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$\Lambda_L\Lambda_L$-Bis(μ-L-cysteinato)-1:2κ^3S:N,S;1:-3κ^3S:N,S-tetrakis(ethylenediamine)-2κ^4N,N';3κ^4N,N'-dicobalt(III)silver(I) tris(perchlorate) pentahydrate

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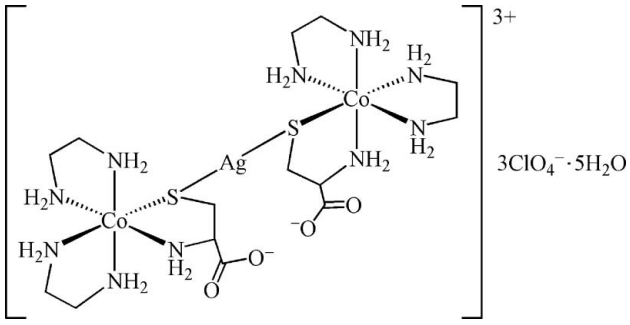
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.023; wR factor = 0.060; data-to-parameter ratio = 7.3.

In the crystal structure of the title compound, $\Lambda_L\Lambda_L$-[$AgCo_2$-$(C_3H_5NO_2S)_2(C_2H_8N_2)_4$]$(ClO_4)_3\cdot5H_2O$, the Ag^I atom, which lies on a twofold rotation axis, is linearly coordinated by two thiolate S atoms from two Λ_L-$[Co(C_3H_5NO_2S)(C_2H_8N_2)_2]^+$ octahedral units, forming an S-bridged Co^{III}–Ag^I–Co^{III} trinuclear unit. The compound has two uncoordinated carboxylate groups.

Related literature

For related literature, see: Konno (2004); Konno *et al.* (2001).



Experimental

Crystal data

$[AgCo_2(C_3H_5NO_2S)_2(C_2H_8N_2)_4]$-$(ClO_4)_3\cdot5H_2O$
M_r = 1092.86
Monoclinic, $C2$
a = 16.542 (2) Å
b = 9.050 (2) Å
c = 13.728 (2) Å
β = 111.507 (10)°
V = 1912.0 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.77 mm^{-1}
T = 296 (2) K
0.40 × 0.18 × 0.18 mm

Data collection

Rigaku AFC-7S diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.537, T_{max} = 0.741
2426 measured reflections
2346 independent reflections
2219 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
3 standard reflections
every 150 reflections
intensity decay: 14.4%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.05
2346 reflections
322 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.001 (18)

Table 1
Selected geometric parameters (Å, °).

Ag1—S1	2.3938 (9)	Co1—N5	1.975 (3)
Co1—N3	1.960 (3)	Co1—N4	1.980 (3)
Co1—N2	1.964 (3)	Co1—S1	2.2642 (10)
Co1—N1	1.972 (3)		
S1^i—Ag1—S1	172.38 (5)	N1—Co1—N5	175.53 (14)
N3—Co1—N2	175.89 (16)	N4—Co1—S1	177.46 (10)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O12^{ii}	0.90	2.30	3.14 (2)	155
N1—H2···O11	0.90	2.19	3.034 (19)	157
N1—H2···O7	0.90	2.23	3.066 (18)	155
N2—H3···O15	0.90	2.04	2.899 (5)	160
N2—H4···O13^{iii}	0.90	2.28	3.057 (19)	144
N3—H5···O4	0.90	2.25	3.146 (13)	174
N3—H6···O10^{iv}	0.90	2.21	3.083 (12)	162
N4—H7···O2^{v}	0.90	2.03	2.868 (4)	155
N4—H8···O7	0.90	2.49	3.117 (16)	128
N4—H8···O17^{v}	0.90	2.50	3.138 (13)	128
N5—H9···O15	0.90	2.36	3.201 (5)	155
N5—H10···O16	0.90	2.25	3.079 (6)	152
O15—H22···O1^{v}	0.85 (5)	1.89 (3)	2.711 (5)	162 (7)
O16—H26···O2^{v}	0.86 (10)	2.12 (4)	2.891 (7)	149 (7)
O17—H27···O1^{vi}	0.85 (2)	2.2 (2)	2.822 (12)	126 (19)
O17—H28···O1	0.85 (2)	2.12 (12)	2.884 (12)	149 (19)

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *CrystalStructure* (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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2256).

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supplementary materials

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$\Lambda_L\Lambda_L$-Bis(μ-L-cysteinato)-1:2κ^3S:*N*,*S*;1:3κ^3S:*N*,*S*-tetrakis(ethylenediamine)-2κ^4N,*N*';3κ^4N,*N*'-dicobalt(III)silver(I) tris(perchlorate) pentahydrate

M. Tamura, N. Yoshinari, A. Igashira-Kamiyama and T. Konno

Comment

Thiolato groups coordinated to a metal center possess relatively strong Lewis basicity, which allows them to bind with a second metal center (Konno, 2004). Previously, Konno *et al.* (2001) reported Λ_L-[Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ (*L*-cys = *L*-cysteinate, en = ethylenediamine) reacts with $AgNO_3$ to give an S-bridged $(Co^{III}Ag^I)_n$ coordination polymer, {Λ_L-[Ag{Co(*L*-cys-*N*,*S*)(en)$_2$}](NO$_3$)$_2$}$_n$·H$_2$O (II). In this compound, the Λ_L-[Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ unit binds with two Ag^I atoms through sulfur and with another Ag^I atom through a carboxylate group, to give a sheet-like structure. In this paper, we report on the structure of $\Lambda_L\Lambda_L$-[Ag{Co(*L*-cys-*N*,*S*)(en)$_2$}$_2$](ClO$_4$)$_3$·5H$_2$O (I), which was obtained by the 2:1 reaction of Λ_L-[Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ with $AgClO_4$.

The cation is composed of two octahedral [Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ units that are linked by an Ag^I atom through the S atoms to form a linear-type S-bridged $Co^{III}Ag^ICo^{III}$ trinuclear structure in [Ag{Co(*L*-cys-*N*,*S*)(en)$_2$}$_2$]$^{3+}$ (Fig. 1). The Ag^I atom, which is locate on a twofold axis, adopts an almost linear coordination geometry, unlike an angular geometry found in (II) (S—Ag—S = 149.62 (7) °). Furthermore, the Ag—S bonds in (I) are appreciably shorter than those in (II) (Ag—S = 2.501 (3), 2.511 (3) Å). These differences are ascribed to the fact that the Ag^I center in (II) is coordinated by a carboxylate group (Ag—O = 2.598 (1), 2.490 (8) Å), besides two thiolato groups. Other bond distances and angles in (I) are similar to those in (II) (Table 1). The two [Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ units in (I) have an Λ configuration because of the configuration of the mononuclear Λ_L-[Co(*L*-cys-*N*,*S*)(en)$_2$]$^+$ reactant. The *L*-cys *N*,*S*-chelate ring adopts a λ conformation; the two en *N*,*N*-chelate rings adopt δ and λ conformations.

The cation is connected with to four adjacent cations through N–H···O hydrogen bonds between coordinated amine groups and non-coordinated carboxylate groups to give a sheet-like structure (Fig. 2). The sheets are further linked through the perchlorate anions and water molecules through hydrogen bonds.

Experimental

Treatment of Λ_L-[Co(*L*-Hcys-*N*,*S*)(en)$_2$](ClO$_4$)$_2$ with a mixture of 0.5 molar equiv. of $AgClO_4$ and 0.5 equiv. of NaOH in water at room temperature gave a red solution, from which red crystals (I) were isolated by adding an aqueous solution of $NaClO_4$.

Refinement

H atoms bonded to C and N atoms were placed at calculated positions [C—H = 0.97 (methylene) and 0.98 (methine) Å, and N—H = 0.90 Å] and refined as riding with $U_{iso}(H) = 1.2U_{eq}$ (*C*,*N*). H atoms of water molecules were found in a difference Fourier map and were refined with restrained geometrical parameters [O—H = 0.85 (2) Å, H···H = 1.38 (2) Å, and $U_{iso} = 1.5U_{eq}(O)$]. One H atom of one water molecule is disordered over two positions (H23/H24), which were refined with site occupancies of 0.5. Atom H26 of a water molecule was refined with a restrained geometrical parameter to form an ideal hydrogen bond [H26···O2^{v} = 2.00 (5) Å; symmetry code: (v) −*x* + 1/2, *y* + 1/2, −*z* + 1]. One perchrolate anion is disordered over two positions (O7—O10 and O11—O14), which were refined with site occupancies of 0.5. Atoms O7, O8, O9 and O10, disordered on a twofold axis of the Cl2, were refined with site occupancies of 0.5.

Figures

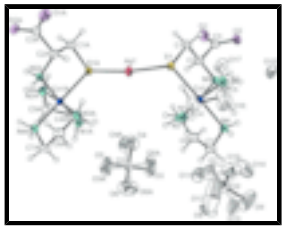

Fig. 1. A view of the molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. Both of the disordered components of ClO_4^- anions are shown. The suffixes A correspond to symmetry code (- *x*, *y*, − *z*). H atoms of water molecules have been omitted.

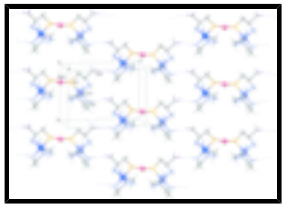

Fig. 2. A view of the two-dimensional sheet like structure in (I). Dashed lines indicate N–H···O hydrogen bonds. Perchlorate anions and water molecules have been omitted.

$\Lambda_L\Lambda_L$—Bis(μ-*L*-cysteinato)- 1:2κ^3*S*:*N*,*S*;1:3κ^3*S*:*N*,*S*- tetrakis(ethylenediamine)-2κ^4*N*,*N*';3κ^4*N*,*N*'-dicobalt(III)silver(I) tris(perchlorate) pentahydrate

Crystal data

$[AgCo_2(C_3H_5N_1O_2S_1)_2(C_2H_8N_2)_4](Cl_1O_4)_3{\cdot}5H_2O$	F_{000} = 1116
M_r = 1092.86	D_x = 1.898 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71069 Å
Hall symbol: C 2y	Cell parameters from 25 reflections
a = 16.542 (2) Å	θ = 14.6–15.0º
b = 9.050 (2) Å	μ = 1.77 mm^{-1}
c = 13.728 (2) Å	*T* = 296 (2) K
β = 111.507 (10)º	Rod, dark red
V = 1912.0 (6) Å^3	0.40 × 0.18 × 0.18 mm
Z = 2	

Data collection

Rigaku AFC-7S diffractometer	R_{int} = 0.015
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.5º
T = 296(2) K	h = 0→21
ω–2θ scans	k = 0→11
Absorption correction: ψ scan (North *et al.*, 1968)	l = −17→16
T_{min} = 0.537, T_{max} = 0.741	3 standard reflections
2426 measured reflections	every 150 reflections
2346 independent reflections	intensity decay: 14.4%
2219 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.023	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.6577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.060	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
2346 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
322 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
13 restraints	Extinction coefficient: 0.0150 (5)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983)
Secondary atom site location: difference Fourier map	Flack parameter: 0.001 (18)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)

Ag1	0.0000	0.31917 (5)	0.0000	0.04457 (14)	
Co1	0.21020 (3)	0.48714 (5)	0.22914 (3)	0.02666 (12)	
S1	0.14873 (5)	0.30161 (10)	0.11542 (6)	0.03258 (19)	
O1	0.0811 (2)	0.0540 (4)	0.3873 (3)	0.0581 (9)	
O2	0.22302 (18)	0.1037 (4)	0.4561 (2)	0.0458 (7)	
N1	0.2271 (2)	0.6004 (4)	0.1154 (2)	0.0395 (7)	
H1	0.1798	0.5912	0.0564	0.047*	
H2	0.2340	0.6967	0.1327	0.047*	
N2	0.3263 (2)	0.4071 (4)	0.2530 (3)	0.0396 (7)	
H3	0.3576	0.4039	0.3222	0.048*	
H4	0.3216	0.3145	0.2277	0.048*	
N3	0.09835 (19)	0.5808 (4)	0.2088 (3)	0.0383 (7)	
H5	0.0783	0.6268	0.1463	0.046*	
H6	0.0595	0.5112	0.2089	0.046*	
N4	0.2594 (2)	0.6494 (4)	0.3304 (2)	0.0364 (6)	
H7	0.2765	0.6141	0.3961	0.044*	
H8	0.3061	0.6878	0.3207	0.044*	
N5	0.1989 (2)	0.3614 (3)	0.3410 (2)	0.0322 (6)	
H9	0.2515	0.3238	0.3787	0.039*	
H10	0.1825	0.4186	0.3842	0.039*	
C1	0.1504 (3)	0.1644 (4)	0.2126 (3)	0.0372 (8)	
H11	0.1051	0.0919	0.1813	0.045*	
H12	0.2059	0.1135	0.2369	0.045*	
C2	0.1364 (2)	0.2377 (4)	0.3044 (3)	0.0317 (7)	
H13	0.0771	0.2771	0.2810	0.038*	
C3	0.1481 (2)	0.1233 (4)	0.3914 (3)	0.0361 (8)	
C4	0.3050 (3)	0.5450 (7)	0.0968 (4)	0.0573 (13)	
H14	0.2897	0.4603	0.0502	0.069*	
H15	0.3280	0.6216	0.0648	0.069*	
C5	0.3707 (3)	0.5023 (7)	0.2000 (4)	0.0551 (12)	
H16	0.4181	0.4487	0.1904	0.066*	
H17	0.3943	0.5896	0.2417	0.066*	
C6	0.1082 (3)	0.6900 (5)	0.2938 (4)	0.0477 (10)	
H18	0.0610	0.7610	0.2716	0.057*	
H19	0.1078	0.6402	0.3562	0.057*	
C7	0.1931 (3)	0.7657 (4)	0.3154 (4)	0.0456 (10)	
H20	0.1900	0.8290	0.2571	0.055*	
H21	0.2078	0.8261	0.3779	0.055*	
Cl1	0.0000	0.86644 (15)	0.0000	0.0397 (3)	
O3	0.0194 (6)	0.8851 (10)	0.1120 (5)	0.070 (2)	0.50
O4	0.0409 (7)	0.7347 (13)	−0.0117 (9)	0.112 (4)	0.50
O5	−0.0919 (4)	0.8481 (10)	−0.0499 (6)	0.067 (2)	0.50
O6	0.0282 (5)	0.9912 (12)	−0.0383 (7)	0.079 (2)	0.50
Cl2	0.37527 (6)	0.98034 (14)	0.19897 (9)	0.0495 (2)	
O7	0.3094 (11)	0.898 (2)	0.2056 (16)	0.115 (6)	0.50
O8	0.3534 (12)	1.1056 (13)	0.1333 (12)	0.121 (6)	0.50
O9	0.4166 (17)	1.056 (3)	0.2960 (10)	0.168 (10)	0.50
O10	0.4352 (8)	0.8937 (16)	0.1788 (16)	0.097 (6)	0.50
O11	0.2889 (9)	0.919 (2)	0.1446 (11)	0.084 (4)	0.50

O12	0.3949 (13)	1.028 (5)	0.1154 (12)	0.218 (17)	0.50
O13	0.3750 (11)	1.080 (2)	0.2633 (16)	0.159 (10)	0.50
O14	0.4421 (13)	0.887 (2)	0.248 (2)	0.193 (13)	0.50
O15	0.4028 (2)	0.3330 (6)	0.4736 (3)	0.0604 (9)	
H22	0.403 (4)	0.389 (6)	0.524 (4)	0.091*	
H23	0.419 (11)	0.247 (6)	0.497 (7)	0.091*	0.50
H24	0.454 (3)	0.309 (17)	0.482 (8)	0.091*	0.50
O16	0.1116 (4)	0.4563 (10)	0.4944 (4)	0.115 (2)	
H25	0.083 (6)	0.438 (14)	0.534 (6)	0.173*	
H26	0.156 (4)	0.510 (12)	0.530 (7)	0.173*	
O17	0.0413 (7)	0.2037 (15)	0.5497 (11)	0.096 (3)	0.50
H27	−0.013 (3)	0.20 (2)	0.538 (15)	0.144*	0.50
H28	0.053 (12)	0.131 (15)	0.517 (16)	0.144*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0396 (2)	0.0497 (3)	0.0313 (2)	0.000	−0.00251 (16)	0.000
Co1	0.0272 (2)	0.0267 (2)	0.0234 (2)	0.00172 (18)	0.00598 (16)	−0.00014 (18)
S1	0.0351 (4)	0.0334 (4)	0.0248 (4)	−0.0001 (4)	0.0058 (3)	−0.0024 (4)
O1	0.0459 (17)	0.067 (2)	0.064 (2)	−0.0068 (15)	0.0227 (15)	0.0198 (17)
O2	0.0473 (15)	0.0469 (16)	0.0363 (13)	0.0033 (14)	0.0072 (11)	0.0092 (13)
N1	0.0432 (16)	0.0415 (17)	0.0322 (14)	−0.0023 (15)	0.0119 (13)	0.0047 (14)
N2	0.0345 (15)	0.0474 (19)	0.0366 (16)	0.0048 (14)	0.0124 (13)	0.0015 (15)
N3	0.0332 (15)	0.0337 (15)	0.0421 (17)	0.0054 (13)	0.0068 (13)	−0.0008 (14)
N4	0.0412 (16)	0.0320 (15)	0.0321 (14)	−0.0028 (13)	0.0086 (12)	−0.0044 (13)
N5	0.0379 (15)	0.0315 (15)	0.0264 (13)	0.0027 (12)	0.0109 (12)	−0.0027 (11)
C1	0.044 (2)	0.0312 (18)	0.0295 (17)	0.0022 (16)	0.0056 (15)	0.0003 (15)
C2	0.0305 (17)	0.0318 (17)	0.0316 (17)	0.0029 (14)	0.0100 (14)	0.0057 (14)
C3	0.0417 (18)	0.031 (2)	0.0365 (17)	0.0003 (16)	0.0159 (15)	0.0012 (15)
C4	0.062 (3)	0.072 (3)	0.050 (2)	0.008 (2)	0.035 (2)	0.016 (2)
C5	0.038 (2)	0.074 (3)	0.060 (3)	0.001 (2)	0.0259 (19)	0.007 (3)
C6	0.048 (2)	0.042 (2)	0.054 (3)	0.0119 (19)	0.019 (2)	−0.0067 (19)
C7	0.059 (3)	0.0250 (17)	0.050 (2)	0.0016 (16)	0.016 (2)	−0.0096 (16)
Cl1	0.0393 (6)	0.0405 (7)	0.0334 (6)	0.000	0.0064 (5)	0.000
O3	0.093 (5)	0.078 (5)	0.034 (3)	−0.023 (5)	0.017 (3)	−0.007 (3)
O4	0.117 (9)	0.099 (7)	0.088 (7)	0.074 (6)	−0.002 (6)	−0.025 (6)
O5	0.038 (3)	0.080 (6)	0.069 (4)	−0.008 (4)	0.002 (3)	−0.008 (4)
O6	0.073 (5)	0.083 (6)	0.090 (6)	−0.017 (5)	0.039 (4)	0.026 (6)
Cl2	0.0404 (5)	0.0508 (6)	0.0594 (6)	−0.0013 (5)	0.0209 (4)	−0.0041 (5)
O7	0.107 (13)	0.077 (8)	0.215 (19)	−0.032 (9)	0.120 (14)	−0.020 (13)
O8	0.185 (17)	0.056 (6)	0.096 (10)	0.015 (7)	0.021 (9)	0.039 (6)
O9	0.25 (2)	0.159 (18)	0.050 (6)	−0.088 (18)	0.008 (11)	−0.023 (8)
O10	0.060 (7)	0.075 (7)	0.174 (16)	−0.003 (6)	0.063 (10)	−0.041 (10)
O11	0.054 (5)	0.083 (8)	0.108 (9)	−0.021 (5)	0.021 (6)	−0.006 (8)
O12	0.135 (15)	0.45 (5)	0.067 (7)	−0.13 (2)	0.039 (9)	0.004 (18)
O13	0.097 (9)	0.140 (13)	0.173 (19)	0.042 (9)	−0.028 (10)	−0.103 (14)
O14	0.112 (12)	0.132 (15)	0.26 (3)	0.089 (11)	−0.015 (15)	−0.002 (18)

O15	0.062 (2)	0.076 (3)	0.0410 (16)	−0.007 (2)	0.0156 (15)	−0.0118 (19)
O16	0.104 (4)	0.169 (7)	0.089 (3)	−0.027 (4)	0.054 (3)	−0.029 (4)
O17	0.083 (6)	0.113 (9)	0.109 (9)	−0.020 (6)	0.054 (6)	−0.028 (7)

Geometric parameters (Å, °)

Ag1—S1^{i}	2.3938 (9)	C2—H13	0.9800
Ag1—S1	2.3938 (9)	C4—C5	1.486 (7)
Co1—N3	1.960 (3)	C4—H14	0.9700
Co1—N2	1.964 (3)	C4—H15	0.9700
Co1—N1	1.972 (3)	C5—H16	0.9700
Co1—N5	1.975 (3)	C5—H17	0.9700
Co1—N4	1.980 (3)	C6—C7	1.492 (6)
Co1—S1	2.2642 (10)	C6—H18	0.9700
S1—C1	1.815 (4)	C6—H19	0.9700
O1—C3	1.256 (5)	C7—H20	0.9700
O2—C3	1.245 (5)	C7—H21	0.9700
N1—C4	1.490 (5)	Cl1—O6	1.396 (8)
N1—H1	0.9000	Cl1—O4	1.409 (8)
N1—H2	0.9000	Cl1—O5	1.430 (6)
N2—C5	1.486 (6)	Cl1—O3	1.462 (6)
N2—H3	0.9000	Cl2—O13	1.264 (15)
N2—H4	0.9000	Cl2—O7	1.351 (14)
N3—C6	1.492 (5)	Cl2—O14	1.359 (16)
N3—H5	0.9000	Cl2—O10	1.370 (11)
N3—H6	0.9000	Cl2—O12	1.372 (15)
N4—C7	1.479 (5)	Cl2—O8	1.410 (10)
N4—H7	0.9000	Cl2—O9	1.430 (15)
N4—H8	0.9000	Cl2—O11	1.459 (14)
N5—C2	1.482 (5)	O15—H22	0.85 (5)
N5—H9	0.9000	O15—H23	0.84 (2)
N5—H10	0.9000	O15—H24	0.84 (2)
C1—C2	1.516 (5)	O16—H25	0.85 (9)
C1—H11	0.9700	O16—H26	0.86 (10)
C1—H12	0.9700	O17—H27	0.85 (2)
C2—C3	1.538 (5)	O17—H28	0.85 (2)
S1^{i}—Ag1—S1	172.38 (5)	N5—C2—C1	108.2 (3)
N3—Co1—N2	175.89 (16)	N5—C2—C3	111.8 (3)
N3—Co1—N1	93.59 (14)	C1—C2—C3	109.7 (3)
N2—Co1—N1	84.87 (14)	N5—C2—H13	109.0
N3—Co1—N5	90.38 (13)	C1—C2—H13	109.0
N2—Co1—N5	91.31 (14)	C3—C2—H13	109.0
N1—Co1—N5	175.53 (14)	O2—C3—O1	126.4 (4)
N3—Co1—N4	84.43 (14)	O2—C3—C2	117.3 (3)
N2—Co1—N4	91.80 (14)	O1—C3—C2	116.3 (3)
N1—Co1—N4	91.68 (15)	C5—C4—N1	107.5 (4)
N5—Co1—N4	90.76 (13)	C5—C4—H14	110.2
N3—Co1—S1	93.46 (10)	N1—C4—H14	110.2

N2—Co1—S1	90.35 (11)	C5—C4—H15	110.2
N1—Co1—S1	89.86 (11)	N1—C4—H15	110.2
N5—Co1—S1	87.84 (9)	H14—C4—H15	108.5
N4—Co1—S1	177.46 (10)	N2—C5—C4	107.3 (4)
C1—S1—Co1	96.81 (12)	N2—C5—H16	110.3
C1—S1—Ag1	105.49 (13)	C4—C5—H16	110.3
Co1—S1—Ag1	120.00 (4)	N2—C5—H17	110.3
C4—N1—Co1	110.1 (3)	C4—C5—H17	110.3
C4—N1—H1	109.6	H16—C5—H17	108.5
Co1—N1—H1	109.6	C7—C6—N3	106.6 (3)
C4—N1—H2	109.6	C7—C6—H18	110.4
Co1—N1—H2	109.6	N3—C6—H18	110.4
H1—N1—H2	108.2	C7—C6—H19	110.4
C5—N2—Co1	109.5 (3)	N3—C6—H19	110.4
C5—N2—H3	109.8	H18—C6—H19	108.6
Co1—N2—H3	109.8	N4—C7—C6	107.2 (3)
C5—N2—H4	109.8	N4—C7—H20	110.3
Co1—N2—H4	109.8	C6—C7—H20	110.3
H3—N2—H4	108.2	N4—C7—H21	110.3
C6—N3—Co1	110.4 (2)	C6—C7—H21	110.3
C6—N3—H5	109.6	H20—C7—H21	108.5
Co1—N3—H5	109.6	O6—Cl1—O4	113.6 (7)
C6—N3—H6	109.6	O6—Cl1—O5	110.9 (5)
Co1—N3—H6	109.6	O4—Cl1—O5	108.5 (6)
H5—N3—H6	108.1	O6—Cl1—O3	109.1 (5)
C7—N4—Co1	109.7 (2)	O4—Cl1—O3	106.8 (6)
C7—N4—H7	109.7	O5—Cl1—O3	107.5 (5)
Co1—N4—H7	109.7	O13—Cl2—O14	107.9 (13)
C7—N4—H8	109.7	O7—Cl2—O10	111.0 (10)
Co1—N4—H8	109.7	O13—Cl2—O12	115 (2)
H7—N4—H8	108.2	O14—Cl2—O12	102.4 (17)
C2—N5—Co1	115.1 (2)	O7—Cl2—O8	117.5 (11)
C2—N5—H9	108.5	O10—Cl2—O8	111.5 (10)
Co1—N5—H9	108.5	O7—Cl2—O9	108.9 (12)
C2—N5—H10	108.5	O10—Cl2—O9	109.2 (13)
Co1—N5—H10	108.5	O8—Cl2—O9	97.6 (11)
H9—N5—H10	107.5	O13—Cl2—O11	112.1 (11)
C2—C1—S1	110.2 (3)	O14—Cl2—O11	118.9 (13)
C2—C1—H11	109.6	O12—Cl2—O11	100.4 (9)
S1—C1—H11	109.6	H22—O15—H23	109 (4)
C2—C1—H12	109.6	H22—O15—H24	109 (4)
S1—C1—H12	109.6	H25—O16—H26	108 (9)
H11—C1—H12	108.1	H27—O17—H28	108 (4)
N3—Co1—S1—C1	−98.88 (17)	N1—Co1—N4—C7	79.2 (3)
N2—Co1—S1—C1	82.67 (17)	N5—Co1—N4—C7	−104.6 (3)
N1—Co1—S1—C1	167.53 (16)	N3—Co1—N5—C2	75.3 (3)
N5—Co1—S1—C1	−8.63 (16)	N2—Co1—N5—C2	−108.4 (3)
N3—Co1—S1—Ag1	13.43 (11)	N4—Co1—N5—C2	159.7 (2)
N2—Co1—S1—Ag1	−165.03 (11)	S1—Co1—N5—C2	−18.1 (2)

N1—Co1—S1—Ag1	−80.16 (11)	Co1—S1—C1—C2	34.0 (3)
N5—Co1—S1—Ag1	103.68 (10)	Ag1—S1—C1—C2	−89.7 (3)
N3—Co1—N1—C4	−173.1 (3)	Co1—N5—C2—C1	44.4 (3)
N2—Co1—N1—C4	10.7 (3)	Co1—N5—C2—C3	165.4 (2)
N4—Co1—N1—C4	102.4 (3)	S1—C1—C2—N5	−51.5 (3)
S1—Co1—N1—C4	−79.7 (3)	S1—C1—C2—C3	−173.7 (3)
N1—Co1—N2—C5	16.7 (3)	N5—C2—C3—O2	−32.8 (5)
N5—Co1—N2—C5	−165.6 (3)	C1—C2—C3—O2	87.2 (4)
N4—Co1—N2—C5	−74.8 (3)	N5—C2—C3—O1	150.2 (4)
S1—Co1—N2—C5	106.5 (3)	C1—C2—C3—O1	−89.7 (4)
N1—Co1—N3—C6	−105.3 (3)	Co1—N1—C4—C5	−35.7 (5)
N5—Co1—N3—C6	76.8 (3)	Co1—N2—C5—C4	−40.6 (5)
N4—Co1—N3—C6	−14.0 (3)	N1—C4—C5—N2	49.3 (6)
S1—Co1—N3—C6	164.6 (3)	Co1—N3—C6—C7	38.9 (4)
N3—Co1—N4—C7	−14.3 (3)	Co1—N4—C7—C6	39.3 (4)
N2—Co1—N4—C7	164.1 (3)	N3—C6—C7—N4	−50.3 (5)

Symmetry codes: (i) −*x*, *y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O12^{ii}	0.90	2.30	3.14 (2)	155
N1—H2···O11	0.90	2.19	3.034 (19)	157
N1—H2···O7	0.90	2.23	3.066 (18)	155
N2—H3···O15	0.90	2.04	2.899 (5)	160
N2—H4···O13^{iii}	0.90	2.28	3.057 (19)	144
N3—H5···O4	0.90	2.25	3.146 (13)	174
N3—H6···O10^{iv}	0.90	2.21	3.083 (12)	162
N4—H7···O2^{v}	0.90	2.03	2.868 (4)	155
N4—H8···O7	0.90	2.49	3.117 (16)	128
N4—H8···O17^{v}	0.90	2.50	3.138 (13)	128
N5—H9···O15	0.90	2.36	3.201 (5)	155
N5—H10···O16	0.90	2.25	3.079 (6)	152
O15—H22···O1^{v}	0.85 (5)	1.89 (3)	2.711 (5)	162 (7)
O15—H24···O15^{vi}	0.84 (2)	2.23 (5)	3.027 (8)	158 (12)
O16—H25···O17	0.85 (9)	2.27 (11)	2.794 (15)	120 (10)
O16—H26···O2^{v}	0.86 (10)	2.12 (4)	2.891 (7)	149 (7)
O17—H27···O1^{vii}	0.85 (2)	2.2 (2)	2.822 (12)	126 (19)
O17—H28···O1	0.85 (2)	2.12 (12)	2.884 (12)	149 (19)

Symmetry codes: (ii) −*x*+1/2, *y*−1/2, −*z*; (iii) *x*, *y*−1, *z*; (iv) *x*−1/2, *y*−1/2, *z*; (v) −*x*+1/2, *y*+1/2, −*z*+1; (vi) −*x*+1, *y*, −*z*+1; (vii) −*x*, *y*, −*z*+1.

Fig. 1

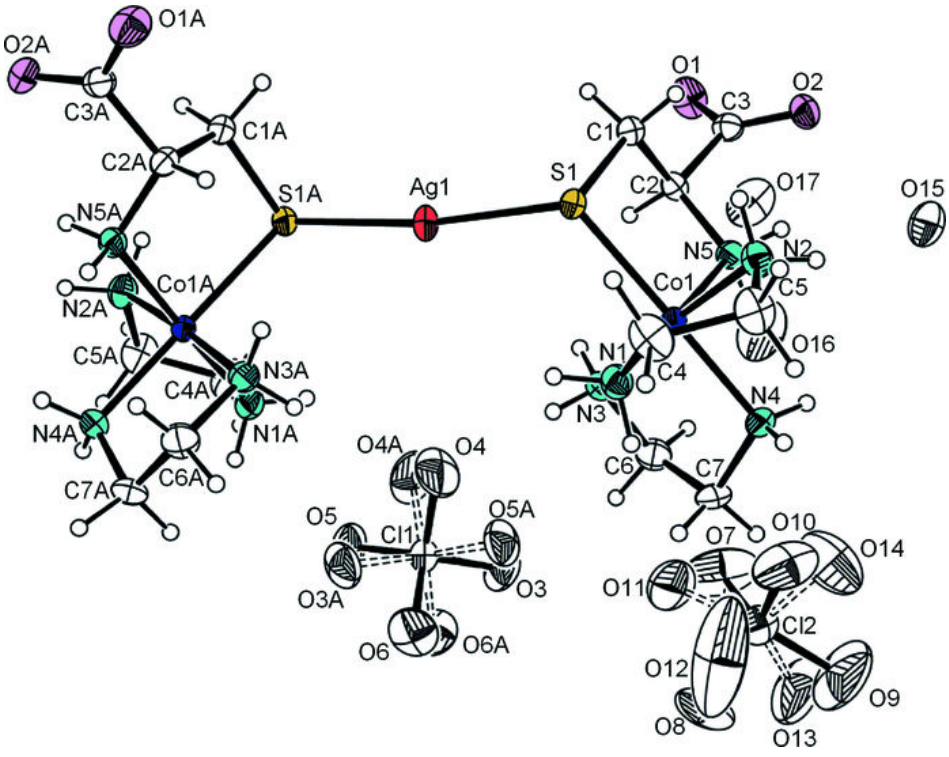
O1A
O2A
C3A
C1A
C2A
S1A
Ag1
S1
O1
C3
O2
C1
C2
O17
O15
N5A
N5
N2
N2A
Co1A
Co1
C5
C5A
N3A
C4A
C4
O16
N1
N4A
N1A
N3
N4
O4A
O4
C6
C7
C7A
C6A
O5
Cl1
O5A
O7
O10
O14
O3A
O3
O11
Cl2
O6
O6A
O12
O9
O8
O13

Fig. 2