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# Bis(1,10-phenanthroline-$\kappa^2N,N'$)(sulfato-$\kappa^2O,O'$)cobalt(II) propane-1,3-diol solvate

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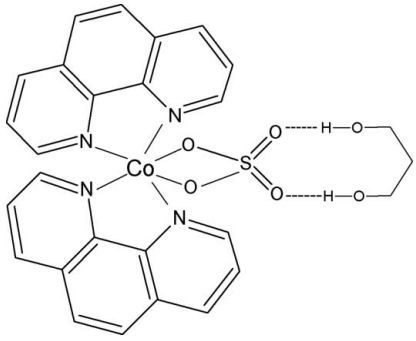
Key indicators: single-crystal X-ray study; $T$ = 223 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.038; $wR$ factor = 0.101; data-to-parameter ratio = 15.8.

The title compound, $[Co(SO_4)(C_{12}H_8N_2)_2]\cdot C_3H_8O_2$, was obtained unexpectedly as a by-product during an attempt to synthesize a mixed-ligand complex of $Co^{II}$ with 1,10-phenanthroline (phen) and melamine *via* a solvothermal reaction. The $Co^{II}$ metal ions are in a distorted octahedral coordination environment formed by four N atoms from two chelating phen ligands and two O atoms from a bidentate sulfate ligand. The two chelating $N_2C_2$ groups are almost perpendicular to each other [dihedral angle = 80.06 (8)°]. A twofold rotation axis passes through the Co and S atoms, and also through the central C atom of the propane-1,3-diol solvent molecule. Intermolecular O—H···O hydrogen bonds help to stabilize the structure.

## Related literature

For related cobalt compounds with monodentate, bidentate-bridging sulfate ligands, see: Hennig *et al.* (1975); Li & Zhou (1987); Song *et al.* (2008); Zheng & Lin (2003). For related complexes with bidentate-chelating ligands, see: Lu *et al.* (2006); Paul *et al.* (2002); Wang *et al.* (2009). For an isostructural structure, see: Zhong *et al.* (2006). For a related structure, see: Chen *et al.* (2005). For applications of transition metal complexes of phen, see: Li *et al.* (2004); Wang *et al.* (2000).




## Experimental

### Crystal data

$[Co(SO_4)(C_{12}H_8N_2)_2]\cdot C_3H_8O_2$
$M_r$ = 591.49
Monoclinic, $C2/c$
$a$ = 18.285 (4) Å
$b$ = 12.422 (3) Å
$c$ = 13.211 (3) Å
$\beta$ = 121.82 (3)°
$V$ = 2549.7 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.81 mm$^{-1}$
$T$ = 223 K
0.60 × 0.40 × 0.34 mm

### Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*: Jacobson, 1998)
$T_{min}$ = 0.823, $T_{max}$ = 1.000
7099 measured reflections
2898 independent reflections
2540 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.101
$S$ = 1.06
2898 reflections
183 parameters
21 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.72 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$B$···O2 | 0.82 | 1.92 | 2.737 (3) | 179 |

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); 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: ZQ2024).

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# supplementary materials

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# Bis(1,10-phenanthroline-$\kappa^2N,N'$)(sulfato-$\kappa^2O,O'$)cobalt(II) propane-1,3-diol solvate

**K.-L. Zhong**

## Comment

Metal-organic complexes have been widely applied in fields of research and production because of their capability of showing novel optical, electronical, magnetical properties. M-phen transition metal complexes (phen = phenantroline) possess important actions in the areas of extraction, plating, bio-inorganic chemistry, analytical chemistry and functional materials (Wang *et al.*, 2000; Li *et al.*, 2004).

Although many transtion metal complexes with sulfate ions as monodentate, bidentate and bidentate-bridging ligands have been structurally characterized (Hennig *et al.*, 1975; Zheng & Lin, 2003; Song *et al.*, 2008), as far as we know, the reports on complexes with bidentate-chelating sulfate ligands are few (Paul *et al.*, 2002; Lu *et al.*, 2006; Wang *et al.*, 2009). Here, we report the crystal structure of the new complex $[CoSO_4(C_{12}H_8N_2)_2].C_3H_8O_2$ unexpectedly obtained during an attempt to synthesize a mixed-ligand complex of cobalt with phen and melamine *via* a solvothermal reaction, which is analogue with a previously reported $Co^{II}$ complex (Zhong *et al.*, 2006).

In the crystal structure of the title complex, the $Co^{II}$ metal ion is six-coordinated in a distorted octahedral environement by four N atoms from two chelating phen ligands and two O atoms from a bidentate-chelating sulfate ligand (Fig. 1). The Co—O bond distance [2.1323 (15) Å], the O—Co—O bite angle [66.54 (8)°], the Co—N bond distances [2.1295 (16)–2.1341 (17) Å] and the N—Co—N bite angle [77.99 (6)°] are very similar to those seen in the previously reported cobalt complex $[CoSO_4(C_{12}H_8N_2)_2].C_2H_6O_2$ (II)[Zhong *et al.*, 2006]. The dihedral angle between the two chelating $N_2C_2$ groups is 80.06 (8)°, this is larger than that found in (II) [70.16 (6)°]. A twofold rotation axis (symmetry code: $-x + 1, y, -z + 1/2$) passes through the Co and S atoms, and also through the mid-carbon of the propane-1,3-diol solvent molecule. The crystal structure is further stabilized by intermolecular O3—H3B···O2 hydrogen bonds (Fig. 1 and Table 1).

## Experimental

Red prism-shaped crystals of the title compound was unexpectedly obtained as a by-product during an attempt to synthesize a mixed-ligand cobalt complex with phen and melamine *via* a propane-1,3-diol/water solvothermal reaction. 0.2 mmol phen, 0.1 mmol melamine, 0.1 mmol $CoSO_4.7H_2O$, 2.0 ml 1,3-propanediol and 1.0 ml water were mixed and placed in a thick Pyrex tube, which was sealed and heated to 413 K for 96 h, whereupon red-prisms of the title complex were obtained.

## Refinement

The non-H atoms were refined anisotropically. The H atoms of phen were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of central C atom of propane-1,3-diol were constrained, with C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, whereas other H atoms were placed in geometrically idealized positions and refined as riding atoms, with C—H = 0.97 Å and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$.

## Figures

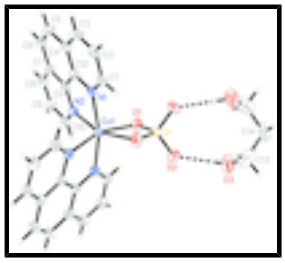

Fig. 1. The molecular structure of the title complex showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. The dashed lines represent O—H···O interactions. Unlabeled atoms are related to the labelled atoms by the symmetry operator (-*x* + 1, *y*, - *z* + 1/2).

## Bis(1,10-phenanthroline-κ$^2$*N*,*N*')(sulfato- κ$^2$*O*,*O*')cobalt(II) propane-1,3-diol solvate

*Crystal data*

| | |
|---|---|
| $[Co(SO_4)(C_{12}H_8N_2)_2]\cdot C_3H_8O_2$ | $F(000) = 1220$ |
| $M_r = 591.49$ | $D_x = 1.541$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 3592 reflections |
| *a* = 18.285 (4) Å | θ = 3.2–27.5° |
| *b* = 12.422 (3) Å | μ = 0.81 mm$^{-1}$ |
| *c* = 13.211 (3) Å | *T* = 223 K |
| β = 121.82 (3)° | Prism, red |
| *V* = 2549.7 (13) Å$^3$ | 0.60 × 0.40 × 0.34 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Rigaku Mercury CCD diffractometer | 2898 independent reflections |
| Radiation source: fine-focus sealed tube | 2540 reflections with $I > 2\sigma(I)$ |
| Graphite Monochromator | $R_{int} = 0.021$ |
| Detector resolution: 28.5714 pixels mm$^{-1}$ | $\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$ |
| ω scans | $h = -23\rightarrow23$ |
| Absorption correction: multi-scan (*REQAB*: Jacobson, 1998) | $k = -16\rightarrow13$ |
| $T_{min} = 0.823$, $T_{max} = 1.000$ | $l = -17\rightarrow14$ |
| 7099 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.101$ | $w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 1.0504P]$ where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| $S$ = 1.06 | $(\Delta/\sigma)_{max} < 0.001$ |
| 2898 reflections | $\Delta\rho_{max}$ = 0.72 e Å$^{-3}$ |
| 183 parameters | $\Delta\rho_{min}$ = −0.45 e Å$^{-3}$ |
| 21 restraints | Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0057 (6) |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.5000 | 0.81835 (3) | 0.2500 | 0.02201 (14) |
| S1 | 0.5000 | 1.03618 (5) | 0.2500 | 0.02331 (17) |
| O1 | 0.44793 (9) | 0.96187 (12) | 0.14805 (12) | 0.0329 (3) |
| C11 | 0.34382 (12) | 0.68292 (14) | 0.14757 (16) | 0.0224 (4) |
| N2 | 0.40420 (10) | 0.71189 (13) | 0.12195 (14) | 0.0238 (3) |
| C10 | 0.39507 (13) | 0.67410 (16) | 0.02169 (18) | 0.0284 (4) |
| H10A | 0.4356 | 0.6935 | 0.0028 | 0.034* |
| C8 | 0.26687 (13) | 0.57717 (16) | −0.03144 (17) | 0.0304 (4) |
| H8A | 0.2213 | 0.5328 | −0.0832 | 0.036* |
| O2 | 0.55612 (10) | 1.10269 (14) | 0.22920 (16) | 0.0446 (4) |
| C6 | 0.21399 (13) | 0.58852 (17) | 0.10868 (18) | 0.0310 (4) |
| H6A | 0.1679 | 0.5434 | 0.0604 | 0.037* |
| C12 | 0.35267 (11) | 0.72718 (15) | 0.25388 (16) | 0.0223 (4) |
| C7 | 0.27424 (12) | 0.61511 (16) | 0.07446 (17) | 0.0264 (4) |
| C4 | 0.29234 (12) | 0.69936 (16) | 0.28497 (17) | 0.0270 (4) |
| C9 | 0.32726 (14) | 0.60646 (18) | −0.05671 (18) | 0.0331 (4) |
| H9A | 0.3235 | 0.5817 | −0.1257 | 0.040* |
| C5 | 0.22322 (12) | 0.62810 (18) | 0.21042 (18) | 0.0322 (5) |
| H5A | 0.1841 | 0.6086 | 0.2319 | 0.039* |
| N1 | 0.41806 (10) | 0.79727 (13) | 0.31789 (14) | 0.0250 (3) |
| C1 | 0.42581 (13) | 0.84107 (17) | 0.41526 (18) | 0.0291 (4) |
| H1A | 0.4706 | 0.8892 | 0.4597 | 0.035* |
| C2 | 0.36899 (14) | 0.81726 (18) | 0.45310 (19) | 0.0335 (5) |
| H2A | 0.3762 | 0.8491 | 0.5215 | 0.040* |
| C3 | 0.30319 (13) | 0.74709 (18) | 0.38888 (18) | 0.0335 (5) |

| | | | | |
|---|---|---|---|---|
| H3A | 0.2653 | 0.7306 | 0.4135 | 0.040* |
| O3 | 0.56334 (16) | 1.31539 (16) | 0.1809 (2) | 0.0659 (6) |
| H3B | 0.5610 | 1.2514 | 0.1944 | 0.099* |
| C14 | 0.5000 | 1.4456 (3) | 0.2500 | 0.0562 (10) |
| C13 | 0.5774 (2) | 1.3764 (3) | 0.2780 (3) | 0.0723 (9) |
| H13A | 0.6268 | 1.4227 | 0.3033 | 0.087* |
| H13B | 0.5907 | 1.3286 | 0.3436 | 0.087* |
| H14 | 0.496 (3) | 1.442 (4) | 0.174 (2) | 0.143 (19)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0211 (2) | 0.0208 (2) | 0.0239 (2) | 0.000 | 0.01172 (16) | 0.000 |
| S1 | 0.0212 (3) | 0.0200 (3) | 0.0303 (3) | 0.000 | 0.0146 (3) | 0.000 |
| O1 | 0.0315 (7) | 0.0277 (8) | 0.0270 (7) | 0.0012 (6) | 0.0068 (6) | 0.0011 (6) |
| C11 | 0.0222 (9) | 0.0193 (9) | 0.0227 (9) | 0.0027 (7) | 0.0098 (7) | 0.0026 (7) |
| N2 | 0.0253 (8) | 0.0218 (8) | 0.0254 (8) | 0.0006 (6) | 0.0141 (7) | 0.0004 (6) |
| C10 | 0.0334 (10) | 0.0272 (11) | 0.0284 (10) | −0.0004 (8) | 0.0189 (9) | −0.0014 (8) |
| C8 | 0.0306 (10) | 0.0278 (11) | 0.0241 (9) | −0.0033 (8) | 0.0085 (8) | −0.0045 (8) |
| O2 | 0.0435 (9) | 0.0362 (9) | 0.0676 (12) | −0.0093 (8) | 0.0386 (9) | 0.0028 (8) |
| C6 | 0.0243 (9) | 0.0314 (11) | 0.0298 (10) | −0.0075 (8) | 0.0092 (8) | 0.0014 (8) |
| C12 | 0.0202 (8) | 0.0222 (9) | 0.0218 (8) | 0.0026 (7) | 0.0092 (7) | 0.0028 (7) |
| C7 | 0.0251 (9) | 0.0245 (10) | 0.0247 (9) | 0.0007 (8) | 0.0098 (8) | 0.0020 (7) |
| C4 | 0.0251 (9) | 0.0291 (10) | 0.0271 (9) | 0.0023 (8) | 0.0139 (8) | 0.0045 (8) |
| C9 | 0.0397 (11) | 0.0332 (11) | 0.0252 (9) | 0.0002 (9) | 0.0162 (9) | −0.0043 (8) |
| C5 | 0.0259 (9) | 0.0382 (12) | 0.0328 (10) | −0.0041 (9) | 0.0157 (8) | 0.0046 (9) |
| N1 | 0.0249 (8) | 0.0252 (8) | 0.0253 (8) | 0.0004 (6) | 0.0135 (7) | −0.0008 (6) |
| C1 | 0.0304 (10) | 0.0283 (11) | 0.0270 (9) | −0.0003 (8) | 0.0140 (8) | −0.0050 (8) |
| C2 | 0.0409 (12) | 0.0361 (12) | 0.0282 (10) | 0.0029 (9) | 0.0213 (10) | −0.0025 (8) |
| C3 | 0.0347 (10) | 0.0419 (13) | 0.0318 (10) | 0.0004 (9) | 0.0229 (9) | 0.0030 (9) |
| O3 | 0.1116 (18) | 0.0412 (11) | 0.0867 (15) | −0.0012 (11) | 0.0808 (15) | 0.0034 (10) |
| C14 | 0.085 (3) | 0.0301 (18) | 0.068 (3) | 0.000 | 0.050 (2) | 0.000 |
| C13 | 0.077 (2) | 0.072 (2) | 0.069 (2) | −0.0252 (18) | 0.0392 (17) | −0.0071 (17) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Co1—N1$^{i}$ | 2.1295 (16) | C6—C7 | 1.432 (3) |
| Co1—N1 | 2.1295 (16) | C6—H6A | 0.9300 |
| Co1—O1$^{i}$ | 2.1323 (15) | C12—N1 | 1.355 (3) |
| Co1—O1 | 2.1323 (15) | C12—C4 | 1.408 (3) |
| Co1—N2 | 2.1341 (17) | C4—C3 | 1.410 (3) |
| Co1—N2$^{i}$ | 2.1341 (17) | C4—C5 | 1.428 (3) |
| Co1—S1 | 2.7058 (9) | C9—H9A | 0.9300 |
| S1—O2 | 1.4519 (15) | C5—H5A | 0.9300 |
| S1—O2$^{i}$ | 1.4519 (15) | N1—C1 | 1.334 (3) |
| S1—O1 | 1.4901 (15) | C1—C2 | 1.401 (3) |
| S1—O1$^{i}$ | 1.4901 (15) | C1—H1A | 0.9300 |
| C11—N2 | 1.363 (2) | C2—C3 | 1.360 (3) |

| | | | |
|---|---|---|---|
| C11—C7 | 1.402 (3) | C2—H2A | 0.9300 |
| C11—C12 | 1.436 (3) | C3—H3A | 0.9300 |
| N2—C10 | 1.330 (2) | O3—C13 | 1.392 (3) |
| C10—C9 | 1.401 (3) | O3—H3B | 0.8200 |
| C10—H10A | 0.9300 | C14—C13$^{i}$ | 1.525 (4) |
| C8—C9 | 1.361 (3) | C14—C13 | 1.525 (4) |
| C8—C7 | 1.414 (3) | C14—H14 | 0.97 (3) |
| C8—H8A | 0.9300 | C13—H13A | 0.9700 |
| C6—C5 | 1.356 (3) | C13—H13B | 0.9700 |
| N1$^{i}$—Co1—N1 | 165.87 (9) | C9—C8—H8A | 120.4 |
| N1$^{i}$—Co1—O1$^{i}$ | 100.94 (6) | C7—C8—H8A | 120.4 |
| N1—Co1—O1$^{i}$ | 90.91 (6) | C5—C6—C7 | 120.98 (18) |
| N1$^{i}$—Co1—O1 | 90.91 (6) | C5—C6—H6A | 119.5 |
| N1—Co1—O1 | 100.94 (6) | C7—C6—H6A | 119.5 |
| O1$^{i}$—Co1—O1 | 66.54 (8) | N1—C12—C4 | 123.01 (17) |
| N1$^{i}$—Co1—N2 | 93.19 (6) | N1—C12—C11 | 117.63 (16) |
| N1—Co1—N2 | 77.99 (6) | C4—C12—C11 | 119.33 (17) |
| O1$^{i}$—Co1—N2 | 157.72 (6) | C11—C7—C8 | 117.41 (18) |
| O1—Co1—N2 | 96.36 (6) | C11—C7—C6 | 119.39 (18) |
| N1$^{i}$—Co1—N2$^{i}$ | 77.99 (6) | C8—C7—C6 | 123.19 (18) |
| N1—Co1—N2$^{i}$ | 93.19 (6) | C12—C4—C3 | 116.81 (18) |
| O1$^{i}$—Co1—N2$^{i}$ | 96.36 (6) | C12—C4—C5 | 119.71 (18) |
| O1—Co1—N2$^{i}$ | 157.72 (6) | C3—C4—C5 | 123.45 (18) |
| N2—Co1—N2$^{i}$ | 103.42 (9) | C8—C9—C10 | 119.69 (19) |
| N1$^{i}$—Co1—S1 | 97.06 (5) | C8—C9—H9A | 120.2 |
| N1—Co1—S1 | 97.06 (5) | C10—C9—H9A | 120.2 |
| O1$^{i}$—Co1—S1 | 33.27 (4) | C6—C5—C4 | 120.73 (18) |
| O1—Co1—S1 | 33.27 (4) | C6—C5—H5A | 119.6 |
| N2—Co1—S1 | 128.29 (5) | C4—C5—H5A | 119.6 |
| N2$^{i}$—Co1—S1 | 128.29 (5) | C1—N1—C12 | 118.30 (16) |
| O2—S1—O2$^{i}$ | 110.64 (15) | C1—N1—Co1 | 127.99 (14) |
| O2—S1—O1 | 111.10 (9) | C12—N1—Co1 | 113.67 (12) |
| O2$^{i}$—S1—O1 | 110.18 (9) | N1—C1—C2 | 122.42 (19) |
| O2—S1—O1$^{i}$ | 110.18 (9) | N1—C1—H1A | 118.8 |
| O2$^{i}$—S1—O1$^{i}$ | 111.10 (9) | C2—C1—H1A | 118.8 |
| O1—S1—O1$^{i}$ | 103.45 (12) | C3—C2—C1 | 119.41 (19) |
| O2—S1—Co1 | 124.68 (7) | C3—C2—H2A | 120.3 |
| O2$^{i}$—S1—Co1 | 124.68 (7) | C1—C2—H2A | 120.3 |
| O1—S1—Co1 | 51.72 (6) | C2—C3—C4 | 120.05 (18) |
| O1$^{i}$—S1—Co1 | 51.72 (6) | C2—C3—H3A | 120.0 |
| S1—O1—Co1 | 95.01 (7) | C4—C3—H3A | 120.0 |
| N2—C11—C7 | 123.19 (17) | C13—O3—H3B | 109.5 |
| N2—C11—C12 | 116.97 (16) | C13$^{i}$—C14—C13 | 111.4 (3) |
| C7—C11—C12 | 119.82 (17) | C13$^{i}$—C14—H14 | 100 (3) |

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|---|---|---|---|
| C10—N2—C11 | 117.47 (17) | C13—C14—H14 | 77 (3) |
| C10—N2—Co1 | 128.88 (13) | O3—C13—C14 | 112.8 (2) |
| C11—N2—Co1 | 113.62 (12) | O3—C13—H13A | 109.0 |
| N2—C10—C9 | 123.06 (18) | C14—C13—H13A | 109.0 |
| N2—C10—H10A | 118.5 | O3—C13—H13B | 109.0 |
| C9—C10—H10A | 118.5 | C14—C13—H13B | 109.0 |
| C9—C8—C7 | 119.17 (19) | H13A—C13—H13B | 107.8 |
| $N1^{i}$—Co1—S1—O2 | −9.86 (10) | C11—N2—C10—C9 | −0.4 (3) |
| N1—Co1—S1—O2 | 170.14 (10) | Co1—N2—C10—C9 | −178.16 (15) |
| $O1^{i}$—Co1—S1—O2 | 89.33 (12) | N2—C11—C12—N1 | 2.5 (3) |
| O1—Co1—S1—O2 | −90.67 (12) | C7—C11—C12—N1 | −176.19 (17) |
| N2—Co1—S1—O2 | −109.61 (10) | N2—C11—C12—C4 | −179.60 (17) |
| $N2^{i}$—Co1—S1—O2 | 70.39 (10) | C7—C11—C12—C4 | 1.7 (3) |
| $N1^{i}$—Co1—S1—$O2^{i}$ | 170.14 (10) | N2—C11—C7—C8 | −1.0 (3) |
| N1—Co1—S1—$O2^{i}$ | −9.86 (10) | C12—C11—C7—C8 | 177.62 (17) |
| $O1^{i}$—Co1—S1—$O2^{i}$ | −90.67 (12) | N2—C11—C7—C6 | 179.73 (18) |
| O1—Co1—S1—$O2^{i}$ | 89.33 (12) | C12—C11—C7—C6 | −1.7 (3) |
| N2—Co1—S1—$O2^{i}$ | 70.39 (10) | C9—C8—C7—C11 | 0.8 (3) |
| $N2^{i}$—Co1—S1—$O2^{i}$ | −109.61 (10) | C9—C8—C7—C6 | −179.9 (2) |
| $N1^{i}$—Co1—S1—O1 | 80.81 (9) | C5—C6—C7—C11 | 0.1 (3) |
| N1—Co1—S1—O1 | −99.19 (9) | C5—C6—C7—C8 | −179.1 (2) |
| $O1^{i}$—Co1—S1—O1 | 180.0 | N1—C12—C4—C3 | −0.9 (3) |
| N2—Co1—S1—O1 | −18.94 (9) | C11—C12—C4—C3 | −178.66 (17) |
| $N2^{i}$—Co1—S1—O1 | 161.06 (9) | N1—C12—C4—C5 | 177.55 (18) |
| $N1^{i}$—Co1—S1—$O1^{i}$ | −99.19 (9) | C11—C12—C4—C5 | −0.2 (3) |
| N1—Co1—S1—$O1^{i}$ | 80.81 (9) | C7—C8—C9—C10 | −0.5 (3) |
| O1—Co1—S1—$O1^{i}$ | 180.0 | N2—C10—C9—C8 | 0.3 (3) |
| N2—Co1—S1—$O1^{i}$ | 161.06 (9) | C7—C6—C5—C4 | 1.4 (3) |
| $N2^{i}$—Co1—S1—$O1^{i}$ | −18.94 (9) | C12—C4—C5—C6 | −1.3 (3) |
| O2—S1—O1—Co1 | 118.19 (9) | C3—C4—C5—C6 | 177.0 (2) |
| $O2^{i}$—S1—O1—Co1 | −118.83 (9) | C4—C12—N1—C1 | 0.6 (3) |
| $O1^{i}$—S1—O1—Co1 | 0.0 | C11—C12—N1—C1 | 178.38 (17) |
| $N1^{i}$—Co1—O1—S1 | −101.54 (8) | C4—C12—N1—Co1 | 178.28 (14) |
| N1—Co1—O1—S1 | 86.20 (8) | C11—C12—N1—Co1 | −3.9 (2) |
| $O1^{i}$—Co1—O1—S1 | 0.0 | $N1^{i}$—Co1—N1—C1 | 128.19 (17) |
| N2—Co1—O1—S1 | 165.15 (7) | $O1^{i}$—Co1—N1—C1 | −19.01 (17) |
| $N2^{i}$—Co1—O1—S1 | −42.22 (19) | O1—Co1—N1—C1 | −85.28 (18) |
| C7—C11—N2—C10 | 0.7 (3) | N2—Co1—N1—C1 | −179.54 (18) |
| C12—C11—N2—C10 | −177.90 (17) | $N2^{i}$—Co1—N1—C1 | 77.41 (18) |
| C7—C11—N2—Co1 | 178.87 (14) | S1—Co1—N1—C1 | −51.81 (17) |
| C12—C11—N2—Co1 | 0.2 (2) | $N1^{i}$—Co1—N1—C12 | −49.27 (13) |
| $N1^{i}$—Co1—N2—C10 | −14.97 (17) | $O1^{i}$—Co1—N1—C12 | 163.52 (13) |
| N1—Co1—N2—C10 | 176.18 (18) | O1—Co1—N1—C12 | 97.25 (14) |

| | | | |
|---|---|---|---|
| O1$^{i}$—Co1—N2—C10 | 114.64 (19) | N2—Co1—N1—C12 | 2.99 (13) |
| O1—Co1—N2—C10 | 76.30 (17) | N2$^{i}$—Co1—N1—C12 | −100.06 (14) |
| N2$^{i}$—Co1—N2—C10 | −93.38 (17) | S1—Co1—N1—C12 | 130.73 (13) |
| S1—Co1—N2—C10 | 86.62 (17) | C12—N1—C1—C2 | −0.1 (3) |
| N1$^{i}$—Co1—N2—C11 | 167.15 (13) | Co1—N1—C1—C2 | −177.43 (15) |
| N1—Co1—N2—C11 | −1.71 (12) | N1—C1—C2—C3 | −0.1 (3) |
| O1$^{i}$—Co1—N2—C11 | −63.2 (2) | C1—C2—C3—C4 | −0.3 (3) |
| O1—Co1—N2—C11 | −101.58 (13) | C12—C4—C3—C2 | 0.7 (3) |
| N2$^{i}$—Co1—N2—C11 | 88.74 (13) | C5—C4—C3—C2 | −177.6 (2) |
| S1—Co1—N2—C11 | −91.26 (13) | C13$^{i}$—C14—C13—O3 | 64.6 (2) |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3B···O2 | 0.82 | 1.92 | 2.737 (3) | 179. |

**Fig. 1**