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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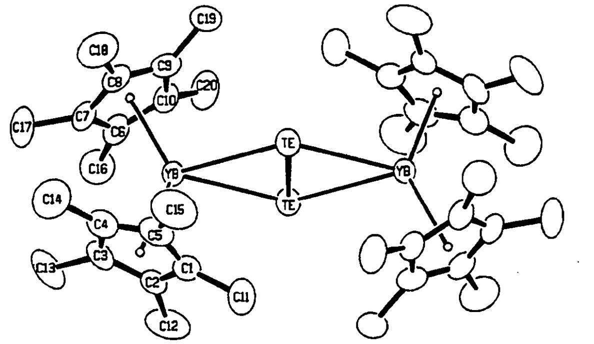

Fig. 1. *ORTEP* (Johnson, 1965) drawing of molecule; 50% probability ellipsoids.

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

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Abstract. $[UO_2Cl_2\{(CH_3)_3CNHCHO\}_3]$, $M_r = 644·38$, orthorhombic, *Pbca*, $a = 12·793$ (3), $b = 18·306$ (6), $c = 21·275$ (5) Å, $V = 4983$ (4) Å^3, $Z = 8$, $D_x = 1·718$ Mg m^{-3}, λ(Mo $K\bar{\alpha}$) = 0·71073 Å, $\mu = 6·42$ mm^{-1}, $F(000) = 2480$, $T = 295$ K, $R = 0·041$ 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

Table 1. *Positional parameters and their estimated standard deviations*

	x	y	z	B(Å^2)
U	0·71933 (6)	0·13483 (4)	0·07461 (4)	2·99 (1)*
Cl(1)	0·5029 (4)	0·1356 (3)	0·0854 (2)	3·6 (1)*
Cl(2)	0·9072 (4)	0·1424 (5)	0·1340 (3)	6·1 (2)*
O(1)	0·644 (1)	0·1080 (7)	−0·0283 (6)	3·6 (3)
O(2)	0·848 (1)	0·1353 (8)	−0·0069 (6)	4·0 (3)
O(3)	0·678 (1)	0·1514 (8)	0·1826 (6)	3·9 (3)
O(1–1)	0·714 (1)	0·2302 (7)	0·0609 (6)	3·7 (3)
O(1–2)	0·721 (1)	0·0391 (7)	0·0846 (6)	3·9 (3)
N(10)	0·541 (1)	0·0413 (9)	−0·0937 (7)	3·7 (4)
N(20)	0·970 (1)	0·1834 (9)	−0·0749 (8)	4·2 (4)
N(30)	0·623 (1)	0·150 (1)	0·2846 (7)	3·9 (4)
C(10)	0·603 (2)	0·048 (1)	−0·0467 (9)	4·0 (5)
C(11)	0·499 (2)	0·099 (1)	−0·132 (1)	4·5 (6)
C(12)	0·588 (2)	0·145 (2)	−0·161 (1)	7·9 (8)
C(13)	0·440 (2)	0·059 (1)	−0·186 (1)	6·6 (7)
C(14)	0·425 (2)	0·147 (1)	−0·094 (1)	7·5 (7)
C(20)	0·896 (2)	0·187 (1)	−0·0292 (9)	4·0 (5)
C(21)	0·019 (2)	0·115 (1)	−0·096 (1)	4·5 (6)
C(22)	0·938 (2)	0·063 (1)	−0·122 (1)	7·4 (7)
C(23)	0·093 (2)	0·136 (2)	−0·151 (1)	7·2 (7)
C(24)	0·079 (2)	0·077 (2)	−0·044 (1)	10 (1)
C(30)	0·608 (2)	0·149 (1)	0·225 (1)	5·3 (6)
C(31)	0·726 (2)	0·145 (1)	0·3158 (9)	3·8 (4)
C(32)	0·796 (2)	0·211 (1)	0·2985 (9)	4·2 (5)
C(33)	0·781 (2)	0·075 (1)	0·297 (1)	6·3 (6)
C(34)	0·706 (2)	0·147 (1)	0·387 (1)	5·8 (6)

* $B_{eq} = \sum_i \sum_j \mathbf{a}_i \mathbf{a}_j \beta_{ij}$.

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

Environment of the U atom

U–O(1–1)	1·77 (1)	O(1–1)–U–O(1–2)	176·9 (6)
U–O(1–2)	1·77 (2)	Cl(1)–U–Cl(2)	147·4 (2)
U–O(1)	2·44 (1)		
U–O(2)	2·39 (1)		
U–O(3)	2·38 (1)		
U–Cl(1)	2·779 (5)		
U–Cl(2)	2·719 (6)		

Ligands	1	2	3
O(1)–C(10)	1·28 (3)	1·23 (3)	1·27 (3)
C(10)–N(10)	1·28 (3)	1·36 (3)	1·29 (3)
N(10)–C(11)	1·43 (3)	1·46 (3)	1·48 (3)
C(11)–C(12)	1·54 (3)	1·52 (3)	1·56 (3)
C(11)–C(13)	1·57 (3)	1·55 (3)	1·52 (3)
C(11)–C(14)	1·52 (3)	1·54 (4)	1·53 (3)
O(1)–C(10)–N(10)	126 (3)	126 (3)	127 (3)
N(10)–C(11)–C(12)	111 (2)	111 (2)	111 (2)
N(10)–C(11)–C(13)	105 (2)	106 (2)	110 (2)
N(10)–C(11)–C(14)	111 (2)	114 (2)	107 (2)
C(12)–C(11)–C(13)	108 (2)	107 (2)	109 (2)
C(12)–C(11)–C(14)	111 (2)	109 (2)	108 (2)
C(13)–C(11)–C(14)	111 (2)	111 (2)	111 (2)

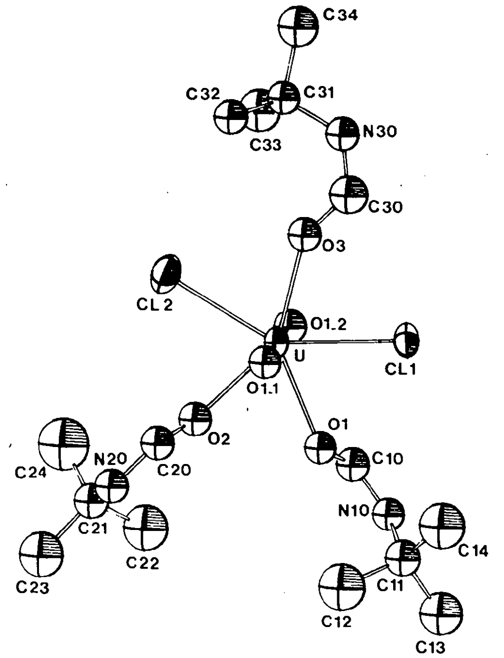

Fig. 1. *ORTEP* drawing (Johnson, 1976) of the molecule with numbering scheme.

positions, not refined but constrained to ride their C atoms (C—H = 0·95 Å and $B = 1{\cdot}3B$ of C atom), $R = 0{\cdot}041$, $wR = 0{\cdot}043$, $w = 4F_o^2/[(\sigma I)^2 + (pF_o^2)^2]$, $p = 0{\cdot}04$, $(\Delta/\sigma)_{max} = 0{\cdot}01$, $S = 1{\cdot}39$. In final difference Fourier synthesis, no peak greater than 0·8 e Å^{-3}; no correction for extinction; computations on a PDP 11/23 Plus with programs from Enraf–Nonius *SDP* (Frenz, 1983). Atomic parameters are given in Table 1, and the molecular structure is shown in Fig. 1.* Selected bond distances and angles are in Table 2.

Related literature. In the $UO_2Cl_2L_n$ complexes, n depends on the bulkiness of the ligands. $n = 2$ with the hexamethylphosphoramide (Julien, Rodier & Khodadad, 1977).

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* Lists of structure factors, anisotropic thermal parameters, complete bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44910 (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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