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Diaquatetrakis(dimethyl sulfoxide-κO)cobalt(II) bis[diamminetetrakis(thiocyanato-κN)chromate(III)] dimethyl sulfoxide hexasolvate dihydrate

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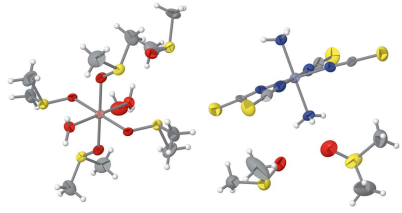
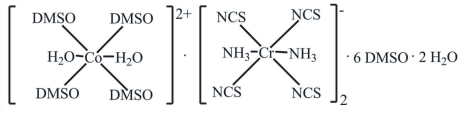
Structural data: full structural data are available from iucrdata.iucr.org

The solvated title salt, $[Co(C_2H_6OS)_4(H_2O)_2][Cr(NCS)_4(NH_3)_2]\cdot 6C_2H_6OS\cdot 2H_2O$, is build up from a complex $[Co(DMSO)_4(H_2O)_2]^{2+}$ cation (where DMSO is dimethyl sulfoxide), two Reinecke's Salt anions, *i.e.* $[Cr(NCS)_4(NH_3)_2]^-$, as the complex counter-ions, together with solvent molecules (six DMSO and two water). The crystal packing consists of a branched three-dimensional system of hydrogen bonds involving the DMSO and water solvent molecules, the S atoms of the thiocyanate ligands, and the coordinating NH_3 and H_2O molecules.

3D view



Chemical scheme



Structure description

The Co^{II} atom of the complex cation lies on an inversion centre and, as shown in Fig. 1, adopts a slightly distorted octahedral coordination geometry. Four O atoms from DMSO ligands constitute the equatorial plane, with the O atoms of two coordinating water molecules in axial positions.

The Cr^{III} atom of the anion is also six-coordinate involving six N atoms, four from thiocyanate ligands in the equatorial plane and two from ammine ligands in axial positions. The bond lengths and angles in the title complex agree well with those reported in closely related compounds (Schubert *et al.*, 1981; Tang *et al.*, 1993; Foust & Janickis, 1980; Anbalagan *et al.*, 2009; Nikitina *et al.*, 2008). The title complex is most closely related to the salt $[Mn(DMSO)_4(H_2O)_2][Cr(NCS)_4(NH_3)_2]\cdot 6DMSO\cdot 2H_2O$ (Gerasimova *et al.*, 2009).

In the crystal structure of the title salt, cations are linked to anions and anions are linked to other anions both directly and through the DMSO and water solvent molecules acting as bridges. The extensive series of hydrogen bonds (Table 1) generates a three-dimensional network of anions, cations and solvent molecules (Fig. 2).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···S6^{i}	0.89	2.76	3.647 (7)	176
N5—H5B···O5^{ii}	0.89	2.17	3.019 (8)	160
N6—H6A···O4^{iii}	0.89	2.03	2.874 (8)	158
N6—H6B···O4	0.89	2.22	3.037 (9)	152
N6—H6C···O6	0.89	2.22	3.069 (8)	160
O1W—H1WA···S6^{iv}	0.85	2.55	3.293 (7)	147
O1W—H1WB···O6^{iv}	0.85	1.89	2.711 (9)	163
C3—H3E···S6^{v}	0.96	2.97	3.590 (9)	124

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

Synthesis and crystallization

Cobalt powder (0.159 g, 2.70 mmol), $NH_4[Cr(NCS)_4(NH_3)_2]\cdot H_2O$ (1.943 g, 5.4 mmol) and DMSO (20 ml) were heated in air at 323–333 K and stirred magnetically until the metal powder had completely dissolved. 2-Propanol was added dropwise after a few days to obtain a fine-grained red precipitate. Good quality single crystals suitable for X-ray analysis were obtained by recrystallization from DMSO with the addition of a few ml of Et_2O. These were filtered off, washed with dry 2-propanol and finally dried in *vacuo* at room temperature (yield: 0.78 g, 37.5%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_2H_6OS)_4(H_2O)_2][Cr(NCS)_4(NH_3)_2]\cdot 6C_2H_6OS\cdot 2H_2O$
M_r	1549.05
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	294
a, b, c (Å)	11.752 (3), 12.212 (4), 13.257 (3)
α, β, γ (°)	85.95 (2), 87.98 (2), 70.17 (2)
V (Å^3)	1785.3 (9)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.11
Crystal size (mm)	0.6 × 0.4 × 0.2
Data collection	
Diffractometer	Siemens P3/PC
Absorption correction	Analytical [Katayama (1986) in *WinGX* (Farrugia, 2012)]
T_{min}, T_{max}	0.604, 0.842
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6478, 6138, 3459
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.195, 1.04
No. of reflections	6138
No. of parameters	352
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.23, −1.03

Computer programs: *P3* (Siemens, 1991), *XDISK* in *SHELXTL-Plus* (Sheldrick, 1992), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Anbalagan, K., Tamilselvan, M., Nirmala, S. & Sudha, L. (2009). *Acta Cryst.* E**65**, m836–m837.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Foust, A. S. & Janickis, V. (1980). *Inorg. Chem.* **19**, 1048–1050.
Gerasimova, E. A., Utkina, T. V., Peresypkina, E. V., Virovets, A. V. & Cherkasova, T. G. (2009). *Russ. J. Inorg. Chem.* **54**, 692–697.
Katayama, C. (1986). *Acta Cryst.* A**42**, 19–23.
Nikitina, V. M., Nesterova, O. V., Kokozay, V. N., Goreshnik, E. A. & Jezierska, J. (2008). *Polyhedron*, **27**, 2426–2430.
Schubert, U., Zimmer-Gasser, B., Dash, K. C. & Chaudhury, G. R. (1981). *Cryst. Struct. Commun.* **10**, 251–254.
Sheldrick, G. M. (1992). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Siemens (1991). *P3/P4-PC Diffractometer Program*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tang, K., Kastner, M. E., Cooper, J. N., Kanaskie, M. & Monoski, A. (1993). *Acta Cryst.* C**49**, 1265–1267.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

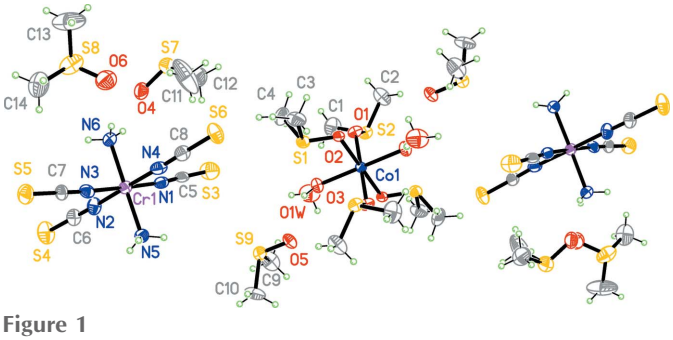


Figure 1
The asymmetric unit of the title compound, shown with 30% probability displacement ellipsoids.

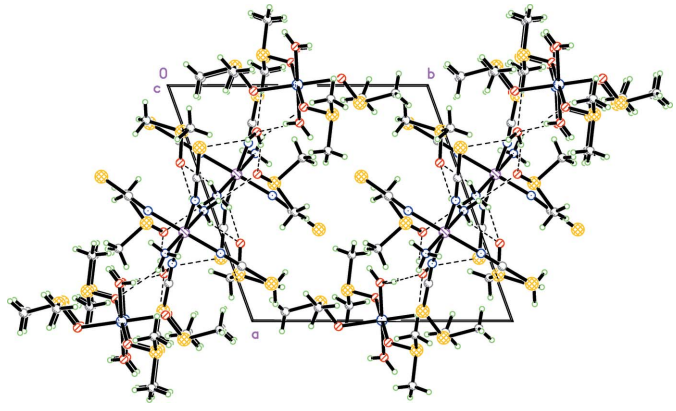


Figure 2
The crystal packing of the title compound. Cation–anion chains are joined by hydrogen bonds (dashed lines) to the DMSO and H_2O solvent molecules.

full crystallographic data

IUCrData (2016). **1**, x161571 [https://doi.org/10.1107/S2414314616015716]

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Crystal data

$[Co(C_2H_6OS)_4(H_2O)_2]$
$[Cr(NCS)_4(NH_3)_2]\cdot 6C_2H_6OS\cdot 2H_2O$
M_r = 1549.05
Triclinic, $P\overline{1}$
a = 11.752 (3) Å
b = 12.212 (4) Å
c = 13.257 (3) Å
α = 85.95 (2)°
β = 87.98 (2)°
γ = 70.17 (2)°
V = 1785.3 (9) Å^3
Z = 1
$F(000)$ = 807
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2015 reflections
θ = 3.5–25.0°
μ = 1.11 mm^{-1}
T = 294 K
Block, colourless
0.6 × 0.4 × 0.2 mm

Data collection

Siemens P3/PC diffractometer
Graphite monochromator
Detector resolution: 16.1827 pixels mm^{-1}
θ–2θ scans
Absorption correction: analytical [analytical correction (Katayama 1986) in *WinGX* (Farrugia, 2012)]
T_{min} = 0.604, T_{max} = 0.842
6478 measured reflections
6138 independent reflections
3459 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.1°, θ_{min} = 1.8°
h = −8→14
k = −14→14
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.195
S = 1.04
6138 reflections
352 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.5000	0.0000	0.0220 (3)
Cr1	−0.62334 (11)	0.13962 (9)	0.24820 (8)	0.0275 (3)
S1	−0.07654 (17)	0.28560 (14)	0.07475 (14)	0.0304 (4)
S2	0.12683 (18)	0.59160 (14)	0.17553 (13)	0.0308 (4)
S3	−0.3879 (2)	0.3817 (2)	0.2914 (2)	0.0599 (7)
S4	−0.9581 (2)	0.3312 (2)	0.45589 (19)	0.0635 (7)
S5	−0.8412 (2)	−0.12533 (19)	0.23569 (18)	0.0513 (6)
S6	−0.2658 (2)	−0.0376 (2)	0.05798 (18)	0.0518 (6)
S7	−0.1953 (2)	0.01062 (19)	0.47090 (19)	0.0531 (6)
S8	−0.4153 (3)	−0.2743 (2)	0.44568 (18)	0.0626 (7)
S9	−0.49827 (18)	0.64195 (18)	0.07185 (15)	0.0411 (5)
N1	−0.5327 (5)	0.2493 (5)	0.2657 (4)	0.0300 (14)
N2	−0.7566 (6)	0.2290 (5)	0.3392 (5)	0.0388 (16)
N3	−0.7121 (5)	0.0272 (5)	0.2342 (4)	0.0304 (14)
N4	−0.4888 (6)	0.0534 (5)	0.1567 (5)	0.0375 (16)
N5	−0.7122 (6)	0.2396 (5)	0.1241 (4)	0.0335 (14)
H5A	−0.7178	0.1931	0.0771	0.050*
H5B	−0.6711	0.2848	0.0990	0.050*
H5C	−0.7861	0.2840	0.1426	0.050*
N6	−0.5326 (6)	0.0345 (5)	0.3673 (4)	0.0365 (15)
H6A	−0.5855	0.0258	0.4142	0.055*
H6B	−0.4840	0.0669	0.3937	0.055*
H6C	−0.4887	−0.0349	0.3459	0.055*
O1W	−0.1997 (6)	0.7216 (5)	0.2060 (5)	0.067 (2)
H1WA	−0.2318	0.7664	0.1551	0.100*
H1WB	−0.2532	0.7245	0.2515	0.100*
O1	0.0946 (5)	0.4937 (4)	0.1327 (3)	0.0309 (11)
O2	0.0271 (4)	0.3229 (4)	0.0310 (3)	0.0271 (11)
O3	−0.1606 (4)	0.5446 (4)	0.0842 (3)	0.0290 (11)
H3A	−0.1635	0.5746	0.1414	0.044*
H3B	−0.2310	0.5814	0.0596	0.044*
O4	−0.3298 (5)	0.0593 (5)	0.4896 (4)	0.0486 (15)
O5	−0.3876 (4)	0.5990 (4)	0.0043 (4)	0.0362 (12)
O6	−0.3761 (6)	−0.2221 (6)	0.3498 (5)	0.068 (2)
C1	0.0615 (9)	0.6080 (8)	0.2977 (6)	0.062 (3)
H1A	−0.0246	0.6443	0.2925	0.093*
H1B	0.0938	0.6559	0.3341	0.093*
H1C	0.0798	0.5328	0.3330	0.093*
C2	0.2785 (8)	0.5278 (7)	0.2116 (7)	0.050 (2)

H2A	0.3288	0.5070	0.1524	0.076*
H2B	0.2876	0.4591	0.2550	0.076*
H2C	0.3022	0.5824	0.2470	0.076*
C3	−0.0346 (8)	0.1364 (6)	0.0480 (7)	0.049 (2)
H3C	−0.0360	0.1304	−0.0237	0.074*
H3D	−0.0905	0.1032	0.0808	0.074*
H3E	0.0455	0.0950	0.0725	0.074*
C4	−0.0561 (9)	0.2702 (8)	0.2070 (6)	0.061 (3)
H4A	−0.0622	0.3441	0.2315	0.091*
H4B	0.0223	0.2146	0.2225	0.091*
H4C	−0.1173	0.2435	0.2391	0.091*
C5	−0.4680 (6)	0.3038 (6)	0.2776 (5)	0.0301 (16)
C6	−0.8409 (8)	0.2721 (7)	0.3870 (6)	0.0385 (19)
C7	−0.7661 (7)	−0.0362 (6)	0.2354 (5)	0.0291 (16)
C8	−0.3949 (8)	0.0144 (6)	0.1159 (5)	0.0361 (18)
C9	−0.5010 (9)	0.7771 (8)	0.1143 (7)	0.060 (3)
H9A	−0.4347	0.7643	0.1591	0.090*
H9B	−0.5759	0.8128	0.1495	0.090*
H9C	−0.4939	0.8276	0.0573	0.090*
C10	−0.6211 (8)	0.6956 (7)	−0.0121 (8)	0.056 (3)
H10A	−0.6269	0.6328	−0.0489	0.084*
H10B	−0.6086	0.7544	−0.0586	0.084*
H10C	−0.6946	0.7286	0.0257	0.084*
C11	−0.1800 (11)	−0.0291 (14)	0.3457 (10)	0.122 (6)
H11A	−0.2114	−0.0913	0.3398	0.183*
H11B	−0.0960	−0.0546	0.3264	0.183*
H11C	−0.2241	0.0368	0.3022	0.183*
C12	−0.1471 (9)	0.1326 (8)	0.4536 (8)	0.067 (3)
H12A	−0.1447	0.1632	0.5180	0.101*
H12B	−0.2026	0.1915	0.4103	0.101*
H12C	−0.0679	0.1095	0.4232	0.101*
C13	−0.3090 (12)	−0.4163 (9)	0.4675 (11)	0.106 (5)
H13A	−0.2356	−0.4111	0.4928	0.159*
H13B	−0.2921	−0.4549	0.4052	0.159*
H13C	−0.3416	−0.4600	0.5162	0.159*
C14	−0.5386 (10)	−0.3128 (8)	0.4146 (8)	0.068 (3)
H14A	−0.6029	−0.2444	0.3904	0.102*
H14B	−0.5659	−0.3477	0.4734	0.102*
H14C	−0.5152	−0.3675	0.3627	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0229 (7)	0.0162 (6)	0.0226 (7)	−0.0010 (5)	0.0027 (5)	−0.0031 (5)
Cr1	0.0321 (7)	0.0245 (6)	0.0240 (6)	−0.0068 (5)	0.0012 (5)	−0.0028 (4)
S1	0.0295 (10)	0.0218 (8)	0.0378 (10)	−0.0066 (8)	0.0001 (8)	0.0006 (7)
S2	0.0398 (11)	0.0252 (9)	0.0263 (9)	−0.0088 (8)	0.0005 (8)	−0.0054 (7)
S3	0.0625 (16)	0.0475 (13)	0.0787 (17)	−0.0294 (12)	−0.0204 (13)	0.0010 (12)

S4	0.0650 (17)	0.0701 (16)	0.0529 (14)	−0.0178 (14)	0.0334 (13)	−0.0293 (12)
S5	0.0531 (14)	0.0431 (12)	0.0645 (15)	−0.0253 (11)	0.0003 (12)	−0.0022 (10)
S6	0.0393 (13)	0.0578 (13)	0.0565 (14)	−0.0125 (11)	0.0195 (11)	−0.0209 (11)
S7	0.0456 (14)	0.0470 (12)	0.0621 (15)	−0.0115 (11)	0.0013 (11)	0.0049 (11)
S8	0.096 (2)	0.0466 (13)	0.0441 (13)	−0.0210 (14)	−0.0135 (13)	−0.0082 (10)
S9	0.0321 (11)	0.0432 (11)	0.0420 (11)	−0.0075 (9)	0.0049 (9)	0.0072 (9)
N1	0.018 (3)	0.036 (3)	0.025 (3)	0.004 (3)	0.002 (2)	0.001 (3)
N2	0.050 (4)	0.038 (3)	0.030 (3)	−0.017 (3)	0.004 (3)	−0.006 (3)
N3	0.023 (3)	0.031 (3)	0.032 (3)	−0.002 (3)	0.004 (3)	−0.006 (3)
N4	0.038 (4)	0.030 (3)	0.036 (4)	−0.002 (3)	0.004 (3)	−0.001 (3)
N5	0.036 (4)	0.033 (3)	0.028 (3)	−0.007 (3)	0.000 (3)	0.000 (2)
N6	0.037 (4)	0.033 (3)	0.033 (3)	−0.005 (3)	−0.003 (3)	0.005 (3)
O1W	0.073 (5)	0.056 (4)	0.057 (4)	0.000 (4)	−0.002 (4)	−0.020 (3)
O1	0.042 (3)	0.023 (2)	0.028 (3)	−0.011 (2)	−0.005 (2)	−0.0024 (19)
O2	0.020 (2)	0.025 (2)	0.030 (3)	−0.001 (2)	−0.002 (2)	0.0054 (19)
O3	0.027 (3)	0.029 (2)	0.030 (3)	−0.006 (2)	0.005 (2)	−0.010 (2)
O4	0.055 (4)	0.042 (3)	0.044 (3)	−0.011 (3)	0.016 (3)	−0.002 (3)
O5	0.024 (3)	0.043 (3)	0.036 (3)	−0.003 (2)	0.001 (2)	−0.008 (2)
O6	0.065 (5)	0.063 (4)	0.061 (4)	−0.005 (4)	0.016 (4)	−0.006 (3)
C1	0.078 (7)	0.068 (6)	0.034 (5)	−0.016 (6)	0.011 (5)	−0.019 (4)
C2	0.050 (5)	0.048 (5)	0.059 (6)	−0.020 (4)	0.007 (4)	−0.025 (4)
C3	0.044 (5)	0.024 (4)	0.081 (6)	−0.013 (4)	0.001 (5)	−0.006 (4)
C4	0.072 (7)	0.066 (6)	0.035 (5)	−0.015 (5)	0.015 (5)	0.007 (4)
C5	0.025 (4)	0.023 (3)	0.041 (4)	−0.005 (3)	−0.016 (3)	−0.002 (3)
C6	0.047 (5)	0.041 (4)	0.027 (4)	−0.014 (4)	0.016 (4)	−0.010 (3)
C7	0.037 (4)	0.027 (4)	0.024 (4)	−0.013 (4)	−0.004 (3)	0.002 (3)
C8	0.046 (5)	0.032 (4)	0.029 (4)	−0.011 (4)	0.004 (4)	−0.005 (3)
C9	0.057 (6)	0.063 (6)	0.063 (6)	−0.019 (5)	0.004 (5)	−0.037 (5)
C10	0.035 (5)	0.035 (4)	0.091 (7)	−0.002 (4)	−0.027 (5)	0.000 (5)
C11	0.073 (8)	0.218 (17)	0.098 (10)	−0.065 (10)	0.027 (7)	−0.097 (11)
C12	0.062 (7)	0.068 (6)	0.075 (7)	−0.029 (6)	−0.016 (5)	0.019 (5)
C13	0.121 (11)	0.046 (6)	0.152 (13)	−0.025 (7)	−0.071 (10)	0.009 (7)
C14	0.085 (8)	0.059 (6)	0.074 (7)	−0.041 (6)	0.003 (6)	−0.012 (5)

Geometric parameters (Å, º)

Co1—O1	2.097 (5)	N6—H6A	0.8900
Co1—O1^{i}	2.097 (5)	N6—H6B	0.8900
Co1—O2	2.089 (4)	N6—H6C	0.8900
Co1—O2^{i}	2.088 (4)	O1W—H1WA	0.8499
Co1—O3	2.084 (4)	O1W—H1WB	0.8500
Co1—O3^{i}	2.084 (4)	O3—H3A	0.8600
Cr1—N1	2.003 (7)	O3—H3B	0.8600
Cr1—N2	1.998 (6)	C1—H1A	0.9600
Cr1—N3	2.007 (7)	C1—H1B	0.9600
Cr1—N4	1.999 (6)	C1—H1C	0.9600
Cr1—N5	2.065 (6)	C2—H2A	0.9600
Cr1—N6	2.045 (6)	C2—H2B	0.9600

S1—O2	1.523 (5)	C2—H2C	0.9600
S1—C3	1.777 (7)	C3—H3C	0.9600
S1—C4	1.767 (8)	C3—H3D	0.9600
S2—O1	1.521 (5)	C3—H3E	0.9600
S2—C1	1.763 (8)	C4—H4A	0.9600
S2—C2	1.755 (9)	C4—H4B	0.9600
S3—C5	1.571 (8)	C4—H4C	0.9600
S4—C6	1.606 (8)	C9—H9A	0.9600
S5—C7	1.617 (8)	C9—H9B	0.9600
S6—C8	1.620 (8)	C9—H9C	0.9600
S7—O4	1.506 (6)	C10—H10A	0.9600
S7—C11	1.748 (11)	C10—H10B	0.9600
S7—C12	1.762 (10)	C10—H10C	0.9600
S8—O6	1.509 (7)	C11—H11A	0.9600
S8—C13	1.771 (10)	C11—H11B	0.9600
S8—C14	1.739 (10)	C11—H11C	0.9600
S9—O5	1.513 (5)	C12—H12A	0.9600
S9—C9	1.772 (8)	C12—H12B	0.9600
S9—C10	1.766 (8)	C12—H12C	0.9600
N1—C5	1.189 (9)	C13—H13A	0.9600
N2—C6	1.145 (9)	C13—H13B	0.9600
N3—C7	1.154 (9)	C13—H13C	0.9600
N4—C8	1.173 (9)	C14—H14A	0.9600
N5—H5A	0.8900	C14—H14B	0.9600
N5—H5B	0.8900	C14—H14C	0.9600
N5—H5C	0.8900		

O1^{i}—Co1—O1	180.0	H3A—O3—H3B	103.1
O2—Co1—O1	87.58 (18)	S2—C1—H1A	109.5
O2^{i}—Co1—O1^{i}	87.58 (17)	S2—C1—H1B	109.5
O2^{i}—Co1—O1	92.42 (17)	S2—C1—H1C	109.5
O2—Co1—O1^{i}	92.42 (18)	H1A—C1—H1B	109.5
O2^{i}—Co1—O2	180.0	H1A—C1—H1C	109.5
O3^{i}—Co1—O1^{i}	89.13 (19)	H1B—C1—H1C	109.5
O3^{i}—Co1—O1	90.87 (19)	S2—C2—H2A	109.5
O3—Co1—O1^{i}	90.87 (19)	S2—C2—H2B	109.5
O3—Co1—O1	89.13 (19)	S2—C2—H2C	109.5
O3^{i}—Co1—O2	89.38 (17)	H2A—C2—H2B	109.5
O3—Co1—O2	90.62 (17)	H2A—C2—H2C	109.5
O3^{i}—Co1—O2^{i}	90.62 (17)	H2B—C2—H2C	109.5
O3—Co1—O2^{i}	89.38 (17)	S1—C3—H3C	109.5
O3—Co1—O3^{i}	180.0	S1—C3—H3D	109.5
N1—Cr1—N3	178.4 (2)	S1—C3—H3E	109.5
N1—Cr1—N5	91.4 (2)	H3C—C3—H3D	109.5
N1—Cr1—N6	90.0 (2)	H3C—C3—H3E	109.5
N2—Cr1—N1	91.1 (2)	H3D—C3—H3E	109.5
N2—Cr1—N3	88.7 (2)	S1—C4—H4A	109.5
N2—Cr1—N4	178.7 (3)	S1—C4—H4B	109.5

N2—Cr1—N5	90.4 (2)	S1—C4—H4C	109.5
N2—Cr1—N6	91.7 (2)	H4A—C4—H4B	109.5
N3—Cr1—N5	90.2 (2)	H4A—C4—H4C	109.5
N3—Cr1—N6	88.4 (3)	H4B—C4—H4C	109.5
N4—Cr1—N1	87.6 (2)	N1—C5—S3	177.1 (6)
N4—Cr1—N3	92.5 (2)	N2—C6—S4	179.0 (8)
N4—Cr1—N5	89.2 (2)	N3—C7—S5	179.4 (7)
N4—Cr1—N6	88.8 (2)	N4—C8—S6	179.0 (7)
N6—Cr1—N5	177.5 (2)	S9—C9—H9A	109.5
O2—S1—C3	104.2 (3)	S9—C9—H9B	109.5
O2—S1—C4	105.4 (4)	S9—C9—H9C	109.5
C4—S1—C3	99.8 (4)	H9A—C9—H9B	109.5
O1—S2—C1	105.9 (4)	H9A—C9—H9C	109.5
O1—S2—C2	105.0 (3)	H9B—C9—H9C	109.5
C2—S2—C1	97.8 (5)	S9—C10—H10A	109.5
O4—S7—C11	104.8 (5)	S9—C10—H10B	109.5
O4—S7—C12	105.7 (4)	S9—C10—H10C	109.5
C11—S7—C12	98.3 (6)	H10A—C10—H10B	109.5
O6—S8—C13	107.0 (6)	H10A—C10—H10C	109.5
O6—S8—C14	106.6 (5)	H10B—C10—H10C	109.5
C14—S8—C13	98.5 (6)	S7—C11—H11A	109.5
O5—S9—C9	106.8 (4)	S7—C11—H11B	109.5
O5—S9—C10	104.8 (4)	S7—C11—H11C	109.5
C10—S9—C9	98.2 (4)	H11A—C11—H11B	109.5
C5—N1—Cr1	172.9 (5)	H11A—C11—H11C	109.5
C6—N2—Cr1	171.4 (7)	H11B—C11—H11C	109.5
C7—N3—Cr1	173.8 (6)	S7—C12—H12A	109.5
C8—N4—Cr1	164.3 (7)	S7—C12—H12B	109.5
Cr1—N5—H5A	109.5	S7—C12—H12C	109.5
Cr1—N5—H5B	109.5	H12A—C12—H12B	109.5
Cr1—N5—H5C	109.5	H12A—C12—H12C	109.5
H5A—N5—H5B	109.5	H12B—C12—H12C	109.5
H5A—N5—H5C	109.5	S8—C13—H13A	109.5
H5B—N5—H5C	109.5	S8—C13—H13B	109.5
Cr1—N6—H6A	109.5	S8—C13—H13C	109.5
Cr1—N6—H6B	109.5	H13A—C13—H13B	109.5
Cr1—N6—H6C	109.5	H13A—C13—H13C	109.5
H6A—N6—H6B	109.5	H13B—C13—H13C	109.5
H6A—N6—H6C	109.5	S8—C14—H14A	109.5
H6B—N6—H6C	109.5	S8—C14—H14B	109.5
H1WA—O1W—H1WB	109.7	S8—C14—H14C	109.5
S2—O1—Co1	127.9 (3)	H14A—C14—H14B	109.5
S1—O2—Co1	119.5 (2)	H14A—C14—H14C	109.5
Co1—O3—H3A	119.3	H14B—C14—H14C	109.5
Co1—O3—H3B	124.5		

C1—S2—O1—Co1	122.0 (5)	C3—S1—O2—Co1	160.4 (4)
C2—S2—O1—Co1	−135.1 (4)	C4—S1—O2—Co1	−95.1 (4)

Symmetry code: (i) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*A*···S6^{ii}	0.89	2.76	3.647 (7)	176
N5—H5*B*···O5^{iii}	0.89	2.17	3.019 (8)	160
N6—H6*A*···O4^{iv}	0.89	2.03	2.874 (8)	158
N6—H6*B*···O4	0.89	2.22	3.037 (9)	152
N6—H6*C*···O6	0.89	2.22	3.069 (8)	160
O1*W*—H1*WA*···S6^{v}	0.85	2.55	3.293 (7)	147
O1*W*—H1*WB*···O6^{v}	0.85	1.89	2.711 (9)	163
C3—H3*E*···S6^{vi}	0.96	2.97	3.590 (9)	124

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