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A Dimer of Dichlorodioxobis(tetrahydrofuran)uranium(VI)

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Abstract. $[UO_2Cl_2(C_4H_8O)_2]$, $M_r = 485{\cdot}1$, orthorhombic, $Pnma$, $a = 23{\cdot}585\ (7)$, $b = 9{\cdot}602\ (2)$, $c = 12{\cdot}377\ (3)$ Å, $V = 2803\ (2)$ Å^3, $Z = 8$ (unit formulae), $D_x = 2{\cdot}30$ Mg m^{-3}, $\lambda(\text{Mo } K\bar{\alpha}) = 0{\cdot}71073$ Å, $\mu = 11{\cdot}36$ mm^{-1}, $F(000) = 1712$, $T = 295$ K. Final $R = 0{\cdot}038$ for 470 observed reflections. Di-μ-Cl-$[UO_2Cl_2(THF)_2]_2$ dimeric units exist (THF = tetrahydrofuran), in which each U atom is seven-coordinated in a pentagonal-bipyramidal geometry. The two independent U atoms and their eight equatorial atoms (four O of the THF molecules and four Cl atoms), all on special positions (m) of the $Pnma$ space group, are coplanar. The linear UO_2^{2+} ions and the four planar THF groups lie perpendicularly to this plane. The U(1)···U(2) distance is 4·619 (5) Å, the U—Cl distances range from 2·65 (2) to 2·83 (2) Å (Cl atoms shared by U atoms) and the average U—O$_{\text{THF}}$ distance is 2·40 (3) Å.

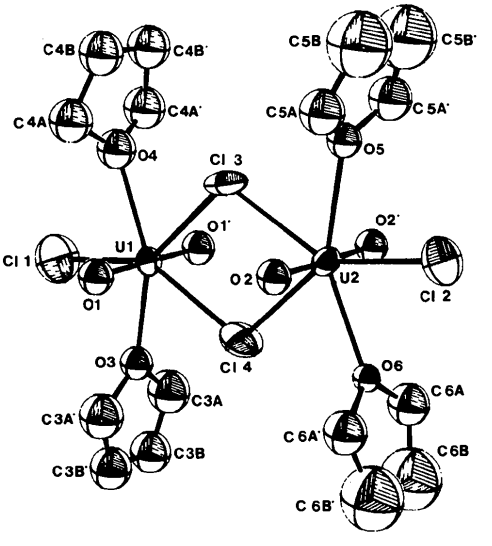

Fig. 1. Drawing of the title compound showing the atom numbering (primed atoms are related by the symmetry plane at $y = \frac{1}{4}$).

Table 1. *Positional and isotropic thermal parameters and their e.s.d.'s*

	x	y	z	B(Å^2)
U(1)	0·2093 (1)	0·250	0·5040 (2)	3·03 (8)*
Cl(1)	0·099 (1)	0·250	0·453 (2)	3·4 (8)*
O(1)	0·209 (1)	0·434 (7)	0·504 (3)	4·5 (7)
O(3)	0·206 (2)	0·250	0·317 (3)	5 (1)
C(3*A*)	0·212 (3)	0·368 (6)	0·242 (5)	8 (2)
C(3*B*)	0·210 (3)	0·321 (5)	0·134 (4)	9 (2)
O(4)	0·160 (2)	0·250	0·679 (4)	5 (1)
C(4*A*)	0·146 (2)	0·377 (5)	0·739 (4)	7 (1)
C(4*B*)	0·160 (2)	0·331 (5)	0·854 (4)	7 (2)
Cl(3)	0·286 (1)	0·250	0·679 (1)	4·7 (6)*
Cl(4)	0·321 (1)	0·250	0·427 (1)	6·1 (7)*
U(2)	0·3982 (2)	0·250	0·6027 (2)	3·12 (8)*
O(2)	0·397 (1)	0·431 (3)	0·602 (2)	3·5 (6)
Cl(2)	0·506 (1)	0·250	0·659 (2)	6·0 (7)*
O(5)	0·402 (2)	0·250	0·804 (3)	4 (1)
C(5*A*)	0·409 (2)	0·376 (5)	0·862 (4)	6 (1)
C(5*B*)	0·423 (3)	0·331 (7)	0·972 (6)	14 (3)
O(6)	0·450 (2)	0·250	0·440 (3)	3 (1)
O(6*A*)	0·469 (2)	0·367 (5)	0·377 (4)	7 (2)
O(6*B*)	0·494 (3)	0·323 (7)	0·273 (6)	14 (3)

* $B_{\text{eq}} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

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

U(1)–O(1)	1·76 (3)	U(2)–O(2)	1·74 (2)
U(1)–Cl(1)	2·66 (3)	U(2)–Cl(2)	2·65 (2)
U(1)–Cl(3)	2·83 (2)	U(2)–Cl(3)	2·81 (2)
U(1)–Cl(4)	2·80 (2)	U(2)–Cl(4)	2·83 (2)
U(1)–O(3)	2·32 (3)	U(2)–O(5)	2·49 (4)
U(1)–O(4)	2·46 (5)	U(2)–O(6)	2·36 (4)
U(1)···U(2)	4·619 (5)		
O(1)–U(1)–O(1)′	179 (1)	O(2)–U(2)–O(2)′	178 (2)

Experimental. Crystal obtained by an unexpected oxidation of bis(acetylacetonato)dichlorouranium(IV) in a THF solution; yellow crystal 0·55 × 0·35 × 0·25 mm; data collected on an Enraf–Nonius CAD-4 diffractometer using graphite-monochromated Mo $K\alpha$ radiation and ω–2θ scanning; cell parameters derived from 25 reflections ($8 < \theta < 12°$); 1354 reflections with $2 < \theta < 23°$ (h 0→10, k 0→12, l 0→24), 470 with $I > 3\sigma(I)$; three standard reflections monitored every hour showed a decay of 1·5% in 12 h; Lorentz and polarization corrections; empirical absorption correction using *DIFABS* (Walker & Stuart, 1983), transmission coefficients: min. 0·839 and max. 1·490; structure solved by the heavy-atom method and refined by full-matrix least squares (F); anisotropic thermal parameters for U and Cl; H atoms introduced in calculated positions (C—H = 0·95 Å, $B = 5$ Å^2), not refined but constrained to ride their C atoms; $R = 0{\cdot}038$, $wR = 0{\cdot}046$ ($w = 1$), $S = 2{\cdot}1$, $(\Delta/\sigma)_{\max} = 0{\cdot}03$, $\Delta\rho_{\max} = 0{\cdot}83$ e Å^{-3}; atomic scattering factors including anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974); program: Enraf–Nonius *SDP-Plus* (Frenz, 1983); PDP 11/23 Plus; Fig. 1 plotted using *ORTEP* (Johnson, 1976).

The structure of the title compound is shown in Fig. 1. Atomic parameters are given in Table 1, selected bond lengths and angles in Table 2.*

Related literature. This compound is a by-product obtained during the synthesis of [U(acac)$_2$Cl$_2$(THF)$_2$] (Doretti, Zanella, Faleschini & Faraglia, 1973).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, all bond lengths and angles and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44016 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Mononuclear Gold(I) Complex Containing a Covalently Bound Ylide Ligand. The Structure of Chloro[methyl(methylene)diphenylphosphoranyl-*C*]gold(I)

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Abstract. [AuCl{P(CH$_2$)(CH$_3$)(C$_6$H$_5$)$_2$}], $M_r = 432{\cdot}5$, monoclinic, $P2_1/n$, $a = 15{\cdot}313$ (4), $b = 11{\cdot}726$ (3), $c = 16{\cdot}712$ (4) Å, $\beta = 103{\cdot}62$ (2)°, $V = 2916$ (1) Å^3, $Z = 8$, $D_x = 2{\cdot}03$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 103{\cdot}24$ cm^{-1}, $F(000) = 1616$, $T = 298$ K. Final $R = 0{\cdot}0452$ for 2657 unique observed reflections. The structure of a mononuclear gold(I) complex containing a covalently bound phosphonium ylide ligand is reported. The asymmetric unit contains two crystallographically independent molecules, each consisting of a dimethyldiphenylphosphonium ylide linked by a methylene group to an Au$^{\rm I}$ center. The Au atoms are two-coordinate, linear, with a chloride ligand *trans* to the ylide group.

Experimental. The gold(I) ylide dimer, [Au(CH$_2$)$_2$P(C$_6$H$_5$)$_2$]$_2$, was prepared by a modification of the literature procedure (Schmidbaur & Franke, 1975). The mononuclear gold(I) complex, ClAu(CH$_2$)P(CH$_3$)(C$_6$H$_5$)$_2$, was prepared in good yield by introducing a

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