

## References

- ATKINSON, I. M., KEENE, F. R. & SEARLE, G. H. (1991). *J. Chem. Soc. Dalton Trans.* pp. 45–51.
- BOER, J. L. DE & DUSENBERG, A. J. M. (1984). Enraf–Nonius CAD-4F diffractometer software update, February 1984. Groningen and Utrecht, The Netherlands.
- JOHNSON, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- SARGESON, A. M. (1966). *Transition Met. Chem.* **3**, 303–343.
- SEARLE, G. H. & KEENE, F. R. (1989). *Inorg. Chim. Acta*, **155**, 125–138.
- SEARLE, G. H. & TIEKINK, E. R. T. (1989a). *Inorg. Chim. Acta*, **156**, 57–63.
- SEARLE, G. H. & TIEKINK, E. R. T. (1989b). *Acta Cryst.* **C45**, 1300–1303.
- SHELDRICK, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.

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## Complexes Between Uranyl Nitrate and Benzo-15-crown-5: Structures of the (2/1) and (1/1) Complexes of Benzo-15-crown-5–Diaquadintratodioxouranium(VI)

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**Abstract.** (1) [UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>].2C<sub>14</sub>H<sub>20</sub>O<sub>5</sub>, *M<sub>r</sub>* = 966.69, monoclinic, *P*2<sub>1</sub>/*n*, *a* = 10.891 (3), *b* = 8.312 (2), *c* = 20.507 (6) Å, β = 97.21 (2)°, *V* = 1842 (1) Å<sup>3</sup>, *Z* = 2, *D<sub>x</sub>* = 1.74 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71073 Å, μ = 42.56 cm<sup>-1</sup>, *F*(000) = 956, *T* = 295 K, *R* = 0.024 for 1994 unique reflections. (2) [UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>].C<sub>14</sub>H<sub>20</sub>O<sub>5</sub>, *M<sub>r</sub>* = 698.38, triclinic, *P*1̄, *a* = 8.477 (2), *b* = 8.809 (2), *c* = 16.700 (3) Å, α = 105.18 (2)°, β = 82.42 (2)°, γ = 110.08 (2)°, *V* = 1129 (1) Å<sup>3</sup>, *Z* = 2, *D<sub>x</sub>* = 2.05 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71073 Å, μ = 68.86 cm<sup>-1</sup>, *F*(000) = 668, *T* = 295 K, *R* = 0.033 for 2431 unique reflections. In both complexes, the crown ether molecules are hydrogen bonded to the two water molecules of the hexagonal bipyramidal [UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]. In complex (1), two crown ether molecules are linked to one U complex to form a molecular structure whereas in complex (2), each crown ether molecule is shared by two U complexes to form polymer chains.

**Introduction.** Most *f*-element salts, and particularly U salts, are known to form a large variety of adducts with crown ethers (Moody & Ryan, 1979; Rogers, 1988; Rogers, Kurihara & Benning, 1987). During the recrystallization of the adducts of uranyl nitrate with benzo-15-crown-5 from ethanol solution, well shaped crystals with different morphology and colour were obtained. These crystals have been studied by X-ray diffraction and shown to be the 1/1 and 1/2 adducts.

**Experimental.** Suitable crystals of both complexes were obtained by slow evaporation from ethanol solution of uranyl nitrate and benzo-15-crown-5.

Table 1. Data collection and refinement parameters for [UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>](benzo-15-crown-5)<sub>2</sub> (1) and [UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>](benzo-15-crown-5) (2)

	Complex (1)	Complex (2)
Crystal colour	Yellow	Yellow
Crystal size (mm)	0.35 × 0.35 × 0.20	0.40 × 0.35 × 0.20
2θ range for data collection (°)	2–50	2–44
Standard reflections	330, 404, 305	033, 133, 236
Variation (%) of standard reflections over period (h) of data collection	0.2, 44	0.3, 43
<i>hkl</i> range, <i>h</i>	0, 12	8, –8
<i>k</i>	0, 9	9, –9
<i>l</i>	–24, 24	0, 17
Absorption corrections (maximum/minimum transmission)	0.996/0.792	0.999/0.491
Total No. of reflections measured	3676	2871
No. of unique reflections	3233	2755
<i>R<sub>int</sub></i>	0.018	0.015
No. of reflections with <i>I</i> > 3σ( <i>I</i> )	1994	2431
No. of parameters	162	219
<i>R</i>	0.024	0.033
<i>wR</i> ( <i>w</i> = 1)	0.030	0.051
<i>S</i>	2.23	3.52
(Δ/ <i>σ</i> ) <sub>max</sub>	0.02	0.03
Maximum electron density (e Å <sup>-3</sup> ) in final difference map	0.849	0.658

Details of data collection and structure refinement for both compounds are summarized in Table 1. All data were collected at room temperature on an Enraf–Nonius CAD-4 diffractometer by the ω/2θ-scan method using variable scan speed (1.54–10° min<sup>-1</sup>), scan width of (0.80 + 0.35tanθ)° and graphite monochromator. Lattice parameters were determined from the setting angles of 25 selected reflections with θ between 8 and 12°. Three standard reflections were measured after each hour to monitor crystal decay; no significant variations were observed for both compounds. The data were corrected for Lorentz–polarization effects, as well as absorption using an empirical correction based on ψ scans

Table 2. Fractional coordinates and isotropic or equivalent isotropic thermal parameters ( $\text{\AA}^2$ ) for  $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2](\text{benzo-15-crown-5})_2$  (1) and  $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2](\text{benzo-15-crown-5})$  (2)

U, O and N atoms were refined anisotropically;  $B_{\text{eq}} = (4/3)\sum_i \beta_i a_i^2$ .

	x	y	z	$B_{\text{iso}}/B_{\text{eq}}$
<b>Complex (1)</b>				
U	0.000	0.000	0.000	2.136 (5)
O(21)	-0.0572 (4)	0.1673 (6)	-0.0464 (2)	3.4 (1)
O(22)	0.1244 (4)	-0.0827 (7)	-0.0843 (2)	3.4 (1)
O(23)	0.2140 (4)	0.1181 (7)	0.0094 (3)	4.2 (1)
O(24)	0.1076 (4)	0.1800 (8)	0.0861 (3)	4.8 (1)
O(25)	0.2894 (5)	0.2841 (8)	0.0861 (3)	5.6 (1)
N	0.2929 (5)	0.6972 (8)	0.4378 (3)	3.6 (1)
O(3)	0.9642 (4)	0.3305 (6)	0.1794 (2)	3.3 (1)
O(6)	0.7639 (5)	0.4414 (7)	0.0972 (3)	4.1 (1)
O(9)	0.6312 (4)	0.1533 (7)	0.0682 (3)	4.4 (1)
O(12)	0.6967 (5)	-0.0299 (7)	0.1835 (3)	4.4 (1)
O(15)	0.9448 (5)	0.0446 (6)	0.2220 (2)	4.0 (1)
C(1)	1.0329 (7)	0.1380 (9)	0.2577 (4)	3.2 (1)
C(2)	1.0458 (6)	0.2929 (9)	0.2339 (3)	3.0 (1)
C(4)	0.9631 (7)	0.492 (1)	0.1563 (4)	4.6 (1)
C(5)	0.8843 (6)	0.496 (2)	0.0902 (4)	4.6 (1)
C(7)	0.6910 (8)	0.411 (1)	0.0360 (4)	4.5 (2)
C(8)	0.5847 (8)	0.308 (1)	0.0484 (4)	4.8 (2)
C(10)	0.5464 (7)	0.054 (1)	0.0982 (4)	4.3 (2)
C(11)	0.6136 (8)	-0.086 (1)	0.1292 (4)	4.3 (2)
C(13)	0.7827 (8)	-0.149 (1)	0.2077 (4)	5.0 (2)
C(14)	0.8825 (8)	-0.075 (1)	0.2562 (4)	4.4 (2)
C(16)	1.1077 (7)	0.084 (1)	0.3132 (4)	4.2 (2)
C(17)	1.1968 (8)	0.188 (1)	0.3432 (4)	4.9 (2)
C(18)	1.2112 (8)	0.339 (1)	0.3205 (4)	5.0 (2)
C(19)	1.1350 (7)	0.393 (1)	0.2651 (4)	4.3 (2)
<b>Complex (2)</b>				
U	0.09654 (6)	0.08350 (5)	0.27603 (3)	1.725 (9)
O(30)	0.109 (1)	-0.197 (1)	0.2650 (6)	3.6 (2)
O(29)	0.102 (1)	0.362 (1)	0.2855 (6)	3.0 (2)
O(21)	0.260 (1)	0.119 (1)	0.1992 (6)	3.7 (3)
O(22)	-0.067 (1)	0.057 (1)	0.3541 (6)	3.9 (3)
O(23)	-0.084 (1)	-0.147 (1)	0.1728 (6)	3.6 (2)
O(24)	-0.108 (1)	0.094 (1)	0.1856 (7)	5.5 (3)
O(25)	-0.253 (1)	-0.119 (1)	0.0945 (7)	6.1 (3)
N(1)	-0.152 (1)	-0.055 (1)	0.1485 (7)	3.9 (3)
O(26)	0.293 (1)	0.056 (1)	0.3674 (8)	7.1 (3)
O(27)	0.296 (1)	0.306 (1)	0.3813 (6)	3.8 (2)
O(28)	0.458 (1)	0.255 (2)	0.4548 (7)	6.2 (3)
N(2)	0.354 (2)	0.209 (1)	0.4044 (7)	3.8 (3)
O(3)	-0.087 (1)	0.510 (1)	0.8687 (6)	3.0 (2)
O(6)	-0.377 (1)	0.424 (1)	0.7840 (5)	2.9 (2)
O(9)	-0.270 (1)	0.279 (1)	0.6301 (5)	2.8 (2)
O(12)	0.065 (1)	0.444 (1)	0.6090 (5)	2.8 (2)
O(15)	0.175 (1)	0.496 (1)	0.7700 (5)	2.8 (2)
C(1)	0.206 (1)	0.600 (1)	0.8505 (8)	2.2 (2)
C(2)	0.067 (2)	0.608 (1)	0.9015 (8)	2.3 (2)
C(4)	-0.236 (2)	0.544 (2)	0.9125 (9)	3.5 (3)
C(5)	-0.384 (2)	0.411 (2)	0.8697 (9)	3.6 (3)
C(7)	-0.487 (2)	0.277 (2)	0.733 (1)	3.9 (3)
C(8)	-0.442 (2)	0.278 (2)	0.6437 (9)	3.5 (3)
C(10)	-0.202 (2)	0.296 (2)	0.547 (1)	3.8 (3)
C(11)	-0.020 (2)	0.304 (2)	0.5456 (9)	3.7 (3)
C(13)	0.230 (2)	0.440 (2)	0.6230 (9)	3.5 (3)
C(14)	0.286 (2)	0.561 (2)	0.7050 (9)	3.4 (3)
C(16)	0.367 (2)	0.687 (2)	0.8763 (9)	3.3 (3)
C(17)	0.385 (2)	0.786 (2)	0.958 (1)	4.0 (3)
C(18)	0.251 (2)	0.798 (2)	1.0079 (9)	3.7 (3)
C(19)	0.087 (2)	0.708 (2)	0.9822 (9)	3.4 (3)

(North, Phillips & Mathews, 1968). For both compounds, the Patterson function revealed the position of the U atom and the subsequent difference electron density maps gave the positions of all non-H atoms. The structures were refined by full-matrix least squares (on  $F$ ) with anisotropic thermal parameters for U, N and O atoms. H atoms, introduced at calculated positions ( $C-H = 0.95 \text{ \AA}$  and  $B = 6 \text{ \AA}^2$ ), were not refined but constrained to ride on their C

Table 3. Selected bond distances ( $\text{\AA}$ ), bond angles ( $^\circ$ ) and hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) for complexes (1) and (2)

Complex (1)		Complex (2)	
<b>U environment</b>			
U—O(21)	1.754 (4)	U—O(21)	1.764 (5)
U—O(22)	2.425 (3)	U—O(22)	1.770 (5)
U—O(23)	2.514 (3)	U—O(23)	2.486 (5)
U—O(24)	2.492 (4)	U—O(24)	2.484 (6)
		U—O(26)	2.514 (6)
		U—O(27)	2.548 (5)
		U—O(29)	2.402 (5)
		U—O(30)	2.466 (5)
O(21)—U—O(22)	91.7 (1)	O(21)—U—O(22)	177.4 (3)
O(21)—U—O(23)	89.7 (1)	O(21)—U—O(23)	90.2 (2)
O(21)—U—O(24)	90.7 (2)	O(21)—U—O(24)	91.6 (3)
O(22)—U—O(23)	64.5 (1)	O(21)—U—O(26)	90.0 (3)
		O(21)—U—O(27)	88.3 (2)
		O(21)—U—O(29)	86.0 (3)
		O(21)—U—O(30)	91.2 (2)
<b>Benzo-15-crown-15</b>			
C(1)—C(2)	1.391 (7)	C(1)—C(2)	1.37 (1)
C(2)—O(3)	1.373 (6)	C(2)—O(3)	1.381 (8)
O(3)—C(4)	1.424 (9)	O(3)—C(4)	1.46 (1)
C(4)—C(5)	1.510 (7)	C(4)—C(5)	1.50 (1)
C(5)—O(6)	1.411 (6)	C(5)—O(6)	1.46 (1)
O(6)—C(7)	1.422 (6)	O(6)—C(7)	1.44 (1)
C(7)—C(8)	1.486 (8)	C(7)—C(8)	1.50 (1)
C(8)—O(9)	1.424 (7)	C(8)—O(9)	1.45 (1)
O(9)—C(10)	1.434 (6)	O(9)—C(10)	1.45 (1)
C(10)—C(11)	1.475 (7)	C(10)—C(11)	1.52 (1)
C(11)—O(12)	1.423 (6)	C(11)—O(12)	1.44 (1)
O(12)—C(13)	1.408 (7)	O(12)—C(13)	1.463 (9)
C(13)—C(14)	1.506 (8)	C(13)—C(14)	1.52 (1)
C(14)—O(15)	1.438 (6)	C(14)—O(15)	1.441 (9)
O(15)—C(1)	1.372 (6)	O(15)—C(1)	1.415 (8)
C(1)—C(16)	1.389 (7)	C(1)—C(16)	1.38 (1)
C(16)—C(17)	1.383 (8)	C(16)—C(17)	1.40 (1)
C(17)—C(18)	1.357 (9)	C(17)—C(18)	1.34 (1)
C(18)—C(19)	1.393 (8)	C(18)—C(19)	1.40 (1)
C(19)—C(2)	1.373 (7)	C(19)—C(2)	1.40 (1)
<b>Hydrogen-bond geometry</b>			
O(22)···O(3)	2.917 (7)	O(29)···O(6)	2.782 (7)
O(22)···O(9)	2.705 (7)	O(29)···O(9)	3.020 (7)
O(22)···O(15)	2.848 (6)	O(29)···O(12)	2.727 (7)
		O(30)···O(3)	3.028 (7)
		O(30)···O(9)	2.719 (7)
		O(30)···O(15)	2.881 (7)
O(3)···O(22)···O(9)	99.6 (2)	O(6)···O(29)···O(12)	106.6 (2)
O(9)···O(22)···O(15)	106.2 (2)	O(3)···O(30)···O(9)	93.7 (2)
		O(9)···O(30)···O(15)	99.8 (2)

Symmetry code: (i)  $-x, -y, 1-z$ .

atoms. All calculations were performed on a MicroVAX II computer with the *Enraf-Nonius Structure Determination Package* (Frenz, 1985). Atomic scattering factors including anomalous-scattering contributions were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).

**Discussion.** Fractional atomic coordinates are listed in Table 2,\* and selected bond distances and angles in Table 3. The atom-labelling schemes are shown in Figs. 1 and 2 for (1) and (2) respectively.

\* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond angles and distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55432 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU0322]

The complex (2) is isostructural with  $[\text{UO}_2(\text{NO}_3)_2 \cdot (\text{H}_2\text{O})_2](15\text{-crown-5})$  (Gutberlet, Dreissig, Luger, Bechthold, Maung & Knöchel, 1989).

Both structures consist of  $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2]$  and (benzo-15-crown-5) units with a ratio of metal to crown ether of 1/2 for complex (1) and 1/1 for complex (2). In (1), the U atom lies on a crystallographic centre of inversion, whereas no local symmetry is imposed on the site occupied by the U atom in (2). In both complexes, the linear uranyl ion is equatorially surrounded by six O atoms from two bidentate nitrate and two water molecules. The U—O distances [uranyl 1.75 and 1.77 (average), nitrate 2.50 and 2.50, and water 2.42 and 2.43 Å, for (1) and (2) respectively] are normal and agree with

those found in similar complexes (Charpin, Lance, Nierlich & Vigner, 1987; Ritger, Burns & Bombieri, 1983).

Although H atoms have not been observed, the  $\text{O}\cdots\text{O}$  contacts near 3 Å are indicative of hydrogen bonding between some O atoms of the crown ether and the water ligand. In both compounds, each water molecule is involved in three possible hydrogen bonds with one water molecule. In (1), two crown ether molecules are linked to one U complex to form a molecular structure as shown in Fig. 3, whereas in (2), each crown ether molecule is shared by two U units to form a polymer chain as shown in Fig. 4.

In both complexes, the bond lengths and angles of the crown ether molecules are similar to those found in other such compounds (Rogers *et al.*, 1987; Gutberlet *et al.*, 1989). The C—C bonds average 1.41 (2) and 1.44 (2) Å, and the mean C—O distances are 1.47 (3) and 1.48 (3) Å for (1) and (2), respectively.

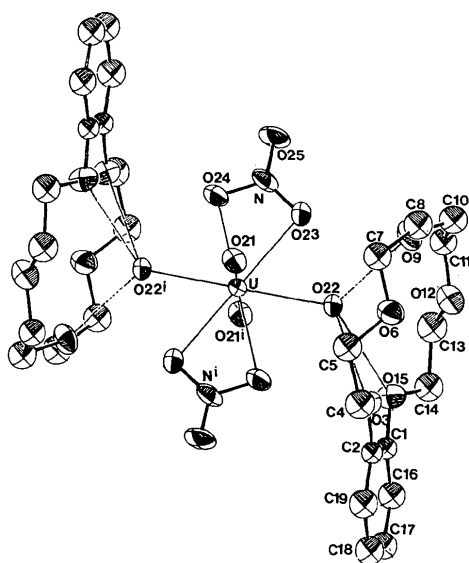


Fig. 1. ORTEP drawing (Johnson, 1976) of  $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2] \cdot (\text{benzo-15-crown-5})_2$  (1).

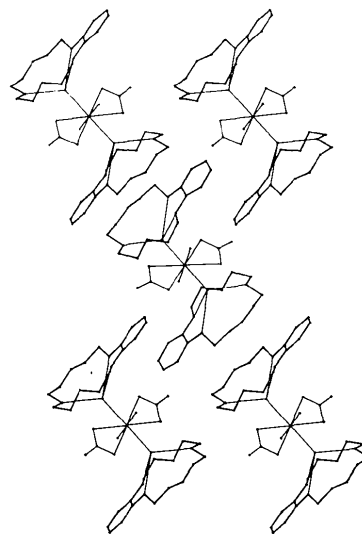


Fig. 3. Molecular packing of complex (1).

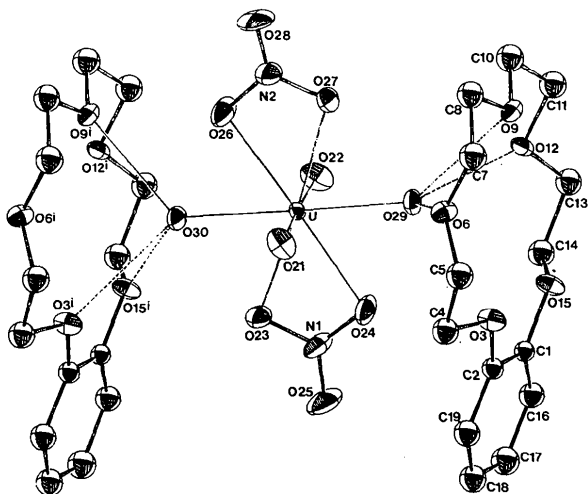


Fig. 2. Drawing of  $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2] \cdot (\text{benzo-15-crown-5})$  (2).

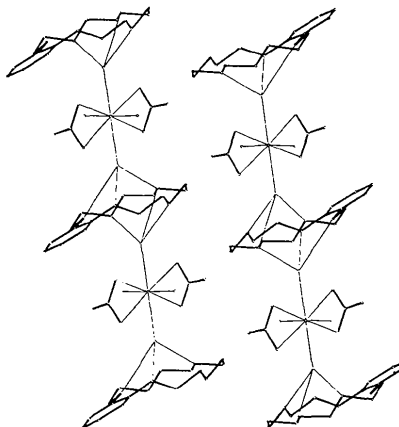


Fig. 4. Molecular packing of complex (2).

Table 4. Torsion angles ( $^{\circ}$ ) for complexes (1) and (2)

	Complex (1)	Complex (2)
C(4)—O(3)—C(2)—C(1)	173.6 (6)	-166 (1)
C(2)—O(3)—C(4)—C(5)	170.0 (6)	-174 (1)
C(7)—O(6)—C(5)—C(4)	-168.2 (8)	164 (1)
C(5)—O(6)—C(7)—C(8)	162.4 (8)	-165 (1)
C(10)—O(9)—C(8)—C(7)	164.5 (6)	-174 (1)
C(8)—O(9)—C(10)—C(11)	-167.6 (7)	177 (1)
C(13)—O(12)—C(11)—C(10)	-167.6 (6)	168 (1)
C(11)—O(12)—C(13)—C(14)	167.4 (6)	-164 (1)
C(14)—O(15)—C(11)—C(2)	-149.5 (7)	141 (1)
C(1)—O(15)—C(14)—C(13)	174.4 (6)	-177 (1)
O(15)—C(1)—C(2)—O(3)	2.5 (9)	1 (1)
O(3)—C(4)—C(5)—O(6)	58.8 (9)	-62 (1)
O(6)—C(7)—C(8)—O(9)	-68.9 (8)	61 (1)
O(9)—C(10)—C(11)—O(12)	68.1 (8)	-60 (1)
O(12)—C(13)—C(14)—O(15)	-61.3 (8)	67 (1)

Torsion angles for both compounds are given Table 4: the molecular conformation is essentially the same as that observed in the complex  $\text{NaI}(\text{benzo-15-crown-5})\cdot\text{H}_2\text{O}$  (Bush & Truter, 1972) and is best described as a sequence of  $\pm 64$  (4) and  $\pm 60$  (2) $^{\circ}$  for the aliphatic C—C bond [except for the C—C bond linked to the aromatic ring: 2.5 (9) and 1 (1) $^{\circ}$ ] and  $\pm 166$  (6) and 167 (7) $^{\circ}$  for the C—O—C—C torsion

angles, for (1) and (2) respectively. The five O atoms are not quite coplanar.

## References

- BUSH, M. A. & TRUTER, M. R. (1972). *J. Chem. Soc. Perkin Trans. 2*, pp. 341–344.
- CHARPIN, P., LANCE, M., NIERLICH, M. & VIGNER, D. (1987). *Acta Cryst.* **C43**, 442–445.
- FRENZ, B. A. (1985). *Enraf-Nonius Structure Determination Package*. Version 3.0. Enraf-Nonius, Delft, The Netherlands.
- GUTBERLET, T., DREISSIG, W., LUGER, P., BECHTHOLD, H.-C., MAUNG, R. & KNÖCHEL, A. (1989). *Acta Cryst.* **C45**, 1146–1149.
- JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- MOODY, D. C. & RYAN, R. R. (1979). *Cryst. Struct. Commun.* **8**, 933–936.
- NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- RITGER, P. L., BURNS, J. H. & BOMBIERI, G. (1983). *Inorg. Chim. Acta*, **77**, L217–L219.
- ROGERS, R. D. (1988). *Acta Cryst.* **C44**, 638–641.
- ROGERS, R. D., KURIHARA, L. K. & BENNING, M. M. (1987). *J. Incl. Phenom.* **5**, 645–658.

*Acta Cryst.* (1993). **C49**, 19–22

## Structure of $\mu$ -[Cystamine-*N,N,N',N'*-tetraacetato(4-)]-bis(5-methylimidazole)-dicopper(II) Dihydrate

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**Abstract.**  $\mu$ -[(Dithiodi-2,1-ethanediy)dinitrilo-tetraacetato(4-)-*N,O,O'',S:N',O''''',O''''''',S'*]-bis-[(5-methylimidazole-*N*<sup>3</sup>)copper(II)] dihydrate,

$[\text{Cu}_2(\text{C}_{12}\text{H}_{16}\text{N}_2\text{O}_8\text{S}_2)(\text{C}_4\text{H}_6\text{N}_2)_2]\cdot 2\text{H}_2\text{O}$ ,  $M_r = 707.7$ , monoclinic,  $C2/c$ ,  $a = 22.503$  (5),  $b = 7.491$  (2),  $c = 17.367$  (2) Å,  $\beta = 110.76$  (1) $^{\circ}$ ,  $V = 2737$  (2) Å<sup>3</sup>,  $Z =$

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