feature often found among perchlorates of bulky organic cations, namely large vibrational thermal motion. The average Cl—O distances, corrected or uncorrected for thermal motion, for the two ions are rather short, 1·36 (1) and 1·39 (1) Å. The largest deviations for the two ions from the tetrahedral angle (109·5°) amount to 5·2 and 10·0°, which are about 5 and 10 times the e.s.d.'s. The difference maps did not give any further information about the state of these ions.

Some rather short O···H and C···H contacts exist between the perchlorate O and methylene H atoms [O(3)···H(1A), O(4)···H(5A), O(5)···H(3B), 2·34 (1) (3×) Å] and the phenyl C and H atoms of different rings [C(16)···H(24), 2·53 (1) Å]. The van der Waals values for O—H and C—H are 2·4 and 2·5 Å, respectively (Gieren & Dederer, 1977; Baur, 1972). The H atoms were, however, located by geometrical methods, the phenyl and methylene groups assumed to be rigid bodies.

The packing of the ions is shown in Fig. 3. The two perchlorate ions, not bonded to Ni, are situated one on each side of the complex cation.

Magnetic-susceptibility measurements were performed at room temperature with a Faraday balance (Blom & Hörlin, 1977). As expected the compound is diamagnetic.

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Studies on the Metal—Amide Bond.
III.* The Structure of the Copper(II) Deprotonated Complex of N,N'-Ethylenedi-2-pyridinecarboxamide

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Abstract

Aqua(N,N'-ethylenedi-2-pyridinecarboxamido)copper-(II) monohydrate, $[Cu(C_{14}H_{12}N_4O_2)(H_2O)].H_2O$, $C_{14}H_{14}CuN_4O_3.H_2O$, is monoclinic, space group $P2_1/c$, with $a = 17·298$ (15), $b = 13·505$ (9), $c = 14·119$ (22) Å, $\beta = 115·8$ (2)°, $Z = 8$. The structure was refined to $R = 0·099$ for 3112 non-zero photographic reflexions. The crystal contains two distinct geometric isomers. In each the ligand acts as an approximately planar N_4 quadridentate ligand, coordinating the Cu atom [Cu—N(amide) average 1·920 (7), Cu—N(pyridine) average 2·053 (7) Å, N(amide)—Cu—N(amide) average 82·5 (3), N(pyridine)—Cu—N(pyridine) 110·8 (3), 112·7 (3)°], with a water molecule occupying the apex of a distorted square pyramid [Cu—O 2·361 (8) and 2·317 (8) Å]. The Cu atoms are 0·22 and 0·28 Å above the N_4 planes. The two isomers differ in the degree and nature of folding of the quadridentate ligands from planarity. The molecules pack in a series of planes parallel to (10Ī) with the coordinated and lattice water molecules

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* Part II: Chapman, Stephens & Vagg (1980).

hydrogen bonding amide O atoms of neighbouring molecules.

Introduction

As part of a systematic study on the nature of the coordination of amide groups to transition-metal ions we have prepared a series of quadridentate ligands containing the picolinamide unit (Barnes, Chapman, Vagg & Watton, 1978). The coordination chemistry of one of these, N,N'-(o-phenylene)di-2-pyridine-carboxamide, pdpH$_2$, has been outlined (Chapman & Vagg, 1979) and the crystal structure of its deprotonated Cu^{II} chelate reported (Chapman, Stephens & Vagg, 1980). Our work has shown the more flexible ligand N,N'-ethylenedi-2-pyridinecarboxamide, edpH$_2$ (I), to readily form complexes with transition metals in both neutral and deprotonated forms. Here we report the results of an analysis of the deprotonated Cu^{II} complex of that ligand, $[Cu(edp)(H_2O)]$. H$_2$O.

(I)
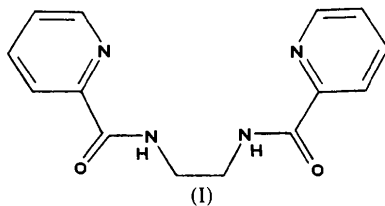
Experimental

The reaction of edpH$_2$ with a hot aqueous solution of Cu^{II} acetate and sodium acetate yielded large violet-blue rhomboids of [Cu(edp)(H$_2$O)]. H$_2$O on cooling.

Crystal data

C$_{14}$H$_{14}$CuN$_4$O$_3$.H$_2$O, $M_r = 367\cdot8$, monoclinic, $a = 17\cdot298$ (15), $b = 13\cdot505$ (9), $c = 14\cdot119$ (22) Å, $\beta = 115\cdot8$ (2)°, $U = 2969\cdot6$ Å^3, $D_m = 1\cdot67$ (by flotation), $D_c = 1\cdot645$ Mg m^{-3}, $Z = 8$, $F(000) = 1512$, $\mu(Cu\,K\alpha) = 2\cdot37$ mm^{-1}. Systematic absences: $0k0$ when $k = 2n + 1$ and $h0l$ when $l = 2n + 1$; space group $P2_1/c$.

Cell parameters were determined from oscillation photographs with Cu $K\alpha$ radiation. With the Weissenberg equi-inclination technique 5323 non-zero reflexions were recorded on layers 0–3kl, h0–3l and hk0–4. Their intensities were read visually and corrected for Lorentz and polarization effects but not for absorption or extinction. The observed structure factor amplitudes were placed on a common scale by internal correlation to yield a data set of 3112 unique reflexions.

Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All calcula-

tions were carried out on a Univac 1106 computer with programs written by FSS.

Structure determination

The structure was solved by the heavy-atom method. Isotropic refinement was by full-matrix least squares in which the function minimized was $\sum w\Delta^2$. Weights, initially unity, in the final cycles were given by

Table 1. *Final atomic coordinates (fractional, $\times 10^4$) for non-hydrogen atoms, with e.s.d.'s in parentheses, and equivalent isotropic thermal parameters* (Å^2)

	x	y	z	U_{eq}*
Cu(1)	172 (1)	1323 (1)	1678 (1)	0·149
O(W1)	−690 (4)	1632 (5)	2561 (6)	0·159
O(11)	1734 (4)	3674 (4)	2844 (7)	0·161
O(12)	1206 (4)	−1423 (4)	2211 (6)	0·141
N(111)	−265 (5)	2677 (5)	978 (6)	0·133
N(121)	−589 (4)	171 (5)	830 (6)	0·130
N(11)	1167 (5)	2103 (5)	2525 (5)	0·127
N(12)	961 (4)	253 (5)	2281 (7)	0·130
C(11)	1902 (6)	1602 (7)	3331 (9)	0·165
C(12)	1839 (6)	484 (7)	3047 (9)	0·146
C(111)	308 (6)	3402 (6)	1516 (8)	0·127
C(112)	92 (6)	4384 (6)	1278 (9)	0·149
C(113)	−715 (7)	4637 (8)	501 (10)	0·175
C(114)	−1278 (8)	3918 (8)	−46 (10)	0·176
C(115)	−1021 (6)	2930 (8)	212 (9)	0·170
C(121)	−164 (6)	−712 (7)	1092 (8)	0·145
C(122)	−526 (6)	−1574 (7)	605 (9)	0·134
C(123)	−1379 (7)	−1573 (8)	−183 (9)	0·166
C(124)	−1819 (6)	−680 (8)	−434 (8)	0·155
C(125)	−1411 (6)	158 (7)	95 (8)	0·147
C(011)	1145 (5)	3070 (6)	2374 (8)	0·120
C(012)	756 (5)	−646 (6)	1940 (8)	0·124
Cu(2)	4926 (1)	3911 (1)	3178 (1)	0·146
O(W2)	5834 (4)	4243 (5)	2402 (7)	0·164
O(21)	3260 (4)	6206 (5)	2265 (6)	0·159
O(22)	3806 (4)	1226 (5)	2717 (6)	0·156
N(211)	5328 (4)	5221 (5)	3994 (6)	0·119
N(221)	5660 (5)	2757 (5)	4031 (7)	0·139
N(21)	3939 (5)	4714 (5)	2351 (7)	0·138
N(22)	4138 (5)	2850 (5)	2539 (7)	0·141
C(21)	3221 (7)	4214 (7)	1508 (10)	0·175
C(22)	3264 (6)	3110 (7)	1792 (8)	0·146
C(211)	4713 (5)	5950 (6)	3532 (7)	0·121
C(212)	4870 (6)	6931 (7)	3871 (9)	0·109
C(213)	5667 (7)	7154 (7)	4716 (9)	0·130
C(214)	6262 (7)	6432 (8)	5186 (9)	0·176
C(215)	6061 (6)	5454 (7)	4794 (9)	0·149
C(221)	5200 (6)	1897 (6)	3814 (8)	0·141
C(222)	5501 (7)	1036 (7)	4362 (9)	0·158
C(223)	6337 (7)	1047 (8)	5215 (9)	0·171
C(224)	6823 (6)	1919 (9)	5412 (9)	0·172
C(225)	6474 (6)	2743 (7)	4810 (9)	0·164
C(021)	3899 (6)	5606 (7)	2636 (8)	0·141
C(022)	4284 (6)	1965 (7)	2934 (8)	0·141
O(W3)	−2203 (4)	607 (5)	1753 (6)	0·173
O(W4)	7340 (4)	3160 (5)	3153 (6)	0·163

* $U_{eq} = (U_1 U_2 U_3)^{1/3}$.

$w = (15\cdot0 + 0\cdot5|F_o| + 0\cdot011|F_o|^2)^{-1}$. Reflexions for which $|F_o| < 0\cdot33|F_c|$ were omitted from the refinement. Positions for H atoms on the pyridine rings were calculated with C—H $= 1\cdot0$ Å. A difference synthesis was used to locate the methylene H atoms and those of the water molecules. All H atoms were assigned thermal parameters $B = 6\cdot0$ Å^2 and were not refined.

With the large number of variable parameters (416) block matrices were used during anisotropic refinement. The three matrices contained (1) the overall scale and thermal factors and the parameters for (2) the first and (3) the second chelate molecules. Refinement was terminated when the maximum shift in any parameter was $<0\cdot1\sigma$. 3103 reflexions were included in the final cycle. A final difference synthesis showed maximum positive electron densities of $1\cdot3$ e Å^{-3} associated with the Cu atoms. R, based on 3112 reflexions, was $0\cdot099$ and $R'[=(\sum w\varDelta^2/\sum w|F_o|^2)^{1/2}]$ was $0\cdot128$. Atomic coordinates are given in Table 1.*

Discussion

The structure contains two chelate molecules of very similar stereochemistries which are nonetheless crystallographically distinct. A drawing of each molecule, with the atom labelling, is given in Fig. 1

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* Lists of structure factors, hydrogen atom coordinates and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35629 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths (Å) and angles (°) with e.s.d.'s in parentheses*

	m − 1		m − 2	
Cu(m)-O(Wm)	2·361 (8)		2·317 (8)	
C(m1)-C(m2)	1·553 (13)		1·536 (13)	

	n − 1	n − 2	n − 1	n − 2
Cu(m)· N(mn)	1·926 (7)	1·914 (7)	1·928 (7)	1·911 (7)
Cu(m)-N(mn1)	2·060 (7)	2·052 (7)	2·059 (7)	2·040 (7)
N(mn1)-C(mn1)	1·365 (10)	1·365 (11)	1·386 (10)	1·365 (11)
N(mn1)-C(mn5)	1·327 (11)	1·346 (11)	1·317 (11)	1·357 (11)
N(mn) C(Omn)	1·321 (11)	1·297 (11)	1·282 (12)	1·296 (11)
N(mn)-C(mn)	1·452 (11)	1·464 (11)	1·457 (12)	1·459 (11)
O(mn)-C(Omn)	1·247 (11)	1·263 (10)	1·284 (10)	1·247 (11)
C(mn1)-C(Omn)	1·496 (11)	1·521 (11)	1·499 (11)	1·531 (12)
C(mn1)-C(mn2)	1·379 (11)	1·358 (12)	1·395 (12)	1·368 (13)
C(mn2)-C(mn3)	1·390 (14)	1·408 (13)	1·407 (14)	1·423 (14)
C(mn3)-C(mn4)	1·353 (16)	1·387 (15)	1·362 (15)	1·403 (16)
C(mn4) C(mn5)	1·404 (14)	1·371 (14)	1·416 (13)	1·370 (14)

	m = 1		m = 2	
N(m11)-Cu(m)-N(m21)	112·7 (3)		110·8 (3)	
N(m1)-Cu(m)-N(m2)	82·3 (3)		82·8 (3)	
N(m1)·C(m1)-C(m2)	108·2 (6)		108·0 (8)	
N(m2)· C(m2)-C(m1)	109·4 (7)		109·8 (6)	

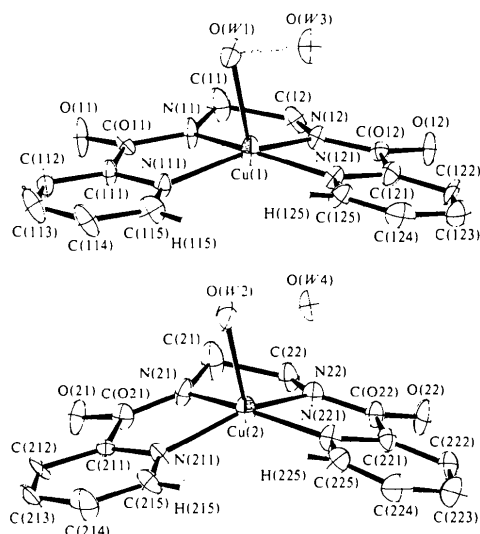|	n − 1	n − 2	n − 1	n − 2
O(Wm) Cu(m) N(mn)	100·1 (3)	113·0 (3)	102·1 (3)	114·4 (3)
O(Wm)-Cu(m)-N(mn1)	84·9 (3)	92·9 (3)	88·0 (3)	92·9 (3)
N(m11)- Cu(m)-N(mn)	81·6 (3)	157·7 (3)	81·4 (3)	154·9 (3)
N(m21)-Cu(m)-N(mn)	161·6 (3)	80·7 (3)	161·2 (3)	80·7 (3)
Cu(m)-N(mn1)-C(mn1)	110·2 (3)	111·8 (3)	110·1 (3)	111·5 (3)
Cu(m)-N(mn1)-C(mn5)	130·1 (5)	130·8 (5)	130·5 (5)	130·4 (5)
C(mn1)-N(mn1)-C(mn5)	119·2 (4)	117·4 (5)	119·3 (4)	117·9 (5)
Cu(m)··N(mn)-C(Omn)	119·1 (4)	121·0 (3)	119·5 (5)	121·6 (4)
Cu(m)-N(mn)-C(mn)	118·2 (6)	118·5 (5)	116·6 (6)	117·5 (5)
O(mn)-C(Omn)-C(mn1)	120·8 (8)	119·0 (7)	118·3 (8)	119·4 (8)
N(mn1)-C(mn1)-C(Omn)	116·5 (6)	114·6 (6)	115·1 (6)	115·2 (7)
N(mn1) C(mn1)-C(mn2)	120·0 (6)	122·5 (7)	121·2 (7)	123·7 (7)
C(Omn)-N(mn) ·C(mn)	122·7 (7)	120·1 (5)	123·3 (8)	118·6 (5)
O(mn) -C(Omn)-N(mn)	127·0 (8)	129·3 (7)	128·3 (8)	130·4 (7)
N(mn)-C(Omn)-C(mn1)	112·2 (8)	111·7 (7)	113·4 (8)	110·1 (8)
C(Omn)-C(mn1)-C(mn2)	123·4 (8)	122·9 (8)	123·7 (8)	121·0 (8)
C(mn1)-C(mn2)-C(mn3)	120·1 (8)	119·5 (8)	117·8 (8)	117·7 (8)
C(mn2)-C(mn3)-C(mn4)	120·0 (8)	118·2 (7)	120·9 (7)	119·3 (8)
C(mn3)-C(mn4)-C(mn5)	117·8 (8)	119·0 (7)	118·1 (7)	119·6 (8)
C(mn4)-C(mn5)-N(mn1)	122·9 (8)	123·4 (8)	122·6 (8)	122·3 (8)

Fig. 1. Perspective drawings of the two molecular formula units (Johnson, 1965) and the labelling of the atoms. H atoms other than those in the 6 positions of the pyridyl rings have been omitted for clarity. Thermal ellipsoids of non-hydrogen atoms are scaled to include 50% probability.

(Johnson, 1965). Bond lengths and angles are given in Table 2.

In each molecule the ligand has an approximately planar N$_4$ arrangement quadridentate to the Cu atom with a water molecule occupying the apex of a distorted square pyramid. The dimensions of each Cu coordination sphere are in accord with those of the related [Cu(pdp)(H$_2$O)] (Chapman, Stephens & Vagg, 1980). In the present structure the Cu—O lengths [2·361 (8) and 2·317 (8) Å] are significantly longer than the 2·286 (2) Å in the benzene-substituted analogue, whilst the Cu—N(amide) and Cu—N(pyridine) lengths agree well in both structures. The Cu atoms are 0·22 and 0·28 Å above the two N$_4$ planes (Table 3, planes 1 and 9), again similar to [Cu(pdp)H$_2$O].

The closest approaches to the metal atoms in what would constitute octahedral coordination are 3·55 (1) Å for Cu(1) by C(122) at $(\bar{x}, \bar{y}, \bar{z})$, and 3·73 (1) Å for Cu(2) by C(214) at $(1 - x, 1 - y, 1 - z)$. Both values lie outside the sum of the van der Waals radii (Huheey, 1978). In each molecule only one

Table 3. *Least-squares planes*

Least-squares planes and their equations given by $lX' + mY' + nZ' - p = 0$, where X', Y' and Z' are orthogonal coordinates related to the atomic coordinates X, Y and Z by $X' = X\sin\beta$, $Y' = Y$ and $Z' = Z + X\cos\beta$. Deviations (Å) of relevant atoms from the planes are given in square brackets ($\sigma = 0.005$–0.012 Å).

	l	m	n	p
Plane (1): N(11), N(12), N(111), N(121)				
	−0.3886	0.0364	0.9207	1.7995

[N(11) 0.071; N(12) −0.070; N(111) −0.051; N(121) 0.051; Cu(1) 0.22]

Plane (2): N(11), N(12), C(11), C(12)				
	−0.3786	−0.0670	0.9232	1.6581

[N(11) −0.06; N(12) 0.06; C(11) 0.09; C(12) −0.09; Cu(1) 0.19; C(O11) −0.31; C(O12) −0.04; N(111) −0.28; N(121) 0.16]

Plane (3): N(111), C(111)–C(115)				
	−0.3747	0.0173	0.9270	1.6692

[N(111) 0.014; C(111), C(114) <|0.001|; C(112) −0.012; C(113) 0.012; C(115) −0.014; Cu(1) 0.34; C(O11) 0.04]

Plane (4): N(121), C(121)–C(125)				
	−0.3255	−0.1649	0.9311	1.7818

[N(121) −0.018; C(121) 0.011; C(122), C(012) <|0.001|; C(123) −0.04; C(124) −0.002; C(125) 0.013; Cu(1) −0.08]

Plane (5): N(111), N(11), C(111), C(O11)				
	−0.4037	0.1002	0.9094	1.9799

[N(111) −0.013; N(11) 0.013; C(111) 0.022; C(O11) −0.022; Cu(1) 0.13; O(11) −0.11]

Plane (6): N(121), N(12), C(121), C(O12)				
	−0.3291	−0.1531	0.9318	1.7760

[N(121) −0.005; N(12) 0.005; C(121) 0.008; C(O12) −0.008; Cu(1) −0.05; O(12) −0.04]

Plane (7): C(111), N(11), O(11)				
	−0.3558	0.1379	0.9243	2.2268

[C(O11) 0.010; Cu(1) −0.005; N(111) −0.12; C(11) 0.04]

Plane (8): C(121), N(12), O(12)				
	−0.3157	−0.1698	0.9335	1.7994

[C(O12) 0.003; Cu(1) −0.096; N(121) −0.04; C(12) −0.09]

Plane (9): N(21), N(22), N(211), N(221)				
	0.4325	0.0811	−0.8980	2.7685

[N(21) 0.086; N(22) −0.088; N(211) −0.065; N(221) 0.066; Cu(2) 0.28]

Plane (10): N(21), N(22), C(21), C(22)				
	0.3945	−0.0503	−0.9175	1.8497

[N(21) −0.07; N(22) 0.07; C(21) 0.12; C(22) −0.12; Cu(2) 0.20; C(O21) −0.55; C(O22) −0.19; N(211) −0.42; N(221) 0.13]

Plane (11): N(211), C(211)–C(215)				
	0.3903	0.1828	−0.9024	3.0511

[N(211) 0.013; C(211) −0.011; C(212) 0.002; C(213) 0.006; C(214) −0.004; C(215), C(O21) −0.005; Cu(2) 0.21]

Table 3 (*cont.*)

	l	m	n	p
Plane (12): N(221), C(221)–C(225)				
	0.3656	−0.2791	−0.8879	0.9399

[N(221), C(223) −0.021; C(221) 0.005; C(222), C(225) 0.016; C(224) 0.006; Cu(2) −0.30; C(O22) −0.05]

Plane (13): N(211), N(21), C(211), C(O21)				
	0.4019	0.2833	−0.8708	3.9414

[N(211) −0.021; N(21) 0.023; C(211) 0.037; C(O21) −0.039; Cu(2) −0.035; O(21) 0.17]

Plane (14): N(221), N(22), C(221), C(O22)				
	0.3462	−0.2585	−0.9019	0.8102

[N(221) −0.006; N(22) 0.006; C(221) 0.010; C(O22) −0.010; Cu(2) −0.22; O(22) −0.057]

Plane (15): C(211), N(21), O(21)				
	0.3221	0.3404	−0.8834	3.8838

[C(O21) 0.007; Cu(2) −0.25; N(211) −0.19; C(21) −0.016]

Plane (16): C(221), N(22), O(22)				
	0.3257	−0.2823	−0.9024	0.5921

[C(O22) 0.008; Cu(2) −0.28; N(221) −0.057; C(22) −0.18]

Angles (°) between selected planes ($\sigma = 0.3$–$1.0°$)

Planes		Planes	
(1), (2):	6.4	(9), (10):	7.9
(1), (3):	1.4	(9), (11):	6.3
(1), (4):	12.1	(9), (12):	21.1
(3), (4):	10.8	(11), (12):	26.8

of the two amide five-membered chelate rings is planar, the other showing the Cu atom to deviate significantly from that plane (Table 3, planes, 5, 6, 13 and 14). The central en chelate rings of each molecule (planes 2 and 10) are necessarily non-planar.

The lattice and coordinated water molecules are involved in hydrogen bonding with the amide O atoms of neighbouring chelate molecules. Details are given in Table 4. As a result, the molecules pack in a series of planes parallel to ($10\bar{1}$) with the hydrogen-bonding network linking these planes (Fig. 2). Again this structural arrangement is similar to that for [Cu(pdp)(H$_2$O)]. An interesting aspect of this packing mode is the pseudo-body-centred relationship between molecule (1) and the second molecule at $(1 - x, 1 - y, 1 - z)$. This was evident in the Patterson synthesis by a vector at $0.5, 0.5, 0.5$ which was one-third of the intensity of the origin peak. Considering the closely similar geometries of both molecules, the fact that the compound does not crystallize in a body-centred space group implies either that this is prohibited by packing forces such as the hydrogen bonding, or that there is a real difference in the molecular structures of the two isomers. The bonding dimensions (Table 2) show few dissimilarities between the two molecules.

Table 4. *Proposed hydrogen bonds* (Å)

Donor–acceptor distances are given with e.s.d.'s in parentheses.

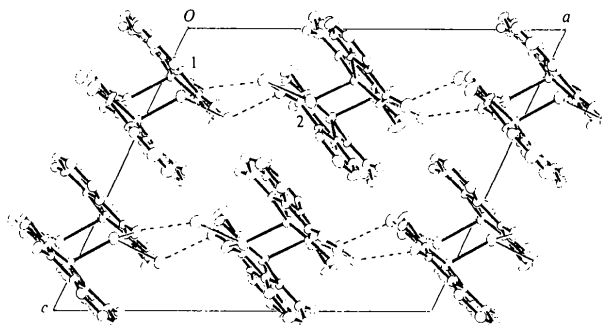|	Acceptor at	
O(W1)–H(W11)···O(12)	($\bar{x}, \frac{1}{2} + y, \frac{1}{2} - z$)	2·836 (9)
O(W1) H(W12)···O(W3)	(x,y,z)	2·732 (9)
O(W2)–H(W21)···O(22)	($1 - x, \frac{1}{2} + y, \frac{1}{2} - z$)	2·770 (9)
O(W2)–H(W22)···O(W4)	(x,y,z)	2·765 (9)
O(W3)–H(W31)···O(11)	($x, y - \frac{1}{2}, \frac{1}{2} - z$)	2·718 (10)
O(W3)–H(W32)···O(21)	($x, y - \frac{1}{2}, \frac{1}{2} - z$)	2·851 (10)
O(W4)–H(W41)···O(12)	($1 - x, \frac{1}{2} + y, \frac{1}{2} - z$)	2·836 (10)
O(W4)–H(W42)···O(21)	($1 - x, y - \frac{1}{2}, \frac{1}{2} - z$)	2·801 (10)

Fig. 2. The packing of the molecules showing the hydrogen-bonding network. Broken lines indicate that one of the atoms involved in the bond is from a molecule in the next cell along b. The two primary molecules in the asymmetric unit are numbered accordingly.

Fig. 2 shows that the quadridentate ligand in molecule (1) is more nearly planar than in molecule (2). This observation is confirmed by the angles between selected planes in each molecule (Table 3). In particular, the pyridine rings (planes 3 and 4) in molecule (1), with a dihedral angle of 10·8°, twist in the same direction relative to the N_4 coordination plane (plane 1). However, in the second molecule the pyridine rings (planes 11 and 12), which make a dihedral angle of 26·8°, are rotated both to a greater extent and in opposite directions. The effect is shown in the slightly larger O(W)–Cu–N angles in the second molecule (Table 2). The unequal rotation of the two pyridyl groups in each molecule (1·4 and 12·1°; 6·3 and 21·1°) signifies a distortion towards a trigonal-bipyramidal geometry at the Cu atoms, as in [Cu(pdp)(H$_2$O)] (Chapman, Stephens & Vagg, 1980). In that structure steric interaction of the two H atoms in the 6 positions of the pyridyl rings (H···H = 1·98 Å) was seen as the cause of this distortion. In [Cu(edp)(H$_2$O)].H$_2$O the more flexible central ethylene link in the ligand allows a greater separation of these H atoms [H(115)···H(125) = 2·27, H(215)···H(225) = 2·24 Å] resulting in a less planar function of the ligand. This steric effect has been noticed previously in complexes of related ligands (Bailey, McKenzie & Mullins, 1970; Gibson & McKenzie, 1971).

The reason for the structural variance in the two molecules is not readily evident. The differences observed would appear to be greater than those expected from packing effects alone. However, an explanation may lie in the ability of Cu^{II} to adopt a variety of distorted five-coordinate stereochemistries which in this case may result from the hydrogen-bonding requirements in the crystal.

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