

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

## **cyclo-Tetrakis( $\mu_2$ -3-sulfidopropyl- $\kappa^3C^1,S:S$ )tetrakis[chloridocobalt(III)]. Retraction**

Shafique Ahmad Awan,<sup>a</sup> M. Nawaz Tahir,<sup>b\*</sup> Iram Khushi  
Muhammad,<sup>c</sup> Saeed Ahmad<sup>c</sup> and Muhammad Ilyas Tariq<sup>d</sup>

<sup>a</sup>PAEC, PO Box No. 1114, Islamabad GPO 44000, Pakistan, <sup>b</sup>Department of Physics, University of Sargodha, Sargodha, Pakistan, <sup>c</sup>Department of Chemistry, University of Engineering and Technology, Lahore 54890, Pakistan, and <sup>d</sup>Department of Chemistry, University of Sargodha, Sargodha, Pakistan  
Correspondence e-mail: dmntahir\_uos@yahoo.com

Received 18 May 2012; accepted 18 May 2012

The paper by Awan *et al.* [*Acta Cryst.* (2011), E67, m576–m577] is retracted. It has subsequently been shown that the crystal studied was an already known zinc compound,  $[Zn_4Cl_4(C_2H_6NS)_4]$ .

---

We wish to withdraw the paper by Awan *et al.* (2011) on a compound reported to be  $[Co_4Cl_4(C_3H_6S)_4]$ . It has subsequently been shown that the crystal studied was a related zinc compound,  $[Zn_4Cl_4(C_2H_6NS)_4]$ , which was reported by Fleischer *et al.* (2006).

### References

- Awan, S. A., Tahir, M. N., Muhammad, I. K., Ahmad, S. & Tariq, M. I. (2011). *Acta Cryst.* E67, m576–m577.  
Fleischer, H., Hardt, S. & Schollmeyer, D. (2006). *Inorg. Chem.* 45, 8318–8325.

## cyclo-Tetrakis( $\mu_2$ -3-sulfidopropyl- $\kappa^3C^1,S:S$ )tetrakis[chloridocobalt(III)]

Shafique Ahmad Awan,<sup>a</sup> M. Nawaz Tahir,<sup>b\*</sup> Iram Khushi Muhammad,<sup>c</sup> Saeed Ahmad<sup>c</sup> and Muhammad Ilyas Tariq<sup>d</sup>

<sup>a</sup>PAEC, PO Box # 1114, Islamabad GPO 44000, Pakistan, <sup>b</sup>Department of Physics, University of Sargodha, Sargodha, Pakistan, <sup>c</sup>Department of Chemistry, University of Engineering and Technology, Lahore 54890, Pakistan, and <sup>d</sup>Department of

Chemistry, University of Sargodha, Sargodha, Pakistan

Correspondence e-mail: dmntahir\_uos@yahoo.com

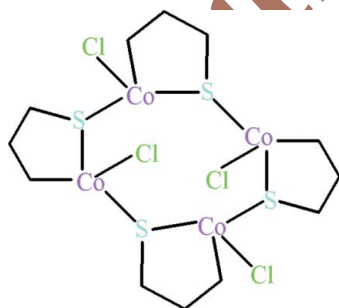
Received 2 April 2011; accepted 7 April 2011

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.011$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.125; data-to-parameter ratio = 19.7.

In the centrosymmetric title compound,  $[Co_4Cl_4(C_3H_6S)_4]$ , the two independent  $Co^{III}$  ions are each coordinated in a distorted tetrahedral geometry by one C, one Cl and two S atoms. The molecules are stabilized by  $C-H \cdots Cl$  hydrogen bonds. In the crystal, intermolecular  $C-H \cdots Cl$  and  $C-H \cdots S$  hydrogen bonds with  $R_2^2(8)$ ,  $R_4^2(8)$  and  $R_2^2(6)$  ring motifs generate a polymeric network.

### Related literature

For related background see: Shahid *et al.* (2009); Altaf *et al.* (2010). For related structures, see: Duan *et al.* (1997); Tremel *et al.* (1992). For graph-set notation, see: Bernstein *et al.* (1995).



### Experimental

#### Crystal data

$[Co_4Cl_4(C_3H_6S)_4]$   
 $M_r = 674.07$   
 Monoclinic,  $C2/c$   
 $a = 23.6135$  (12) Å  
 $b = 7.8465$  (3) Å  
 $c = 16.8693$  (9) Å  
 $\beta = 130.440$  (4)°

$V = 2378.9$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.54$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.24 \times 0.16 \times 0.14$  mm

#### Data collection

Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{min} = 0.675$ ,  $T_{max} = 0.683$

13736 measured reflections  
 2152 independent reflections  
 1782 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.058$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.125$   
 $S = 1.04$   
 2152 reflections

109 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.70$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.62$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Co1—Cl1	2.228 (2)	Co2—S1	2.305 (2)
Co1—S1	2.3570 (17)	Co2—S2 <sup>i</sup>	2.3648 (16)
Co1—S2	2.318 (2)	Co2—C6 <sup>i</sup>	2.051 (6)
Co1—C3	2.038 (6)	S1—C1	1.826 (7)
Co2—Cl2	2.236 (3)	S2—C4	1.837 (8)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C3—H3A <sup>ii</sup> ···S2 <sup>ii</sup>	0.97	2.57	3.539 (8)	175
C3—H3B···Cl2 <sup>iii</sup>	0.97	2.74	3.512 (7)	138
C3—H3B···Cl2 <sup>iv</sup>	0.97	2.81	3.412 (6)	121
C6—H6A···Cl1 <sup>i</sup>	0.97	2.62	3.379 (7)	135
C6—H6B···Cl1 <sup>v</sup>	0.97	2.48	3.343 (7)	148

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP III (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2349).

### References

- Altaf, M., Stoeckli-Evans, H., Batool, S. S., Isab, A. A., Ahmad, S., Saleem, M., Awan, S. A. & Shaheen, M. A. (2010). *J. Coord. Chem.* **63**, 1176–1185.  
 Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (2009). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Burnett, M. N. & Johnson, C. K. (1996). *ORTEP III*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

Duan, C.-Y., Liu, Z.-H., You, X.-Z., Xue, F. & Mak, T. C. W. (1997). *Chem. Commun.* pp. 381–382.  
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
Shahid, M., Rüffer, T., Lang, H., Awan, S. A. & Ahmad, S. (2009). *J. Coord. Chem.* **62**, 440–445.

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.  
Tremel, W., Krebs, B., Greiwe, K., Simon, W., Stephan, H.-O. & Henkel, G. (1992). *Z. Naturforsch. Teil B*, **47**, 1580–1592.

Article retracted

## supporting information

*Acta Cryst.* (2011). E67, m576–m577 [doi:10.1107/S1600536811013067]

**cyclo-Tetrakis( $\mu_2$ -3-sulfidopropyl- $\kappa^3C^1, S:S$ )tetrakis[chloridocobalt(III)]**

**Shafique Ahmad Awan, M. Nawaz Tahir, Iram Khushi Muhammad, Saeed Ahmad and Muhammad Ilyas Tariq**

**S1. Comment**

Recently, we have reported the crystal structure of zinc(II) and mercury(II) complexes of pyrrolidinedithiocarbamate (PDTC) (Shahid *et al.*, 2009) & (Altaf, *et al.*, 2010). In the present study, we attempted to prepare a cobalt(II) complex with PDTC, but surprisingly the title compound (I, Fig. 1) was isolated, the crystal structure of which is being presented.

The crystal structure of (II) i.e., tetranuclear molecular square[Co(HL)]<sub>4</sub><sup>4+</sup> [H<sub>2</sub>L = tetra(2-pyridyl)thiocarbazone] (Duan *et al.*, 1997) and (III) i.e., bis(tetraethylammonium) hexakis( $\mu_2$ -phenylthiolato)-tetrachloro-tetra-cobalt acetonitrile solvate (Tremel *et al.*, 1992) have been published which are related to the title compound (I).

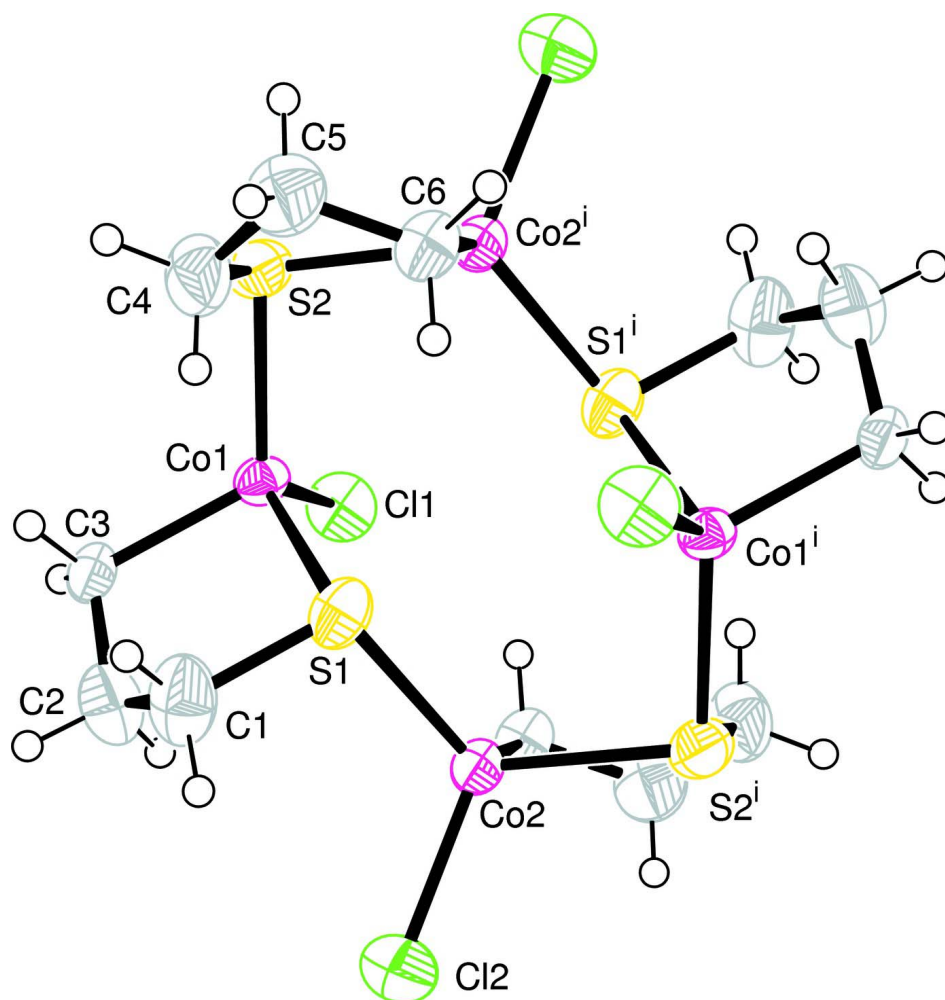
The crystal structure of the title compound (I) is centrosymmetric. The coordination around two independent Co<sup>iii</sup> ions is distorted tetrahedral from one C, Cl and two S-atoms. The range of Co—C [2.038 (6)–2.051 (6) Å] is shorter compared to Co—S [2.305 (2)–2.3648 (16) Å]. The Co—Cl bonds have values of 2.228 (2) and 2.236 (2) Å. The important bond distances are given in Table 1. The molecules are stabilized in the form of a polymeric network due to C—H···Cl and C—H···S intermolecular H-bonds (Table 2) forming  $R_2^2(8)$ ,  $R_4^2(8)$  and  $R_2^2(6)$  ring motifs (Bernstein *et al.*, 1995).

**S2. Experimental**

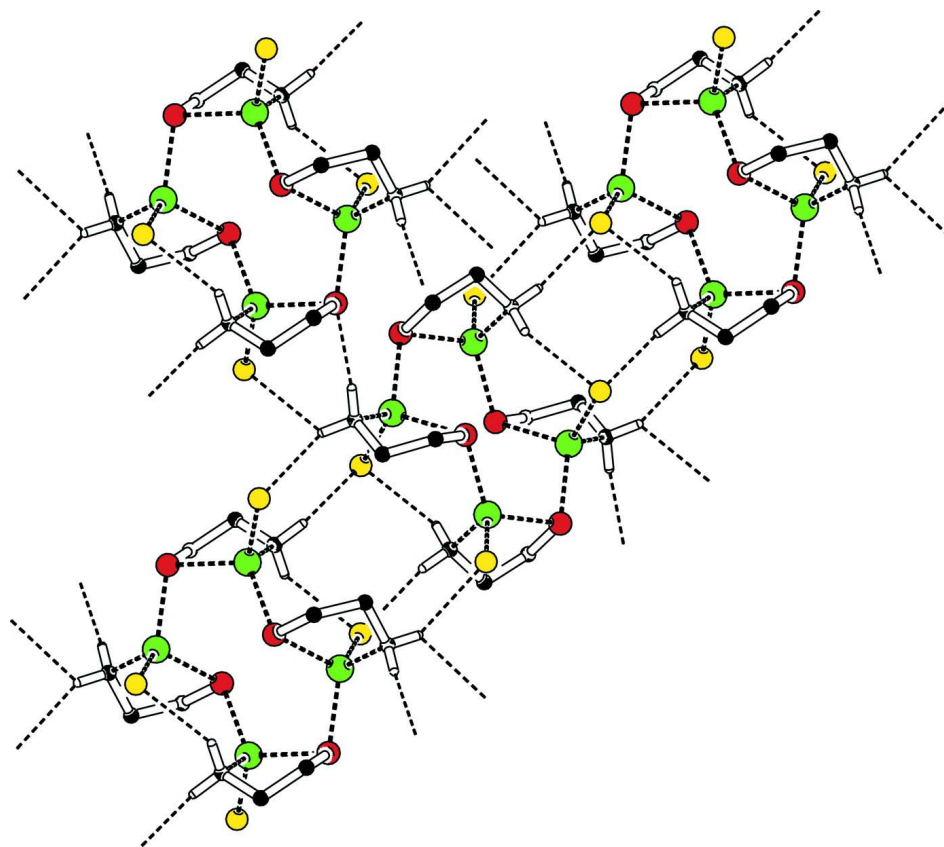
The title compound was prepared by adding two equivalents of ammonium pyrrolidinedithiocarbamate (PDTC) in 15 ml methanol to a solution of CoCl<sub>2</sub>·6H<sub>2</sub>O in 10 ml methanol. The addition of PDTC in the pink colored metal ion solution resulted in the formation of green precipitates immediately. After stirring for half an hour, the precipitates were filtered off and dried. The blackish brown crystals of the title compound (I) were prepared by dissolving 0.03 g precipitates in 3 ml DMSO on heating in a vial and then cooling the resulting solution at room temperature.

**S3. Refinement**

The H-atoms were positioned geometrically (C—H = 0.97 Å) and were included in the refinement in the riding model approximation, with  $U_{iso}(H) = xU_{eq}(C)$ , where  $x = 1.2$  for all H-atoms.

**Figure 1**

View of the centrosymmetric title compound. Symmetry code  $i = -x + 1/2, -y - 1/2, -z + 1$ . The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii.

**Figure 2**

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form a polymeric network with ring motifs. H-atoms not involved in H-bondings are omitted for clarity.

***cyclo*-Tetrakis( $\mu_2$ -3-sulfidopropyl- $\kappa^3C^1, S:S$ )tetrakis[chloridocobalt(III)]**

*Crystal data*

[Co<sub>4</sub>Cl<sub>4</sub>(C<sub>3</sub>H<sub>6</sub>S)<sub>4</sub>]  
*M<sub>r</sub>* = 674.07  
 Monoclinic, *C2/c*  
 Hall symbol: -C 2yc  
*a* = 23.6135 (12) Å  
*b* = 7.8465 (3) Å  
*c* = 16.8693 (9) Å  
 $\beta$  = 130.440 (4)°  
*V* = 2378.9 (2) Å<sup>3</sup>  
*Z* = 4

*F*(000) = 1344  
*D<sub>x</sub>* = 1.882 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å  
 Cell parameters from 1782 reflections  
 $\theta$  = 2.3–25.2°  
 $\mu$  = 3.54 mm<sup>-1</sup>  
*T* = 296 K  
 Prisms, white  
 0.24 × 0.16 × 0.14 mm

*Data collection*

Bruker Kappa APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 8.10 pixels mm<sup>-1</sup>  
 $\omega$  scans

Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2005)  
*T<sub>min</sub>* = 0.675, *T<sub>max</sub>* = 0.683  
 13736 measured reflections  
 2152 independent reflections  
 1782 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.058

$\theta_{\max} = 25.2^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -28 \rightarrow 28$

$k = -9 \rightarrow 8$   
 $l = -20 \rightarrow 20$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.125$   
 $S = 1.04$   
 2152 reflections  
 109 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 15.5359P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.70 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.17597 (4)	-0.17781 (9)	0.30876 (5)	0.0323 (2)
Co2	0.14629 (4)	-0.12119 (9)	0.50575 (5)	0.0336 (2)
Cl1	0.09923 (9)	-0.3988 (2)	0.25283 (12)	0.0555 (5)
Cl2	0.07469 (11)	0.0860 (3)	0.49043 (15)	0.0694 (7)
S1	0.21157 (8)	-0.0272 (2)	0.45587 (11)	0.0460 (4)
S2	0.28224 (8)	-0.2358 (2)	0.33225 (11)	0.0481 (5)
C1	0.1631 (4)	0.1666 (8)	0.3814 (5)	0.066 (3)
C2	0.0959 (4)	0.1316 (9)	0.2708 (5)	0.061 (2)
C3	0.1163 (3)	-0.0287 (7)	0.2182 (4)	0.0362 (17)
C4	0.3356 (4)	-0.0372 (9)	0.3904 (6)	0.064 (3)
C5	0.4140 (4)	-0.0689 (10)	0.4862 (6)	0.065 (3)
C6	0.4164 (3)	-0.1622 (7)	0.5638 (4)	0.0417 (17)
H1A	0.14799	0.22914	0.41469	0.0787*
H1B	0.19711	0.23811	0.38263	0.0787*
H2A	0.05934	0.07031	0.26878	0.0733*
H2B	0.07391	0.23855	0.23404	0.0733*
H3A	0.14572	0.09690	0.20863	0.0435*
H3B	0.07165	-0.00820	0.15024	0.0435*
H4A	0.33533	0.02242	0.33979	0.0769*
H4B	0.31166	0.03559	0.40757	0.0769*
H5A	0.43922	-0.13460	0.46849	0.0783*
H5B	0.43980	0.03894	0.51537	0.0783*
H6A	0.39644	-0.09200	0.58805	0.0502*
H6B	0.46733	-0.19168	0.62322	0.0502*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0275 (4)	0.0399 (4)	0.0300 (4)	-0.0012 (3)	0.0189 (3)	-0.0025 (3)
Co2	0.0338 (4)	0.0373 (4)	0.0312 (4)	-0.0014 (3)	0.0217 (3)	0.0004 (3)
C11	0.0496 (9)	0.0537 (9)	0.0545 (9)	-0.0089 (7)	0.0299 (8)	-0.0081 (7)
C12	0.0683 (11)	0.0733 (11)	0.0725 (12)	0.0219 (9)	0.0483 (10)	0.0114 (9)
S1	0.0485 (8)	0.0520 (8)	0.0377 (7)	-0.0099 (7)	0.0281 (7)	-0.0045 (6)
S2	0.0407 (8)	0.0667 (10)	0.0398 (8)	0.0055 (7)	0.0274 (7)	0.0030 (7)
C1	0.091 (5)	0.045 (4)	0.054 (4)	-0.010 (4)	0.044 (4)	-0.004 (3)
C2	0.066 (4)	0.047 (4)	0.056 (4)	0.003 (3)	0.033 (4)	0.008 (3)
C3	0.034 (3)	0.045 (3)	0.030 (3)	-0.003 (2)	0.021 (2)	0.005 (2)
C4	0.056 (4)	0.064 (4)	0.074 (5)	0.000 (3)	0.043 (4)	0.022 (4)
C5	0.056 (4)	0.067 (4)	0.074 (5)	-0.010 (3)	0.043 (4)	0.003 (4)
C6	0.038 (3)	0.047 (3)	0.037 (3)	-0.012 (2)	0.023 (3)	-0.005 (2)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Co1—C11	2.228 (2)	C5—C6	1.469 (11)
Co1—S1	2.3570 (17)	C1—H1A	0.9700
Co1—S2	2.318 (2)	C1—H1B	0.9700
Co1—C3	2.038 (6)	C2—H2A	0.9700
Co2—C12	2.236 (3)	C2—H2B	0.9700
Co2—S1	2.305 (2)	C3—H3A	0.9700
Co2—S2 <sup>i</sup>	2.3648 (16)	C3—H3B	0.9700
Co2—C6 <sup>i</sup>	2.051 (6)	C4—H4A	0.9700
S1—C1	1.826 (7)	C4—H4B	0.9700
S2—C4	1.837 (8)	C5—H5A	0.9700
C1—C2	1.495 (10)	C5—H5B	0.9700
C2—C3	1.492 (11)	C6—H6A	0.9700
C4—C5	1.490 (13)	C6—H6B	0.9700
Co1...H4A <sup>ii</sup>	3.3200	S2...H4A <sup>ii</sup>	3.0500
C11...C3	3.473 (6)	C2...C12 <sup>iv</sup>	3.570 (7)
C11...C6 <sup>iii</sup>	3.343 (7)	C3...C11	3.473 (6)
C11...C6 <sup>i</sup>	3.379 (7)	C3...S1	3.103 (5)
C12...C1	3.623 (11)	C3...S2	3.686 (7)
C12...C3 <sup>iv</sup>	3.512 (7)	C3...C1	2.455 (9)
C12...C6 <sup>i</sup>	3.492 (6)	C3...C12 <sup>iv</sup>	3.512 (7)
C12...C3 <sup>v</sup>	3.412 (6)	C3...C12 <sup>viii</sup>	3.412 (6)
C12...S1	3.744 (4)	C3...S2 <sup>ix</sup>	3.539 (8)
C12...C2 <sup>iv</sup>	3.570 (7)	C6...C11 <sup>i</sup>	3.379 (7)
C11...H4A <sup>ii</sup>	2.8900	C6...C12 <sup>i</sup>	3.491 (6)
C11...H2B <sup>vi</sup>	2.8800	C6...C11 <sup>x</sup>	3.343 (7)
C11...H6A <sup>i</sup>	2.6200	H1A...C12	2.9600
C11...H6B <sup>iii</sup>	2.4800	H1B...H3A	2.5900
C12...H1A	2.9600	H1B...S1 <sup>vii</sup>	3.1000
C12...H3B <sup>v</sup>	2.8100	H2A...H2A <sup>iv</sup>	2.4400



Cl2...H3B <sup>iv</sup>	2.7400	H2B...C11 <sup>xi</sup>	2.8800
Cl2...H5B <sup>vii</sup>	2.9600	H3A...H1B	2.5900
S1...Cl2	3.744 (4)	H3A...S2 <sup>ix</sup>	2.5700
S1...S2	3.785 (3)	H3B...Cl2 <sup>iv</sup>	2.7400
S1...C2	2.774 (7)	H3B...Cl2 <sup>viii</sup>	2.8100
S1...C3	3.103 (5)	H4A...Co1 <sup>ix</sup>	3.3200
S1...Co1 <sup>i</sup>	3.8074 (16)	H4A...C11 <sup>ix</sup>	2.8900
S1...S1 <sup>i</sup>	3.773 (2)	H4A...S2 <sup>ix</sup>	3.0500
S2...C3 <sup>ii</sup>	3.539 (8)	H4B...S1	3.0000
S2...S1	3.785 (3)	H4B...H6A	2.5200
S2...C3	3.686 (7)	H5B...Cl2 <sup>vii</sup>	2.9600
S1...H4B	3.0000	H6A...H4B	2.5200
S1...H1B <sup>vii</sup>	3.1000	H6A...C11 <sup>i</sup>	2.6200
S2...H3A <sup>ii</sup>	2.5700	H6B...C11 <sup>x</sup>	2.4800
Cl1—Co1—S1	118.22 (8)	C2—C1—H1B	109.00
Cl1—Co1—S2	114.37 (8)	H1A—C1—H1B	108.00
Cl1—Co1—C3	108.9 (2)	C1—C2—H2A	110.00
S1—Co1—S2	108.14 (7)	C1—C2—H2B	109.00
S1—Co1—C3	89.52 (17)	C3—C2—H2A	110.00
S2—Co1—C3	115.5 (2)	C3—C2—H2B	109.00
Cl2—Co2—S1	111.09 (9)	H2A—C2—H2B	108.00
Cl2—Co2—S2 <sup>i</sup>	113.44 (8)	Co1—C3—H3A	110.00
Cl2—Co2—C6 <sup>i</sup>	109.0 (2)	Co1—C3—H3B	110.00
S1—Co2—S2 <sup>i</sup>	115.39 (8)	C2—C3—H3A	110.00
S1—Co2—C6 <sup>i</sup>	117.5 (2)	C2—C3—H3B	110.00
S2 <sup>i</sup> —Co2—C6 <sup>i</sup>	88.68 (15)	H3A—C3—H3B	108.00
Co1—S1—Co2	110.96 (8)	S2—C4—H4A	109.00
Co1—S1—C1	93.3 (2)	S2—C4—H4B	109.00
Co2—S1—C1	104.4 (4)	C5—C4—H4A	109.00
Co1—S2—C4	102.5 (4)	C5—C4—H4B	109.00
Co1—S2—Co2 <sup>i</sup>	99.94 (8)	H4A—C4—H4B	108.00
Co2 <sup>i</sup> —S2—C4	93.3 (2)	C4—C5—H5A	110.00
S1—C1—C2	113.0 (5)	C4—C5—H5B	110.00
C1—C2—C3	110.6 (8)	C6—C5—H5A	109.00
Co1—C3—C2	108.5 (4)	C6—C5—H5B	110.00
S2—C4—C5	112.1 (5)	H5A—C5—H5B	108.00
C4—C5—C6	110.6 (9)	C5—C6—H6A	110.00
Co2 <sup>i</sup> —C6—C5	107.9 (4)	C5—C6—H6B	110.00
S1—C1—H1A	109.00	H6A—C6—H6B	108.00
S1—C1—H1B	109.00	Co2 <sup>i</sup> —C6—H6A	110.00
C2—C1—H1A	109.00	Co2 <sup>i</sup> —C6—H6B	110.00
Cl1—Co1—S1—Co2	-7.06 (11)	S2 <sup>i</sup> —Co2—S1—C1	-148.1 (2)
Cl1—Co1—S1—C1	-113.8 (3)	C6 <sup>i</sup> —Co2—S1—Co1	10.1 (2)
S2—Co1—S1—Co2	-139.02 (7)	C6 <sup>i</sup> —Co2—S1—C1	109.3 (3)
S2—Co1—S1—C1	114.2 (3)	Cl2—Co2—S2 <sup>i</sup> —Co1 <sup>i</sup>	-145.79 (9)
C3—Co1—S1—Co2	104.3 (2)	Cl2—Co2—S2 <sup>i</sup> —C4 <sup>i</sup>	110.9 (4)

C3—Co1—S1—C1	-2.5 (4)	S1—Co2—S2 <sup>i</sup> —Co1 <sup>i</sup>	-16.01 (8)
Cl1—Co1—S2—C4	-174.3 (3)	S1—Co2—S2 <sup>i</sup> —C4 <sup>i</sup>	-119.3 (4)
Cl1—Co1—S2—Co2 <sup>i</sup>	-78.66 (7)	Cl2—Co2—C6 <sup>i</sup> —C5 <sup>i</sup>	-87.1 (6)
S1—Co1—S2—C4	-40.3 (3)	S1—Co2—C6 <sup>i</sup> —C5 <sup>i</sup>	145.4 (5)
S1—Co1—S2—Co2 <sup>i</sup>	55.34 (7)	Co1—S1—C1—C2	30.3 (8)
C3—Co1—S2—C4	58.1 (3)	Co2—S1—C1—C2	-82.3 (7)
C3—Co1—S2—Co2 <sup>i</sup>	153.74 (17)	Co1—S2—C4—C5	130.1 (7)
Cl1—Co1—C3—C2	95.3 (5)	Co2 <sup>i</sup> —S2—C4—C5	29.2 (7)
S1—Co1—C3—C2	-24.5 (5)	S1—C1—C2—C3	-56.3 (9)
S2—Co1—C3—C2	-134.5 (5)	C1—C2—C3—Co1	51.0 (7)
Cl2—Co2—S1—Co1	-116.41 (8)	S2—C4—C5—C6	-57.7 (9)
Cl2—Co2—S1—C1	-17.1 (2)	C4—C5—C6—Co2 <sup>i</sup>	54.4 (7)
S2 <sup>i</sup> —Co2—S1—Co1	112.67 (7)		

Symmetry codes: (i)  $-x+1/2, -y-1/2, -z+1$ ; (ii)  $-x+1/2, y-1/2, -z+1/2$ ; (iii)  $x-1/2, -y-1/2, z-1/2$ ; (iv)  $-x, y, -z+1/2$ ; (v)  $x, -y, z+1/2$ ; (vi)  $x, y-1, z$ ; (vii)  $-x+1/2, -y+1/2, -z+1$ ; (viii)  $x, -y, z-1/2$ ; (ix)  $-x+1/2, y+1/2, -z+1/2$ ; (x)  $x+1/2, -y-1/2, z+1/2$ ; (xi)  $x, y+1, z$ .

#### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C3—H3 <i>A</i> $\cdots$ S2 <sup>ix</sup>	0.97	2.57	3.539 (8)	175
C3—H3 <i>B</i> $\cdots$ Cl2 <sup>iv</sup>	0.97	2.74	3.512 (7)	138
C3—H3 <i>B</i> $\cdots$ Cl2 <sup>viii</sup>	0.97	2.81	3.412 (6)	121
C6—H6 <i>A</i> $\cdots$ Cl1 <sup>i</sup>	0.97	2.62	3.379 (7)	135
C6—H6 <i>B</i> $\cdots$ Cl1 <sup>x</sup>	0.97	2.48	3.343 (7)	148

Symmetry codes: (i)  $-x+1/2, -y-1/2, -z+1$ ; (iv)  $-x, y, -z+1/2$ ; (viii)  $x, -y, z-1/2$ ; (ix)  $-x+1/2, y+1/2, -z+1/2$ ; (x)  $x+1/2, -y-1/2, z+1/2$ .