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***trans*-Chloridobis(ethane-1,2-diamine- $\kappa^2N,N'$ )(thiocyanato- $\kappa N$ )cobalt(III) diamminetetrakis(thiocyanato- $\kappa N$ )chromate(III)**

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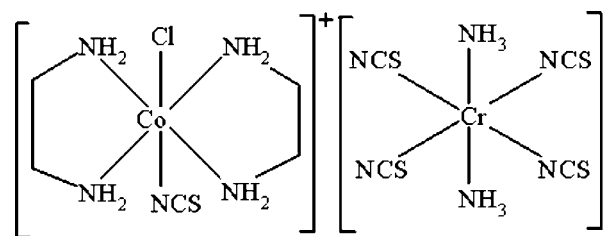
Received 21 January 2014; accepted 19 February 2014

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.009$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.141; data-to-parameter ratio = 32.2.

The title ionic complex  $[CoCl(NCS)(C_2H_8N_2)_2][Cr(NCS)_4(NH_3)_2]$ , which crystallizes as a non-merohedral twin, is built up of a complex cation  $[CoCl(NCS)(en)_2]^+$  (*en* is ethane-1,2-diamine) and the Reinecke's salt anion  $[Cr(NCS)_4(NH_3)_2]^-$  as complex counter-ion. A network of  $N-H \cdots S$  and  $N-H \cdots Cl$  hydrogen bonds, as well as short  $S \cdots S$  contacts [3.538 (2) and 3.489 (3) Å], between the NCS groups of the complex anions link the molecules into a three-dimensional supramolecular network. Intensity statistic indicated twinning by non-merohedry with refined weights of twin components are 0.5662:0.4338.

### Related literature

For background to the ammonium salt route for direct synthesis of coordination compounds, see: Kovbasyuk *et al.* (1997); Pryma *et al.* (2003); Buvaylo *et al.* (2005). For the salt route for direct synthesis of coordination compounds, see: Vassilyeva *et al.* (1997); Makhankova *et al.* (2002). For direct synthesis of heterometallic complexes with ethylenediamine, see: Nesterova (Pryma) *et al.* (2004); Nesterova *et al.* (2005, 2008). For the application of Reinecke's salt in the direct synthesis of heterometallic complexes, see: Nikitina *et al.* (2008, 2009). For the structures of related complexes, see: Schubert *et al.* (1981); Tang *et al.* (1993); Foust & Janicki (1980); Anbalagan *et al.* (2009).



### Experimental

#### Crystal data

$[CoCl(NCS)(C_2H_8N_2)_2][Cr(NCS)_4(NH_3)_2]$   
 $M_r = 591.05$   
 Triclinic,  $P\bar{1}$   
 $a = 8.8290$  (15) Å  
 $b = 10.745$  (3) Å  
 $c = 13.275$  (3) Å  
 $\alpha = 106.98$  (2)°  
 $\beta = 93.131$  (17)°  
 $\gamma = 90.646$  (17)°  
 $V = 1202.1$  (5) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.71$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.27 \times 0.24 \times 0.08$  mm

#### Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)  
 $T_{min} = 0.855$ ,  $T_{max} = 0.883$   
 8238 measured reflections  
 8238 independent reflections  
 6185 reflections with  $I > 2\sigma(I)$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.141$   
 $S = 1.03$   
 8238 reflections  
 256 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 1.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.72$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
N1—H1A⋯S3 <sup>iii</sup>	0.97	2.60	3.485 (5)	152
N1—H1B⋯S5 <sup>iii</sup>	0.97	2.70	3.598 (5)	154
N2—H2A⋯S3	0.97	2.54	3.473 (4)	163
N2—H2B⋯S4 <sup>iv</sup>	0.97	2.54	3.411 (4)	150
N4—H4A⋯Cl1 <sup>v</sup>	0.97	2.59	3.398 (4)	141
N10—H10B⋯S1 <sup>iv</sup>	0.89	2.81	3.696 (6)	171
N11—H11C⋯S5 <sup>vi</sup>	0.89	2.70	3.578 (5)	168

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: BR2236).

## References

- Anbalagan, K., Tamilselvan, M., Nirmala, S. & Sudha, L. (2009). *Acta Cryst. E* **65**, m836–m837.
- Buvaylo, E. A., Kokozay, V. N., Vassilyeva, O. Yu., Skelton, B. W., Jezierska, J., Brunel, L. C. & Ozarowski, A. (2005). *Chem. Commun.* pp. 4976–4978.
- Foust, A. S. & Janickis, V. (1980). *Inorg. Chem.* **19**, 1048–1050.
- Kovbasyuk, L. A., Babich, O. A. & Kokozay, V. N. (1997). *Polyhedron*, **16**, 161–163.
- Makhankova, V. G., Vassilyeva, O. Yu., Kokozay, V. N., Skelton, B. W., Sorace, L. & Gatteschi, D. (2002). *J. Chem. Soc. Dalton Trans.* pp. 4253–4259.
- Nesterova, O. V., Lipetskaya, A. V., Petrusenko, S. R., Kokozay, V. N., Skelton, B. W. & Jezierska, J. (2005). *Polyhedron*, **24**, 1425–1434.
- Nesterova, O. V., Petrusenko, S. R., Kokozay, V. N., Skelton, B. W., Jezierska, J., Linert, W. & Ozarowski, A. (2008). *Dalton Trans.* pp. 1431–1436.
- Nesterova (Pryma), O. V., Petrusenko, S. R., Kokozay, V. N., Skelton, B. W. & Linert, W. (2004). *Inorg. Chem. Commun.* **7**, 450–454.
- Nikitina, V. M., Nesterova, O. V., Kokozay, V. N., Dyakonenko, V. V., Shishkin, O. V. & Jezierska, J. (2009). *Polyhedron*, **28**, 1265–1272.
- Nikitina, V. M., Nesterova, O. V., Kokozay, V. N., Goreschnik, E. A. & Jezierska, J. (2008). *Polyhedron*, **27**, 2426–2430.
- Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd, Abingdon, England.
- Pryma, O. V., Petrusenko, S. R., Kokozay, V. N., Skelton, B. W., Shishkin, O. V. & Teplytska, T. S. (2003). *Eur. J. Inorg. Chem.* pp. 1426–1432.
- Schubert, U., Zimmer-Gasser, B., Dash, K. C. & Chaudhury, G. R. (1981). *Cryst. Struct. Commun.* **10**, 251–254.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Tang, K., Kastner, M. E., Cooper, J. N., Kanaskie, M. & Monoski, A. (1993). *Acta Cryst. C* **49**, 1265–1267.
- Vassilyeva, O. Yu., Kokozay, V. N., Zhukova, N. I. & Kovbasyuk, L. A. (1997). *Polyhedron*, **16**, 263–266.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## supplementary materials

*Acta Cryst.* (2014). E70, m110–m111 [doi:10.1107/S1600536814003869]

***trans*-Chloridobis(ethane-1,2-diamine- $\kappa^2N,N'$ )(thiocyanato- $\kappa N$ )cobalt(III)  
diamminetetrakis(thiocyanato- $\kappa N$ )chromate(III)**

**Julia A. Rusanova, Valentyna V. Semenaka and Roman I. Zubatyuk**

### 1. Introduction

### 2. Experimental

#### 2.1. Synthesis and crystallization

Cobalt powder (0.074 g, 1.25 mmol),  $\text{NH}_4[\text{Cr}(\text{NCS})_4(\text{NH}_3)_2]\cdot\text{H}_2\text{O}$  (0.443 g, 1.25 mmol),  $\text{en}\cdot 2\text{HCl}$  (0.166 g, 1.25 mmol) and methanol (20 ml) were heated in air to 323–333 K and stirred magnetically during 7 h. The resulting blue solution was slowly evaporated at room temperature until light-brown crystals suitable for crystallographic study were formed. The crystals were filtered off, washed with dry  $\text{PrOH}$  and finally dried *in vacuo* at room temperature. Yield: 0.12 g, 17.1%.

#### 2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All of the hydrogen atoms were positioned geometrically and refined using a riding model approximation with  $U_{\text{iso}} = 1.2$  or  $1.5 U_{\text{eq}}$  of the carrier atom. A rotating model was used for  $\text{NH}_3$  and  $\text{CH}_3$  groups. Intensity statistic indicated a nonmerohedral twinning with refined weights of twin components are 0.5662:0.4338.

### 3. Results and discussion

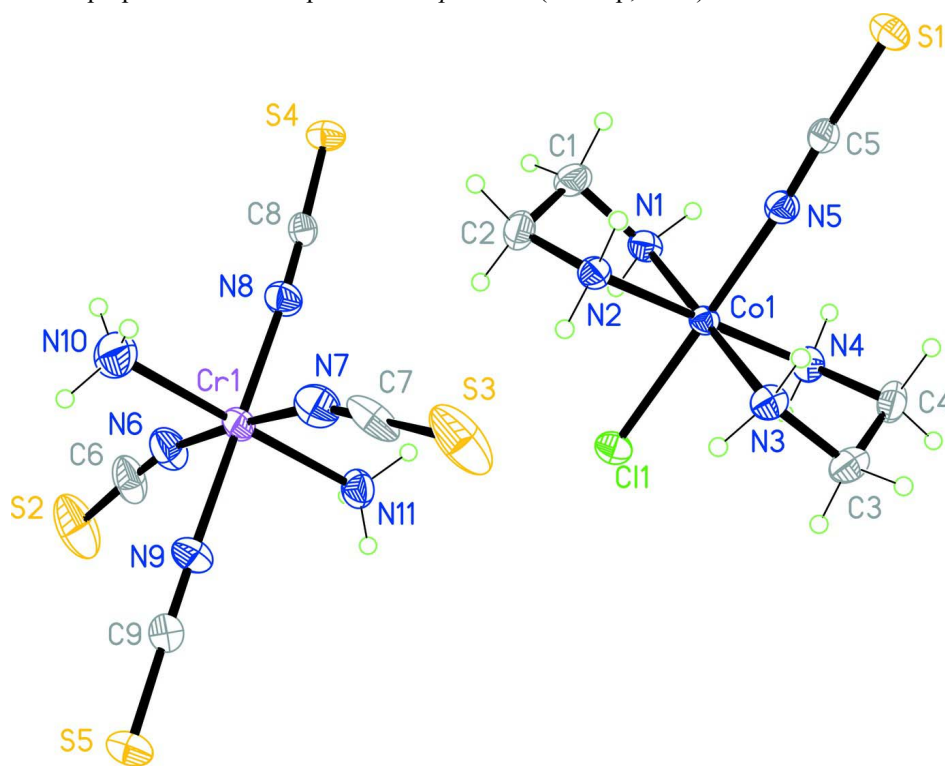
In order to continue our research on direct synthesis of coordination compounds (Kovbasyuk *et al.*, 1997; Pryma *et al.*, 2003; Buvaylo *et al.*, 2005; Vassilyeva *et al.*, 1997; Makhankova *et al.*, 2002; Nesterova (Pryma) *et al.*, 2004; Nesterova *et al.*, 2005, 2008; Nikitina *et al.*, 2008, 2009) in this paper we present a novel Co/Cr heterometallic ionic complex which has been synthesized using zerovalent cobalt, Reinecke's salt and non-aqueous solution of ethylenediamine as a starting materials.

As it shown on Fig.1 Co atom in complex cation is in distorted square bipyramidal coordination environment with one NCS group and chlorine atom at the axial positions and four N atoms from two ethylenediamine molecules in equatorial plane. The Cr centers are in the similar to Co coordination environment and coordinated to six N atoms - four NCS-groups in equatorial position and two  $\text{NH}_3$  molecules in axial position. The bond distances and angles in the title molecule agree well with the corresponding bond distances and angles reported in closely related compounds (Schubert *et al.*, 1981, Tang *et al.*, 1993, Foust *et al.*, 1980, Anbalagan *et al.*, 2009, Nikitina *et al.*, 2008, 2009). There are short interanionic  $\text{S}\cdots\text{S}$  contacts between NCS-groups of the complex anions with the distances 3.538 (1) ( $\text{S5}\cdots\text{S5}$ ) and 3.489 (1) Å ( $\text{S2}\cdots\text{S2}$ ) whereas sum of standard Van-der-Vaals radius of the sulfur atom is 3.68 Å. Two NCS-groups of the ligand which involve S2 and S3 atoms show relatively large thermal displacements ( $U_{\text{eq}}$  is 0.1063 (9) Å<sup>2</sup> and 0.0984 (8) Å<sup>2</sup>, resp.). Also these NCS-groups show notably non-linear Cr–N–C bond angles (166.2 (5)° and 163.2 (5)°). This might be caused by inter-

molecular contacts involving S2 and S3. S...S contacts as well as a network of hydrogen bonds link the molecule into threedimensional supramolecular network. The crystal packing of the title compound is presented on Fig 2.

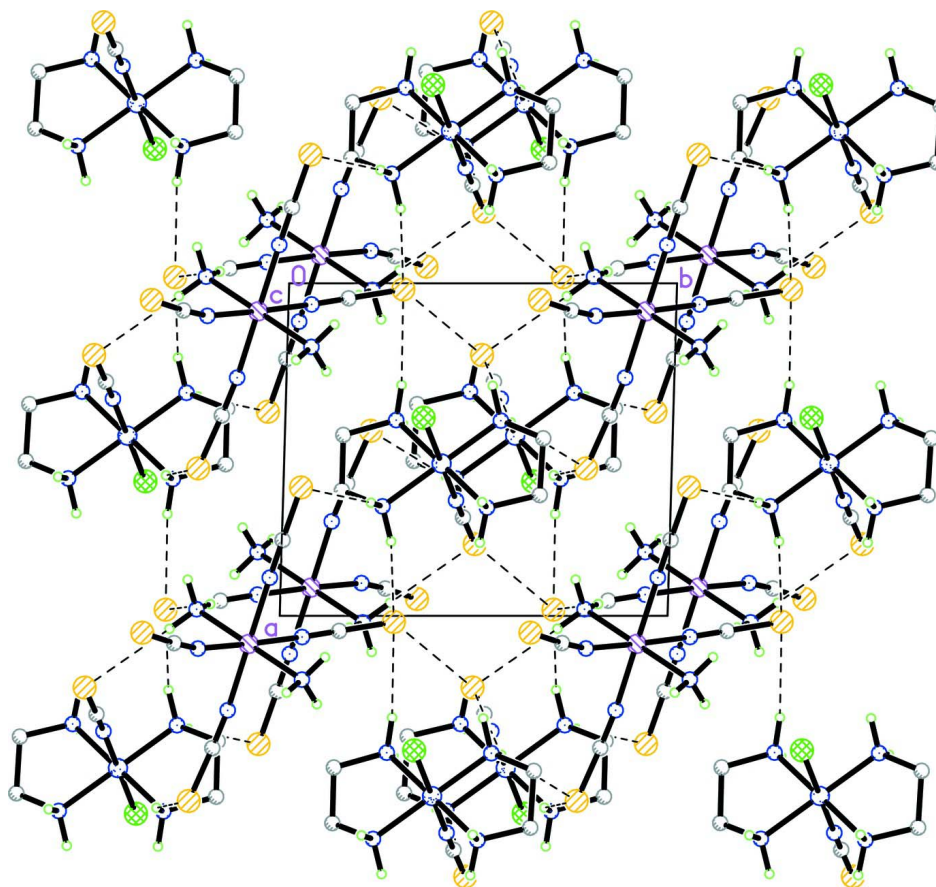
### Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).



**Figure 1**

Crystal structure of the complex, showing the atom numbering, with 30% probability displacement ellipsoids

**Figure 2**

The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

***trans*-Chloridobis(ethane-1,2-diamine- $\kappa^2N,N'$ )(thiocyanato- $\kappa N$ )cobalt(III) diamminetetrakis(thiocyanato- $\kappa N$ )chromate(III)**

*Crystal data*

[CoCl(NCS)(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>][Cr(NCS)<sub>4</sub>(NH<sub>3</sub>)<sub>2</sub>]

$M_r = 591.05$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 8.8290(15) \text{ \AA}$

$b = 10.745(3) \text{ \AA}$

$c = 13.275(3) \text{ \AA}$

$\alpha = 106.98(2)^\circ$

$\beta = 93.131(17)^\circ$

$\gamma = 90.646(17)^\circ$

$V = 1202.1(5) \text{ \AA}^3$

$Z = 2$

$F(000) = 602$

$D_x = 1.633 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.7107 \text{ \AA}$

Cell parameters from 3528 reflections

$\theta = 3.1\text{--}27.3^\circ$

$\mu = 1.71 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, light brown

$0.27 \times 0.24 \times 0.08 \text{ mm}$

*Data collection*

Oxford Diffraction Xcalibur Sapphire3  
diffractometer

Radiation source: Enhance (Mo) X-ray Source  
Graphite monochromator

Detector resolution:  $16.1827 \text{ pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2010)

$T_{\min} = 0.855$ ,  $T_{\max} = 0.883$

8238 measured reflections

8238 independent reflections  
 6185 reflections with  $I > 2\sigma(I)$   
 $\theta_{\max} = 28.6^\circ$ ,  $\theta_{\min} = 2.9^\circ$

$h = -11 \rightarrow 11$   
 $k = -13 \rightarrow 13$   
 $l = -17 \rightarrow 17$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.141$   
 $S = 1.03$   
 8238 reflections  
 256 parameters  
 0 restraints

Primary atom site location: structure-invariant  
 direct methods  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 0.5674P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.19 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.54186 (7)	0.40606 (6)	0.75563 (4)	0.02775 (16)
Cr1	0.08452 (9)	-0.07796 (8)	0.76057 (7)	0.0385 (2)
Cl1	0.40444 (16)	0.35647 (13)	0.87609 (9)	0.0438 (3)
S1	0.78440 (16)	0.49754 (14)	0.48138 (10)	0.0452 (3)
S2	0.0503 (3)	-0.3524 (2)	0.9791 (2)	0.1063 (9)
S3	0.0184 (2)	0.2947 (2)	0.6471 (2)	0.0984 (8)
S4	0.55652 (16)	-0.22096 (14)	0.61991 (10)	0.0442 (3)
S5	-0.38612 (16)	0.04575 (16)	0.91039 (11)	0.0518 (4)
N1	0.6708 (5)	0.2569 (4)	0.7487 (3)	0.0370 (9)
H1A	0.7764	0.2817	0.7471	0.044*
H1B	0.6599	0.2272	0.8104	0.044*
N2	0.4114 (4)	0.2859 (4)	0.6452 (3)	0.0343 (9)
H2A	0.3061	0.2971	0.6623	0.041*
H2B	0.4225	0.3036	0.5783	0.041*
N3	0.4130 (5)	0.5558 (4)	0.7636 (3)	0.0371 (9)
H3A	0.4180	0.5815	0.6996	0.045*
H3B	0.3084	0.5323	0.7701	0.045*
N4	0.6745 (5)	0.5263 (4)	0.8661 (3)	0.0367 (9)
H4A	0.6582	0.5137	0.9342	0.044*
H4B	0.7801	0.5104	0.8513	0.044*
N5	0.6529 (5)	0.4460 (4)	0.6499 (3)	0.0362 (9)
N6	0.0981 (6)	-0.2081 (5)	0.8404 (4)	0.0603 (14)
N7	0.0637 (6)	0.0593 (5)	0.6873 (4)	0.0561 (13)
N8	0.2839 (5)	-0.1270 (4)	0.6994 (4)	0.0461 (11)
N9	-0.1149 (5)	-0.0282 (5)	0.8214 (4)	0.0515 (12)
N10	-0.0200 (6)	-0.2146 (5)	0.6325 (4)	0.0695 (15)
H10A	-0.1087	-0.2397	0.6501	0.104*

H10B	0.0388	-0.2832	0.6125	0.104*
H10C	-0.0353	-0.1801	0.5796	0.104*
N11	0.1914 (5)	0.0620 (4)	0.8881 (3)	0.0472 (11)
H11A	0.1242	0.1198	0.9190	0.071*
H11B	0.2652	0.1023	0.8656	0.071*
H11C	0.2306	0.0238	0.9344	0.071*
C1	0.6231 (7)	0.1510 (5)	0.6512 (4)	0.0502 (14)
H1C	0.6687	0.1659	0.5908	0.060*
H1D	0.6558	0.0677	0.6578	0.060*
C2	0.4560 (7)	0.1507 (5)	0.6370 (4)	0.0482 (13)
H2C	0.4101	0.1210	0.6910	0.058*
H2D	0.4220	0.0926	0.5685	0.058*
C3	0.4661 (6)	0.6663 (5)	0.8567 (4)	0.0444 (13)
H3C	0.4223	0.6579	0.9200	0.053*
H3D	0.4360	0.7484	0.8463	0.053*
C4	0.6367 (7)	0.6613 (5)	0.8674 (4)	0.0459 (13)
H4C	0.6814	0.6831	0.8093	0.055*
H4D	0.6757	0.7230	0.9330	0.055*
C5	0.7041 (5)	0.4652 (4)	0.5783 (4)	0.0323 (10)
C6	0.0819 (7)	-0.2700 (6)	0.8967 (6)	0.0664 (19)
C7	0.0454 (6)	0.1544 (7)	0.6701 (5)	0.0591 (17)
C8	0.3977 (5)	-0.1639 (4)	0.6657 (4)	0.0334 (10)
C9	-0.2279 (6)	0.0020 (5)	0.8567 (4)	0.0374 (11)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0309 (3)	0.0296 (3)	0.0247 (3)	0.0017 (2)	0.0031 (3)	0.0106 (3)
Cr1	0.0263 (4)	0.0419 (5)	0.0462 (5)	0.0008 (3)	0.0036 (4)	0.0108 (4)
Cl1	0.0507 (8)	0.0489 (7)	0.0341 (7)	-0.0010 (6)	0.0105 (6)	0.0143 (6)
S1	0.0434 (8)	0.0541 (8)	0.0429 (7)	-0.0030 (6)	0.0120 (6)	0.0201 (6)
S2	0.0773 (14)	0.1127 (18)	0.167 (2)	-0.0156 (12)	-0.0050 (15)	0.1033 (18)
S3	0.0516 (11)	0.1282 (18)	0.163 (2)	0.0142 (11)	0.0175 (12)	0.1146 (18)
S4	0.0379 (7)	0.0539 (8)	0.0404 (7)	0.0099 (6)	0.0089 (6)	0.0116 (6)
S5	0.0381 (8)	0.0682 (10)	0.0514 (8)	0.0099 (7)	0.0136 (6)	0.0190 (7)
N1	0.040 (2)	0.037 (2)	0.040 (2)	0.0086 (18)	0.0094 (19)	0.0181 (19)
N2	0.034 (2)	0.037 (2)	0.030 (2)	-0.0024 (17)	0.0018 (17)	0.0074 (17)
N3	0.043 (2)	0.038 (2)	0.032 (2)	0.0060 (18)	0.0011 (19)	0.0116 (18)
N4	0.040 (2)	0.038 (2)	0.033 (2)	-0.0029 (18)	-0.0041 (18)	0.0126 (17)
N5	0.042 (2)	0.035 (2)	0.033 (2)	0.0034 (18)	0.0054 (19)	0.0111 (18)
N6	0.051 (3)	0.056 (3)	0.083 (4)	0.000 (2)	0.013 (3)	0.033 (3)
N7	0.047 (3)	0.068 (3)	0.057 (3)	0.005 (3)	0.003 (2)	0.024 (3)
N8	0.033 (2)	0.050 (3)	0.055 (3)	0.005 (2)	0.008 (2)	0.014 (2)
N9	0.034 (3)	0.062 (3)	0.059 (3)	0.004 (2)	0.013 (2)	0.016 (2)
N10	0.049 (3)	0.073 (4)	0.073 (4)	-0.004 (3)	-0.002 (3)	0.002 (3)
N11	0.041 (3)	0.049 (3)	0.048 (3)	-0.010 (2)	-0.003 (2)	0.012 (2)
C1	0.068 (4)	0.032 (3)	0.051 (3)	0.011 (3)	0.021 (3)	0.009 (2)
C2	0.065 (4)	0.034 (3)	0.042 (3)	-0.011 (3)	0.004 (3)	0.007 (2)
C3	0.060 (4)	0.037 (3)	0.036 (3)	0.012 (2)	0.004 (2)	0.008 (2)
C4	0.064 (4)	0.031 (3)	0.041 (3)	-0.011 (2)	-0.003 (3)	0.008 (2)

C5	0.032 (3)	0.030 (2)	0.033 (3)	-0.0010 (19)	-0.001 (2)	0.007 (2)
C6	0.035 (3)	0.049 (4)	0.122 (6)	0.001 (3)	0.004 (4)	0.038 (4)
C7	0.029 (3)	0.105 (5)	0.063 (4)	0.003 (3)	0.008 (3)	0.053 (4)
C8	0.034 (3)	0.030 (2)	0.039 (3)	-0.001 (2)	0.000 (2)	0.014 (2)
C9	0.038 (3)	0.039 (3)	0.039 (3)	0.000 (2)	-0.003 (2)	0.017 (2)

*Geometric parameters (Å, °)*

Co1—C11	2.2378 (14)	N3—H3B	0.9700
Co1—N1	1.960 (4)	N3—C3	1.492 (6)
Co1—N2	1.954 (4)	N4—H4A	0.9700
Co1—N3	1.962 (4)	N4—H4B	0.9700
Co1—N4	1.965 (4)	N4—C4	1.488 (6)
Co1—N5	1.900 (4)	N5—C5	1.144 (6)
Cr1—N6	1.987 (5)	N6—C6	1.149 (8)
Cr1—N7	1.995 (5)	N7—C7	1.122 (8)
Cr1—N8	1.990 (4)	N8—C8	1.150 (6)
Cr1—N9	1.990 (5)	N9—C9	1.135 (6)
Cr1—N10	2.058 (5)	N10—H10A	0.8900
Cr1—N11	2.080 (4)	N10—H10B	0.8900
S1—C5	1.623 (5)	N10—H10C	0.8900
S2—C6	1.629 (7)	N11—H11A	0.8900
S3—C7	1.640 (7)	N11—H11B	0.8900
S4—C8	1.615 (5)	N11—H11C	0.8900
S5—C9	1.616 (5)	C1—H1C	0.9700
S2—S2 <sup>i</sup>	3.489 (3)	C1—H1D	0.9700
S5—S5 <sup>ii</sup>	3.538 (2)	C1—C2	1.477 (8)
N1—H1A	0.9700	C2—H2C	0.9700
N1—H1B	0.9700	C2—H2D	0.9700
N1—C1	1.489 (7)	C3—H3C	0.9700
N2—H2A	0.9700	C3—H3D	0.9700
N2—H2B	0.9700	C3—C4	1.508 (8)
N2—C2	1.485 (6)	C4—H4C	0.9700
N3—H3A	0.9700	C4—H4D	0.9700
N1—Co1—C11	90.78 (12)	H4A—N4—H4B	108.5
N1—Co1—N3	179.61 (17)	C4—N4—Co1	107.7 (3)
N1—Co1—N4	93.44 (17)	C4—N4—H4A	110.2
N2—Co1—C11	88.77 (12)	C4—N4—H4B	110.2
N2—Co1—N1	86.23 (17)	C5—N5—Co1	171.6 (4)
N2—Co1—N3	94.07 (17)	C6—N6—Cr1	166.2 (5)
N2—Co1—N4	179.54 (17)	C7—N7—Cr1	163.2 (5)
N3—Co1—C11	88.98 (13)	C8—N8—Cr1	175.0 (4)
N3—Co1—N4	86.27 (17)	C9—N9—Cr1	179.0 (5)
N4—Co1—C11	91.54 (12)	Cr1—N10—H10A	109.5
N5—Co1—C11	178.03 (13)	Cr1—N10—H10B	109.5
N5—Co1—N1	89.78 (17)	Cr1—N10—H10C	109.5
N5—Co1—N2	89.38 (17)	H10A—N10—H10B	109.5
N5—Co1—N3	90.47 (17)	H10A—N10—H10C	109.5
N5—Co1—N4	90.31 (17)	H10B—N10—H10C	109.5



N6—Cr1—N7	176.5 (2)	Cr1—N11—H11A	109.5
N6—Cr1—N8	92.1 (2)	Cr1—N11—H11B	109.5
N6—Cr1—N9	88.1 (2)	Cr1—N11—H11C	109.5
N6—Cr1—N10	90.7 (2)	H11A—N11—H11B	109.5
N6—Cr1—N11	90.3 (2)	H11A—N11—H11C	109.5
N7—Cr1—N10	91.1 (2)	H11B—N11—H11C	109.5
N7—Cr1—N11	87.9 (2)	N1—C1—H1C	110.1
N8—Cr1—N7	90.8 (2)	N1—C1—H1D	110.1
N8—Cr1—N9	179.7 (2)	H1C—C1—H1D	108.4
N8—Cr1—N10	89.1 (2)	C2—C1—N1	108.0 (4)
N8—Cr1—N11	90.47 (19)	C2—C1—H1C	110.1
N9—Cr1—N7	88.9 (2)	C2—C1—H1D	110.1
N9—Cr1—N10	90.9 (2)	N2—C2—H2C	110.2
N9—Cr1—N11	89.51 (19)	N2—C2—H2D	110.2
N10—Cr1—N11	179.0 (2)	C1—C2—N2	107.6 (4)
Co1—N1—H1A	110.1	C1—C2—H2C	110.2
Co1—N1—H1B	110.1	C1—C2—H2D	110.2
H1A—N1—H1B	108.4	H2C—C2—H2D	108.5
C1—N1—Co1	108.2 (3)	N3—C3—H3C	110.3
C1—N1—H1A	110.1	N3—C3—H3D	110.3
C1—N1—H1B	110.1	N3—C3—C4	107.1 (4)
Co1—N2—H2A	109.9	H3C—C3—H3D	108.5
Co1—N2—H2B	109.9	C4—C3—H3C	110.3
H2A—N2—H2B	108.3	C4—C3—H3D	110.3
C2—N2—Co1	108.7 (3)	N4—C4—C3	107.1 (4)
C2—N2—H2A	109.9	N4—C4—H4C	110.3
C2—N2—H2B	109.9	N4—C4—H4D	110.3
Co1—N3—H3A	109.8	C3—C4—H4C	110.3
Co1—N3—H3B	109.8	C3—C4—H4D	110.3
H3A—N3—H3B	108.2	H4C—C4—H4D	108.5
C3—N3—Co1	109.4 (3)	N5—C5—S1	176.7 (5)
C3—N3—H3A	109.8	N6—C6—S2	176.6 (6)
C3—N3—H3B	109.8	N7—C7—S3	179.0 (7)
Co1—N4—H4A	110.2	N8—C8—S4	177.7 (5)
Co1—N4—H4B	110.2	N9—C9—S5	178.3 (5)
Co1—N1—C1—C2	-38.5 (5)	Co1—N4—C4—C3	42.6 (5)
Co1—N2—C2—C1	-38.6 (5)	N1—C1—C2—N2	50.6 (5)
Co1—N3—C3—C4	35.7 (5)	N3—C3—C4—N4	-51.3 (5)

Symmetry codes: (i)  $-x, -y-1, -z+2$ ; (ii)  $-x-1, -y, -z+2$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ S3 <sup>iii</sup>	0.97	2.60	3.485 (5)	152
N1—H1B $\cdots$ S5 <sup>iii</sup>	0.97	2.70	3.598 (5)	154
N2—H2A $\cdots$ S3	0.97	2.54	3.473 (4)	163
N2—H2B $\cdots$ S4 <sup>iv</sup>	0.97	2.54	3.411 (4)	150
N4—H4A $\cdots$ C11 <sup>v</sup>	0.97	2.59	3.398 (4)	141

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N10—H10B···S1 <sup>iv</sup>	0.89	2.81	3.696 (6)	171
N11—H11C···S5 <sup>vi</sup>	0.89	2.70	3.578 (5)	168

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