



Title	meso-Tetrakis(ethylenediamine)-1 κ^4 N,N';3 κ^4 N,N'-di- μ -sulfidoacetato-1:2 κ^3 O,S:S;2:3 κ^3 S:S,0-dicobalt(III)silver(I) triperchlorate
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Citation	Acta Crystallographica Section E. 2006, E62(6), p. m1229-m1231
Version Type	VoR
URL	https://hdl.handle.net/11094/54379
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Nobuto Yoshinari, Asako Igashira-Kamiyama and Takumi Konno

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***meso*-Tetrakis(ethylenediamine)-1 κ^4 N,N';3 κ^4 N,N'-di- μ -sulfidoacetato-1:2 κ^3 O,S:S;2:3 κ^3 S:S,O-dicobalt(III)-silver(I) triperchlorate**

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Key indicators

Single-crystal X-ray study
 $T = 296\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
Disorder in solvent or counterion
 R factor = 0.032
 wR factor = 0.085
Data-to-parameter ratio = 14.0

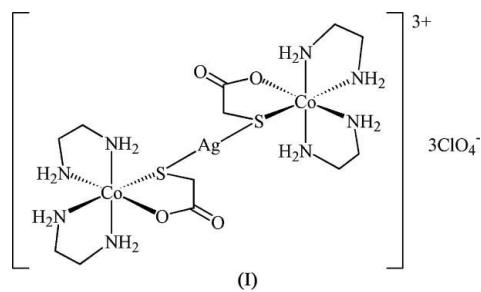
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound, $[\text{AgCo}_2(\text{C}_2\text{H}_4\text{O}_2\text{S})(\text{C}_2\text{H}_8\text{N}_2)_2](\text{ClO}_4)_3$, the Ag^{I} atom is located on an inversion center and is linearly coordinated by two sulfide S atoms from Δ - and Λ - $[\text{Co}^{\text{III}}(\text{C}_2\text{H}_4\text{O}_2\text{S})(\text{C}_2\text{H}_8\text{N}_2)_2]^+$ octahedral units, forming a *meso* configurational S-bridged $\text{Co}^{\text{III}}-\text{Ag}^{\text{I}}-\text{Co}^{\text{III}}$ trinuclear structure.

Received 17 April 2006
Accepted 29 April 2006

Comment

Thiolato groups coordinated to a metal center possess a relatively strong Lewis basicity, which allows them to bind with a second metal center (Konno, 2004). Heeg *et al.* (1980) reported that the thiolato group in $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2](\text{ClO}_4)$ (tga = mercaptoacetate, en = ethylenediamine) binds with an Ag^{I} ion to afford an S-bridged $\text{Co}^{\text{III}}-\text{Ag}^{\text{I}}-\text{Co}^{\text{III}}$ trinuclear complex, *racemic*- $[\text{Ag}[\text{Co}(\text{tga})(\text{en})_2]](\text{ClO}_4)_3$, (II). In (II), the two $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^+$ units have the same chiral configuration (Δ or Λ) to form a *racemic* ($\Delta\Delta/\Lambda\Lambda$) compound. In this paper, we report the structure of the *meso* ($\Delta\Lambda$) compound of $[\text{Ag}[\text{Co}(\text{tga})(\text{en})_2]](\text{ClO}_4)_3$, (I).



The asymmetric unit of (I) contains half a centrosymmetric complex cation, an ordered perchlorate anion, and half a centrosymmetrically disordered perchlorate anion. The entire complex cation is composed of two approximately octahedral $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^+$ units that are linked by an Ag^{I} atom through $\text{Ag}-\text{S}$ bonds, forming a linear-type S-bridged $\text{Co}^{\text{III}}-\text{Ag}^{\text{I}}-\text{Co}^{\text{III}}$ trinuclear structure in $[\text{Ag}[\text{Co}(\text{tga})(\text{en})_2]]^{3+}$ (Fig. 1). The two $[\text{Co}(\text{tga})(\text{en})_2]^+$ units in (I) have the opposite chiral configurations (Δ and Λ) to give a *meso* compound ($\Delta\Lambda$), which is distinct from the structure of (II) (Heeg *et al.*, 1980). In (I), the Ag atom is located on a crystallographic inversion center and thus adopts a strictly linear coordination geometry, while compound (II) contains an angular Ag^{I} atom [$\text{S}-\text{Ag}-\text{S} = 169.34(9)\text{ }^\circ$]. In addition, the $\text{Ag}-\text{S}$ bonds in (I) [$\text{Ag}1-\text{S}1 = 2.3954(10)\text{ \AA}$] are appreciably longer than those in (II) [$\text{Ag}-\text{S} = 2.370(1)\text{ \AA}$]. This could be ascribed to the contact of perchlorate anions with the Ag^{I} center [$\text{Ag}\cdots\text{O} = 3.090(5)$ and $3.124(7)\text{ \AA}$ in (I) (Konno *et al.*, 2002)]. The other bond

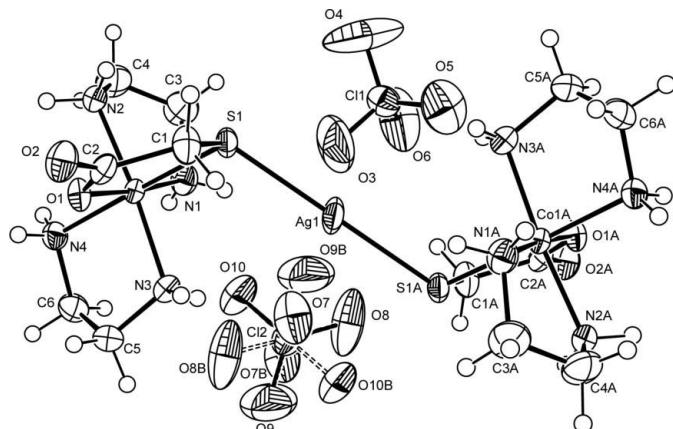


Figure 1

A view of the molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. Both the disordered components of ClO_4^- anions are shown. The suffixes A and B correspond to symmetry codes $(1 - x, 1 - y, 1 - z)$ and $(1 - x, -y, 1 - z)$, respectively.

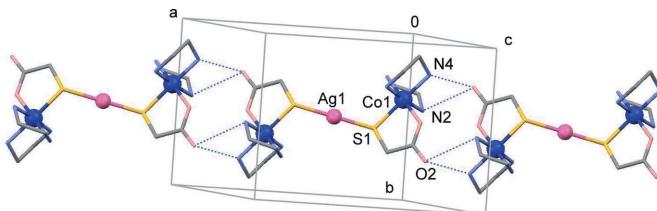


Figure 2

A view of the one-dimensional chain structure formed along the a axis in (I). Dashed lines indicate $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds. H atoms have been omitted for clarity.

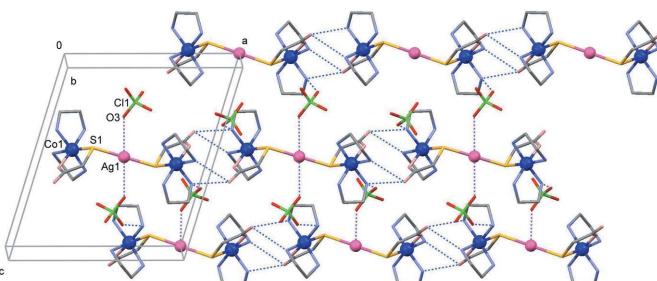


Figure 3

Packing diagram of (I). Dashed lines indicate $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (blue) and $\text{Ag}\cdots\text{O}$ interactions (purple). H atoms and the minor components of disordered ClO_4^- anions have been omitted for clarity.

distances and angles in (I) are similar to those in (II) (Table 1). In each $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^{2+}$ unit of (I), the tga O,S -chelate ring is almost planar, while the two en N,N' -chelate rings have a *gauche* conformation with *lel* (λ for Δ and δ for Λ) and *ob* (δ for Δ and λ for Λ) forms. This conformational feature is the same as that in (II).

The crystal structure of (I) is stabilized by several intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions (Table 2). It is noteworthy that each complex cation is connected with two adjacent cations through eight $\text{N}-\text{H}\cdots\text{O}=\text{C}$ hydrogen bonds to construct a one-dimensional chain structure (Fig. 2). The one-dimensional chains are

further bridged by ordered perchlorate anions through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds besides the $\text{Ag}\cdots\text{O}$ bonding interaction (Fig. 3).

Experimental

$[\text{Ag}[\text{Co}(\text{tga})(\text{en})_2]_2](\text{ClO}_4)_3$ was prepared by a method described in the literature (Heeg *et al.*, 1980), and crystals of the *meso* compound (I) were grown from aqueous NaClO_4 , instead of the use of aqueous HClO_4 .

Crystal data

$[\text{AgCo}_2(\text{C}_2\text{H}_4\text{O}_2\text{S})_2(\text{C}_2\text{H}_8\text{N}_2)_4](\text{ClO}_4)_3$
 $M_r = 944.69$
Monoclinic, $P2_1/n$
 $a = 12.486 (3)$ Å
 $b = 8.974 (2)$ Å
 $c = 14.410 (2)$ Å
 $\beta = 106.857 (14)^\circ$

$V = 1545.2 (6)$ Å³
 $Z = 2$
 $D_x = 2.030 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 2.16 \text{ mm}^{-1}$
 $T = 296 (2)$ K
Prism, red
 $0.35 \times 0.35 \times 0.25$ mm

Data collection

Rigaku AFC-7S diffractometer
 $\omega-2\theta$ scans
Absorption correction: ψ scan
(North *et al.*, 1968)
 $T_{\min} = 0.492$, $T_{\max} = 0.583$
3700 measured reflections
3542 independent reflections

2788 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 27.5^\circ$
3 standard reflections
every 150 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.085$
 $S = 1.03$
3542 reflections
253 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.5353P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.59 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.42 \text{ e } \text{\AA}^{-3}$

Table 1
Selected geometric parameters (Å, °).

Ag1—S1	2.3954 (10)	Co1—N2	1.952 (3)
Ag1—O3	3.090 (5)	Co1—N3	1.965 (3)
Ag1—O7	3.124 (7)	Co1—N4	1.983 (3)
Co1—O1	1.897 (2)	Co1—S1	2.2458 (10)
Co1—N1	1.957 (3)		
S1—Ag1—S1 ⁱ	180.0	O1—Co1—N1	175.06 (12)
N4—Co1—S1	176.16 (10)	N2—Co1—N3	175.04 (13)

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

Table 2
Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H4 ⁱⁱ —O2 ⁱⁱ	0.92 (5)	2.27 (5)	3.053 (4)	143 (4)
N4—H8 ⁱⁱ —O2 ⁱⁱ	0.87 (4)	2.53 (4)	3.004 (4)	115 (3)
N1—H2 ⁱⁱⁱ —O4 ⁱⁱⁱ	0.78 (5)	2.34 (5)	3.057 (6)	152 (5)
N2—H3 ^{iv} —O6 ^{iv}	0.81 (4)	2.26 (4)	2.993 (5)	151 (3)

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

H atoms bound to C atoms were placed at calculated positions ($C-H = 0.97 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms bound to N atoms were refined freely, giving $N-H = 0.78(5)-0.92(5) \text{ \AA}$. Atoms O7, O8, O9 and O10, disordered about the inversion center at atom Cl2, were refined with a fixed occupancy of 0.5.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: Crystal structure (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

Acta Cryst. (2006). E62, m1229–m1231 [doi:10.1107/S1600536806015868]

meso-Tetrakis(ethylenediamine)-1κ⁴N,N';3κ⁴N,N'-di-μ-sulfido-acetato-1:2κ³O,S:S;2:3κ³S:S,O-dicobalt(III)silver(I) triperchlorate

Nobuto Yoshinari, Asako Igashira-Kamiyama and Takumi Konno

S1. Comment

Thiolato groups coordinated to a metal center possess a relatively strong Lewis basicity, which allows them to bind with a second metal center (Konno, 2004). Heeg *et al.* (1980) reported that the thiolato group in $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2](\text{ClO}_4)$ (tga = mercaptoacetate, en = ethylenediamine) binds with an Ag^{l} ion to afford an S-bridged $\text{Co}^{\text{III}}-\text{Ag}^{\text{l}}-\text{Co}^{\text{III}}$ trinuclear complex, *racemic*- $[\text{Ag}\{\text{Co}(\text{tga})(\text{en})_2\}_2](\text{ClO}_4)_3$, (II). In (II), the two $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^+$ units have the same chiral configuration (Δ or Λ) to form a *racemic* ($\Delta\Delta/\Lambda\Lambda$) compound. In this paper, we report the structure of the *meso* ($\Delta\Lambda$) compound of $[\text{Ag}\{\text{Co}(\text{tga})(\text{en})_2\}_2](\text{ClO}_4)_3$, (I).

The asymmetric unit of (I) contains half a complex cation, an ordered perchlorate anion, and half a centrosymmetrically disordered perchlorate anion. The entire complex cation is composed of two approximately octahedral $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^+$ units that are linked by an Ag^{l} atom through $\text{Ag}-\text{S}$ bonds, forming a linear-type S-bridged $\text{Co}^{\text{III}}-\text{Ag}^{\text{l}}-\text{Co}^{\text{III}}$ trinuclear structure in $[\text{Ag}\{\text{Co}(\text{tga})(\text{en})_2\}_2]^{3+}$ (Fig. 1). The two $[\text{Co}(\text{tga})(\text{en})_2]^+$ units in (I) have the opposite chiral configurations (Δ and Λ) to give a *meso* compound ($\Delta\Lambda$), which is distinct from the structure of (II) (Heeg *et al.*, 1980). In (I), the Ag atom is located on a crystallographic inversion center and thus adopts a strictly linear coordination geometry, while compound (II) contains an angular Ag^{l} atom [$\text{S}-\text{Ag}-\text{S} = 169.34(9)^\circ$]. In addition, the $\text{Ag}-\text{S}$ bonds in (I) [$\text{Ag}^{\text{l}}-\text{S} = 2.3954(10)$ Å] are appreciably longer than those in (II) [$\text{Ag}-\text{S} = 2.370(1)$ Å]. This could be ascribed to the contact of perchlorate anions with the Ag^{l} center [$\text{Ag}\cdots\text{O} = 3.090(5)$ and $3.124(7)$ Å] in (I) (Konno *et al.*, 2002). The other bond distances and angles in (I) are similar to those in (II) (Table 1). In each $[\text{Co}^{\text{III}}(\text{tga})(\text{en})_2]^+$ unit of (I), the tga O,S -chelate ring is almost planar, while the two en N,N' -chelate rings have a *gauche* conformation with *lel* (λ for Δ and δ for Λ) and *ob* (δ for Δ and λ for Λ) forms. This conformational feature is the same as that in (II).

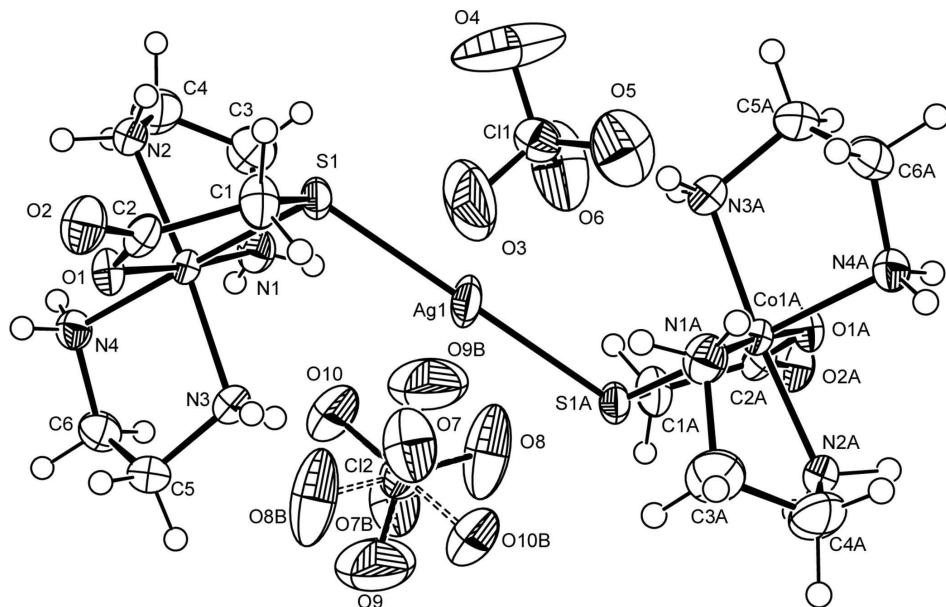
The crystal structure of (I) is stabilized by several intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions (Table 2). It is noteworthy that each complex cation is connected with two adjacent cations through eight $\text{N}-\text{H}\cdots\text{O}=\text{C}$ hydrogen bonds to construct a one-dimensional chain structure (Fig. 2). The one-dimensional chains are further bridged by ordered perchlorate anions through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds besides the $\text{Ag}\cdots\text{O}$ bonding interaction (Fig. 3).

S2. Experimental

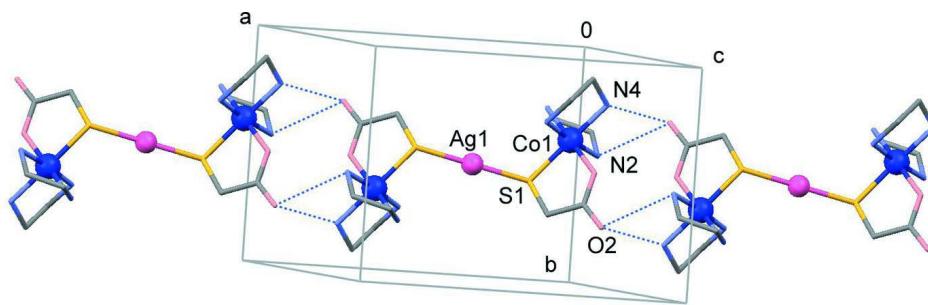
$[\text{Ag}\{\text{Co}(\text{tga})(\text{en})_2\}_2](\text{ClO}_4)_3$ was prepared by a method described in the literature (Heeg *et al.*, 1980), and crystals of the *meso* compound (I) were grown from aqueous NaClO_4 , instead of the use of aqueous HClO_4 .

S3. Refinement

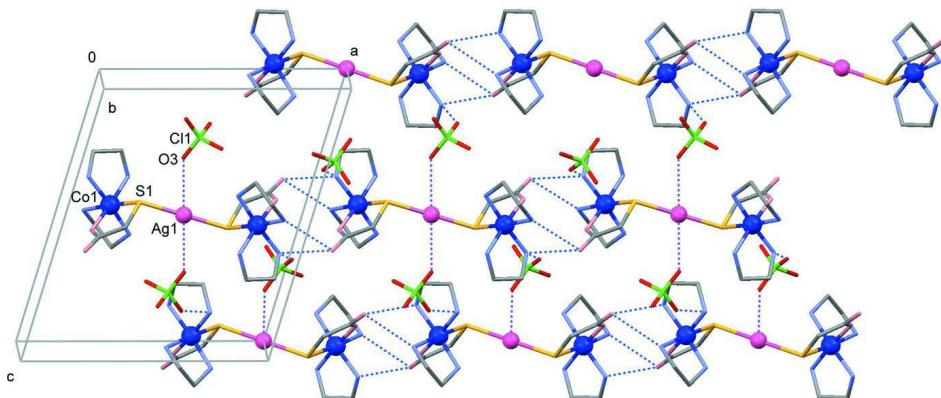
H atoms bound to C atoms were placed at calculated positions ($\text{C}-\text{H} = 0.97$ Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms bound to N atoms were refined freely, giving $\text{N}-\text{H} = 0.78(5) - 0.92(5)$ Å. Atoms O7, O8, O9 and O10, disordered about the inversion center of atom Cl2, were refined with a fixed occupancy of 0.5.

**Figure 1**

A view of the molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. Both the disordered components of ClO_4^- anions are shown. The suffixes A and B correspond to symmetry codes $(1 - x, 1 - y, 1 - z)$ and $(1 - x, -y, 1 - z)$, respectively.

**Figure 2**

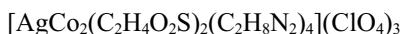
A view of the one-dimensional chain structure formed along the *a* axis in (I). Dashed lines indicate $\text{N}—\text{H}\cdots\text{O}$ hydrogen bonds. H atoms have been omitted for clarity.

**Figure 3**

Packing diagram of (I). Dashed lines indicate N–H···O hydrogen bonds (blue) and Ag···O interactions (purple). H atoms and the minor components of disordered ClO_4^- anions have been omitted for clarity.

meso-Tetrakis(ethylenediamine)-1 κ^4 N,N';3 κ^4 N,N'-di- μ -sulfidoacetato-1:2 κ^3 O,S:S;2:3 κ^3 S:S,O-dicobalt(III)silver(I) triperchlorate

Crystal data



$M_r = 944.69$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 12.486 (3)$ Å

$b = 8.974 (2)$ Å

$c = 14.410 (2)$ Å

$\beta = 106.857 (14)^\circ$

$V = 1545.2 (6)$ Å³

$Z = 2$

Data collection

Rigaku AFC-7S
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω – 2θ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.492$, $T_{\max} = 0.583$

3700 measured reflections

$F(000) = 952$

$D_x = 2.030 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 25 reflections

$\theta = 14.7$ – 15.0°

$\mu = 2.16 \text{ mm}^{-1}$

$T = 296$ K

Prism, red

0.35 × 0.35 × 0.25 mm

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.085$

$S = 1.03$

3542 reflections

253 parameters

0 restraints

3542 independent reflections

2788 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$

$h = 0$ – 16

$k = 0$ – 11

$l = -18$ – 17

3 standard reflections every 150 reflections

intensity decay: –0.1%

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.5353P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.59 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	0.5000	0.5000	0.5000	0.04000 (12)	
Co1	0.19574 (3)	0.37190 (5)	0.47184 (3)	0.02058 (11)	
Cl1	0.47295 (8)	0.38249 (11)	0.22391 (7)	0.0417 (2)	
Cl2	0.5000	0.0000	0.5000	0.0454 (3)	
S1	0.30444 (6)	0.55848 (9)	0.44754 (6)	0.02741 (17)	
O1	0.14597 (18)	0.4998 (3)	0.55573 (17)	0.0284 (5)	
O2	0.1355 (2)	0.7241 (3)	0.61434 (19)	0.0392 (6)	
O3	0.4350 (4)	0.3429 (8)	0.3006 (3)	0.127 (2)	
O4	0.3938 (6)	0.4563 (6)	0.1514 (4)	0.152 (3)	
O5	0.5711 (4)	0.4729 (5)	0.2582 (3)	0.0879 (13)	
O6	0.5030 (4)	0.2534 (4)	0.1830 (4)	0.1032 (16)	
O7	0.5009 (6)	0.1547 (8)	0.5280 (6)	0.070 (2)	0.50
O8	0.5780 (6)	-0.0101 (10)	0.4459 (8)	0.098 (3)	0.50
O9	0.5190 (10)	-0.0930 (13)	0.5775 (9)	0.133 (4)	0.50
O10	0.3886 (6)	-0.0226 (10)	0.4341 (6)	0.079 (2)	0.50
N1	0.2377 (3)	0.2483 (4)	0.3760 (2)	0.0335 (6)	
H1	0.304 (4)	0.252 (4)	0.380 (3)	0.033 (10)*	
H2	0.225 (4)	0.164 (5)	0.382 (3)	0.051 (15)*	
N2	0.0707 (2)	0.4379 (4)	0.3635 (2)	0.0301 (6)	
H3	0.076 (3)	0.526 (4)	0.355 (3)	0.021 (9)*	
H4	0.007 (4)	0.431 (5)	0.382 (3)	0.062 (14)*	
N3	0.3122 (2)	0.2950 (4)	0.5846 (2)	0.0293 (6)	
H5	0.345 (4)	0.373 (5)	0.623 (3)	0.043 (12)*	
H6	0.357 (3)	0.248 (4)	0.569 (3)	0.029 (10)*	
N4	0.1015 (2)	0.2121 (3)	0.5023 (2)	0.0294 (6)	
H7	0.058 (4)	0.257 (5)	0.533 (3)	0.041 (11)*	
H8	0.058 (3)	0.166 (4)	0.452 (3)	0.029 (10)*	
C1	0.2712 (3)	0.6901 (4)	0.5306 (3)	0.0348 (8)	
H9	0.3378	0.7079	0.5842	0.042*	
H10	0.2492	0.7841	0.4973	0.042*	
C2	0.1778 (3)	0.6359 (4)	0.5704 (2)	0.0279 (7)	
C3	0.1761 (4)	0.3000 (6)	0.2771 (3)	0.0502 (11)	

H11	0.2142	0.3845	0.2591	0.060*
H12	0.1724	0.2208	0.2305	0.060*
C4	0.0624 (3)	0.3432 (6)	0.2775 (3)	0.0501 (11)
H13	0.0185	0.2549	0.2800	0.060*
H14	0.0257	0.3976	0.2188	0.060*
C5	0.2609 (3)	0.1903 (5)	0.6400 (3)	0.0400 (8)
H15	0.3175	0.1246	0.6798	0.048*
H16	0.2266	0.2453	0.6819	0.048*
C6	0.1748 (3)	0.1024 (4)	0.5673 (3)	0.0381 (8)
H17	0.2100	0.0376	0.5308	0.046*
H18	0.1318	0.0415	0.5993	0.046*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.01916 (17)	0.0438 (2)	0.0608 (3)	0.00068 (16)	0.01763 (17)	0.0042 (2)
Co1	0.01564 (18)	0.0233 (2)	0.0231 (2)	0.00048 (16)	0.00621 (15)	0.00018 (16)
Cl1	0.0511 (5)	0.0386 (5)	0.0386 (5)	0.0029 (4)	0.0182 (4)	-0.0003 (4)
Cl2	0.0390 (7)	0.0425 (7)	0.0540 (8)	0.0042 (6)	0.0123 (6)	-0.0046 (7)
S1	0.0204 (3)	0.0301 (4)	0.0348 (4)	-0.0011 (3)	0.0127 (3)	0.0022 (3)
O1	0.0242 (10)	0.0308 (12)	0.0349 (12)	-0.0034 (10)	0.0156 (9)	-0.0029 (10)
O2	0.0356 (13)	0.0373 (14)	0.0489 (15)	0.0054 (11)	0.0187 (12)	-0.0101 (12)
O3	0.091 (3)	0.229 (7)	0.078 (3)	-0.029 (4)	0.054 (3)	0.013 (4)
O4	0.183 (6)	0.082 (3)	0.120 (4)	0.034 (4)	-0.066 (4)	0.022 (3)
O5	0.098 (3)	0.077 (3)	0.089 (3)	-0.037 (2)	0.027 (2)	-0.029 (2)
O6	0.118 (4)	0.056 (2)	0.166 (5)	-0.025 (2)	0.089 (3)	-0.046 (3)
O7	0.077 (5)	0.050 (4)	0.100 (6)	-0.003 (3)	0.051 (4)	-0.024 (4)
O8	0.057 (4)	0.104 (7)	0.149 (8)	-0.014 (4)	0.055 (5)	-0.079 (6)
O9	0.115 (9)	0.123 (9)	0.136 (10)	-0.001 (7)	-0.006 (7)	0.075 (8)
O10	0.039 (3)	0.101 (6)	0.085 (5)	0.000 (4)	-0.001 (3)	0.011 (5)
N1	0.0306 (16)	0.0368 (18)	0.0350 (16)	0.0019 (14)	0.0125 (13)	-0.0055 (14)
N2	0.0203 (13)	0.0368 (17)	0.0325 (15)	0.0003 (13)	0.0067 (11)	0.0070 (14)
N3	0.0225 (13)	0.0328 (16)	0.0309 (15)	0.0024 (12)	0.0053 (11)	0.0022 (13)
N4	0.0250 (13)	0.0322 (16)	0.0306 (15)	-0.0052 (12)	0.0076 (12)	0.0012 (12)
C1	0.0328 (17)	0.0236 (16)	0.053 (2)	-0.0027 (14)	0.0209 (16)	-0.0052 (16)
C2	0.0197 (14)	0.0319 (17)	0.0319 (16)	0.0056 (13)	0.0071 (12)	-0.0016 (14)
C3	0.051 (2)	0.072 (3)	0.0290 (19)	0.008 (2)	0.0136 (17)	-0.0048 (19)
C4	0.043 (2)	0.072 (3)	0.0286 (19)	0.002 (2)	-0.0003 (16)	0.001 (2)
C5	0.0345 (18)	0.052 (2)	0.0327 (18)	0.0036 (17)	0.0083 (15)	0.0145 (17)
C6	0.040 (2)	0.0314 (19)	0.045 (2)	0.0009 (15)	0.0154 (17)	0.0112 (16)

Geometric parameters (\AA , $^\circ$)

Ag1—S1 ⁱ	2.3954 (10)	N1—C3	1.483 (5)
Ag1—S1	2.3954 (10)	N1—H1	0.82 (4)
Ag1—O3	3.090 (5)	N1—H2	0.78 (5)
Ag1—O7	3.124 (7)	N2—C4	1.480 (5)
Co1—O1	1.897 (2)	N2—H3	0.81 (4)

Co1—N1	1.957 (3)	N2—H4	0.92 (5)
Co1—N2	1.952 (3)	N3—C5	1.492 (5)
Co1—N3	1.965 (3)	N3—H5	0.91 (4)
Co1—N4	1.983 (3)	N3—H6	0.78 (4)
Co1—S1	2.2458 (10)	N4—C6	1.479 (4)
C11—O3	1.370 (4)	N4—H7	0.89 (4)
C11—O4	1.381 (4)	N4—H8	0.87 (4)
C11—O6	1.400 (4)	C1—C2	1.522 (4)
C11—O5	1.432 (4)	C1—H9	0.9700
Cl2—O9 ⁱⁱ	1.358 (9)	C1—H10	0.9700
Cl2—O8 ⁱⁱ	1.416 (7)	C3—C4	1.473 (6)
Cl2—O8	1.416 (7)	C3—H11	0.9700
Cl2—O7	1.445 (7)	C3—H12	0.9700
Cl2—O7 ⁱⁱ	1.445 (7)	C4—H13	0.9700
Cl2—O10 ⁱⁱ	1.454 (7)	C4—H14	0.9700
Cl2—O10	1.454 (7)	C5—C6	1.491 (5)
S1—C1	1.813 (4)	C5—H15	0.9700
O1—C2	1.283 (4)	C5—H16	0.9700
O2—C2	1.225 (4)	C6—H17	0.9700
		C6—H18	0.9700
S1—Ag1—S1 ⁱ	180.0	C4—N2—H4	111 (3)
S1 ⁱ —Ag1—O3	99.35 (10)	Co1—N2—H4	108 (3)
S1—Ag1—O3	80.65 (10)	H3—N2—H4	103 (4)
S1 ⁱ —Ag1—O7	77.11 (14)	C5—N3—Co1	109.5 (2)
S1—Ag1—O7	102.89 (14)	C5—N3—H5	110 (3)
O3—Ag1—O7	69.98 (19)	Co1—N3—H5	109 (3)
O1—Co1—N2	89.57 (12)	C5—N3—H6	105 (3)
N4—Co1—S1	176.16 (10)	Co1—N3—H6	112 (3)
O1—Co1—N1	175.06 (12)	H5—N3—H6	110 (4)
N2—Co1—N1	85.56 (13)	C6—N4—Co1	108.9 (2)
O1—Co1—N3	89.21 (12)	C6—N4—H7	110 (3)
N2—Co1—N3	175.04 (13)	Co1—N4—H7	106 (3)
N1—Co1—N3	95.70 (14)	C6—N4—H8	110 (2)
O1—Co1—N4	88.36 (12)	Co1—N4—H8	115 (2)
N2—Co1—N4	90.48 (13)	H7—N4—H8	107 (4)
N1—Co1—N4	92.51 (15)	C2—C1—S1	112.8 (2)
N3—Co1—N4	84.67 (12)	C2—C1—H9	109.0
O1—Co1—S1	88.45 (7)	S1—C1—H9	109.0
N2—Co1—S1	91.63 (10)	C2—C1—H10	109.0
N1—Co1—S1	90.85 (11)	S1—C1—H10	109.0
N3—Co1—S1	93.15 (9)	H9—C1—H10	107.8
O3—Cl1—O4	113.3 (4)	O2—C2—O1	122.8 (3)
O3—Cl1—O6	108.9 (4)	O2—C2—C1	118.7 (3)
O4—Cl1—O6	107.4 (4)	O1—C2—C1	118.5 (3)
O3—Cl1—O5	109.3 (3)	C4—C3—N1	108.0 (3)
O4—Cl1—O5	110.0 (3)	C4—C3—H11	110.1
O6—Cl1—O5	107.9 (3)	N1—C3—H11	110.1

O9—Cl2—O8	115.4 (7)	C4—C3—H12	110.1
O9—Cl2—O7	112.0 (6)	N1—C3—H12	110.1
O8—Cl2—O7	105.4 (4)	H11—C3—H12	108.4
O9—Cl2—O10	110.9 (6)	C3—C4—N2	108.7 (3)
O8—Cl2—O10	108.2 (5)	C3—C4—H13	110.0
O7—Cl2—O10	104.2 (5)	N2—C4—H13	110.0
C1—S1—Co1	96.81 (11)	C3—C4—H14	110.0
C1—S1—Ag1	109.97 (12)	N2—C4—H14	110.0
Co1—S1—Ag1	113.22 (4)	H13—C4—H14	108.3
C2—O1—Co1	122.5 (2)	C6—C5—N3	106.9 (3)
Cl1—O3—Ag1	125.0 (3)	C6—C5—H15	110.3
Cl2—O7—Ag1	156.5 (5)	N3—C5—H15	110.3
C3—N1—Co1	109.3 (3)	C6—C5—H16	110.3
C3—N1—H1	107 (3)	N3—C5—H16	110.3
Co1—N1—H1	113 (3)	H15—C5—H16	108.6
C3—N1—H2	110 (4)	N4—C6—C5	106.3 (3)
Co1—N1—H2	112 (3)	N4—C6—H17	110.5
H1—N1—H2	105 (4)	C5—C6—H17	110.5
C4—N2—Co1	109.9 (2)	N4—C6—H18	110.5
C4—N2—H3	115 (3)	C5—C6—H18	110.5
Co1—N2—H3	109 (3)	H17—C6—H18	108.7
O1—Co1—S1—C1	3.03 (15)	N2—Co1—N1—C3	15.0 (3)
N2—Co1—S1—C1	92.55 (16)	N3—Co1—N1—C3	-169.8 (3)
N1—Co1—S1—C1	178.14 (16)	N4—Co1—N1—C3	105.3 (3)
N3—Co1—S1—C1	-86.10 (16)	S1—Co1—N1—C3	-76.6 (3)
O1—Co1—S1—Ag1	118.21 (8)	O1—Co1—N2—C4	-170.1 (3)
N2—Co1—S1—Ag1	-152.26 (10)	N1—Co1—N2—C4	10.7 (3)
N1—Co1—S1—Ag1	-66.67 (10)	N4—Co1—N2—C4	-81.7 (3)
N3—Co1—S1—Ag1	29.09 (10)	S1—Co1—N2—C4	101.5 (3)
O3—Ag1—S1—C1	-171.75 (17)	O1—Co1—N3—C5	76.1 (3)
O7—Ag1—S1—C1	121.42 (19)	N1—Co1—N3—C5	-104.3 (3)
O3—Ag1—S1—Co1	81.19 (12)	N4—Co1—N3—C5	-12.3 (3)
O7—Ag1—S1—Co1	14.37 (15)	S1—Co1—N3—C5	164.5 (2)
N2—Co1—O1—C2	-89.0 (3)	O1—Co1—N4—C6	-106.3 (2)
N3—Co1—O1—C2	95.8 (3)	N2—Co1—N4—C6	164.2 (3)
N4—Co1—O1—C2	-179.5 (3)	N1—Co1—N4—C6	78.6 (3)
S1—Co1—O1—C2	2.7 (2)	N3—Co1—N4—C6	-16.9 (3)
O4—Cl1—O3—Ag1	-105.1 (4)	Co1—S1—C1—C2	-7.6 (3)
O6—Cl1—O3—Ag1	135.6 (4)	Ag1—S1—C1—C2	-125.4 (2)
O5—Cl1—O3—Ag1	18.0 (5)	Co1—O1—C2—O2	170.4 (3)
S1 ⁱ —Ag1—O3—Cl1	-65.0 (4)	Co1—O1—C2—C1	-8.9 (4)
S1—Ag1—O3—Cl1	115.0 (4)	S1—C1—C2—O2	-168.2 (3)
O7—Ag1—O3—Cl1	-137.6 (4)	S1—C1—C2—O1	11.2 (4)
O9—Cl2—O7—Ag1	170.9 (10)	Co1—N1—C3—C4	-37.7 (5)
O8—Cl2—O7—Ag1	44.6 (12)	N1—C3—C4—N2	47.0 (5)
O10 ⁱⁱ —Cl2—O7—Ag1	110.8 (11)	Co1—N2—C4—C3	-34.6 (4)
O10—Cl2—O7—Ag1	-69.2 (11)	Co1—N3—C5—C6	38.8 (4)

S1 ⁱ —Ag1—O7—Cl2	—91.0 (11)	Co1—N4—C6—C5	42.3 (3)
S1—Ag1—O7—Cl2	89.0 (11)	N3—C5—C6—N4	—52.6 (4)
O3—Ag1—O7—Cl2	14.1 (10)		

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
N2—H4 \cdots O2 ⁱⁱⁱ	0.92 (5)	2.27 (5)	3.053 (4)	143 (4)
N4—H8 \cdots O2 ⁱⁱⁱ	0.87 (4)	2.53 (4)	3.004 (4)	115 (3)
N1—H2 \cdots O4 ^{iv}	0.78 (5)	2.34 (5)	3.057 (6)	152 (5)
N2—H3 \cdots O6 ^v	0.81 (4)	2.26 (4)	2.993 (5)	151 (3)

Symmetry codes: (iii) $-x, -y+1, -z+1$; (iv) $-x+1/2, y-1/2, -z+1/2$; (v) $-x+1/2, y+1/2, -z+1/2$.