Finally, it is interesting to note that the {SOP-(OEt)$_2$} ligand always adopts a bridging position to form an Mo$_2$OSP five-membered ring (Lu, Huang, Huang & Lu, 1984; Lu, Huang, Lin & Huang, 1987). We are unaware of any examples of {SOP(OEt)$_2$} chelating to an Mo atom to form an MoSOP four-membered ring. This leads us to believe that the [Mo$_3$S$_4${μ-SOP(OEt)$_2$}$_3$.L$_3$] cluster compound may be stable.

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Structure of *catena*-Bis[μ-chloro-chloro-μ-quinoxaline-*N*,*N'*-copper(II)]

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Abstract. [Cu(C$_8$H$_6$N$_2$)Cl$_2$]$_n$, $M_r = 264.60$, monoclinic, $C2/m$, $a = 13.237$ (5), $b = 6.935$ (3), $c = 9.775$ (3) Å, $\beta = 107.88$ (2)°, $V = 853.9$ (5) Å^3, $Z = 4$, $D_m = 2.01$ (2), $D_x = 2.06$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, μ(Mo $K\alpha$) = 30.0 cm^{-1}, $F(000) = 524$, $T = 295$ K, final $R = 0.025$ for 979 unique reflections. The polymeric structure is composed of double chains in which quinoxaline molecules form bridges between Cu atoms along the b axis and the two chains are bound together by two Cl atoms. The coordination polyhedron about the Cu atom is a trigonal bipyramid with three Cl atoms in the equatorial plane with the quinoxaline N atoms occupying the apical positions.

Introduction. Quinoxaline, like other nitrogen heterocycles with two N atoms in the molecule, has a tendency to form polymeric structures in which quinoxaline forms a bridge between two metal atoms (Lumme, Lindroos & Lindell, 1987; Richardson, Hatfield, Stoklosa & Wasson, 1973).

The metal-bridging capabilities of pyrazine, which quinoxaline chemically resembles, have been well studied (Santoro, Mighell & Reimann, 1970; Darriet, Haddad, Duesler & Hendrickson, 1979; Havnes, Rettig, Sams, Thompson & Trotter, 1987). Unlike pyrazine only a few structures of quinoxaline metal complexes have been determined. To learn more about the coordination behaviour of polymeric quinoxaline (= Q) compounds, we have determined the structure of Cu(Q)Cl$_2$, the results of which we present here.

Experimental. Quinoxaline (0.5 mmol) in ethanol (100 cm^3) was added to CuCl$_2$.2H$_2$O (0.5 mmol) in ethanol (100 cm^3). The mixture was carefully heated (at ~ 313 K) for 6 h and allowed to stand for several weeks. The green crystals that formed were filtered and washed successively with ethanol and ether. The crystal selected for data collection had dimensions 0.2 × 0.2 × 0.4 mm. The density was determined by flotation. The unit-cell parameters were determined by a least-squares fit of the setting angles of 25 reflections with $13.2 \leq 2\theta \leq 27.7°$, measured on a Nicolet *P3F* diffractometer. The intensity measurements were carried out at room temperature (295 K) with graphite-monochromatized Mo $K\alpha$ radiation and the ω–2θ scan technique. The scan rate varied from 2.0 to 29.3° min^{-1}.

A set of 1056 unique reflections was obtained from 1113 reflections measured in the range $3 \leq 2\theta \leq 55°$ (h 0→19, k 0→11, l −14→14). 979 reflections with $F_o > 4\sigma(F_o)$ were considered as observed and used in refinement. Three strong reflections (133, 204 and

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal factors* (Å^2) *with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i{}^*a_j{}^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Cu	0·04175 (3)	0	0·34227 (3)	0·0212 (2)
Cl(1)	−0·12463 (5)	0	0·37025 (7)	0·0252 (3)
Cl(2)	0·18073 (6)	0	0·25847 (8)	0·0314 (4)
N(1)	0·0393 (1)	0·2978 (3)	0·3308 (2)	0·0220 (8)
C(1)	0·1050 (2)	0·3987 (3)	0·4342 (2)	0·0256 (10)
C(2)	−0·1518 (2)	0·3991 (3)	−0·0202 (2)	0·0272 (10)
C(3)	−0·0911 (2)	0·2994 (3)	0·0961 (2)	0·0272 (9)
C(4)	−0·0261 (1)	0·3975 (3)	0·2170 (2)	0·0208 (9)
H(1)	0·153 (2)	0·336 (5)	0·512 (3)	
H(2)	−0·191 (2)	0·328 (4)	−0·102 (3)	
H(3)	−0·093 (2)	0·162 (5)	0·100 (3)	

Table 2 *Bond distances* (Å) *and angles* (°)

The coordination sphere of copper

Cu—Cl(1)	2·300 (2)	Cl(1)—Cu—Cl(2)	166·04 (3)
Cu—Cl(1ⁱⁱ)	2·685 (1)	Cl(1)—Cu—Cl(1ⁱⁱ)	88·53 (4)
Cu—Cl(2)	2·232 (2)	Cl(1)—Cu—N(1)	90·41 (4)
Cu—N(1)	2·068 (2)	Cl(2)—Cu—N(1)	88·89 (5)
Cu—N(1ⁱ)	2·068 (2)	Cl(1ⁱⁱ)—Cu—N(1)	92·95 (5)
Cu···Cuⁱⁱ	3·580 (1)	N(1)—Cu—N(1ⁱ)	174·07 (8)
		Cu—Cl(1)—Cuⁱⁱ	91·47 (4)

The quinoxaline molecule

N(1)—C(1)	1·314 (3)	C(1)—N(1)—C(4)	117·4 (2)
C(1)—C(1ⁱ)	1·405 (3)	N(1)—C(1)—C(1ⁱ)	122·2 (2)
N(1)—C(4)	1·369 (2)	N(1)—C(4)—C(3)	120·6 (2)
C(4)—C(4ⁱ)	1·420 (3)	N(1)—C(4)—C(4ⁱ)	120·4 (2)
C(3)—C(4)	1·406 (3)	C(2)—C(3)—C(4)	120·5 (2)
C(2)—C(3)	1·362 (3)	C(3)—C(2)—C(2ⁱ)	120·5 (2)
C(2)—C(2ⁱ)	1·399 (3)		
C(1)—H(1)	0·94 (3)		
C(2)—H(2)	0·95 (3)		
C(3)—H(3)	0·95 (3)		

Symmetry code: (i) $x, -y, z$; (ii) $-x, -y, 1 - z$.

51̄5) monitored periodically during data collection exhibited no significant intensity variation. The intensities were corrected for Lorentz and polarization effects and also for absorption by the ψ-scan technique. The transmission factor varied from 1·000 to 0·788.

The space group (monoclinic $C2/m$, No. 12) was established on the basis of both the systematic absences (hkl, $h + k = 2n + 1$) and the structure analysis. The structure was solved by direct methods and subsequent $\Delta\rho$ maps using programs *SHELXS86* (Sheldrick, 1986) and *SHELX76* (Sheldrick, 1976) on a VAX 8650 computer. Least-squares planes were calculated with *MPLN* (Truter & Vickery, 1973). The atomic scattering factors were as supplied in *SHELX76*, and for Cu from Cromer & Mann (1968). The non-H atoms were refined anisotropically by least squares (on F) with U fixed to 0·05 Å^2 for the H atoms; convergence occurred at R = 0·025 and wR = 0·034, where $w = 2·4853/[\sigma^2(F_o) + 0·000171(F_o{}^2)]$; 73 parameters were refined. After the last cycle, maximum and minimum Δ/σ were

± 0·001. The maximum and minimum peaks in the final $\Delta\rho$ map were +0·54 and −0·63 e Å^{-3}, respectively.

Discussion. The atomic coordinates and equivalent isotropic thermal parameters for the non-H atoms are listed in Table 1.* The bond lengths and angles are listed in Table 2. The *ORTEP* drawing (Johnson, 1965) in Fig. 1 shows the environment of the Cu atom. The coordination polyhedron around the Cu atom is a trigonal bipyramid with three Cl atoms forming the equatorial plane and N atoms of the two quinoxaline molecules the apices of the bipyramid. The Cu atom has two strong bonds to atoms Cl(1) and Cl(2) and one weaker bond of 2·685 (1) Å to Cl(1ⁱⁱ). The coordination polyhedron is similar to that in triaquabis(quinoxaline)copper(II) perchlorate
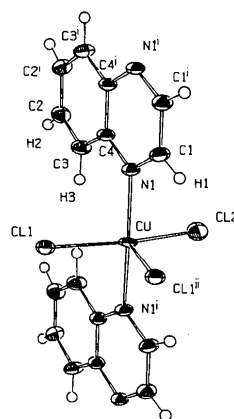
Fig. 1. An *ORTEP* drawing showing the environment of the central metal atom with thermal ellipsoids at 50% probability.
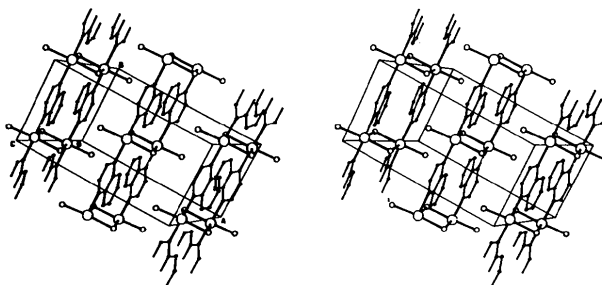

Fig. 2. Stereoview of the packing of the molecules as viewed along the c axis.

(Lumme, Lindroos & Lindell, 1988), where the equatorial plane consists of three O atoms, and one of the Cu—O bonds is distinctly longer. The asymmetry of the equatorial plane is due to the steric effect of the large quinoxaline molecules.

The title compound has an infinite double-chain structure in which quinoxaline molecules form bridges between Cu atoms along the b axis. Two such chains are linked together with two Cl atoms, so that the distance between the Cu atoms in different chains is 3·580 (1) Å (Fig. 2). The Cu—Cu distance is similar to dimeric chloro-bridged structures (Marsh, Hatfield & Hodgson, 1982; Klein, Stevens, O'Connor, Majeste & Trefonas, 1983). Two hydrogen bonds connect the double chains to each other in the direction of the a and c axes, and there is a further hydrogen bond in the direction of the chain.

The aromatic ring of the quinoxaline molecule is planar, the maximum deviation from the least-squares plane being 0·008 (3) Å for C(3). The heterocyclic ring exhibits a slight boat conformation with the N atoms −0·026 (2) Å from the least-squares plane. The C atoms are coplanar [deviations 0·013 (2) and 0·012 (2) Å for C(1) and C(4) respectively]. The aromatic and heterocyclic rings are slightly tilted toward each other, so that the quinoxaline molecule has an open-book form. The dihedral angle is 4·9 (5)°. The bond lengths and angles in the quinoxaline molecule are similar to those measured in other structures (Lumme, Lindroos & Lindell,

1987, 1988; Padmaja, Ramakumar & Viswamitra, 1987; Lipkowski, Andreetti & Sgarabotto, 1977).

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Structure of Bis(3,4-hexanedione dioximato)bis(thiourea)copper(II)

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Abstract. [Cu(C$_6$H$_{11}$N$_2$O$_2$)$_2$(CH$_4$N$_2$S)$_2$], M_r = 502·11, monoclinic, $C2/c$, a = 15·065 (4), b = 10·216 (3), c = 15·513 (4) Å, β = 103·86 (2)°, V = 2318·0 (11) Å^3, Z = 4, D_m = 1·43, D_x = 1·44 g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ = 32·77 cm^{-1}, F(000) = 1052, room temperature, R = 0·034, wR = 0·037 for 985 reflections with $I \geq 3\sigma(I)$. The structure consists of centro-symmetric monomeric molecules [Cu(hd)$_2$(tu)$_2$] (hd = 3,4-hexanedione dioximate anion, tu = thiourea). The coordination polyhedron of copper(II) is a square bipyramid with four dioxime N atoms in the equatorial plane and two thiourea S atoms in axial positions, in contrast with the pentacoordinate copper dioxime complexes reported so far.