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# Aqua(iminodiacetato-$\kappa^3O,N,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)cobalt(II) monohydrate

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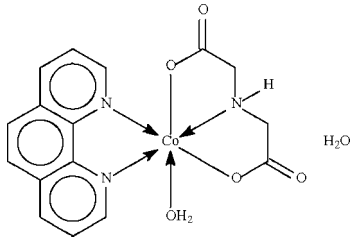
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.048; $wR$ factor = 0.126; data-to-parameter ratio = 14.7.

The iminodiacetate dianion in the title compound, $[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$, chelates to the cobalt(II) atom, its N and two O atoms occupying the *fac* sites of the distorted octahedron around the metal atom. The metal atom is also chelated by the *N*-heterocycle. The dianion, and coordinated and uncoordinated water molecules interact through hydrogen bonds, generating a layer motif. The crystal studied was a racemic twin with a 0.62 (2):0.38 (2) domain ratio.

## Related literature

For structural examples of the *N*-heterocycle adducts of cobalt iminodiacetate, see: Su & Xu (2004); Xu *et al.* (1989).




## Experimental

### Crystal data

$[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
$M_r$ = 406.26
Monoclinic, *Pn*
$a$ = 6.7884 (3) Å
$b$ = 12.0903 (5) Å
$c$ = 10.4945 (4) Å
$\beta$ = 108.357 (3)°
$V$ = 817.49 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.09 mm$^{-1}$
$T$ = 100 (2) K
0.35 × 0.02 × 0.02 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.701, $T_{max}$ = 0.979
6417 measured reflections
3639 independent reflections
2997 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
$S$ = 1.00
3639 reflections
248 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$
Absolute structure: Flack (1983), 1746 Friedel pairs
Flack parameter: 0.38 (2)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$w$—H11···O2$^{i}$ | 0.84 (5) | 1.82 (4) | 2.656 (5) | 174 (6) |
| O1$w$—H12···O4$^{ii}$ | 0.84 (6) | 1.87 (4) | 2.682 (5) | 162 (6) |
| O2$w$—H21···O1$^{i}$ | 0.84 (5) | 1.98 (4) | 2.815 (5) | 174 (7) |
| O2$w$—H22···O4 | 0.84 (6) | 2.05 (5) | 2.871 (5) | 165 (6) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2563).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, m41 [ **doi:10.1107/S1600536808041226** ]

# Aqua(iminodiacetato-$\kappa^3O,N,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)cobalt(II) monohydrate

**H. L. Ng, C. H. Ng and S. W. Ng**

## Comment

(type here to add)

## Experimental

An aqueous solution of cobalt(II) chloride (0.24 g, 1 mmol) was mixed with an aqueous solutin of disodium iminodiacetate monohydrate (0.20 g, 1 mmol); this was added to a water-methanol solution of 1,10-phenanthroline (0.20 g, 1 mmol). The solution was set aside for the growth of orange crystals.

## Refinement

Carbon-bound hydrogen atoms were placed at calculated positions (C–H 0.95–0.99 Å) and were treated as riding on their parent atoms, with $U$(H) set to 1.2 times $U_{eq}(C)$. The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their temperature factors were freely refined. The amino H-atom could not be located, and was treated as riding.

The structure is a racemic twin. The explicit refinement of the Flack parameter gave the twin component as 0.38 (2).

## Figures

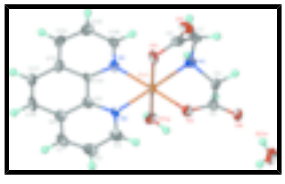


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Co(C_{12}H_8N_2)(C_4H_5NO_4)(H_2O)\cdot H_2O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

## Aqua(iminodiacetato-κ$^3$*O,N,O'*)(1,10- phenanthroline-κ$^2$*N,N'*)cobalt(II) monohydrate

*Crystal data*

| | |
|---|---|
| $[Co(C_4H_5NO_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$ | $F_{000}$ = 418 |
| $M_r$ = 406.26 | $D_x$ = 1.650 Mg m$^{-3}$ |
| Monoclinic, *Pn* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: P 2yac | Cell parameters from 1265 reflections |
| *a* = 6.7884 (3) Å | θ = 2.6–24.5º |
| *b* = 12.0903 (5) Å | μ = 1.09 mm$^{-1}$ |
| *c* = 10.4945 (4) Å | *T* = 100 (2) K |

| | |
|---|---|
| β = 108.357 (3)º | Prism, orange |
| $V$ = 817.49 (6) Å$^3$ | 0.35 × 0.02 × 0.02 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 3639 independent reflections |
| Radiation source: fine-focus sealed tube | 2997 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.048 |
| $T$ = 100(2) K | $\theta_{max}$ = 27.5º |
| ω scans | $\theta_{min}$ = 1.7º |
| Absorption correction: Multi-scan (SADABS; Sheldrick, 1996) | $h$ = −8→8 |
| $T_{min}$ = 0.701, $T_{max}$ = 0.979 | $k$ = −15→15 |
| 6417 measured reflections | $l$ = −13→13 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | $w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.126 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.00 | $\Delta\rho_{max}$ = 0.86 e Å$^{-3}$ |
| 3639 reflections | $\Delta\rho_{min}$ = −0.49 e Å$^{-3}$ |
| 248 parameters | Extinction correction: none |
| 8 restraints | Absolute structure: Flack (1983), 1746 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.38 (2) |
| Secondary atom site location: difference Fourier map | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.49999 (10) | 0.85733 (5) | 0.50000 (8) | 0.01527 (16) |
| O1 | 0.4183 (7) | 0.8730 (3) | 0.6730 (4) | 0.0222 (9) |
| O2 | 0.3360 (6) | 1.0019 (3) | 0.7965 (4) | 0.0254 (8) |
| O3 | 0.7258 (6) | 0.9787 (3) | 0.5790 (3) | 0.0196 (9) |
| O4 | 0.7806 (5) | 1.1607 (3) | 0.5786 (3) | 0.0190 (7) |
| O1W | 0.5702 (6) | 0.8446 (3) | 0.3211 (4) | 0.0194 (9) |
| H11 | 0.652 (7) | 0.896 (3) | 0.317 (5) | 0.029* |
| H12 | 0.493 (7) | 0.830 (4) | 0.243 (2) | 0.029* |
| O2W | 0.9365 (7) | 1.2706 (3) | 0.3875 (4) | 0.0307 (9) |
| H21 | 0.939 (10) | 1.225 (4) | 0.327 (4) | 0.046* |
| H22 | 0.870 (9) | 1.243 (4) | 0.435 (5) | 0.046* |

| | | | | |
|---|---|---|---|---|
| N1 | 0.3129 (7) | 1.0058 (4) | 0.4480 (4) | 0.0162 (10) |
| H1 | 0.2104 | 0.9968 | 0.3727 | 0.019* |
| N2 | 0.6902 (8) | 0.7165 (4) | 0.5733 (5) | 0.0171 (10) |
| N3 | 0.2824 (7) | 0.7278 (4) | 0.4343 (4) | 0.0168 (11) |
| C1 | 0.3389 (7) | 0.9654 (4) | 0.6867 (5) | 0.0193 (10) |
| C2 | 0.2335 (7) | 1.0313 (4) | 0.5604 (5) | 0.0202 (10) |
| H2A | 0.0826 | 1.0160 | 0.5320 | 0.024* |
| H2B | 0.2533 | 1.1112 | 0.5814 | 0.024* |
| C3 | 0.4607 (8) | 1.0907 (4) | 0.4324 (5) | 0.0183 (10) |
| H3A | 0.4062 | 1.1653 | 0.4414 | 0.022* |
| H3B | 0.4760 | 1.0849 | 0.3419 | 0.022* |
| C4 | 0.6704 (8) | 1.0754 (4) | 0.5382 (5) | 0.0177 (10) |
| C5 | 0.8890 (9) | 0.7128 (5) | 0.6410 (5) | 0.0217 (13) |
| H5 | 0.9625 | 0.7806 | 0.6638 | 0.026* |
| C6 | 0.9974 (10) | 0.6143 (5) | 0.6811 (6) | 0.0256 (13) |
| H6 | 1.1410 | 0.6154 | 0.7310 | 0.031* |
| C7 | 0.8948 (9) | 0.5164 (5) | 0.6478 (5) | 0.0246 (13) |
| H7 | 0.9666 | 0.4485 | 0.6736 | 0.030* |
| C8 | 0.6812 (10) | 0.5167 (5) | 0.5748 (5) | 0.0221 (13) |
| C9 | 0.5835 (10) | 0.6199 (5) | 0.5401 (7) | 0.0210 (14) |
| C10 | 0.5597 (10) | 0.4182 (5) | 0.5380 (6) | 0.0269 (14) |
| H10 | 0.6247 | 0.3481 | 0.5601 | 0.032* |
| C11 | 0.3534 (10) | 0.4234 (4) | 0.4720 (6) | 0.0230 (12) |
| H11A | 0.2754 | 0.3570 | 0.4500 | 0.028* |
| C12 | 0.2518 (10) | 0.5267 (5) | 0.4351 (5) | 0.0205 (13) |
| C13 | 0.3668 (10) | 0.6250 (4) | 0.4676 (6) | 0.0128 (12) |
| C14 | 0.0390 (9) | 0.5374 (4) | 0.3682 (5) | 0.0220 (12) |
| H14 | −0.0462 | 0.4734 | 0.3459 | 0.026* |
| C15 | −0.0462 (10) | 0.6399 (4) | 0.3350 (6) | 0.0238 (14) |
| H15 | −0.1902 | 0.6475 | 0.2884 | 0.029* |
| C16 | 0.0795 (8) | 0.7328 (5) | 0.3699 (6) | 0.0182 (11) |
| H16 | 0.0175 | 0.8035 | 0.3467 | 0.022* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0158 (3) | 0.0120 (3) | 0.0173 (3) | 0.0003 (3) | 0.0041 (2) | −0.0001 (3) |
| O1 | 0.033 (3) | 0.0132 (18) | 0.024 (2) | 0.0052 (16) | 0.0135 (19) | 0.0029 (14) |
| O2 | 0.0220 (19) | 0.032 (2) | 0.0207 (17) | 0.0070 (16) | 0.0052 (14) | −0.0024 (16) |
| O3 | 0.017 (2) | 0.0178 (19) | 0.021 (2) | 0.0012 (15) | 0.0013 (16) | 0.0033 (15) |
| O4 | 0.0219 (18) | 0.0127 (17) | 0.0210 (17) | −0.0021 (14) | 0.0048 (14) | 0.0012 (13) |
| O1W | 0.014 (2) | 0.023 (2) | 0.0183 (19) | −0.0049 (15) | 0.0022 (16) | 0.0039 (15) |
| O2W | 0.049 (3) | 0.0175 (19) | 0.029 (2) | −0.0081 (18) | 0.0165 (19) | −0.0030 (15) |
| N1 | 0.010 (2) | 0.022 (3) | 0.012 (2) | −0.0009 (18) | −0.0025 (17) | 0.0020 (19) |
| N2 | 0.019 (2) | 0.011 (2) | 0.022 (2) | 0.0010 (19) | 0.0077 (19) | −0.0011 (19) |
| N3 | 0.021 (2) | 0.015 (2) | 0.014 (2) | 0.0008 (19) | 0.0053 (19) | −0.0012 (18) |
| C1 | 0.012 (2) | 0.027 (3) | 0.017 (2) | 0.001 (2) | 0.0017 (19) | −0.001 (2) |
| C2 | 0.015 (2) | 0.021 (2) | 0.025 (3) | 0.0072 (19) | 0.008 (2) | 0.003 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.017 (3) | 0.013 (2) | 0.022 (2) | −0.002 (2) | 0.002 (2) | 0.0032 (19) |
| C4 | 0.020 (3) | 0.016 (3) | 0.017 (2) | 0.001 (2) | 0.007 (2) | 0.001 (2) |
| C5 | 0.019 (3) | 0.026 (3) | 0.018 (3) | 0.002 (2) | 0.003 (2) | −0.004 (2) |
| C6 | 0.017 (3) | 0.034 (3) | 0.022 (3) | 0.008 (3) | 0.002 (2) | 0.004 (2) |
| C7 | 0.027 (3) | 0.021 (3) | 0.026 (3) | 0.012 (2) | 0.008 (2) | 0.008 (2) |
| C8 | 0.027 (3) | 0.020 (3) | 0.023 (3) | 0.004 (2) | 0.013 (2) | 0.007 (2) |
| C9 | 0.023 (3) | 0.018 (3) | 0.024 (3) | 0.001 (2) | 0.009 (2) | 0.000 (2) |
| C10 | 0.041 (4) | 0.011 (2) | 0.033 (3) | 0.004 (2) | 0.017 (3) | 0.002 (2) |
| C11 | 0.029 (3) | 0.013 (2) | 0.030 (3) | −0.001 (2) | 0.014 (2) | 0.001 (2) |
| C12 | 0.029 (3) | 0.015 (3) | 0.022 (3) | −0.004 (2) | 0.013 (3) | 0.000 (2) |
| C13 | 0.016 (3) | 0.010 (3) | 0.013 (2) | 0.003 (2) | 0.006 (2) | 0.0001 (19) |
| C14 | 0.019 (3) | 0.019 (3) | 0.027 (3) | −0.007 (2) | 0.006 (2) | −0.002 (2) |
| C15 | 0.019 (3) | 0.025 (3) | 0.027 (3) | −0.005 (2) | 0.006 (2) | −0.003 (2) |
| C16 | 0.012 (2) | 0.016 (3) | 0.023 (3) | 0.003 (2) | 0.001 (2) | −0.003 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Co1—O1 | 2.067 (4) | C3—C4 | 1.516 (7) |
| Co1—O1W | 2.083 (4) | C3—H3A | 0.9900 |
| Co1—O3 | 2.095 (4) | C3—H3B | 0.9900 |
| Co1—N3 | 2.113 (5) | C5—C6 | 1.394 (8) |
| Co1—N2 | 2.129 (5) | C5—H5 | 0.9500 |
| Co1—N1 | 2.167 (5) | C6—C7 | 1.362 (8) |
| O1—C1 | 1.269 (6) | C6—H6 | 0.9500 |
| O2—C1 | 1.240 (6) | C7—C8 | 1.411 (8) |
| O3—C4 | 1.260 (6) | C7—H7 | 0.9500 |
| O4—C4 | 1.267 (6) | C8—C9 | 1.406 (9) |
| O1W—H11 | 0.84 (5) | C8—C10 | 1.430 (8) |
| O1W—H12 | 0.84 (6) | C9—C13 | 1.429 (8) |
| O2W—H21 | 0.84 (5) | C10—C11 | 1.355 (9) |
| O2W—H22 | 0.84 (6) | C10—H10 | 0.9500 |
| N1—C2 | 1.476 (6) | C11—C12 | 1.420 (8) |
| N1—C3 | 1.480 (6) | C11—H11A | 0.9500 |
| N1—H1 | 0.8800 | C12—C14 | 1.399 (9) |
| N2—C5 | 1.313 (8) | C12—C13 | 1.403 (8) |
| N2—C9 | 1.360 (8) | C14—C15 | 1.365 (8) |
| N3—C16 | 1.331 (7) | C14—H14 | 0.9500 |
| N3—C13 | 1.368 (7) | C15—C16 | 1.389 (8) |
| C1—C2 | 1.518 (6) | C15—H15 | 0.9500 |
| C2—H2A | 0.9900 | C16—H16 | 0.9500 |
| C2—H2B | 0.9900 | | |
| O1—Co1—O1W | 177.6 (2) | C4—C3—H3A | 109.6 |
| O1—Co1—O3 | 87.34 (16) | N1—C3—H3B | 109.6 |
| O1W—Co1—O3 | 93.54 (15) | C4—C3—H3B | 109.6 |
| O1—Co1—N3 | 90.07 (17) | H3A—C3—H3B | 108.1 |
| O1W—Co1—N3 | 89.20 (16) | O3—C4—O4 | 124.0 (5) |
| O3—Co1—N3 | 175.53 (17) | O3—C4—C3 | 118.3 (5) |
| O1—Co1—N2 | 93.20 (16) | O4—C4—C3 | 117.7 (4) |
| O1W—Co1—N2 | 88.95 (17) | N2—C5—C6 | 123.2 (6) |

| | | | |
|---|---|---|---|
| O3—Co1—N2 | 97.62 (17) | N2—C5—H5 | 118.4 |
| N3—Co1—N2 | 78.88 (15) | C6—C5—H5 | 118.4 |
| O1—Co1—N1 | 81.23 (15) | C7—C6—C5 | 119.1 (6) |
| O1W—Co1—N1 | 96.68 (15) | C7—C6—H6 | 120.4 |
| O3—Co1—N1 | 79.47 (17) | C5—C6—H6 | 120.4 |
| N3—Co1—N1 | 103.74 (19) | C6—C7—C8 | 119.5 (5) |
| N2—Co1—N1 | 173.79 (18) | C6—C7—H7 | 120.2 |
| C1—O1—Co1 | 114.9 (3) | C8—C7—H7 | 120.2 |
| C4—O3—Co1 | 114.3 (3) | C9—C8—C7 | 117.5 (5) |
| Co1—O1W—H11 | 109 (3) | C9—C8—C10 | 119.0 (5) |
| Co1—O1W—H12 | 130 (3) | C7—C8—C10 | 123.5 (5) |
| H11—O1W—H12 | 109 (5) | N2—C9—C8 | 121.7 (6) |
| H21—O2W—H22 | 109 (5) | N2—C9—C13 | 118.4 (6) |
| C2—N1—C3 | 111.9 (4) | C8—C9—C13 | 119.9 (6) |
| C2—N1—Co1 | 107.7 (3) | C11—C10—C8 | 121.0 (5) |
| C3—N1—Co1 | 103.8 (3) | C11—C10—H10 | 119.5 |
| C2—N1—H1 | 111.0 | C8—C10—H10 | 119.5 |
| C3—N1—H1 | 111.0 | C10—C11—C12 | 121.0 (6) |
| Co1—N1—H1 | 111.0 | C10—C11—H11A | 119.5 |
| C5—N2—C9 | 118.9 (5) | C12—C11—H11A | 119.5 |
| C5—N2—Co1 | 128.7 (4) | C14—C12—C13 | 116.9 (5) |
| C9—N2—Co1 | 112.4 (4) | C14—C12—C11 | 123.6 (5) |
| C16—N3—C13 | 117.0 (5) | C13—C12—C11 | 119.5 (6) |
| C16—N3—Co1 | 129.6 (4) | N3—C13—C12 | 123.5 (6) |
| C13—N3—Co1 | 113.4 (4) | N3—C13—C9 | 116.9 (6) |
| O2—C1—O1 | 123.4 (5) | C12—C13—C9 | 119.6 (6) |
| O2—C1—C2 | 118.9 (4) | C15—C14—C12 | 119.9 (5) |
| O1—C1—C2 | 117.6 (4) | C15—C14—H14 | 120.0 |
| N1—C2—C1 | 113.4 (4) | C12—C14—H14 | 120.0 |
| N1—C2—H2A | 108.9 | C14—C15—C16 | 119.5 (6) |
| C1—C2—H2A | 108.9 | C14—C15—H15 | 120.3 |
| N1—C2—H2B | 108.9 | C16—C15—H15 | 120.3 |
| C1—C2—H2B | 108.9 | N3—C16—C15 | 123.3 (5) |
| H2A—C2—H2B | 107.7 | N3—C16—H16 | 118.4 |
| N1—C3—C4 | 110.3 (4) | C15—C16—H16 | 118.4 |
| N1—C3—H3A | 109.6 | | |
| O3—Co1—O1—C1 | 66.7 (4) | Co1—O3—C4—C3 | −4.4 (6) |
| N3—Co1—O1—C1 | −116.9 (4) | N1—C3—C4—O3 | 31.4 (6) |
| N2—Co1—O1—C1 | 164.2 (4) | N1—C3—C4—O4 | −149.6 (4) |
| N1—Co1—O1—C1 | −13.1 (4) | C9—N2—C5—C6 | −0.1 (8) |
| O1—Co1—O3—C4 | −96.3 (4) | Co1—N2—C5—C6 | −178.6 (4) |
| O1W—Co1—O3—C4 | 81.5 (4) | N2—C5—C6—C7 | 0.8 (9) |
| N2—Co1—O3—C4 | 170.9 (3) | C5—C6—C7—C8 | −0.6 (8) |
| N1—Co1—O3—C4 | −14.7 (4) | C6—C7—C8—C9 | −0.3 (8) |
| O1—Co1—N1—C2 | −1.0 (3) | C6—C7—C8—C10 | −178.6 (5) |
| O1W—Co1—N1—C2 | 177.7 (3) | C5—N2—C9—C8 | −0.9 (8) |
| O3—Co1—N1—C2 | −89.9 (3) | Co1—N2—C9—C8 | 177.9 (4) |
| N3—Co1—N1—C2 | 86.9 (3) | C5—N2—C9—C13 | 179.4 (5) |
| O1—Co1—N1—C3 | 117.8 (3) | Co1—N2—C9—C13 | −1.9 (6) |

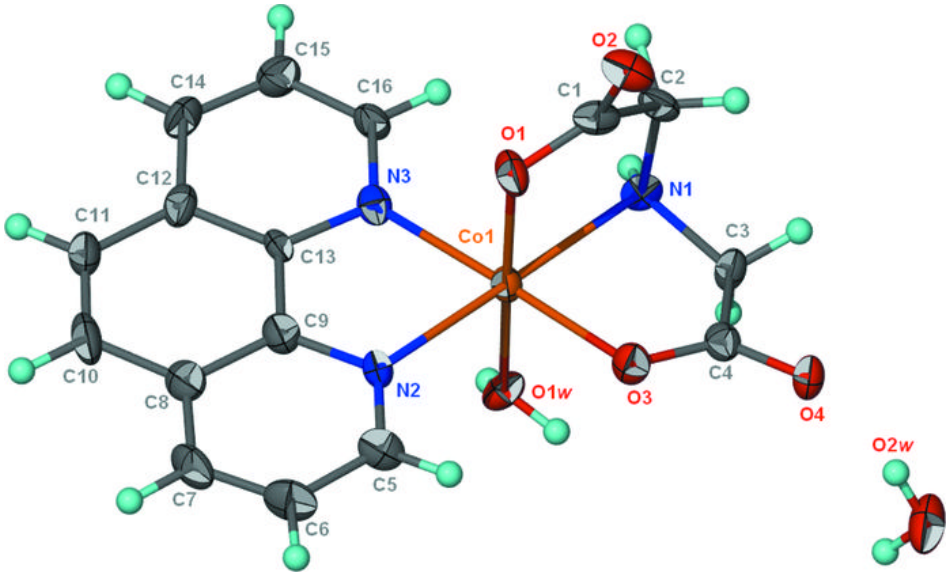
| | | | |
|---|---|---|---|
| O1W—Co1—N1—C3 | −63.4 (3) | C7—C8—C9—N2 | 1.0 (8) |
| O3—Co1—N1—C3 | 28.9 (3) | C10—C8—C9—N2 | 179.4 (5) |
| N3—Co1—N1—C3 | −154.3 (3) | C7—C8—C9—C13 | −179.2 (5) |
| O1—Co1—N2—C5 | −90.5 (5) | C10—C8—C9—C13 | −0.8 (7) |
| O1W—Co1—N2—C5 | 90.7 (5) | C9—C8—C10—C11 | −0.7 (8) |
| O3—Co1—N2—C5 | −2.8 (5) | C7—C8—C10—C11 | 177.6 (5) |
| N3—Co1—N2—C5 | −180.0 (5) | C8—C10—C11—C12 | 1.1 (8) |
| O1—Co1—N2—C9 | 90.9 (4) | C10—C11—C12—C14 | −179.3 (5) |
| O1W—Co1—N2—C9 | −88.0 (4) | C10—C11—C12—C13 | 0.0 (8) |
| O3—Co1—N2—C9 | 178.6 (4) | C16—N3—C13—C12 | 1.3 (8) |
| N3—Co1—N2—C9 | 1.4 (4) | Co1—N3—C13—C12 | 179.6 (4) |
| O1—Co1—N3—C16 | 84.0 (5) | C16—N3—C13—C9 | −178.2 (5) |
| O1W—Co1—N3—C16 | −93.7 (5) | Co1—N3—C13—C9 | 0.1 (6) |
| N2—Co1—N3—C16 | 177.2 (5) | C14—C12—C13—N3 | −1.7 (8) |
| N1—Co1—N3—C16 | 3.0 (5) | C11—C12—C13—N3 | 179.0 (5) |
| O1—Co1—N3—C13 | −94.1 (4) | C14—C12—C13—C9 | 177.8 (5) |
| O1W—Co1—N3—C13 | 88.3 (4) | C11—C12—C13—C9 | −1.5 (7) |
| N2—Co1—N3—C13 | −0.8 (4) | N2—C9—C13—N3 | 1.2 (7) |
| N1—Co1—N3—C13 | −175.0 (3) | C8—C9—C13—N3 | −178.5 (5) |
| Co1—O1—C1—O2 | −158.4 (4) | N2—C9—C13—C12 | −178.3 (5) |
| Co1—O1—C1—C2 | 24.6 (6) | C8—C9—C13—C12 | 1.9 (7) |
| C3—N1—C2—C1 | −101.0 (5) | C13—C12—C14—C15 | 1.4 (8) |
| Co1—N1—C2—C1 | 12.5 (5) | C11—C12—C14—C15 | −179.2 (5) |
| O2—C1—C2—N1 | 157.4 (4) | C12—C14—C15—C16 | −0.9 (9) |
| O1—C1—C2—N1 | −25.4 (6) | C13—N3—C16—C15 | −0.7 (8) |
| C2—N1—C3—C4 | 77.1 (5) | Co1—N3—C16—C15 | −178.7 (4) |
| Co1—N1—C3—C4 | −38.8 (4) | C14—C15—C16—N3 | 0.5 (9) |
| Co1—O3—C4—O4 | 176.7 (4) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*w*—H11···O2$^{i}$ | 0.84 (5) | 1.82 (4) | 2.656 (5) | 174 (6) |
| O1*w*—H12···O4$^{ii}$ | 0.84 (6) | 1.87 (4) | 2.682 (5) | 162 (6) |
| O2*w*—H21···O1$^{i}$ | 0.84 (5) | 1.98 (4) | 2.815 (5) | 174 (7) |
| O2*w*—H22···O4 | 0.84 (6) | 2.05 (5) | 2.871 (5) | 165 (6) |
| N1—H1···O2$^{ii}$ | 0.88 | 2.41 | 3.126 (6) | 139 |

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

**Fig. 1**


C15
C14
C16
O2
C2
C1
O1
C12
N3
N1
C11
Co1
C3
C13
C9
C10
N2
O1w
O3
C4
O4
C8
O2w
C7
C5
C6