Tableau 2. *Distances interatomiques* (Å), *angles de liaison* (°) *et écarts-type*

(1) Environnement de l'uranium

U–O(1)	1,760 (12)	O(1)–U–O(2)	177,4 (6)
U–O(2)	1,778 (13)	O(5)–U–O(4*B*)	73,8 (5)
U–O(5)	2,309 (13)	O(3*B*)–U–O(4*B*)	69,5 (4)
U–O(3*A*)	2,396 (11)	O(3*B*)–U–O(3*A*)	71,5 (4)
U–O(4*A*)	2,362 (13)	O(3*A*)–U–O(4*A*)	69,8 (4)
U–O(3*B*)	2,403 (14)	O(4*A*)–U–O(5)	75,4 (4)
U–O(4*B*)	2,384 (12)		

(2) *β*-Dicétones

	A	*B*
O(4)–C(9)	1,27 (2)	1,25 (2)
C(9)–C(8)	1,35 (3)	1,36 (3)
C(8)–C(1)	1,42 (3)	1,38 (3)
C(1)–O(3)	1,25 (2)	1,25 (2)
C(9)–C(10)	1,47 (3)	1,54 (3)
C(10)–F(1)	1,33 (2)	1,27 (3)
C(10)–F(2)	1,32 (3)	1,26 (3)
C(10)–F(3)	1,28 (3)	1,28 (4)
C(1)–C(2)	1,49 (2)	1,48 (3)
$\langle$C–C$\rangle_{\text{phényl}}$	1,37 (3)	1,37 (3)
O(4)–C(9)–C(8)	125 (2)	129 (2)
C(9)–C(8)–C(1)	124 (2)	123 (2)
C(8)–C(1)–O(3)	123 (2)	122 (2)
$\langle$C–C–C$\rangle_{\text{phényl}}$	120 (2)	120 (2)
$\langle$F–C(10)–F$\rangle$	106 (2)	106 (2)

(3) hmpa

P–O(5)	1,492 (13)	O(5)–P–N(1)	109,8 (9)
P–N(1)	1,63 (2)	O(5)–P–N(2)	113,7 (9)
P–N(2)	1,62 (2)	O(5)–P–N(3)	108,9 (9)
P–N(3)	1,61 (2)	P–N(1)–C(11)	125 (2)
N(1)–C(11)	1,39 (4)	P–N(1)–C(12)	12 (2)
N(1)–C(12)	1,42 (4)	P–N(2)–C(21)	127 (2)
N(2)–C(21)	1,40 (4)	P–N(2)–C(22)	118 (2)
N(2)–C(22)	1,43 (4)	P–N(3)–C(31)	121 (2)
N(3)–C(31)	1,47 (4)	P–N(3)–C(32)	113 (2)
N(3)–C(32)	1,47 (4)		

dicétones se placent de manière à ce que les phényls se trouvent voisins. L'angle entre les plans des deux phényls *A* et *B* est de 106°.

Les groupements CF_3. Les fluors des groupements CF_3 sont difficiles à localiser avec précision étant donné leurs très grandes amplitudes de vibration. Les valeurs moyennes des distances C—F de 1,31 (3) Å pour la molécule *B* sont cependant raisonnables et en bon accord avec celles trouvées dans la littérature.

Le ligande hexaméthylphosphoramide. L'atome de phosphore se situe pratiquement dans le plan moyen du pentagone [distance du phosphore au plan moyen 0,125 (5) Å]. L'angle U—O(5)—P vaut 166 (2)°, beaucoup plus éloigné de la linéarité que dans $UO_2(NO_3)_2$(hmpa)$_2$ (Charpin, Lance, Soulié & Vigner, 1985) dans lequel l'angle U—O—P est de 174 (2)°. Cet angle qui correspond à une rotation du phosphore vers O(4*B*) pourrait s'expliquer par l'encombrement stérique des autres ligandes.

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Bis(2-ethylaminopyridine 1-oxido)copper(II)

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Abstract. [$Cu(C_7H_9N_2O)_2$], $M_r = 337{\cdot}9$, orthorhombic, *Pbca*, $a = 9{\cdot}077$ (3), $b = 15{\cdot}372$ (7), $c = 10{\cdot}827$ (4) Å, $V = 1511$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}49$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 15{\cdot}1$ cm^{-1}, $F(000) = 700$, $T = 298$ K, final $R = 0{\cdot}036$ for 953 observed reflections. The complex has $\bar{1}$ (C_i) symmetry. Deprotonated 2-ethylaminopyridine 1-oxide acts as a bidentate ligand with Cu coordinated in a pure

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nondistorted square-planar configuration. Cu—O 1·918 (2), Cu—N 1·899 (2) Å, angle O(1)—Cu—N(2) 83·53 (8)°.

Introduction. Molecular complexes of Cu^{II} have recently received considerable attention because of their solubility in lipids and their anti-inflammatory activity. This activity seems to be associated with a square-planar coordination of the central Cu. Cu is a suitable metal for pharmaceutical purposes, because it is essential for normal metabolism of human tissues and is of relatively low toxicity (Sorenson, 1976; Leuthauser, Oberley, Oberley, Sorenson & Ramakrishna, 1981).

West & Roberts (1984) have prepared and spectrally characterized molecular planar Cu^{II} complexes of deprotonated 2-alkylaminopyridine *N*-oxides and 2-aminopicoline *N*-oxides. We can now confirm that, as suggested, the title complex has a square-planar coordination and *O*,*N*-chelation in a *trans* arrangement.

Experimental. A tan material was synthesized by Professor D. X. West of Illinois State University. Recrystallization from $CHCl_3$; Syntex $P2_1$ diffractometer: cell parameters by least squares from setting angles of 15 reflections; variable θ–2θ scan, scan rate 1·0–15° min^{-1}, $2\theta_{max} = 65°$; two standards measured every 50 reflections, no significant change; corrections for Lorentz and polarization effects, not for absorption; index range h 0–13, k 0–20, l 0–16. 3058 reflections measured; 953 $[I > 3\sigma(I)]$ considered observed. Atomic scattering factors from Cromer & Mann (1968), and Stewart, Davidson & Simpson (1965). Structure determined by direct methods with *MULTAN*80 (Main *et al.*, 1980). Eight non-H atoms located on *E* map; remainder including Cu and H atoms from difference Fourier synthesis; full-matrix least-squares refinement on *F* of all atoms, isotropic temperature factors for H and anisotropic for non-H atoms. $R = 0{\cdot}036$, $wR = 0{\cdot}038$, $S = 1{\cdot}352$, $(\Delta/\sigma)_{max} = 1{\cdot}00$, $(\Delta/\sigma)_{average} = 0{\cdot}17$. No peaks > 0·3 e $Å^{-3}$ in final difference Fourier map. *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) used.

Discussion. Positional and thermal parameters of the title compound are listed in Table 1.* The atomic numbering and bond distances and angles are shown in Fig. 1.

The structure of the centrosymmetric formula unit is shown in Fig. 2. Cu is coordinated solely to two chelating ligands in a *trans*-square-planar configuration. Clearly, the ethyl groups can prevent the Cu atom from completing the coordination sphere with anion or solvent molecules, whereas in the corresponding dimethylamino complex the methyl groups cannot hinder the long-range coordination of the ClO_4^- ion (West, Pavkovic & Brown, 1980). Cu is bonded to O(1) and N(2) with bond lengths of 1·918 (2) and 1·899 (2) Å. This is a shorter Cu—N(amine) bond

Table 1. *Final positional parameters and equivalent isotropic temperature factors* ($Å^2 \times 10^2$)

$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$

	x	y	z	U_{eq}
Cu	0·5	0·0	0·0	3·52
O(1)	0·6305 (2)	0·0900 (1)	0·0553 (2)	4·73
N(1)	0·6273 (3)	0·1583 (1)	−0·230 (2)	4·37
N(2)	0·4595 (2)	0·0794 (1)	−0·1301 (2)	4·10
C(1)	0·5338 (3)	0·1524 (2)	−0·1229 (2)	3·96
C(2)	0·5336 (3)	0·2258 (2)	−0·2018 (3)	4·90
C(3)	0·6205 (4)	0·2963 (2)	−0·1787 (3)	6·01
C(4)	0·7126 (4)	0·2966 (2)	−0·0770 (3)	6·32
C(5)	0·7145 (3)	0·2272 (2)	−0·0000 (3)	5·84
C(6)	0·3605 (3)	0·0660 (2)	−0·2348 (3)	5·28
C(7)	0·4389 (4)	0·0399 (2)	−0·3526 (3)	6·52

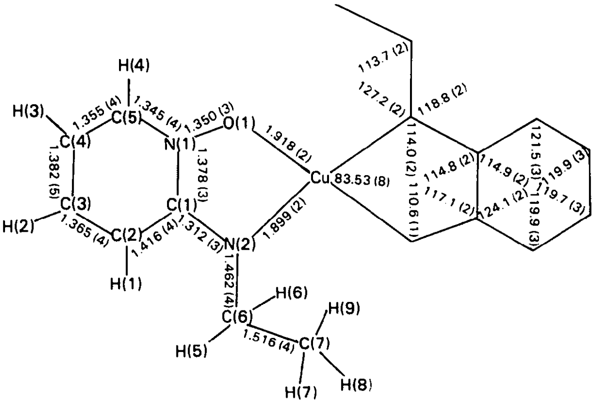

Fig. 1. Schematic diagram of the complex showing bond distances (Å) and angles (°).

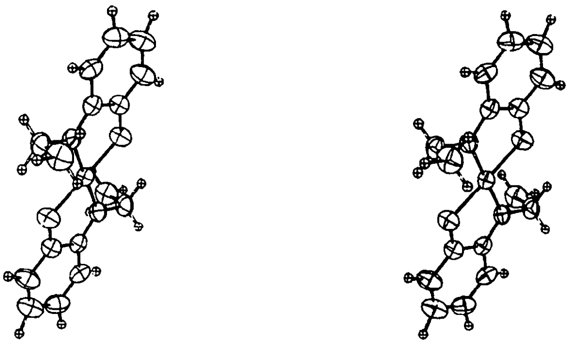

Fig. 2. Stereoscopic view of the structure. Thermal ellipsoids are drawn at the 50% probability level (Johnson, 1971).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42862 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

length than in bis(2-dimethylaminopyridine 1-oxide)-copper diperchlorate [2·052 (2) Å] or dinitrato-(*N,N,N',N'*-tetramethylethylenediamine)copper(II) [2·003 (2) Å] (Pavkovic, Miller & Brown, 1977). The Cu—O(1) (*N*-oxide oxygen) bonding distance is about the same as in the dimethyl complex, but shorter than in picolinato *N*-oxide and nicotinato *N*-oxide Cu complexes. The N(1)—O(1) distances in the coordinated compounds are in the range 1·330–1·352 Å (Knuuttila, 1983; Knuuttila, 1982), whereas uncoordinated N—O is only 1·314 Å (Knuuttila & Knuuttila, 1983). Coordination suppresses the double-bond character of N—O when the steric conditions are favorable.

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Crystal Phases Obtained from Aqueous Solutions of Sodium Dodecyl Sulfate. The Structure of a Monoclinic Phase of Sodium Dodecyl Sulfate Hemihydrate

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Abstract. $Na^+.C_{12}H_{25}SO_4^-.\frac{1}{2}H_2O$, $M_r=297·4$, monoclinic, $C2$, $a=9·847\,(1)$, $b=5·248\,(1)$, $c=30·798\,(6)$ Å, $\beta=91·29\,(1)°$, $V=1591·1\,(5)$ Å^3, $Z=4$, $D_x=1·24$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha)=1·5418$ Å, $\mu=2·1$ mm^{-1}, $F(000)=644$, $T=285$–288 K, $R=0·073$ for 1387 observed reflections. This analysis has been carried out since crystal phases which are grown from aqueous micellar solutions can contain structural features common to micelles. The sodium dodecyl sulfate (SDS) molecules are arranged in the crystal to form a lamellar structure with layers alternately polar and apolar. In the polar region the sulfate groups are held together by sodium ions and water molecules through strong ionic interactions and hydrogen bonds. Very weak van der Waals interactions are present in the apolar region. By comparison of this structure with another crystal phase of SDS containing less water, obtained from organic solvent, it emerges that the lamellar size decreases with increasing surface area of the polar head.

Introduction. Many important aspects of micellar systems such as shape, size and water content of their interior are not yet clear (Dill, Koppel, Cantor, Dill, Bendedouch & Chen, 1984; Menger & Doll, 1984). Therefore, the knowledge of the surfactant structure and aggregation modes in the solid phase is important, in order to obtain models to use in the study of micellar solutions.

SDS forms micellar aggregates in aqueous solution at concentrations over the critical micellar concentration [$8·1\times10^{-3}$ mol dm^{-3} (Mukerjee & Mysels, 1971)]. The SDS anion is amphiphilic since it possesses the sulfate group as polar head and the nonpolar hydrocarbon chain ending with a methyl group. A structure determination of SDS has already been made on crystals grown from organic solvent [chloroform–methanol mixture, 9:1 *v:v* (Sundell, 1977)]. In spite of the poor atomic resolution, especially for some carbon

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