The bonds between Cd and bridging thiocyanato are essentially identical, to within experimental accuracy, to those found in the literature (Cavalca, Nardelli & Fava, 1960; Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1972; Haasnoot, de Keyzer & Verschoor, 1983). A significant difference is found in the Cd—N(2) bond which is much longer (2·53 Å) in the ethylenethiourea complex (Cavalca, Nardelli & Fava, 1960). The Cd—N(2) distance is shorter than the Cd—N(1) distance [2·340 (8) vs 2·415 (8) Å], as found in other polymeric Cd compounds (Haasnoot, de Keyzer & Verschoor, 1983). The Cd—N(2)—C(3) angle is 164·3 (8)°.

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Structures of catena-Di-μ-chloro- and catena-Di-μ-bromo-(2,2-bipyridine)copper(II)

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Abstract. (I) $[CuCl_2(C_{10}H_8N_2)]_\infty$, $M_r = 290.63$, triclinic, $P\bar{1}$, $a = 7.288$ (2), $b = 9.640$ (2), $c = 9.771$ (2) Å, $\alpha = 55.36$ (3), $\beta = 69.29$ (2), $\gamma = 70.48$ (3)°, $V = 520$ (1) Å^3, $Z = 2$, $D_x = 1.855$ Mg m^{-3}, $\lambda(Mo K\alpha) = 0.71073$ Å, $\mu = 2.585$ mm^{-1}, $F(000) = 290$, $T = 291$ K, $R = 0.0425$ for 1450 unique observed reflections. The crystal consists of alternating spaced chains, oriented along the x axis. The coordination polyhedron around the Cu atom can be described as a distorted octahedron. The basal plane is formed by the two N atoms of the 2,2'-bipyridine ligand and two Cl atoms. The axial sites are occupied by Cl atoms from the other monomeric units. Cu—N(1) = 2·029 (3), Cu—N(2) = 2·027 (3), Cu—Cl(1) = 2·267 (1), Cu—Cl(2) = 2·267 (1), Cu—Cl(1^i) = 3·035 (1), Cu—Cl(2^{ii}) = 3·106 (1), Cu—Cu^i = 3·876 (1) and Cu—Cu^{ii} = 3·802 (1) Å. (II) [CuBr$_2$-($C_{10}H_8N_2$)]$_\infty$, $M_r = 379.55$, monoclinic, $C2/c$, $a = 16.966$ (4), $b = 9.287$ (2), $c = 7.490$ (2) Å, $\beta = 111.60$ (2)°, $V = 1097$ (2) Å^3, $Z = 4$, $D_x = 2.297$ Mg m^{-3}, $\lambda(Mo K\alpha) = 0.71073$ Å, $\mu = 9.117$ mm^{-1}, $F(000) = 724$, $T = 291$ K, $R = 0.0716$ for 708 unique observed reflections. The crystal consists of alternating spaced chains along the z axis. The coordination polyhedron around the Cu atom can be described as a distorted octahedron. The basal plane is formed by the two N atoms of the 2,2'-bipyridine ligand and two Br atoms. The axial sites are occupied by Br atoms from the other monomeric units. Cu—N(1) = 2·030 (6), Cu—Br(1) = 2·410 (1), Cu—Br(1$''$) = 3·175 (1), Cu—Cu$''$ = 3·974 (1) Å.

Introduction. As far as their structure is concerned, copper(II) compounds display a rich variety of

geometries. This is due to a great number of coordination polyhedra, related to the possibility of distortion of the coordination sphere around the Cu atom. These plasticity properties are due to the Jahn–Teller effect.

Copper(II) complexes of formula Cu(NN)X_2 are known to have different geometries with coordination numbers of four, five and six (X = Cl, Br). For example, [CuBr$_2$(maep)]$_2$ [maep = 2-(2-methylaminoethyl)pyridine] has been shown to be a pentacoordinated species with a trigonal bipyramidal geometry at the copper ion (Wilson, Hatfield & Hodgson, 1976), while [CuBr$_2$(dpm)]$_2$ (dpm = di-2-pyridylmethane) is better described as a distorted square pyramid (Garland, Grandjean, Spodine & Manzur, 1987). [CuCl$_2$(py)$_2$]$_\infty$ is a linear polymer, where the copper ion completes its octahedral coordination sphere by binding to chloride ions from adjacent molecules (Jeter & Hatfield, 1972). Doubly substituted pyridine or thiazole blocks more bonding sites and leads to four-coordinate copper monomers (Landee & Greeney, 1986).

The present work describes the structure of two polymeric complexes, [CuCl$_2$(bpy)]$_\infty$ and [CuBr$_2$(bpy)]$_\infty$ (bpy = 2,2'-bipyridine).

Experimental. The complexes were prepared by addition of 1 mmol of anhydrous CuBr$_2$ or CuCl$_2$ to a degassed solution containing 1 mmol of ligand in freshly distilled methanol. The resultant solution was refluxed under N$_2$. When the reaction mixture was cooled a microcrystalline solid was obtained. The complexes were recrystallized from dimethylacetamide (chloride complex) and a dimethylacetamide–acetonitrile mixture (bromide complex).

Crystal dimensions: in (I) 0·10 × 0·22 × 0·30 mm, in (II) 0·15 × 0·22 × 0·25 mm. Nonius CAD-4 κ-geometry diffractometer, cell dimensions calculated by least-squares refinement on setting angles of 25 reflections with 9·96 ≤ 2θ ≤ 24·0° for (I) and 10·74 ≤ 2θ ≤ 25·0° for (II); 1951 integrated reflections for (I) and 1043 for (II) collected up to (sinθ)/λ = 0·595 Å^{-1}; ω–2θ scan technique, scan width (1·0 + 0·35tanθ)°, 0 ≤ h ≤ 8, −10 ≤ k ≤ 11, −10 ≤ l ≤ 11 for (I) and 0 ≤ h ≤ 20, 0 ≤ k ≤ 10, −8 ≤ l ≤ 7 for (II); (I) 2·7% and (II) 0·5% decay in intensities of three standard reflections during 29 h (I) and 15 h (II) of irradiation; no absorption correction and no time decay corrections applied; (I) 1830 unique reflections after averaging (R_{int} = 0·013) and (II) 957 unique reflections after averaging (R_{int} = 0·026); (I) 1450 and (II) 708 with F^2 > 3σ(F^2); structure solution by $MULTAN$80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); refined by full-matrix least squares based on F_o, weights based on counting statistics: 1/w = σ^2(F) = $\frac{1}{4}$[σ^2(I) + (0·04I)^2]/I for (I) and 1/w = σ^2(F) = $\frac{1}{4}$[σ^2(I) + (0·08I)^2]/I for (II) (Stout & Jensen, 1968); atomic scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974); H atoms

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

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j.$$

	x	y	z	B_{eq}
[CuCl$_2$(C$_{10}$H$_8$N$_2$)]				
Cu	0·75485 (9)	0·06697 (6)	0·93296 (6)	2·92 (1)
Cl(1)	0·9541 (2)	−0·1934 (1)	1·0210 (1)	3·78 (3)
Cl(2)	0·5455 (2)	−0·0202 (1)	1·1917 (1)	3·82 (3)
N(1)	0·9056 (5)	0·1643 (4)	0·6872 (4)	2·73 (9)
N(2)	0·6085 (5)	0·3123 (4)	0·8323 (4)	2·69 (9)
C(1)	0·8379 (6)	0·3288 (5)	0·5819 (5)	2·6 (1)
C(2)	0·9161 (7)	0·4096 (6)	0·4086 (5)	3·7 (1)
C(3)	1·0643 (8)	0·3198 (7)	0·3424 (6)	4·5 (2)
C(4)	1·1364 (8)	0·1524 (6)	0·4497 (6)	4·2 (1)
C(5)	1·0549 (8)	0·0781 (5)	0·6210 (5)	3·6 (1)
C(6)	0·4605 (8)	0·3802 (6)	0·9173 (5)	3·7 (1)
C(7)	0·3773 (8)	0·5514 (6)	0·8388 (6)	4·2 (1)
C(8)	0·4459 (8)	0·6549 (6)	0·6701 (7)	4·4 (2)
C(9)	0·5951 (7)	0·5859 (6)	0·5803 (6)	3·7 (1)
C(10)	0·6739 (6)	0·4144 (5)	0·6656 (5)	2·6 (1)
[CuBr$_2$(C$_{10}$H$_8$N$_2$)]				
Br(1)	0·90825 (8)	−0·1095 (1)	0·0491 (2)	3·33 (3)
Cu	1·000	−0·0726 (2)	0·250	2·64 (4)
N(1)	0·9270 (5)	0·240 (1)	0·106 (1)	2·2 (2)
C(1)	0·8534 (7)	0·234 (1)	−0·038 (2)	3·5 (3)
C(2)	0·8050 (8)	0·350 (2)	−0·124 (2)	4·7 (3)
C(3)	0·8370 (9)	0·484 (2)	−0·056 (2)	4·9 (3)
C(4)	0·9147 (8)	0·495 (1)	0·092 (2)	3·7 (3)
C(5)	0·9587 (7)	0·370 (1)	0·170 (1)	2·7 (2)

placed at idealized positions with C—H distances of 0·95 Å and with fixed thermal parameters [4·0 Å^2 for (I) and 4·5 Å^2 for (II)] and not refined; anisotropic thermal parameters for all other atoms; refinement converged to R = 0·0425, wR = 0·0573, goodness of fit S = 1·947 for 137 refined parameters for (I) and R = 0·0716, wR = 0·0897, goodness of fit S = 1·999 for 70 refined parameters for (II); largest shift to e.s.d. in last cycle 0·01 for (I) and 0·01 for (II); largest residual peak in difference Fourier map 1·26 and 0·76 e Å^{-3} for (I) and (II) respectively. All computer programs from the Enraf–Nonius *SDP* described by Frenz (1978).

We consider that the high R value for (II) is due to the absorption of the Br atom, because no intensity correction was made.

Discussion. Table 1 lists the fractional atomic coordinates of non-H atoms, Table 2 bond lengths and angles.* The crystal can be described as consisting of linear polymers. The structure of the monomeric units is illustrated in Fig. 1, which also shows the atomic numbering scheme. When the interatomic contacts to neighbouring formula units are considered, the geometry about the Cu atom is distorted tetragonal. The coordination octahedron is defined by two N atoms

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44714 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Intramolecular bond lengths* (Å) *and bond angles* (°) *and selected intermolecular bond lengths* (Å) *with e.s.d.'s in parentheses*

[CuCl₂(C₁₀H₈N₂)]

Cu–Cl(1)	2·267 (1)	N(2)–C(10)	1·338 (4)
Cu–Cl(2)	2·267 (1)	C(1)–C(2)	1·384 (5)
Cu–Cl(1ⁱ)	3·035 (1)	C(1)–C(10)	1·481 (4)
Cu–Cl(2ⁱⁱ)	3·106 (1)	C(2)–C(3)	1·360 (6)
Cu–Cuⁱ	3·876 (1)	C(3)–C(4)	1·371 (6)
Cu–Cuⁱⁱ	3·802 (1)	C(4)–C(5)	1·373 (5)
Cu–N(1)	2·079 (3)	C(6)–C(7)	1·379 (5)
Cu–N(2)	2·027 (2)	C(8)–C(9)	1·378 (6)
N(1)–C(1)	1·341 (4)	C(9)–C(10)	1·376 (5)
N(1)–C(5)	1·342 (4)	C(7)–C(8)	1·358 (6)
N(2)–C(6)	1·339 (4)		

N(1)–Cu–N(2)	80·0 (1)	N(1)–Cu–N(2)	80·0 (1)
Cl(1)–Cu–Cl(2)	92·71 (3)	Cu–N(1)–C(1)	115·0 (2)
N(1)–Cu–Cl(1)	93·82 (8)	Cu–N(1)–C(5)	126·5 (2)
N(1)–Cu–Cl(2)	171·57 (8)	C(1)–N(1)–C(5)	118·4 (3)
Cl(1)–Cu–N(2)	172·60 (8)	Cu–N(2)–C(6)	126·3 (2)
Cl(1)–Cu–Cl(1ⁱ)	89·57 (3)	Cu–N(2)–C(10)	115·2 (2)
Cl(1ⁱ)–Cu–N(2)	85·94 (8)	C(6)–N(2)–C(10)	118·4 (3)
Cl(1ⁱ)–Cu–N(1)	85·76 (8)	N(1)–C(1)–C(2)	121·7 (3)
N(2)–Cu–Cl(2)	93·83 (8)	N(1)–C(1)–C(10)	114·8 (3)
Cl(1ⁱ)–Cu–Cl(2)	99·62 (3)	C(2)–C(1)–C(10)	123·5 (3)
Cl(2ⁱⁱ)–Cu–Cl(2)	89·05 (3)	C(1)–C(2)–C(3)	119·4 (3)
Cl(2ⁱⁱ)–Cu–N(1)	84·55 (8)	C(2)–C(3)–C(4)	119·2 (3)
Cl(2ⁱⁱ)–Cu–N(2)	83·33 (8)	C(3)–C(4)–C(5)	119·3 (3)
Cl(2ⁱⁱ)–Cu–Cl(1ⁱ)	166·63 (3)	N(1)–C(5)–C(4)	122·0 (3)
Cl(2ⁱⁱ)–Cu–Cl(1)	100·24 (3)	N(2)–C(6)–C(7)	122·0 (3)
Cuⁱ–Cu–Cuⁱⁱ	143·3 (2)		

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

[CuBr₂(C₁₀H₈N₂)]

Cu–Br(1)	2·410 (1)	N(1)–C(5)	1·332 (11)
Cu–Br(1″)	3·175 (1)	C(1)–C(2)	1·362 (14)
Cu–Cu″	3·974 (1)	C(2)–C(3)	1·38 (2)
Cu–N(1)	2·030 (6)	C(3)–C(4)	1·380 (14)
N(1)–C(1)	1·316 (11)	C(4)–C(5)	1·390 (13)

Br(1)–Cu–Br(1′)	91·02 (6)	Cu–N(1)–C(1)	127·6 (6)
Br(1)–Cu–N(1)	94·45 (18)	Cu–N(1)–C(5)	114·3 (5)
N(1)–Cu–N(1′)	80·22 (36)	C(1)–N(1)–C(5)	118·0 (7)
Br(1″)–Cu–N(1)	86·14 (17)	N(1)–C(1)–C(2)	125·1 (9)
Br(1″)–Cu–Br(1)	98·32 (3)	C(1)–C(2)–C(3)	117·0 (1)
Br(1″)–Cu–Br(1′)	90·36 (3)	C(2)–C(3)–C(4)	119·3 (9)
Br(1″)–Cu–N(1′)	84·41 (17)	C(3)–C(4)–C(5)	118·9 (9)
Cu″–Cu–Cu‴	140·38 (57)	N(1)–C(5)–C(4)	121·5 (8)
Br(1)–Cu–N(1′)	173·87 (18)		

Symmetry operations: (′) $-x+1, y, \frac{1}{2}-z$; (″) $x, -y, \frac{1}{2}+z$; (‴) $x, -y, -z$.

provided by the 2,2′-bipyridine and by four Cl or Br atoms, two of which link the monomeric units between them. Each Cl or Br atom has a short distance to a Cu atom and a long distance to a vicinal Cu atom. A view of the alternating spaced chain is shown in Fig. 2.

The basal plane around each Cu atom is formed by the two *cis* N atoms from the 2,2′-bipyridine and two *cis* Cl or Br atoms, while the apical positions are occupied by halogen atoms from other monomeric units. The Cu atom in (II) is placed on the 2_1 axis, so the primed positions are generated by symmetry. Cu–N(1) = 2·029 (3), Cu–N(2) = 2·027 (3), Cu–Cl(1) = 2·267 (1), Cu–Cl(2) = 2·267 (1), Cu–Cl(1ⁱ) = 3·035 (1), Cu–Cl(2ⁱⁱ) = 3·106 (1) Å for (I), and Cu–N(1) = 2·030 (6), Cu–Br(1) = 2·410 (1), Cu–Br(1″) = 3·175 (1) Å for (II).

The C–N bonds are comparable with those found in (2,2′-bipyridine)salicylaldehydatocopper(II) perchlorate (Garland, Le Marouille & Spodine, 1986). The

C–N bonds of the 2,2′-bipyridine molecule range from 1·316 (11) to 1·332 (11) Å for the bromo complex, and from 1·335 (4) to 1·343 (5) Å for the chloro complex. The same bonds in the mixed copper(II) complexes have values between 1·339 (5) and 1·357 (5) Å. The same is observed for the C–C bond lengths. All the pyridine rings are planar.

The two long axial distances for (I) are Cu–Cl(1ⁱ) = 3·036 (1) and Cu–Cl(2ⁱⁱ) = 3·106 (1) Å, while for (II) Cu–Br(1″) = Cu–Br(1‴) = 3·175 (1) Å. These are shorter than the axial distance found for the alternately spaced linear chain compound, *catena*-dichloro(3,6-dithiooctane)copper(II), $R_0 = 3·234$ (1) Å (Olmstead, Musker, ter Haar & Hatfield, 1982). The long bridging bond distance for di-μ-chloro-copper(II)

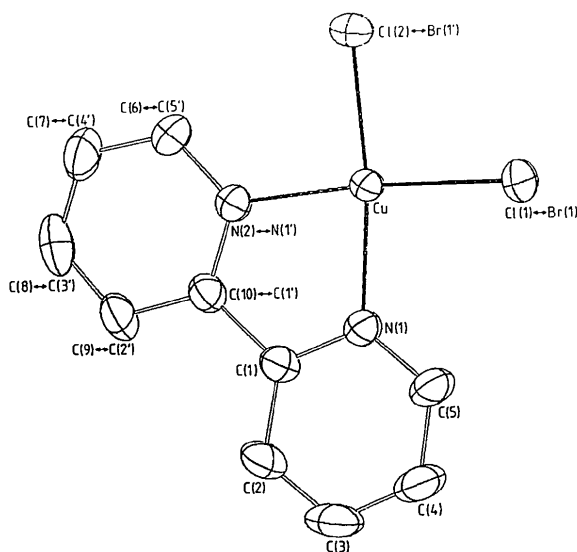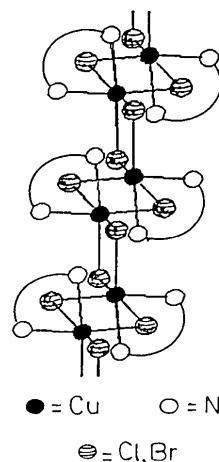Fig. 1. A perspective view of the halogenated monomeric molecule with H atoms excluded for clarity.

● = Cu   ○ = N

⊖ = Cl,Br

Fig. 2. A schematic view of the halogenated polymeric molecule.

uniform chain compounds has values in the 2·75–3·21 Å range (Hatfield, 1985). For di-μ-chloro-copper(II) dimers this same distance is 2·45–3·02 Å. The values reported for di-μ-bromo-copper(II) dimers are between 2·80 and 3·87 Å (Hatfield, 1985; Garland et al., 1987).

The Cu—Cu distance in the two Cu_2Cl_2 planar units of (I) are 3·802 (1) and 3·876 (1) Å, and 3·974 (1) Å for the Cu_2Br_2 planar units of (II). The Cu atoms form an angle of 143·31 (2)° in the chain along the x axis of (I) and an angle of 140·38 (7)° in the chain along the z axis of (II). The dihedral angles between the two alternating planar units of (I) and (II) are 89·1 and 89·8° respectively.

The unweighted mean plane through the four donor atoms N(1), N(1'), Br(1) and Br(1') shows a lack of planarity with displacements of −0·062, 0·062, 0·047 and −0·047 Å respectively. The Cu atom is placed on this plane, while the two apical Br atoms, Br(1'') and Br(1''') are symmetrically located from this plane at a distance of 3·157 Å.

In the case of the homologous plane for the chloro complex, the displacements of N(1), N(2), Cl(1) and Cl(2) donor atoms are 0·095, −0·095, −0·076 and 0·076 Å respectively. The Cu atom is displaced by 0·017 from this plane in the direction of the apical Cl(1^i). The two apical Cl(1^i) and Cl(2^{ii}) are at a distance of 3·027 and 3·052 Å from this plane.

The dihedral angle between the planes through Cu, N(1) and N(1') and Cu, Br(1), Br(1') is 4·3° for compound (II), and the homologous planes for compound (I) form a dihedral angle of 6·9°. This indicates no tendency to tetrahedrality.

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(Dioxane)dineopentylmagnesium: a Polymeric Structure

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Abstract. catena-Poly[(dineopentylmagnesium)-μ-(dioxane-O:O')], [Mg(C_5H_{11})$_2$($C_4H_8O_2$)], $M_r = 254\cdot71$, monoclinic, $C2/c$, $a = 17\cdot040$ (4), $b = 9\cdot362$ (1), $c = 10\cdot833$ (5) Å, $\beta = 98\cdot64$ (2)°, $V = 1708\cdot6$ Å^3, $Z = 4$, $D_x = 0\cdot990$ Mg m^{-3}, $\lambda(Mo\,K\alpha) = 0\cdot71073$ Å, $\mu = 0\cdot091$ mm^{-1}, $F(000) = 568$, $T = 293$ (1) K, $R = 0\cdot042$ for 1213 observed reflections with $I > 3\sigma(I)$. The structure has dineopentylmagnesium units linked through dioxanes (having chair conformations) to form polymeric chains that run parallel to the z axis. An Mg atom is bonded in an approximately tetrahedral fashion to two O atoms [Mg—O 2·132 (1) Å], one from each of two dioxane molecules, and to two neopentyl C atoms [Mg—C 2·133 (2) Å] with an unusually large C—Mg—C angle [139·95 (9)°].

Introduction. The title compound has been isolated on several occasions in our laboratory from reaction mixtures in which dioxane was an accidental and only minor component. The usual preparation of