is the possibility of representing each symmetry operation as an ordered product

$$a_k^{\nu k}a_{k-1}^{\nu k-1}\ldots\ a_i^{\nu i}\ldots a_1^{\nu 1}a_0^{\nu 0} \tag{3}$$

$(0\le\nu_i<n_i$, $n_i$ order of $N_i/N_{i-1})$ of powers of the generators $a_i$.

The general positions can be understood as a set of representatives of the cosets $S/T$, where $S$ means the whole space group, $T$ means the set of all translations. The set of all translations of a space group is always an invariant subgroup belonging to a chain (2). First one can generate the set of translations. The generation of the general positions then is second step, which shall be considered here.*

In general there are different possible chains $N_0, N_1, \ldots, N_k$. Therefore the choice of generators is not unique and one can impose further conditions on crystallographic grounds: *e.g.* one can choose the generators in such a way that *primarily* rotations are preferred, always using, in non-cubic space groups, the rotations of highest order. In cubic space groups there is no principal axis and the ordering scheme should reflect the aspects of the cubic system. In all cases an ordering scheme is preferred in which important subgroups can be seen at a glance.

It is noteworthy that the proposed ordering scheme was often obeyed in the 'old' *Internationale Tabellen* (1935) with

* If a 'centred' lattice (*i.e.* a lattice defined by a multiple cell) belongs to a space group, then the centring translations can be added to the listed general positions, as is customary in *Internationale Tabellen* (1935) and I. T. For the systematic generation of all general positions belonging to a given unit cell these fractional translations have to be introduced as the first generators after the integral translations. Note that both integral and fractional centring translations are lattice translations whereas the translation component $\tau_\alpha$ in (1) is a fractional, but not a lattice translation.

minor changes (interchange of columns and lines), but not in the new ones, where the scheme varies even for a change of origin.

Table 1. *Ordering scheme of symmetry operations in* ($m3m$–$O_h$)

In the $T$ block the first line contains the principal 180° rotations, the second and third lines contain the eight 120° rotations.

In the $T2_d$ block, $2_d$ and $2_z\,2_d$ represent 180° rotations with axes $x\,\bar{x}\,0$ and $x\,x\,0$ respectively. The 90° rotations are

$$2_x2_d=4_z\ ;\qquad 2_y2_d=4_z^3\ ;\qquad 2_y3^22_d=4_x$$
$$2_z3^22_d=4_x^3\ ;\qquad 2_x32_d=4_y;\qquad 2_x32_d=4_y$$

All other operations in the $T2_d$ block are binary.

The last two blocks only produce a change of sign of the coordinates coming from the first two blocks.

The transformed positions may be recognized in the corresponding scheme proposed for $Pn3n-O_h^2$ (Table 3).

| | | | | |
|---|---|---|---|---|
| $e$ | $2_z$ | $2_x$ | $2_y=2_z2_x$ | |
| $3$ | $2_z3$ | $2_x3$ | $2_y3$ | $T$ |
| $3^2$ | $2_z3^2$ | $2_x3^2$ | $2_y3^2$ | |
| $2_d$ | $2_z2_d$ | $2_x2_d$ | $2_y2_d$ | |
| $32_d$ | $2_z32_d$ | $2_x32_d$ | $2_y32_d$ | $T2_d$ |
| $3^22_d$ | $2_z3^22_d$ | $2_x3^22_d$ | $2_y3^22_d$ | |
| $\bar{1}$ | $2_z\bar{1}$ | $2_x\bar{1}$ | $2_y\bar{1}$ | |
| $3\bar{1}$ | $2_z3\bar{1}$ | $2_x3\bar{1}$ | $2_y3\bar{1}$ | $T\bar{1}$ |
| $3^2\bar{1}$ | $2_z3^2\bar{1}$ | $2_x3^2\bar{1}$ | $2_y3^2\bar{1}$ | |
| $m=2_d\bar{1}$ | $2_zm$ | $2_xm$ | $2_ym$ | |
| $3m$ | $2_z3m$ | $2_x3m$ | $2_y3m$ | $Tm$ |
| $3^2m$ | $2_z3^2m$ | $2_x3^2m$ | $2_y3^2m$ | |

*Examples*

In the following, the identity operation is a trivial generator.

In the space group $P4$–$C_4^1$ one can choose the 180° rotation as the first generator and the 90° rotation as the second

$$\begin{array}{cccc} xyz, & \bar{x}\bar{y}z, & \bar{y}xz, & y\bar{x}z \\ e & 2^1=4^2 & 4^1 & 4^3=2^14^1 \end{array} \qquad (4)$$

The sites produced by generators are underlined. Generation of 4 in two steps (as well as $6=3\cdot2$) has some advantage: The first and second column of (4) represent the invariant subgroup $P2$–$C_2^1$.†

A more complicated example from the I.T. pilot edition (1969) may demonstrate the advantages of this way. We choose the following generators in $P4/mbm$–$D_{4h}^5$:2 in $00z$; 4 in $00z$, $2_1$ in $x\tfrac{1}{4}0$, and $\bar{1}$ in 000. The ordering of general positions is given by

$$\begin{array}{l} x,y,z\ ;\ \bar{x},\bar{y},z\ ;\ \bar{y},x,z\ ;\ y,\bar{x},z \\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\bar{z};\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\bar{z};\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\bar{z} \\ \bar{x},\bar{y},\bar{z}\ ;\ x,y,\bar{z}\ ;\ y,\bar{x},\bar{z}\ ;\ \bar{y},x,\bar{z} \\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,z\,. \end{array} \qquad (5)$$

† The cyclic group of order four is noted 4; its symmetry operations are $4^1$, $4^2$, $4^3$ and $e$. The superscript 1 is dropped in the following when there is no confusion. $6=3\cdot2$ means that the cyclic group of order six is the direct product of the cyclic groups 3 and 2. One has $6^1=3^22^1$.

Here the symmetry operations are $e$, 2, 4, $4^3$, $2_1$, $22_1$, $42_1$, $4^32_1$ followed by those multiplied by $\bar{1}$.

The symmetry relations of $P4/mbm$ with some of its subgroups are obvious: $P4$–$C_4^1$ [first line of (5)], $P42_12$–$D_4^2$ (first plus second line), $P4/m$–$C_{4h}^1$ (first and third line) and $P4bm$–$C_{4v}^2$ (first and fourth line). In the same way the first column of (5) corresponds to space group $P2_1/b$–$C_{2h}^5$ and the sum of the first and second columns to space group $Pbam$–$D_{2h}^9$.

In Table 1 we give the ordering scheme for the general positions of space groups of $m3m$–$O_h$ which also covers those of 23–$T$, 432–$O$, $m3$–$T_h$ and $\bar{4}3m$–$T_d$. The meaning of the symbols is as follows

| | |
|---|---|
| $e$ | identity, |
| $2_z$, $2_x$, $2_y$ | 180° rotations around axes in $00z$, $x00$, $0y0$ respectively, |
| 3 | 120° rotation around axis in $xxx$, |
| $2_d$ | 180° rotation around axis in $x\bar{x}0$, |
| $m$ | reflection in a symmetry plane, its normal being in $x\bar{x}0$. |

Note that

$$2_x2_d=4_z;\quad 2_y2_d=4_z^3 \qquad (6)$$

Although these operations are indicated in point-group notation, it is understood that they represent the whole symbol $(\alpha|\tau_\alpha)$, *i.e.* $2_z$ represents the symbol $(2_z|\tau_z)$ and so on. Table 1 is composed of four blocks, of three lines each. The first block contains the 12 operations of the tetrahedral group 23–$T$. The second, third and fourth blocks are $T$-blocks multiplied on the right by $2_d$, $\bar{1}$ and $2_d\bar{1}=m$ respectively. It is easily seen that the combination of blocks $T$ with one of the other three blocks gives rise to another cubic space group: (432–$O$) = blocks one and two; ($m3$–$T_h$) = blocks one and three; ($\bar{4}3m$–$T_d$) = blocks one and four.

The first column of the blocks gives rise to rhombohedral subgroups and finally the first lines of the blocks represent tetragonal and orthorhombic space groups (Table 2). As an example, the general positions are given for $Pn3n$–$O_h^2$ (Table 3).

Table 2. *Subgroup relations*

| | Blocks | Point-group | Example |
|---|---|---|---|
| | 1+2+3+4 | $m3m$——$O_h$ | $Pn3n$——$O_h^2$ |
| | 1+2 | 432——$O$ | $P432$——$O^1$ |
| | 1+3 | $m3$——$T_h$ | $Pn3$——$T_h^2$ |
| | 1+4 | $\bar{4}3m$——$T_d$ | $P\bar{4}3n$——$T_d^4$ |
| | 1 | 23——$T$ | $P23$——$T^1$ |
| First column of | 1+2+3+4 | $\bar{3}m$——$D_{3d}$ | $R\bar{3}c$——$D_{3d}^6$ |
| | 1+2 | 32——$D_3$ | $R32$——$D_3^7$ |
| | 1+3 | $\bar{3}$——$C_{3i}$ | $R\bar{3}$——$C_{3i}^2$ |
| | 1+4 | $3m$——$C_{3v}$ | $R3c$——$C_{3v}^6$ |
| | 1 | 3——$C_3$ | $R3$——$C_3^4$ |
| First line | 1+2+3+4 | $4/mmm$–$D_{4h}$ | $P4/nnc$—$D_{4h}^4$ |
| | 1+2 | 422——$D_4$ | $P422$——$D_4^1$ |
| | 1+4 | $\bar{4}2m$——$D_{2d}$ | $P\bar{4}2_1c$——$D_{2d}^2$ |
| | 1+3 | $mmm$—$D_{2h}$ | $Pnnn$——$D_{2h}^2$ |
| | 1 | 222——$D_2$ | $P222$——$D_2^1$ |

In many cases the subgroups outlined in the Table correspond to the standard notation in I. T. only after a shift of the origin. For instance for the group $P222$ in the first line of block one (Table 3) the standard notation: $xyz$, $\bar{x}\bar{y}z$, $x\bar{y}\bar{z}$, $\bar{x}y\bar{z}$, is only obtained after a shift of $\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}$ of the origin.

Table 3. *Ordering of general positions in Pn3n–$O_h^2$*

| | | | | Block No. |
|---|---|---|---|---|
| $x\,y\,z$ | $\frac{1}{2}-x, \frac{1}{2}-y, z$ | $x, \frac{1}{2}-y, \frac{1}{2}-z$ | $\frac{1}{2}-x, y, \frac{1}{2}-z$ | |
| $z\,x\,y$ | $\frac{1}{2}-z, \frac{1}{2}-x, y$ | $z, \frac{1}{2}-x, \frac{1}{2}-y$ | $\frac{1}{2}-z, x, \frac{1}{2}-y$ | 1 |
| $y\,z\,x$ | $\frac{1}{2}-y, \frac{1}{2}-z, x$ | $y, \frac{1}{2}-z, \frac{1}{2}-x$ | $\frac{1}{2}-y, z, \frac{1}{2}-x$ | |
| $\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z$ | $y, x, \frac{1}{2}-z$ | $\frac{1}{2}-y, x, z$ | $y, \frac{1}{2}-x, z$ | |
| $\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}-x$ | $z, y, \frac{1}{2}-x$ | $\frac{1}{2}-z, y, x$ | $z, \frac{1}{2}-y, x$ | 2 |
| $\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-y$ | $x, z, \frac{1}{2}-y$ | $\frac{1}{2}-x, z, y$ | $x, \frac{1}{2}-z, y$ | |
| $\bar{x}\,\bar{y}\,\bar{z}$ | $\frac{1}{2}+x, \frac{1}{2}+y, \bar{z}$ | $\bar{x}, \frac{1}{2}+y, \frac{1}{2}+z$ | $\frac{1}{2}+x, \bar{y}, \frac{1}{2}+z$ | |
| $\bar{z}\,\bar{x}\,\bar{y}$ | $\frac{1}{2}+z, \frac{1}{2}+x, \bar{y}$ | $\bar{z}, \frac{1}{2}+x, \frac{1}{2}+y$ | $\frac{1}{2}+z, \bar{x}, \frac{1}{2}+y$ | 3 |
| $\bar{y}\,\bar{z}\,\bar{x}$ | $\frac{1}{2}+y, \frac{1}{2}+z, \bar{x}$ | $\bar{y}, \frac{1}{2}+z, \frac{1}{2}+x$ | $\frac{1}{2}+y, \bar{z}, \frac{1}{2}+x$ | |
| $\frac{1}{2}+y, \frac{1}{2}+x, \frac{1}{2}+z$ | $\bar{y}, \bar{x}, \frac{1}{2}+z$ | $\frac{1}{2}+y, \bar{x}, \bar{z}$ | $\bar{y}, \frac{1}{2}+x, \bar{z}$ | |
| $\frac{1}{2}+z, \frac{1}{2}+y, \frac{1}{2}+x$ | $\bar{z}, \bar{y}, \frac{1}{2}+x$ | $\frac{1}{2}+z, \bar{y}, \bar{x}$ | $\bar{z}, \frac{1}{2}+y, \bar{x}$ | 4 |
| $\frac{1}{2}+x, \frac{1}{2}+z, \frac{1}{2}+y$ | $\bar{x}, \bar{z}, \frac{1}{2}+y$ | $\frac{1}{2}+x, \bar{z}, \bar{y}$ | $\bar{x}, \frac{1}{2}+z, \bar{y}$ | |

The decomposition of space groups in cosets shown in the examples given, can be carried out in the same manner in the other space groups of the same point groups. In a space group of $4/mm$–$D_{4h}$ [see (5)] there are in the first line the representatives $\{4\}$ of the corresponding subgroup belonging to point group 4–$C_4$, in the other lines the representatives of the cosets $\{4\}(2_x|\tau_x)$, $\{4\}(\bar{1}|\tau_{\bar{1}})$, and $\{4\}(m_x|\tau_m,)$ where $(m_x|\tau_m)=(2_x|\tau_x)\,(\bar{1}|\tau_{\bar{1}})$. Therefore the corresponding subgroups are given by

$\{4\}+\{4\}(2_x|\tau_x)$, a space group belonging to 422–$D_4$,
$\{4\}+\{4\}(\bar{1}|\tau_{\bar{1}})$, a space group belonging to $4/m$–$C_{4h}$ and
$\{4\}+\{4\}(m_x|\tau_m)$, a space group belonging to $4mm$–$C_{4v}$.

Similarly (see Table 3), for a space group of $m3m$–$O_h$

$$\{m3m\text{–}O_h\}=\{T\}+\{T\}(2_d|\tau)+\{T\}(\bar{1}|\tau_{\bar{1}})+\{T\}(m|\tau)_m$$

where

$$(m|\tau_m)=(2_d|\tau')\,(\bar{1}|\tau_{\bar{1}})\,.$$

Subgroups, the representatives of which are $\{T\}+\{T\}(2'|\tau')$, $\{T\}+\{T\}(\bar{1}|\tau_{\bar{1}})$, and $\{T\}+\{T\}(m|\tau_m)$, belong to point groups 432–$O$, $m3$–$T_h$, and $\bar{4}3m$–$T_d$ respectively.

We would like to thank Dr J. Neubüser, Aachen, who suggested the use of subnormal chains for ordering the 'general positions', for critically reading the manuscript and for fruitful discussions, and also the referee for improvements of style and for suggesting the notation $2_d$ for a diagonal binary axis.

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## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J.N. King, 13 White Friars, Chester CH1 1NZ, England).*

### Professor Kathleen Lonsdale 1903-1971

Professor Dame Kathleen Lonsdale died on 1 April, 1971. She was Professor of Chemistry and Head of the Department of Crystallography, University College, London from 1949 to 1968. Her many contributions to crystallography included her work as General Editor of the three volumes of *International Tables for X-ray Crystallography*. She was one of the first women to be elected Fellow of the Royal Society and the first woman President of the British Association for the Advancement of Science. As President of the International Union of Crystallography she chaired the sessions of the Seventh General Assembly in Moscow, 1966.

A full obituary will be published in *Acta Crystallographica*, Section A in due course.

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The Executive Committee of the International Union of Crystallography has pleasure in announcing the publication of a new series of standard reference books entitled *Molecular Structures and Dimensions*. The aim of the series is to make the results of structural investigations by diffraction and related methods readily available to all scientists interested in molecular structures. It is designed to be easily usable by specialist crystallographers and by academic and industrial research workers in the related fields of chemistry, biochemistry, molecular biology and pharmacology. The new series is a continuation and extension of the *Tables of Interatomic Distances in Molecules and Ions* (Chemical Society Special Publication), which covered the literature up to the end of 1959.

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