$V = 336.98$ Å^3
$Z = 1$
$D_x = 8.942$ Mg m^{-3}

Powder
Orange

Data collection

Flat cone powder diffractometer with a multi-counter detector system
Absorption correction: none

32 groups of reflections with $I > 2\sigma(I)$ measured
$\theta_{\max} = 35.58°$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 5$

Refinement

Refinement on I
$R_I = 0.043$ where $R_I = \Sigma|I_o - I_c|/\Sigma I_o$
32 groups of reflections

9 parameters
Scattering lengths from Sears (1992)

Table 3. *Fractional atomic coordinates and isotropic displacement parameters (Å^2) for (II)*

	Occupancy	Wyckoff position	x	y	z	$B_{\rm iso}$
Bi,Ti	1.0	8(*g*)	0	0.254 (3)	0.234 (3)	1.9 (2)
O1	0.96	8(*f*)	0.300 (4)	x	0	3.1 (3)
O2	1.0	4(*d*)	0	1/2	0.380 (7)	2.3 (5)
O3	0.16	2(*a*)	0	0	0	0 (4)
O4	0.08	2(*b*)	0	0	1/2	5 (21)

Table 4. *Selected geometric parameters (Å) for (II)*

Bi,Ti—O1	2.20 (3)	Bi,Ti—O2	2.76 (4)
Bi,Ti—O1	2.69 (3)	Bi,Ti—O3	2.37 (2)
Bi,Ti—O2	2.07 (3)	Bi,Ti—O4	2.47 (2)

Weight losses of slowly cooled samples were less than 0.2%. Determination of active oxygen (Cornwell, 1971) showed that no oxidation of bismuth had occurred. Therefore, any significant change of composition during the heating procedure can be excluded. All subsequent investigations were performed with homogeneous samples only. Neither their X-ray nor their neutron powder patterns showed reflections of other phases.

The crystal data were determined using a Siemens D5000 powder diffractometer with secondary monochromator, Cu $K\alpha_1$ radiation, $\lambda = 1.54056$ Å. The patterns were registered using a step scan (10 s per step) and corrected by least-squares calculations for zero-point shift using the program *XRAYPOWD* (Martin, 1991). The diffractometer was calibrated using silicon as external standard. The neutron diffraction data were collected at the BER II reactor at the Berlin Neutron Scattering Center (BENSC) of the Hahn-Meitner-Institut, Berlin, Germany.

Occupancy factors, connected appropriately by constraints according to the sample composition, were varied stepwise. The refinement of the structural and displacement parameters on groups of overlapping reflections was performed with our own trial-and-error program (*TRITM*; unpublished), which has been used successfully for evaluating powder data before (*e.g.* Trömel, Maetz & Müllner, 1977; von Beckh, Zegreanu & Trömel, 1981).

Lists of neutron diffraction intensities have been deposited with the IUCr (Reference: JZ1066). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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$PdTe_2$

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Abstract

The structure of palladium(IV) telluride has been determined by single-crystal X-ray methods. The structure type is $Cd(OH)_2$-(C6). $PdTe_2$ has a layered structure with the layers stacking along the [001] direction. The Pd^{4+} cations are octahedrally coordinated. The layers are

formed by the octahedra sharing edges along the [100], [010] and [110] directions. The Pd—Te bond distance is 2.693 (2) Å.

Comment

$PdTe_2$ has been previously characterized by powder diffraction (Thomassen, 1929; Grønvold & Røst, 1956).

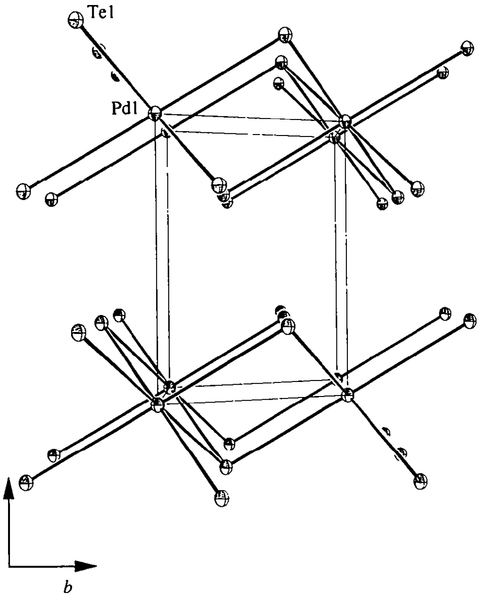

Fig. 1. Unit cell of $PdTe_2$ viewed along [010]. Displacement ellipsoids are shown at the 50% probability level.

Experimental

$PdTe_2$ was obtained in quantitative yield from the reaction of $PdCl_2$ with Te at 723 K in a fused silica tube.

Crystal data

$PdTe_2$
$M_r = 361.62$
Trigonal
$P\bar{3}m1$
$a = 4.024\,(3)$ Å
$c = 5.113\,(4)$ Å
$V = 71.70\,(2)$ Å^3
$Z = 1$
$D_x = 8.374$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 24 reflections
$\theta = 28$–$33°$
$\mu = 26.053$ mm^{-1}
$T = 113\,(2)$ K
Plate
0.212 × 0.171 × 0.012 mm
Black

Data collection

Picker diffractometer
θ–2θ scans
Absorption correction: analytical
$T_{\min} = 0.131$, $T_{\max} = 0.737$
1130 measured reflections
148 independent reflections
$R_{\rm int} = 0.0664$

$\theta_{\max} = 35.08°$
$h = -6 \rightarrow 5$
$k = -6 \rightarrow 6$
$l = -8 \rightarrow 8$
6 standard reflections monitored every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0262$
$wR(F^2) = 0.0648$
$S = 1.325$
148 reflections
7 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0400F_o^2)^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 5.43$ e Å^{-3}
$\Delta\rho_{\min} = -2.11$ e Å^{-3}

Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.285 (26)
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)*

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

	x	y	z	$U_{\rm eq}$
Pd1	0	0	0	0.0063 (3)
Te1	1/3	2/3	0.26628 (8)	0.0068 (3)

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

Pd1—Te1	2.693 (2)	Te1—Pd1—Te1$^{\rm i}$	96.69 (4)

Symmetry code: (i) $x-1, y-1, z$.

Initial cell parameters and symmetry information for $PdTe_2$ were determined from Weissenberg photographs taken at 298 K. Intensity data were processed (Waters & Ibers, 1977) and corrected for absorption (de Meulenaer & Tompa, 1965) on an IBM RS/6000 series computer. The earlier structure solution was refined with the use of the program *SHELXL*93 (Sheldrick, 1993). The final refinement included anisotropic displacement parameters and an extinction parameter. The final difference electron-density map shows no feature with a height greater than 1.7% of that of a Pd atom, the largest peak being near Te1.

Data collection: local program. Cell refinement: local program. Data reduction: local program. Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1994). Software used to prepare material for publication: *SHELXTL/PC*.

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Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1127). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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