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# *catena*-Poly[[diaqua(1*H*-imidazo[4,5-*f*][1,10]phenanthroline)cobalt(II)]-$\mu$-sulfato]

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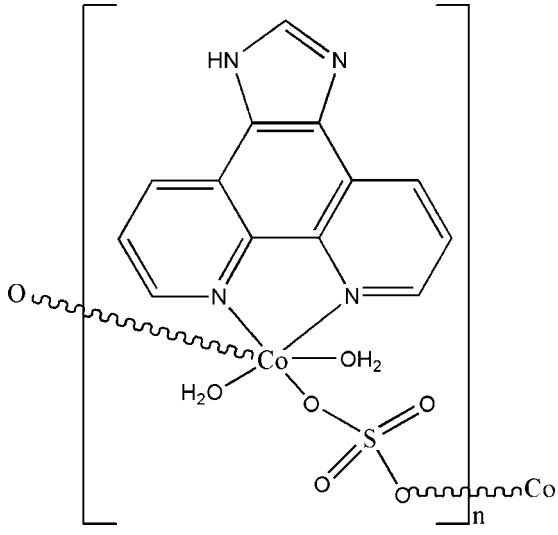
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.063; $wR$ factor = 0.100; data-to-parameter ratio = 10.9.

The $Co^{II}$ ion in the title complex, $[Co(SO_4)(C_{13}H_8N_4)(H_2O)_2]_n$, has a slightly distorted octahedral coordination environment formed by two O atoms from two symmetry-related bridging sulfate ligands, two N atoms from a bis-chelating 1*H*-imidazo[4,5-*f*][1,10]phenanthroline (IPL) ligand and two O atoms from coordinated water molecules. The bridging sulfate ligands connect $Co^{II}$ ions to form a one-dimensional chain along the *b*-axis direction. In the crystal structure, intermolecular O—H···O, O—H···N and N—H···O hydrogen bonds link the chains into a three-dimensional network.

## Related literature

For general background on coordination polymers, see: Ghosh *et al.* (2004). For related IPL coordination complexes, see: Xiong *et al.* (1999). For related structures of coordination polymers, see: Liu *et al.* (2008).




## Experimental

### Crystal data

$[Co(SO_4)(C_{13}H_8N_4)(H_2O)_2]$
$M_r$ = 411.26
Monoclinic, $P2_1/c$
$a$ = 10.916 (4) Å
$b$ = 7.017 (2) Å
$c$ = 19.690 (7) Å
$\beta$ = 99.353 (7)°
$V$ = 1488.2 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.34 mm$^{-1}$
$T$ = 298 K
0.27 × 0.15 × 0.10 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.714, $T_{max}$ = 0.878
7263 measured reflections
2639 independent reflections
1216 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.108

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.100
$S$ = 1.24
2639 reflections
242 parameters
16 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.80 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2*C*···O5 | 0.83 (5) | 1.91 (3) | 2.698 (7) | 159 (7) |
| O1—H1*C*···O5$^{i}$ | 0.82 (5) | 2.00 (4) | 2.749 (6) | 150 (7) |
| O2—H2*B*···O6$^{ii}$ | 0.82 (5) | 2.18 (3) | 2.957 (7) | 158 (6) |
| O1—H1*B*···N4$^{iii}$ | 0.84 (5) | 1.91 (5) | 2.731 (7) | 168 (7) |
| N3—H3*A*···O4$^{iv}$ | 0.86 | 1.95 | 2.795 (6) | 168 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2814).

## References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ghosh, A. K., Ghoshal, D., Lu, T. H., Mostafa, G. & Chaudhuri, N. R. (2004). *Cryst. Growth Des.* **4**, 581–857.
Liu, J. Q., Wang, Y. Y., Ma, L. F., Zhang, W. H., Zeng, X. R., Shi, Q. Z. & Peng, S. M. (2008). *Inorg. Chim. Acta*, **361**, 2327–2334.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Xiong, Y., He, X.-F., Zou, X.-H., Wu, J.-Z., Chen, X.-M., Ji, L.-N., Li, R.-H., Zhou, J.-Y. & Yu, K.-B. (1999). *J. Chem. Soc. Dalton Trans.* pp. 19–24.

# supporting information

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## *catena*-Poly[[diaqua(1*H*-imidazo[4,5-*f*][1,10]phenanthroline)cobalt(II)]-$\mu$-sulfato]

**Jian Yu**

### S1. Comment

A wide range of extended one-dimensional, two-dimensional or three-dimenional frameworks with different interesting structural features, resulting from coordination bonding, hydrogen bonding, aromatic $\pi\cdots\pi$ stacking interactions play an important role in electron-transfer processes in some biological systems (Ghosh *et al.*, 2004). 1H-imidazo[4,5-f][1,10]-phenanthroline (IPL) is a rich conjugated molecular building block and has been employed to construct frameworks (Xiong *et al.*, 1999). Herein, we describe the preparation and crystal structure of the title complex (I).

The $Co^{II}$ ion in the title complex, has a slightly distorted octahedral coordination formed by two O atoms from symmetry related bridging sulfate ligands, two N atoms from a bis-chelate IPL ligand and two O atoms from coordinated water molecules (Figure 1). The Co—N and Co—O bond lengths are not significantly different from the values observed in related complexes (Liu *et al.*, 2008). The bridging sulfate ligands connect $Co^{II}$ ions into a 1-D zigzag chain parallel to [0 1 0]. In the crystal structure, intermolecular O-H···O, O-H···N and N-H···O hydrogen bonds link one dimensional chains into a three dimensional network (Fig. 2). In addition, significant $\pi\cdots\pi$ stacking interactions with centroid to centroid distances in the range 3.465 (4)-3.548 (4)Å help stabilize the crystal structure.

### S2. Experimental

The title compound was prepared by hydrothermal conditions. IPL (22mg, 0.1 mmol) in an aqueous solution (10 mL) was mixed with an aqueous solution (5mL) of $Co(SO_4)_2$ (31mg, 0.12mmol). After stirring for 30 min in air, the mixture was placed into 25 mL Teflon-lined autoclave and heated at 383K for 96h. The autoclave was cooled at a rate 5° $h^{-1}$. The title complex as pink crystal was collected by filtration, washed with water, and dried in air.

### S3. Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å; N-H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}$. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O-H = 0.82 (1) Å).

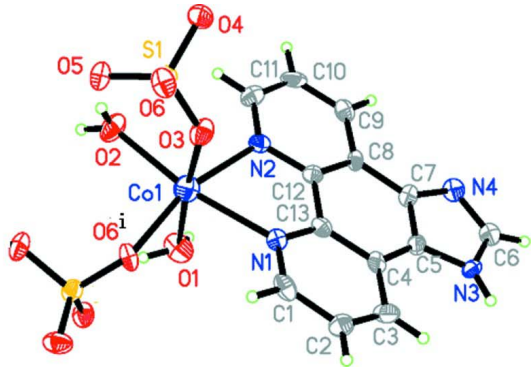


**Figure 1**

Molecular structure of the title compound showing the atom-labeling scheme [Symmetry codes: (i) -x+1,y+1/2,-z+1/2]. Displacement ellipsoids are shown at the 30% probability level.

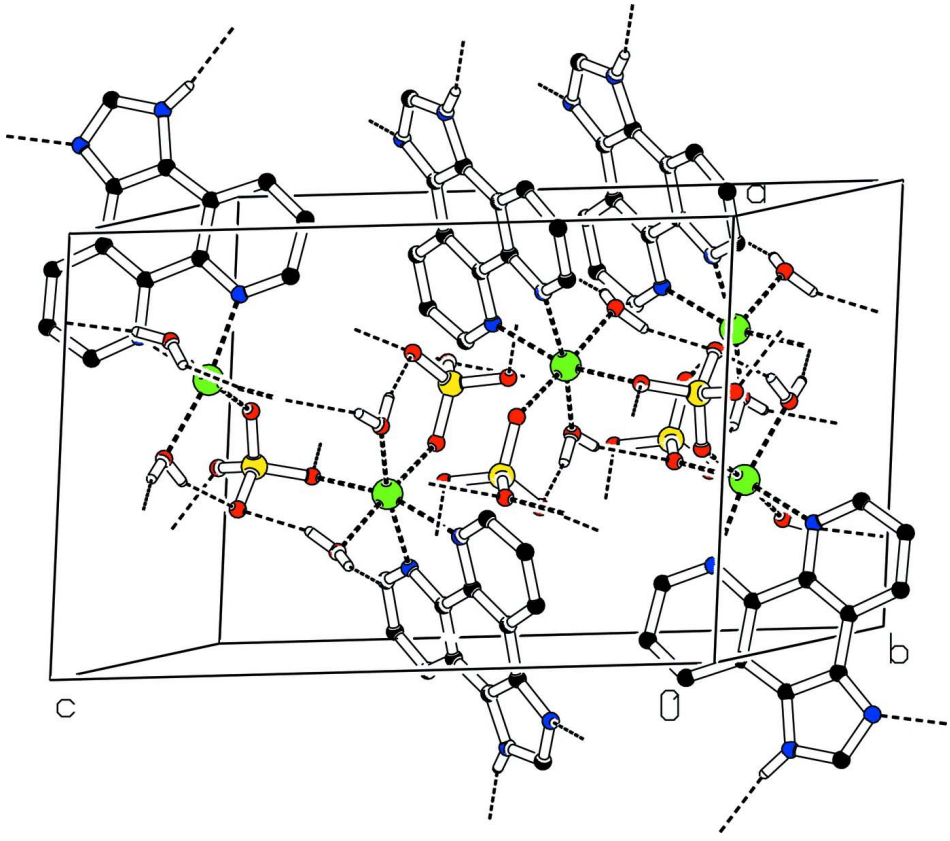


**Figure 2**

Part of the crystal structure showing hydrogen bonds as dashed lines.

***catena*-Poly[[diaqua(1*H*-imidazo[4,5-f][1,10] phenanthroline)cobalt(II)]-$\mu$-sulfato]**

*Crystal data*

| | |
|---|---|
| $[Co(SO_4)(C_{13}H_8N_4)(H_2O)_2]$ | $a$ = 10.916 (4) Å |
| $M_r$ = 411.26 | $b$ = 7.017 (2) Å |
| Monoclinic, $P2_1/c$ | $c$ = 19.690 (7) Å |
| Hall symbol: -P 2ybc | $\beta$ = 99.353 (7)° |

$V$ = 1488.2 (9) Å$^3$
$Z$ = 4
$F$(000) = 836
$D_x$ = 1.835 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2639 reflections
$\theta$ = 2.1–25.1°
$\mu$ = 1.34 mm$^{-1}$
$T$ = 298 K
Block, pink
0.27 × 0.15 × 0.10 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.714, $T_{max}$ = 0.878
7263 measured reflections
2639 independent reflections
1216 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.108
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 2.1°
$h$ = −13→11
$k$ = −7→8
$l$ = −22→23

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.100
$S$ = 1.24
2639 reflections
242 parameters
16 restraints
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
$w = 1/[\sigma^2(F_o^2) + 0.5747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.80 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.

**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 $F^2 > 2$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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.34886 (10) | 0.82399 (16) | 0.17466 (5) | 0.0429 (4) |
| S1 | 0.56896 (17) | 0.4999 (3) | 0.16741 (9) | 0.0274 (5) |
| N1 | 0.1702 (5) | 0.6658 (8) | 0.1762 (3) | 0.0245 (14) |
| N2 | 0.2484 (5) | 0.8137 (8) | 0.0647 (2) | 0.0250 (14) |
| N3 | −0.2426 (5) | 0.6042 (7) | 0.0324 (3) | 0.0267 (16) |
| H3A | −0.2918 | 0.5566 | 0.0579 | 0.032* |
| N4 | −0.1771 (5) | 0.7193 (8) | −0.0599 (2) | 0.0291 (16) |
| O1 | 0.2408 (5) | 1.0847 (8) | 0.1803 (2) | 0.0445 (15) |
| O2 | 0.5124 (5) | 0.9751 (8) | 0.1509 (3) | 0.0412 (14) |
| O3 | 0.4411 (4) | 0.5535 (6) | 0.1725 (2) | 0.0350 (14) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.5748 (4) | 0.4383 (7) | 0.09768 (19) | 0.0386 (14) |
| O5 | 0.6524 (4) | 0.6627 (7) | 0.18635 (19) | 0.0323 (12) |
| O6 | 0.6059 (4) | 0.3399 (6) | 0.21441 (19) | 0.0307 (12) |
| C1 | 0.1378 (7) | 0.5856 (9) | 0.2311 (3) | 0.031 (2) |
| H1A | 0.1966 | 0.5749 | 0.2708 | 0.037* |
| C2 | 0.0173 (7) | 0.5157 (10) | 0.2320 (3) | 0.0332 (19) |
| H2A | −0.0017 | 0.4581 | 0.2715 | 0.040* |
| C3 | −0.0704 (7) | 0.5316 (10) | 0.1759 (3) | 0.034 (2) |
| H3 | −0.1503 | 0.4864 | 0.1764 | 0.041* |
| C4 | −0.0385 (6) | 0.6200 (9) | 0.1152 (3) | 0.0238 (18) |
| C5 | −0.1175 (6) | 0.6462 (10) | 0.0526 (3) | 0.0265 (18) |
| C6 | −0.2719 (6) | 0.6509 (10) | −0.0334 (3) | 0.0278 (18) |
| H6 | −0.3512 | 0.6371 | −0.0585 | 0.033* |
| C7 | −0.0817 (6) | 0.7170 (10) | −0.0066 (3) | 0.0254 (18) |
| C8 | 0.0452 (6) | 0.7759 (9) | −0.0039 (3) | 0.0216 (18) |
| C9 | 0.0918 (7) | 0.8457 (9) | −0.0621 (3) | 0.0286 (18) |
| H9 | 0.0403 | 0.8592 | −0.1043 | 0.034* |
| C10 | 0.2155 (7) | 0.8930 (10) | −0.0542 (3) | 0.036 (2) |
| H10 | 0.2491 | 0.9375 | −0.0917 | 0.043* |
| C11 | 0.2904 (7) | 0.8744 (9) | 0.0098 (3) | 0.032 (2) |
| H11 | 0.3740 | 0.9063 | 0.0138 | 0.039* |
| C12 | 0.1267 (6) | 0.7589 (9) | 0.0569 (3) | 0.0226 (18) |
| C13 | 0.0858 (6) | 0.6824 (10) | 0.1185 (3) | 0.0237 (17) |
| H1B | 0.213 (6) | 1.151 (9) | 0.146 (2) | 0.052 (12)* |
| H2B | 0.549 (6) | 1.076 (5) | 0.159 (3) | 0.041 (7)* |
| H1C | 0.291 (5) | 1.130 (10) | 0.212 (2) | 0.049 (9)* |
| H2C | 0.570 (4) | 0.898 (7) | 0.160 (3) | 0.041 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0385 (7) | 0.0469 (8) | 0.0425 (6) | 0.0000 (7) | 0.0044 (5) | −0.0012 (6) |
| S1 | 0.0247 (11) | 0.0297 (13) | 0.0272 (10) | 0.0014 (11) | 0.0024 (8) | −0.0027 (10) |
| N1 | 0.025 (4) | 0.023 (4) | 0.025 (3) | 0.001 (3) | 0.002 (3) | 0.001 (3) |
| N2 | 0.028 (4) | 0.023 (4) | 0.025 (3) | 0.002 (3) | 0.008 (3) | −0.002 (3) |
| N3 | 0.020 (4) | 0.037 (4) | 0.025 (3) | −0.005 (3) | 0.007 (3) | −0.001 (3) |
| N4 | 0.028 (4) | 0.028 (4) | 0.029 (3) | 0.005 (3) | −0.001 (3) | 0.004 (3) |
| O1 | 0.052 (4) | 0.041 (4) | 0.036 (4) | 0.018 (3) | −0.008 (3) | 0.007 (3) |
| O2 | 0.031 (4) | 0.027 (4) | 0.067 (4) | −0.004 (3) | 0.013 (3) | 0.006 (3) |
| O3 | 0.022 (3) | 0.029 (4) | 0.053 (3) | 0.006 (3) | 0.002 (3) | 0.000 (2) |
| O4 | 0.040 (3) | 0.054 (4) | 0.023 (3) | −0.009 (3) | 0.009 (3) | −0.005 (2) |
| O5 | 0.025 (3) | 0.031 (3) | 0.039 (3) | −0.005 (3) | −0.002 (2) | 0.002 (3) |
| O6 | 0.035 (3) | 0.026 (3) | 0.027 (2) | 0.004 (3) | −0.007 (2) | 0.004 (2) |
| C1 | 0.042 (5) | 0.027 (5) | 0.020 (4) | 0.001 (4) | −0.007 (4) | 0.002 (3) |
| C2 | 0.036 (5) | 0.035 (5) | 0.031 (4) | −0.003 (5) | 0.010 (4) | 0.004 (4) |
| C3 | 0.033 (5) | 0.042 (6) | 0.029 (4) | 0.005 (4) | 0.012 (4) | −0.003 (4) |
| C4 | 0.025 (4) | 0.011 (5) | 0.034 (4) | 0.003 (4) | 0.003 (4) | −0.006 (3) |
| C5 | 0.023 (4) | 0.025 (5) | 0.031 (4) | −0.001 (4) | 0.003 (4) | −0.006 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.024 (4) | 0.024 (5) | 0.034 (4) | 0.009 (4) | −0.002 (4) | −0.002 (4) |
| C7 | 0.022 (4) | 0.021 (5) | 0.032 (4) | 0.001 (4) | 0.002 (4) | 0.004 (4) |
| C8 | 0.018 (4) | 0.016 (5) | 0.029 (4) | 0.000 (3) | −0.001 (3) | −0.002 (3) |
| C9 | 0.035 (5) | 0.018 (5) | 0.032 (4) | 0.002 (4) | 0.001 (4) | −0.001 (4) |
| C10 | 0.051 (6) | 0.036 (6) | 0.028 (4) | −0.002 (4) | 0.025 (4) | −0.002 (4) |
| C11 | 0.030 (5) | 0.033 (5) | 0.036 (5) | 0.000 (4) | 0.012 (4) | 0.005 (4) |
| C12 | 0.023 (5) | 0.021 (5) | 0.024 (4) | 0.005 (4) | 0.005 (4) | 0.000 (3) |
| C13 | 0.029 (4) | 0.015 (4) | 0.027 (4) | 0.003 (4) | 0.004 (3) | −0.003 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O3 | 2.152 (4) | O2—H2C | 0.83 (5) |
| Co1—O6$^{i}$ | 2.162 (4) | O6—Co1$^{ii}$ | 2.162 (4) |
| Co1—O2 | 2.192 (5) | C1—C2 | 1.406 (9) |
| Co1—O1 | 2.190 (5) | C1—H1A | 0.9300 |
| Co1—N1 | 2.249 (5) | C2—C3 | 1.343 (8) |
| Co1—N2 | 2.263 (5) | C2—H2A | 0.9300 |
| S1—O4 | 1.451 (4) | C3—C4 | 1.438 (8) |
| S1—O3 | 1.465 (4) | C3—H3 | 0.9300 |
| S1—O6 | 1.469 (4) | C4—C5 | 1.397 (8) |
| S1—O5 | 1.471 (5) | C4—C13 | 1.417 (9) |
| N1—C1 | 1.317 (7) | C5—C7 | 1.382 (8) |
| N1—C13 | 1.347 (7) | C6—H6 | 0.9300 |
| N2—C11 | 1.312 (7) | C7—C8 | 1.438 (8) |
| N2—C12 | 1.368 (7) | C8—C12 | 1.375 (8) |
| N3—C6 | 1.325 (7) | C8—C9 | 1.414 (8) |
| N3—C5 | 1.391 (7) | C9—C10 | 1.374 (9) |
| N3—H3A | 0.8600 | C9—H9 | 0.9300 |
| N4—C6 | 1.322 (7) | C10—C11 | 1.393 (9) |
| N4—C7 | 1.353 (8) | C10—H10 | 0.9300 |
| O1—H1B | 0.84 (5) | C11—H11 | 0.9300 |
| O1—H1C | 0.82 (5) | C12—C13 | 1.462 (8) |
| O2—H2B | 0.82 (5) | | |

| | | | |
|---|---|---|---|
| O3—Co1—O6$^{i}$ | 91.96 (17) | N1—C1—C2 | 122.4 (7) |
| O3—Co1—O2 | 91.30 (19) | N1—C1—H1A | 118.8 |
| O6$^{i}$—Co1—O2 | 97.5 (2) | C2—C1—H1A | 118.8 |
| O3—Co1—O1 | 174.6 (2) | C3—C2—C1 | 120.3 (7) |
| O6$^{i}$—Co1—O1 | 86.69 (17) | C3—C2—H2A | 119.8 |
| O2—Co1—O1 | 94.1 (2) | C1—C2—H2A | 119.8 |
| O3—Co1—N1 | 88.53 (18) | C2—C3—C4 | 118.8 (7) |
| O6$^{i}$—Co1—N1 | 93.88 (18) | C2—C3—H3 | 120.6 |
| O2—Co1—N1 | 168.6 (2) | C4—C3—H3 | 120.6 |
| O1—Co1—N1 | 86.3 (2) | C5—C4—C13 | 116.6 (6) |
| O3—Co1—N2 | 96.26 (18) | C5—C4—C3 | 126.3 (6) |
| O6$^{i}$—Co1—N2 | 164.44 (18) | C13—C4—C3 | 117.0 (6) |
| O2—Co1—N2 | 95.5 (2) | C7—C5—N3 | 103.5 (6) |
| O1—Co1—N2 | 83.90 (18) | C7—C5—C4 | 125.0 (7) |

| | | | |
|---|---|---|---|
| N1—Co1—N2 | 73.20 (19) | N3—C5—C4 | 131.4 (6) |
| O4—S1—O3 | 109.3 (3) | N4—C6—N3 | 113.4 (6) |
| O4—S1—O6 | 108.6 (3) | N4—C6—H6 | 123.3 |
| O3—S1—O6 | 108.7 (3) | N3—C6—H6 | 123.3 |
| O4—S1—O5 | 110.5 (3) | N4—C7—C5 | 111.8 (6) |
| O3—S1—O5 | 109.9 (3) | N4—C7—C8 | 129.9 (6) |
| O6—S1—O5 | 109.8 (3) | C5—C7—C8 | 118.3 (7) |
| C1—N1—C13 | 119.4 (6) | C12—C8—C9 | 117.9 (6) |
| C1—N1—Co1 | 124.9 (5) | C12—C8—C7 | 119.4 (6) |
| C13—N1—Co1 | 114.9 (4) | C9—C8—C7 | 122.7 (6) |
| C11—N2—C12 | 117.5 (6) | C10—C9—C8 | 118.0 (6) |
| C11—N2—Co1 | 126.7 (5) | C10—C9—H9 | 121.0 |
| C12—N2—Co1 | 115.3 (4) | C8—C9—H9 | 121.0 |
| C6—N3—C5 | 107.3 (5) | C9—C10—C11 | 120.0 (6) |
| C6—N3—H3A | 126.4 | C9—C10—H10 | 120.0 |
| C5—N3—H3A | 126.4 | C11—C10—H10 | 120.0 |
| C6—N4—C7 | 104.1 (5) | N2—C11—C10 | 122.9 (7) |
| Co1—O1—H1B | 124 (5) | N2—C11—H11 | 118.5 |
| Co1—O1—H1C | 94 (5) | C10—C11—H11 | 118.5 |
| H1B—O1—H1C | 121 (7) | N2—C12—C8 | 123.5 (6) |
| Co1—O2—H2B | 140 (5) | N2—C12—C13 | 115.6 (6) |
| Co1—O2—H2C | 105 (5) | C8—C12—C13 | 120.9 (6) |
| H2B—O2—H2C | 101 (7) | N1—C13—C4 | 122.0 (6) |
| S1—O3—Co1 | 133.0 (3) | N1—C13—C12 | 118.2 (6) |
| S1—O6—Co1$^{ii}$ | 132.0 (3) | C4—C13—C12 | 119.7 (6) |

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| O3—Co1—N1—C1 | 79.0 (5) | C13—C4—C5—N3 | −179.2 (7) |
| O6$^{i}$—Co1—N1—C1 | −12.9 (5) | C3—C4—C5—N3 | 2.5 (12) |
| O2—Co1—N1—C1 | 168.3 (9) | C7—N4—C6—N3 | −0.6 (8) |
| O1—Co1—N1—C1 | −99.3 (5) | C5—N3—C6—N4 | 0.7 (8) |
| N2—Co1—N1—C1 | 175.9 (6) | C6—N4—C7—C5 | 0.4 (8) |
| O3—Co1—N1—C13 | −111.3 (5) | C6—N4—C7—C8 | −179.5 (7) |
| O6$^{i}$—Co1—N1—C13 | 156.9 (5) | N3—C5—C7—N4 | 0.0 (8) |
| O2—Co1—N1—C13 | −22.0 (13) | C4—C5—C7—N4 | 177.6 (6) |
| O1—Co1—N1—C13 | 70.4 (5) | N3—C5—C7—C8 | 179.9 (6) |
| N2—Co1—N1—C13 | −14.3 (4) | C4—C5—C7—C8 | −2.5 (11) |
| O3—Co1—N2—C11 | −88.4 (6) | N4—C7—C8—C12 | −179.6 (7) |
| O6$^{i}$—Co1—N2—C11 | 150.2 (7) | C5—C7—C8—C12 | 0.5 (10) |
| O2—Co1—N2—C11 | 3.5 (6) | N4—C7—C8—C9 | −1.8 (12) |
| O1—Co1—N2—C11 | 97.1 (6) | C5—C7—C8—C9 | 178.3 (7) |
| N1—Co1—N2—C11 | −174.9 (6) | C12—C8—C9—C10 | −0.3 (10) |
| O3—Co1—N2—C12 | 99.8 (5) | C7—C8—C9—C10 | −178.2 (6) |
| O6$^{i}$—Co1—N2—C12 | −21.7 (10) | C8—C9—C10—C11 | −1.0 (10) |
| O2—Co1—N2—C12 | −168.3 (5) | C12—N2—C11—C10 | 3.1 (10) |
| O1—Co1—N2—C12 | −74.8 (5) | Co1—N2—C11—C10 | −168.6 (5) |
| N1—Co1—N2—C12 | 13.2 (4) | C9—C10—C11—N2 | −0.5 (11) |
| O4—S1—O3—Co1 | −102.4 (4) | C11—N2—C12—C8 | −4.4 (10) |
| O6—S1—O3—Co1 | 139.3 (3) | Co1—N2—C12—C8 | 168.2 (5) |

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| O5—S1—O3—Co1 | 19.1 (4) | C11—N2—C12—C13 | 176.7 (6) |
| O6$^{i}$—Co1—O3—S1 | −89.7 (4) | Co1—N2—C12—C13 | −10.7 (7) |
| O2—Co1—O3—S1 | 7.9 (4) | C9—C8—C12—N2 | 3.0 (10) |
| N1—Co1—O3—S1 | 176.5 (4) | C7—C8—C12—N2 | −179.0 (6) |
| N2—Co1—O3—S1 | 103.6 (4) | C9—C8—C12—C13 | −178.1 (6) |
| O4—S1—O6—Co1$^{ii}$ | 168.3 (3) | C7—C8—C12—C13 | −0.1 (10) |
| O3—S1—O6—Co1$^{ii}$ | −72.9 (4) | C1—N1—C13—C4 | 1.4 (10) |
| O5—S1—O6—Co1$^{ii}$ | 47.3 (4) | Co1—N1—C13—C4 | −168.9 (5) |
| C13—N1—C1—C2 | 0.1 (10) | C1—N1—C13—C12 | −175.5 (6) |
| Co1—N1—C1—C2 | 169.4 (5) | Co1—N1—C13—C12 | 14.1 (8) |
| N1—C1—C2—C3 | −1.0 (11) | C5—C4—C13—N1 | 179.6 (6) |
| C1—C2—C3—C4 | 0.5 (11) | C3—C4—C13—N1 | −1.9 (10) |
| C2—C3—C4—C5 | 179.3 (7) | C5—C4—C13—C12 | −3.5 (10) |
| C2—C3—C4—C13 | 0.9 (10) | C3—C4—C13—C12 | 175.0 (6) |
| C6—N3—C5—C7 | −0.4 (7) | N2—C12—C13—N1 | −2.3 (9) |
| C6—N3—C5—C4 | −177.7 (7) | C8—C12—C13—N1 | 178.8 (6) |
| C13—C4—C5—C7 | 4.0 (11) | N2—C12—C13—C4 | −179.3 (6) |
| C3—C4—C5—C7 | −174.3 (7) | C8—C12—C13—C4 | 1.7 (10) |

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*C*···O5 | 0.83 (5) | 1.91 (3) | 2.698 (7) | 159 (7) |
| O1—H1*C*···O5$^{i}$ | 0.82 (5) | 2.00 (4) | 2.749 (6) | 150 (7) |
| O2—H2*B*···O6$^{iii}$ | 0.82 (5) | 2.18 (3) | 2.957 (7) | 158 (6) |
| O1—H1*B*···N4$^{iv}$ | 0.84 (5) | 1.91 (5) | 2.731 (7) | 168 (7) |
| N3—H3*A*···O4$^{v}$ | 0.86 | 1.95 | 2.795 (6) | 168 |

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