

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: MU1181). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Harris, C. M. & Lockyer, T. N. (1959). *J. Chem. Soc. A*, pp. 3083–3085.
- Herber, R. H., Croft, M., Coyer, M. J., Bilash, B. & Sahiner, A. (1994). *Inorg. Chem.* **33**, 2422–2426.
- Gould, R. O. & Smith, D. E. (1986). *CADABS. Program for Data Reduction*. Univ. of Edinburgh, Scotland.
- Gould, R. O. & Taylor, P. (1986). *CALC. Program for Molecular Geometry Calculations*. Univ. of Edinburgh, Scotland.
- Macgregor, S. A., McInnes, E. J. L., Sorbie, R. J. & Yellowlees, L. J. (1993). *Molecular Electrochemistry of Inorganic, Bioinorganic and Organometallic Compounds*, edited by A. J. L. Pombeiro & J. A. McCleverty, pp. 503–517. Dordrecht: Kluwer Academic Publishers.
- Osborn, R. S. & Rogers, D. (1974). *J. Chem. Soc. Dalton Trans.* pp. 1002–1004.
- Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination*. Univ. of Cambridge, England.
- Sheldrick, G. M. (1990). *SHELXTL/PC User's Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Walker, N. G. & Stuart, D. (1983). *Acta Cryst.* **A39**, 158–166.
- Yam, V. W.-W., Choi, S. W.-K., Lai, T.-F. & Lee, W.-K. (1993). *J. Chem. Soc. Dalton Trans.* pp. 1001–1002.

Acta Cryst. (1995). **C51**, 2025–2028

N-Benzenesulfonylglycylglycine, (I), and Tetrakis(μ -*N*-benzenesulfonylglycylglycinato)bis[aquacopper(II)](*Cu*—*Cu*)—Water (1/4), (II)

KAKOLI MUKHERJEE, TAPATI BANERJEE AND PRIYOBROTO ROYCHOWDHURY

Department of Physics, University College of Science and Technology, Calcutta 700009, India

TAKASHI YAMANE

Department of Applied Chemistry, Nagoya University, Furo-cho, Chikusa-Ku, Nagoya 464, Japan

(Received 19 April 1993; accepted 19 April 1995)

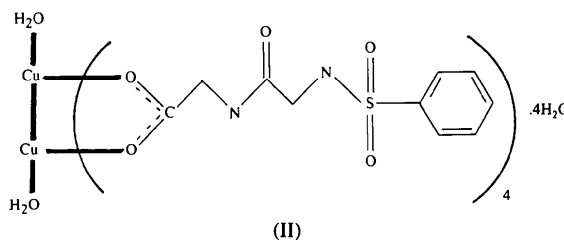
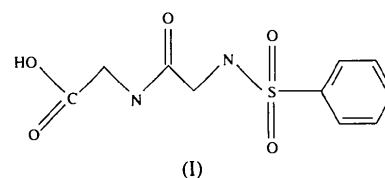
Abstract

Each Cu^{II} ion in $[\{\text{Cu}(\text{H}_2\text{O})\}_2(\mu\text{-C}_{10}\text{H}_{11}\text{N}_2\text{O}_5\text{S})_4]\cdot 4\text{H}_2\text{O}$, (II), is coordinated to its centrosymmetric counterpart, the equatorial carbonyl and carboxylic O atoms of two *N*-benzenesulfonylglycylglycinato moieties and their centrosymmetric counterparts and to an axial water O atom. The centrosymmetrically related Cu^{II} ions

are linked by bridges of 2.641 (1) Å to form dimeric dinuclear units. In both (I) ($\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$) and (II), the terminal and peptide N atoms are in *cis* conformation. The carboxylic group is localized in (I) but a complete delocalization of this group has been observed in the metal complex. When coordinated by the metal ion, the *N*-benzenesulfonylglycylglycine moieties undergo major conformational changes about the N—C α bonds along the peptide backbone.

Comment

Transition metal complexes of amino acids and peptides are of considerable importance because they provide simple models for more complex metal–enzyme and metal–peptide systems. The crystal structures of (I) and (II) have been determined in order to study the effect of a modified amino acid side chain on the coordinating properties of the peptide bond.



In both (I) and (II), the S—N distances are shorter than the corresponding single-bond distance of 1.764 Å in sulfamic acid (Sass, 1960), indicating considerable double-bond character of the bonds. This shortening is more pronounced in the metal complex; a similar finding has been observed in the structure of *N*-benzenesulfonyl-DL-alanine and its copper complex (Chaudhuri, 1984). The enlargement of the S—O bond distances in the metal complex may be due to the increased double-bond character of the S—N(1) bonds in the complex.

The N(1)—C(7) bond distances in both of the structures are shorter than corresponding distances measured in α -glycylglycine [1.484 (2) Å reported by Kvick, Al-Karaghoulis & Koetzle (1977), and 1.497 Å by Biswas, Hughes, Sharma & Wilson (1968)]. Shortening of the N(1)—C(7) bond may be attributed to the conjugation of the benzene sulfonamide group with the glycylglycine moiety. The carbonyl group [C(8)—O(3)] is delocalized in both the free ligand and the complex. The terminal and peptide N atoms are in *cis* conformation in both the free ligand (I) and the complex (II).

Bond distances indicate localization of the terminal carbonyl and carboxylic bonds in (I), but in the complex there is complete delocalization of the π electrons in these bonds. Similar phenomena have been observed in the structures of other metal-peptide complexes (Meester & Hodgson, 1977; Chaudhuri, 1984).

The coordination behaviour of the Cu^{II} ion is very interesting in this complex. Each Cu^{II} ion is coordinated to the carbonyl and carboxylic O atoms of two *N*-benzenesulfonylglycylglycine moieties, their centrosymmetrically related counterparts and to a water O atom

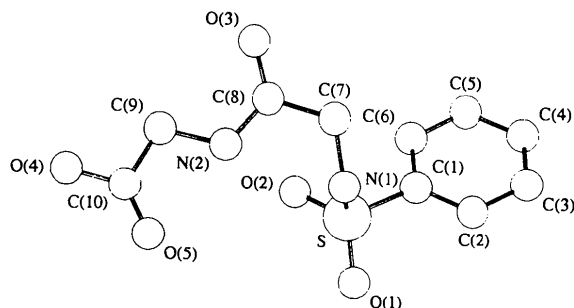


Fig. 1. View of *N*-benzenesulfonylglycylglycine, (I), showing the atom-numbering scheme.

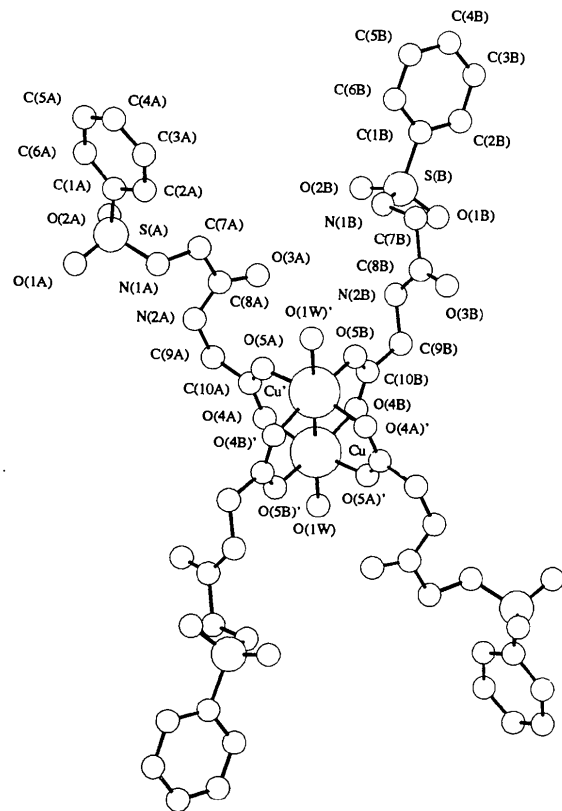


Fig. 2. View of tetrakis(μ -*N*-benzenesulfonylglycylglycine)bis[aqua-copper(II)]-water (1/2), (II), showing the atom-numbering scheme.

(see Fig. 2). The sixth coordination site of the Cu^{II} ion is occupied by a centrosymmetrically related Cu^{II} ion at a distance of 2.649 (1) Å, forming dimeric dinuclear units. This coordination geometry closely resembles that found in the structure of Cu^{II} succinate dihydrate (O'Connor & Maslen, 1966). When coordinated by the metal ion, the *N*-benzenesulfonylglycylglycine moieties undergo major conformational changes about the N(2)—C(9) bonds.

The crystal structures are stabilized by hydrogen bonding. The carbonyl O atom O(3) of the free ligand molecule (I) accepts two hydrogen bonds, one from the N(1) atom of a glide-related molecule and the other from the carboxylic O atom O(4) of the translated-related molecule. In the complex (II), the N(1B) atom is hydrogen bonded to the water molecule. The coordinated water molecule donates a hydrogen bond to the coordinated carboxylic O atom O(5) of ligand B.

Experimental

The compounds were synthesized in the Department of Chemistry, University College of Science, Calcutta, by the method of Mukherjee & Chakraborty (1985). Crystals of (I) were obtained from ethanol. Deep-blue crystals of complex (II) were obtained from hot water. For each compound, the crystal density D_m was measured by flotation (benzene/bromoform mixture).

Ligand (I)

Crystal data

C₁₀H₁₂N₂O₅S

$M_r = 272.3$

Monoclinic

$P2_1/a$

$a = 14.980 (2) \text{ \AA}$

$b = 6.050 (2) \text{ \AA}$

$c = 13.310 (2) \text{ \AA}$

$\beta = 101.21 (7)^\circ$

$V = 1183.26 (5) \text{ \AA}^3$

$Z = 4$

$D_x = 1.53 \text{ Mg m}^{-3}$

$D_m = 1.5 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation

$\lambda = 1.5418 \text{ \AA}$

Cell parameters from 14

reflections

$\theta = 6-20^\circ$

$\mu = 2.56 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Needle

$0.35 \times 0.30 \times 0.30 \text{ mm}$

Colourless

Data collection

Rigaku four-circle AFC-V diffractometer

$\omega/2\theta$ scans

Absorption correction:

none

1757 measured reflections

1715 independent reflections

1525 observed reflections

$[I \geq 2.5\sigma(I)]$

$R_{\text{int}} = 0.01$

$\theta_{\text{max}} = 60^\circ$

$h = 0 \rightarrow 17$

$k = 0 \rightarrow 7$

$l = -15 \rightarrow 15$

3 standard reflections

monitored every 50

reflections

intensity decay: <2%

Refinement

Refinement on F

$R = 0.0615$

$wR = 0.0567$

$S = 1.17$

$(\Delta/\sigma)_{\text{max}} = 0.984$

$\Delta\rho_{\text{max}} = 0.65 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.04 \text{ e \AA}^{-3}$

Extinction correction: none

1525 reflections	Atomic scattering factors	C(8)	0.3284 (2)	0.5390 (7)	0.6291 (3)	0.040 (1)
211 parameters	from <i>International Tables</i>	O(3)	0.2853 (1)	0.7089 (5)	0.6015 (2)	0.0461 (9)
Only coordinates of H atoms	for <i>X-ray Crystallography</i>	N(2)	0.4181 (2)	0.5300 (7)	0.6371 (3)	0.045 (1)
refined	(1974, Vol. IV)	C(9)	0.4696 (2)	0.7208 (8)	0.6181 (4)	0.048 (1)
$w = 20.92/[\sigma^2(F)$		C(10)	0.5641 (2)	0.6541 (7)	0.6041 (3)	0.043 (1)
$+ 0.000037F^2]$		O(4)	0.6086 (2)	0.8305 (6)	0.5839 (3)	0.057 (1)
		O(5)	0.5921 (2)	0.4700 (5)	0.6114 (2)	0.053 (1)

Complex (II)*Crystal data*[Cu(C₁₀H₁₁N₂O₅S)₂(H₂O)]·
2H₂O $M_r = 662.14$

Triclinic

 $P\bar{1}$ $a = 13.716 (3) \text{ \AA}$ $b = 12.374 (3) \text{ \AA}$ $c = 7.992 (4) \text{ \AA}$ $\alpha = 97.66 (3)^\circ$ $\beta = 83.12 (3)^\circ$ $\gamma = 95.82 (2)^\circ$ $V = 1329.6 (8) \text{ \AA}^3$ $Z = 2$ $D_x = 1.65 \text{ Mg m}^{-3}$ $D_m = 1.61 \text{ Mg m}^{-3}$ *Data collection*Rigaku four-circle AFC-V
diffractometer $\omega/2\theta$ scans

Absorption correction:

none

4240 measured reflections

4201 independent reflections

3901 observed reflections

 $[I \geq 2.5\sigma(I)]$ *Refinement*Refinement on F^2 $R = 0.0574$ $wR = 0.0599$ $S = 1.13$

3901 reflections

361 parameters

H-atom parameters not

refined

 $w = 4.67/\sigma^2(F)$ Cu $K\alpha$ radiation $\lambda = 1.5418 \text{ \AA}$ Cell parameters from 16
reflections $\theta = 10\text{--}25^\circ$ $\mu = 3.229 \text{ mm}^{-1}$ $T = 297 \text{ K}$

Plate

 $0.30 \times 0.25 \times 0.20 \text{ mm}$

Deep blue

 $R_{\text{int}} = 0.024$ $\theta_{\text{max}} = 62.5^\circ$ $h = -16 \rightarrow 16$ $k = -14 \rightarrow 14$ $l = -9 \rightarrow 9$

3 standard reflections

monitored every 50

reflections

intensity decay: <2%

 $(\Delta/\sigma)_{\text{max}} = 0.117$ $\Delta\rho_{\text{max}} = 1.23 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -1.07 \text{ e \AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables*for *X-ray Crystallography*

(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

Ligand (I)	x	y	z	U_{eq}
C(1)	0.2547 (2)	0.0498 (7)	0.8534 (3)	0.044 (1)
C(2)	0.2227 (3)	-0.1617 (8)	0.8368 (3)	0.051 (1)
C(3)	0.1378 (3)	-0.2121 (9)	0.8583 (4)	0.055 (2)
C(4)	0.0885 (3)	-0.0556 (9)	0.8971 (4)	0.058 (2)
C(5)	0.1221 (3)	0.1532 (9)	0.9167 (4)	0.063 (2)
C(6)	0.2064 (3)	0.2091 (9)	0.8951 (4)	0.055 (2)
S	0.3587 (1)	0.1237 (2)	0.8181 (1)	0.0469 (3)
O(1)	0.4199 (2)	-0.0571 (6)	0.8382 (3)	0.068 (1)
O(2)	0.3836 (2)	0.3360 (6)	0.8576 (3)	0.061 (1)
N(1)	0.3368 (2)	0.1523 (6)	0.6923 (3)	0.045 (1)
C(7)	0.2785 (2)	0.3334 (7)	0.6497 (3)	0.045 (1)

Complex (II)

Cu	0.9898	0.5462	1.6597 (1)	0.0332 (2)
O(1W)	0.9712 (2)	0.6109 (3)	1.9277 (4)	0.0355 (9)
O(2W)	0.0138 (3)	0.8680 (4)	0.7686 (6)	0.0620 (1)
O(3W)	0.0354 (3)	0.1152 (4)	0.6977 (8)	0.0760 (2)
C(1A)	1.4366 (3)	0.6753 (4)	0.5864 (6)	0.033 (1)
C(2A)	1.3830 (5)	0.5785 (5)	0.5315 (8)	0.060 (2)
C(3A)	1.3924 (6)	0.5403 (6)	0.3599 (9)	0.071 (3)
C(4A)	1.4528 (5)	0.5967 (6)	0.2467 (7)	0.060 (2)
C(5A)	1.5050 (5)	0.6940 (6)	0.3005 (8)	0.057 (2)
C(6A)	1.4963 (4)	0.7329 (5)	0.4727 (7)	0.050 (2)
S(A)	1.4339 (1)	0.7233 (1)	0.8053 (1)	0.0360 (4)
O(1A)	1.5173 (3)	0.6860 (4)	0.8650 (5)	0.058 (1)
O(2A)	1.4225 (4)	0.8379 (3)	0.8235 (5)	0.059 (2)
N(1A)	1.3370 (3)	0.6628 (3)	0.9024 (5)	0.036 (1)
C(7A)	1.2407 (4)	0.7007 (5)	0.8994 (6)	0.043 (2)
C(8A)	1.1889 (3)	0.7327 (4)	1.0746 (6)	0.032 (1)
O(3A)	1.1025 (2)	0.7536 (3)	1.0896 (5)	0.040 (1)
N(2A)	1.2411 (3)	0.7357 (3)	1.2056 (5)	0.033 (1)
C(9A)	1.1960 (4)	0.7490 (4)	1.3792 (6)	0.036 (1)
C(10A)	1.1266 (3)	0.6523 (3)	1.4256 (6)	0.028 (1)
O(4A)	1.0905 (2)	0.6584 (3)	1.5804 (4)	0.033 (1)
O(5A)	1.1102 (2)	0.5753 (2)	1.3127 (4)	0.032 (1)
C(1B)	0.7190 (4)	0.9596 (3)	0.8075 (6)	0.032 (1)
C(2B)	0.6260 (4)	0.9952 (4)	0.8206 (7)	0.042 (2)
C(3B)	0.5930 (4)	1.0247 (4)	0.6736 (8)	0.047 (2)
C(4B)	0.6518 (4)	1.0146 (4)	0.5198 (7)	0.044 (2)
C(5B)	0.7436 (4)	0.9781 (4)	0.5088 (6)	0.042 (2)
C(6B)	0.7798 (4)	0.9502 (4)	0.6528 (6)	0.037 (1)
S(B)	0.7638 (1)	0.9309 (1)	0.9928 (2)	0.0442 (4)
O(1B)	0.6811 (4)	0.9123 (4)	1.1151 (5)	0.062 (2)
O(2B)	0.8397 (5)	1.0142 (4)	1.0327 (7)	0.084 (2)
N(1B)	0.8178 (3)	0.8182 (3)	0.9485 (5)	0.037 (1)
C(7B)	0.7581 (3)	0.7135 (4)	0.9384 (6)	0.031 (1)
C(8B)	0.7515 (3)	0.6576 (3)	1.0993 (6)	0.029 (1)
O(3B)	0.7042 (3)	0.5690 (3)	1.1061 (5)	0.045 (1)
N(2B)	0.7979 (3)	0.7130 (3)	1.2274 (5)	0.031 (1)
C(9B)	0.7878 (3)	0.6781 (4)	1.3949 (6)	0.033 (1)
C(10B)	0.8701 (3)	0.6113 (3)	1.4261 (5)	0.026 (1)
O(4B)	0.8910 (2)	0.6240 (3)	1.5780 (4)	0.033 (1)
O(5B)	0.9080 (2)	0.5483 (3)	1.3054 (4)	0.033 (1)

Table 2. Selected geometric parameters (\AA , $^\circ$)

Complex (II)			
Cu—Cu'	2.649 (1)	Cu—O(1W)	2.179 (3)
Cu—O(4A)	1.968 (3)	Cu—O(4B)	1.958 (3)
Cu—O(5A')	1.946 (3)	Cu—O(5B')	1.980 (3)
O(5A')—Cu—O(5B')	89.5 (2)	O(4A)—Cu—O(1W)	98.4 (2)
O(1W)—Cu—O(5')	92.4 (1)	O(4A)—Cu—O(4B)	88.0 (2)
O(1W)—Cu—O(5A')	93.5 (2)	Cu'—Cu—O(5')	85.2 (1)
O(4B)—Cu—O(5')	168.3 (2)	Cu'—Cu—O(5A')	83.3 (1)
O(4B)—Cu—O(5A')	88.4 (2)	Cu'—Cu—O(1W)	176.0 (1)
O(4B)—Cu—O(1W)	99.2 (2)	Cu'—Cu—O(4B)	83.1 (1)
O(4A)—Cu—O(5')	91.6 (2)	Cu'—Cu—O(4A)	84.8 (1)
O(4A)—Cu—O(5A')	167.9 (2)		

Ligand (I)	A	B
C(1)—C(2)	1.369 (7)	1.379 (8)
C(2)—C(3)	1.391 (7)	1.412 (9)
C(3)—C(4)	1.363 (8)	1.385 (8)
C(4)—C(5)	1.366 (8)	1.369 (8)
C(5)—C(6)	1.390 (7)	1.391 (8)
C(6)—C(1)	1.384 (7)	1.371 (7)
C(1)—S	1.770 (4)	1.768 (5)
S—O(1)	1.419 (5)	1.430 (5)
S—O(2)	1.410 (5)	1.429 (4)
S—N(1)	1.652 (5)	1.623 (4)
N(1)—C(7)	1.446 (6)	1.450 (7)

C(7)—C(8)	1.504 (7)	1.514 (6)	1.529 (7)
C(8)—O(3)	1.231 (6)	1.227 (5)	1.220 (5)
C(8)—N(2)	1.328 (5)	1.332 (7)	1.343 (6)
N(2)—C(9)	1.438 (7)	1.445 (6)	1.448 (7)
C(9)—C(10)	1.518 (5)	1.509 (6)	1.527 (7)
C(10)—O(4)	1.314 (6)	1.272 (6)	1.267 (5)
C(10)—O(5)	1.188 (6)	1.244 (5)	1.253 (5)
C(1)—C(2)—C(3)	118.5 (6)	118.6 (6)	118.2 (5)
C(2)—C(3)—C(4)	120.7 (6)	120.8 (7)	120.5 (5)
C(3)—C(4)—C(5)	120.5 (6)	120.7 (6)	120.5 (5)
C(4)—C(5)—C(6)	120.1 (7)	118.9 (6)	120.7 (5)
C(5)—C(6)—C(1)	118.7 (7)	120.3 (6)	118.2 (5)
C(6)—C(1)—C(2)	121.4 (5)	120.7 (5)	121.9 (5)
C(1)—S—O(1)	109.0 (4)	107.4 (3)	107.8 (3)
C(1)—S—O(2)	108.3 (4)	107.1 (3)	107.2 (3)
C(1)—S—N(1)	106.5 (3)	107.7 (3)	108.4 (2)
S—C(1)—C(2)	119.5 (4)	120.6 (4)	118.5 (4)
S—C(1)—C(6)	119.1 (5)	118.6 (4)	119.5 (4)
O(1)—S—N(1)	105.4 (4)	106.4 (3)	107.7 (3)
O(2)—S—N(1)	105.6 (4)	108.4 (3)	105.5 (3)
S—N(1)—C(7)	117.6 (4)	120.1 (4)	119.4 (4)
O(1)—S—O(2)	121.2 (4)	119.5 (3)	119.8 (3)
N(1)—C(7)—C(8)	114.5 (4)	113.4 (4)	113.4 (4)
C(7)—C(8)—O(3)	119.6 (4)	119.5 (4)	119.7 (4)
C(7)—C(8)—N(2)	118.9 (6)	117.0 (4)	116.0 (4)
O(3)—C(8)—N(2)	121.5 (6)	123.5 (5)	124.3 (5)
C(8)—N(2)—C(9)	121.5 (5)	121.9 (4)	122.5 (4)
N(2)—C(9)—C(10)	110.7 (5)	113.6 (4)	114.3 (4)
C(9)—C(10)—O(4)	109.4 (6)	115.2 (4)	114.6 (4)
C(9)—C(10)—O(5)	124.2 (6)	118.5 (4)	119.0 (4)
O(4)—C(10)—O(5)	126.4 (5)	126.3 (4)	126.4 (4)
C(1)—S—N(1)—C(7)	67.1 (5)	-78.9 (4)	-78.9 (4)
O(1)—S—N(1)—C(7)	-177.3 (5)	166.3 (4)	37.5 (5)
O(2)—S—N(1)—C(7)	-47.9 (6)	36.6 (5)	166.6 (4)
S—N(1)—C(7)—C(8)	95.1 (6)	-122.7 (4)	-99.3 (4)
N(1)—C(7)—C(8)—O(3)	-173.5 (5)	-171.4 (5)	-179.5 (5)
N(1)—C(7)—C(8)—N(2)	9.3 (8)	8.2 (7)	2.1 (6)
C(7)—C(8)—N(2)—C(9)	179.8 (5)	-170.6 (5)	171.7 (4)
O(3)—C(8)—N(2)—C(9)	2.7 (9)	8.9 (7)	-6.7 (8)
C(8)—N(2)—C(9)—C(10)	-164.7 (5)	67.6 (6)	96.4 (5)
N(2)—C(9)—C(10)—O(4)	178.2 (5)	175.7 (4)	147.8 (4)
N(2)—C(9)—C(10)—O(5)	-2.3 (8)	-4.0 (6)	-34.2 (6)

Symmetry code: (') 2 - x, 1 - y, 3 - z.

The structures were solved by direct methods and Fourier syntheses using *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and *SHELX76* (Sheldrick, 1976).

We thank Dr G. N. Mukherjee for the gift of the compounds and the Council of Scientific and Industrial Research for financial support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1088). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Biswas, A. B., Hughes, E. W., Sharma, B. D. & Wilson, J. N. (1968). *Acta Cryst.* **B24**, 40–50.
 Chaudhuri, S. (1984). *J. Chem. Soc. Dalton Trans.* pp. 779–783.
 Kvick, A., Al-Karaghoul, A. R. & Koetzle, T. F. (1977). *Acta Cryst.* **B33**, 3796–3801.
 Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

- Meester, P. & Hodgson, D. (1977). *Acta Cryst.* **B33**, 3505–3510.
 Mukherjee, G. N. & Chakraborty, P. K. (1985). *Indian J. Chem.* **24A**, 841–848.
 O'Connor, B. H. & Maslen, E. N. (1966). *Acta Cryst.* **20**, 824–835.
 Sass, R. L. (1960). *Acta Cryst.* **13**, 320–324.
 Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination.* Univ. of Cambridge, England.

Acta Cryst. (1995). **C51**, 2028–2030

Tetraamminebis(saccharinato-*N*)cadmium

ISABEL PASCUAL

Departamento de Química Inorgánica, Universidad de Zaragoza-CSIC, Facultad de Ciencias, E-50009 Zaragoza, Spain

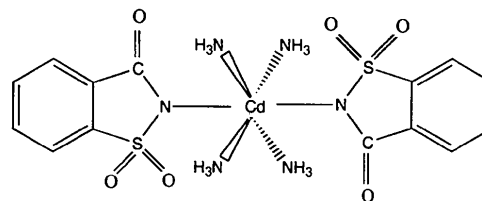
(Received 22 December 1994; accepted 27 February 1995)

Abstract

Single crystals of the title compound, [Cd(C₇H₄NO₃S)₂(NH₃)₄], were prepared from tetraaquabis(saccharinato-*N*)cadmium dihydrate using ammonia flux [saccharin is 1,2-benzisothiazol-3(2*H*)-one 1,1-dioxide]. The complex displays the same geometry as the parent compound, although its packing in the solid state and hydrogen-bonding network are very different as a result of the absence of the water molecules of crystallization. If exposed to air, the product becomes amorphous; several studies suggest a conversion to the parent hydrogen-bonding pattern by the acquisition of water molecules from the moisture in the air.

Comment

The title compound, (I), crystallizes in space group *P*2₁/*c* with four molecules in the unit cell. The structure consists of neutral molecules comprising Cd atoms bonded to a mutually *trans* pair of saccharinate anions through the (deprotonated) N atom and four equatorial ammonia ligands which complete a slightly distorted octahedral coordination sphere. The Cd atom sits on a crystallographic inversion centre, which relates the two saccharinate ligands.



(I)