Thione Compounds of Copper and Silver: Tetrakis[1-methyl-2(1H)-pyridinethione-S]-copper(I) Tetrafluoroborate and Tetrakis-[1-methyl-2(1H)-pyridinethione-S]silver(I) Tetrafluoroborate

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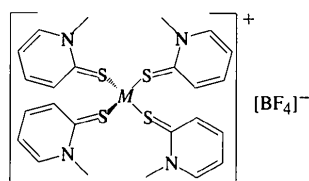*Inorganic Chemistry Laboratory, ETH, CH-8092 Zurich, Switzerland. E-mail: currao@inorg.chem.ethz.ch*

Abstract

The title compounds, $[Cu(C_6H_7NS)_4]BF_4$ and $[Ag(C_6H_7NS)_4]BF_4$, are both mononuclear complexes in which the central metal(I) cation (M^I) is surrounded by the four donor S atoms of the ligands. The M^IS_4 unit adopts a distorted tetrahedral geometry.

Comment

Copper(I) and silver(I) complexes with ligands containing sulfur as donor atoms exhibit a wide variety of stoichiometries and configurations. In mononuclear compounds, copper(I) and silver(I) often adopt linear-dihedral, trigonal-planar or tetrahedral geometries. The title complexes, (I) and (II), show a distorted coordination geometry and consist of discrete $[M(C_6H_7NS)_4]^+$ cations, where all the ligands bind to the metal centre through their S atoms, and BF_4^- anions.

(I): *M* = Cu   (II): *M* = Ag

In complex (I), the Cu—S distances range from 2.331 (1) to 2.379 (1) Å (Fig. 1 and Table 2). The observed distances are typical for compounds of this kind having tetrahedral geometry, as follows from a comparison with both $[Cu\{2(1H)-pyridinethione\}_4]ClO_4$–$2(1H)$-pyridinethione (1/2) (Kokkou, Schramm & Karagiannidis, 1985) and $[Cu_2\{2(1H)-pyridinethione\}_6]Cl_2$ (Constable & Raithby, 1987). In the related compound $[Cu\{2(1H)-pyridinethione\}_3]NO_3$ (Kokkou, Fortier, Rentzeperis & Karagiannidis, 1983), which has a

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trigonal-planar coordination, the Cu—S distances are *ca* 0.07–0.10 Å longer. This influence of the coordination geometry on the Cu—S distances has been discussed by both Hunt, Terry & Amma (1979) and Weininger, Hunt & Amma (1972) with regard to related compounds containing the thiourea ligand. The S—C and C—N distances (Tables 2 and 4) of complexes (I) and (II) are similar to those found in the complexes cited above.
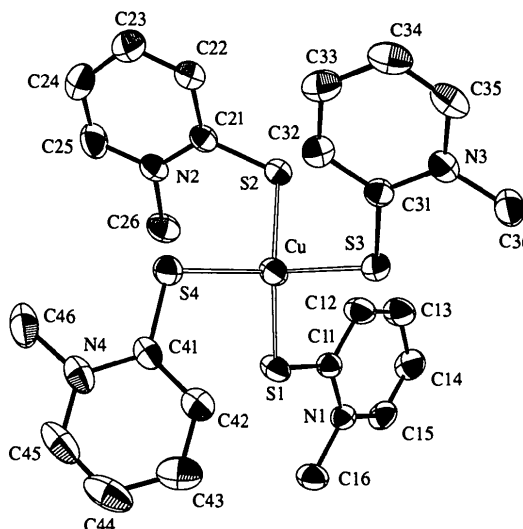
Fig. 1. The structure of complex (I) with the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

The Ag—S distances in complex (II) range from 2.557 (1) to 2.592 (1) Å (Fig. 2 and Table 4). As expected, the Ag—S distances are similar to those found in both $[Ag_2(thiosemicarbazide)_6]Cl_2$ (Bonamartini, Gasparri, Belicchi & Nardelli, 1987) and $[Ag_2(thiourea)_6](ClO_4)_2$ (Udupa & Krebs, 1973) for the terminal ligands. The Ag—S distances in complex (II) are larger then the Cu—S distances in complex (I). This is due to the larger Ag^I radius. The short Au—S distances of 2.281 and 2.291 Å in $[Au\{2(1H)-pyridinethione\}_2]CF_3SO_3$ (Geier, Primo & Mordasini, 1995) are partially due to the dihedral geometry around Au^I (S—Au—S 176.4°), but mainly due to the contraction of the $6s$ orbital of Au^I.

The S—*M*—S angles vary from 100.95 (4) to 121.77 (4)° (Table 2) in (I) and from 100.73 (5) to 119.81 (5)° (Table 4) in (II), which shows clearly the distortion from an ideal tetrahedron. This kind of distortion is found in other similar compounds.

The C—S—Cu and C—S—Ag angles are all less than 120° (Tables 2 and 4). This is usual for such complexes, as follows from a comparison with the work cited above and the work of Truter & Rutherford (1962) on $[Cu(CH_3CSNH_2)_4]Cl$.
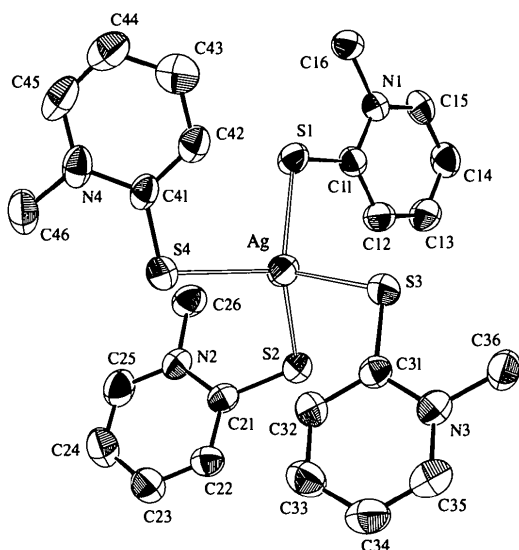
Fig. 2. The structure of complex (II) with the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

In both title structures, the S atom and the associated ring atoms define planes, two of which are almost parallel [3.1 (2) for (I) and 0.6 (2)° for (II)]. The other planes form angles with each other in the range 46–59° in both complexes.

The metal centre does not lie in any of these planes. The orthogonal distance from the metal to the plane defined by the atoms that constitute the ring of a ligand varies from 0.449 (5) to 2.101 (3) Å for (I) and from 0.736 (6) to 2.316 (4) Å for (II). This is also seen in the three compounds mentioned above (Kokkou, Schramm & Karagiannidis, 1985; Battaglia, Corradi, Nardelli & Tani, 1976; Bowmaker *et al.*, 1994) and in [Cu(2-imidazolidinethione)]NO$_3$ (Hunt, Terry & Amma, 1979; Udupa & Krebs, 1973). Only in the case of tris(thiourea)copper(I) chloride (Okaya & Knobler, 1964) do the authors calculate distances in the range 0.171 to 0.945 Å.

The facts that in both structures the C—S—M angles are *ca* 110° and that the metal is not coplanar with the ligands may indicate that the S atom has partially changed its hybridization from sp^2 to sp^3 and that the C—S bond therefore has partial single-bond character.

Experimental

The 2(1*H*)-pyridinethione ligand was prepared according to the literature methods of Gutbier (1900) and Jones & Katritzky (1958). Acetonitrile solutions of [Cu(CH$_3$CN)$_4$]BF$_4$ and the ligand were mixed in a ratio of 1:4. Orange crystals of complex (I) suitable for X-ray analysis were obtained by evaporation of the solvent. The synthesis of complex (II) was carried out by mixing acetonitrile solutions of AgBF$_4$ and the ligand in a ratio of 1:4. Yellow crystals suitable for X-ray analysis were obtained by evaporation of the solvent.

Compound (I)

Crystal data

[Cu(C$_6$H$_7$NS)$_4$]BF$_4$	Mo $K\alpha$ radiation
$M_r = 651.09$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 5 still
$P2_1/c$	exposures on scanner
$a = 13.183$ (6) Å	$\theta = 4–26°$
$b = 7.833$ (2) Å	$\mu = 1.100$ mm^{-1}
$c = 27.801$ (13) Å	$T = 298$ (2) K
$\beta = 90.56$ (4)°	Rectangular prism
$V = 2871$ (2) Å^3	$0.35 \times 0.25 \times 0.20$ mm
$Z = 4$	Orange
$D_x = 1.507$ Mg m^{-3}	
D_m not measured	

Data collection

Scanner Stoe IPDS	4560 observed reflections
diffractometer	[$I > 2\sigma(I)$]
Oscillation scans	$R_{int} = 0.0261$
Absorption correction:	$\theta_{max} = 26.01°$
none	$h = -16 \rightarrow 16$
17 672 measured reflections	$k = -9 \rightarrow 8$
5203 independent reflections	$l = -30 \rightarrow 34$
	No standard reflections

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} < 0.001$
$R(F) = 0.0493$	$\Delta\rho_{max} = 0.546$ e Å^{-3}
$wR(F^2) = 0.1541$	$\Delta\rho_{min} = -0.373$ e Å^{-3}
$S = 1.049$	Extinction correction: none
4560 reflections	Atomic scattering factors
343 parameters	from *International Tables*
H atoms: see text	*for Crystallography* (1992,
$w = 1/[\sigma^2(F_o^2) + (0.0771P)^2$	Vol. C, Tables 4.2.6.8 and
$+ 2.2783P]$	6.1.1.4)
where $P = (F_o^2 + 2F_c^2)/3$	

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

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

	x	y	z	U_{eq}
Cu	0.28090 (3)	0.02368 (6)	0.126717 (14)	0.0560 (2)
S1	0.30758 (6)	0.10325 (13)	0.04706 (3)	0.0616 (3)
N1	0.4579 (2)	0.2208 (4)	-0.00638 (9)	0.0534 (6)
C11	0.4222 (2)	0.1958 (4)	0.03877 (11)	0.0515 (7)
C12	0.4859 (3)	0.2500 (6)	0.07681 (14)	0.0723 (10)
C13	0.5774 (3)	0.3244 (7)	0.0683 (2)	0.0820 (12)
C14	0.6096 (3)	0.3473 (6)	0.0218 (2)	0.0797 (12)
C15	0.5496 (3)	0.2954 (5)	-0.01462 (14)	0.0688 (10)
C16	0.3957 (3)	0.1720 (6)	-0.04836 (13)	0.0723 (10)
S2	0.32599 (6)	0.22136 (12)	0.18828 (3)	0.0608 (2)
N2	0.1520 (2)	0.3987 (4)	0.18318 (10)	0.0585 (7)
C21	0.2150 (2)	0.2992 (4)	0.21001 (11)	0.0515 (7)
C22	0.1837 (3)	0.2647 (5)	0.25730 (12)	0.0592 (8)
C23	0.0954 (3)	0.3258 (6)	0.27526 (15)	0.0724 (10)
C24	0.0333 (3)	0.4240 (7)	0.2460 (2)	0.0854 (12)
C25	0.0623 (3)	0.4582 (6)	0.2010 (2)	0.0786 (11)
C26	0.1783 (3)	0.4465 (6)	0.13392 (14)	0.0751 (10)
S3	0.39287 (6)	-0.19876 (12)	0.14345 (3)	0.0576 (2)
N3	0.4433 (2)	-0.3749 (4)	0.22233 (10)	0.0568 (6)
C31	0.3725 (2)	-0.2736 (4)	0.19987 (11)	0.0494 (7)
C32	0.2852 (3)	-0.2351 (5)	0.22652 (13)	0.0601 (8)
C33	0.2720 (3)	-0.2957 (5)	0.27206 (13)	0.0716 (10)
C34	0.3474 (4)	-0.3949 (6)	0.29329 (14)	0.0778 (11)

	x	y	z	U_{eq}
C35	0.4300 (3)	−0.4323 (5)	0.26795 (14)	0.0718 (10)
C36	0.5346 (3)	−0.4280 (6)	0.1967 (2)	0.0743 (10)
S4	0.10641 (6)	−0.01004 (13)	0.13286 (3)	0.0641 (3)
N4	−0.0369 (2)	−0.0805 (5)	0.06734 (12)	0.0676 (8)
C41	0.0617 (2)	−0.1050 (4)	0.08179 (11)	0.0539 (8)
C42	0.1205 (3)	−0.2101 (5)	0.05272 (13)	0.0620 (8)
C43	0.0812 (4)	−0.2866 (6)	0.0127 (2)	0.0826 (13)
C44	−0.0186 (5)	−0.2581 (8)	−0.0003 (2)	0.096 (2)
C45	−0.0744 (3)	−0.1573 (7)	0.0273 (2)	0.0850 (15)
C46	−0.1036 (3)	0.0298 (8)	0.0951 (2)	0.095 (2)
B	−0.1808 (4)	−0.4642 (8)	0.1146 (2)	0.0754 (12)
F1	−0.2050 (3)	−0.4743 (6)	0.06727 (12)	0.1248 (13)
F2	−0.0880 (3)	−0.4070 (7)	0.1207 (2)	0.159 (2)
F3	−0.2436 (5)	−0.3440 (12)	0.1303 (2)	0.238 (4)
F4	−0.2007 (5)	−0.6003 (9)	0.1371 (3)	0.247 (4)

Table 2. Selected geometric parameters (Å, °) for (I)

Cu—S4	2.3234 (14)	S2—C21	1.701 (3)
Cu—S3	2.3276 (11)	N2—C21	1.357 (4)
Cu—S1	2.3305 (13)	S3—C31	1.698 (3)
Cu—S2	2.3792 (12)	N3—C31	1.371 (4)
S1—C11	1.693 (4)	S4—C41	1.703 (4)
N1—C11	1.360 (4)	N4—C41	1.369 (4)
S4—Cu—S3	121.77 (4)	S1—Cu—S2	118.07 (4)
S4—Cu—S1	105.01 (5)	C11—S1—Cu	112.77 (11)
S3—Cu—S1	106.79 (4)	C21—S2—Cu	106.20 (11)
S4—Cu—S2	105.17 (4)	C31—S3—Cu	109.70 (12)
S3—Cu—S2	100.95 (4)	C41—S4—Cu	108.86 (12)

Compound (II)

Crystal data

$[Ag(C_6H_7NS)_4]BF_4$
$M_r = 695.42$
Monoclinic
$P2_1/c$
$a = 13.350$ (3) Å
$b = 7.755$ (3) Å
$c = 28.028$ (8) Å
$\beta = 90.15$ (2)°
$V = 2901.7$ (15) Å³
$Z = 4$
$D_x = 1.592$ Mg m⁻³
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 6 still exposures on scanner
$\theta = 3.5–24°$
$\mu = 1.030$ mm⁻¹
$T = 200$ (2) K
Rectangular prism
$0.30 \times 0.20 \times 0.20$ mm
Yellow

Data collection

Scanner Stoe IPDS diffractometer
Oscillation scans
Absorption correction: none
14 367 measured reflections
4339 independent reflections

3915 observed reflections [$I > 2\sigma(I)$]
$R_{int} = 0.0306$
$\theta_{max} = 24.15°$
$h = −13 \rightarrow 15$
$k = −8 \rightarrow 8$
$l = −31 \rightarrow 31$
No standard reflections

Refinement

Refinement on F^2
$R(F) = 0.0452$
$wR(F^2) = 0.1282$
$S = 1.075$
3915 reflections
343 parameters
H atoms: see text
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 6.0571P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.841$ e Å⁻³
$\Delta\rho_{min} = −0.492$ 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 (Å²) for (II)

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

	x	y	z	U_{eq}
Ag	0.27816 (3)	0.50956 (5)	0.374259 (12)	0.0462 (2)
S1	0.30974 (9)	0.5985 (2)	0.46092 (4)	0.0477 (3)
N1	0.4650 (3)	0.7196 (5)	0.51004 (13)	0.0417 (8)
C11	0.4212 (3)	0.7016 (6)	0.4659 (2)	0.0400 (10)
C12	0.4737 (4)	0.7737 (7)	0.4271 (2)	0.0505 (12)
C13	0.5654 (4)	0.8531 (7)	0.4331 (2)	0.0561 (13)
C14	0.6066 (4)	0.8655 (7)	0.4782 (2)	0.0550 (12)
C15	0.5551 (4)	0.7989 (7)	0.5156 (2)	0.0505 (12)
C16	0.4118 (4)	0.6563 (7)	0.5524 (2)	0.0512 (12)
S2	0.32642 (9)	0.7370 (2)	0.31056 (4)	0.0458 (3)
N2	0.1478 (3)	0.8949 (5)	0.31703 (13)	0.0440 (9)
C21	0.2133 (3)	0.8036 (6)	0.2894 (2)	0.0405 (10)
C22	0.1831 (4)	0.7695 (6)	0.2423 (2)	0.0469 (11)
C23	0.0932 (4)	0.8244 (7)	0.2253 (2)	0.0571 (13)
C24	0.0281 (4)	0.9156 (8)	0.2548 (2)	0.0670 (15)
C25	0.0575 (4)	0.9473 (7)	0.2999 (2)	0.0598 (14)
C26	0.1733 (4)	0.9400 (7)	0.3666 (2)	0.0562 (13)
S3	0.39684 (9)	0.2635 (2)	0.35224 (4)	0.0458 (3)
N3	0.4419 (3)	0.1152 (5)	0.26940 (13)	0.0430 (9)
C31	0.3721 (3)	0.2076 (5)	0.2949 (2)	0.0390 (10)
C32	0.2837 (3)	0.2525 (6)	0.2708 (2)	0.0447 (11)
C33	0.2682 (4)	0.2076 (7)	0.2241 (2)	0.0546 (12)
C34	0.3419 (4)	0.1151 (7)	0.1996 (2)	0.0576 (13)
C35	0.4256 (4)	0.0703 (7)	0.2228 (2)	0.0533 (12)
C36	0.5340 (4)	0.0566 (7)	0.2928 (2)	0.0536 (12)
S4	0.08845 (9)	0.4637 (2)	0.36946 (4)	0.0529 (3)
N4	−0.0410 (3)	0.3854 (5)	0.43966 (15)	0.0503 (10)
C41	0.0560 (3)	0.3722 (6)	0.4222 (2)	0.0420 (10)
C42	0.1226 (4)	0.2808 (6)	0.4513 (2)	0.0458 (11)
C43	0.0933 (4)	0.2082 (7)	0.4943 (2)	0.0606 (14)
C44	−0.0043 (4)	0.2262 (8)	0.5094 (2)	0.0597 (14)
C45	−0.0690 (4)	0.3130 (8)	0.4820 (2)	0.0599 (15)
C46	−0.1159 (4)	0.4803 (8)	0.4121 (2)	0.067 (2)
B	0.1898 (5)	0.5171 (8)	0.1128 (2)	0.057 (2)
F1	0.2149 (3)	0.5691 (5)	0.06803 (12)	0.0758 (9)
F2	0.2061 (4)	0.3415 (5)	0.1155 (2)	0.1084 (14)
F3	0.0969 (4)	0.5649 (9)	0.1219 (2)	0.157 (3)
F4	0.2581 (5)	0.5949 (10)	0.1421 (2)	0.162 (3)

Table 4. Selected geometric parameters (Å, °) for (II)

Ag—S3	2.5568 (14)	S2—C21	1.701 (5)
Ag—S1	2.5587 (13)	N2—C21	1.366 (6)
Ag—S4	2.5607 (14)	S3—C31	1.697 (4)
Ag—S2	2.5924 (14)	N3—C31	1.376 (6)
S1—C11	1.695 (5)	S4—C41	1.698 (5)
N1—C11	1.375 (6)	N4—C41	1.389 (6)
S3—Ag—S1	109.25 (4)	S4—Ag—S2	107.81 (4)
S3—Ag—S4	119.81 (5)	C11—S1—Ag	110.3 (2)
S1—Ag—S4	104.34 (4)	C21—S2—Ag	102.93 (15)
S3—Ag—S2	100.73 (5)	C31—S3—Ag	107.5 (2)
S1—Ag—S2	115.45 (5)	C41—S4—Ag	105.5 (2)

The analogous PF_6^- salts of (I) and (II) have identical stoichiometries to those of their corresponding title complex. However, the $CF_3SO_3^-$ salt of the silver(I) compound has the composition $[Ag(C_6H_7NS)_3]CF_3SO_3$ (elemental analysis), but no crystal suitable for X-ray analysis could be obtained (Geier, Giusti & Kleemann, 1995). All H atoms were placed in calculated positions with fixed isotropic displacement parameters ($U_{iso} = 0.080$ Å²). No constraints or restraints were used. Some of the standard deviations are large due to some libration of terminal groups, which is observed quite frequently with organometallic compounds. *SHELXL*93 (Sheldrick, 1993) was used to calculate the least-squares mean plane and the corresponding deviations of all the atoms.

For both compounds, data collection: *EXPOSE* (Stoe & Cie, 1993); cell refinement: *CELL* (Stoe & Cie, 1993); data reduction: *CONVERT* (Stoe & Cie, 1993); program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structures: *SHELXL*93; molecular graphics: *ORTEP*II (Johnson, 1976) in *NRCVAX* (Larson *et al.*, 1986); software used to prepare material for publication: *SHELXL*93.

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Diiodobis(nicotinamide-N^1-acetate-O)-zinc(II)

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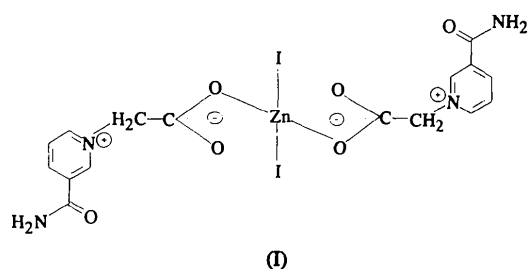
Abstract

In the title compound, [ZnI$_2$(C$_8$H$_8$N$_2$O$_3$)$_2$], the Zn atom, which lies on a twofold axis, exists in a slightly distorted tetrahedral geometry involving two zwitterionic nicotinamide-N^1-acetate substituents [Zn—O1 2.008 (2) Å] and two iodide ligands [Zn—I 2.5848 (3) Å]. Molecules of the complex are connected by intermolecular N—H⋯O hydrogen bonds, with N⋯O distances of 2.965 (3) and 3.133 (3) Å.

Comment

As part of a long-term project involving structural, spectroscopic, thermal and biological activity studies of zinc(II) carboxylates with bioactive N-donor ligands, we have been interested in the product of the reaction between zinc(II) iodoacetate and nicotinamide, *i.e.* diiodobis(nicotinamide-N^1-acetate)zinc(II), (I). We have previously reported the mechanism of the reaction (Zeleňák, Györyová & Císařová, 1995).

(I)

The crystal structure of (I) consists of discrete monomeric units (Fig. 1) with the four-coordinate Zn atom lying on the crystallographic twofold axis. The distorted coordination tetrahedron is formed by two I atoms and two O atoms from the zwitterionic nicotinamide-N^1-acetate ligands. The complexes are linked by intermolecular N—H⋯O hydrogen bonds (Table 3), causing the two N—H distances to be different.

The zwitterionic nicotinamide-N^1-acetate ligands are unidentate with the carboxylate O1 atom bonded to Zn