PTASIEWICZ-BAK, H., MCINTYRE, G. J. & OLOVSSON, I. (1983). *Acta Cryst.* C**39**, 966–968.
SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
STADNICKA, K., GLAZER, A. M. & KORALEWSKI, M. (1987). *Acta Cryst.* B**43**, 319–325.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

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Bis[bis(pentamethylcyclopentadienyl)ytterbium(III)] Ditelluride

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Abstract. $[Yb(C_{10}H_{15})_2]_2Te_2$, $C_{40}H_{60}Te_2Yb_2$, M_r = 1142·20, monoclinic, $P2_1/n$, a = 15·517 (3), b = 10·611 (2), c = 13·166 (3) Å, β = 114·34 (2)°, V = 1975·1 Å^3, Z = 2, D_x = 1·92 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 61·71 cm^{-1}, $F(000)$ = 1088, T = 296 K, R = 0·036 for 3330 [$F^2 > 2\sigma(F^2)$] of 4560 total unique data. The Te_2^{2-} ion is on a center of symmetry and lies perpendicular to and between the two Yb atoms. Each Yb atom is bonded approximately tetrahedrally to two cyclopentadienyl ring centers and the Te_2^{2-} ion. Distances (Å) are: ave. Yb—C 2·626 (17), ave. Yb—Cp(centroid) 2·332 (18), Te—Te 2·7686 (11) Å.

Experimental. The complex was isolated from the reaction of $[Yb\{C_5(CH_3)_5\}_2].(C_2H_5)_2O$ with a large excess of tellurium powder in hexane after stirring for 2 days at room temperature. Black air-sensitive crystals were sealed inside quartz capillaries under argon. Crystal, 0·25 × 0·25 × 0·33 mm, with eight faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 28 reflections, $20 < 2\theta < 54°$; analytical absorption correction, range 2·4–3·8; max. $(\sin\theta/\lambda)$ = 0·65 Å^{-1}; h −20 to 20, k 0 to 13, l −17 to 17; three standard reflections, average decay 0·8%, intensities adjusted accordingly; 8993 data, 4560 unique, $R_{\rm int}$ = 0·023; structure solved by Patterson and Fourier methods; refined on F, f' and f'' terms included, 199 parameters; H atoms not observed in difference maps and were not included; anisotropic thermal parameters for all atoms refined; R = 0·036 for 3330 reflections for which $F^2 > 2\sigma(F^2)$; R = 0·055 all data; wR = 0·052; S = 1·38; $w = 4F_o/[\sigma^2(F_o^2) + (0.06F_o^2)^2]$; max. (shift/$\sigma$) < 0·05; extinction correction $F_{\rm corr} = (1 + 4.8 \times 10^{-8}I)F_o$, extinction parameter estimated after each series of refinements, max. correction 11%; max. and min. of ΔF synthesis 1·6 and −1·4 e Å^{-3}; atomic f, f' and f'' for neutral Yb, Te and C from *International Tables for X-ray Crystallography* (1974); local unpublished programs and *ORTEP* (Johnson, 1965).

Atomic parameters are listed in Table 1, and distances and angles are listed in Table 2.* Fig. 1 shows the molecule and numbering scheme.

Related literature. Comparable Te—Te distances are 2·78 Å in $AuTe_2X$, X = Cl or I (Haendler, Mootz, Rabenau & Rosenstein, 1974), and 2·802 (1) Å in $[Ni\{CH_3C[CH_2P(C_6H_5)_2]_3\}]_2[\mu\text{-}Te_2].2C_4H_8O$ (Di Vaira, Peruzzini & Stoppioni, 1986). The latter is the only structurally characterized compound with the same

Table 1. *Atomic parameters*

$$B_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
Yb	0·16540 (2)	0·07854 (3)	−0·02377 (2)	2·656 (9)
Te	0·05403 (3)	−0·07689 (4)	0·08828 (4)	3·43 (2)
C1	0·1697 (6)	0·2522 (7)	0·1192 (7)	3·7 (2)
C2	0·1706 (5)	0·3167 (6)	0·0264 (7)	3·6 (2)
C3	0·2584 (6)	0·2928 (7)	0·0192 (7)	4·1 (3)
C4	0·3112 (6)	0·2094 (7)	0·1103 (8)	4·4 (3)
C5	0·2554 (6)	0·1844 (7)	0·1702 (7)	4·2 (3)
C6	0·1835 (5)	0·0476 (7)	−0·2110 (6)	3·5 (2)
C7	0·2764 (5)	0·0245 (8)	−0·1270 (6)	3·5 (2)
C8	0·2717 (6)	−0·0846 (7)	−0·0692 (7)	3·7 (2)
C9	0·1786 (6)	−0·1345 (7)	−0·1208 (7)	3·8 (3)
C10	0·1232 (5)	−0·0508 (7)	−0·2093 (6)	3·5 (2)
C11	0·0950 (8)	0·2726 (10)	0·1658 (10)	6·3 (4)
C12	0·0970 (9)	0·4095 (8)	−0·0467 (10)	6·7 (4)
C13	0·2962 (10)	0·3655 (10)	−0·0528 (12)	7·8 (6)
C14	0·4163 (7)	0·1799 (12)	0·1501 (12)	8·1 (5)
C15	0·2877 (10)	0·1090 (11)	0·2775 (9)	7·0 (5)
C16	0·1544 (7)	0·1523 (9)	−0·2991 (8)	5·1 (3)
C17	0·3649 (7)	0·0846 (9)	−0·1232 (9)	5·5 (4)
C18	0·3546 (7)	−0·1478 (10)	0·0237 (7)	5·5 (3)
C19	0·1504 (7)	−0·2631 (7)	−0·0948 (9)	5·1 (4)
C20	0·0263 (6)	−0·0778 (9)	−0·2988 (7)	4·8 (3)

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* Lists of structure factors, anisotropic thermal parameters, additional distances and angles, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44931 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2. *Selected distances* (Å) *and angles* (°)

Cp1 and Cp2 represent the centroids of cyclopentadienyl atoms C1–C5 and C6–C10 respectively.

Cp1–Yb	2·319	Te–Yb–Cp1	107·67
Cp2–Yb	2·344	Te–Yb–Cp2	113·83
C1–Yb	2·616 (7)	Te–Yb–Cp1	109·31
C2–Yb	2·605 (7)	Te–Yb–Cp2	112·59
C3–Yb	2·627 (7)	Cp1–Yb–Cp2	133·32
C4–Yb	2·621 (8)	Te–Yb–Te	52·04 (2)
C5–Yb	2·607 (8)	Yb–Te–Yb	127·96 (2)
C6–Yb	2·614 (7)	Yb–Te–Te	63·82 (2)
C7–Yb	2·659 (7)	Yb–Te–Te	64·14 (2)
C8–Yb	2·625 (7)		
C9–Yb	2·646 (7)		
C10–Yb	2·638 (7)		
Te–Yb	3·1513 (9)		
Te–Yb	3·1598 (7)		
Te–Te	2·7686 (11)		

geometry for the Te_2 unit as that found in the present work. A comparable distance for Yb–Cp is 2·347 (2) Å in $[Yb(C_5Me_5)_2(C_6H_5S)(NH_3)]$ (Zalkin, Henley & Andersen, 1987).

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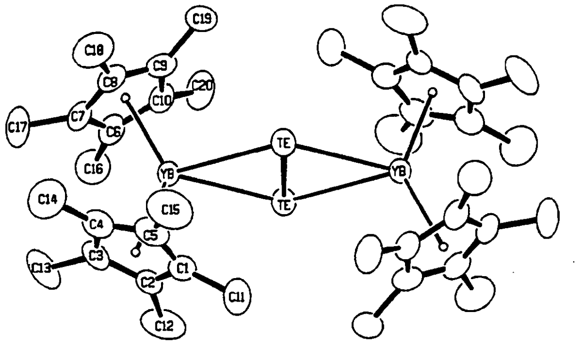

Fig. 1. *ORTEP* (Johnson, 1965) drawing of molecule; 50% probability ellipsoids.

References

Di Vaira, M., Peruzzini, M. & Stoppioni, P. (1986). *J. Chem. Soc. Chem. Commun.* p. 374.

Haendler, H. M., Mootz, D., Rabenau, A. & Rosenstein, G. (1974). *J. Solid State Chem.* **10**, 175–181.

International Tables for X-ray Crystallography (1974). Vol. IV, Table 2.2, pp. 71–102. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Zalkin, A., Henly, T. J. & Andersen, R. A. (1987). *Acta Cryst.* C43, 233–236.

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Structure of Tris(*N*-*tert*-butylformamide)dichlorodioxouranium(VI)

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Abstract. $[UO_2Cl_2\{(CH_3)_3CNHCHO\}_3]$, $M_r = 644{\cdot}38$, orthorhombic, *Pbca*, $a = 12{\cdot}793\,(3)$, $b = 18{\cdot}306\,(6)$, $c = 21{\cdot}275\,(5)$ Å, $V = 4983\,(4)$ Å^3, $Z = 8$, $D_x = 1{\cdot}718$ Mg m^{-3}, $\lambda(\text{Mo}\,K\overline{\alpha}) = 0{\cdot}71073$ Å, $\mu = 6{\cdot}42$ mm^{-1}, $F(000) = 2480$, $T = 295$ K, $R = 0{\cdot}041$ for 1033 unique observed data. The structure is of molecular type. The stereochemistry about the U atom adopts a pentagonal bipyramidal geometry, common in five-coordinate dioxouranium(VI) complexes with the linear UO_2^{2+} axial. The equatorial pentagon is planar (all five atoms are less than 0·2 Å out of the plane) but is not quite regular owing to the presence of two large Cl atoms at 2·779 (5) and 2·719 (6) Å and three O atoms at 2·44 (1), 2·39 (1) and 2·38 (1) Å.

Experimental. Crystals formed on leaving UCl_4–*N*-*tert*-butylformamide solutions for several days; crystal 0·25 × 0·2 × 0·1 mm; Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation; $\omega/2\theta$ scan technique; cell parameters obtained from least-squares procedure on 25 reflections ($8 < \theta < 12°$); decay of 7·7% (in 25·3 h) in intensities of three standard reflections monitored every 100 measurements, linearly corrected; Lorentz and polarization corrections; empirical absorption correction based on ψ scans (North, Phillips & Mathews, 1968), min. transmission 0·60; 2654 reflections collected, 2316 unique, 1033 with $I > 3\sigma(I)$; $3 < 2\theta < 40°$; $0 \le h \le 12$, $0 \le k \le 17$, $0 \le l \le 20$; structure solved by the heavy-atom method and refined by full-matrix least squares on *F*; anisotropic thermal parameters for U and Cl; scattering factors including anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974); H atoms introduced at calculated

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