octahedral angle, obviously imposed by the Fe—N distances and the rather rigid bipyridyl conformation. In similar complexes the same 'deviation' in bonding angles has been observed, as for instance in $[\text{phenH}]^+[\text{Fe(phen)Cl}_4]^-$, where an angle of 75·0° is found (Veidis, Witten, Reiff, Garafalo & Brennan, 1981), and in two copper(II)–bipyridyl complexes where the Cu—N distances are shorter than the Fe—N distances in our compound and consequently the N—Cu—N angle is somewhat larger (80°) (Harrison, Hathaway & Kennedy, 1979). All Cl—Fe—Cl angles are about 96°. The Cl^- ions, in a *fac* arrangement, occupy more space than they would have in the case of a regular octahedral coordination of the iron(III) ion.

The bipyridyl ligand is planar to within ± 0·05 Å. The triazole ligand is also planar; all triazole atoms lie within 0·01 Å of the least-squares plane. The least-squares planes through the bipyridyl and triazole ligands are mutually perpendicular, intersecting at an angle of 91·05 (8)°.

The triazole ligand is coordinated through its N(4) atom. The only other examples containing monodentate N(4)-bonded triazole are $\text{Mn(Htrz)(H}_2\text{O)}_4\text{(SO}_4)$ (Gorter & Engelfriet, 1981) and $\text{Cd(NCS)}_2\text{(Htrz)}_2$ (Haasnoot, de Keyzer & Verschoor, 1983). For the first compound this was considered to be unusual and due to hydrogen bonding of H(N1) to the anion. The second compound showed intermolecular N(1)—H to N(2′) hydrogen bridges. However, in our case hydrogen bonding does not occur, as distances from the parent nitrogen atom [N(31)] to the nearest Cl^- ions or N atoms in neighbouring molecules are larger than 3·3 Å. This implies that coordination through N(4) is independent of hydrogen-bond formation by H(N1), and should not be considered unusual.

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Structure of 2-Amino-4,5-dihydro-3H^+-1,3-thiazolium Trichlorocadmate(II), $\text{C}_3\text{H}_7\text{N}_2\text{S}^+.\text{CdCl}_3^-$

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Abstract. $M_r = 321{\cdot}9$, monoclinic, $P2_1/c$, $a = 14{\cdot}438\ (5)$, $b = 3{\cdot}922\ (2)$, $c = 20{\cdot}952\ (7)$ Å, $\beta = 131{\cdot}72\ (5)^\circ$, $U = 885{\cdot}6$ Å^3, $Z = 4$, $D_m = 2{\cdot}40\ (3)$, $D_x = 2{\cdot}41$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 3{\cdot}50$ mm^{-1}, $F(000) = 616$, room temperature, final $R = 0{\cdot}029$ for 2064 reflections. The polymeric structure consists of ATH^+ and CdCl_3^- anions. The Cd atoms are octahedrally coordinated and linked into infinite chains by double Cl bridges. Two such chains running parallel to each other are themselves linked by Cd—Cl bonds. There is no direct bonding between the metal atom and the organic molecule; each ATH^+ cation is associated with $(\text{CdCl}_3^-)_n$ chains through hydrogen bonds involving all of the H atoms attached to N atoms.

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Introduction. 2-Amino-4,5-dihydro-1,3-thiazole (ATH), the potential inducer of the reverse transformation of tumour cells (Brugarolas & Gosálvez, 1982), contains three donor sites capable of interacting with metal ions *i.e.* amine and heterocyclic N atoms and S.

Our recent studies on the Cu^{II}–ATH system have shown that the heterocyclic N atom, which is a protonation site in the ligand hydrochloride, seems to be the only available binding site for Cu^{2+} ions (Głowiak, Kubiak, Tatarowski, Kozłowski & Gosálvez, 1983). At low pH, which could favour Cu–S bond formation (Kozłowski & Kowalik, 1978), the ligand molecule does not form any direct binding with the metal ion.

To check the possibilities of metal—sulphur bond formation by ATH we have studied also the interaction of Cd^{II} with this ligand and the X-ray structure of such a system is presented here.

Experimental. Clear, colourless crystal from equimolar amounts of cadmium(II) acetate and ATH.HCl at room temperature, dimensions 0·12 × 0·10 × 0·15 mm; density measured in a mixture of $CHBr_3$ and $CHCl_3$; monoclinic from Weissenberg photographs, $P2_1/c$; Syntex $P2_1$ computer-controlled four-circle diffractometer, scintillation counter, graphite monochromator; cell parameters by least squares from setting angles of 15 reflections; 2064 independent reflections; variable θ–2θ scan, scan rate 2·0–29·3° min^{-1} (depending on intensity), $2\theta \leq 65{\cdot}0°$; two standards measured every 30 reflections, no significant change; corrected for Lorentz and polarization, not for absorption; 2064 with $I > 1{\cdot}96\sigma(I)$ used for structure determination, index range h 0→16, k 0→5, l –24→22; calculations performed on a NOVA 1200 computer with programs supplied by Syntex (1976); neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); heavy-atom method, full-matrix least squares (on F); difference synthesis revealed H atoms; non-H atoms refined with anisotropic and H atoms with isotropic temperature factors, 119 variables; $(\Delta/\sigma)_{max}$ 0·1; $(\Delta\rho)_{max}$ 0·3 e Å^{-3}; R = 0·029, R_w = 0·042, S = 4·10, $w = 1/\sigma^2(F)$; no correction for secondary extinction.

Discussion. Final atomic parameters are given in Table 1* and interatomic distances and angles in Table 2. Fig. 1 shows a fragment of the crystal structure viewed along **b** and indicates the numbering system used.

The asymmetric unit consists of a $CdCl_3^-$ anion and an ATH^+ cation. The structure is polymeric. The Cd atoms are separated by one unit-cell translation along **b** and are linked by double Cl bridges forming an infinite –Cd–Cl_2–Cd– ribbon perpendicular to the *ac* plane. A second such chain, generated by the 2_1 axis, runs parallel to the first and is linked to it by Cd—Cl bonds, similar to the polymeric di-μ-chloro-imidazole-cadmium(II) (Nassimbeni & Rodgers, 1976). The octahedral coordination of Cd is completed by a terminal Cd—Cl bond, perpendicular to the –Cd–Cl_2–Cd– plane.

The Cd···Cd separations of adjacent octahedra are 3·922 (2) Å (along **b**) and 4·115 (1) (related by the 2_1 axis). These distances are considerably longer than the values of about 3·36 Å in the linear chain structure of $[(CH_3)_4N][CdCl_3]$ (Morosin, 1972) and similar to those found in ammonium cadmium chloride (Rolies & De Ranter, 1978) and di-μ-chloro-imidazole-cadmium(II) (Nassimbeni & Rodgers, 1976).

The Cd—Cl bond lengths are comparable with values found in related complexes. Cl(1) is bonded to three Cd atoms forming Cd—Cl bonds which are considerably longer than those involving Cl(2), which is bonded only to two Cd atoms. The distance between Cd and Cl(1) of the same asymmetric unit is 2·657 (2) Å. The linkage between adjacent chains occurs by the bonds Cl(1)—Cd($-x, \frac{1}{2}+y, \frac{1}{2}-z$) and Cl(1)—Cd($-x, -\frac{1}{2}+y, \frac{1}{2}-z$) with distances 2·742 (1) and 2·822 (1) Å, respectively (Table 2). Cl(2) is bonded to two Cd atoms and lies at 2·593 (1) and 2·621 (1) Å from Cd and Cd($x, 1+y, z$), respectively. The terminal Cl(3) atom is involved in the shortest Cd—Cl bond of 2·466 (2) Å.

The ATH^+ molecule does not participate in coordination to the metal atom, but forms ionic and hydrogen-bonded contacts with the $CdCl_3^-$ ion.

All bond distances and angles within the ATH^+ cation fall in the expected range. The C(1)—N(1) distance of 1·283 (10) Å is shorter than the C(1)—N(2) and C(2)—N(2) bonds, 1·336 (9) and 1·459 (10) Å, respectively. The similarity of the exocyclic C(1)—N(1) distance to the C(1)—N(2) value and the shortening of the C(1)—S bond in comparison to the C(3)—S distance indicates considerable electron delocalization in the N_{exo}–CS–N_{endo} moiety. This distribution of bond lengths is in good agreement with values obtained from the structure determinations of ATH.HCl (Vedavathi & Vijayan, 1981) and $(ATH)_2CuCl_4$ (Głowiak *et al.*, 1983).

The dihydrothiazole ring is not planar,* with methylene C atoms situated on opposite sides of the NCSN plane at 0·215 (6) and –0·322 (6) Å. The atoms H(1), H(2) and HN(2) lie in the NCSN plane. This conformation is different from that of ATH.HCl, where the dihydrothiazole ring has an envelope-like conformation, similar to those found in $(ATH)_2CuCl_4$.

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles involving H atoms, least-squares-planes' calculations and hydrogen-bond parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38738 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* See deposition footnote.

Table 1. *Fractional coordinates and isotropic temperature factors* (Å^2)

For non-hydrogen atoms $B_{eq} = \frac{1}{3}\sum B_{ii}$.

	x	y	z	B_{eq}/B_{iso}
Cd	0·12026 (3)	0·29287 (8)	0·24491 (2)	1·79 (2)
Cl(1)	−0·1209 (1)	0·2784 (3)	0·1606 (1)	1·62 (6)
Cl(2)	0·0812 (1)	−0·2024 (3)	0·1475 (1)	1·82 (6)
Cl(3)	0·3491 (1)	0·2873 (3)	0·3493 (1)	2·21 (7)
S	0·4291 (1)	0·4390 (4)	0·1603 (1)	2·04 (7)
N(1)	0·3990 (5)	0·2742 (15)	0·0247 (3)	3·2 (4)
N(2)	0·2276 (4)	0·2500 (12)	0·0136 (2)	2·0 (3)
C(1)	0·3475 (4)	0·3052 (13)	0·0560 (3)	1·8 (3)
C(2)	0·1857 (5)	0·3575 (16)	0·0575 (3)	2·5 (4)
C(3)	0·2975 (5)	0·3351 (15)	0·1520 (3)	2·5 (3)
H(1)	0·470 (7)	0·283 (20)	0·060 (5)	6·1 (21)
H(2)	0·364 (5)	0·215 (15)	−0·028 (4)	3·5 (13)
HN(2)	0·190 (6)	0·153 (17)	−0·032 (4)	3·2 (15)
H(21)	0·125 (4)	0·226 (11)	0·045 (3)	1·9 (7)
H(22)	0·151 (5)	0·564 (18)	0·037 (4)	2·6 (13)
H(31)	0·305 (5)	0·154 (16)	0·177 (4)	3·6 (14)
H(32)	0·297 (5)	0·511 (17)	0·184 (4)	3·6 (14)

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

Cd–Cl(1)	2·657 (2)	Cd···Cd^{i}	4·115 (1)
Cd–Cl(2)	2·593 (1)	Cd···Cd^{ii}	4·115 (1)
Cd–Cl(3)	2·466 (2)	Cd^{i}–Cd–Cd^{ii}	56·92 (1)
Cd–Cl(1^{ii})	2·822 (1)		
Cd–Cl(1^{i})	2·742 (1)		
Cd–Cl(2^{iii})	2·621 (1)		
Cl(1)–Cd–Cl(1^{i})	82·42 (4)	Cl(2)–Cd–Cl(2^{iii})	97·55 (4)
Cl(1)–Cd–Cl(1^{ii})	80·91 (4)	Cl(2)–Cd–Cl(1^{i})	169·36 (4)
Cl(1)–Cd–Cl(2)	87·64 (4)	Cl(2)–Cd–Cl(1^{ii})	85·06 (4)
Cl(1)–Cd–Cl(2^{ii})	89·50 (4)	Cl(1^{ii})–Cd–Cl(2^{iii})	169·97 (4)
Cl(1)–Cd–Cl(3)	168·14 (5)	Cl(1^{i})–Cd–Cl(1^{ii})	89·63 (4)
Cl(3)–Cd–Cl(1^{i})	90·39 (4)	Cl(1^{i})–Cd–Cl(2^{iii})	86·17 (4)
Cl(3)–Cd–Cl(1^{ii})	89·67 (4)	Cd–Cl(1)–Cd^{ii}	99·30 (4)
Cl(3)–Cd–Cl(2)	98·78 (5)	Cd–Cl(1)–Cd^{i}	97·32 (4)
Cl(3)–Cd–Cl(2^{iii})	99·46 (5)	Cd^{i}–Cl(1)–Cd^{ii}	89·63 (4)
		Cd–Cl(2)–Cd^{iii}	97·55 (5)
N(1)–C(1)	1·283 (10)	N(1)–C(1)–S	122·2 (5)
C(1)–S	1·735 (5)	N(1)–C(1)–N(2)	125·5 (6)
C(1)–N(2)	1·336 (9)	C(1)–N(2)–C(2)	115·6 (5)
N(2)–C(2)	1·459 (10)	N(2)–C(2)–C(3)	106·3 (5)
S–C(3)	1·836 (8)	C(1)–S–C(3)	91·2 (3)
C(2)–C(3)	1·511 (8)	S–C(3)–C(2)	104·2 (4)
		S–C(1)–N(2)	112·3 (4)

Symmetry code: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (iii) $x, 1+y, z$.

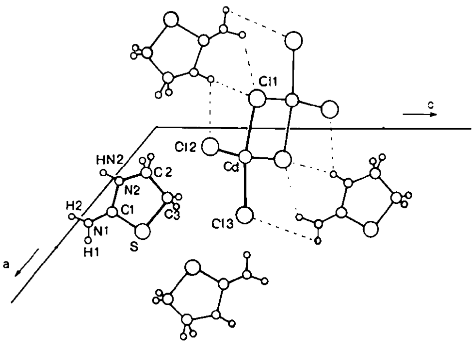

Fig. 1. A fragment of the crystal structure viewed along **b** showing the atom numbering.

N(2) in the heterocyclic ring is the protonation site, as has been observed earlier (Vedavathi & Vijayan, 1981; Głowiak *et al.*, 1983). Both N atoms make some significant short contacts with Cl atoms, which can be considered as hydrogen bonds.*

It is interesting to note that all H atoms bound to N and all Cl atoms are involved in hydrogen bonds of different strengths, with parameters in the ranges: $2 \cdot 4 < \mathrm{H} \cdots \mathrm{Cl} < 3 \cdot 3$ Å and $105 < \mathrm{N{-}H} \cdots \mathrm{Cl} < 165°$. The heterocyclic NH group is involved in hydrogen bonding to Cl(2) with HN(2)···Cl 2·94 (9) Å. Two weaker interactions involving the same NH group and two symmetry-related Cl(1) atoms at NH···Cl distances 2·75 (7) and 3·11 (7) Å are also present. These trifurcated N–H···Cl interactions have the net effect of 'completing the cage', similar to that described by Nassimbeni & Rodgers (1976) in polymeric di-μ-chloro-imidazolecadmium(II). A similar trifurcated N–H···Cl interaction is postulated for H(2).

One of the principal features of this crystal structure is the columnar packing along **b**. These columns are stabilized by the hydrogen-bond network involving HN(2) and H(2). The stability of the columns is further enhanced by the formation of a bifurcated hydrogen bond between H(1) and symmetry-related Cl(3) atoms. This network also connects the columnar stacks together and stabilizes the whole crystal structure.

S atoms, with short S···S contacts of 3·454 (2) Å, also play an important role in the molecular packing.

The results presented above indicate that also in the case of Cd, which is considered to be a softer acid than Cu, the heterocyclic S atom does not participate in the direct binding of the metal ion. Thus, in the proper pH range, the main binding site of metal ions such as Cu^{II}, Zn^{II} or Cd^{II} seems to be heterocyclic N only, as was suggested earlier (Głowiak *et al.*, 1983).

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* See deposition footnote.

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