Crystal and Molecular Structure of Bis-(*N*-n-hexyl-7-methylsalicylaldiminato)copper(II)

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The crystal structure of the title compound has been determined by Fourier methods from *X*-ray diffraction photographic data. Crystals are monoclinic, space group $P2_1/c$, with $Z = 2$ in a unit cell of dimensions: $a = 7{\cdot}760(2)$, $b = 15{\cdot}909(5)$, $c = 10{\cdot}605(7)$ Å, $\beta = 100{\cdot}8°(3)$. The structure was refined by least squares to R 0·102 for 1390 independent reflections. The configuration around the copper ion is square planar. The dihedral angle between the mean planes of the benzene and chelate rings is 2·5°. The co-ordination plane is tilted 38° from the benzene, 37° from the salicylaldimine, and 15° from the n-hexyl planes. The molecular geometry is as expected, although some steric effects may be due to the presence of the *N*-hexyl and 7-methyl groups.

In recent years, a number of compounds of transition metals with Schiff's bases derived from salicylaldehyde and various amino-acids have been synthesised and studied by *X*-ray diffraction techniques. It has been found that d^7, d^8, and d^9 for Co^{II}, Ni^{II}, and Cu^{II} species, have near tetrahedral geometry in identical crystal environments. Although the copper atom is more resistant to adopting a tetrahedral configuration, its co-ordination geometry strongly depends upon the nature and type of ligand, steric effects, hydrogen bonding, and the strain induced by nitrogen substituents. In addition, distortion due to the electronic configuration of the copper, which has electron density along the *z* axis, causes ligand repulsion. Thus, four-co-ordinate copper takes up either a square planar or a distorted tetrahedral configuration, although some structures [1-5] have been reported as having flattened tetrahedral and distorted square pyramidal [6] configurations. Recently, Waters *et al.*[7] have reported a molecule having two slightly different asymmetric units and also some structures having an asymmetric unit consisting of two molecules with minor differences in their geometry.

We have determined the crystal structure of bis-(*N*-n-hexyl-7-methylsalicylaldiminato)copper(II) [8] in order to study the effects on the molecular geometry, of the bulky substituent *N*-n-hexyl and of the 7-methyl group on the contiguous salicylaldimine residue.

EXPERIMENTAL

Crystals were reddish-brown rhombs.

Crystal Data.—$C_{28}H_{40}N_2O_2Cu$, $M = 499{\cdot}5$, Monoclinic, $a = 7{\cdot}760(2)$, $b = 15{\cdot}909(5)$, $c = 10{\cdot}605(7)$ Å, $\beta = 100{\cdot}8°(3)$, $U = 1286$ Å^3, $D_m = 1{\cdot}32$ g cm^{-3}, $Z = 2$, $D_c = 1{\cdot}28$ g cm^{-3}, $F(000) = 534$. Space group $P2_1/c$ from systematic absences. Cu-K_α radiation, $\lambda = 1{\cdot}5418$ Å, μ-(Cu-K_α)[9] $= 14{\cdot}75$ cm^{-1}.

Integrated intensities were collected from a crystal of dimensions *ca.* 0·27 × 0·25 × 0·20 mm rotating along the *b* axis. Ten layers of equi-inclination Weissenberg photographs were obtained utilising nickel filtered Cu-K_α radiation and multiple-film technique. In all, 1390 independent reflections were estimated by the microphotometer method. Out of these, 785 reflections were estimated also by the counter method. In the latter case, all reflections which had very high and strong-to-medium intensity were estimated to get better values from the two sets of data.

In the counter estimation, observations were taken on a General Electric diffractometer having a xenon-filled proportional counter and using Cu-K_α filtered radiation. Diffractometer settings for the ω—2θ scan method were calculated from the formula of ref. 10.

The intensities of 4 standard reflections were monitored every 4 h. The scale factor was calculated from these standard values and applied to the intensities measured during the interval.

Calculations.—By use of the data reduction program of Wadhawan,[11] intensities were reduced to relative amplitudes, $|F_{rel}|$, by applying Lorentz and polarisation corrections. Secondary extinction corrections were applied at the final stages of the least-squares refinement. No absorption corrections were applied. Calculations for structure factors and Fourier synthesis [12] were carried out on an IBM 7044 computer by use of the modified programs of Block and Holden. All calculations for the full-matrix least-squares refinement [13] and for bond lengths and angles [14] were carried out by use of the modified version of Busing, Martin, and Levy programs.[14] Atomic scattering factors

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[13] W. R. Busing, K. O. Martin, and H. A. Levy, 'ORFLS, Fortran Crystallographic Least-squares Program,' Oak Ridge, National Laboratory, Tennessee Report ORNL TM 305, modified by W. C. Hamilton, J. A. Ibers, C. K. Johnson, S. Srikanta, and S. K. Sikka for the CDC 3600 computer.

[14] W. R. Busing, K. O. Martin, and H. A. Levy, 'ORFFE, A Fortran Crystallographic Function and Error Program,' Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A., modified by C. K. Johnson and S. Srikanta for the CDC 3600 computer.

were taken from ref. 15 for copper, from ref. 16 for oxygen and nitrogen, from ref. 17 for carbon, and from Table II of ref. 18 for hydrogen. Projections of the contents of the unit cell and the orientation of thermal ellipsoids of the asymmetric unit were obtained using the modified program of Johnson.[19]

Structure Determination.—Space group $P2_1/c$ with $Z = 2$ requires that the molecule be centrosymmetric with a copper atom at the centre of symmetry. A Fourier synthesis was therefore calculated with the copper at 0,0,0, and the oxygen and nitrogen atoms were then easily located. Further three-dimensional Fourier syntheses enabled the positions of all 17 non-hydrogen atoms to be determined. A structure-factor calculation with these positions gave R 0·25.

Three cycles of full-matrix least-squares refinement[13] with individual anisotropic temperature factors reduced R to 0·19. At this stage, hydrogen atoms were introduced at calculated positions, assuming C–H 1·05 Å, with fixed isotropic temperature factors, but were not refined.

TABLE 1

Final positional and thermal parameters ($\times 10^4$) * with estimated standard deviations in parentheses (photographic data)

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cu	0(0)	5000(0)	5000(0)	137(5)	30(1)	91(3)	0(0)	51(4)	0(0)
O	1195(14)	3967(7)	4952(11)	129(24)	29(5)	107(13)	13(9)	21(17)	15(7)
N	2065(15)	5610(8)	4536(11)	90(21)	21(5)	72(11)	1(11)	28(18)	7(8)
C(1)	2005(18)	3780(9)	4021(14)	62(23)	25(7)	75(15)	5(15)	16(23)	1(10)
C(2)	2106(22)	2923(11)	3693(20)	86(31)	39(8)	115(24)	20(16)	28(27)	7(12)
C(3)	2897(21)	2667(11)	2694(18)	126(30)	33(8)	119(21)	1(17)	9(29)	1(12)
C(4)	3702(24)	3248(12)	2015(17)	175(35)	45(9)	86(17)	39(19)	18(27)	1(12)
C(5)	3709(24)	4088(12)	2389(14)	191(35)	42(9)	61(14)	18(15)	26(25)	5(11)
C(6)	2899(18)	4390(10)	3385(14)	69(23)	34(7)	66(13)	5(14)	27(22)	1(10)
C(7)	3054(19)	5278(10)	3793(15)	98(26)	27(6)	76(14)	1(14)	1(22)	8(9)
C(8)	4496(23)	5790(10)	3395(16)	142(33)	33(8)	68(16)	1(14)	26(24)	7(10)
C(9)	2413(19)	6465(9)	5066(14)	112(27)	26(7)	64(14)	8(14)	20(21)	2(8)
C(10)	1726(22)	7158(11)	4162(16)	140(31)	35(8)	96(18)	1(13)	1(21)	1(8)
C(11)	2160(24)	8040(10)	4779(16)	200(37)	29(7)	85(16)	12(14)	17(23)	7(10)
C(12)	1611(22)	8784(12)	3897(17)	130(33)	36(9)	104(18)	2(14)	15(23)	1(8)
C(13)	2216(25)	9617(12)	4465(19)	177(39)	21(8)	155(22)	1(14)	20(23)	5(10)
C(14)	1637(30)	10379(13)	3540(23)	264(52)	36(9)	145(27)	5(16)	27(17)	16(8)

* The temperature factor for an atom is of the form $\exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)]$.

TABLE 2

Bond lengths and bond angles with estimated standard deviations in parentheses

(*a*) Bond lengths (Å)

Cu–O	1·893(11)	C(4)–C(5)	1·394(27)
Cu–N	2·012(12)	C(5)–C(6)	1·410(24)
O–C(1)	1·300(20)	C(6)–C(7)	1·475(22)
N–C(7)	1·309(21)	C(7)–C(8)	1·507(24)
N–C(9)	1·477(19)	C(9)–C(10)	1·492(22)
C(1)–C(2)	1·414(23)	C(10)–C(11)	1·558(24)
C(1)–C(6)	1·433(22)	C(11)–C(12)	1·520(24)
C(2)–C(3)	1·382(29)	C(12)–C(13)	1·494(26)
C(3)–C(4)	1·390(27)	C(13)–C(14)	1·571(29)

(*b*) Bond angles (deg.)

O–Cu–N	89·7(5)	C(5)–C(6)–C(1)	118·4(14)
C(1)–O–Cu	121·9(10)	C(1)–C(6)–C(7)	122·0(14)
C(7)–N–C(9)	120·9(13)	C(8)–C(7)–N	120·0(14)
C(7)–N–Cu	122·4(10)	C(6)–C(7)–N	122·5(14)
C(9)–N–Cu	116·6(10)	C(6)–C(7)–C(8)	117·3(14)
O–C(1)–C(6)	123·3(13)	N–C(9)–C(10)	117·8(11)
C(2)–C(1)–C(6)	118·9(15)	C(9)–C(10)–C(11)	112·7(13)
C(1)–C(2)–C(3)	121·7(17)	C(10)–C(11)–C(12)	113·2(14)
C(2)–C(3)–C(4)	120·6(17)	C(11)–C(12)–C(13)	114·3(14)
C(3)–C(4)–C(5)	117·9(17)	C(12)–C(13)–C(14)	114·1(15)
C(4)–C(5)–C(6)	121·1(17)		

TABLE 3

(*a*) Equations of mean planes through the molecule in the form $lx + my + nz = p$ where x, y, and z are orthogonal co-ordinates in Å measured along a, b, and the normal to 001. Deviations (Å) of relevant atoms from the planes are listed in square brackets

Plane (I): Co-ordination group

$$0{\cdot}222x + 0{\cdot}095y + 0{\cdot}970z = 5{\cdot}591$$

Plane (II): Salicylaldimine residue

$$0{\cdot}76x + 0{\cdot}101y + 0{\cdot}670z = 2{\cdot}786$$

[C(2) −0·009, C(5) −0·009, N −0·009, C(1) −0·026, C(3) −0·075, C(4) −0·060, C(6) 0·028, C(7) 0·183, O −0·023]

Plane (III): Benzene ring

$$0{\cdot}737x - 0{\cdot}129y + 0{\cdot}663z = 2{\cdot}593$$

[C(1) −0·030, C(3) −0·017, C(5) −0·012, C(2) 0·027, C(4) −0·024, C(6) 0·001]

Plane (IV): n-Hexyl chain

$$-0{\cdot}032x + 0{\cdot}120y + 0{\cdot}99z = 6{\cdot}099$$

[C(9) 0·323, C(11) 0·348, C(13) 0·318, C(10) −0·466, C(12) −0·405, C(14) −0·458]

Plane (V): Chelate ring

$$0{\cdot}721x - 0{\cdot}099y + 0{\cdot}686z = 2{\cdot}889$$

[O −0·027, N −0·027, C(6) −0·027, C(7) 0·138, C(1) −0·058]

(*b*) Dihedral angles (deg.) between planes

(I)–(II)	36·5	(II)–(IV)	50·7
(I)–(III)	37·4	(II)–(V)	9·5
(I)–(IV)	14·7	(III)–(IV)	51·8
(I)–(V)	35·5	(III)–(V)	2·5
(II)–(III)	5·5	(IV)–(V)	49·8

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[18] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 1965, 42, 3175.

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A Hughes weighting scheme and secondary extinction corrections were applied and the final R was 0·102. The function minimised was $\Sigma w(|F_o| - |F_c|)$.[2] Final parameters of non-hydrogen atoms with their estimated standard deviations are in Table 1. Observed and calculated structure amplitudes are listed in Supplementary Publication No. SUP 20733 (2 pp., 1 microfiche).* Table 2 contains bond distances and valence angles, together with their estimated standard deviations. The equation of various planes through the molecule and deviations of relevant atoms are given in Table 3.

RESULTS AND DISCUSSION

The ligands have a transplanar configuration around the central metal ion and are illustrated in Figures 1 and 2.

In Table 4 some interatomic distances are compared with those in other copper salicylaldimine complexes. In spite of the additional bulk of the n-hexyl and the 7-methyl groups on the salicylaldimine (sim), only minor differences exist. Thus the overall values of bond lengths and angles and the geometry of the co-ordination sphere of the present molecule are similar to those for other copper–salicylaldimine molecules.

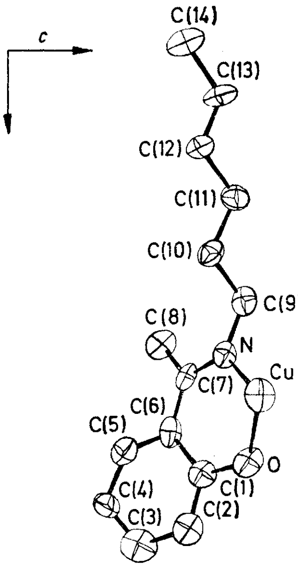

FIGURE 1 Vibration ellipsoids of the asymmetric unit viewed down a

In the present case, Cu–N bond (2·012 Å) is longer by *ca.* 0·11 Å than that in $(\text{sim})_2\text{Cu}$ [20] which has no substitution in the salicylaldimine residue. Similar lengthening of this bond has also been reported in $(N\text{-Et-sim})_2\text{Cu}$ [7] (2·00 Å), $(N\text{-Bu}^t\text{-sim})_2\text{Cu}$ [3] (2·01 Å), and in $(N\text{-Bu}^n\text{-sim})_2\text{Cu}$ (2·019 Å).[21]

The difference of 0·12 Å between Cu–N and Cu–O (Table 2) bonds compares well with previous values for N-alkyl- and N-aryl-salicylaldiminato-compounds.[1, 22, 23] However, in some recently studied [24–26] Cu(sim)_2 complexes, these bond lengths have been found to be nearly identical (Table 4).

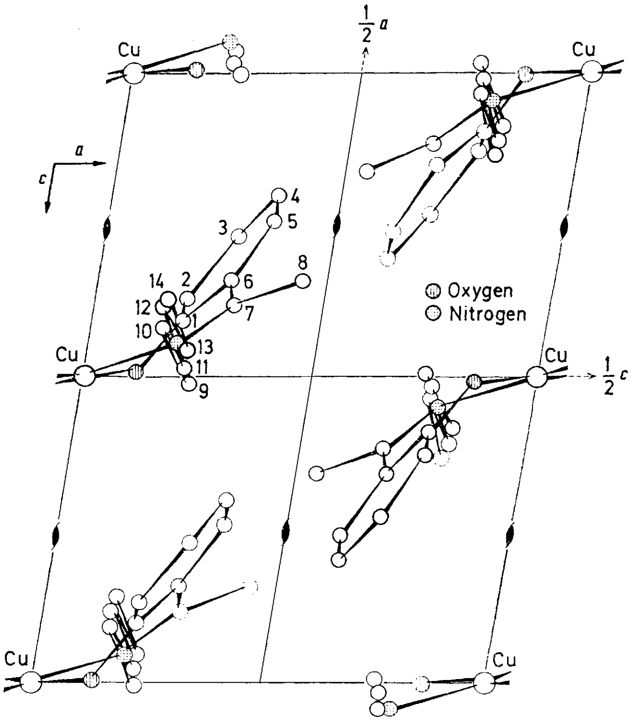

FIGURE 2 Projection of the unit cell contents on the 010 plane

The mean values of the bonds and angles of the benzene ring (1·40 Å and 120° respectively) are similar to those for other metal–sim compounds.[27, 28] The C(7)–N bond length (1·309 Å) agrees with the mean value of 1·30 ± 0·04 Å suggested for C=N,[29] revealing the presence of more double-bond character. There are some short C · · · O contacts (Table 5) which might be a consequence of the steric effect of the n-hexyl group.

The bond angle Cu–N–C(9) (117°, Table 2) is comparable to those in $(N\text{-Me-sim})_2\text{Cu}$ [7] (121°), $(N\text{-}\beta\text{-dimethylaminoethylsim})_2\text{Cu}$ [25] (118°), $(N\text{-Bu}^n\text{-sim})_2\text{Cu}$ [21] (120°), and $(N\text{-2-pyridylsim})_2\text{Cu}$ (120°). The short non-bonding interaction due to the close contact C(8) · · · C(9) (2·81 Å, Table 5) has resulted in increase of the angle

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* For details see Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue. (Items less than 10 pp. are sent as full size copies.)

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C(7)–N–C(9) to 121° whereas the average value in other sim compounds is 116°. The bond lengths and angles of the linear chain carbon atoms of the present molecule compare well with those in other Cu-sim molecules having linear chains on nitrogen.[21,25,30–34]

TABLE 4

Some bond lengths (Å) in various salicylaldiminato–copper(II) molecules

Compound	Cu–O	Cu–N
Present compound	1·893(11)	2·012(12)
[a]	1·91	1·90
[b]	1·92(1)	1·94(1)
[c]	1·908(9)	1·957(9)
[d]	1·901(6)	1·989(7)
[e] (i)	1·90(2)	1·99(2)
(ii)	1·87	1·92
(i) †	1·89	1·99
(ii) †	1·90	1·94
[f] (i)	1·92	1·98
(ii)	1·87	1·98
[g] (i)	1·93	1·97
(ii)	1·89	2·01
[h] (i)	1·875(9)	1·918(9)
(ii)	1·906	1·966
(i) *	1·895	1·964
(ii) *	1·885	1·948
[i] (i)	1·887(9)	2·005(9)
(ii)	1·887	2·000
(i) †	1·886	1·987
(ii) †	1·860	2·003
[j] (i)	1·943(3)	1·948(3)
(ii)	1·930(3)	1·944(3)
[k] (i)	1·870(6)	1·979(10)
(ii)	1·887(7)	1·990(8)
[l]	1·86(2)	1·99(2)
[m] (i)	1·903(6)	1·960(6)
(ii)	1·893(6)	2·010(6)
[n]	1·901(7)	2·019(7)
[o] (i)	1·888(5)	1·970(6)
(ii)	1·889(5)	1·961(5)
[p]	1·878(3)	1·993(4)
[q] (i)	1·888(6)	2·002(6)
(ii)	1·889(7)	2·008(6)
[r]	1·965(6)	1·975(8)
[s]	1·928(6)	1·949(7)
[t]	1·936(6)	1·913(7)
[u] (i)	1·914(10)	1·966(10)
(ii)	1·910(10)	1·956(10)
Mean	1·889	1·973

(i) and (ii) are values from two asymmetric units of the molecule.

* From independent work, ref. 33. † From two independent molecules of the asymmetric unit.

[a] Bis(salicylaldiminato)copper(II), ref. 20. [b] Bis(salicylaldoximato)copper(II), M. A. Jarksi and E. C. Lingafelter, *Acta Cryst.*, 1964, **17**, 1109. [c] Bis-(5-chlorosalicylaldoximato)-copper(II) ref. 37. [d] α-Form, bis(*N*-methylsalicylaldiminato)copper(II), ref. 1. [e] γ-Form, bis(*N*-methylsalicylaldiminato)copper(II), ref. 4. [f] Bis(*N*-2-hydroxyethylsalicylaldiminato)copper(II), ref. 27. [g] Bis-(*N*-α-phenylethylsalicylaldiminato)copper(II), Z. A. Starikova, *Acta Cryst*, 1966, **A21**, 154. [h] Bis-(*N*-ethylsalicylaldiminato)copper(II), monoclinic, refs. 32 and 33. [i] Bis-(*N*-ethylsalicylaldiminato)copper(II), orthorhombic, ref. 7. [j] Bis-(*N*-β-dimethylaminoethylsalicylaldiminato)copper(II), ref. 25. [k] Bis-(*N*-isopropylsalicylaldiminato)copper(II), ref. 28. [l] Bis-(*N*-n-propylsalicylaldiminato)copper(II), ref. 34. [m] Bis-(*N*-t-butylsalicylaldiminato)copper(II), ref. 3. [n] Bis-(*N*-n-butylsalicylaldiminato)copper(II), ref. 21. [o] 1,3,5-trinitrobenzene–bis-(*N*-t-butylsalicylaldiminato)copper(II), 1 : 1, E. E. Castellano, O. J. R. Hodder, C. K. Prout, and P. J. Sadler, *J. Chem. Soc.* (*A*), 1971, 2620. [p] Bis-(*N*-phenylsalicylaldiminato)copper(II), ref. 36. [q] Bis-(*N*-phenylsalicylaldiminato)copper(II) pyridine solvate, D. Hall, S. V. Sheat-Rumball, and T. N. Waters, *J. Chem. Soc.* (*A*), 1968, 2721. [r] Tetranuclear tetrakis(aquo)-(*N*-2-pyridylsalicylaldiminato)copper(II) Tetranitrate, ref. 24. [s] Aquo-*N*-salicylideneglycinato-copper(II) hemihydrate, T. Ueki, T. Ashida, Y. Sasada, and M. Kakudo, *Acta Cryst.*, 1967, **22**, 870. [t] Aquo-*N*-salicylideneglycinatocopper(II) tetrahydrate, ref. 26. [u] Aquo-*N*-salicylidene-α-aminoisobutyrato-copper(II), ref. 6.

TABLE 5

Intramolecular distances (Å); primed atoms are related to the unprimed atoms by centre of symmetry

Cu · · · C(1)	2·81	C(2) · · · C(6)	2·46
Cu · · · C(7)	2·91	C(3) · · · C(5)	2·44
Cu · · · C(9)	2·96	C(3) · · · C(6)	2·89
Cu · · · C(6)	3·19	C(4) · · · C(6)	2·49
O · · · N	2·74	C(5) · · · C(7)	2·58
O · · · N′	2·76	C(5) · · · C(8)	2·95
O · · · C(9′)	2·86	C(6) · · · C(8)	2·55
O · · · C(7)	2·91	C(7) · · · C(10)	3·21
O · · · C(10′)	3·17	C(8) · · · C(9)	2·81
N · · · C(1)	2·97	C(8) · · · C(10)	3·27
N · · · C(10)	2·51	C(9) · · · C(11)	2·55
C(1) · · · C(3)	2·47	C(10) · · · C(12)	2·61
C(1) · · · C(7)	2·55	C(11) · · · C(13)	2·53
C(1) · · · C(4)	2·83	C(12) · · · C(14)	2·56
C(2) · · · C(4)	2·43		

The O · · · N distance, or ' bite ' of the chelate[35] ring, is 2·75 Å (Table 5), which is comparable with values of 2·77 (*N*-Ph-sim)$_2$Cu,[36] 2·78 (*N*-Me-sim)$_2$Cu,[1] and 2·78 Å for (*N*-OH-5-Cl-sim)$_2$Cu.[37] This would be expected since for a given metal the chelate ' bite ' is the same in molecules with the same co-ordination configuration.

The dihedral angle between the mean n-hexyl and benzene planes is 52°. Although the angle of tilt between the mean planes of the benzene [Plane (III), Table 3] and the chelate ring [Plane (V)] is only 2·5°, the displacements of atoms such as Cu, N, and C(7) from these planes differ substantially. C(7) is significantly out of the chelate plane (0·14 Å) and the salicylaldimine plane (0·18 Å). The copper atoms deviate by nearly −0·60 Å from the plane defined by salicylaldimine and copper, thereby giving rise to stepped configuration at the metal atom (Table 3). The persistent unduly tight-packing relations between the n-hexyl group and the 7-methyl-salicylaldimine residue and the folding of the chelate rings have resulted in cumulative bond strain on the molecular conformation. As a consequence, Cu–N is larger and N–C(9) shorter than values observed in other copper–sim molecules having less-bulky substituents on the nitrogen.

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The packing contacts of the n-hexyl hydrogen atoms with contiguous atoms of the salicylaldimine residue and the 7-methyl group hydrogen atoms will also play a major role in determining the molecular conformation. The insertion of hydrogen atoms into the structure will require further tightening in the intramolecular packing and quite specialised orientation of the methylene groups of the n-hexyl chain and of 7-methyl group are needed to exclude H · · · H and H · · · O separations.

It is thus concluded that both inter- and intramolecular interactions, van der Waals forces, and the steric effects due to the presence of the n-hexyl and 7-methyl groups influence packing, molecular conformation, and stability.

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