best by comparing the atom positions relative to the center of the cluster unit. Stated simply the octahedron of metal atoms is expanded and the surrounding cluster of chlorine atoms, both bridging and terminal, is contracted as a result of this process. Consequently, the Nb–Cl(terminal) bond is shortened most because the Nb and Cl atoms move directly toward each other.

If local coordinates on the metal atoms are chosen so that the *z* axes point toward the center of the octahedron, then the metal MO's most strongly affected by the removal of electrons are those constructed from the d_{z^2} set, *viz*, a_{1g}, e_g*, and t_{2g}*.[12] Of this set only a_{1g} is bonding and occupied with electrons in the $Nb_6Cl_{18}^{4-}$ cluster. From the dimensional changes discussed above it appears that the d_{z^2} orbitals may be extracted from metal–metal bonding upon oxidation and used for tighter binding of the terminal Cl atoms. Thus a comparison of the structural data for $Nb_6Cl_{18}^{n-}$ species suggests that a_{1g} is in all cases the bonding MO of highest energy or that the a_{1g} and a_{2u} levels cross over with successive removal of electrons in the oxidation process.

Also included in Table III are structural data for $Ta_6Cl_{18}^{2-}$ as recently determined from a study of $H_2Ta_6Cl_{18} \cdot 6H_2O$.[24] The most noteworthy features of these data are the Ta–Ta distance which is 0.06 Å shorter and the Ta–Cl(terminal) distance which is 0.05 Å longer than the corresponding distances in the isoelectronic $Nb_6Cl_{18}^{2-}$. Since the M–Cl(bridging) distances are nearly equivalent, the principal difference appears to be stronger metal–metal bonding and weaker M–Cl(terminal) bonding in the tantalum cluster compared to the niobium cluster. Chemical evidence[2] does suggest that the tantalum clusters are more stable toward degradation than their niobium counterparts.

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[24] C. B. Thaxton and R. A. Jacobson, *Inorg. Chem.*, **10**, 1460 (1971).

CONTRIBUTION FROM THE DEPARTMENTS OF CHEMISTRY, UNIVERSITY OF WATERLOO, WATERLOO, ONTARIO, CANADA,
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The Crystal and Molecular Structure of the Five-Coordinated Copper(II) Complex with *N*-β-Dimethylaminoethylsalicylaldimine

BY P. C. CHIEH AND GUS J. PALENIK*

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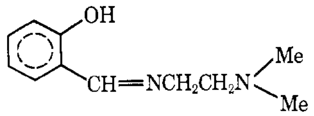
The green compound bis(*N*-β-dimethylaminoethylsalicyladiminato)copper(II), $Cu[OC_6H_4CHNCH_2CH_2N(CH_3)_2]_2$, crystallizes as monoclinic plates with a = 13.079 (5), b = 11.816 (11), c = 15.071 (8) Å, and β = 102.52 (6)°. The space group is $P2_1/n$ with four molecules per unit cell, d_m = 1.295 (5) g/cm³, and d_c = 1.302 (2) g/cm³. Diffractometer data were measured using Cu Kα radiation and the structure has been refined by least-squares methods with anisotropic thermal parameters to a final R of 0.048 for 3081 observed reflections. The crystal consists of discrete molecules of the complex with the copper atom surrounded by five of the six possible donor atoms; the β nitrogen of one ligand is uncoordinated. The molecule is severely distorted but appears to be closer to a trigonal-bipyramidal rather than a square-pyramidal configuration. Some pertinent distances are Cu to O of 1.930 (3) and 1.943 (3) Å, Cu to the azomethine nitrogens of 1.944 (3) and 1.948 (3) Å, and Cu to a dimethylamino nitrogen of 2.553 (4) Å. The long Cu to N distance is in the equatorial plane in the trigonal-bipyramidal configuration which is rather unusual for five-coordinated copper compounds with this configuration.

Introduction

A Cu(II) ion in a regular octahedral field is unstable[1] and is expected to distort to remove the degeneracy of the e_g orbitals. The result is either a compressed or elongated octahedron with the latter being far more common. The final distribution of electrons is unsymmetrical, producing changes in the molecular dimensions of symmetrical chelating ligands.[2,3] Whether the final configuration (the elongated or compressed octahedron) is a function of the type of ligand atoms is an intriguing question. During our study of Cu(II) and high-spin Mn(III) complexes which are susceptible to these distortions, we prepared the bis(*N*-β-dimethylaminoethylsalicylaldiminato)copper(II) complex. The ligand, **1**, is a potential anionic tridentate ligand; we hoped the copper(II) complex would be octahedral. The results of our crystal structure analysis have revealed that the Cu(II) ion is pentacoordinated with one of the dimethylamino groups not bonded to the Cu(II) ion. The resulting configuration is severely distorted from either idealized pentacoordinated configuration and contains several unusual features not observed in other copper complexes.[4]



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Experimental Section

Bis(*N*-β-dimethylaminoethylsalicylaldiminato)copper(II) crystallizes from cyclohexane as green plates elongated along *b* with (001) well developed. Weissenberg, precession, and rotation photographs were taken to obtain preliminary cell constants and to determine the space group. A second crystal with dimensions of 0.16 × 0.18 × 0.16 mm (along *a*, *b*, *c*, respectively) was used for the intensity measurements and for obtaining refined cell

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(1) H. A. Jahn and E. Teller, *Proc. Roy. Soc., Ser. A*, **161**, 220 (1937).

(2) M. V. Veidis, G. H. Schreiber, T. E. Gough, and G. J. Palenik, *J. Amer. Chem. Soc.*, **91**, 1859 (1969).

(3) M. Mathew and G. J. Palenik, *J. Coord. Chem.*, in press.

(4) A preliminary account of this study was presented at the American Crystallographic Association Meeting, Ottawa, Ontario, Canada, Aug 1970.

dimensions. A least-squares fit of 20 Cu Kβ (λ 1.39217 Å) 2θ values was used to obtain the lattice parameters. The pertinent data are presented in Table I.

TABLE I
CRYSTAL DATA FOR
BIS(N-β-DIMETHYLAMINOETHYLSALICYALDIMINATO)COPPER(II),
$Cu(C_{11}H_{15}N_2O)_2$ (MOL WT 446.05)

a = 13.079 (5) Å	Space group $P2_1/n$ (C_{2h}^5)
b = 11.816 (11) Å	d_m = 1.295 (5) g/cm^3
c = 15.071 (8) Å	d_o = 1.302 (2) g/cm^3
β = 102.52 (6)°	Z = 4
U = 2274.0 Å^3	μ(Cu Kα) = 15.7 cm^{-1}

The crystal was mounted on a glass fiber and aligned on a General Electric single-crystal orienter with b^* parallel to the φ axis of the orienter. The intensity measurements were made using a wide beam (4° takeoff angle) of Cu Kα_1 radiation (λ 1.54051 Å), using the stationary-crystal, stationary-counter method. A 20-sec count was taken for all reflections with a 0.7-mil Ni foil in front of the scintillation counter window. Four standard reflections were measured after every 100 reflections and were used to correct for a decrease in their intensity with time (maximum change was 6%). A total of 9740 measurements with $2\theta < 135°$ were made and reduced to a set of 4235 independent reflections after averaging of symmetry-equivalent forms. An experimental background curve was derived by the systematic measurement of areas of reciprocal space which were known to contain no reflections and then averaging the values obtained at a given 2θ angle. The 3081 reflections with I (total counts) greater than B (background counts) + $3\sqrt{I}$ were considered to be observed. The remaining 1154 reflections were considered to be unobserved and were given a value of $^1/_2(3\sqrt{I})$ and flagged with a minus sign.

A correction for the α_1–α_2 splitting was made on the basis of previous comparisons of moving-crystal *vs.* stationary-counter measurements. No correction for absorption was made because of the relatively small value of μ (15.7 cm^{-1}) and the small size of the crystal. These data were then reduced to a set of structure amplitudes on an arbitrary scale in the usual manner.

TABLE II
FINAL POSITIONAL AND THERMAL PARAMETERS FOR THE NONHYDROGEN ATOMS[a]

Atoms	x/a	y/b	z/c	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	21,403 (4)	8860 (5)	15,718 (4)	433 (3)	593 (4)	343 (2)	−84 (7)	236 (4)	−186 (6)
OA1	875 (2)	42 (2)	1,563 (2)	51 (2)	70 (2)	33 (1)	−13 (3)	30 (2)	−23 (3)
CA1	380 (3)	28 (3)	2,224 (2)	35 (2)	67 (3)	33 (2)	21 (4)	12 (3)	6 (4)
CA2	462 (3)	886 (4)	2,888 (3)	50 (3)	77 (3)	39 (2)	12 (5)	40 (4)	−12 (5)
CA3	−122 (4)	775 (5)	3,573 (3)	77 (4)	116 (5)	51 (2)	6 (7)	66 (5)	−25 (6)
CA4	−737 (4)	−124 (5)	3,621 (4)	72 (4)	135 (6)	60 (3)	−17 (8)	76 (5)	−3 (7)
CA5	−820 (4)	−939 (5)	2,974 (3)	51 (3)	121 (5)	64 (3)	−38 (7)	39 (5)	26 (7)
CA6	−288 (3)	−886 (4)	2,284 (3)	44 (2)	83 (4)	44 (2)	−19 (6)	19 (4)	−1 (5)
CAN	1,087 (4)	1873 (4)	2,881 (3)	64 (3)	68 (3)	46 (2)	12 (6)	40 (4)	−25 (5)
NA1	1,745 (3)	2007 (3)	2,378 (2)	61 (2)	60 (3)	38 (2)	−11 (4)	29 (3)	−15 (3)
CE1	2,285 (4)	3090 (4)	2,373 (3)	88 (4)	62 (4)	53 (3)	−26 (6)	41 (5)	−33 (5)
CE2	2,002 (4)	3559 (4)	1,413 (4)	85 (4)	59 (3)	66 (3)	−5 (6)	37 (6)	−1 (5)
NA2	2,284 (3)	2757 (3)	764 (2)	56 (2)	66 (3)	41 (2)	−16 (4)	11 (3)	0 (4)
CM1	3,390 (4)	2876 (5)	727 (4)	67 (3)	98 (5)	64 (3)	−46 (7)	43 (5)	6 (6)
CM2	1,619 (5)	2916 (5)	−139 (4)	89 (4)	120 (6)	58 (3)	−32 (8)	−29 (6)	33 (7)
OB1	3,593 (2)	959 (3)	2,230 (2)	53 (2)	79 (3)	39 (1)	7 (4)	−2 (3)	−16 (3)
CB1	4,390 (3)	459 (4)	2,009 (3)	49 (3)	64 (3)	41 (2)	5 (5)	4 (4)	30 (4)
CB2	4,337 (3)	−180 (3)	1,221 (3)	39 (2)	65 (3)	44 (2)	8 (5)	30 (4)	40 (4)
CB3	5,254 (3)	−695 (4)	1,058 (3)	54 (3)	98 (5)	56 (2)	27 (6)	56 (4)	45 (5)
CB4	6,199 (4)	−559 (5)	1,646 (4)	46 (3)	143 (6)	82 (3)	53 (7)	53 (5)	101 (8)
CB5	6,252 (4)	84 (6)	2,396 (4)	45 (3)	148 (7)	80 (4)	10 (7)	−10 (5)	67 (8)
CB6	5,394 (4)	599 (5)	2,592 (3)	49 (3)	109 (5)	59 (3)	6 (6)	−22 (5)	19 (6)
CBN	3,380 (3)	−366 (3)	548 (3)	47 (3)	61 (3)	35 (2)	2 (5)	39 (4)	17 (4)
NB1	2,459 (2)	−20 (3)	588 (2)	43 (2)	53 (2)	30 (1)	−1 (4)	21 (3)	3 (3)
CE3	1,587 (3)	−343 (4)	−165 (2)	43 (2)	71 (3)	28 (2)	−3 (5)	8 (3)	−15 (4)
CE4	1,196 (3)	−1529 (4)	−60 (3)	53 (3)	68 (3)	41 (2)	−8 (5)	23 (4)	−29 (4)
NB2	1,932 (3)	−2403 (3)	−160 (3)	69 (3)	66 (3)	81 (3)	15 (5)	47 (5)	−30 (5)
CM3	1,930 (8)	−2547 (6)	−1,131 (6)	240 (11)	125 (7)	130 (6)	34 (14)	245 (14)	−91 (10)
CM4	1,685 (5)	−3471 (5)	224 (5)	108 (5)	71 (5)	110 (5)	0 (8)	26 (8)	1 (7)

[a] All values are multiplied by 10^4 except for the Cu atom parameters which are multiplied by 10^5. The thermal parameter is of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$. The estimated standard deviations are in parentheses.

Determination and Refinement of the Structure

The position of the copper atom was deduced from a sharpened three-dimensional Patterson function. A minimum function was computed using the Cu–Cu inversion vector but the interpretation was difficult because of the distorted nature of the complex (*vide infra*). Only five atoms with reasonable distances and angles relative to the Cu(II) ion were located in the minimum function. A Fourier synthesis using the copper and five light atoms for phasing revealed the entire structure. The positional parameters and an individual isotropic thermal parameter for each atom were refined by full-matrix least-squares methods to an R of 0.10. The thermal parameters were converted to an anisotropic form and further least-squares refinement using a block approximation (3×3 and 6×6) reduced R to 0.07.

A difference Fourier synthesis gave distinct positions for all the nonmethyl group hydrogens. Additional least-squares refinement followed by a second difference Fourier synthesis gave probable positions for all but one methyl hydrogen atom. The hydrogen atoms were refined with an individual isotropic thermal parameter and behaved reasonably well although some of the thermal parameters became very small. The refinement was terminated with a final R ($R = \Sigma|F_o - F_c|/\Sigma|F_o|$) of 0.048.

The least-squares refinement minimized $\Sigma w(\Delta F)^2$ where $\sqrt{w} = F_o/8$ if $F_o < 8$, $\sqrt{w} = 1$ if $8 < F_o < 32$, and $\sqrt{w} = 32\ F_o$ if $F_o > 32$. The scattering factors were from the usual source[5] with the scattering factor for Cu being corrected for the real part of the anomalous dispersion. The final positional and thermal parameters for the nonhydrogen atoms are given in Table II with the hydrogen atom positions being given in Table III.[6] The atomic numbering and some bond distances and angles are given in

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(5) "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1969, p 202.

(6) A listing of structure factor amplitudes will appear following these pages in the microfilm edition of this volume of the journal. Single copies may be obtained from the Business Operations Office, Books and Journals Division, American Chemical Society, 1155 Sixteenth St., N.W., Washington, D. C. 20036, by referring to author, title of article, volume, and page number. Remit check or money order for $3.00 for photocopy or $2.00 for microfiche.

TABLE III

FINAL POSITIONAL ($\times 10^3$) AND ISOTROPIC THERMAL PARAMETERS FOR THE HYDROGEN ATOMS

Atoms	*x/a*	*y/b*	*z/c*	*B*, Å^2
HA3	−1 (4)	125 (4)	399 (3)	3.6 (1.2)
HA4	−93 (5)	−20 (5)	408 (4)	5.5 (8.0)
HA5	−112 (4)	−145 (4)	304 (3)	3.3 (1.4)
HA6	−30 (3)	−146 (4)	188 (3)	1.8 (2.1)
HAN	97 (4)	256 (4)	323 (3)	2.8 (1.5)
HE1	301 (4)	298 (4)	253 (3)	2.4 (1.7)
HF1	209 (4)	366 (4)	272 (3)	3.3 (1.4)
HE2	124 (4)	364 (4)	126 (3)	3.4 (1.3)
HF2	233 (3)	434 (4)	134 (3)	2.1 (1.9)
HB3	516 (3)	−108 (3)	56 (2)	0.8 (3.0)
HB4	675 (5)	−91 (5)	152 (4)	5.1 (9.0)
HB5	674 (5)	20 (5)	279 (4)	5.6 (7.0)
HB6	540 (4)	104 (4)	310 (3)	3.9 (1.1)
HBN	348 (3)	−86 (3)	4 (2)	0.5 (3.2)
HE3	181 (3)	−27 (3)	−67 (2)	0.4 (3.4)
HF3	105 (3)	21 (4)	−17 (3)	1.8 (2.2)
HE4	108 (3)	−159 (4)	53 (3)	2.0 (2.1)
HF4	51 (4)	−165 (4)	−44 (3)	2.3 (1.8)
H11	348 (4)	359 (4)	50 (3)	2.2 (1.8)
H12	385 (4)	280 (4)	141 (3)	3.7 (1.2)
H13	357 (4)	225 (4)	36 (3)	2.4 (1.7)
H21	167 (4)	376 (4)	−33 (3)	3.7 (1.2)
H22	184 (4)	232 (4)	−50 (3)	3.6 (1.2)
H23	83 (4)	266 (5)	−16 (4)	4.4 (1.0)
H31	238 (5)	−313 (6)	−112 (4)	6.8 (6.0)
H33	217 (6)	−190 (6)	−136 (5)	7.5 (5.0)
H41	224 (5)	−408 (6)	22 (5)	7.2 (5.0)
H42	100 (5)	−386 (5)	−18 (4)	5.3 (8.0)
H43	157 (6)	−332 (6)	73 (5)	8.1 (4.0)

Figures 1 and 2. A stereoscopic view of the complex is given in Figure 3.[7]

Discussion

The crystal consists of discrete molecules in which the pentacoordinated copper(II) atom is surrounded by the two oxygen atoms, the two azomethine nitrogen atoms, but only one of the two β-nitrogen atoms. The overall geometry is very distorted and the complex is not easily classified as either a trigonal-bipyramidal or square-pyramidal arrangement. Although structural data on five-coordinated copper complexes are sparse,[8] many of the five-coordinated structures reported recently[9-13] are also severely distorted.

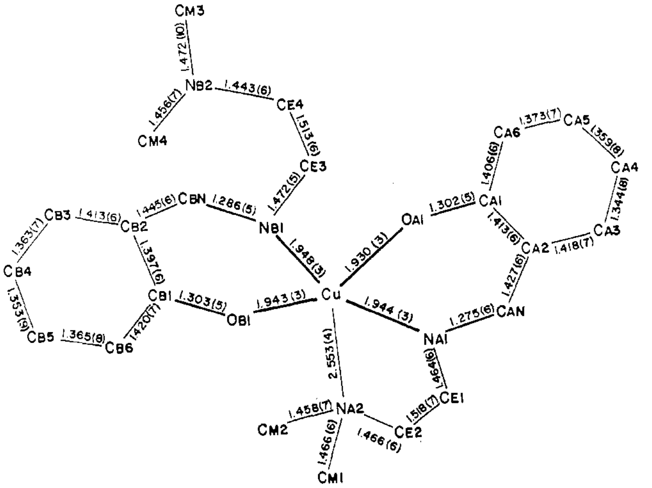

Figure 1.—The atomic numbering, bond distances, and estimated standard deviations in bis(N-β-dimethylaminoethylsalicylaldiminato)copper(II).

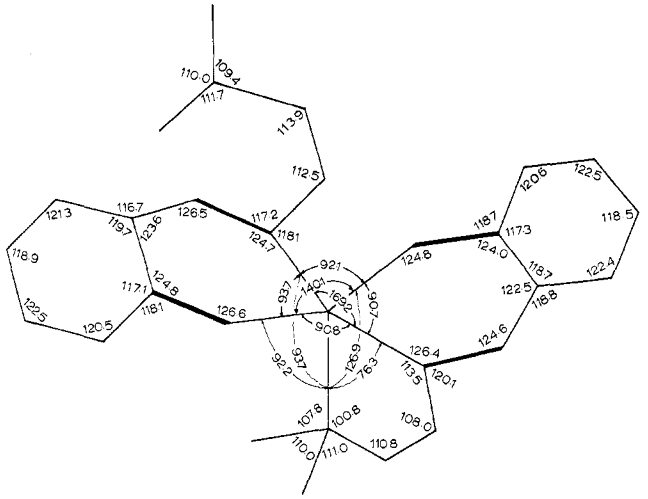

Figure 2.—The bond angles in bis(N-β-dimethylaminoethylsalicylaldiminato)copper(II). The numbering is identical with that in Figure 1. The estimated standard deviations are 0.1° for light atom–copper–light atom angles, 0.3° for copper–light atom–light atom angles, and 0.4° for angles involving only light atoms.

A square-bipyramidal arrangement would be similar to the structure reported for bis(N-β-diethylaminoethyl-5-chlorosalicylaldiminato)nickel(II).[14] The NA2 atom would be axial, with the OA1, OB1, NA1, and NB1 atoms in the basal plane. There are appreciable distortions from an ideal square pyramid; *i.e.*, NA2–Cu–OA1 is 126.9 (1)°, rather than 90°, OB1–Cu–OA1 is 140.1 (1)°, rather than 180°, and the four basal atoms (see Table IV) are nonplanar, making this description unappealing.

The alternative symmetrical configuration, the trigonal-bipyramidal arrangement, would have NA1 and NB1 as the axial atoms, with OA1, OB1, and NA2 in the equatorial plane. The three equatorial angles [OA1–Cu–OB1 of 140.1 (1)°, OA1–Cu–NA2 of 126.9 (1)°, and OB1–Cu–NA2 of 92.2 (1)°] show large deviations from the ideal value of 120°. Similarly, the NA1–Cu–NB1 angle of 169.2 (1)° is slightly smaller than the ideal value of 180°. The two Cu–O distances (average 1.936 Å) are only slightly shorter than the two axial Cu–N distances (average 1.946 Å), suggesting an axial compression of the trigonal-bipyramidal arrangement. A similar effect was noted in the $CuCl_5^{3-}$ ion where the equatorial bonds are 0.095 Å longer than the axial bonds.[12] Furthermore, the long equatorial Cu–NA2 distance of 2.553 (4) Å is similar to the long Cu–Cl distance [2.703 (5) Å *vs.* 2.273 (5) and 2.319 (5) Å] in the equatorial plane of the trigonal-bipyramidal $Cu_2Cl_8^{4-}$ ion.[13] Therefore, the trigonal-bi-

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[7] The stereoscopic drawing was prepared using the ORTEP program written by C. K. Johnson, Oak Ridge National Laboratories, Nashville, Tenn. The estimated standard deviations were calculated using a revised version of Pippy and Ahmed's program "Scan of Interatomic Distances and Angles." All other programs were written by G. J. P.

[8] A survey of the stereochemistry of copper(II) was given recently by B. J. Hathaway and D. E. Billing, *Coord. Chem. Rev.*, **5**, 143 (1970), and W. E. Hatfield and R. Whyman, *Transition Metal Chem.*, **5**, 47 (1969).

[9] B. F. Hoskins and F. D. Whillans, *J. Chem. Soc. A*, 123 (1970).

[10] G. Marongin, E. C. Lingafelter, and P. Paoletti, *Inorg. Chem.*, **8**, 2763 (1969).

[11] P. C. Jain and E. C. Lingafelter, *J. Amer. Chem. Soc.*, **89**, 6131 (1967).

[12] K. N. Raymond, D. W. Meek, and J. A. Ibers, *Inorg. Chem.*, **7**, 1111 (1968).

[13] D. J. Hodgson, P. K. Hale, and W. E. Hatfield, *ibid.*, **10**, 1061 (1971).

[14] P. L. Orioli, M. Di Vaira, and L. Sacconi, *J. Amer. Chem. Soc.*, **88**, 4383 (1966).

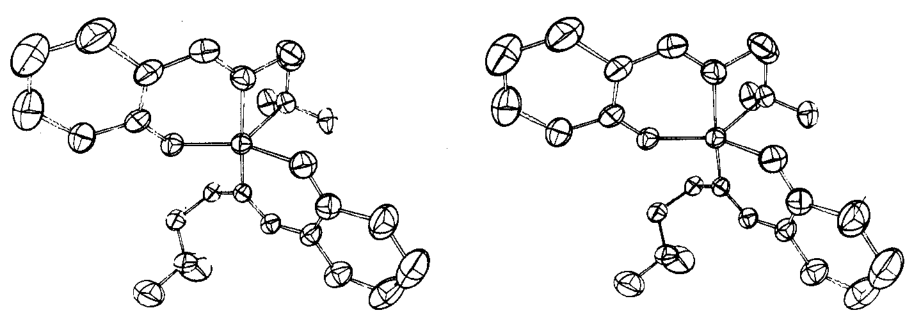

Figure 3.—A stereoscopic pair illustrating the thermal ellipsoids (50% probability) and the geometry of the complex The view shows the trigonal-bipyramidal nature of the complex.

TABLE IV

Least-Squares Planes[a]

	Plane				
Atoms	I	II	III	IV	V
Cu	238	−174*	−18*	619	−88
OA1	−427*	185*		9	
NA1	430*	101*		141	
CAN		51*		−33	
CA1		−37*		6*	
CA2		−127*		1*	
CA3				−8*	
CA4				8*	
CA5				−1*	
CA6				−6*	
OB1	−415*		25*		−22
NB1	411*		2*		−12
CBN			16*		37
CB1			−9*		−16*
CN2			−16*		12*
CB3					0*
CB4					−7*
CB5					2*
CB6					9*
Parameters for the Planes[b]					
l	−345	5208	2656	6585	
m	7323	5115	8292	−4857	
n	−6801	6835	−4919	5749	
p	−11,212	−20,569	3552	17,011	

[a] The deviations (×10³) from the plane (in Å) are given for the specified atom. [b] Equation of the plane in the form: deviation (Å) = $lX + mY + nZ - p$, where X, Y, and Z are the orthogonal coordinates (in Å) relative to a, b, and c^* and p is the distance (in Å) of the plane from the origin. The atoms used to define the plane are noted by an asterisk following the deviation.

pyramidal arrangement appears to be a more reasonable description of the complex, although the distortions from ideality in both cases are sufficiently large to make a preference for one description relative to the other a matter of personal taste.

Although the Cu–O and Cu–N (azomethine nitrogens) distances are slightly shorter than reported for other five-coordinated Cu(II) complexes (or the Ni(II) complex[14]), the Cu–NA2 distance is longer than normal. Steric hindrance is an unreasonable explanation since the corresponding Ni–N distance was 2.199 Å[14] and a study of the bis(*N*,*N*-dimethylethylenediamine)-copper(II) cation[15] showed that the two Cu–N bonds differed by only 0.08 Å. The lengthening of the Cu–NA2 bond may be related to the unsymmetrical electron distribution in the Cu(II) ion but additional studies are required before any definitive conclusions can be drawn.

The bond distances in the two ligands are equivalent. The two benzene rings are planar (see Table IV) with an average C–C distance of 1.385 Å, in agreement with the value of 1.392 Å found in benzene.[16] The C–N bonds to the azomethine nitrogen atoms average 1.280 Å in excellent agreement with the value of 1.30 ± 0.04 Å proposed for a C–N double bond.[17] Similarly the C–C bonds from the benzene ring (average of 1.436 Å) suggest a slight shortening relative to an sp²–sp² C–C single bond. The C–O bonds (average 1.302 Å) are shorter than a C–O single bond but are significantly longer than the C–O bond found in a phenol salt[18] or in a C–O double bond. However, all the distances in the two ligands are similar to the values found in other salicylaldiminato complexes.[19]

In contrast to the identical dimensions in the two ligands, the conformations of the two chelate systems are different. The chelate ring in molecule A involving the azomethine nitrogen and the oxygen atom of the salicylaldiminato group is distorted from planarity while the similar ring in molecule B is approximately planar. Similarly, the benzene ring in molecule A is tilted by 10.2° with respect to the chelate ring while in molecule B the corresponding angle is only 1.8°. These differences in the conformation of the two ligands are undoubtedly related to the facts that molecule A is functioning as a tridentate ligand while molecule B is only coordinated in a bidentate fashion and that strains are involved when the ligand attempts to coordinate all three potential donor atoms.

The shortest intermolecular contacts are tabulated in Table V and indicate no unusual interactions. The packing of the molecules must be governed by van der Waals forces, especially with the lack of any hydrogen bonding or similar intermolecular attractive force.

TABLE V

SHORTEST INTERMOLECULAR DISTANCES (Å)

From atom	To atom	Equiv position	Distance
Cu	CE1	$^1/_2 - x, -^1/_2 - y, ^1/_2 - z$	3.676 (5)
Cu	HF1	$^1/_2 - x, -^1/_2 - y, ^1/_2 - z$	2.94 (5)
OA1	CE3	$-x, -y, -z$	3.457 (5)
OA1	HF3	$-x, -y, -z$	2.91 (4)
OB1	HF1	$^1/_2 - x, -^1/_2 - y, ^1/_2 - z$	2.87 (5)
CA6	H12	$^1/_2 - x, -^1/_2 - y, ^1/_2 - z$	2.86 (5)
CB2	HAN	$^1/_2 - x, -^1/_2 - y, ^1/_2 - z$	2.85 (4)
CB3	CB3	$1 - x, -y, -z$	3.520 (7)

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