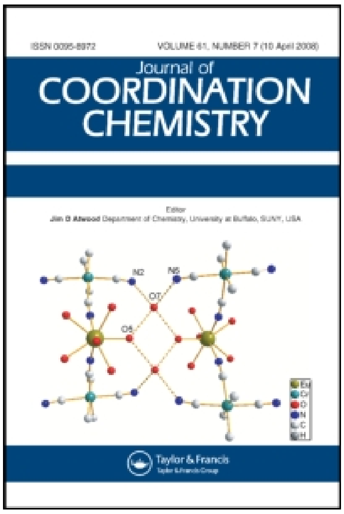

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OBSERVATIONS ON THE CONFORMATION OF IMINODIACETATE(2-) ION IN MIXED LIGAND COPPER(II) COMPLEXES WITH NITROGEN HETEROCYCLES AS SECONDARY LIGANDS. CRYSTAL STRUCTURE OF (2,2'-BYPIRIDINE)(IMINODIACETATO)COPPER(II) HEXAHYDRATE

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OBSERVATIONS ON THE CONFORMATION OF IMINODIACETATE(2-) ION IN MIXED LIGAND COPPER(II) COMPLEXES WITH NITROGEN HETEROCYCLES AS SECONDARY LIGANDS. CRYSTAL STRUCTURE OF (2,2′-BYPIRIDINE)(IMINODIACETATO)COPPER(II) HEXAHYDRATE

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(2,2′-Bipyridine)(iminodiacetato)copper(II) hexahydrate, [Cu(IDA)(2,2′-bipy)]·$6H_2O$, has been obtained and studied by X-ray diffraction. The compound (triclinic system, space group *P*1, *Z* = 2; *R* = 0.036 and *R* = 0.040 for 7541 independent reflections) consists of asymmetric dinuclear entities, $[Cu(IDA)(2,2'\text{-bipy})]_2$, and uncoordinated H_2O molecules in a hydrogen bonding network. Both Cu(II) atoms of each dinuclear entity are chemically very similar. Each Cu(II) atom exhibits a flattened, square pyramidal coordination. Two N atoms of 2,2′-bipy and the N and one O atoms of IDA are at the square base; another O atom of the same terdentate IDA is at the apical position. Two weak interactions between each Cu(II) atom and one O atom from IDA which chelates the second contribute to the dinuclear entity. On the basis of these results and the known structure of other Cu(II) complexes with IDA and imidazole or 4,4′-bipy, an attempt to rationalize the nearly coplanar or perpendicular conformation of the two five-membered IDA-Cu(II) chelate rings in such mixed-ligand copper(II) complexes is made.

KEYWORDS: Copper(II), iminodiacetate(2-) ions, conformation, nitrogen heterocyclic ligands, 2,2′-bipyridine, crystal structure

INTRODUCTION

Structural, spectroscopic and magnetic interests have promoted studies of several mixed-ligand copper(II) complexes with the iminodiacetate(2-) ion (IDA) as

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primary ligand and water,[1] imidazole (ImH)[2,3] or 4,4′-bipyridine (4,4′-bipy)[4] as secondary ligand. In these complexes the terdentate IDA ligand exhibits two nearly coplanar or perpendicular chelate rings. In an attempt to rationalize the influence of *N*-heterocyclic ligands (imidazole and bipyridines) on the two chelate ring conformations of IDA in such mixed-ligand copper(II) complexes, (2,2′-bipyridine)(iminodiacetato)copper(II) hexahydrate has been synthesized and studied by X-ray diffraction methods.

EXPERIMENTAL

Synthesis of the title compound

The title compound was obtained by recrystallization of equimolar amounts (0.233 g, 1 mmol) of $[Cu(IDA)(H_2O)_2]$[1] and 2,2′-bipyridine (0.156 g, 1 mmol, Sigma Chem. Co.) in 150 cm^3 of water. By slow evaporation, well-shaped the crystals of the desired product appeared and these were filtered off, washed with a little cold water and air-dried. Yield: > 90%. Elemental analysis suggested the formula $[Cu(IDA)(2,2'\text{-bipy})]\cdot nH_2O$ with n = 5–5.5. Calcd. for $C_{14}H_{23}CuN_3O_9$ (n = 5): C, 38.14: H, 5.26; N, 9.53%. Found: C, 38.72; H, 4.97; N, 9.74%. However, TG-DTA diagrams (Rigaku Thermoflex 2000) showed the loss of all water molecules (%) from room temperature to 355 K (expl. 21.52%, calcd. for n = 6, 23.55%). Anhydrous [Cu(IDA)(2,2′-bipy)] is stable up to 450K. The hexahydrate composition was finally established by crystal structure analysis.

X-ray data collection and structure solution and refinement

A blue prismatic crystal of $[Cu\{HN(CH_2COO)_2\}(2,2'\text{-bipy})]\cdot 6H_2O$ of approximate size 0.15 × 0.15 × 0.25 mm was mounted on a glass fibre. Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 25 reflections in the range of $7.9 < \theta < 15.0$ in an Enraf-Nonius CAD4 diffractometer.[5] Data were collected at 293 K using MoKα radiation (λ = 0.70930 Å) and the $\omega/2\theta$ scan technique. Of 8425 unique reflections measured in the range $3 < \theta < 27$, 7541 independent reflections with $I > 3\sigma(I)$ were used and corrected for Lorentz and polarization effects. An empirical absorption correction[6] was used (absorption: min. 0.849, max. 1.273, av. 1.001). A summary of the crystal is given in Table 1.

The structure was solved by direct methods[7] and refined on F by a full-matrix least-squares procedure using anisotropic displacement parameters for all non-hydrogen atoms. The hydrogen atoms were located on a difference Fourier map with exception of H(210) which was positioned according to idealized geometry (N-H = 0.95 Å) and those of the six water molecules not found. The H-atoms were added to the structure factor calculations with fixed contributions (B_{iso} = 5.0 Å^2) but their positional parameters were not refined. A secondary extinction coefficient (1.25 × 10^{-6}) correction was applied.[8] After all shift/e.s.d. ratios were <0.01, the refinement converged to agreement factors R = 0.036 and

Table 1 Crystal data for [Cu(IDA)(2,2′-bipy)]·$6H_2O$.

Crystal size	0.15 × 0.15 × 0.25 mm
Chemical formula	$C_{14}H_{25}CuN_3O_{10}$
Formula weight	458.91
Crystal system	triclinic
Space group	$P1$
Unit cell dimensions	a = 10.593(1) b = 12.454(1) c = 7.923(1)Å α = 102.64(1) β = 107.40(1) γ = 83.68(1)° V = 972.0(1)$Å^3$
Z	2
$d_{calcd.}$	1.568 g cm^{-3}
$F(000)$	478
$\mu_{MoK\alpha}$	11.792 cm^{-1}

R_w = 0.040 for 503 parameters.* Atomic scattering factors were taken from International Tables for X-ray Crystallography.[9] Molecular graphics used were those of SCHAKAL.[10]

RESULTS AND DISCUSSION

Positional parameters are given in Table 2. Bond lengths and angles are shown in Table 3. The compound consists of a three-dimensional network of non-centrosymmetric dinuclear entities $[Cu(IDA)(2,2'\text{-bipy})]_2$ water molecules in accordance with the formula [Cu(IDA)(2,2′-bipy)]·$6H_2O$ (Figs. 1 and 2). In these asymmetric units, both Cu(II) atoms are very similar from a chemical point of view. Each Cu(II) atom exhibits a very flattened, square-pyramidal coordination sphere where two N atoms from 2,2′-bipy and the N and one O atoms from the same IDA ligand form a distorted square base. The Cu(1) and Cu(2) atoms are slightly displaced from its mean square plane (0.078 and 0.063 Å, respectively) toward the fifth donor, one O carboxylate atom of the corresponding chelating IDA ligand. The Cu-O_{apex} bonds are typically longer (2.23(2) Å) than the Cu-O and Cu-N bonds in the square plane (2.00(5) Å). The dinuclear entity arises from two additional very weak interactions, Cu(1)...O(22) and Cu(2)...O(12), with longest distances of 3.00(1)Å, correlating each copper(II) atom with an IDA oxygen atom of the other fragment of the asymmetric unit. The stability of these entities and the crystal packing is reinforced by a hydrogen bonding network involving the N-H of the IDA ligand and probably most of water molecule H atoms with oxygen atoms of IDA or water.

In the new mixed-ligand Cu(II) complex, the 2,2′-bipy ligand has a nearly planar conformation (max. dev. 0.035(5) Å for C 213) with analogous internal geometry and Cu-N bonds that match those reported for related examples.[11,12,13] Cu(1) and Cu(2) are displaced out of the mean planes of the bidentate nitrogen heterocycles

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* Further details of the structure determination and full lists of thermal parameters, H atom positions, and observed and calculated structure factors are available from the authors upon request.

Table 2 Positional parameters and estimated standard deviations.*

Atom	*x*/*a*	y/*b*	*z*/*c*	B(Å^2)
Cu1	0.000	0.000	0.000	1.989(8)
Cu2	-0.28148(4)	-0.23216(4)	0.25259(6)	1.994(8)
O1	0.0513(3)	0.0792(3)	-0.4909(4)	4.09(7)
O2	0.5029(4)	0.5332(3)	0.5011(5)	5.1(1)
O3	-0.3523(4)	-0.3031(3)	-0.2808(5)	7.20(9)
O4	-0.7861(4)	0.2468(3)	-0.2433(5)	4.86(9)
O5	-0.1641(4)	0.2868(3)	-0.5844(4)	5.6(1)
O6	-0.1197(5)	0.4843(3)	-0.1583(4)	5.3(1)
O7	0.6008(4)	0.3951(3)	1.2277(5)	5.20(9)
O8	-0.8882(4)	-0.6085(4)	-0.9771(5)	6.3(1)
O9	-0.5103(3)	0.2575(3)	-0.1018(5)	4.37(8)
O10	-0.7654(4)	-0.4845(3)	-0.6441(5)	5.13(9)
O11	-0.1490(3)	-0.0925(2)	-0.0729(3)	2.65(5)
O12	-0.3512(2)	-0.1033(2)	-0.0429(4)	2.99(6)
O14	-0.0738(3)	0.0949(2)	-0.2213(3)	2.86(6)
O15	-0.1840(4)	0.2524(3)	-0.2683(4)	4.45(7)
O21	-0.1298(2)	-0.1386(2)	0.3273(3)	2.38(5)
O22	0.0684(3)	-0.1297(3)	0.2967(4)	3.76(7)
O24	-0.1993(3)	-0.3257(2)	0.4768(3)	2.79(6)
O25	-0.0990(3)	-0.4898(2)	0.5141(4)	3.74(7)
O110	-0.8388(4)	-0.5750(3)	-0.4038(5)	5.9(1)
O120	-0.4260(5)	0.3662(4)	-0.3056(6)	7.4(1)
N11	-0.1163(2)	0.1169(2)	0.1166(3)	1.49(5)
N12	0.1090(3)	-0.1069(3)	-0.1260(4)	2.33(6)
N13	0.1714(3)	0.0679(3)	0.1123(4)	2.84(7)
N21	-0.1644(3)	-0.3452(3)	0.1466(4)	2.68(7)
N22	-0.3911(3)	-0.1226(2)	0.3820(4)	2.18(6)
N23	-0.4598(3)	-0.3046(2)	0.1360(4)	1.73(6)
C11	-0.2504(4)	-0.0336(3)	-0.0151(4)	2.45(7)
C12	-0.2449(4)	0.0621(3)	0.0876(5)	3.09(7)
C13	-0.1371(4)	0.2163(3)	0.0293(4)	2.72(8)
C14	-0.1292(4)	0.1801(3)	-0.1729(4)	2.54(7)
C15	0.0629(5)	-0.2006(3)	-0.2531(5)	3.20(9)
C16	0.1427(4)	-0.2653(4)	-0.3374(5)	2.83(8)
C17	0.2779(4)	-0.2357(4)	-0.3036(6)	3.44(9)
C18	0.3190(3)	-0.1489(4)	-0.1799(5)	2.73(8)
C19	0.2355(3)	-0.0808(3)	0.0939(4)	2.30(7)
C21	-0.0336(3)	-0.1792(3)	0.2728(5)	2.10(7)
C22	-0.0444(3)	-0.2958(3)	0.1539(5)	2.22(7)
C23	-0.1399(4)	-0.4402(3)	0.2340(5)	2.44(7)
C24	-0.1450(4)	-0.4182(3)	0.4205(6)	2.62(8)
C25	-0.3483(3)	-0.0355(3)	0.5009(5)	2.35(8)
C26	-0.4312(4)	0.0336(3)	0.5991(5)	3.33(9)
C27	-0.5536(4)	0.0081(4)	0.5645(5)	2.86(8)
C28	-0.6070(4)	-0.0909(3)	0.4348(5)	2.80(8)
C29	-0.5167(3)	-0.1510(3)	0.3460(5)	2.02(7)
C110	0.2692(3)	0.0215(3)	0.0459(5)	2.23(7)
C111	0.3956(4)	0.0590(4)	0.0930(5)	3.10(9)
C112	0.4237(5)	0.1597(3)	0.2385(6)	3.54(9)
C113	0.3219(5)	0.2075(3)	0.3005(6)	3.4(1)
C114	0.2030(4)	0.1584(4)	0.2380(6)	2.91(9)
C210	-0.3573(3)	-0.2524(3)	0.2087(4)	2.22(7)
C211	-0.6821(3)	-0.2960(3)	0.1487(5)	2.89(8)
C212	-0.7053(4)	-0.3854(4)	0.0313(6)	3.16(9)
C213	-0.6090(4)	-0.4379(4)	-0.0546(6)	3.38(9)
C214	-0.4821(4)	-0.3960(3)	0.0027(5)	2.98(8)

*Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as (4/3) × $[a^2 \times B(1,1) + b^2 \times B(2,2) + c^2 \times B(3,3) + ab(\cos \text{gamma}) \times B(1,2) + ac(\cos \text{beta}) \times B(1,3) + bc(\cos \text{alpha}) \times B(2,3)]$.

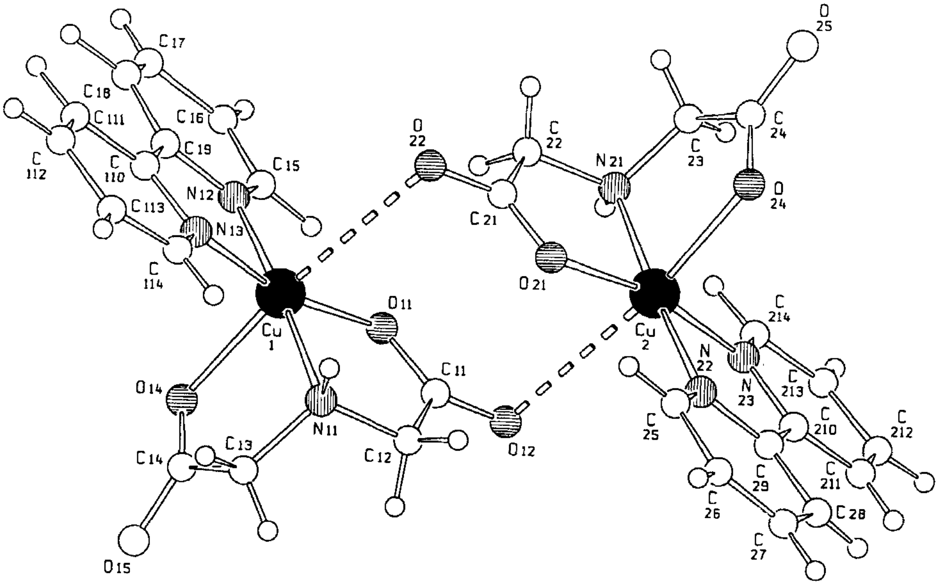

Figure 1 Illustration of the structure of the asymmetric entity $[Cu(IDA)(2,2'\text{-bipy})]_2$ and the atom numbering scheme.

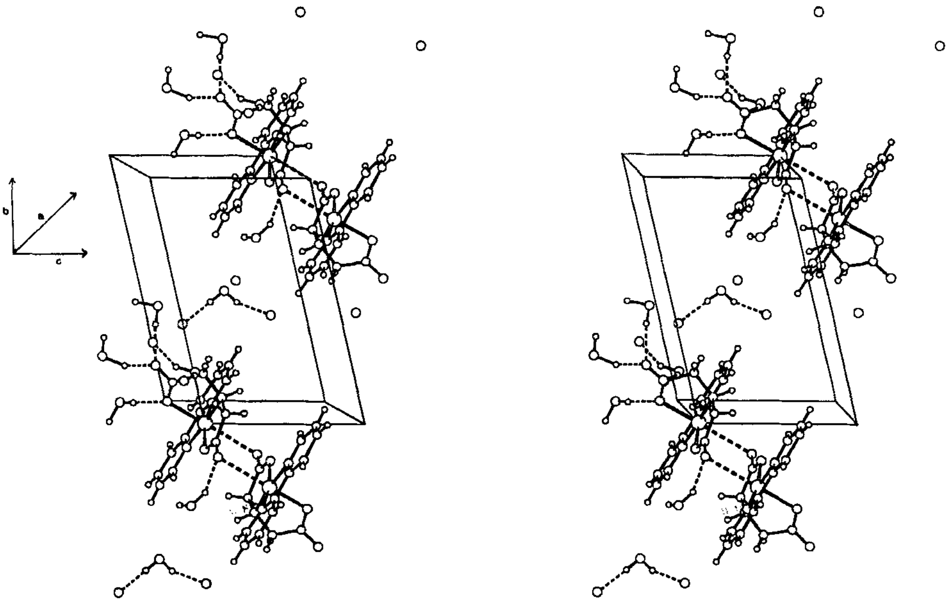

Figure 2 Stereo view of the unit cell showing some hydrogen bonds (looking down the *a* axis with the *b* axis vertical and the *c* axis horizontal).

Table 3 Bond lengths (Å) and angles (deg.) of [Cu(IDA)(2,2'-bipy)].6H_2.

Cu(II) environment			
Cu(1) – O(1)	1.927(3)	O(11) – Cu(1) – O(14)	96.4(2)
Cu(1) – O(14)	2.229(3)	O(11) – Cu(1) – O(22)	78.4(1)
Cu(1) – O(22)	3.007(4)	O(11) – Cu(1) – N(11)	86.0(2)
Cu(1) – N(11)	2.047(3)	O(11) – Cu(1) – N(12)	94.8(1)
Cu(1) – N(12)	1.967(3)	O(11) – Cu(1) – N(13)	166.0(1)
Cu(1) – N(13)	1.961(3)	O(14) – Cu(1) – O(22)	173.7(2)
Cu(2) – O(12)	2.991(3)	O(14) – Cu(1) – N(11)	81.6(2)
Cu(2) – O(21)	1.957(3)	O(14) – Cu(1) – N(12)	94.5(1)
Cu(2) – O(24)	2.242(3)	O(14) – Cu(1) – N(13)	97.4(1)
Cu(2) – N(21)	1.986(3)	O(22) – Cu(1) – N(11)	94.6(1)
Cu(2) – N(22)	2.003(3)	O(22) – Cu(1) – N(12)	89.4(1)
Cu(2) – N(23)	2.050(3)	O(22) – Cu(1) – N(13)	88.1(1)
Cu(1) – Cu(2)	5.409(1)	N(11) – Cu(1) – N(12)	176.0(1)
		N(11) – Cu(1) – N(13)	99.1(1)
		N(12) – Cu(1) – N(13)	81.1(1)
		O(12) – Cu(2) – O(21)	78.86(9)
		O(12) – Cu(2) – O(24)	171.89(9)
		O(12) – Cu(2) – N(21)	96.0(1)
		O(12) – Cu(2) – N(22)	89.2(2)
		O(12) – Cu(2) – N(23)	88.3(2)
		O(21) – Cu(2) – N(21)	94.1(2)
		O(21) – Cu(2) – N(21)	84.9(1)
		O(21) – Cu(2) – N(22)	94.4(2)
		O(21) – Cu(2) – N(23)	166.7(1)
		O(24) – Cu(2) – N(21)	79.3(1)
		O(24) – Cu(2) – N(22)	95.4(1)
		O(24) – Cu(2) – N(23)	99.1(1)
		N(21) – Cu(2) – N(22)	174.5(1)
		N(21) – Cu(2) – N(23)	100.0(1)
		N(22) – Cu(2) – N(23)	81.8(2)
IDA		Cu(1) – N(13) – C(114)	129.9(3)
		Cu(1) – N(12) – C(15)	125.2(3)
N(11) – C(12)	1.525(5)	Cu(1) – N(11) – C(12)	105.8(2)
C(12) – C(11)	1.489(6)	Cu(1) – N(11) – C(13)	109.0(2)
C(11) – O(12)	1.232(5)	C(12) – N(11) – C(13)	112.9(3)
C(11) – O(11)	1.296(5)	N(11) – C(12) – C(11)	114.5(3)
N(11) – C(13)	1.510(5)	N(11) – C(13) – C(14)	110.3(3)
C(13) – C(14)	1.592(5)	C(12) – C(11) – O(11)	116.4(3)
C(14) – O(14)	1.199(5)	C(13) – C(14) – O(14)	121.1(3)
C(14) – O(15)	1.281(5)	C(12) – C(11) – O(12)	118.1(4)
N(21) – C(22)	1.453(5)	C(13) – C(14) – O(15)	112.4(3)
C(22) – C(21)	1.544(5)	C(11) – O(11) – C(1)	117.0(2)
C(21) – O(22)	1.248(5)	C(14) – O(14) – Cu(1)	111.2(2)
C(21) – O(21)	1.239(4)	Cu(2) – N(23) – C(214)	125.2(3)
		Cu(2) – N(21) – C(22)	109.8(2)
N(21) – C(23)	1.458(5)	N(21) – C(22) – C(21)	110.8(4)
C(23) – C(24)	1.459(6)	C(22) – C(21) – O(22)	117.3(3)
C(24) – O(25)	1.249(5)	C(22) – C(21) – O(21)	118.1(4)
C(24) – O(24)	1.281(4)	C(21) – O(21) – Cu(2)	115.3(2)
		Cu(2) – N(21) – C(23)	110.4(3)
		N(21) – C(23) – C(24)	116.2(3)
		C(23) – C(24) – O(25)	119.1(3)
		C(23) – C(24) – O(24)	116.8(4)
		C(24) – O(24) – Cu(2)	110.6(3)
		Cu(2) – N(22) – C(23)	125.7(2)

Table 3 *Continued.*

2,2’-bipy			
N(12)—C(15)	1.390(4)	N(12)—C(15)—C(16)	120.8(4)
C(15)—C(16)	1.327(6)	C(15)—C(16)—C(17)	120.0(4)
C(16)—C(17)	1.449(6)	C(16)—C(17)—C(18)	117.6(4)
C(17)—C(18)	1.305(5)	C(17)—C(18)—C(19)	122.2(3)
C(18)—C(19)	1.381(5)	C(18)—C(19)—N(12)	120.5(3)
C(19)—N(12)	1.349(5)	C(19)—N(12)—C(15)	118.8(3)
N(13)—C(110)	1.321(5)	N(13)—C(114)—C(113)	127.4(4)
C(110)—C(19)	1.491(4)	C(114)—C(113)—C(112)	119.2(3)
C(110)—C(111)	1.383(6)	C(113)—C(112)—C(111)	116.8(5)
C(111)—C(112)	1.495(5)	C(112)—C(111)—C(110)	115.8(4)
C(112)—C(113)	1.343(7)	C(111)—C(110)—N(13)	126.4(3)
C(113)—C(114)	1.367(6)	C(110)—N(13)—C(114)	114.3(3)
C(114)—N(13)	1.329(6)	C(110)—C(19)—N(12)	112.0(4)
N(22)—C(25)	1.294(4)	C(110)—C(19)—C(18)	127.5(3)
C(25)—C(26)	1.438(6)	C(19)—C(110)—N(13)	114.8(3)
C(26)—C(27)	1.303(6)	C(19)—C(110)—C(111)	118.7(3)
C(27)—C(28)	1.466(5)	C(19)—N(12)—Cu(1)	116.0(2)
C(28)—C(29)	1.409(6)	C(110)—N(13)—Cu(1)	115.7(2)
C(29)—N(22)	1.345(5)	N(22)—C(25)—C(26)	122.0(6)
N(23)—C(210)	1.366(5)	C(25)—C(26)—C(27)	118.6(3)
C(210)—C(29)	1.484(4)	C(26)—C(27)—C(28)	122.0(4)
C(210)—C(211)	1.392(5)	C(27)—C(28)—C(29)	113.9(4)
C(211)—C(212)	1.280(5)	C(28)—C(29)—N(22)	123.1(4)
C(212)—C(213)	1.416(6)	C(29)—N(22)—C(25)	120.3(4)
C(213)—C(214)	1.404(6)	N(23)—C(214)—C(213)	117.5(4)
C(214)—N(23)	1.360(4)	C(214)—C(213)—C(212)	118.9(4)
		C(213)—C(212)—C(211)	121.2(4)
		C(212)—C(211)—C(210)	121.2(4)
		C(211)—C(210)—N(23)	119.0(3)
		C(210)—N(23)—C(214)	122.0(4)
		C(29)—C(210)—C(211)	126.6(3)
		C(29)—C(210)—N(23)	114.4(3)
		C(210)—C(29)—C(28)	120.1(3)
		C(210)—C(29)—N(22)	116.7(3)
		Cu(2)—N(23)—C(210)	112.9(2)
		Cu(2)—N(22)—C(29)	113.8(2)

(0.14 and 0.17 Å, respectively). These ligands are slightly twisted (7.0(4)° and 8.2(4)°) *versus* the corresponding Cu(1) and Cu(2) square planes. On the other hand, the IDA ligand forms two nearly perpendicular, five-membered chelate rings, sharing the Cu-N(IDA) bond.

It is instructive to compare the relative conformation of the two IDA chelate rings in the parent diaqua-complex [Cu(IDA)(H_2O)$_2$] and in related, mixed-ligand complexes of known structure with one IDA and a nitrogen heterocycle (ImH, 2,2′-bipy, 4,4′-bipy) as secondary ligand (Table 4). In all of these compounds the Cu(II) ion shows an elongated octahedral coordination (I and II) or has a pyramidal coordination (III to V) with one additional semi-coordination bond (IV) or a weaker Cu. . .O interaction (III and V). All Cu(II) complexes with nitrogen-heterocycle ligands in Table 3 have an *N*-heterocycle donor *trans* to the *N*(IDA) donor. We think that the coordination of only one *N*-heterocycle per Cu(II) atom (II and III) will cause a *trans*-stabilizing effect which leads to a Cu-N(IDA) bond of less than 2.000 Å and promotes a nearly coplanar conformation of the two IDA-Cu chelate

Table 4 IDA Chelate ring conformation and related data in mixed-ligand complexes.

	Compound	Cu(II) coordination	Conf. of IDA chelate rings**	Length of Cu-N(IDA)(A)	Ref.
I	$[Cu(IDA)(H_2O)_2]$	4 + 1	⊥	2.014(3)	1
II	$[Cu(IDA)(ImH)(CH_3OH)]\cdot 0.37H_2O$	4 + 2	—	1.977(7)	2
III	$[Cu_2(IDA)_2(4,4'\text{-bipy})]$	4 + 1(+ 1)*	—	1.994(4)	4
IV	$[Cu(IDA)(ImH)_2]_2\cdot 2H_2O$	4 + 1(+ 1)*	⊥	2.049(1)	3
V	$[Cu(IDA)(2,2'\text{-bipy})]\cdot 6H_2O$	4 + 1(+ 1)*	⊥	2.016(3) average	this work

*Semi-coordination bond or weak interaction. **⊥ Nearly perpendicular, — = nearly coplanar.

rings. The entry of a second *N*-heterocyclic donor per Cu(II) atom from one univalent ligand (ImH in IV) as well as from one *cis*-bidentate ligand (2,2′-bipy in V) is always made *cis versus* the former one, and which imposes a nearly perpendicular conformation of the two IDA-Cu chelate rings. In these cases the Cu-N(IDA) bond is longer than 2.000 Å.

The crystal structure of the parent diaqua-compound $[Cu(IDA)(H_2O)_2]$ shows one near H_2O molecule *cis* to N(IDA) and a second remote one at an apical site of an elongated, octahedral Cu(II) coordination polyhedron. The *trans*-position to the *N*(IDA) donor is now occupied by one oxygen donor of an adjacent IDA ligand and the IDA chelates the Cu(II) with its rings nearly perpendicular.[1] The observed preference of the former incoming *N*-heterocycle donor for a *trans* position to the *N*(IDA) donor seems to be ruled out for water. However, in spite of the Cu(II) coordination to two water molecules in I (clearly different to the two ImH ligands in the tetragonal coordination plane in IV), the nearly perpendicular conformation of the IDA chelate rings in I also gives a Cu-N(IDA) bond length > 2.000 Å.

On the basis of the above considerations of mixed-ligand Cu(II) complexes with IDA and *N*-heterocycles as secondary ligands, we conclude that the nearly coplanar or nearly perpendicular configuration of the Cu(II)-IDA chelate rings is promoted by the preference of the former incoming *N*-heterocyclic donor for a *trans* position to N-(IDA) and by the in-plane *cis* coordination of two *N*-heterocyclic donor atoms with the Cu-N(IDA) bond.

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