

Fig. 1. ORTEP (Johnson, 1976) drawing of the [Fe(tdta)]<sup>-</sup> anion (50% probability thermal ellipsoids) with the atom-numbering scheme. H atoms are omitted for clarity.

solution because of rapid racemization or rearrangement. The trimethylenediamine moiety takes a symmetric skew-boat form with  $\delta$  conformation. This differs from Li[Fe(tdta)] (Li salt) and other metal–tdta complexes, which have a twist-boat conformation (Yamamoto, Mikata, Miyoshi & Yoneda, 1988, and references therein).

The Fe–N [av. 2.175 (2) Å] and Fe–O [av. 1.973 (2) Å] distances in the present complex (Na salt) are shorter than those of the Li salt [2.194 (3) and 1.989 (3) Å, respectively]. The deviations of the bond angles around the Fe<sup>III</sup> atom from 90 and 180° in the Na salt are smaller than those in the Li salt,

e.g. O(3)—Fe—O(5), 105.8 (1)° [112.5 (1)° in the Li salt]; N(1)—Fe—N(2), 92.9 (1)° [94.3 (1)°]; in-plane, O—Fe—N, 80.1 (1) and 82.7 (1)° [77.8 (1) and 78.8 (1)°], and so on. This fact seems to indicate that in the Na salt the molecular geometry of the Fe<sup>III</sup> complex has less steric hindrance in the solid in comparison with the Li salt.

The Na atom is surrounded octahedrally by three O atoms of the tdta moiety [O(2) ( $-\frac{1}{2} + x, \frac{1}{2} - y, 2 - z$ ), O(4) and O(8) ( $\frac{1}{2} - x, 1 - y, \frac{1}{2} + z$ )] and three water O atoms. The Na—O distances are in the range 2.343 (3)–2.515 (3) Å. Hydrogen bonds also exist between the water molecules and the O atoms in the tdta moiety, O(1)⋯O(11) [2.817 (4) Å], O(6)⋯O(11) [2.792 (4) Å] and O(7)⋯O(13) [2.882 (4) Å].

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## Structure of [2,6-Bis(2-benzimidazolyl)pyridine]dichlorocopper(II) Dimethylformamide

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**Abstract.** [CuCl<sub>2</sub>(C<sub>19</sub>H<sub>13</sub>N<sub>5</sub>)]·C<sub>3</sub>H<sub>7</sub>NO, *M<sub>r</sub>* = 518.9, monoclinic, *P*2<sub>1</sub>/*n*, *a* = 9.150 (1), *b* = 12.908 (3), *c* = 18.964 (4) Å,  $\beta$  = 93.33 (1)°, *V* = 2236.0 (7) Å<sup>3</sup>, *Z* = 4, *D<sub>m</sub>* = 1.54 (2), *D<sub>x</sub>* = 1.54 Mg m<sup>-3</sup>,  $\lambda$ (Mo *K* $\alpha$ ) = 0.71069 Å,  $\mu$  = 1.25 mm<sup>-1</sup>, *F*(000) = 1060, room

temperature, *R* = 0.069 for 1918 reflections. The structure shows Cu<sup>II</sup> in a square-pyramidal environment with the planar tridentate ligand and one chloride in the equatorial plane, and the second chloride more weakly bound (as shown by the

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Cu—Cl bond distance) in the axial position. The disordered dimethylformamide is not bound to the copper but is hydrogen bonded to a benzimidazole group.

**Introduction.** In the course of our attempts to prepare dioxygen complexes of copper we have studied the chemistry of copper(II) with a series of planar tridentate nitrogen ligands of which 2,6-bis(2-benzimidazolyl)pyridine (bzimpy) is a typical example (Piguet, Bocquet, Müller & Williams, 1989). The crystal structure of the title compound [2,6-bis(2-benzimidazolyl)pyridine]dichlorocopper(II)dimethylformamide was determined in order to confirm the tridentate coordination of the bzimpy ligand and to compare its properties with [CuCl<sub>2</sub>(terpy)] (terpy = 2,2':6',2''-terpyridyl) (Henke, Kremer & Reinen, 1983).

**Experimental.** Preparation of crystals: 0.311 g (1 mmol) of ligand, bzimpy, synthesized by the method of Addison & Burke (1981), was dissolved in 20 ml ethanol and then mixed with 0.17 g (1 mmol) of CuCl<sub>2</sub>·2H<sub>2</sub>O in the same solvent. The resulting precipitate was separated by filtration and recrystallized from 300 ml hot DMF. Green crystals suitable for X-ray diffraction were obtained in 70% yield. Density was measured by flotation.

An emerald-green prism 0.13 × 0.15 × 0.22 mm (sealed in a capillary under argon) was measured using a Philips PW 1100 diffractometer,  $\omega/2\theta$  scan, scan width (1.2 + 0.25 tan  $\theta$ )°, scan speed 0.03° s<sup>-1</sup>. Graphite-monochromated Mo K $\alpha$  radiation. 2979 reflections were measured (6 < 2 $\theta$  < 44°;  $h = -9, 9; k = 0, 13; l = 0, 19$ ). 2734 unique reflections ( $R_{\text{int}} = 0.026$ ) of which 1918 were taken to be observed [ $|F_o| \geq 3\sigma(F_o)$ ,  $|F_o| \geq 6.0$ ]. Three standard reflections measured every 60 min showed a variation of less than 1.6 $\sigma(I)$  and no correction for change in intensity was applied. Cell parameters were from least-squares refinement of 27 centred reflections (21 < 2 $\theta$  < 28°). Data were corrected for Lorentz and polarization effects and for spherical absorption ( $\mu r = 0.21$ ; max. and min. transmission factors 0.734 and 0.732). The structure was solved by direct methods using MULTAN80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). All other calculations used a local version of XRAY76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) and ORTEPII (Johnson, 1976). Scattering factors for neutral atoms were from Cromer & Mann (1968), and anomalous-dispersion corrections for Cu and Cl from *International Tables for X-ray Crystallography* (1974). Hydrogen atoms were in calculated positions for the ligand. All non-hydrogen atoms refined with anisotropic displacement parameters except for the carbon atoms of DMF. The

dimethylformamide molecule is disordered about a twofold axis joining the nitrogen and oxygen atoms. Two privileged positions for the carbon atoms were identified, and were refined with the sum of the populations of the two symmetry-related sites constrained to unity. The sites occupied by C(20), C(21) and C(22) had a population of 0.7 and those occupied by C(201), C(211) and C(221) a population of 0.3. Apart from the population parameters, no constraints were applied to the refinement of the dimethylformamide molecule, and the resulting bond lengths and angles for the two molecules showed no features of particular interest. Full-matrix least-squares refinement based on  $F$  using weights  $w = (|F_o|/48)^2$  for  $|F_o| \leq 48$ ,  $w = (48/|F_o|)^2$  for  $|F_o| > 48$  gave final values of  $R = 0.069$ ,  $wR = 0.056$ ,  $S = 1.50$  for 262 variables and 1918 contributing reflections;  $(\Delta/\sigma)_{\text{max}} = 0.058$ ,  $(\Delta/\sigma)_{\text{ave}} = 0.011$ . The final difference Fourier map showed maxima and minima of +0.89 and -0.54 e Å<sup>-3</sup> in the region of the disordered dimethylformamide.

**Discussion.** Atomic coordinates and equivalent isotropic temperature factors are given in Table 1, and selected bond lengths and bond angles in Table 2.\* Fig. 1. gives an ORTEP view of the complex and the hydrogen-bonded dimethylformamide molecule, and shows the atomic numbering scheme.

The complex [CuCl<sub>2</sub>(bzimpy)] shows a square-pyramidal geometry very similar to that observed for [CuCl<sub>2</sub>(terpy)]· $n$ H<sub>2</sub>O ( $n = 0, 1$ ; Henke, Kremer & Reinen, 1983) and [Cu(mbzimpy)(CH<sub>3</sub>CN)](ClO<sub>4</sub>)<sub>2</sub> [mbzimpy = 2,6-bis(1-methyl-2-benzimidazolyl)pyri-

\* Lists of structure factors, atomic positional and anisotropic displacement parameters, bond distances and angles, and other information in the printed form of the Standard Crystallographic File Structure of Brown (1985) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52894 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

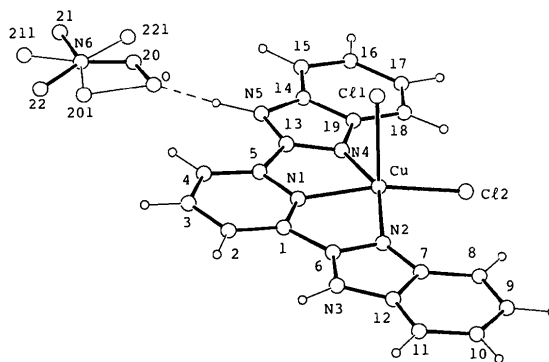


Fig. 1. ORTEP view of the complex hydrogen bonded to a disordered dimethylformamide, and atomic numbering scheme for [CuCl<sub>2</sub>(bzimpy)]·DMF.

Table 1. Positional, equivalent isotropic atomic displacement parameters and population parameters (PP) for [CuCl<sub>2</sub>(bzimpy)].DMF

	x	y	z	U <sub>eq</sub> * (Å <sup>2</sup> )	PP
Cu	0.3578 (1)	0.01600 (8)	0.59966 (6)	0.0409 (6)	
Cl(1)	0.1615 (2)	0.1372 (2)	0.6439 (1)	0.053 (1)	
Cl(2)	0.4604 (3)	-0.0510 (2)	0.6981 (1)	0.062 (2)	
N(1)	0.3022 (7)	0.0565 (5)	0.4999 (3)	0.035 (4)	
N(2)	0.2271 (7)	-0.1060 (5)	0.5664 (3)	0.039 (4)	
N(3)	0.0634 (8)	-0.1665 (6)	0.4838 (4)	0.047 (5)	
N(4)	0.4999 (7)	0.1340 (6)	0.5848 (4)	0.044 (4)	
N(5)	0.5448 (7)	0.2744 (6)	0.5182 (4)	0.046 (5)	
C(1)	0.1976 (8)	0.0021 (7)	0.4634 (4)	0.040 (5)	
C(2)	0.143 (1)	0.0359 (7)	0.3978 (5)	0.045 (5)	
C(3)	0.196 (1)	0.1266 (8)	0.3709 (5)	0.054 (6)	
C(4)	0.3063 (9)	0.1821 (7)	0.4096 (5)	0.046 (6)	
C(5)	0.3529 (8)	0.1443 (7)	0.4748 (4)	0.036 (5)	
C(6)	0.1593 (9)	-0.0897 (7)	0.5025 (4)	0.039 (5)	
C(7)	0.1698 (9)	-0.1985 (7)	0.5899 (5)	0.042 (5)	
C(8)	0.198 (1)	-0.2522 (8)	0.6537 (5)	0.058 (7)	
C(9)	0.117 (1)	-0.3435 (8)	0.6631 (6)	0.074 (8)	
C(10)	0.017 (1)	-0.3793 (8)	0.6098 (7)	0.081 (8)	
C(11)	-0.008 (1)	-0.3280 (8)	0.5463 (6)	0.067 (7)	
C(12)	0.068 (1)	-0.2375 (7)	0.5390 (5)	0.046 (6)	
C(13)	0.4675 (9)	0.1871 (7)	0.5253 (4)	0.041 (5)	
C(14)	0.639 (1)	0.2806 (7)	0.5782 (5)	0.051 (6)	
C(15)	0.745 (1)	0.3547 (8)	0.5984 (5)	0.058 (6)	
C(16)	0.825 (1)	0.3365 (9)	0.6602 (6)	0.064 (7)	
C(17)	0.797 (1)	0.2477 (9)	0.7025 (6)	0.062 (7)	
C(18)	0.690 (1)	0.1764 (8)	0.6840 (5)	0.053 (6)	
C(19)	0.6108 (9)	0.1936 (7)	0.6197 (5)	0.044 (6)	
N(6)	0.5999 (9)	0.5324 (7)	0.3497 (4)	0.070 (5)	
O	0.4946 (9)	0.4108 (7)	0.4132 (5)	0.109 (7)	
C(20)	0.58249	0.48250	0.40781	0.06890	0.71
C(201)	0.50269	0.45602	0.32957	0.16100	0.29
C(21)	0.70633	0.62036	0.34766	0.08580	0.62
C(211)	0.62818	0.59868	0.29116	0.09240	0.38
C(22)	0.51157	0.50602	0.28458	0.11790	0.76
C(221)	0.69476	0.55013	0.42080	0.08750	0.24

$$* U_{eq} = \frac{1}{3} \sum U_{ii}$$

respect to the pyridine nucleus. The ease with which the benzimidazole groups may be rotated about the pyridine-benzimidazole bonds has been shown by the structure of the complex formed by the bis-*N*-methylated derivative of bzimpy (mbzimpy) with copper(I), [Cu<sub>2</sub>(mbzimpy)<sub>2</sub>]<sup>2+</sup>, where the inclination of the benzimidazole planes with respect to the pyridines varies between 18 and 45° (Piguet, Bernardinelli & Williams, 1989).

The equatorial chloride ligand Cl(2) lies 0.094 Å above the plane of the bzimpy. The copper atom is 0.306 Å above the plane of the bzimpy [towards Cl(1)] and 0.260 Å above the N<sub>3</sub>Cl plane defined by the three coordinating nitrogen atoms and Cl(2). The Cu—Cl(1) bond makes an angle of 82.4° to the N<sub>3</sub>Cl plane, and is appreciably longer than the equatorial Cu—Cl(2) bond. This difference [0.344 (4) Å] is significantly greater than observed for [CuCl<sub>2</sub>(terpy)] (0.271 Å) and comparable with that in [CuCl<sub>2</sub>(terpy)].H<sub>2</sub>O (0.333 Å). This suggests a considerable difference in Lewis acidity between the axial and equatorial sites of the Cu(bzimpy)<sup>2+</sup> moiety, as was previously deduced from its behaviour in solution (Piguet, Bocquet, Müller & Williams, 1989).

The hydrogen atoms bound to the non-coordinating nitrogen atoms of the benzimidazole rings are involved in hydrogen bonding. H(105), bound to N(5), is hydrogen bonded to the oxygen of the dimethylformamide [N(5)⋯O = 2.68 (1) Å, angle N(5)—H(105)—O *ca* 172°], and H(103), bound to N(3), is hydrogen bonded to Cl(1) of the complex related by the symmetry operation  $-x, -y, 1-z$  [N(3)⋯Cl(1) = 3.109 (7) Å, angle N(3)—H(103)—Cl(1) *ca* 160°] so as to form chains along the *a* axis. The hydrogen bonded N⋯Cl distance is comparable with the values reported for other structures (Barlein & Mostad, 1981; Menabue, Pellacani, Albinati, Ganazzoli, Cariati & Rassu, 1982), and is close to the O⋯(axial)Cl distance (3.2 Å) in [CuCl<sub>2</sub>(terpy)].H<sub>2</sub>O (Henke, Kremer & Reinen, 1983) where hydrogen bonding was also postulated. No interaction between the chains was found in the molecular packing.

Table 2. Selected bond distances (Å) and angles (°) for [CuCl<sub>2</sub>(bzimpy)]

Cu—N(1)	2.000 (6)	N(2)—C(6)	1.35 (1)
Cu—N(2)	2.055 (7)	C(6)—C(1)	1.45 (1)
Cu—N(4)	2.033 (7)	C(1)—N(1)	1.34 (1)
Cu—Cl(1)	2.559 (3)	N(1)—C(5)	1.32 (1)
Cu—Cl(2)	2.215 (3)	C(5)—C(13)	1.49 (1)
C(13)—N(4)	1.34 (1)		
N(1)—Cu—N(2)	78.3 (3)	N(2)—Cu—N(4)	153.9 (3)
N(1)—Cu—N(4)	78.7 (3)	N(2)—Cu—Cl(1)	99.3 (2)
N(1)—Cu—Cl(1)	90.3 (2)	N(2)—Cu—Cl(2)	99.8 (2)
N(1)—Cu—Cl(2)	166.2 (2)	N(4)—Cu—Cl(1)	93.1 (2)
Cl(1)—Cu—Cl(2)	103.53 (9)	N(4)—Cu—Cl(2)	99.6 (2)
Cu—N(2)—C(6)	112.7 (5)	Cu—N(4)—C(13)	112.8 (5)
N(2)—C(6)—C(1)	118.3 (7)	N(4)—C(13)—C(5)	117.8 (8)
C(6)—C(1)—N(1)	110.4 (7)	C(13)—C(5)—N(1)	109.6 (7)
C(1)—N(1)—Cu	119.0 (5)	C(5)—N(1)—Cu	119.3 (5)

dine; Sanni, Behm, Beurskens, van Albada, Reedijk, Lenstra, Addison & Palaniandavar, 1988]. The coordination of the ligand bzimpy is very similar to that found in these structures, with three almost equal Cu—N distances and an average N—Cu—N bite angle of 78.5°. The geometry of the ligand bzimpy itself is very close to planarity, the greatest deviation from the least-squares plane through the 24 non-hydrogen atoms being 0.09 Å, with a standard deviation of 0.04 Å. This very small deviation from planarity is due mainly to a slight inclination (1.6 and 2.8°) of the benzimidazole planes with

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## Synthesis and Structure of Cytosine Cobalt Dichloride

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**Abstract.** Bis[4-amino-2(1*H*)-pyrimidinone]dichloro-cobalt,  $[\text{CoCl}_2(\text{C}_4\text{H}_5\text{N}_3\text{O})_2]$ ,  $M_r = 352.04$ , triclinic,  $P\bar{1}$ ,  $a = 12.663$  (3),  $b = 7.553$  (2),  $c = 7.061$  (2) Å,  $\alpha = 93.07$  (8),  $\beta = 72.93$  (8),  $\gamma = 88.28$  (8)°,  $V = 643.9$  (9) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 1.816$  Mg m<sup>-3</sup>,  $\lambda(\text{Ag K}\alpha) = 0.56087$  Å,  $\mu = 0.9$  mm<sup>-1</sup>,  $F(000) = 354$ ,  $T = 298$  K,  $R = 0.062$ ,  $wR = 0.71$  for 1885 reflections  $> 1\sigma(F)$ . The crystal structure of the title compound consists of two crystallographically independent cytosine molecules attached together through the direct bonding of the  $\text{Co}^{2+}$  ion with two N atoms of the pyrimidine rings. In addition to N atoms, cobalt ions are coordinated to two Cl atoms forming a slightly distorted tetrahedral environment, unlike the  $[\text{CuCl}_2(\text{C}_4\text{H}_5\text{N}_3\text{O})_2]$  complex in which the Cu atom is in a square-planar coordination. The bond distances of cobalt to the Cl(1), Cl(2), N(3) and N(3') atoms are 2.303 (2), 2.296 (2), 2.057 (5) and 2.053 (5) Å, respectively. The packing of the Cyt(I)– $\text{CoCl}_2$ –Cyt(II) complex in the crystal, ensured by short intermolecular contacts presumably mediated by hydrogen bonding involving Cl, O, C and N atoms, has very little effect on the internal bonds and angles of the cytosine groups or on their planarity.

**Introduction.** It was observed that the interaction of metals with nucleic acids produces different effects. Some metals are effective in destroying the native structure of DNA, others are effective in maintaining it.

It was reported that  $\text{Mg}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mn}^{2+}$  and  $\text{Zn}^{2+}$  act as stabilizers of the calf-thymus

DNA macromolecule while  $\text{Cu}^{2+}$  induces the reverse effect (Eichhorn, 1962). The destabilization of the DNA molecule by certain metal ions, notably  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$  and  $\text{Hg}^{2+}$ , is attributed to the ability of these latter atoms to lodge at the center of the heterocyclic base pairs, thereby disrupting their hydrogen bonding. The stabilizing effect is due to the binding of these ions to the sugar–phosphate backbone of DNA (Eichhorn & Shin, 1968).

Selective binding of alkali ions to GC-rich DNA fragments was first suggested by kinetic studies (Eichhorn & Shin, 1968) and was later confirmed by X-ray analysis of the structure of cytosine calcium chloride, in which the alkali ion is found to be directly coordinated to the cytosine base (Ogawa, Kumihashi, Tomita & Shirotake, 1980). Direct cytosine–Cu–cytosine binding was first suggested by NMR studies (Venner & Zimmer, 1966) then conclusively confirmed by X-ray analysis of  $\text{CuCl}_2(\text{C}_4\text{H}_5\text{N}_3\text{O})_2$  (Sundaralingam & Carrabine, 1971; Tran Qui & Palacios, 1990).

Recently, in the course of our attempts to synthesize other cytosine complexes with stabilizing metal ions,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$  and  $\text{Mn}^{2+}$ , we have succeeded in crystallizing and isolating an unknown cobalt complex. X-ray photographs show this crystal to be triclinic [unlike the monoclinic symmetry observed for the copper complex (Tran Qui & Palacios, 1990)]. Although this difference appeared as the crystal structure determination progressed, the cobalt and copper compounds are stereoisomers.  $\text{Co}^{2+}$  in  $\text{CoCl}_2(\text{C}_4\text{H}_5\text{N}_3\text{O})_2$  is found, unexpectedly, to be