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INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

(READY OCTOBER, 1952)

Published for

THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY

by THE KYNOCH PRESS, *Birmingham, England*

Volume I

SYMMETRY GROUPS

Editors: N. F. M. HENRY and K. LONSDALE

Demy quarto, bound in cloth. xii+558 pages, with 237 figures, index, and dictionary in five languages

Historical introduction by M. v. Laue

At the London Conference of Crystallography in 1946 it was decided to replace the old *International Tables for Crystal Structure Determination* (1935) by a new work. This was necessitated by the great development of the science of crystallography in recent years and its growing importance to the chemist, the physicist, the metallurgist, the biologist and the mineralogist. Much of the material in the former tables was of permanent usefulness, but experience had shown that it could be much more conveniently arranged, that some of the old material was not in common use, and that the growth of the subject had produced a demand for much new material.

The Commission of the International Union of Crystallography charged with this work now has the following members:

Chairman: K. Lonsdale (University College, Gower Street, London, W.C.1, England)

M. J. Buerger (U.S.A.)

N. F. M. Henry (U.K.)

J. S. Kasper (U.S.A.)

C. H. MacGillavry (Netherlands)

The new *International Tables for X-ray Crystallography* have been planned to be of the maximum practical usefulness in the determination of crystal structures and in allied problems, primarily those involving the use of X-ray methods; but their value for teaching purposes has also been kept in mind. The tables are written in English, but a dictionary of terms in English, French, German, Russian and Spanish is included.

The Commission is keeping in mind the possibility of issuing supplementary material later where the development of crystallographic methods renders this desirable.

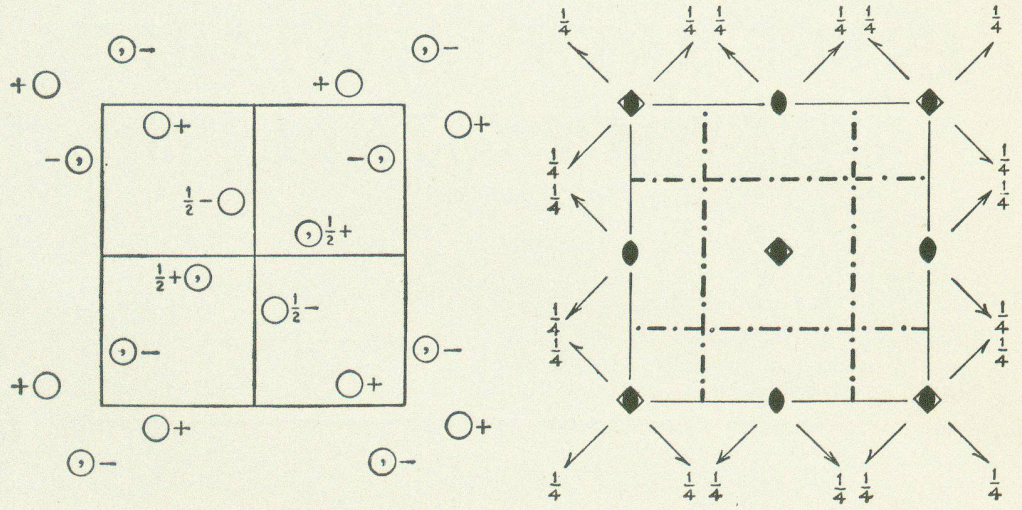
Volume I, now ready, deals with crystal symmetry and the crystallographic groups, and the detailed contents are given on the back page of this prospectus. Volumes II and III, which are in preparation and which will be sold separately, will cover Mathematical Tables and Physical and Chemical Tables respectively.

The whole work is being financially subsidised by UNESCO, to whom the thanks of the Commission are particularly due.

The price of Volume I is £5 5s. (five guineas), inclusive of postage and packing, and orders may be sent on the enclosed order form to the publishers.

$P\bar{4}n2$ D_{2d}^{8}

No. 118 $P\,\bar{4}\,n\,2$ $\bar{4}\,2\,m$ Tetragonal



Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	*i*	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$.	*hkl*: No conditions 0*kl*: $k+l=2n$ *hhl*: No conditions *h*00: $(h=2n)$ *hh*0: No conditions
				Special: as above, plus
4	*h*	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$.	*hkl*: $h+k+l=2n$
4	*g*	2	$x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$.	no extra conditions
4	*f*	2	$x,\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}+x,x,\frac{3}{4}$; $\frac{1}{2}-x,\bar{x},\frac{3}{4}$.	
4	*e*	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	*hkl*: $h+k+l=2n$
2	*d*	222	$0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{1}{4}$.	
2	*c*	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	
2	*b*	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	*a*	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

$P\bar{4}b2$
D_{2d}^{7}

Origin at $\bar{4}$. $\quad | \; x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\bar{z};\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\bar{z} \; |$

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)+\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$B=4\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)-\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$h+k=2n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$h+k=2n+1$ $\quad A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $l=0$

$A=B=0$ if $h=0$ or $k=0$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$P\bar{4}n2$
D_{2d}^{8}

Origin at $\bar{4}$.

$| \; x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}-z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}-z \; |$

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$B=4\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)-\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$h+k+l=2n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

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$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

CONTENTS

In 1951 an important work was published, indispensable for chemists, crystallographers, mineralogists, metallurgists, and all those interested in the solid state, entitled:

STRUCTURE REPORTS

FOR 1947–1948

VOLUME 11

General Editor: A. J. C. WILSON
University of Wales, Cardiff, Great Britain.

Section Editors: C. S. BARRETT (Metals)
University of Chicago, U.S.A.

J. M. BIJVOET (Inorganic Compounds)
University of Utrecht, Holland.

J. MONTEATH ROBERTSON (Organic Compounds)
University of Glasgow, Great Britain.

STRUCTURE REPORTS is an international undertaking sponsored by the International Union of Crystallography, and supported financially by UNESCO and British, American and Dutch research organizations and industrial firms. It is divided into three sections: Metals, Inorganic Compounds, Organic Compounds, and contains extensive Subject, Formula, and Author Indexes. It is a continuation of the pre-war publication *Strukturbericht*, the last issue of which was vol. VII for 1939.

It is intended to make up the gap between this issue and the first volume (11) of STRUCTURE REPORTS in three volumes: vol. 10 for 1945—1946, vol. 9 for 1942—1944 and vol. 8 for 1940—1941. Further announcements will be made as these become available.

The next volume to appear will be 12 for 1949, which will be ready about September 1952.

STRUCTURE REPORTS describes structure determinations which were published in the periods indicated and it gives all the structural data embodied in the articles so completely that only those in need of minute detail will find it profitable to consult the original papers.

Published for the

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

by

N.V. A. OOSTHOEK'S UITGEVERS MIJ., UTRECHT (HOLLAND)

Phosphorus Pentoxide

Preliminary account

P_2O_5 F.W. = 141·96

I. Crystal structure of the third form of phosphorus pentoxide. CAROLINA H. MACGILLAVRY, H. C. J. DE DECKER and L. M. NYLAND, 1949. *Nature*, **164**, 448.

II. Phosphorpentoxide. C. H. J. DE DECKER, 1941. Thesis (Utrecht).

III. Phosphorpentoxide. CAROLINA H. MACGILLAVRY and C. H. J. DE DECKER, 1942. *Chem. Weekbl.*, **39**, 227.

Orthorhombic, $a = 9{\cdot}23$ Å, $b = 7{\cdot}18$ Å, $c = 4{\cdot}94$ Å (I, II), $U = 327$ Å^3, $Z = 4$, $D_x = 2{\cdot}88$ g/cm^3.

Space group Pnam (D_{2h}^{16}) (I). No details.

Atomic positions (I)

4 PI, 4 PII, 4 OI, 4 OII, 4 OIII in (*c*): $\pm\,(x, y, \frac{1}{4};\ \frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{4})$

8 OIV in (*d*): $\pm\,(x, y, z;\ \frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}-z;\ \bar{x}, \bar{y}, \frac{1}{2}+z;\ \frac{1}{2}-x, \frac{1}{2}+y, \bar{z})$

with

	x	*y*	*z*
PI	0·244	0·288	...
PII	—0·098	—0·156	...
OI	—0·219	—0·011	...
OII	—0·142	0·346	...
OIII	0·055	—0·089	...
OIV	0·136	0·282	0·000

Physical properties

II, III. With water, in a very short time, crystals of this form split in two mutually perpendicular directions, leaving microscopic laths.

Discussion of the structure

I. The structure consists of corrugated sheets, parallel to (100). One such sheet is shown in fig. 1, projected along the *a* axis. Two sheets run throughout the unit cell. The linking in the sheet is of the same general type as in vanadium pentoxide (**1**), the difference being that the tetrahedra in phosphorus pentoxide are much less deformed than those in vanadium pentoxide. The binding in the sheet is less anisotropic and the packing denser.

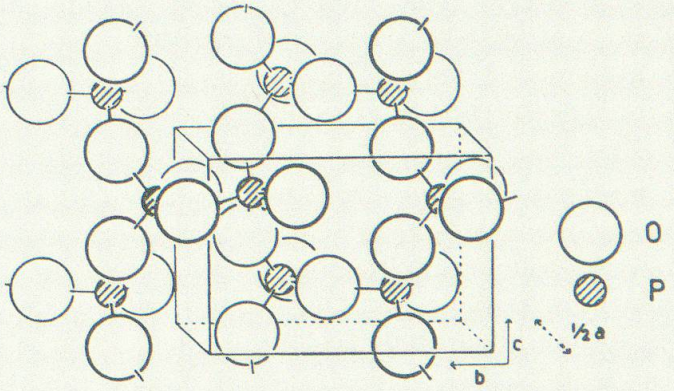

Fig. 1. Structure of orthorhombic P_2O_4. One of the two sheets of connected PO_4 tetrahedra is shown.

Details of analysis

In preparing the second form of P_2O_5 some crystals of this third form were obtained. These crystals were proved to be identical with those of Hill *et al.* (**2**).

Rotation and Weissenberg diagrams, Cu*K* and Mo*K* radiation, around *c* axis (II). No further details.

1. $D8_7$ type, *Strukturbericht*, **4**, 22.
2. W. L. Hill, G. T. Faust and S. B. Hendricks, 1943. *J. Am. Chem. Soc.*, **65**, 794.

Violarite

Iron Nickel Sulphide

I. The discovery of nickel in Egypt. G. L. Nassim, 1949. *Econ. Geol.*, **44**, 143—150.

Cubic, $a = 9{\cdot}47$ Å, spinel type.

Spacings and intensities are close to those of linnaeite (**1**, **2**). Analysis of mineral not given.

1. *Strukturbericht*, **1**, 421.
2. W. F. de Jong and H. W. V. Willems, 1927. *Z. anorg. allg. Chem.*, **161**, 312.

Neptunium Oxides

I. Higher oxides of the actinide elements. The preparation of Np_3O_8. J. J. Katz and D. M. Green, 1949. *J. Amer. Chem. Soc.*, **71**, 2106.

Chocolate-brown Np_3O_8 is prepared by oxidation of Np (V) hydroxide with nitrogen dioxide at 300°. Chemical analysis gives $NpO_{2{\cdot}64\pm3}$. X-ray diagrams show that Np_3O_8 is isotypic with U_3O_8 (**1**). The unit cell of Np_3O_8 is 110·7 Å^3 and that of U_3O_8 110·4 Å^3, whereas it might be expected that the volume of the unit cell of the neptunium compound would be smaller than that of uranium