Table 1. Positional parameters and equivalent isotropic displacement parameters $\left(\AA^{2}\right)$

| $\begin{gathered} B_{\mathrm{cq}}=(4 / 3)\left[a^{2} B_{11}+\mathrm{b}^{2} B_{22}+\mathrm{c}^{2} B_{33}+\mathrm{ab}(\cos \gamma) B_{1_{2}}+a c(\cos \beta) B_{1,}+\right. \\ b c(\cos \alpha) B_{2, \mathrm{y}} \end{gathered}$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $x$ | $y$ | $z$ | $B_{\text {cq }}$ |
| Sn | 0.51399 (5) | 0.06664 (5) | 0.78956 (3) | 2.261 (7) |
| Ol | 0.5984 (6) | -0.0926 (5) | 0.8511 (3) | 3.1 (1) |
| O2 | 0.5522 (5) | -0.2481 (5) | 0.7748 (3) | 3.0 (1) |
| O3 | 0.8697 (7) | -0.3398 (7) | 0.9403 (4) | 4.7 (2) |
| N | 0.7781 (8) | -0.2506 (7) | 0.9151 (4) | 3.4 (1) |
| Cl | 0.3028 (8) | 0.0222 (8) | 0.8118 (4) | 2.6 (1) |
| C2 | 0.2139 (9) | 0.1313 (9) | 0.8185 (5) | 3.4 (2) |
| C3 | 0.0765 (9) | 0.107 (1) | 0.8415 (5) | 3.9 (2) |
| C4 | 0.0340 (9) | -0.020 (1) | 0.8569 (5) | 4.2 (2) |
| C5 | 0.124 (1) | -0.123 (1) | 0.8488 (6) | 4.8 (2) |
| C6 | 0.2592 (9) | -0.1012 (8) | 0.8252 (5) | 3.5 (2) |
| C7 | 0.5926 (8) | 0.1979 (8) | 0.8654 (4) | 2.6 (1) |
| C8 | 0.7090 (9) | 0.2747 (9) | 0.8539 (5) | 3.5 (2) |
| C9 | 0.755 (1) | 0.357 (1) | 0.9071 (6) | 4.5 (2) |
| C10 | 0.687 (1) | 0.364 (1) | 0.9700 (5) | 4.6 (2) |
| C11 | 0.570 (1) | 0.288 (1) | 0.9813 (5) | 5.0 (3) |
| C12 | 0.526 (1) | 0.2035 (9) | 0.9295 (4) | 3.8 (2) |
| C13 | 0.6480 (8) | 0.0255 (7) | 0.7045 (5) | 2.7 (1) |
| C14 | 0.608 (1) | 0.0080 (9) | 0.6378 (5) | 3.9 (2) |
| C15 | 0.706 (1) | -0.015 (1) | 0.5850 (5) | 5.1 (2) |
| C16 | 0.846 (1) | -0.024 (1) | 0.6045 (6) | 4.9 (2) |
| C17 | 0.885 (1) | -0.005 (1) | 0.6701 (6) | 5.0 (2) |
| C18 | 0.7883 (9) | 0.019 (1) | 0.7205 (5) | 4.1 (2) |
| C19 | 0.6145 (8) | -0.2068 (7) | 0.8274 (4) | 2.4 (1) |
| C20 | 0.7186 (9) | -0.2909 (8) | 0.8611 (5) | 3.2 (2) |
| C21 | 0.936 (1) | -0.294 (1) | 1.0024 (6) | 6.3 (3) |

Table 2. Selected bond distances $(\AA)$ and angles ( ${ }^{\circ}$ )

| $\mathrm{Sn}-\mathrm{Ol}$ | 2.185 (5) | $\mathrm{Sn}-\mathrm{O}^{\prime}$ | 2.367 (5) |
| :---: | :---: | :---: | :---: |
| $\mathrm{Sn}-\mathrm{Cl}$ | 2.152 (7) | $\mathrm{Sn}-\mathrm{C} 7$ | 2.134 (7) |
| $\mathrm{Sn}-\mathrm{Cl} 3$ | 2.139 (7) | $\mathrm{Ol}-\mathrm{Cl} 9$ | 1.273 (8) |
| C19-02 | 1.254 (8) | C19-C20 | 1.48 (1) |
| $\mathrm{C} 20-\mathrm{N}$ | 1.26 (1) | $\mathrm{N}-\mathrm{O} 3$ | 1.371 (8) |
| O3-C21 | 1.44 (1) |  |  |
| $\mathrm{Ol}-\mathrm{Sn}-\mathrm{O}^{\prime}$ | 173.2 (2) | $\mathrm{Ol}-\mathrm{Sn}-\mathrm{Cl}$ | 95.3 (2) |
| $\mathrm{Ol}-\mathrm{Sn}-\mathrm{C} 7$ | 88.2 (2) | $\mathrm{Ol}-\mathrm{Sn}-\mathrm{Cl} 3$ | 92.1 (2) |
| $\mathrm{O}^{\prime}-\mathrm{Sn}-\mathrm{Cl}$ | 90.9 (2) | O2'-Sn-C7 | 86.9 (2) |
| O2'-Sn-C13 | 85.7 (2) | $\mathrm{Cl}-\mathrm{Sn}-\mathrm{C} 7$ | 110.0 (3) |
| $\mathrm{Cl}-\mathrm{Sn}-\mathrm{Cl} 3$ | 134.0 (3) | $\mathrm{C} 7-\mathrm{Sn}-\mathrm{Cl} 3$ | 115.6 (3) |
| $\mathrm{Sa}-\mathrm{Ol}-\mathrm{Cl} 9$ | 123.1 (4) | $\mathrm{Sn}-\mathrm{O}^{\prime}-\mathrm{Cl} 9^{\prime}$ | 146.0 (5) |
| $\mathrm{O} 1-\mathrm{C} 19-\mathrm{O} 2$ | 123.0 (7) | $\mathrm{Ol}-\mathrm{Cl} 9-\mathrm{C} 20$ | 117.8 (6) |
| $\mathrm{O} 2-\mathrm{C} 19-\mathrm{C} 20$ | 119.1 (6) | $\mathrm{N}-\mathrm{C} 20-\mathrm{C} 19$ | 118.9 (7) |
| $\mathrm{O} 3-\mathrm{N}-\mathrm{C} 20$ | 111.8 (7) | $\mathrm{N}-\mathrm{O} 3-\mathrm{C} 21$ | 111.6 (7) |
| Symmetry code: (') $1-x, \frac{1}{2}-y, \frac{3}{2}-z$. |  |  |  |



Fig. 1. Structure of the asymmetric unit of the polymer.

Related literature. Tiekink (1991) has reviewed the structures of triorganotin carboxylates.

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# Structure of $\left[\mathrm{IrCl}_{\mathbf{2}}(\mathbf{C O})\left(\mathbf{P E t}_{\mathbf{3}}\right)_{\mathbf{2}}(\mathbf{S O C l})\right]$ 

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#### Abstract

Carbonyldichloro(sulfur monoxide chloride)bis(triethylphosphine)iridium(III), $\quad\left[\mathrm{IrCl}_{2}(\mathrm{CO})\right.$ $\left.\left(\mathrm{C}_{6} \mathrm{H}_{15} \mathrm{P}\right)_{2}(\mathrm{SOCl})\right], \quad M_{r}=610.96$, monoclinic, $P 2_{1} / c$, $a=14.5752$ (17),$\quad b=9.7304$ (8), $\quad c=15.163$ (5) $\AA$,


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Table 1. Atomic coordinates and equivalent isotropic thermal parameters $\left(\AA^{2}\right)$

| $U_{\text {eq }}=(1 / 3) \sum_{i} \sum_{j} U_{i j} a_{i}^{*} a_{j}^{*} \mathbf{a}_{i} \cdot \mathbf{a}_{j}$. |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $x$ | $y$ | $z$ | $U_{\text {eq }}$ |
| Ir | 0.258880 (20) | -0.08396 (4) | 0.192210 (20) | 0.03610 (23) |
| P (2) | 0.16359 (18) | 0.0920 (3) | 0.24370 (18) | 0.0438 (15) |
| $\mathrm{Cl}(1)$ | 0.35738 (18) | -0.0608 (3) | 0.33320 (18) | 0.0515 (16) |
| $\mathrm{Cl}(2)$ | 0.34329 (21) | 0.0982 (4) | 0.13402 (21) | 0.0648 (19) |
| P(1) | 0.36319 (19) | -0.2549 (4) | 0.14951 (21) | 0.0545 (18) |
| S | 0.17658 (22) | -0.0676 (4) | 0.05226 (19) | 0.0592 (18) |
| $\mathrm{Cl}(3)$ | 0.04967 (23) | -0.1759 (5) | 0.06788 (25) | 0.085 (3) |
| $\mathrm{O}(1)$ | 0.2188 (7) | -0.1410 (11) | -0.0163 (5) | 0.078 (6) |
| C(2) | 0.1859 (7) | -0.2261 (13) | 0.2331 (7) | 0.046 (6) |
| $\mathrm{O}(2)$ | 0.1477 (6) | -0.3067 (9) | 0.2589 (6) | 0.063 (6) |
| C(III) | 0.3076 (9) | -0.4027 (12) | 0.0913 (8) | 0.059 (7) |
| C(112) | 0.3641 (9) | -0.5219 (12) | 0.0760 (8) | 0.062 (8) |
| C(121) | 0.4326 (11) | -0.3339 (22) | 0.2425 (13) | 0.135 (16) |
| $\mathrm{C}(122)$ | 0.3755 (16) | -0.4124 (21) | 0.3022 (11) | 0.126 (16) |
| C(131) | 0.4327 (14) | -0.1731 (21) | 0.0628 (15) | 0.065 (14) |
| C(132) | 0.5196 (16) | -0.251 (3) | 0.0512 (17) | 0.089 (17) |
| C(133) | 0.4801 (20) | -0.220 (4) | 0.1215 (22) | 0.051 (11) |
| C(134) | 0.476 (3) | -0.191 (5) | 0.028 (3) | 0.061 (12) |
| C(211) | 0.2302 (8) | 0.2228 (13) | 0.3102 (8) | 0.061 (8) |
| C(212) | 0.1753 (10) | 0.3368 (14) | 0.3458 (9) | 0.075 (9) |
| C(221) | 0.0853 (8) | 0.1828 (12) | 0.1596 (8) | 0.056 (7) |
| C(222) | 0.1335 (9) | 0.2889 (13) | 0.1054 (9) | 0.071 (9) |
| C(231) | 0.0826 (8) | 0.0238 (14) | 0.3152 (8) | 0.058 (7) |
| C(232) | 0.1250 (9) | -0.0363 (15) | 0.4011 (8) | 0.068 (8) |

Table 2. Bond lengths $(\AA)$ and angles $\left({ }^{\circ}\right)$

| $\mathrm{Ir}-\mathrm{P}(1)$ | 2.399 (3) | $\mathrm{P}(2)-\mathrm{C}(231) \quad 1.82$ | 1.829 (12) |
| :---: | :---: | :---: | :---: |
| $\mathrm{Ir}-\mathrm{P}(2)$ | 2.398 (3) | $\mathrm{S}-\mathrm{Cl}(3) \quad 2.16$ | 2.168 (5) |
| $\mathrm{Ir}-\mathrm{Cl}(1)$ | 2.426 (3) | $\mathrm{S}-\mathrm{O}(1) \quad 1.46$ | 1.462 (10) |
| $\mathrm{Ir}-\mathrm{Cl}(2)$ | 2.391 (3) | $\mathrm{C}(2)-\mathrm{O}(2) \quad 1.06$ | 1.065 (14) |
| Ir -S | 2.304 (3) | $\mathrm{C}(111)-\mathrm{C}(112) \quad 1.45$ | 1.458 (18) |
| $\mathrm{Ir}-\mathrm{C}(2)$ | 1.898 (11) | $\mathrm{C}(121)-\mathrm{C}(122) \quad 1.5$ | 1.51 (3) |
| $\mathrm{P}(1)-\mathrm{C}(111)$ | 1.822 (13) | $\mathrm{C}(131)-\mathrm{C}(132) \quad 1.50$ | 1.50 (3) |
| $\mathrm{P}(1)-\mathrm{C}(121)$ | 1.798 (19) | $\mathrm{C}(133)-\mathrm{C}(134) \quad 1.45$ | 1.45 (6) |
| $\mathrm{P}(1)-\mathrm{C}(131)$ | 1.932 (22) | $\mathrm{C}(211)-\mathrm{C}(212) \quad 1.50$ | 1.507 (19) |
| $\mathrm{P}(1)-\mathrm{C}(133)$ | 1.84 (3) | $\mathrm{C}(221)-\mathrm{C}(222) \quad 1.5$ | 1.544 (18) |
| $\mathrm{P}(2)-\mathrm{C}(211)$ | 1.823 (12) | $\mathrm{C}(231)-\mathrm{C}(232) \quad 1.4$ | 1.486 (18) |
| $\mathrm{P}(2)-\mathrm{C}(221)$ | 1.825 (12) |  |  |
| $\mathrm{P}(2)-\mathrm{Ir}-\mathrm{P}(1)$ | 175.67 (10) | $\mathrm{Ir}-\mathrm{P}(2)-\mathrm{C}(22 \mathrm{I})$ | 117.0 (4) |
| $\mathrm{Cl}(1)-\mathrm{Ir}-\mathrm{P}(1)$ | 88.78 (10) | $\mathrm{Ir}-\mathrm{P}(2)-\mathrm{C}(231)$ | 112.3 (4) |
| $\mathrm{Cl}(2)-\mathrm{Ir}-\mathrm{P}(1)$ | 92.30 (11) | $\mathrm{C}(111)-\mathrm{P}(1)-\mathrm{C}(121)$ | 1) 102.2 (7) |
| $\mathrm{P}(1)-\mathrm{Ir}-\mathrm{S}$ | 94.12 (11) | $\mathrm{C}(111)-\mathrm{P}(1)-\mathrm{C}(131)$ | (1) 103.6 (8) |
| $\mathrm{P}(1)-\mathrm{Ir}-\mathrm{C}(2)$ | 89.1 (3) | $\mathrm{C}(111)-\mathrm{P}(1)-\mathrm{C}(133)$ | ) 113.7 (11) |
| $\mathrm{P}(2)-\mathrm{Ir}-\mathrm{Cl}(1)$ | 87.05 (10) | $\mathrm{C}(121)-\mathrm{P}(1)-\mathrm{C}(131)$ | (3) 114.7 (9) |
| $\mathrm{P}(2)-\mathrm{Ir}-\mathrm{Cl}(2)$ | 86.46 (10) | $\mathrm{C}(211)-\mathrm{P}(2)-\mathrm{C}(221)$ | 1) 106.7 (6) |
| $\mathrm{P}(2)-\mathrm{Ir}-\mathrm{S}$ | 89.79 (11) | $\mathrm{C}(211)-\mathrm{P}(2)-\mathrm{C}(231)$ | 1) 105.3 (6) |
| $\mathrm{P}(2)-\mathrm{Ir}-\mathrm{C}(2)$ | 92.3 (3) | $\mathrm{C}(221)-\mathrm{P}(2)-\mathrm{C}(231)$ | ) 101.4 (6) |
| $\mathrm{Cl}(1)-\mathrm{Ir}-\mathrm{Cl}(2)$ | 88.99 (10) | $\mathrm{Ir}-\mathrm{S}-\mathrm{Cl}(3)$ | 102.44 (17) |
| $\mathrm{Cl}(1)-\mathrm{Ir}-\mathrm{S}$ | 169.49 (11) | $\mathrm{Ir}-\mathrm{S}-\mathrm{O}(1)$ | 113.9 (4) |
| $\mathrm{Cl}(1)-\mathrm{Ir}-\mathrm{C}(2)$ | 94.1 (3) | $\mathrm{Cl}(3)-\mathrm{S}-\mathrm{O}(1)$ | 106.5 (4) |
| $\mathrm{Cl}(2)-\mathrm{Ir}-\mathrm{S}$ | 80.81 (11) | $\mathrm{Ir}-\mathrm{C}(2)-\mathrm{O}(2)$ | 177.0 (10) |
| $\mathrm{Cl}(2)-\mathrm{Ir}-\mathrm{C}(2)$ | 176.6 (3) | $\mathrm{P}(1)-\mathrm{C}(111)-\mathrm{C}(112)$ | 2) $\quad 118.7$ (9) |
| $\mathrm{S}-\mathrm{Ir}-\mathrm{C}(2)$ | 96.0 (3) | $\mathrm{P}(1)-\mathrm{C}(121)-\mathrm{C}(122)$ | ) 112.8 (14) |
| $\mathrm{Ir}-\mathrm{P}(1)-\mathrm{C}(111)$ | 114.9 (4) | $\mathrm{P}(1)-\mathrm{C}(131)-\mathrm{C}(132)$ | ) 113.4 (16) |
| $\mathrm{Ir}-\mathrm{P}(1)-\mathrm{C}(121)$ | 113.4 (6) | $\mathrm{P}(1)-\mathrm{C}(133)-\mathrm{C}(134)$ | 4) 110.2 (26) |
| $\mathbf{I r}-\mathbf{P}(1)-\mathbf{C}(131)$ | 107.7 (7) | $\mathrm{P}(2)-\mathrm{C}(211)-\mathrm{C}(212)$ | 2) 116.3 (9) |
| $\mathbf{I r}-\mathbf{P}(1)-\mathbf{C}(133)$ | 124.8 (10) | $\mathrm{P}(2)-\mathrm{C}(221)-\mathrm{C}(222)$ | 2) $\quad 114.1$ (8) |
| $\mathrm{Ir}-\mathrm{P}(2)-\mathrm{C}(211)$ | 112.9 (4) | $\mathrm{P}(2)-\mathrm{C}(23 \mathrm{I})-\mathrm{C}(232)$ | 2) 115.8 (9) |

Experimental. The title compound was prepared by oxidative addition of $\mathrm{SOCl}_{2}$ to $\left[\mathrm{IrCl}(\mathrm{CO})\left(\mathrm{PEt}_{3}\right)_{2}\right]$; crystals were obtained from $\mathrm{CH}_{2} \mathrm{Cl}_{2}$ /hexane. A colourless irregular column-shaped crystal, $0.25 \times$ $0.30 \times 0.75 \mathrm{~mm}$, was mounted on a CAD-4 diffractometer (graphite-monochromated Mo $K \alpha$ Xradiation). Cell parameters were refined against the positions of 25 centred reflections with $28<2 \theta<$ $30^{\circ}$. For data collection $T=183 \mathrm{~K}, \omega-2 \theta$-scan mode, $2 \theta_{\text {max }}=50^{\circ}, h-17 \rightarrow 17, k 0 \rightarrow 11, l 0 \rightarrow 18$. Two standard reflections varied randomly by $\pm 7 \%$
but did not indicate significant crystal movement or decay. Of the 4130 reflections collected, 3739 were unique ( $R_{\text {int }} 0.043$ ) and 2803 with $F>6 \sigma(F)$ were used for structure solution (from a Patterson synthesis followed by iterative cycles of least-squares refinement and difference Fourier synthesis) and refinement [using full-matrix least squares on $F$ (SHELX76; Sheldrick, 1976)]. At isotropic convergence, corrections (maximum 1.448, minimum 0.771) for absorption were applied empirically using DIFABS (Walker \& Stuart, 1983). One of the ethyl groups on $\mathrm{P}(1)$ was disordered: a model involving two partly occupied orientations [C(131) and C(132) $0.53, \mathrm{C}(133)$ and $\mathrm{C}(134)$ 0.47] was applied. Anisotropic thermal parameters were refined for all non- H atoms except C atoms in the minor component of the disorder; H atoms were included in fixed calculated positions; no secondary-extinction parameter. At final convergence, $R=0.0448, w R=0.0504, S=1.11$ for 208 parameters, $(\Delta / \sigma)_{\text {max }}=0.03$ in final cycle, maximum and minimum residues in the final $\Delta F$ synthesis were 1.98 and $-2.35 \mathrm{e} \AA^{-3}$, respectively. The weighting scheme $w^{-1}=\sigma^{2}(F)+0.000137 F^{2}$ gave satisfactory agreement analyses. Scattering factors were inlaid (Sheldrick, 1976) except for Ir (Cromer \& Mann, 1968). Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1, while selected bond lengths and angles appear in Table 2.* The atom-numbering scheme for the molecule is shown in Fig. 1, which was generated using the version of ORTEP included in the GX crystallographic program system (Mallinson \& Muir,


Fig. 1. A general view of the molecule showing the atomnumbering scheme. Thermal ellipsoids are drawn at the $30 \%$ probability level, except those of C and H which have artificial radii of 0.15 and $0.10 \AA$, respectively, for clarity. Only the major component of the disordered ethyl group is shown.
1985). Molecular geometry calculations were performed using CALC (Gould \& Taylor, 1985).

Related literature. Other small molecules such as $\mathrm{PF}_{4} \mathrm{Cl}, \mathrm{CF}_{3} \mathrm{Br}$ and $\mathrm{CF}_{3} \mathrm{I}$ undergo oxidative addition at $\mathrm{Ir}^{\mathrm{I}}$ and $\mathrm{Rh}^{\mathrm{I}}$ centres and we have determined the structures of some of the resulting $\mathrm{Ir}^{\mathrm{III}}$ and $\mathrm{Rh}^{\mathrm{III}}$ products (Blake, Cockman, Ebsworth, Henderson, Holloway, Pilkington \& Rankin, 1987; Blake, Ebsworth, Holloway \& Rieland, 1992).

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# Structure of Pentakis( $N, N$-dimethylformamide)dioxouranium(VI) Tetrafluoroborate 

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#### Abstract

UO}_{2}\left(\mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}\right)_{5}\right]\left(\mathrm{BF}_{4}\right)_{2}, \quad M_{r}=809.11\), monoclinic, $C 2 / c, a=21.077$ (5), $b=13.296$ (3), $c=$ 11.525 (2) $\AA, \beta=112.24$ (2) ${ }^{\circ}, V=2989$ (1) $\AA^{3}, Z=$ $4, D_{x}=1.798 \mathrm{~g} \mathrm{~cm}^{-3}, \lambda\left(\mathrm{Mo}^{\prime} K \alpha_{1}\right)=0.71073 \AA, \mu=$ $52.34 \mathrm{~cm}^{-1}, F(000)=1560, T=295 \mathrm{~K}, R=0.029$ for 1935 independent observed reflections with $I>$ $3 \sigma(I)$. The structure consists of packed $\mathrm{UO}_{2}(\mathrm{dmf})_{s}$ cations [ $\mathrm{dmf}=\left(\mathrm{CH}_{3}\right)_{2} \mathrm{NCHO}$ ] and $\mathrm{BF}_{4}$ anions. The linear $\mathrm{UO}_{2}$ group is equatorially surrounded by five O atoms belonging to dmf molecules. The uranyl distance of 1.762 (3) $\AA$ is typical for the $\mathrm{UO}_{2}$ group and the equatorial $\mathrm{U}-\mathrm{O}$ distances fall in the range 2.334 (5)-2.383 (3) $\AA$.


Experimental. A yellow single crystal of dimensions $0.35 \times 0.35 \times 0.30 \mathrm{~mm}$, grown during the reaction between tetrafluoroboric acid and $\mathrm{UO}_{3}$ in aqueous dmf solution, was used for data collection on an Enraf-Nonius CAD-4 diffractometer with graphite monochromator. Lattice parameters were determined by least-squares procedure from the setting angles of 25 reflections with $\theta=8-12^{\circ}$. Data were collected up to $2 \theta=50^{\circ}$ and measured for $0 \leq h \leq$ $25,0 \leq k \leq 15,-13 \leq l \leq 13$, with $\omega-2 \theta$ scans, $\omega$-scan width $(0.80+0.35 \tan \theta)^{\circ}$ at $1.54-10^{\circ} \mathrm{min}^{-1}$. Three standard reflections measured every hour ( $\overline{151}$, 731,423 ) showed a loss of intensity of $4.7 \%$ in 36 h ; a linear correction was applied. Lorentz-polarization correction and an empirical absorption correction using the program DIFABS (Walker \& Stuart, 1983), maximum and minimum transmission 0.801 and
1.298, were applied. 2832 reflections were measured, 2626 unique ( $R_{\text {int }}=0.024$ ), of which 1935 with $I>$ $3 \sigma(I)$ were used in structure solution and refinement. The structure was solved by the heavy-atom method and refined by full-matrix least-squares procedures based on $F$, with anisotropic thermal parameters. 178 parameters were refined; H atoms not introduced. All calculations were performed on a MicroVAX II computer with the Enraf-Nonius Structure Determination Package (Frenz, 1985). The U atom lies on the diad axis, as do the O and N atoms of a dmf molecule $[\mathrm{O}(2)$ and $\mathrm{N}(2)$ introduced in refinements with an occupation factor of 0.5]. Atomic scattering factors including anomalous-scattering contributions were taken from International Tables for X-ray Crystallography (1974, Vol. IV). Minimized function: $\sum w\left(\left|F_{o}\right|-\left|F_{c}\right|\right)^{2}$, where $w=4 F_{o} / \sigma^{2}(I)$ with $\sigma^{2}(I)=$ $\left[\sigma^{2}\left(I_{c}\right)+\left(p F_{o}\right)^{2}\right], p=0.04$. Final $R=0.029, w R=$ $0.034, S=3.60,(\Delta / \sigma)_{\max }=0.01$, highest peak in the final difference Fourier map $=0.499$ e $\AA^{-3}$. The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1.* Bond lengths and angles are listed in Table 2. A perspective view of the molecular structure with the atom-numbering scheme is shown in Fig. 1.

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[^1]:    * Lists of structure factors, anisotropic thermal parameters, and bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55132 ( 11 pp .). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU0327]

