375. *The Crystal Structure of Bis-1-aminocyclopentanecarboxylatocopper*(II).

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The crystal structure of bis-1-aminocyclopentanecarboxylatocopper(II) has been determined by *X*-ray diffraction methods; refinement was carried out by least-squares procedures with anisotropic thermal parameters and full three-dimensional data. There are two molecules in the monoclinic unit cell (space group, $P2_1/a$) with dimensions $a = 10{\cdot}824 \pm 0{\cdot}012$, $b = 5{\cdot}496 \pm 0{\cdot}006$, $c = 10{\cdot}789 \pm 0{\cdot}014$ Å, $\beta = 94° \; 17' \pm 7'$. The centrosymmetric molecules $(C_6H_{10}NO_2)_2Cu$ are held together by hydrogen bonds. The copper atoms have an essentially square-planar co-ordination of two nitrogen atoms at 1·98 Å and two oxygen atoms at 1·91 Å. The longer fifth and sixth bonds which are found in bivalent copper compounds are not present; the nearest neighbours in the octahedral sites of the copper atom are oxygen atoms 3·17 Å away.

THE copper(II) complexes of α-amino-acids exhibit three types of visible absorption spectrum in the solid state.[1] The hydrated compounds of simple α-amino-acids, which are freely soluble in water, have absorption spectra similar to those of their aqueous solutions. The structure of one of these compounds, di-DL-prolinatocopper(II) dihydrate, is known;[2] the copper atom has distorted octahedral co-ordination with two water molecules at longer distances in the " octahedral " sites. Compounds of the second group are only sparingly soluble in water and form anhydrous solids; they have one broader band at about 590 mμ in their visible absorption spectra. In bis-α-aminobutyratocopper(II), which belongs to this group, the copper atom is said to have a distorted octahedral environment, the two longer bonds being to oxygen atoms of the carboxyl groups from adjacent molecules.[3] The copper(II) complexes of α-aminoisobutyric acid and 1-aminocyclopentanecarboxylic acid, which belong to the third group, separate from water, in which they are very soluble, as anhydrous solids. The visible absorption spectra of the solid compounds have two overlapping bands at 510 and 590 mμ. By analogy with 1,3-diketone derivatives of bivalent copper, Graddon and Munday[1] suggested that these amino-acid complexes contain truly four-co-ordinated copper atoms. The crystal structure of bis-1-aminocyclopentanecarboxylatocopper(II), $(H_2N{\cdot}C_5H_8{\cdot}CO_2)_2Cu$, has been determined to test this hypothesis.

EXPERIMENTAL

Crystals of bis-1-aminocyclopentanecarboxylatocopper(II) were obtained from aqueous solution as blue plates lying on their (001) faces. Single-crystal oscillation and Weissenberg photographs indicated that the crystals belong to the monoclinic system. From the systematic absences ($h0l$ absent if $h = 2n + 1$, and $0k0$ absent if $k = 2n + 1$) the space group was uniquely determined as $P2_1/a$. Accurate cell dimensions were determined from zero-layer Weissenberg photographs about the *a*- and the *b*-axis, with sodium chloride powder lines for calibration;[4] least-squares procedures were used to obtain the final parameters. Intensities were estimated visually from equi-inclination Weissenberg photographs taken about each of the three principal axes for all layers which could be obtained with copper radiation. After the Lorentz and polarisation corrections had been applied, the intensities were placed on a common arbitrary scale by internal correlation. Because of the low absorption coefficient ($\mu = 26{\cdot}7$ cm.$^{-1}$) and the small size of the crystal used ($0{\cdot}2 \times 0{\cdot}1 \times 0{\cdot}05$ mm.), the intensities were not corrected for absorption; 781 of the 855 possible reflections gave measurable intensities.

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[1] Graddon and Munday, *J. Inorg. Nuclear Chem.*, 1961, **23**, 231.
[2] Mathieson and Welsh, *Acta Cryst.*, 1953, **5**, 599.
[3] Stosick, *J. Amer. Chem. Soc.*, 1945, **67**, 362.
[4] Fridricksons, *J. Amer. Mineral.*, 1959, **44**, 200.

Structure factors, Fourier syntheses, and the anisotropic least-squares refinement were calculated on UTECOM (a Deuce electronic digital computer) with programmes written by Dr. J. S. Rollett. The programme for differential synthesis was written by one of us (G. A. B.).

Scattering factors of Berghius *et al.*[5] were used for all atoms, the values for copper being corrected for anomalous dispersion.[6]

Crystal Data.—$C_{12}H_{20}CuN_2O_4$; M = 319·69; monoclinic; a = 10·824 ± 0·012, b = 5·496 ± 0·006, c = 10·789 ± 0·014 Å; β = 94° 17′ ± 7′; U = 640·04 Å^3; D_m = 1·64 ± 0·01 g.cm.$^{-3}$ (by flotation); Z = 2; D_c = 1·660 g.cm.$^{-3}$; $F(000)$ = 330; space group $P2_1/a$ (C_{2h}^5; No. 14). Radiation, copper, unfiltered; single-crystal oscillation and Weissenberg photographs. Data for structure analysis from $hk0 \longrightarrow hk\,6$, $h0l \longrightarrow h3l$, $0kl \longrightarrow 6kl$.

Structure Determination.—Since there are four general equivalent positions in the space group $P2_1/a$ [fractional co-ordinates $\pm$ (x, y, z; $\frac{1}{2} + x$, $\frac{1}{2} - y$, z)], the copper atoms must occupy special positions on centres of symmetry. The copper atoms (at 0, 0, 0 and $\frac{1}{2}$, $\frac{1}{2}$, 0) contribute only to those reflections with $h + k = 2n$; the signs of the contributions to these structure factors are positive. A Fourier synthesis was calculated with these reflections, and the resulting electron density map led to positions for all the light atoms (excluding hydrogen). The structure factors calculated with co-ordinates for all atoms and a temperature factor $\exp\,(-B \sin^2 \theta/\lambda^2)$ with B = 3·0 Å^2 gave a discrepancy factor, R, of 0·41. Refinement was carried out by using observed and calculated differential syntheses until no further shifts in co-ordinates were indicated; individual isotropic thermal parameters for each atom were introduced. After six cycles, the R value had dropped to 0·19.

Further refinement was carried out by an anisotropic least-squares procedure in which $\sum w(|F_o| - |F_c)^2$ was minimised. Each reflection was weighted as follows: $|F_o| \leqslant 4F_{\text{min.}}$, $w = (|F_o|/4F_{\text{min.}})^2$; $|F_o| > 4F_{\text{min.}}$, $w = (4F_{\text{min.}}/|F_o|)^2$. The refinement was complete after four cycles; the largest shifts in the parameters were less than half the corresponding estimated standard deviations and R had been reduced to 0·13 (based on the 781 observed reflections).

The final atomic co-ordinates together with their root-mean-square estimated standard deviations are given in Table 1. Table 2 contains the thermal parameters of the atoms; the temperature factor for each atom was calculated from the expression: $\exp - (b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)$. The calculated structure factors and the observed structure amplitudes are given in Table 3.

TABLE 1.

Atomic co-ordinates.

Atom	x/a	y/b	z/c	σ (Å)	Atom	x/a	y/b	z/c	σ (Å)
Cu	0·5000	0·5000	0·0000	—	C(1)	0·4496	0·1777	0·1922	0·013
N	0·3787	0·3360	0·0999	0·012	C(2)	0·3715	−0·0352	0·2394	0·017
O(1)	0·6037	0·2289	0·0470	0·010	C(3)	0·3388	0·0323	0·3645	0·024
O(2)	0·6239	−0·0845	0·1713	0·011	C(4)	0·3759	0·2966	0·3891	0·021
C(0)	0·5626	0·0885	0·1351	0·015	C(5)	0·4868	0·3132	0·3098	0·015

TABLE 2.

Thermal parameters.

Atom	10^4b_{11}	10^4b_{22}	10^4b_{33}	10^4b_{12}	10^4b_{13}	10^4b_{23}	Atom	10^4b_{11}	10^4b_{22}	10^4b_{33}	10^4b_{12}	10^4b_{13}	10^4b_{23}
Cu	49	276	65	−64	19	−39	C(1)	75	225	51	−32	37	10
N	49	243	81	85	−20	−32	C(2)	137	136	122	21	89	−115
O(1)	65	324	88	108	39	113	C(3)	164	693	114	66	154	−21
O(2)	81	286	109	108	31	128	C(4)	90	558	147	−34	59	68
C(0)	74	252	72	27	21	60	C(5)	121	264	57	−111	43	−5

DISCUSSION

The crystal consists of molecules of the composition $(H_2N{\cdot}C_5H_8{\cdot}CO_2)_2Cu$ with the amino-acid acting as a chelate group. There is hydrogen bonding between the amino-group of one molecule and the carboxyl-oxygen atom of another [O(2′)–N distance = 2·95 Å, σ = 0·02 Å; the angle C(1)–N–O(2′) = 111°]. Each molecule is involved in four such hydrogen bonds to the four molecules separated from it by (a/2, b/2), thus forming

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[5] Burghuis, Haanappel, Potters, Loopstra, MacGillavry, and Veenendaal, *Acta Cryst.*, 1955, **8**, 478.

[6] Dauben and Templeton, *Acta Cryst.*, 1955, **8**, 841.

TABLE 3.

Calculated structure factors and observed structure amplitudes (scale ½ absolute).

l	F_c	$\lvert F_o \rvert$
	0,0,l	
1	51	29
2	6	5
3	17	16
4	2	3
5	22	21
6	19	17
7	9	8
8	7	9
9	5	6
10	8	8
11	4	4
13	3	3
	0,1,l	
1	−30	26
2	−5	4
3	−20	20
4	−14	14
5	−2	2
6	−4	4
11	−3	3
	0,2,l	
0	11	13
1	12	12
2	5	5
3	7	8
4	16	14
5	17	15
6	14	14
7	12	12
8	15	17
9	9	9
10	3	3
11	6	5
12	4	4
13	3	2
	0,3,l	
1	10	11
2	4	4
5	6	6
6	8	9
7	7	6
	0,4,l	
0	11	11
1	8	9
2	12	12
3	16	16
4	13	13
5	9	10
6	4	4
7	2	3
8	4	4
9	3	6
	0,5,l	
1	5	4
2	3	3
	0,6,l	
0	5	5
1	3	3
2	2	4
3	5	4
4	4	4
5	2	3
	1,1,l	
−11	5	5
−10	9	8
−9	11	11
−8	5	6
−7	9	10
−6	14	14
−5	12	9
−4	23	20
−3	26	22
−2	18	14
−1	15	16
0	1	2
1	15	13
2	49	41
3	41	34
4	17	15
6	4	4
	1,1,l	
7	14	13
8	11	11
9	8	9
10	9	10
11	5	5
12	4	4
	1,2,l	
−6	−10	9
−5	−6	7
−3	3	4
−2	2	3
−1	10	11
0	4	7
1	−3	6
1	8	9
2	5	4
3	−4	6
4	−4	5
5	5	6
8	5	6
9	6	6
	1,3,l	
−9	5	6
−7	4	6
−6	13	12
−5	18	17
−4	18	16
−3	12	11
−2	16	16
−1	26	25
0	8	11
1	11	12
2	16	14
4	11	10
5	16	16
6	12	11
7	11	11
8	5	6
	1,4,l	
−6	4	5
−5	2	3
−4	−4	4
−3	−7	6
0	−4	5
2	−6	6
3	5	4
4	10	10
6	−6	6
	1,5,l	
−7	7	5
−6	5	5
−2	7	7
−1	9	8
0	9	9
1	4	4
2	3	4
3	7	7
4	4	4
6	6	6
7	6	5
8	3	3
	1,6,l	
−6	−2	3
−3	−1	3
3	3	3
	2,0,l	
−10	10	10
−9	11	11
−8	15	14
−7	30	26
−6	18	16
−5	14	12
−4	18	19
−3	18	16
−2	41	31
−1	19	13
0	50	40
1	49	38
2	−10	10
3	16	15
4	19	15
	2,0,l	
5	13	12
6	18	17
8	−4	4
9	4	6
10	7	7
11	6	7
12	4	4
13	4	3
	2,1,l	
−10	6	7
−7	5	5
−4	−12	11
−3	−11	12
−2	−6	7
−1	7	8
0	14	16
1	−24	22
2	−14	11
3	−8	9
4	−15	13
5	4	4
6	2	4
7	−5	5
9	4	6
10	4	6
	2,2,l	
−11	6	5
−10	3	4
−8	12	11
−7	11	10
−6	3	4
−5	3	3
−4	5	6
−3	14	14
−2	25	24
−1	21	19
0	8	7
1	17	19
2	17	19
3	10	11
4	22	22
5	21	20
6	14	14
7	12	14
8	12	10
9	11	10
10	5	6
	2,3,l	
−9	−3	3
−8	−4	3
−7	−5	5
−4	−3	3
−2	7	6
−1	6	6
0	6	6
1	8	7
4	3	4
5	4	4
6	6	6
8	−3	4
	2,4,l	
−8	3	4
−7	6	6
−6	7	8
−5	11	11
−4	14	16
−3	14	16
−2	13	14
−1	6	6
0	7	9
1	12	12
2	9	10
3	7	9
4	4	6
5	3	4
6	5	4
7	4	4
8	5	5
9	5	5
	2,5,l	
−1	−5	5
0	−5	6
	2.6,l	
−5	4	3
−4	4	4
−1	−1	2
0	4	5
1	8	6
2	7	5
3	6	4
4	4	4
5	3	3
	3,1,l	
−10	4	5
−9	6	6
−8	7	7
−7	8	8
−6	21	19
−5	27	22
−4	19	17
−3	12	10
−2	−1	4
−1	9	9
0	34	32
1	22	20
2	21	18
3	30	26
4	18	15
5	11	9
6	11	9
7	10	9
8	10	9
9	6	6
	3,2,l	
−8	5	7
−6	−7	8
−5	−5	6
−4	4	4
−3	2	3
−2	−7	9
−1	−5	8
0	7	9
1	12	12
2	19	19
3	9	9
4	−9	11
5	−8	9
6	−3	4
8	4	5
	3,3,l	
−11	6	5
−10	6	5
−9	8	8
−8	10	9
−6	5	5
−5	16	15
−4	13	13
−3	13	14
−2	12	12
−1	19	18
0	21	20
1	11	10
2	10	9
4	3	3
5	11	10
6	7	7
7	6	7
8	7	7
	3,4,l	
−2	−5	6
−1	−4	5
2	−2	3
3	−6	7
4	3	4
	3,5,l	
−6	3	4
−3	6	7
−2	8	8
−1	7	7
0	6	7
3	10	10
4	10	10
5	5	4
6	5	5
	3,6,l	
−6	−3	3
1	2	5
2	1	5
3	1	4
6	1	2
	4,0,l	
−10	11	10
−9	19	18
−8	8	9
−7	14	14
−6	19	18
−5	6	5
−4	32	23
−3	34	28
−2	16	13
−1	8	8
0	−16	19
1	3	3
2	12	10
3	13	12
4	18	15
5	10	9
6	17	14
7	15	14
10	5	5
11	4	4
	4,1,l	
−7	4	6
−6	−4	3
−5	−5	6
−4	− 7	7
−3	−23	24
−2	−11	13
−1	−3	3
0	−1	2
1	−5	6
2	−4	3
3	14	12
4	9	9
5	9	8
6	6	6
7	−5	6
	4,2,l	
−8	6	7
−7	8	7
−6	5	7
−5	5	5
−4	7	7
−3	18	17
−2	29	26
−1	28	28
0	15	17
1	16	15
2	29	27
3	20	20
4	13	13
5	13	13
6	6	7
7	7	7
8	8	7
9	5	5
10	4	5
	4,3,l	
−5	3	4
−4	1	3
−3	5	6
−2	9	9
−1	8	9
0	−3	4
1	−6	6
2	−2	3
4	6	7
6	4	5
	4,4,l	
−8	4	4
−7	8	8
−6	11	11
−5	7	8
−4	5	7
−3	4	5
−2	6	8
−1	9	10
	4,4,l	
0	7	8
1	8	9
2	9	10
3	4	5
6	5	5
7	6	6
8	5	6
	4,5,l	
−2	3	3
0	−3	5
4	3	3
5	1	3
	4,6,l	
−4	4	4
−1	2	5
0	5	5
1	5	5
2	4	4
	5,1,l	
−8	8	8
−7	16	15
−6	15	14
−5	14	13
−4	14	13
−3	11	12
−2	17	15
−1	19	18
0	23	23
1	21	20
2	5	4
3	10	10
4	19	16
5	14	11
6	11	10
7	8	6
8	6	7
9	7	6
10	5	5
	5,2,l	
−7	7	7
−3	−3	3
−2	−4	5
−1	−4	6
1	6	5
2	5	6
3	3	4
4	−4	7
5	−2	3
6	5	5
	5,3,l	
−10	6	5
−9	6	6
−8	11	10
−7	7	6
−5	9	9
−4	10	11
−3	7	9
−2	9	9
−1	5	7
0	11	12
1	16	15
2	13	13
3	8	8
4	5	6
5	7	8
6	5	6
9	4	5
10	4	4
	5,4,l	
−4	−6	6
0	7	7
1	6	6
3	−7	7
5	4	6
6	4	5
8	2	5
	5,5,l	
−6	4	3
−4	6	6
−3	10	7

TABLE 3. (*Continued.*)

l	F_c	$\lvert F_o\rvert$
	5,5,l	
−2	7	6
−1	5	4
0	4	5
1	4	4
2	4	3
3	6	6
4	7	7
	5,6,l	
−3	2	3
−2	1	2
1	1	4
3	1	3
	6,0,l	
−12	3	3
−11	6	6
−10	9	8
−9	12	10
−8	5	5
−7	−6	7
−6	7	8
−5	11	11
−4	15	15
−3	27	24
−2	4	4
−1	4	4
0	12	13
1	6	5
2	13	12
3	12	14
4	9	9
5	9	9
6	15	12
7	18	14
8	9	8
	6,1,l	
−12	−2	5
−8	−7	8
−4	9	10
−2	−8	10
−1	1	2
0	−2	3
1	2	3
2	6	7
3	9	9
4	9	9
5	5	5
6	5	5
	6,2,l	
−8	7	7
−7	6	8
−6	10	11
−5	17	18
−4	14	14
−3	10	10
−2	17	18
−1	18	19
0	17	20
1	13	13
2	12	11
3	14	14
	6,2,l	
4	8	7
5	8	7
6	5	4
8	4	5
	6,3,l	
−4	4	4
−3	5	6
−1	−6	8
0	−6	7
1	−5	6
3	3	5
6	−5	5
	6,4,l	
−8	6	6
−7	4	4
−6	7	8
−5	6	6
−2	3	4
−1	8	10
0	9	10
1	5	6
2	6	7
3	7	7
4	7	8
5	6	6
6	5	4
7	4	4
8	4	3
	6,5,l	
1	3	3
2	3	3
5	−1	4
	6,6,l	
−4	4	2
−3	5	3
−2	3	3
−1	4	3
0	4	3
1	3	2
	7,1,l	
−9	6	7
−8	6	6
−7	12	13
−6	12	14
−5	3	5
−4	7	8
−3	15	16
−2	17	21
−1	19	21
0	13	16
1	11	13
2	12	11
3	8	8
4	9	8
5	7	6
6	5	6
7	6	5
8	6	6
	7,2,l	
−5	−4	3
−2	4	5
−1	8	9
0	−2	4
1	−8	8
2	−7	7
	7,3,l	
−8	6	5
−7	8	8
−6	5	8
−5	5	8
−4	10	11
−3	6	7
−2	6	8
−1	3	3
1	10	5
2	14	13
3	10	12
4	7	8
5	6	6
6	6	6
	7,4,l	
−4	−5	6
−3	−4	5
−2	4	4
−1	4	3
0	5	6
1	4	4
5	3	5
	7,5,l	
−6	6	5
−5	5	4
−4	4	5
−2	5	4
−1	5	3
0	5	6
1	4	3
2	3	3
	7,6,l	
−1	1	1
0	−2	3
	8,0,l	
−11	2	3
−10	6	5
−8	5	4
−5	8	9
−4	7	8
−3	12	13
−2	11	11
−1	9	10
0	21	21
1	17	19
2	11	12
3	12	13
4	9	12
5	7	11
6	7	7
7	7	7
	8,0,l	
8	5	6
9	3	4
	8,1,l	
−5	4	6
−4	9	12
−3	9	10
−2	−2	3
−1	3	5
0	6	7
4	−4	7
	8,2,l	
−8	7	5
−7	9	9
−6	9	10
−5	13	16
−4	14	16
−3	5	7
−2	8	8
−1	10	11
0	7	9
1	7	7
3	3	5
4	9	8
5	8	6
	8,3,l	
−3	−2	2
−2	−4	5
−1	−7	8
1	4	5
2	3	4
	8,4,l	
−5	4	4
−4	4	6
−3	5	5
−2	6	5
−1	5	5
0	7	8
1	6	4
2	5	4
3	6	5
4	7	7
	9,1,l	
−10	5	4
−9	7	5
−8	6	5
−6	8	9
−5	8	10
−4	5	6
−3	8	8
−2	9	11
−1	9	12
0	12	13
1	10	9
2	9	10
3	8	10
	9,2,l	
−5	−5	5
	9,2,l	
−3	3	5
−2	4	5
−1	6	6
1	−7	8
	9,3,l	
−6	5	5
−5	6	7
−4	8	10
−3	7	8
−2	7	8
−1	7	8
1	4	5
2	8	8
3	6	6
4	5	6
	9,5,l	
−1	3	2
0	5	3
	10,0,l	
−9	4	2
−8	4	4
−7	10	10
−6	7	8
−5	3	4
−4	7	8
−3	10	11
−2	12	11
−1	7	8
0	8	10
1	11	13
2	10	12
3	12	12
4	9	10
5	4	11
6	1	7
	10,1,l	
0	5	5
4	−7	8
	10,2,l	
−6	6	6
−5	4	5
−4	6	8
−3	6	6
−2	4	4
−1	6	6
0	3	4
	10,3,l	
−4	−3	3
−3	−4	5
1	4	6
	10,4,l	
−5	3	2
−4	5	5
−3	6	5
−2	6	6
	10,4,l	
−1	5	3
0	4	4
	11,1,l	
−6	5	5
−5	7	9
−4	6	8
−3	3	4
−2	4	5
−1	5	5
0	8	9
1	7	6
	11,3,l	
−5	3	3
−4	4	5
−3	6	6
−2	7	7
−1	8	7
0	6	6
	11,4,l	
−1	−2	2
	12,0,l	
−7	6	5
−6	9	7
−5	5	6
−4	7	6
−3	8	7
−2	8	6
−1	3	3
2	5	5
3	7	6
4	6	5
5	2	6
6	1	2
	12,1,l	
−6	−1	7
−2	−2	3
0	−1	6
	12,2,l	
−5	4	3
−3	4	5
−2	4	3
−1	4	3
0	5	5
1	5	4
2	6	4
3	5	4
	12,3,l	
−1	4	2
0	2	2
	13,1,l	
−4	5	3
−3	5	4
−2	4	3
−1	5	3
0	4	3

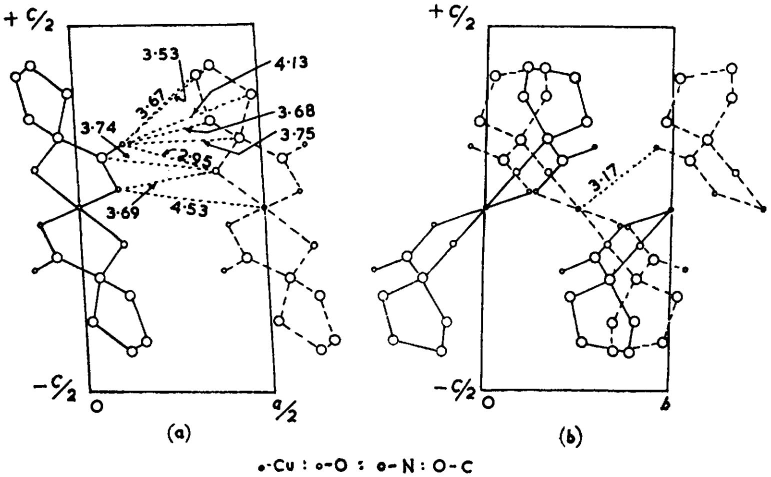
sheets of molecules parallel to the (001) plane. All other intermolecular distances (shown in Fig. 1) are those expected for van der Waals contacts. The ready cleavage of the crystals parallel to the (001) plane is consistent with this molecular arrangement. Two absorption bands (at 3200 and 3320 cm.$^{-1}$) in the infrared spectrum of this and related compounds have been interpreted in terms of hydrogen bonding.[1]

The bond distances and angles in the molecule are shown in Fig. 2 (the estimated standard deviations in the bond angles are 0·5° for the angles around the copper atom and 1—2° for the other angles). The values for individual bonds and angles agree well with those previously reported [7] for related compounds.

Since the copper atom is located on a centre of symmetry, its four nearest neighbours (two oxygen and two nitrogen atoms) must lie in a plane containing the copper atom.

[7] Sutton *et al.*, " Interatomic Distances and Configuration in Molecules and Ions," Chem. Soc. Special Publ. No. 11, London, 1958.

Two further oxygen atoms are situated at distances of 3·17 Å along approximately octahedral directions from the copper atom (see Fig. 1); the O–Cu–O line makes an angle of 19° with the normal to the plane. These are carboxyl-oxygen atoms from two molecules whose centres are separated from the copper atom by *b*. This distance (3·17 Å) appears to be too great to allow appreciable bonding between the copper and oxygen atoms.



(a) (b)

•-Cu : o-O : o-N : O-C

FIG. 1. Arrangement of molecules in the crystal and intermolecular distances (Å). The molecules shown by broken lines are centred at ½, ½, 0.

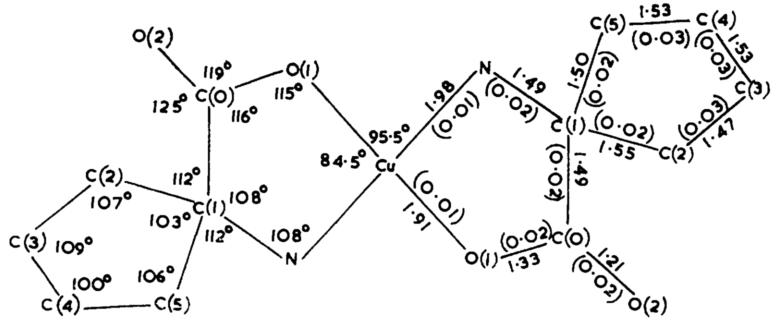


FIG. 2. Bond lengths (Å) and bond angles; estimated standard deviations of lengths are given in parentheses.

The copper atom must be considered to have square-planar co-ordination in this compound; thus, the prediction [1] of this configuration from measurements of the absorption spectrum has been confirmed.

Molecular models of the compound do not suggest any steric hindrance to the addition of water molecules in order to complete a distorted octahedral environment about the copper atom similar to that found for di-(±)-prolinatocopper(II) dihydrate.[2] In aqueous solution two molecules of water are associated with the complex to complete an octahedral co-ordination of the copper atom.[1] It appears, therefore, that the square-planar arrangement about the copper atom in bis-1-aminocyclopentanecarboxylatocopper(II) results from a greater efficiency in the packing of the anhydrous compound than would be possible with a dihydrate.

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