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Bis(2-amino-4-chloromethylthiazolium) Tetrachlorocuprate at 200 and 100 K and Bis(2-amino-4-methylthiazolium) Tetrachlorocuprate at 100 K

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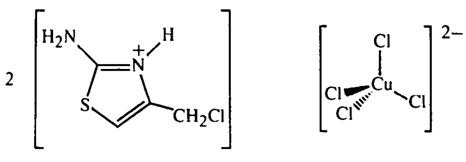
Abstract

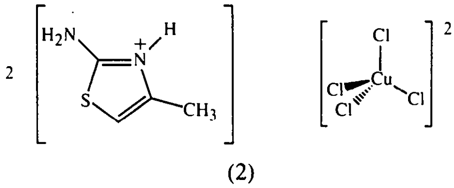
The title compounds, (C$_4$H$_6$ClN$_2$S)$_2$[CuCl$_4$] and (C$_4$H$_7$N$_2$S)$_2$[CuCl$_4$], show thermochromic properties. In both compounds, the thiazole ring is protonated at the N atom.

Comment

Thermochromism is often associated with temperature-dependent changes in the coordination geometry of the chromophore (Bloomquist & Willett, 1982; Sone & Fukuda, 1987). The title compounds, (1) and (2), are thermochromic coordination compounds; the thermochromism is expected to be caused by deformation of the [CuCl$_4$]$^{2-}$ group as a function of temperature. The crystals are amber at room temperature and yellow between 120 and 77 K. The colour change with temperature is a reversible process. In this paper we report the crystal structure of compound (1) at 200 and 100 K and compound (2) at 100 K.



(1)



(2)

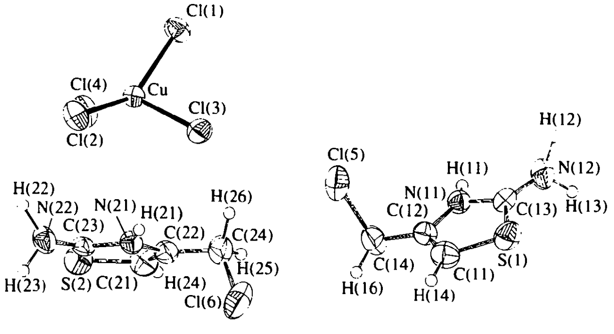


Fig. 1. *EUCLID* (Spek, 1982) plot of compound (1) at 200 K showing the atom-numbering scheme. The ellipsoids are drawn at 50% probability.

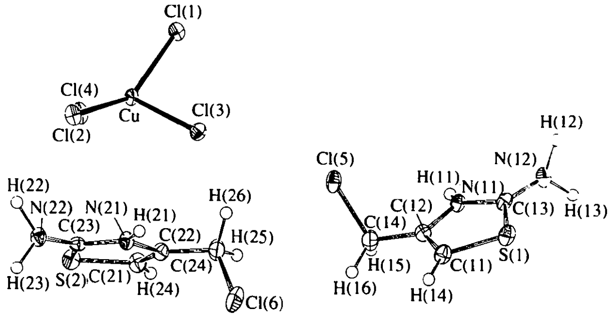


Fig. 2. *EUCLID* (Spek, 1982) plot of compound (1) at 100 K showing the atom-numbering scheme. The ellipsoids are drawn at 50% probability.

Comparison of the crystal structure of (2) at 100 K with that determined at 295 K (Fernández, Morán, Doadrio, Conradi, Willing & Müller, 1987) shows that the maximum angle difference in the anion is

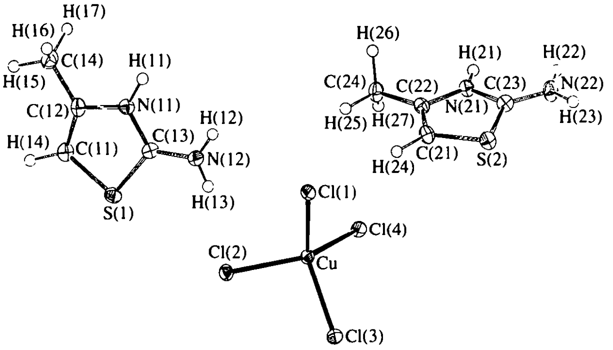


Fig. 3. *EUCLID* (Spek, 1982) plot of compound (2) at 100 K showing the atom-numbering scheme. The ellipsoids are drawn at 50% probability.

for the Cl(3)—Cu—Cl(1) angle. This angle, θ, is 130.6 (1)° at 295 K and 132.15 (4)° at 100 K. Similarly, in the crystal structures of (1) at 200 and 100 K, the greatest difference is for the Cl(2)—Cu—Cl(1) angle [θ = 142.24 (4) and 143.09 (4)° at 200 and 100 K, respectively]. Lowering the temperature results in a deformation of the tetrahedron around the Cu atom. Using the expression $\nu_{\max} = 144.5\theta - 9784\,\text{cm}^{-1}$ (from Harlow, Wells, Watt & Simonsen, 1975), it is possible to obtain the differences between the absorption maximum of the ligand field spectrum at the two temperatures:

θ (200 K) = 142.24 (4)° ($\nu_{\max} = 10769.7\,\text{cm}^{-1}$),
θ (100 K) = 143.09 (4)° ($\nu_{\max} = 10892.5\,\text{cm}^{-1}$),
$\Delta\nu = 122.8\,\text{cm}^{-1}$ for compound (1), and

θ (295 K) = 130.6 (1)° ($\nu_{\max} = 9087.7\,\text{cm}^{-1}$),
θ (100 K) = 132.15 (4)° ($\nu_{\max} = 9311.7\,\text{cm}^{-1}$),
$\Delta\nu = 224\,\text{cm}^{-1}$ for compound (2).

Based on these differences, the change of colour (amber–yellow) may be explained. These observed structural changes also confirm that thermochromism in this kind of coordination compound can be attributed to the changes in the coordination geometry of the Cu atom.

Experimental

Compound (1) was synthesized by reaction of a solution of 2-amino-4-chloromethylthiazole in a mixture of ethanol and hydrochloric acid (6*M*) with a solution of $CuCl_2.2H_2O$ in hydrochloric acid (6*M*) in a similar manner to that described by Fernández, Morán, Doadrio, Conradi, Willing & Müller (1987) for related compounds. Compound (2) was synthesized in a similar way. A solution of 3 g of $CuCl_2.2H_2O$ in 50 ml of hydrochloric acid (6*M*) was added with stirring to a solution of 3.6 g of 2-amino-4-methylthiazole in a 1:1 mixture of 50 ml of ethanol and hydrochloric acid (6 *M*). The mixture was heated gently until the total volume was reduced by half. The cold solution yielded many crystals after 24 h. These were filtered off, washed with ether and recrystallized from a 1:1 mixture of ethanol and hydrochloric acid (6 *M*).

Compound (1) at 200 K

Crystal data

$(C_4H_6ClN_2S)_2[CuCl_4]$
$M_r = 504.58$
Triclinic
$P\bar{1}$
$a = 8.233$ (2) Å
$b = 10.953$ (2) Å
$c = 11.636$ (7) Å
$\alpha = 63.85$ (3)°
$\beta = 80.76$ (2)°
$\gamma = 84.79$ (2)°
$V = 929.4$ (6) Å^3
$Z = 2$
$D_x = 1.803$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15$–$20°$
$\mu = 2.257$ mm^{-1}
$T = 200$ (2) K
Prismatic
0.21 × 0.15 × 0.12 mm
Amber

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.582$, $T_{\max} = 1.000$
5665 measured reflections
5417 independent reflections

4098 observed reflections [$I > 2\sigma(I)$]
$R_{\text{int}} = 0.010$
$\theta_{\max} = 29.97°$
$h = 0 \rightarrow 11$
$k = -15 \rightarrow 15$
$l = -15 \rightarrow 16$
3 standard reflections monitored every 200 reflections
intensity decay: 12%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0426$
$wR(F^2) = 0.1269$
$S = 1.247$
5417 reflections
197 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0892P)^2 + 0.0314P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.022$
$\Delta\rho_{\max} = 0.595$ e Å^{-3}
$\Delta\rho_{\min} = -1.086$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

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

	x	y	z	U_{eq}
Cu	0.29886 (3)	0.21857 (3)	0.69685 (3)	0.0348 (1)
Cl(1)	0.06357 (8)	0.10135 (6)	0.77644 (7)	0.0473 (2)
Cl(2)	0.43449 (8)	0.38281 (6)	0.70605 (7)	0.0499 (2)
Cl(3)	0.22969 (9)	0.34089 (7)	0.49880 (6)	0.0507 (2)
Cl(4)	0.47068 (9)	0.04776 (6)	0.79902 (8)	0.0548 (2)
Cl(5)	0.09986 (12)	0.23710 (8)	1.22579 (8)	0.0641 (2)
S(1)	−0.14784 (11)	0.42002 (7)	0.81560 (7)	0.0563 (2)
N(11)	−0.0939 (3)	0.2050 (2)	1.0124 (2)	0.0388 (4)
N(12)	−0.3332 (3)	0.1974 (3)	0.9309 (3)	0.0594 (7)
C(14)	0.1701 (4)	0.2372 (4)	1.0714 (4)	0.0638 (8)
C(12)	0.0388 (3)	0.2866 (3)	0.9879 (3)	0.0455 (6)
C(13)	−0.2015 (3)	0.2594 (2)	0.9282 (2)	0.0413 (5)
C(11)	0.0293 (4)	0.4057 (3)	0.8853 (3)	0.0562 (7)
Cl(6)	0.5742 (2)	0.36889 (12)	0.14253 (10)	0.0839 (3)
S(2)	0.84805 (10)	0.10028 (7)	0.53857 (8)	0.0549 (2)
N(21)	0.6586 (3)	0.2983 (2)	0.4284 (2)	0.0389 (4)
N(22)	0.8209 (3)	0.3360 (3)	0.5573 (3)	0.0535 (6)

C(24)	0.5090 (4)	0.2297 (4)	0.2970 (4)	0.0650 (9)
C(22)	0.6311 (3)	0.2016 (3)	0.3861 (3)	0.0452 (6)
C(23)	0.7726 (3)	0.2614 (2)	0.5073 (2)	0.0361 (5)
C(21)	0.7229 (4)	0.0901 (3)	0.4365 (3)	0.0553 (7)

Compound (1) at 100 K

Crystal data

$(C_4H_6ClN_2S)_2[CuCl_4]$
$M_r = 504.58$
Triclinic
$P\bar{1}$
$a = 8.168$ (2) Å
$b = 10.919$ (4) Å
$c = 11.437$ (8) Å
$\alpha = 64.24$ (5)°
$\beta = 80.03$ (3)°
$\gamma = 84.72$ (3)°
$V = 904.7$ (8) Å^3
$Z = 2$
$D_x = 1.852$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15$–20°
$\mu = 2.319$ mm^{-1}
$T = 100$ (2) K
Prismatic
0.21 × 0.15 × 0.12 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.875$, $T_{\max} = 1.000$
3417 measured reflections
3171 independent reflections

2751 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.015$
$\theta_{\max} = 24.97$°
$h = 0 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$
3 standard reflections monitored every 200 reflections
intensity decay: 12%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0283$
$wR(F^2) = 0.0797$
$S = 1.087$
3171 reflections
197 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 1.5174P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.861$
$\Delta\rho_{\max} = 0.764$ e Å^{-3}
$\Delta\rho_{\min} = -0.517$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

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

	x	y	z	$U_{\rm eq}$
Cu	0.29680 (4)	0.22133 (3)	0.69792 (3)	0.0137 (1)
Cl(1)	0.05996 (9)	0.10175 (7)	0.77786 (7)	0.0185 (2)
Cl(2)	0.43307 (9)	0.38650 (7)	0.70719 (7)	0.0193 (2)
Cl(3)	0.22812 (9)	0.34353 (7)	0.49761 (7)	0.0194 (2)
Cl(4)	0.46890 (9)	0.05073 (7)	0.80152 (7)	0.0208 (2)
Cl(5)	0.09662 (10)	0.23833 (7)	1.23378 (7)	0.0236 (2)
S(1)	−0.14561 (10)	0.42449 (7)	0.81731 (7)	0.0216 (2)
N(11)	−0.0938 (3)	0.2063 (3)	1.0144 (2)	0.0166 (5)
N(12)	−0.3323 (3)	0.2004 (3)	0.9295 (3)	0.0237 (6)
C(14)	0.1725 (4)	0.2382 (4)	1.0758 (3)	0.0258 (7)
C(12)	0.0402 (4)	0.2884 (3)	0.9907 (3)	0.0192 (6)
C(13)	−0.2007 (4)	0.2611 (3)	0.9290 (3)	0.0175 (6)
C(11)	0.0316 (4)	0.4089 (3)	0.8886 (3)	0.0215 (7)
Cl(6)	0.56993 (12)	0.36699 (9)	0.14419 (8)	0.0325 (2)
S(2)	0.84760 (10)	0.09628 (8)	0.54525 (8)	0.0209 (2)
N(21)	0.6575 (3)	0.2942 (3)	0.4327 (2)	0.0169 (5)
N(22)	0.8189 (3)	0.3358 (3)	0.5621 (3)	0.0212 (6)
C(24)	0.5086 (4)	0.2239 (4)	0.2997 (3)	0.0259 (7)
C(22)	0.6304 (4)	0.1964 (3)	0.3909 (3)	0.0193 (6)
C(23)	0.7709 (3)	0.2591 (3)	0.5128 (3)	0.0146 (6)
C(21)	0.7231 (4)	0.0847 (3)	0.4413 (3)	0.0226 (7)

Compound (2) at 100 K

Crystal data

$(C_4H_7N_2S)_2[CuCl_4]$
$M_r = 435.69$
Triclinic
$P\bar{1}$
$a = 7.750$ (3) Å
$b = 8.474$ (3) Å
$c = 13.683$ (7) Å
$\alpha = 104.49$ (4)°
$\beta = 100.02$ (3)°
$\gamma = 102.83$ (3)°
$V = 822.8$ (6) Å^3
$Z = 2$
$D_x = 1.759$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15$–20°
$\mu = 2.220$ mm^{-1}
$T = 100$ (2) K
Prismatic
0.14 × 0.12 × 0.12 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.735$, $T_{\max} = 0.989$
5716 measured reflections
2859 independent reflections

2323 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.029$
$\theta_{\max} = 24.93$°
$h = 0 \rightarrow 9$
$k = -10 \rightarrow 9$
$l = -16 \rightarrow 15$
3 standard reflections monitored every 200 reflections
intensity decay: 12%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0284$
$wR(F^2) = 0.0758$
$S = 1.128$
2859 reflections
204 parameters
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.495P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.092$
$\Delta\rho_{\max} = 0.599$ e Å^{-3}
$\Delta\rho_{\min} = -0.540$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

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

	x	y	z	$U_{\rm eq}$
Cu	0.04273 (5)	0.56510 (4)	0.73951 (3)	0.0152 (1)
Cl(1)	−0.24922 (9)	0.50663 (9)	0.65045 (5)	0.0174 (2)
Cl(2)	−0.01280 (9)	0.36141 (9)	0.81998 (5)	0.0193 (2)
Cl(3)	0.29126 (9)	0.51632 (9)	0.68978 (5)	0.0187 (2)
Cl(4)	0.12985 (10)	0.84939 (9)	0.78438 (5)	0.0189 (2)
S(1)	−0.33589 (10)	0.24912 (10)	0.98316 (6)	0.0196 (2)
N(11)	−0.6411 (3)	0.2974 (3)	0.9189 (2)	0.0162 (5)
N(12)	−0.4328 (4)	0.3620 (4)	0.8193 (2)	0.0200 (6)
C(11)	−0.5073 (4)	0.2096 (4)	1.0488 (2)	0.0211 (7)

C(12)	−0.6595 (4)	0.2406 (4)	1.0057 (2)	0.0183 (6)
C(13)	−0.4779 (4)	0.3091 (4)	0.8965 (2)	0.0161 (6)
C(14)	−0.8363 (4)	0.2231 (5)	1.0367 (3)	0.0252 (7)
S(2)	−0.23738 (10)	−0.10552 (9)	0.41566 (6)	0.0196 (2)
N(21)	−0.2679 (3)	0.1000 (3)	0.5770 (2)	0.0179 (5)
N(22)	−0.2005 (4)	0.2287 (4)	0.4495 (2)	0.0246 (6)
C(23)	−0.2328 (4)	0.0969 (4)	0.4842 (2)	0.0181 (6)
C(22)	−0.2976 (4)	−0.0548 (4)	0.5983 (2)	0.0176 (6)
C(21)	−0.2867 (4)	−0.1787 (4)	0.5187 (2)	0.0201 (6)
C(24)	−0.3348 (5)	−0.0652 (4)	0.7011 (2)	0.0240 (7)

Table 4. *Bond lengths (Å) and angles (°) for the $[CuCl_4]^{2-}$ anion in (1) and (2)*

	(1)		(2)	
	100 K	200 K	100 K	295 K*
Cu—Cl(1)	2.258 (1)	2.2552 (9)	2.256 (1)	2.257 (1)
Cu—Cl(2)	2.254 (1)	2.2513 (8)	2.272 (1)	2.235 (1)
Cu—Cl(3)	2.235 (2)	2.234 (2)	2.239 (1)	2.264 (1)
Cu—Cl(4)	2.242 (2)	2.239 (1)	2.243 (1)	2.234 (1)
Cl(2)—Cu—Cl(1)	143.09 (4)	142.24 (4)	95.31 (4)	95.6 (1)
Cl(3)—Cu—Cl(1)	94.70 (6)	94.99 (4)	132.15 (4)	130.6 (1)
Cl(3)—Cu—Cl(2)	96.88 (6)	97.04 (4)	98.66 (4)	98.8 (1)
Cl(4)—Cu—Cl(1)	97.12 (5)	97.61 (4)	101.28 (5)	101.7 (1)
Cl(4)—Cu—Cl(2)	96.02 (5)	95.99 (3)	137.64 (4)	137.1 (1)
Cl(3)—Cu—Cl(4)	140.23 (5)	139.66 (4)	98.40 (4)	99.0 (1)

* Data from Fernández *et al.* (1987) (modified atom-labelling scheme).

The diffractometer was equipped with a low-temperature device (Cosier & Glazer, 1986). Data were collected (*CAD*-4 *Software*; Enraf–Nonius, 1989) with profile analysis over all reflections (Lehmann & Larsen, 1974; Grant & Gabe, 1978). Cell refinement was performed using *CRYSDA* (Beurskens *et al.*, 1992) and data reduction was achieved using *DATAR* (local program). The structure was solved by Patterson methods using the *DIRDIF* (Beurskens *et al.*, 1992) phase-expansion procedure (*SHELXS*86; Sheldrick, 1990). Isotropic least-squares refinement was performed using a local version of *SHELX*76 (Sheldrick, 1976; Van der Maelen Uría, 1991). Refinement was completed using *SHELXL*93 (Sheldrick, 1993). For compound (1), the apparently anomalous difference between the transmission factors of the absorption corrections of the 100 and 200 K data sets is thought to arise from the nature of the refined absorption correction method. For compound (1) at 100 and 200 K, C—H and NH_2 (planar) H atoms were included using a riding model; the coordinates of N—H11/21 were refined freely. A common isotropic *U* was included for all H atoms. For compound (2), C—H H atoms were riding, while all N—H H atoms were refined freely; all H-atom displacement parameters were refined freely. Further geometrical calculations were made with *PARST* (Nardelli, 1983). Molecular graphics were produced using *EUCLID* (Spek, 1982) and *SHELXL*93 was used to to prepare the material for publication. All calculations were made at the University of Oviedo on VAX computers of the Scientific Computer Center and the X-ray group.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: JZ1065). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Disodium [*N*,*N*′-(1,3-Propanediyl)bis(oxamato-*N*,*O*)]cuprate(II) Hexahydrate

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Abstract

In order to obtain structural parameters for a comparison with polynuclear metal complexes derived from the $[Cu(C_7H_6N_2O_6)]^{2-}$ complex anion, the X-ray study of the title compound, $Na_2[Cu(C_7H_6N_2O_6)].6H_2O$, has been carried out. The molecular structure parameters are in agreement with the geometrical parameters of derived polynuclear complexes, in particular, with respect to the loss of planarity of the CuN_2O_2 moiety.

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