Crystal and Molecular Structure of Bis(*N*-n-decyl-*o*-hydroxyacetophenoniminato)copper(II) †

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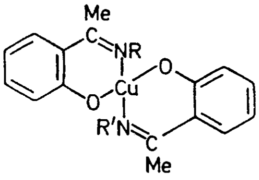
The title compound crystallizes in the triclinic space group $P\bar{1}$, with a = 7.990(8), b = 17.963(10), c = 6.689(10) Å, α = 80.1(6), β = 110.9(4), γ = 100.0(6)°, Z = 1. The structure was solved by the heavy-atom method and refined to R 0.083 for 1 753 observed visually estimated data. Copper is four-co-ordinate planar with Cu–O 1.975 and Cu–N 2.047 Å. In the co-ordination polyhedron copper is displaced from the *o*-hydroxyacetophenone plane by 1.17 Å giving rise to a ' step ' between the two halves of the molecule. The plane of the n-decyl chain makes a dihedral angle of 106° with the co-ordination plane. The carbon atoms of this chain have no contacts sufficiently close to the copper atom to affect its electronic configuration, but the presence of methyl and methylene groups causes distortion in the chelate ring.

MANY crystal structures of salicylaldiminatocopper(II) [(sim)Cu] and of *o*-hydroxyacetophenoniminatocopper(II) [(hapim)Cu] have been studied.[1] In an earlier paper [2] we reported Cu–O and Cu–N distances in 21 salicylaldiminato–copper complexes. Sinn and co-workers [3] have explained the co-ordination mechanism in various (sim)Cu complexes in terms of electronic spectra. A few crystal structures of (sim)Cu and of (hapim)Cu complexes with nitrogen carrying a long linear chain have been studied, *e.g.* four (hapim)Cu structures with methyl,[4] n-butyl,[5] n-hexyl,[2] and n-octyl.[4] The present structure determination of (I) with n-decyl as the chain has been carried out in an attempt to elucidate further the molecular conformation, extent of distortion, and steric effects due to the presence of a long linear chain on the nitrogen of the hapim moiety. A preliminary account of part of this work has been reported earlier.[6]



(I)

EXPERIMENTAL

Crystal Data.—$C_{36}H_{56}N_2O_2Cu$, Triclinic, M = 611.5, a = 7.99(8), b = 17.963(10), c = 6.689(10) Å, α = 80.1(6), β = 110.9(4), γ = 100.0(6)°, U = 876 Å^3, D_m = 1.156 (by flotation), Z = 1, D_c = 1.157. Space group $P\bar{1}$. Cu-K_α radiation λ = 1.5418 Å; μ(Cu-K_α) = 11.25 cm^{-1}. Integrated intensity, visually estimated photographic data.

A well-defined crystal of dimensions *ca.* 0.30 × 0.25 × 0.20 mm was mounted along its needle (c) axis. Integrated intensities for the layers hk0—4 were collected by the multiple-film equi-inclination Weissenberg technique. Two settings were used for all non-zero layers. Another crystal of approximately the same dimensions was mounted along its a axis and its zero and first-layer Weissenberg photographs used for scaling of the intensity data. Intensities were estimated visually. Of 2 003 independent reflections accessible with Cu-K_α radiation, 250 reflections were considered unobserved and were assigned intensity 5.0. Neither absorption nor dispersion corrections were applied.

Structure Determination.—The crystal structure analysis was carried out on a CDC 3600 computer. A structure-factor calculation with copper at the origin and B 3.0 gave R 0.65. A Fourier synthesis [7] based on the phases determined by copper showed peaks corresponding to oxygen and nitrogen atoms. A series of Fourier syntheses led to the location of all non-hydrogen atoms of the molecule; R was then 0.23. Further refinement, by full-matrix least-squares [8] with unit weights, reduced R to 0.18. Because of computer store limitations (139 variables) it was necessary to refine some parameters in alternate cycles. The scale factors and β_{33} were not varied together as they gave a single matrix. R was reduced to 0.116, but some reflections had large ΔF. A Hughes-type weighting scheme [9] with $|F_{\min}|$ 6.0, and secondary extinction corrections with initial value of g 0.0, were applied. A further four cycles of refinement reduced R to 0.103.

Subsequent calculations were carried out on an ICL 1905E computer, with programs described in ref. 10. The expected positions of the hydrogen atoms (assuming C–H 1.0 Å) were calculated with the modified program of Watenpaugh.[11] Three cycles of refinement of isotropic temperature factors and positional parameters of the hydrogen atoms followed by two cycles of refinement of non-hydrogen atoms gave R 0.083, with shifts in the fifth or fourth decimal place except in C(11) and C(12) where they were in the third decimal place in the co-ordinates. The weighting scheme $\sqrt{w} = 1/|F_o|$ was used. Observed and

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TABLE 1

Atomic parameters ($\times 10^4$) of non-hydrogen atoms, with estimated standard deviations in parentheses *

	x/a	y/b	z/c	β_{11}	β_{22}	β_{33}	β_{23}	β_{13}	β_{12}
Cu	0 000	0 000	0 000	366(3)	43(1)	284(5)	−45(2)	318(5)	44(2)
O	2 074(6)	804(2)	257(7)	372(10)	47(1)	165(17)	−46(7)	331(20)	21(6)
N	1 361(7)	−456(2)	3 063(9)	329(11)	32(1)	251(21)	−21(7)	294(21)	73(6)
C(1)	2 550(7)	1 170(3)	1 996(11)	245(11)	49(2)	261(28)	−19(11)	290(24)	39(7)
C(2)	3 072(8)	1 980(3)	1 616(12)	302(13)	45(2)	291(28)	−73(11)	316(28)	7(8)
C(3)	3 506(10)	2 435(4)	3 222(13)	369(16)	47(2)	300(30)	−24(11)	373(32)	14(9)
C(4)	3 334(10)	2 070(4)	5 194(16)	334(15)	58(3)	500(37)	−99(15)	295(36)	21(10)
C(5)	2 917(8)	1 273(3)	5 663(12)	297(13)	47(2)	325(31)	−82(11)	315(28)	40(8)
C(6)	2 546(7)	810(3)	4 023(10)	263(10)	37(2)	177(24)	−37(8)	253(22)	38(6)
C(7)	2 286(7)	−55(3)	4 646(11)	262(11)	40(2)	269(26)	−23(9)	228(24)	43(7)
C(8)	3 195(11)	−407(4)	6 990(12)	444(19)	54(3)	162(28)	12(12)	188(31)	70(11)
C(9)	1 246(10)	−1 327(3)	3 487(11)	411(16)	42(2)	195(27)	−8(9)	316(30)	75(9)
C(10)	1 825(8)	−1 529(3)	1 814(11)	295(13)	43(2)	214(26)	−18(10)	223(25)	53(8)
C(11)	1 580(9)	−2 398(3)	1 909(13)	300(14)	42(2)	393(32)	−17(11)	220(29)	40(8)
C(12)	1 966(10)	−2 614(3)	110(14)	358(15)	40(2)	454(35)	−28(12)	411(35)	55(8)
C(13)	1 782(11)	−3 471(4)	306(15)	396(17)	40(2)	461(36)	−22(12)	357(37)	27(9)
C(14)	2 406(10)	−3 673(3)	−1 395(14)	403(17)	39(2)	446(34)	−65(11)	447(37)	52(9)
C(15)	2 143(10)	−4 546(3)	−1 239(14)	380(16)	39(2)	535(37)	−73(12)	448(37)	66(9)
C(16)	2 696(10)	−4 811(3)	−2 883(14)	399(17)	46(2)	414(35)	−86(13)	527(39)	52(9)
C(17)	2 388(12)	−5 654(4)	−2 835(15)	448(21)	52(3)	469(42)	−53(15)	480(45)	56(11)
C(18)	2 942(12)	−5 899(4)	−4 465(15)	516(24)	74(3)	392(38)	−90(17)	447(44)	100(15)

* The thermal parameters are of the form exp $-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{23}kl + \beta_{13}hl + \beta_{12}hk)$.

calculated structure factors are listed in Supplementary Publication No. SUP 21661 (3 pp., 1 microfiche).* Atomic parameters together with their estimated standard deviations for non-hydrogen atoms are given in Table 1, and for hydrogen atoms in Table 2. Bond lengths and interbond angles are given in Table 3. Some important intramolecular non-bonding distances <3.5 Å are included in Table 3. The thermal ellipsoid plot[12] for non-hydrogen atoms is shown in Figure 1, and a projection of the contents of a unit cell on (001) in Figure 2.

TABLE 2

Fractional co-ordinates ($\times 10^3$) and isotropic thermal parameters (Å^2) for hydrogen atoms *

Atom	x	y	z	B
H(2)	332(11)	226(4)	022(15)	9.4(2.0)
H(3)	401(9)	298(4)	318(13)	4.9(1.6)
H(4)	356(10)	230(4)	625(14)	5.2(1.9)
H(5)	288(10)	098(4)	690(14)	5.7(2.1)
H(81)	300(12)	−012(5)	808(16)	8.0(2.4)
H(82)	252(13)	−087(5)	745(16)	7.2(2.6)
H(83)	441(12)	−042(4)	814(14)	10.1(2.1)
H(91)	236(8)	−148(4)	526(12)	3.9(1.4)
H(92)	012(12)	−157(5)	306(17)	8.7(2.5)
H(101)	319(10)	−123(4)	201(14)	10.6(1.9)
H(102)	090(8)	−130(3)	027(11)	4.0(1.4)
H(111)	218(11)	−253(4)	322(15)	5.0(2.0)
H(112)	026(11)	−264(4)	167(15)	8.1(1.9)
H(121)	323(9)	−236(3)	017(12)	4.2(1.5)
H(122)	116(11)	−237(4)	−125(14)	6.4(1.9)
H(131)	248(9)	−373(3)	168(12)	4.4(1.4)
H(132)	046(12)	−354(5)	−005(15)	7.9(2.2)
H(141)	358(8)	−346(3)	−137(14)	4.4(2.0)
H(142)	156(10)	−343(5)	−297(18)	6.0(2.3)
H(151)	295(12)	−471(5)	056(16)	8.4(2.3)
H(152)	067(11)	−478(4)	−145(16)	8.5(2.4)
H(161)	401(12)	−459(4)	−258(14)	9.6(1.9)
H(162)	182(12)	−464(4)	−459(15)	6.4(1.9)
H(171)	318(9)	−593(4)	−130(12)	4.3(1.5)
H(172)	130(13)	−585(5)	−297(18)	7.7(2.4)
H(181)	370(8)	−555(3)	−481(12)	3.5(1.5)
H(182)	199(12)	−579(5)	−586(17)	7.7(2.5)
H(183)	341(10)	−652(4)	−423(13)	10.3(2.0)

* Numbering of hydrogen atom corresponds to those of the carbon atoms to which they are bonded.

TABLE 3

Interatomic distances (Å) and interbond angles (°) of the (*o*-hydroxyacetophenoniminato)copper skeleton. Values for the n-decyl chain are included in Table 5

Cu–O	1.975(5)	O–Cu–N	88.1(2)
Cu–N	2.047(5)	Cu–O–C(1)	144.3(4)
O–C(1)	1.337(8)	Cu–N–C(7)	124.2(4)
C(1)–C(2)	1.446(8)	O–C(1)–C(2)	144.3(6)
C(2)–C(3)	1.370(10)	O–C(1)–C(6)	123.6(6)
C(3)–C(4)	1.410(12)	C(2)–C(1)–C(6)	122.1(6)
C(4)–C(5)	1.419(10)	C(1)–C(2)–C(3)	120.9(6)
C(5)–C(6)	1.406(9)	C(2)–C(3)–C(4)	116.0(7)
C(6)–C(1)	1.399(9)	C(3)–C(4)–C(5)	124.7(8)
C(6)–C(7)	1.536(7)	C(4)–C(5)–C(6)	118.4(6)
C(7)–C(8)	1.546(10)	C(5)–C(6)–C(1)	117.6(6)
C(7)–N	1.304(8)	C(5)–C(6)–C(7)	117.1(5)
		C(1)–C(6)–C(7)	125.2(5)
		C(6)–C(7)–N	115.7(5)
		C(6)–C(7)–C(8)	120.5(5)
		C(8)–C(7)–N	123.7(6)

Most significant close approach distances are: Cu ··· C(10) 3.185, O ··· C(9′) 3.081, O ··· C(10′) 3.322, C(7) ··· C(9) 2.449, C(8) ··· C(9) 2.908, and intermolecular O ··· C(5) 3.317 Å [C(5) at $x,y,z-1$].

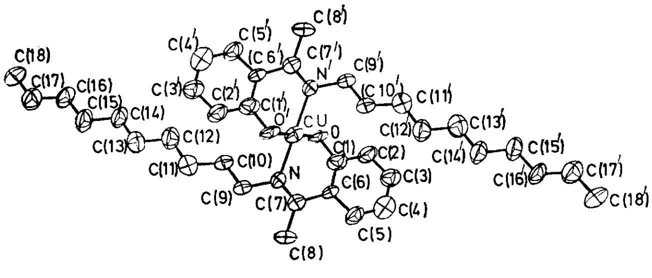

FIGURE 1 Thermal ellipsoid plot (50% probability) for non-hydrogen atoms in (I)

DISCUSSION

The structure is not close packed (Figure 2) and the molecules are arranged in chains with the n-decyl groups

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* See Notice to Authors No. 7 in *J.C.S. Dalton*, 1975, Index issue. (Items less than 10 pp. are supplied as full-size copies.)

[12] C. K. Johnson, 'Program ORTEP,' 1965.

oriented nearly parallel to the *b* axis to give plane-to-plane stacks along this direction. There are several intramolecular close contacts which affect the molecular conformation, especially of the chelate ring. The Cu–N and Cu–O bond lengths are longer than the usual range.[2] However, the Cu–N value is not much different to that (2.019 Å) in (n-butylsim)Cu,[13] and similarly, the Cu–O distance is close to that (1.965 Å) in (2-pyridylsim)Cu-$(NO_3)_4$.[14] As a consequence, the bite distance [15] (N · · · O) has also increased from the range found in other (hapim)-Cu complexes, indicating a relatively weak interaction between these atoms. The difference (0.072 Å) in the Cu–N and Cu–O bond lengths is in excellent agreement with that (0.076 Å) in (n-octylhapim)Cu [4] and (0.073 Å) in (methylhapim)Cu.[4] There are some significant intramolecular van der Waals contacts [*e.g.* O · · · C(9′) 3.08 and O · · · C(10′) 3.32 Å] and an intermolecular close approach of 3.32 Å for O · · · C(5) with the angle C(5) · · · H(5) · · · O 155°. The O–C(1) bond length (1.337 Å) is in agreement with the value (1.341 Å) reported for salicylaldehyde azine.[16] The C(7)—C(8) bond length (1.546 Å) is identical to that in dichloro(*NN′*-ethylenehapim)-Cu.[17] The double-bond character of C(7)⁚N is apparent and agrees well with the suggested C⁚N value [18] and the results of bond-order calculations.[19] In the present case the bond length C(6)—C(7) (1.536 Å) is longer and the angle C(6)–C(7)–N (115.7°) undoubtedly smaller, as compared to those in other (hapim)Cu molecules. Consequently the angle C(1)–C(6)–C(7) is increased to 125.2° from the normal range (120—122°) in other (hapim)Cu complexes.

TABLE 4

Least-squares planes for various groupings of atoms. Equations of the planes are expressed in orthogonalized space as $lX + mY + nZ - p = 0$, where X is along the *a* axis, Y in the (*a*, *b*) plane, and Z is along c^* axis. Deviations of atoms (Å) are in square brackets

Plane (I): Cu, N, O

$$0.7000X - 0.6111Y - 0.3695Z + 0 = 0$$

[C(1) −0.978, C(6) −1.408, C(7) −0.703, C(8) −0.772, C(9) 0.880, C(10) 2.210]

Plane (II): O, N, C(1), C(6)—(8)

$$-0.9850X + 0.1718Y - 0.0157Z + 0.8112 = 0$$

[O −0.265, N 0.193, C(1) 0.000, C(6) 0.266, C(7) 0.089, C(8) −0.283, Cu 0.811, C(9) −0.149, C(10) −1.131, C(11) −1.451, C(12) −2.318]

Plane (III): C(1)—(6)

$$0.9508X + 0.0991Y - 0.2935Z + 1.3064 = 0$$

[C(1) 0.030, C(2) 0.000, C(3) −0.031, C(4) 0.033, C(5) −0.002, C(6) −0.029, Cu 1.306, O 0.126, N 0.219, C(7) −0.208, C(9) −0.084]

Plane (IV): O, N, C(1)—(8)

$$-0.9873X + 0.0600Y - 0.1472Z + 1.1667 = 0$$

[O −0.095, N 0.362, C(1) −0.057, C(2) −0.188, C(3) −0.102, C(4) 0.178, C(5) 0.245, C(6) 0.098, C(7) 0.036, C(8) −0.477, Cu 1.166]

Plane (5): C(9)—(18)

$$-0.7688X - 0.0548Y - 0.6372Z + 1.6978 = 0$$

[C(9) −0.010, C(10) −0.034, C(11) −0.027, C(12) 0.090, C(13) 0.033, C(14) −0.013, C(15) −0.013, C(16) −0.036, C(17) 0.018, C(18) −0.006, Cu 1.697]

Dihedral angles (°) between normals to planes: (I)–(II) 14.21, (I)–(III) 128.1, (I)–(IV) 132.3, (I)–(V) 105.6, (II)–(III) 16.6, (II)–(IV) 9.9, (II)–(V) 40.7, (III)–(IV) 8.9, (III)–(V) 24.1, (IV)–(V) 31.8.

The dimensions of the benzene ring are as expected. The C(3) and C(4) atoms of the ring are the farthest from the metal ion at the origin and have high anisotropy (Table 1) with the major axis of vibration (Figure 1) in-plane oscillation. No attempt has been made to treat the molecule or any part of it as a rigid body. The thermal parameters of the n-decyl carbon atoms increase markedly towards the end of the chain, which accounts for the departure of their bond lengths and angles from ideal values.

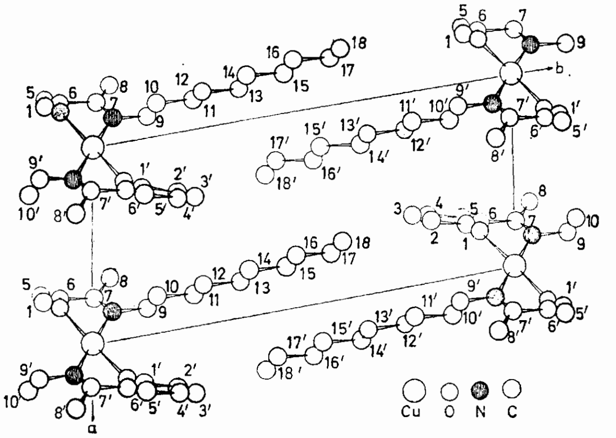

FIGURE 2 Projection of the unit-cell contents on 001

A tabulated list of bond lengths, interbond angles, and other important crystallographic features of the *N*-linear chain group of (hapim)Cu and (sim)Cu complexes [2,4,5,13,20–25] has been deposited as part of the Supplementary publication. Mean bond lengths and inter bond angles are within 3σ, but some individual values vary significantly. The greatest variation is for N–C(9), whose value is probably influenced by steric hindrance from methylene groups of the chain to different

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TABLE 5

Bond lengths (Å), bond angles (°), and other crystallographic details of various *N*-linear substituted *o*-hydroxyacetophenoniminato (hapim) and salicylaldiminato (sim) complexes of copper(II) *

Bonds/angles	(decyl-hapim)Cu	(octyl-hapim)Cu	(hexyl-hapim)Cu †	(butyl-hapim)Cu	(methyl-hapim)Cu	(butyl-sim)-Cu	(propyl-sim)-Cu	(ethylsim)-Cu orthorh.	(ethylsim)-Cu monocl.	(methylsim)-Cu *d*, *e*
References	Present work	4	2	5	4	13	20	24	21, 23	22, 25
N–C(9)	1.534(7)	1.475(3)	1.477(19)	1.486(4)	(a) 1.471(5) (*b*1) 1.472(5) (*b*2) 1.464(6)	1.484	1.46(3)	(i) 1.48 (ii) 1.50 (iii) 1.46 (iv) 1.48	(i) 1.476(18) (ii) 1.530(14) (c, i) 1.476 (*c*, ii) 1.497	(*d*) 1.521 (*e*1) 1.49, 1.47 (*e*2) 1.45, 1.52
C(9)–C(10)	1.473(10)	1.518(6)	1.492(22)	1.506(5)		1.553	1.52(3)	(i) 1.52 (ii) 1.46 (iii) 1.47 (iv) 1.50	(i) 1.513(24) (ii) 1.502(20) (*c*, i) 1.518 (*c*, ii) 1.489	
C(10)–C(11)	1.531(8)	1.514(4)	1.558(24)	1.533(6)		1.523				
C(11)–C(12)	1.470(11)	1.520(6)	1.420(24)	1.438(9)		1.534				
C(12)–C(13)	1.509(9)	1.512(4)	1.494(26)							
C(13)–C(14)	1.512(12)	1.513(7)	1.571(29)							
C(14)–C(15)	1.536(8)	1.503(5)								
C(15)–C(16)	1.495(12)	1.510(7)								
C(16)–C(17)	1.487(10)									
C(17)–C(18)	1.464(14)									
Cu–N–C(7)	124.3(4)	122.0(2)	122.4(10)	124.0(2)	(*a*) 125.2(3) (*b*1) 123.9(3) (*b*2) 124.4(3)	124.1	124(1)	(i) 122.5 (ii) 125.7 (iii) 124.4 (iv) 124.3	(i) 125.8(8) (ii) 125.6(8) (*c*, i) 124.2 (*c*, ii) 123.6	(*d*) 125.7 (*e*1) 127.5, 127.0 (*e*2) 124.8, 124.5
Cu–N–C(9)	116.8(4)	115.3(2)	116.6(10)	116.6(2)	(*a*) 115.7(2) (*b*1) 117.5(3) (*b*2) 115.6(3)	119.9	122(1)	(i) 120.5 (ii) 120.3 (iii) 121.0 (iv) 120.8	(i) 118.1(9) (ii) 118.5(7) (*c*, i) 117.8 (*c*, ii) 120.5	(*d*) 114.9 (*e*1) 119.4, 121.8 (*e*2) 118.5, 124.2
C(7)–N–C(9)	119.0(5)	122.7(2)	120.9(13)		(*a*) 119.1(3) (*b*1) 118.5(4) (*b*2)	115.9	114(2)	(i) 116.9 (ii) 114.0 (iii) 114.5 (iv) 114.9	(i) 116.3(11) (ii) 115.9(9) (*c*, i) 118.0 (*c*, ii) 115.9	(*e*1) 112.9, 111.2 (*e*2) 115.6, 110.7
N–C(9)–C(10)	103.6(5)	109.6(2)	117.8(11)	114.3(3)		111.5	111(2)	(i) 111.9 (ii) 107.8 (iii) 114.1 (iv) 111.8	(i) 111.1(10) (ii) 110.6(9) (*c*, i) 109.0 (*c*, ii) 110.1	
C(9)–C(10)–C(11)	108.8(5)	113.6(3)	112.7(13)	110.1(4)		113.1	112(2)			
C(10)–C(11)–C(12)	110.0(6)	112.4(3)	113.2(14)	115.2(6)		114.5				
C(11)–C(12)–C(13)	108.4(6)	114.0(3)	114.3(14)							
C(12)–C(13)–C(14)	107.1(7)	113.8(3)	114.1(15)							
C(13)–C(14)–C(15)	106.6(6)	114.6(3)								
C(14)–C(15)–C(16)	113.3(7)	113.5(3)								
C(15)–C(16)–C(17)	112.6(7)									
C(16)–C(17)–C(18)	115.5(7)									
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	(*a*) $P2_1/a$; (*b*) $P1$	$P2_1/c$	$P\bar{1}$	*Pbcm*	$P2_1/c$	(*d*) *Ibam*, $P2_12_12_1$ (*e*)
Z	1	1	2	2	(*a*) 2; (*b*) 2	2	1	8	4	(*d*) 4, (*e*) 8
Step in Å ‡	1.31	1.33	−0.60	0.95	(*a*) 0.96; (*b*1) 0.97	0.37	0.13	0.12	0.27	
Bite § (N · · · O) in Å	2.798	2.687	2.75		(*a*) 2.702 (*b*1) 2.691 (*b*2) 2.726					(*d*) 2.78
Co-ordination	4-Planar	4-Planar	4-Planar	4-Planar	(*a*) 4-Planar (*b*) 5-coord.	4-Planar	4-Planar	4-Intermed. sq. pl. and tetrahedral	Distorted tetrahedral	(*d*) 4-Planar (*e*) 5-Distorted sq. pyramidal

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* Numbering scheme adopted in all cases is the same as in the present molecule, *i.e.* linear chain carbon atoms are numbered sequentially with C(9) bonded to nitrogen. Values are: (i) and (ii) from two asymmetric units of the molecule; (iii) and (iv) from the other two asymmetric units of a second molecule; (*a*) from monoclinic; (*b*1) and (*b*2) from the triclinic dimeric form; (*d*) from the α form, and (*e*1) and (*e*2) from the γ-form of dimeric molecule. † Named in place of (*N*-hexyl-7-methylsim)Cu. ‡ Step is the displacement of Cu from the benzene plane. § Bite is N · · · O interligand distance. Ref. 15.

extents. The angle Cu–N–C(7) in these complexes is smaller by at least 2°, compared to the corresponding value in the non-substituted (hapim)Cu and (sim)Cu complexes.[26,27] There is no direct relationship between the length of the linear chain and the 'step' of copper from the mean benzene plane, but a trend towards increasing 'step' with increasing chain length is apparent. Obviously its value is significant in the (hapim)Cu series. The angle C(7)–N–C(9) in hapim(Cu) complexes is larger than in (sim)Cu complexes. No such relationship is observed for 'bite' distance. There is a tendency to form four-co-ordinate complexes with nearly square planar geometry[2,4,20,22] except in (ethylsim)Cu,[21–24] (methylhapim)Cu, and (methylsim)Cu.[25]

Further details of the molecular geometry are evident from Table 4. The angle between the planes of the decyl group and of the hapim fragment is 32°, which is less by 19° than that in (n-hexylhapim)Cu.[2] This would cause some overlapping of the chelate ring by the adjacent methylene groups of the decyl chain. Copper is located 1.68 Å above the mean decyl plane. The dihedral angle between the co-ordination plane and that of the n-decyl chain is 106°. Thus the high deviation of copper accompanied by a large dihedral angle makes it unlikely that the n-decyl group will affect the electronic configuration of the metal atom.

The C–H bond lengths and inter-bond angles involving hydrogen atoms are as expected. There are no serious packing contacts of hydrogen atoms which could be held responsible for the various crystallographic features already discussed.

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