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Phosphorus Pentoxide at 233 K

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Abstract

The structure of the thermodynamically most stable form of phosphorus pentoxide, o'-$(P_2O_5)_\infty$, consists of infinite layers built from six-membered rings of three-corner linked PO_4^- tetrahedra, as described in 1964 by Cruickshank [*Acta Cryst.* (1964), **17**, 679–680]. The P—O bond distances and P—O—P bond angles reported here differ from Cruickshank's values and show a better agreement with the average ranges of known crystalline phosphate structures.

Comment

The o'-$(P_2O_5)_\infty$ single crystals were prepared from the melt in a tightly covered gold crucible at 635 K over two to three weeks in an electrically heated furnace. The needle-like crystals were extracted from the glassy melt by means of acetone at room temperature over several days. X-ray measurements on the single crystal were performed at 233 (2) K and without any contact with air or water vapour (by immersion of the crystal in paraffin within a glass capillary).

The average bond lengths are 1.570 (4) Å for P—O linked bonds and 1.440 (10) Å for unlinked double bonds.

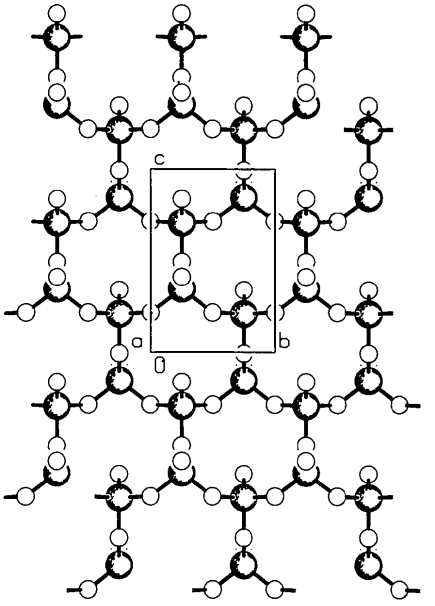

Fig. 1. The structure of a sheet of o'-$(P_2O_5)_\infty$.

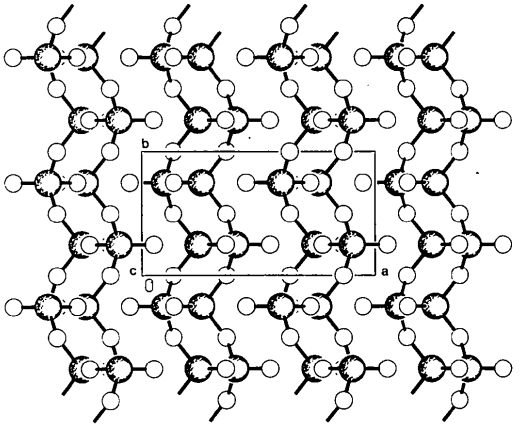

Fig. 2. The stacking of the sheets in P_2O_5.

Experimental

Crystal data

P_2O_5
M_r = 141.94
Orthorhombic
Pnma
a = 9.193 (9) Å
b = 4.890 (4) Å
c = 7.162 (7) Å
V = 322.0 (5) Å^3
Z = 4
D_x = 2.928 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 3.60–16.89°
μ = 1.081 mm^{-1}
T = 233 (2) K
Needle
0.18 × 0.08 × 0.05 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\omega$ scans
Absorption correction: empirical
$T_{min} = 0.874$, $T_{max} = 0.997$
1419 measured reflections
776 independent reflections
532 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.0729$
$\theta_{max} = 34.94°$
$h = 0 \rightarrow 14$
$k = -7 \rightarrow 7$
$l = 0 \rightarrow 11$
3 standard reflections
frequency: 120 min
intensity decay: 2.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.083$
$S = 1.117$
776 reflections
41 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.799$ e Å^{-3}
$\Delta\rho_{min} = -0.691$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0004 (44)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
P1	0.40207 (10)	1/4	0.34571 (13)	0.0055 (2)
P2	0.24238 (10)	1/4	0.70848 (13)	0.0061 (2)
O1	0.2762 (3)	1/4	0.4930 (3)	0.0085 (5)
O2	0.5517 (3)	1/4	0.4104 (4)	0.0095 (5)
O3	0.3612 (3)	1/4	0.8389 (4)	0.0105 (5)
O4	0.3642 (2)	0.0014 (3)	0.2162 (2)	0.0076 (3)

Table 2. *Selected geometric parameters* (Å, °)

P1—O2	1.452 (3)	P2—O3	1.437 (3)
P1—O1	1.566 (3)	P2—O4^{ii}	1.573 (2)
P1—O4	1.568 (2)	P2—O4^{iii}	1.573 (2)
P1—O4^{i}	1.568 (2)	P2—O1	1.574 (3)
O2—P1—O1	119.0 (2)	O3—P2—O4^{ii}	116.77 (10)
O2—P1—O4	113.53 (9)	O3—P2—O4^{iii}	116.77 (10)
O1—P1—O4	103.54 (10)	O3—P2—O1	119.1 (2)
O2—P1—O4^{i}	113.53 (9)	O4^{ii}—P2—O1	99.07 (9)
O1—P1—O4^{i}	103.54 (10)	O4^{iii}—P2—O1	99.07 (9)
O4—P1—O4^{i}	101.66 (15)	P1—O1—P2	143.7 (2)

Symmetry codes: (i) $x, \frac{1}{2}-y, z$; (ii) $\frac{1}{2}-x, -y, \frac{1}{2}+z$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$.

Data collection: *SDP-Plus* (Frenz, 1985). Cell refinement: *SDP-Plus*. Data reduction: *REDU*4 (Stoe & Cie, 1988). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *PLUTON*93 (Spek, 1993). Software used to prepare material for publication: *SHELXL*93.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: DU1085). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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