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The Crystal and Molecular Structure of Bis(2-hydroxyethylimino-salicylaldehydato)copper(II)

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The crystal structure of bis(2-hydroxyethyliminosalicylaldehydato)copper(II) has been determined by means of an X-ray diffraction study of a single-crystal specimen. Four formula units are contained in the monoclinic unit cell, the $P2_1/c$ space group, with lattice parameters of: $a=18.41$ Å, $b=4.82$ Å, $c=19.86$ Å, and $\beta=99.1°$ ($Dm=1.50$ g·cm^{-3}; $Dx=1.50$ g·cm^{-3}). The structure has been refined, by means of three-dimensional difference syntheses and the least-squares method, to $R=0.095$. It has been confirmed that copper(II) links to the 2-hydroxyethyliminopyruvate anion through the phenolic oxygen and the nitrogen of the Schiff base linkage, while the alcoholic oxygen in the ethanol-amine moiety is free from coordination. The two Schiff-base ligands are coordinated around copper(II) in the *trans*-configuration. All the bond distances and angles in the complex are within the range of normal values. The N–Cu–O angles (91.3 and 91.8°) in the chelate rings are close to a right angle, showing that there is less strain in the chelate structure than in the case of a similar chelate of the pyruvate Schiff base (84.6°).

Although the ethanolamine molecule is provided with two functional groups for chelate formation, it can not always be coordinated as a bidentate ligand around a metal ion. The Schiff base derived from salicylaldehyde and ethanolamine is, for instance, coordinated around copper(II) to produce not only a one-to-one-type, but also a one-to-two-type, copper(II) Schiff-base complex, (I), in which the two hydroxyl groups of the ethanol-amine moieties are free from coordination.[1] In addition, the Schiff base derived from pyruvic acid and ethanolamine reacts with copper(II) to form, exclusively, a one-to-two-type copper(II) Schiff base complex, (II); consequently, the corresponding one-to-one-type complex is hardly ever obtained regardless of the molar ratio of copper(II) to the Schiff base employed in the preparation.[2] These findings can be explained by taking into account the rather weak binding ability of alcoholic oxygen, on the one hand, and, on the other hand, the geometrically unfavorable structure[3] of the fused

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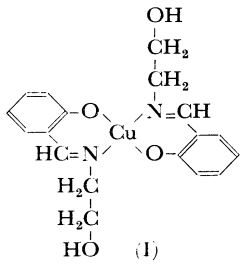
*2 Died Aug. 1, 1968.

1) A. Nakahara, H. Yamamoto and H. Matsumoto, *Sci. Rep., College of General Education, Osaka Univ.*, **12**, 11 (1963).

2) K. Iijima, I. Oonishi, F. Muto, A. Nakahara and Y. Komiyama, This Bulletin, **42**, 1509 (1969).

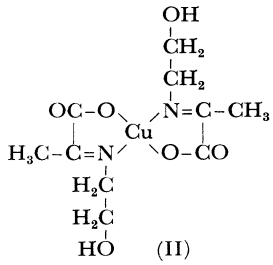
3) A. Nakahara, H. Yamamoto and H. Matsumoto, *ibid.*, **37**, 1137 (1964).

chelate ring in the imaginary one-to-one-type complex of copper(II) 2-hydroxyethyliminopyruvate. In order to estimate the validity of the latter assumption, a comparison of the molecular structure of the copper(II) chelates, I and II, seemed valuable. From this point of view, X-ray studies of the two complexes have recently been performed; the crystal structure of II has already been descrived.[2] This paper will describe the molecular and crystal structure of bis(2-hydroxyethyliminosalicylaldehydato)-copper(II).



(I)

Bis(2-hydroxyethylimino-salicylaldehydato) copper-(II)



(II)

Bis(2-hydroxyethyl-iminopyruvato)cop-per(II)[2]

Experimental

Bis(2-hydroxyethyliminosalicylaldehydato)copper(II) was prepared and purified according to the procedure described in a previous paper.[1] The final pure product appears as thin yellow-brown needles elongated along the *b*-axis. The unit-cell dimensions were determined from the higher-order reflections of Weissenberg photographs (Cu$K\alpha$, λ=1.5418 Å). The systematic absences were $h0l$ for l odd and $0k0$ for k odd. Hence, the space group was unequivocally determined. The crystal data are listed in Table 1. Sets of multiple-film equi-inclination Weissenberg photographs were taken about the *b*-axis (0 to 4th layers), the *a*-axis and the *c*-axis (0th layer). Cu$K\alpha$ radiation was used throughout. The crystal used was a rod with dimensions of 0.07×0.16×0.46 mm. The intensities were estimated visually with a standard film strip and were converted to $|F_o(hkl)|^2$ and $|F_o(hkl)|$ by applying the usual Lorentz, polarization, and spot-shape corrections. No correction was made for absorption and extinction. The range of relative intensities was from 1 to 30000. 2243 independent reflections fell within this range, whereas 1092 others were too weak to be observed.

Table 1. Crystal data

[Cu(HOCH$_2$CH$_2$N=CHC$_6$H$_4$O)$_2$]
Monoclinic
a = 18.41 ± 0.02 Å
b = 4.82 ± 0.01
c = 19.86 ± 0.02
β = 99.1 ± 0.5°
Dx = 1.50 g·cm^{-3}
Dm = 1.50 g·cm^{-3}
Z = 4
Sapce group C_2^{5h}—$P2_1/c$
Linear absorption coefficient for Cu$K\alpha$,
μ = 22.9 cm^{-1}

Structure Analysis

At first, two-dimensional Patterson syntheses projected along the *b*-axis and the *c*-axis were calculated. From these Patterson projections it was apparent that the copper atoms occupy two sets of two-fold positions. They could easily be placed at (000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$) and at ($\frac{1}{2}\frac{1}{2}$0 and $\frac{1}{2}$0$\frac{1}{2}$). Attempts were made to deduce the x and y parameters of the lighter atoms from a three-dimensional Patterson function and from Fourier syntheses of the electron density, $\rho(x,z)$, the signs of which were calculated from the parameter values of the copper atoms. It was possible to locate all the atoms except those belonging to ethanol groups. Two-dimensional difference syntheses revealed ethanol groups, and all the x and y parameters of the lighter atoms were refined by a series of two-dimensional Fourier and difference syntheses to R_{h0l}=0.17. Consideration of the projected bond lengths made the estimation of approximate y coordinates possible. With these coordinates, a subsequent series of three-dimensional Fourier syntheses and difference syntheses reduced the R value to 0.15.

The structure thus obtained was refined by a block-diagonal, least-squares method with a HBLS-4 program written by T. Ashida. In this least-squares calculation, anisotropic temperature factors were introduced and four cycles of refinement were carried out. The following weighting scheme was employed:

$w = 0.2$ if $F_o \leqq F_{\min.}$ (=4.0)
$w = 1.0$ if $F_{\min.} < F_o \leqq F_{\max.}$ (=100.0)
$w = F_{\max.}/F_o$ if $F_o > F_{\max.}$

The final discrepancy factor, $R=\sum||F_o|-|F_c||/\sum|F_o|$, was 0.095 for all the observed reflections. The atomic scattering factors were taken from the International Tables for X-ray Crystallography.[4] The final atomic parameters and their estimated standard deviations are summarized in Table 2. The agreement between the observed and calculated structure amplitudes is reasonable (Table 3).

Description of the Structure and Discussion

The structure projected upon a plane normal to the *b*-axis is shown in Fig. 1. The intramolecular distances and angles are listed with their estimated standard deviations in Tables 4 and 5, and are shown in Figs. 2 and 3. The intramolecular distances and angles were calculated by using program DAPH written by T. Ashida.

4) International Tables for X-Ray Crystallography, Vol. III, Kynoch Press, Birmingham (1962), p. 202.

Table 2. Atomic parameters and their e.s.d.'s* ($\times 10^4$)

The expression of the temperature factor is: $\exp[-(h^2B_{11}+k^2B_{22}+l^2B_{33}+hkB_{12}+hlB_{13}+klB_{23})]$

Atom	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Molecule I									
Cu(1)	0000	0000	0000	25	353	22	2	9	5
O(1)	722(4)	−0590(15)	763(3)	36	382	20	41	4	−15
O(2)	−2024(3)	2236(15)	795(3)	26	405	27	3	18	24
N(1)	−0479(4)	2986(16)	485(4)	19	298	19	−10	9	14
C(1)	872(5)	820(21)	1345(5)	28	315	18	−17	6	0
C(2)	1523(6)	63(28)	1800(5)	32	568	23	27	−1	24
C(3)	1687(6)	1423(27)	2420(5)	36	574	23	−19	−3	27
C(4)	1245(6)	3541(28)	2615(5)	43	569	23	−77	2	−27
C(5)	613(6)	4307(25)	2172(5)	38	454	24	−43	10	−28
C(6)	417(5)	2884(21)	1522(5)	27	307	19	−22	6	19
C(7)	−0235(5)	3892(21)	1096(5)	25	324	20	−9	13	−3
C(8)	−1157(5)	4402(20)	139(5)	22	242	26	12	11	18
C(9)	−1845(5)	2588(22)	119(5)	24	308	24	−5	8	23
Molecule II									
Cu(2)	5000	5000	0000	25	423	27	−2	9	−4
O(3)	5036(4)	1504(17)	4138(4)	27	549	34	66	15	32
O(4)	2689(3)	2256(15)	4064(3)	26	362	25	−15	5	3
N(2)	4106(4)	2652(18)	54(4)	25	315	23	13	3	34
C(10)	5562(5)	1453(25)	3751(5)	28	447	23	−30	8	2
C(11)	5481(7)	3191(29)	3166(6)	44	596	28	−11	17	2
C(12)	6033(7)	3217(29)	2750(6)	45	627	27	−110	14	−30
C(13)	6662(6)	1435(30)	2896(6)	39	751	25	−87	17	−72
C(14)	3270(5)	4711(27)	1546(5)	29	619	24	22	16	61
C(15)	3817(5)	4691(24)	1104(5)	27	426	23	29	12	29
C(16)	3714(5)	2811(22)	546(5)	24	376	23	1	3	57
C(17)	3873(5)	4424(21)	4524(5)	27	276	29	−4	6	20
C(18)	3399(5)	3072(24)	3907(5)	26	454	25	−9	8	1

* e.s.d.'s in parentheses

The new complex, bis(2-hydroxyethyliminosalicylaldehydato)copper(II) is in a *trans*-configuration. The 2-hydroxyethyliminosalicylaldehyde groups are coordinated to copper(II) as a bidentate chelate, through the terminal phenolic oxygen and the nitrogen of the Schiff-base linkage, while the alcohol groups are free from coordination. This is quite reasonable since the donating tendency of the alcohol oxygen has been estimated to be comparatively weak, as in bis(2-hydroxyethyliminopyruvato)-copper(II) tetrahydrate.[2]

The coordination configurations about the copper atoms in the molecules I and II are both square-planar. Square-planar configurations are also found in bis(salicylaldiminato)copper(II),[5] bis(*N*-*n*-butylsalicylaldiminato)copper(II),[6] and bis(*N*-phenylsalicylaldiminato)copper(II),[7] in which all the Cu(II) atoms occupy the positions of a center of symmetry.

The Cu–O distances of 1.872 and 1.869 Å are shorter than the value of 1.92 Å found in bis(2-hydroxymethyliminopyruvato)copper(II) tetrahydrate.[2] The Cu–N distances of 2.011 and 2.015 Å agree with the value of 2.00 Å in bis(2-hydroxymethyliminopyruvato)copper(II) tetrahydrate.[2] The N–Cu–O angles of 91.7 and 91.3° in the chelate rings are close to a right angle, showing that there is less strain in the chelate structure than the case of the similar chelate of the pyruvate Schiff-base (84.6°),[2] because the chelate rings in this Cu(II) complexes are six-membered, while it is five-membered in the latter.[2] The C–C and C–O bond distances in the ethanol moieties agree well with those in bis(2-hydroxymethyliminopyruvato)copper-(II) tetrahydrate,[2] but the N–C bond distances appear to be longer than that observed in the latter. It is interesting to note here that the distances of C(8)–O(1′) and C(17)–O(3′) (both 2.77 Å) are shorter than the corresponding value (3.10 Å) in bis(2-hydroxymethyliminopyruvato)copper(II) tetrahydrate. These differences in the interatomic distances seem to be caused by the difference in the chelate structure described above.

5) E. N. Baker, D. Hall and T. N. Waters, *J. Chem. Soc.*, **1966**, 680.

6) D. Hall, R. H. Sumner and T. N. Waters, *ibid.*, **1969**, 420.

7) L. Wei, R. M. Stogsdill and E. C. Lingafelter, *Acta Crystallogr.*, **17**, 1058 (1964).

TABLE 3. OBSERVED AND CALCULATED STRUCTURE FACTORS

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H,K=-22 0			20 49 60			8 81 -49			H,K= 12 0			10 46 -57			10 58 76			6 152 164			2 190-148			4 67 -64
2 67 74			22 55 67			10 177-167			0 221 224			11 107 110			11 259 265			7 387 421			3 572 601			5 165 202
4 59 62			24 36 70			12 178 163			2 289 310			12 69 -81			12 31 39			8 46 -32			4 141-121			6 139 139
6 95 104			H,K= -9 0			14 128 109			4 224 218			13 70 76			13 164 164			9 244 264			5 272 298			7 128 138
8 59 59			2 180-173			18 35 -39			6 195 189			15 52 60			14 62 -60			11 209 229			6 115 -92			8 121 121
10 27 30			4 92 -89			H,K= 2 0			8 135 116			17 48 57			15 108 104			12 98 94			7 282 283			9 222 245
12 52 68			6 273 254			0 845 846			10 204 189			19 57 67			16 73 -85			13 234 235			8 191-180			10 105 95
H,K=-21 0			8 160 170			2 598 628			12 214 208			H,K=-16 1			17 78 88			14 135 134			9 306 331			11 140 134
4 26 -33			10 76 -70			4 326 377			14 180 198			1 39 -41			19 102 107			15 265 248			10 98 85			12 50 -51
6 13 26			12 22 -16			6 556 589			16 89 86			2 51 56			21 78 90			16 70 76			11 288 301			13 72 80
8 34 -46			16 72 67			8 306 346			18 37 40			3 24 26			23 43 61			17 173 176			13 178 183			14 39 -59
10 26 -28			22 21 -37			10 370 369			H,K= 13 0			4 41 -39			H,K= -8 1			18 19 28			15 143 141			15 94 101
H,K=-20 0			H,K= -8 0			12 176 174			0 106-102			7 27 -30			1 32 -2			19 86 88			17 27 34			17 91 92
2 44 59			2 314 308			14 239 245			2 77 -79			9 51 -60			2 140 116			20 32 36			19 66 68			19 63 64
4 94 95			4 228 248			16 169 174			4 29 -16			12 23 -33			3 129-117			21 41 54			21 74 82			21 32 40
6 138 135			6 171 196			18 160 158			8 58 -58			H,K=-15 1			4 138 123			23 66 84			23 46 63			H,K= 10 1
8 52 58			8 292 321			20 131 130			10 48 -45			1 273 269			5 150 142			H,K= -2 1			H,K= 4 1			0 53 59
10 62 66			10 317 308			22 109 109			14 32 -46			2 84 91			6 85 65			1 223 201			0 306-237			1 67 65
12 64 66			12 229 227			24 45 56			16 20 24			3 220 221			8 79 -82			2 709-712			1 50 26			2 65 -55
14 47 53			14 161 150			H,K= 3 0			H,K= 14 0			4 27 28			9 55 -67			3 431 396			2 82 100			3 31 -29
16 29 32			16 132 125			0 120 102			0 143 156			5 67 62			10 52 54			4 88 66			3 290-244			4 66 -55
H,K=-19 0			18 149 192			2 558-538			2 55 66			6 61 69			11 92-113			5 13 21			4 425 383			5 16 -13
2 23 26			20 121 132			4 241-212			4 26 28			7 80 89			12 74 89			6 28 39			5 11 26			11 157-156
4 33 48			22 73 88			6 80 103			6 91 83			9 127 142			13 28 26			7 79 75			6 43 -45			12 119-116
6 16 24			H,K= -7 0			8 240 187			8 91 79			10 63 65			14 155 169			9 31 -41			7 186 181			14 19 -31
8 82 -84			2 155-131			12 175-168			10 152 157			11 145 143			15 19 -24			10 210-188			8 27 -26			15 45 49
10 57 -54			4 116-109			16 156-155			12 93 92			13 84 79			17 19 -32			11 29 30			9 45 42			16 31 -36
H,K=-18 0			6 351 316			18 89 77			14 89 100			15 67 64			18 58 -65			12 57 -65			10 120-121			17 23 26
2 73 75			8 258 257			20 74 77			16 79 86			17 67 72			19 39 44			13 56 54			11 25 36			18 18 -32
4 138 149			10 19 -4			H,K= 4 0			H,K= 15 0			19 39 49			21 23 30			14 26 28			12 40 29			H,K= 11 1
6 140 128			14 38 -43			0 14 65			0 59 65			21 30 43			23 13 18			18 36 40			13 22 30			0 74 80
8 50 55			16 135 98			2 443 481			4 30 -24			H,K=-14 1			H,K= -7 1			20 63 -67			15 47 45			1 299 320
10 67 80			H,K= -6 0			4 20 56			6 114-105			1 95 100			1 266 277			21 30 31			16 58 63			2 59 63
12 44 46			2 110 155			6 120 177			8 57 -63			2 74 74			2 134-123			22 22 -30			17 39 -49			3 260 248
14 48 52			4 222 246			8 194 185			10 45 52			3 52 -59			3 294 294			H,K= -1 1			19 22 32			4 29 -33
16 55 52			6 347 355			10 421 428			12 26 26			4 83 90			4 27 19			1 540 510			H,K= 5 1			5 248 253
18 64 63			8 188 192			12 401 424			16 31 -40			5 26 -30			5 574 573			2 539-511			0 193 170			6 74 -74
H,K=-17 0			10 375 385			14 119 101			H,K= 16 0			6 64 -66			6 94 80			3 205 234			1 372 361			7 197 188
2 17 17			12 227 216			16 100 -80			0 188 180			8 66 -57			7 206 212			4 80 -69			2 246-230			8 75 75
4 264 263			14 227 218			18 100 80			2 180 182			10 67 -67			8 82 86			5 178 207			3 261 291			9 117 111
6 90 81			16 146 141			20 69 59			4 189 200			14 63 63			9 222 243			6 73 -80			4 285-271			10 19 35
8 34 37			18 105 105			22 93 80			6 64 51			15 22 28			10 81 -91			7 345 378			5 487 453			11 54 56
10 21 -28			20 149 153			H,K= 5 0			8 44 42			H,K=-13 1			11 243 228			8 178 171			6 173-146			12 48 55
H,K=-16 0			22 38 50			0 106 93			10 52 47			1 335 332			12 62 -51			9 272 267			7 304 288			13 140 140
2 225 192			24 22 31			2 152 142			12 53 65			3 222 201			13 219 225			10 98-100			8 57 65			15 52 60
4 128 117			H,K= -5 0			4 299 247			14 67 85			4 25 -37			16 58 -61			11 293 291			9 243 252			17 50 58
6 149 131			2 216 184			6 137 129			H,K= 17 0			5 242 228			17 104 113			13 339 325			11 251 234			19 32 38
8 170 167			4 103 103			8 21 24			0 80 -83			6 62 71			19 110 114			14 75 -76			12 105 -97			H,K= 12 1
10 167 149			6 49 -44			10 56 -59			4 40 46			7 93 92			20 31 -38			15 217 208			13 221 223			1 50 31
12 120 110			8 122 80			14 39 -48			6 31 34			8 105 103			21 72 91			17 186 183			14 177-159			2 118 129
14 76 78			10 99 65			18 30 25			8 38 41			9 165 157			22 15 -30			18 34 36			15 112 117			4 140 144
16 94 88			16 174 157			22 20 23			12 19 22			11 197 207			23 47 63			19 47 48			16 53 54			5 25 -31
18 81 79			18 185 168			H,K= 6 0			14 31 45			13 127 141			H,K= -6 1			20 45 58			17 89 97			6 97 97
20 44 55			H,K= -4 0			0 446 408			H,K= 18 0			15 102 104			1 131-166			21 41 41			19 108 110			7 25 37
H,K=-15 0			2 587 593			2 296 308			0 141 187			16 57 58			2 102 -75			23 60 75			21 49 50			10 34 -27
2 34 -34			4 8 40			4 388 389			2 111 108			17 74 84			3 38 11			H,K= 0 1			23 45 62			11 33 -32
4 83 79			6 320 316			6 311 314			4 64 66			19 63 70			4 104 -83			1 92-124			H,K= 6 1			16 15 23
6 76 72			8 174 217			8 311 338			6 38 29			21 42 55			5 141 124			2 86 50			0 96 71			17 36 45
8 48 51			10 312 308			10 177 165			8 100 104			H,K=-12 1			6 205 221			3 34 24			1 82 -76			18 31 -32
10 75 65			12 126 142			12 270 283			10 67 77			1 73 66			7 51 -47			4 100-150			2 69 40			H,K= 13 1
12 24 29			14 277 282			16 86 88			12 40 47			2 112 101			9 81 77			5 48 38			3 89 76			0 43 -39
14 61 63			16 275 256			18 124 108			H,K= 19 0			4 84 92			10 15 -15			6 91 -88			4 15 23			1 252 258
18 38 37			18 24 23			20 73 70			0 30 -22			5 28 -26			11 25 -22			7 115-116			5 130 104			2 57 -51
20 16 -26			20 126 117			H,K= 7 0			H,K= 20 0			6 73 -70			12 44 -47			8 344-315			6 191-189			3 197 204
H,K=-14 0			22 33 40			0 258-226			0 69 81			7 17 31			13 57 -67			9 190-158			7 141 127			5 181 175
2 306 332			24 29 47			2 247-197			2 88 102			8 95-101			14 28 -36			10 31 -35			9 44 33			6 35 35
4 239 221			H,K= -3 0			4 384 349			4 53 54			9 65 79			15 29 -23			12 74 72			10 43 53			7 190 188
6 59 62			2 676 631			6 141 148			6 39 38			10 91 -86			16 43 51			13 47 39			11 71 67			8 55 62
8 80 80			4 340-300			8 114 112			8 20 25			11 38 44			17 65 70			15 43 29			12 50 51			9 57 63
10 213 188			6 143-119			10 99 97			H,K= 22 0			15 33 32			20 18 27			16 27 -31			13 19 -27			11 98 99
12 216 204			8 270-260			12 95 75			0 58 65			18 54 -62			H,K= -5 1			17 48 50			14 27 -31			13 93 105
14 133 120			10 166-115			14 143-139			2 54 68			20 22 30			1 472 491			19 70 -87			17 44 40			15 79 90
16 89 80			12 239-237			16 43 32			4 47 65			21 24 28			2 338-300			20 22 -40			18 31 -34			17 36 41
18 87 83			14 103 82			20 45 43			H,K=-22 1			H,K=-11 1			3 722 687			21 29 40			H,K= 7 1			H,K= 14 1
22 53 75			18 178 167			H,K= 8 0			7 17 30			1 310 288			4 242-217			22 27 -44			0 335 286			7 31 42
H,K=-13 0			20 72 79			0 242 249			8 29 -40			2 29 26			5 553 572			23 17 26			1 325 300			8 67 81
2 109-116			22 44 -59			2 494 512			9 26 33			3 167 158			6 138 136			H,K= 1 1			2 337 322			10 53 55
6 76 75			H,K= -2 0			4 412 410			H,K=-21 1			5 181 182			7 210 225			0 95 -92			3 176 221			11 41 42
8 52 -52			2 453 452			6 144 159			1 63 74			6 46 34			8 207 201			1 641 609			4 56 41			12 17 29
10 90 -84			4 303 304			8 249 246			2 27 -35			7 238 217			9 187 210			2 390-420			5 311 326			H,K= 15 1
12 158-143			6 246 286			10 225 217			3 58 69			9 235 219			10 204 206			3 276 316			7 202 225			0 47 -48
14 27 31			8 327 338			12 140 145			5 48 60			10 102 -95			11 219 224			4 143 109			9 231 231			1 129 128
16 103 95			10 121 114			16 104 99			7 85 101			11 256 251			13 232 235			5 122 165			10 51 59			3 119 131
20 44 -61			12 113 131			18 67 61			9 67 77			12 26 -30			15 145 131			6 105 90			11 207 193			4 27 -37
H,K=-12 0			14 221 193			20 70 68			11 56 59			13 191 180			16 122-124			7 288 309			12 41 -50			5 107 104
2 44 48			16 212 195			22 28 38			13 46 59			15 189 186			17 67 76			8 36 -55			13 105 110			6 33 -36
4 176 186			18 139 130			H,K= 9 0			H,K=-20 1			17 44 47			18 19 -30			9 309 305			14 27 -21			7 114 112
6 236 242			20 29 24			0 250-224			10 36 39			19 90 104			19 100 102			11 316 320			15 160 167			8 32 -39
8 407 408			22 39 51			2 35 -66			H,K=-19 1			21 77 94			21 93 109			12 20 -25			17 110 116			9 96 94
10 286 276			24 37 46			4 75 -26			1 42 48			23 37 56			23 50 62			13 217 211			19 86 89			11 95 96
12 155 149			H,K= -1 0			6 98 106			2 43 -46			H,K=-10 1			H,K= -4 1			14 60 73			21 47 58			13 72 76
14 72 68			2 12 34			8 30 34			3 65 74			1 86 -78			1 277-232			15 206 199			22 17 27			15 61 72
16 63 61			4 390-399			10 108 114			5 95 99			2 45 -46			3 492 459			17 73 62			H,K= 8 1			16 34 -47
18 52 53			6 62 32			12 40 -40			6 82 -79			4 65 56			4 158-124			20 44 -46			0 167-156			H,K= 16 1
20 28 26			8 153 99			16 31 27			7 91 94			5 37 39			5 155 148			21 93 98			1 292-279			2 27 -38
22 30 44			10 112-104			H,K= 10 0			8 17 -22			6 174 176			7 26 36			23 32 39			2 55 58			H,K= 17 1
H,K=-11 0			12 77 -70			0 270 278			9 86 91			8 97 91			8 25 36			H,K= 2 1			4 53 43			1 110 115
2 79 -96			22 20 -22			2 485 522			11 85 92			12 25 -30			9 23 37			0 193 153			5 138 138			3 50 49
4 82 -86			H,K= 0 0			4 375 395			13 77 82			13 26 24			10 24 -21			1 387-346			6 30 38			4 38 -46
6 156-145			2 676 722			6 183 193			15 65 70			16 48 -42			11 35 39			2 666 628			7 31 45			5 59 60
8 53 43			4 347 347			8 176 171			17 54 74			17 38 -43			12 114 111			3 384-343			8 28 -34			7 87 88
10 59 65			6 72 102			10 240 239			H,K=-18 1			18 48 -64			13 29 -21			4 32 -8			10 40 -48			9 95 97
14 53 -66			8 439 440			12 165 171			2 52 65			19 48 53			14 47 44			5 99 92			11 89 -88			11 57 63
18 57 -70			10 381 414			14 140 148			3 48 52			21 15 27			15 18 -24			6 71 66			12 117-128			13 49 61
20 29 -19			12 339 359			16 39 45			4 35 38			23 27 41			16 19 12			7 39 -23			13 41 -36			H,K= 18 1
22 22 34			14 259 245			18 101 96			6 40 -48			H,K= -9 1			17 53 53			8 111-106			14 39 41			1 39 -36
H,K=-10 0			16 167 166			20 31 36			8 37 -46			1 225 248			19 47 46			9 125-109			15 23 20			2 45 55
2 336 341			18 164 162			H,K= 11 0			H,K=-17 1			2 36 38			20 41 -52			12 36 41			17 25 32			3 15 -25
4 284 267			20 118 112			0 39 -38			1 119 123			3 224 241			21 38 -35			13 41 35			19 22 24			H,K= 19 1
6 200 202			22 87 91			2 136 138			3 111 117			4 172-150			H,K= -3 1			15 70 67			20 32 -38			1 99 104
8 444 435			24 45 57			4 84 -72			4 31 35			5 124 155			1 435 399			16 63 74			H,K= 9 1			2 21 -33
10 256 264			H,K= 1 0			6 35 39			5 43 49			6 48 -60			2 18 -8			17 41 -39			0 93 -89			3 64 71
12 310 297			2 148-181			12 34 -32			7 101 102			7 245 267			3 802 806			18 107 115			1 252 264			5 48 50
14 278 267			4 621 590			16 66 72			8 27 -40			8 54 52			4 136 152			H,K= 3 1			2 24 6			7 68 72
16 184 170			6 100 -66			20 17 -22			9 122 124			9 245 264			5 230 266			1 422 393			3 276 291			9 60 67

TABLE 3. (Continued)

L	FO	FC
H,K= 20 1		
3	30	-35
4	34	-43
H,K= 21 1		
0	35	48
1	69	78
3	69	64
5	53	60
H,K=-20 2		
1	21	-30
2	48	59
4	71	78
6	25	29
7	32	39
8	45	47
10	34	40
12	25	26
H,K=-19 2		
10	35	36
H,K=-18 2		
2	102	97
4	130	122
6	124	117
7	40	53
8	114	104
9	27	31
10	90	90
12	70	69
14	74	76
16	60	60
H,K=-17 2		
4	30	-26
6	38	-43
14	41	48
16	17	19
H,K=-16 2		
2	175	183
3	45	-49
4	141	135
6	58	60
7	55	54
8	112	108
10	96	90
11	34	-35
12	93	95
13	40	-43
14	127	134
16	83	83
18	65	67
H,K=-15 2		
3	63	-62
6	28	30
9	17	24
10	87	-85
12	21	-24
16	23	26
H,K=-14 2		
2	85	76
3	92	-89
4	107	105
5	24	-27
6	134	133
8	152	156
10	142	140
12	118	122
14	111	112
16	99	107
18	83	83
20	43	51
H,K=-13 2		
1	57	46
2	72	66
4	112	-95
5	17	13
6	85	-86
7	51	-45
8	55	49
9	69	-67
10	44	38
12	44	39
20	20	28
21	21	-31
H,K=-12 2		
1	54	-49
2	173	161
3	37	-35
4	184	180
5	50	-51
6	142	140
8	34	32
9	65	59
10	53	51
12	147	146
14	181	184
16	105	101
18	46	41
20	38	44
21	21	-31
H,K=-11 2		
1	26	-21
2	21	-48
3	56	61
6	27	-32
9	97	-101
10	40	-36
11	30	29
13	38	41
14	31	28
16	34	30
H,K=-10 2		
1	57	36
2	161	179
3	93	-91
4	135	136
5	30	-27
6	238	244
7	57	-69
8	257	248
9	151	133
10	88	76
11	88	69
14	35	24
16	43	51
18	64	71
19	36	38
20	69	86
22	30	47
H,K= -9 2		
1	36	42
5	40	-37
6	35	44
7	157	-122
8	37	37
9	22	26
12	107	107
13	143	132
14	31	30
16	71	-78
17	35	39
20	32	46
22	15	24
H,K= -8 2		
2	285	323
3	15	-9
4	261	281
6	327	380
7	100	-86
8	240	250
9	26	27
10	212	206
11	35	51
12	236	222
13	43	-35
14	71	77
15	65	-65
16	110	110
17	43	41
18	100	101
20	55	64
22	36	50
H,K= -7 2		
1	33	35
2	28	38
3	37	-40
4	86	78
5	91	-86
6	169	172
7	88	-75
9	71	74
17	40	42
18	27	29
20	26	37
21	17	-20
H,K= -6 2		
1	133	-116
2	252	284
3	121	98
4	343	372
5	212	-201
6	373	394
7	29	-21
8	191	192
9	17	19
10	214	223
11	65	69
12	263	269
13	102	-98
14	127	123
15	71	-73
16	153	142
18	151	153
20	93	111
21	20	30
22	44	57
H,K= -5 2		
1	46	32
2	132	-116
3	187	149
4	83	86
5	157	-144
6	43	47
7	72	76
8	83	-95
9	52	-62
12	131	-129
13	101	-93
H,K= 2 2		
14	133	-127
H,K= -4 2		
1	44	-43
2	328	363
3	69	-98
4	491	506
5	102	-103
6	315	336
7	41	45
8	265	286
9	64	-64
10	322	353
11	39	36
12	130	123
13	116	-102
14	148	148
15	35	-26
16	111	122
18	123	114
20	85	72
22	48	46
H,K= 3 2		
0	31	39
1	60	56
2	111	94
3	249	258
4	63	-48
5	60	-56
6	79	-70
7	32	-26
8	17	12
10	38	45
11	103	-81
12	40	28
13	48	-49
15	30	-36
16	134	122
18	123	119
20	22	29
21	43	57
22	23	-36
H,K= -2 2		
1	128	143
2	450	525
3	33	-28
4	379	378
5	195	172
6	318	350
7	129	108
8	260	282
10	275	298
11	29	-30
12	170	165
14	166	144
15	122	122
16	134	122
18	123	119
20	22	29
21	43	57
22	24	33
H,K= -1 2		
1	88	112
2	198	248
3	134	129
4	155	133
5	122	122
6	98	-94
7	51	-35
8	91	-95
10	74	64
11	40	-46
12	121	96
13	16	-32
14	137	111
15	28	38
16	54	64
20	25	-40
22	18	18
23	10	-26
H,K= 0 2		
0	107	103
1	125	91
2	191	191
3	16	24
4	217	259
5	88	103
6	376	392
7	98	94
8	234	244
9	12	35
10	193	183
12	145	126
13	23	16
14	139	131
16	147	127
17	44	-56
18	88	81
19	23	39
20	27	33
21	27	38
22	23	27
H,K= 1 2		
0	155	154
1	71	75
2	203	-239
3	128	126
4	24	-17
6	106	93
7	113	-116
8	113	114
9	105	-103
10	198	199
11	74	66
12	54	46
13	47	32
14	31	-33
15	16	11
16	24	30
17	31	-33
19	16	11
22	24	30
H,K= 2 2		
0	383	430
1	105	91
2	321	324
3	70	-59
4	175	207
5	36	16
6	150	-124
7	31	-35
8	258	275
9	64	-64
10	322	353
12	263	273
14	180	191
15	17	20
16	97	87
17	64	-65
18	42	30
19	28	28
20	75	70
22	58	62
H,K= 3 2		
13	59	-73
14	41	42
H,K= 10 2		
0	221	239
3	200	186
4	44	46
5	110	116
7	187	-190
8	62	56
9	29	-19
11	22	13
12	102	89
13	47	50
14	109	96
15	17	-30
16	17	27
17	37	-35
18	72	74
19	20	-21
21	43	57
22	17	14
H,K= 4 2		
0	113	141
1	94	-85
2	126	157
3	89	-100
4	372	415
5	180	-161
6	229	208
7	46	36
8	314	312
9	17	12
10	183	164
12	180	155
14	184	186
15	17	-28
16	142	149
18	127	128
20	74	72
22	45	48
H,K= 5 2		
0	203	-189
1	60	66
2	77	-73
3	69	72
4	284	-295
5	75	77
6	205	-193
7	102	-102
8	63	58
9	80	78
13	35	29
14	58	-65
15	25	-25
17	47	-45
18	40	36
20	25	26
H,K= 6 2		
0	255	209
1	51	29
2	220	222
3	41	44
4	196	199
5	150	-159
6	307	323
7	13	-23
8	266	243
9	127	117
10	209	181
12	142	131
13	43	53
14	107	98
16	60	60
17	-19	-15
18	68	57
19	20	-21
20	60	60
H,K= 7 2		
1	26	-25
2	41	22
4	58	-60
5	29	38
6	139	-126
7	52	46
8	141	-125
9	65	-76
10	55	-47
13	58	55
15	30	33
16	20	-26
19	19	-26
H,K= 8 2		
0	311	319
1	41	24
2	337	364
3	86	-91
4	259	272
5	23	23
6	252	244
8	258	242
9	131	138
10	191	190
12	76	74
14	87	91
15	29	-29
16	122	132
18	74	67
20	63	66
H,K= 9 2		
0	60	55
1	56	-54
2	144	138
3	43	-43
4	107	96
6	54	57
8	41	51
9	37	-38
10	50	-47
11	40	-32
13	59	-73
14	41	42
H,K= 10 2		
1	60	56
2	111	94
3	102	-88
4	237	258
5	125	124
7	89	91
8	20	28
9	43	47
10	28	37
11	28	33
12	26	32
13	54	51
14	96	88
15	38	45
H,K= 11 2		
1	53	-46
2	74	72
3	17	-5
5	28	7
6	26	-31
7	22	-2
9	24	-34
10	60	63
11	24	-25
15	50	48
20	15	-18
H,K= -5 3		
21	36	31
H,K= 2 3		
0	67	-78
1	48	56
2	37	42
3	20	24
5	53	-62
6	23	-15
7	18	-14
8	33	-34
9	44	-53
11	23	24
16	38	-40
21	20	24
H,K= 3 3		
1	191	232
2	56	47
3	223	248
4	17	15
5	258	279
6	114	127
7	172	168
8	103	96
9	127	124
11	125	114
12	24	32
13	118	108
15	78	71
16	46	-24
H,K= 4 3		
0	90	-81
1	41	42
2	24	32
3	24	-29
4	42	-44
5	71	-79
6	196	246
7	176	162
8	249	307
9	102	89
10	71	61
11	35	29
12	88	103
13	131	116
15	130	111
17	88	88
19	21	30
H,K= 5 3		
0	165	169
1	56	-44
2	91	85
3	224	228
4	181	165
5	261	298
6	274	287
8	101	102
9	90	74
10	48	45
11	140	133
12	52	54
13	99	86
15	59	51
16	64	64
17	54	52
19	71	71
H,K= 6 3		
0	83	-80
1	12	20
2	61	-54
3	23	-21
4	84	-68
5	87	88
6	21	21
7	46	-44
8	79	68
9	79	68
10	75	68
11	25	28
12	51	-61
13	69	75
14	37	-42
15	58	56
17	84	83
18	47	47
H,K= 8 3		
0	61	57
1	62	60
2	55	-48
3	54	49
4	115	-115
5	84	67
7	109	-99
8	61	63
9	35	-33
10	24	29
11	75	69
16	37	-41
18	22	-24
H,K= 9 3		
0	59	68
1	73	57
2	27	-21
3	181	186
4	112	-103
5	175	173
6	31	-31
7	137	133
8	57	-63
9	150	158
11	72	74
13	63	66
15	75	77
17	56	59
H,K= 10 3		
0	75	65
1	61	-58
3	41	43
4	41	54
6	90	82
7	35	38
8	17	25
H,K= 11 3		
0	35	-33
1	156	145
2	76	-72
3	161	153
4	24	22
5	80	84
6	73	77
7	97	96
8	28	36
9	119	104
11	103	107
13	66	66
15	33	32
H,K= 12 3		
0	30	37
1	40	-43
2	57	-46
3	41	-43
6	28	-23
8	30	-30
11	36	38
13	38	44
H,K= 13 3		
1	138	130
3	123	118
4	45	50
5	128	110
7	72	68
9	94	86
11	45	46
13	48	52
H,K= 14 3		
0	47	-46
2	32	-34
4	30	-39
6	34	-40
10	34	-39
11	26	35
13	24	34
H,K= 15 3		
1	50	48
3	75	73
4	30	29
6	35	-44
8	53	60
9	35	44
H,K= 16 3		
0	29	-39
2	34	-40
H,K= 17 3		
1	18	24
3	18	19
6	24	31
H,K=-16 4		
1	21	27
2	53	55
4	55	60
6	59	58
7	28	-40
8	54	69
10	47	53

TABLE 3. (Continued)

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H,K=-15	4		6	54	-61	16	62	75	12	27	29	12	78	76	7	13	-11	7	124	-129	0	124	108	13	7	-3
-14	18	28	7	27	-36	18	45	61	14	34	50	14	85	79	8	68	-72	8	117	108	2	83	62	H,K=	12	4
10	22	33	8	27	-34	H,K=	-7	4	15	56	-76	16	54	62	9	34	-31	9	44	-46	3	68	54	0	86	60
11	28	-40	10	81	74	1	95	-86	16	27	40	18	39	51	14	21	41	10	63	67	4	125	107	1	27	-21
12	40	52	12	20	20	3	37	-30	H,K=	-4	4	H,K=	-1	4	H,K=	2	4	12	91	100	6	134	105	2	127	109
H,K=-14	4		13	19	23	5	42	-48	1	24	-27	1	18	35	0	59	73	14	65	61	7	36	35	4	113	95
2	94	82	16	22	-29	9	27	32	2	122	130	3	18	-10	1	13	-9	16	38	36	8	98	82	5	28	30
4	115	109	H,K=	-10	4	11	50	58	4	159	166	5	32	42	2	111	127	H,K=	5	4	10	45	65	6	108	95
6	81	67	2	161	147	12	22	28	6	106	87	6	21	13	3	29	39	0	77	78	14	40	49	8	95	82
7	20	-25	3	74	69	15	34	-39	7	34	24	7	18	-12	4	186	245	2	98	91	H,K=	9	4	10	48	67
8	24	23	4	135	125	17	16	-17	8	126	125	9	79	-68	5	43	46	3	75	70	0	48	-46	11	36	-52
9	33	-44	5	45	33	18	17	-25	10	94	84	11	22	27	6	165	185	4	61	50	2	49	-45	12	49	76
10	56	47	6	103	86	H,K=	-6	4	12	95	89	13	27	36	7	112	-118	6	33	20	3	22	-17	H,K=	13	4
11	42	-50	7	45	39	1	10	-11	14	107	112	15	25	34	8	152	130	7	72	-69	7	38	42	2	29	-30
12	70	73	8	125	114	2	139	146	16	48	54	16	19	-30	9	53	-63	8	27	16	9	50	52	H,K=	14	4
13	24	-26	10	121	117	3	42	-46	18	31	36	H,K=	0	4	10	80	69	9	22	-20	H,K=	10	4	0	72	56
14	42	40	12	99	90	4	135	125	H,K=	-3	4	0	216	221	12	78	65	11	19	-23	0	129	107	2	31	27
H,K=-13	4		14	115	113	5	46	-46	2	27	33	2	236	253	14	86	90	H,K=	6	4	2	123	103	4	36	40
6	30	-34	16	68	72	6	145	123	3	29	-31	3	36	36	16	65	73	0	111	107	3	35	31	6	32	32
9	24	33	H,K=	-9	4	8	113	99	4	31	29	4	124	159	18	36	53	2	91	76	4	124	118	8	47	60
11	35	-37	2	37	31	10	100	85	5	38	48	5	49	50	H,K=	3	4	4	124	112	6	122	106	H,K=	15	4
13	20	-23	7	38	37	11	38	-43	7	41	19	6	177	192	0	26	31	6	179	194	8	124	101	0	27	32
H,K=-12	4		9	31	21	12	81	82	10	38	-61	7	43	-44	2	47	-41	8	115	95	10	68	73	1	22	29
1	38	41	12	30	31	14	52	57	12	20	29	8	91	87	3	51	-45	9	47	54	11	29	-45	4	17	-22
2	86	67	H,K=	-8	4	16	45	54	14	19	29	9	52	-52	4	34	-35	10	47	38	12	34	50	H,K=	16	4
4	116	101	2	117	128	18	28	33	H,K=	-2	4	10	122	122	5	96	-86	12	45	49	14	22	28	0	57	54
6	134	126	4	104	84	H,K=	-5	4	1	22	-26	12	133	131	6	23	-22	13	24	-31	H,K=	11	4	2	65	68
8	92	93	5	26	-28	1	24	-23	2	81	116	14	87	91	7	87	-74	14	81	81	1	55	-53	4	45	56
10	88	92	6	95	80	3	49	-57	3	40	-48	15	29	37	8	47	45	16	56	62	3	13	-4	6	26	43
12	81	67	8	118	99	4	45	27	4	149	167	16	47	53	11	22	32	H,K=	7	4	4	13	8	H,K=	17	4
14	40	36	9	38	44	5	38	-41	5	23	-20	18	49	64	H,K=	4	4	1	75	54	5	13	11	2	19	17
16	31	42	10	95	94	6	24	20	6	163	172	H,K=	1	4	0	114	114	3	78	56	7	13	13			
H,K=-11	4		11	31	44	7	24	31	7	59	62	1	33	-35	1	70	64	4	43	29	8	12	12			
1	90	69	12	58	54	8	25	20	8	108	93	2	25	29	2	91	73	6	73	64	9	12	1			
2	47	44	13	36	39	9	37	43	9	20	27	3	49	-61	3	34	22	9	59	51	10	11	-6			
3	38	23	14	43	40	10	31	42	10	43	49	4	28	23	4	149	138	10	53	57	11	10	9			
4	22	11	15	30	-39	11	22	29	11	49	51	5	23	20	6	113	116	H,K=	8	4	12	9	12			

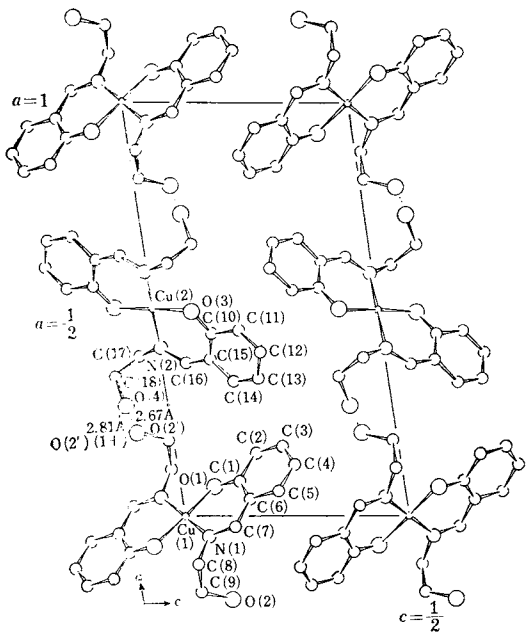


Fig. 1. Projection of the unit cell contents on the (010) plane.

In Table 5 the distances in various related complexes are compared with the values obtained in the present work. These latter values generally agree well with those found in the related compounds. The molecules may be described in terms of a set of various planar groups. Tables 6 (molecule I) and 7 (molecule II) list the equations for various least-square planes, the angles between them, and the deviations of the atoms therefrom. The benzene rings in salicylaldimine groups are almost planar (the maximum deviations of the

TABLE 4. BOND DISTANCES AND THEIR ESTIMATED STANDARD DEVIATIONS*

Molecule I		Molecule II	
Cu(1)–O(1)	1.872(7) Å	Cu(2)–O(3)	1.869(8) Å
N(1)	2.011(8)	N(2)	2.015(9)
C(1)–O(1)	1.331(12)	C(10)–O(3)	1.329(14)
C(2)	1.429(17)	C(11)	1.421(18)
C(6)	1.381(14)	C(15)	1.417(17)
C(3)–C(2)	1.386(19)	C(12)–C(11)	1.408(20)
C(4)	1.397(19)	C(13)	1.434(20)
C(5)–C(4)	1.393(18)	C(14)–C(13)	1.375(20)
C(6)	1.457(16)	C(15)	1.435(18)
C(7)–C(6)	1.439(14)	C(16)–C(15)	1.422(16)
N(1)	1.302(13)	N(2)	1.306(14)
C(8)–N(1)	1.492(12)	C(17)–N(2)	1.465(13)
C(9)	1.534(14)	C(18)	1.534(16)
C(9)–O(2)	1.443(13)	C(18)–O(4)	1.445(14)

* e.s.d.'s in parentheses

atoms from the mean planes are 0.007 Å in the molecule I and 0.014 Å in the molecule II), but the nitrogen atoms are slightly, but significantly, out of the plane (0.104 and 0.092 Å). The two salicylaldimine groups in the molecules I and II are, of course, parallel, as is required by the centrosymmetry, but they are far from coplanar. The perpendicular distances between the two parallel salicylaldimine planes in the molecules I and II are 0.29 and 0.50 Å, while these range from 0.13 to 0.89 Å in other, similar complexes with planar configurations about Cu(II) atoms.[5-7] Each salicylaldimine group makes an angle of 5.5° (in the molecule I) and 9.9° (in the molecule II) with the coordination plane. Thus, the planarity of the molecule I is slightly better than that of the molecule II. This difference seems to be caused by the

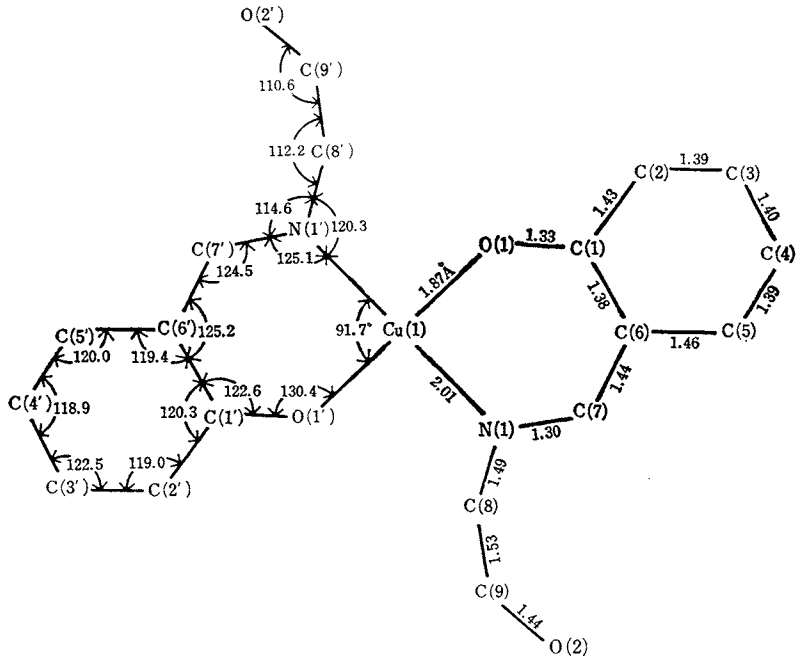


Fig. 2. The environment of the copper atom in the molecule I, showing bond distances and angles.

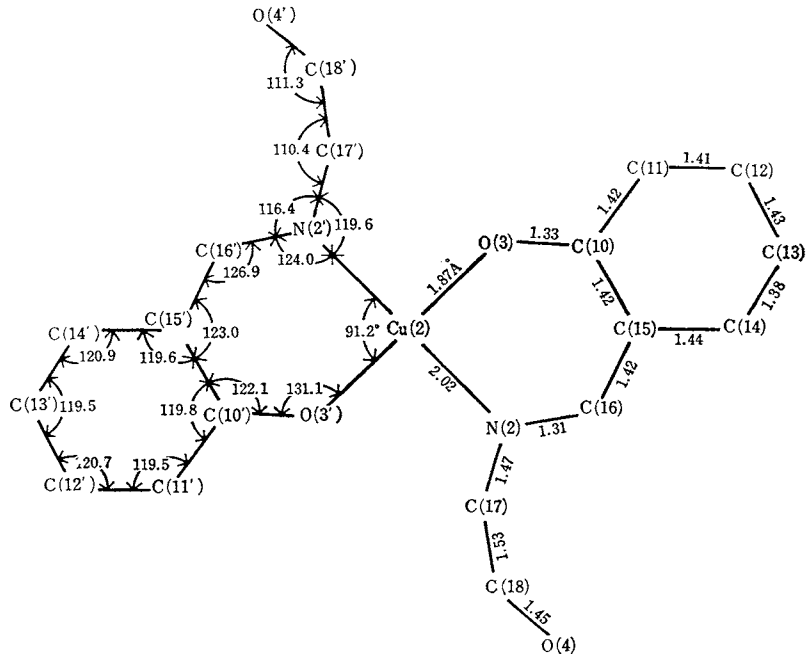


Fig. 3. The environment of the copper atom in the molecule II, showing bond distances and angles.

TABLE 5. BOND ANGLES AND THEIR ESTIMATED STANDARD DEVIATIONS*

Molecule I		Molecule II	
N(1)-Cu(1)-O(1)	91.7(3)°	N(2)-Cu(2)-O(3)	91.2(4)°
Cu(1)-O(1)-C(1)	130.4(7)	Cu(2)-O(3)-C(10)	131.1(8)
O(1)-C(1)-C(6)	122.6(9)	O(3)-C(10)-C(15)	122.1(11)
O(1)-C(1)-C(2)	117.2(9)	O(3)-C(10)-C(11)	118.1(11)
C(2)-C(1)-C(6)	120.3(10)	C(11)-C(10)-C(15)	119.8(11)
C(1)-C(2)-C(3)	119.0(12)	C(10)-C(11)-C(12)	119.5(12)
C(2)-C(3)-C(4)	122.5(12)	C(11)-C(12)-C(13)	120.7(13)
C(3)-C(4)-C(5)	118.9(12)	C(12)-C(13)-C(14)	119.5(13)
C(4)-C(5)-C(6)	120.0(11)	C(13)-C(14)-C(15)	120.9(12)
C(5)-C(6)-C(1)	119.4(10)	C(14)-C(15)-C(10)	119.6(11)
C(5)-C(6)-C(7)	115.3(9)	C(14)-C(15)-C(16)	117.5(11)
C(7)-C(6)-C(1)	125.2(9)	C(16)-C(15)-C(10)	123.0(11)
C(6)-C(7)-N(1)	124.5(9)	C(15)-C(16)-N(2)	126.9(10)
C(7)-N(1)-Cu(1)	125.1(7)	C(16)-N(2)-Cu(2)	124.0(7)
C(7)-N(1)-C(8)	114.6(8)	C(16)-N(2)-N(17)	116.4(9)
C(8)-N(1)-Cu(1)	120.3(6)	C(17)-N(2)-Cu(2)	119.6(6)
N(1)-C(8)-C(9)	112.2(8)	N(2)-C(17)-C(18)	110.4(9)
C(8)-C(9)-O(2)	110.6(8)	C(17)-C(18)-O(4)	111.3(9)

* e.s.d.'s in parentheses

TABLE 6. BOND DISTANCES IN SALICYL COMPLEXES WITH COPPER(II)

	Cu-O	Cu-N	O-C1	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C1-C6	C6-C7	C7-N	N-C8
(1)	1.90	1.99	1.32	1.40	1.39	1.40	1.37	1.39	1.42	1.44	1.31	1.52
(2)	1.92	1.94	1.36	1.39	1.38	1.36	1.36	1.44	1.40	1.45	1.25	—
(3)	1.91	1.96	1.33	1.40	1.38	1.40	1.36	1.40	1.44	1.44	1.26	—
(4)	1.91	1.90	1.31	1.42	1.39	1.41	1.38	1.42	1.38	1.44	1.28	—
(5)	1.90	2.02	1.30	1.41	1.39	1.41	1.38	1.43	1.40	1.46	1.31	1.48
(6)	1.87	2.01	1.33	1.43	1.39	1.40	1.39	1.46	1.38	1.44	1.30	1.49
(7)	1.87	2.02	1.33	1.42	1.41	1.43	1.38	1.44	1.42	1.42	1.31	1.47
(8)	1.88	1.99	1.31	1.42	1.40	1.37	1.37	1.42	1.40	1.44	1.30	1.44
(9)	1.90	1.96	1.29	1.41	1.40	1.39	1.39	1.42	1.42	1.43	1.27	1.48
(10)	1.89	1.95	1.28	1.42	1.40	1.44	1.39	1.38	1.44	1.46	1.28	1.53
(11)	1.89	2.01	1.30	1.43	1.40	1.38	1.40	1.41	1.42	1.46	1.25	1.51
(12)	1.89	1.99	1.33	1.42	1.40	1.39	1.37	1.44	1.42	1.41	1.26	1.49
(13)	1.87	1.98	1.31	1.44	1.43	1.41	1.40	1.44	1.41	1.42	1.33	1.51
(14)	1.93	1.97	1.36	1.44	1.45	1.41	1.42	1.42	—	1.43	1.30	1.56
(15)	1.89	2.01	1.31	1.41	1.40	1.40	1.41	1.42	—	1.45	1.30	1.51

(1) Bis-(*N*-methylsalicylaldiminato)-Cu(II)[8] (2) Bis-(salicylaldoximato)-Cu(II)[9]
(3) Bis-(5-chlorosalicylaldoximato)-Cu(II)[10] (4) Bis-(salicylaldiminato)-Cu(II)[5]
(5) Bis-(*N*-*n*-butylsalicylaldiminato)-Cu(II)[6] (6) Molecule I in present work
(7) Molecule II in present work (8) Bis-(*N*-phenylsalicylaldiminato)-Cu(II)[7]
(9) Bis-(*N*-ethylsalicylaldiminato)-Cu(II)[11] salicyl group I
(10) Bis-(*N*-ethylsalicylaldiminato)-Cu(II)[11] salicyl group II
(11) Bis-(*N*-*t*-buthylsalicylaldiminato)-Cu(II)[12]
(12) Bis-(*N*-isopropylsalicylaldiminato)-Cu(II)[13] salicyl group I
(13) Bis-(*N*-isopropylsalicylaldiminato)-Cu(II)[13] salicyl group II
(14) Bis-(*N*-α-phenylethylsalicylaldiminato)-Cu(II)[14] salicyl group I
(15) Bis-(*N*-α-phenylethylsalicylaldiminato)-Cu(II)[14] salicyl group II

(1), (2), and (3) octahedral (4), (5), (6), (7), and (8) planar
(9), (10), (11), (12), (13), (14), and (15) tetrahedral

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Table 7. Least-squares planes in the molecule I

Coefficients of least-squares plane equations
$AX + BY + CZ + D = 0$

	A	B	C	D
		($\times 10^4$)		
Coordination plane (α)	6440	6861	−3384	0
Chelate ring plane (β)	6253	6618	−4136	11647
Cu-chelate ring plane (β')	6278	6736	−3900	4933
Benzene plane (γ)	5986	6776	−4275	15378
Salicylaldimine plane (δ)	6134	6645	−4269	14444
Cu-salicylaldimine plane (δ')	6128	6723	−4153	9335

X(Å) $= ax + cz\cos\beta$ $\quad Y = by$ $\quad Z = cz\sin\beta$

Angles between the least-squares planes

	β	β'	γ	δ	δ'
			(degree)		
α	4.6	3.2	5.7	5.5	4.8
β		1.5	2.0	1.0	1.0
β'			2.7	2.4	1.7
γ				1.1	1.1
δ					0.8

Distances from least-squares planes

	α	β	β'	γ	δ	δ'
			($\times 10^3$)			
Cu(1)	0	(117)	49	(154)	(144)	93
O(1)	0	−9	−42	(−27)	−15	−52
N(1)	0	29	−1	(104)	61	33
C(1)	(−141)	27	30	3	7	−11
C(2)	(−268)	(77)	(99)	6	31	19
C(3)	(−375)	(74)	(133)	−6	13	21
C(4)	(−384)	(45)	(123)	−1	−8	13
C(5)	(−271)	(8)	(67)	7	−21	−6
C(6)	(−131)	−16	4	−6	−28	−34
C(7)	(− 59)	−17	−14	(40)	−4	−15
C(8)	(36)	(49)	(8)	(174)	(105)	(75)

( ) not included in the least-squares calculations

Table 8. Least-squares planes in the molecule II

Coefficients of least-squares plane equations
$AX + BY + CZ + D = 0$

	A	B	C	D
		(10^4)		
Coordination plane (α)	−5284	7371	−4216	30853
Chelate ring plane (β)	−4308	7280	−5333	24104
Cu-chelate ring plane (β')	−4746	7235	−5013	26896
Benzene plane (γ)	−4084	7219	−5586	23075
Salicylaldimine plane (δ)	−4142	7241	−5515	23175
Cu-salicylaldimine plane (δ')	−4460	7151	−5383	25172

X(Å) $= ax + cz\cos\beta$ $\quad Y = by$ $\quad Z = cz\sin\beta$

Angles between the least-squares planes

	β	β'	γ	δ	δ'
			(degree)		
α	8.5	5.6	10.5	9.9	8.3
β		3.1	2.0	1.4	1.2
β'			5.0	4.5	2.7
γ				0.5	2.5
δ					2.0

Distances from least-squares planes

	α	β	β'	γ	δ	δ'
			($\times 10^3$)			
Cu(2)	0	(199)	64	(288)	(250)	136
O(3)	0	−29	−98	(5)	−17	−105
N(2)	0	36	−18	(92)	62	11
C(10)	(237)	18	20	8	−2	−46
C(11)	(389)	(30)	(67)	−14	−15	−49
C(12)	(661)	(99)	(213)	9	20	33
C(13)	(735)	(105)	(262)	2	17	69
C(14)	(557)	(62)	(185)	−7	−3	41
C(15)	(311)	24	69	2	17	69
C(16)	(112)	−46	31	(−35)	−52	−63
C(17)	(−162)	(−26)	(97)	(56)	(18)	(−29)

( ) not included in the least-squares calculations

difference in the packing of the molecules. The C(8) (in the molecule I) and C(17) (in the molecule II) of ethanolamine groups are displaced from the planes of the chelate ring, the deviations being 0.049 and 0.026 Å. The angles between the C–C single bonds in ethanolamine groups and the planes are 62 and 67° respectively.

The closest approach, less than 3.5 Å, between adjacent molecules occurs between the free alcoholic oxygens of the adjacent molecules. The distances of O(2′)–O(4) and O(2′)–O(4) $(x,-1+y,z)$ are 2.67 and 2.81 Å, as is shown in Fig. 1. These short distances suggest the presence of hydrogen bonds between them. By these hydrogen bonds, the complexes are held together to form layers parallel to the (001) plane. Between adjacent layers there exists no hydrogen bond.

The numerical calculations were carried out on the FACOM231 computer at this University and the HITAC5020E computer at the Computer Center, Tokyo University.

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