# metal-organic compounds

# (Aminoacetato-$\kappa^2 O$,$N$)bis(quinolin-8-olato-$\kappa^2 O$,$N$)cobalt(III) methanol solvate

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In the crystal structure of the title compound, $[Co(C_2H_4-NO_2)(C_9H_6NO)_2] \cdot CH_3OH$, the Co$^{III}$ atom is chelated by two quinolin-8-olate and one glycinate anions in a distorted octahedral coordination geometry. The five-membered chelating glycinate ring assumes an envelope conformation. The complex molecules are assembled by intermolecular N—H···O hydrogen bonding.

## Related literature

For a related structure, see: Li *et al.* (2003).
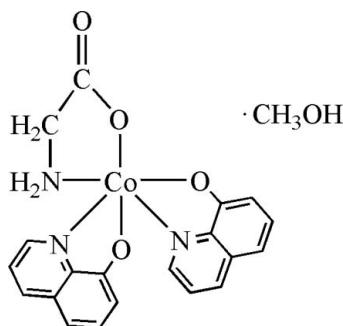


## Experimental

### Crystal data

$[Co(C_2H_4NO_2)(C_9H_6NO)_2] \cdot CH_4O$
$M_r = 453.33$
Triclinic, $P\bar{1}$
$a = 9.8377$ (4) Å
$b = 10.6526$ (4) Å
$c = 10.7369$ (4) Å
$\alpha = 82.047$ (1)°
$\beta = 76.289$ (1)°
$\gamma = 64.941$ (1)°
$V = 989.32$ (7) Å³
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.91$ mm$^{-1}$
$T = 273$ (2) K
$0.20 \times 0.15 \times 0.12$ mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.840$, $T_{max} = 0.899$
11346 measured reflections
3486 independent reflections
3261 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.093$
$S = 1.00$
3486 reflections
281 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.28$ e Å$^{-3}$
$\Delta\rho_{min} = -0.36$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Co1—O1 | 1.9045 (12) | Co1—N1 | 1.9373 (14) |
| Co1—O3 | 1.8926 (13) | Co1—N2 | 1.9179 (15) |
| Co1—O4 | 1.9002 (13) | Co1—N3 | 1.9309 (15) |
| | | | |
| O3—Co1—O4 | 90.60 (6) | O1—Co1—N3 | 85.75 (6) |
| O3—Co1—O1 | 89.93 (6) | N2—Co1—N3 | 92.71 (7) |
| O4—Co1—O1 | 176.81 (5) | O3—Co1—N1 | 85.82 (6) |
| O3—Co1—N2 | 176.47 (5) | O4—Co1—N1 | 92.39 (6) |
| O4—Co1—N2 | 85.88 (6) | O1—Co1—N1 | 90.79 (6) |
| O1—Co1—N2 | 93.56 (6) | N2—Co1—N1 | 94.60 (6) |
| O3—Co1—N3 | 87.07 (7) | N3—Co1—N1 | 172.09 (7) |
| O4—Co1—N3 | 91.14 (6) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5···O2$^i$ | 0.82 | 1.92 | 2.743 (3) | 175 |
| N3—H21···O5 | 0.85 (2) | 2.17 (3) | 2.950 (3) | 153 (2) |
| N3—H22···O3$^{ii}$ | 0.86 (3) | 2.10 (3) | 2.952 (2) | 169 (2) |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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: *SHELXTL*.

## References

Li, D.-X., Xu, D.-J., Gu, J.-M. & Xu, Y.-Z. (2003). *Acta Cryst.* E**59**, m543–m545.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

# supporting information

# (Aminoacetato-*κ²O,N*)bis(quinolin-8-olato-*κ²O,N*)cobalt(III) methanol solvate

**Bu-Qin Jing, Shuang-Ming Meng, Jing Han, Bin Wang and Xue-Mei Li**

## S1. Comment

The 8–hydroxyquinoline (HQ) is a very good ligand, forms complex compounds with various metal ions in solution. The strong chelating action of HQ in solution has been extensively studied and widely used in analytical chemistry. In this work, we use glycin and 8–hydroxyquinoline as bidedtate ligand to synthesize the title complex, (I).

The molecular structure of the title compound is shown in Fig. 1. The Co$^{III}$ atom is chelated by two 8-hydroxyquinoline and one glycin anions in a distorted octahedral coordination geometry. The Co—N bond distances are longer than Co—O bond distances (Table 1), which agrees with that found in a related structure, tris(8-quinolinolato)-cobalt(III) methanol solvate (Li *et al.* 2003). The two 8-hydroxyquinolate rings are almost perpendicular to each other with a dihedral angle of 81.0°. The five-membered chelating ring of the glycin assumes an envelope conformation, with N3 atom at the flap position. The complex molecules are assembled by intermolecular N–H···O hydrogen bonding (Table 2). Lattice methanol molecule is linked with complex *via* O—H···O and N—H···O hydrogen bonding (Fig. 2).

## S2. Refinement

Amino H atoms were located in a difference Fourier map and refined isotropically. Other H atoms were placed in calculated positions and allowed to ride on their attached atoms, with C—H = 0.93–0.97 Å, O–H = 0.82 Å, $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C,*O*).
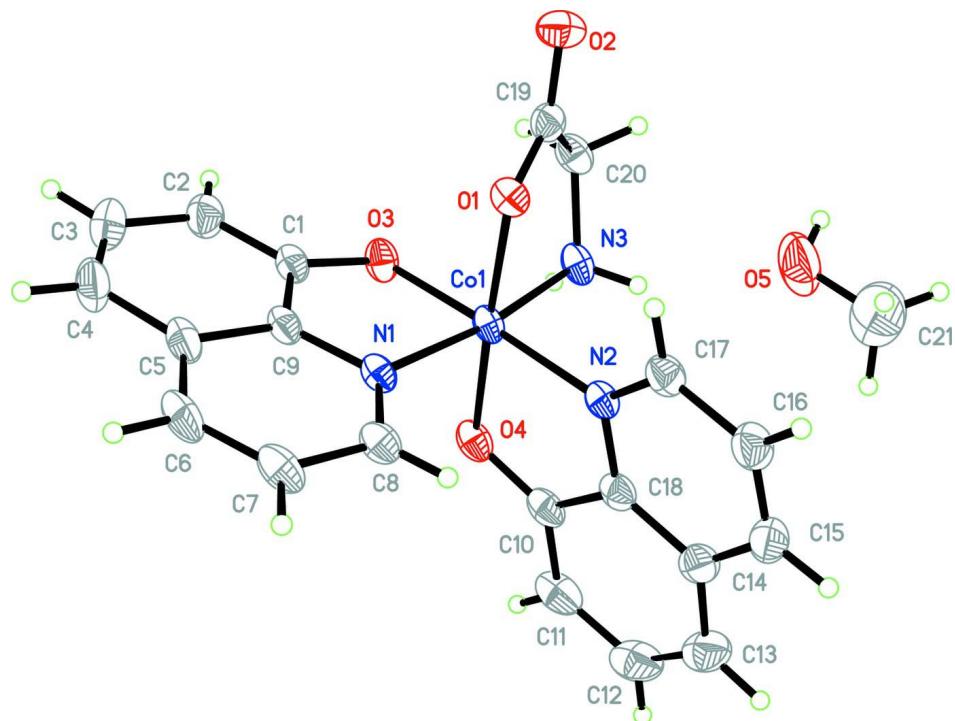
**Figure 1**

The atomic labeling scheme of (I) with displacement ellipsoids at the 30% probability level.
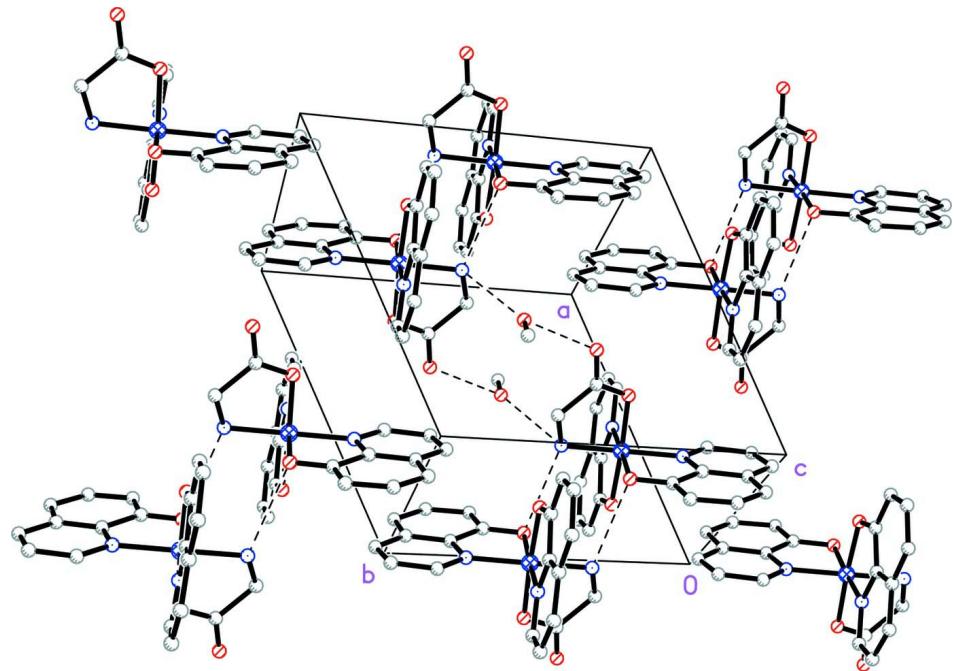


**Figure 2**

A packing diagram of the unit cell showing hydrogen bonds as dashed lines. H atoms, except for those involved in hydrogen bonds, are not included.
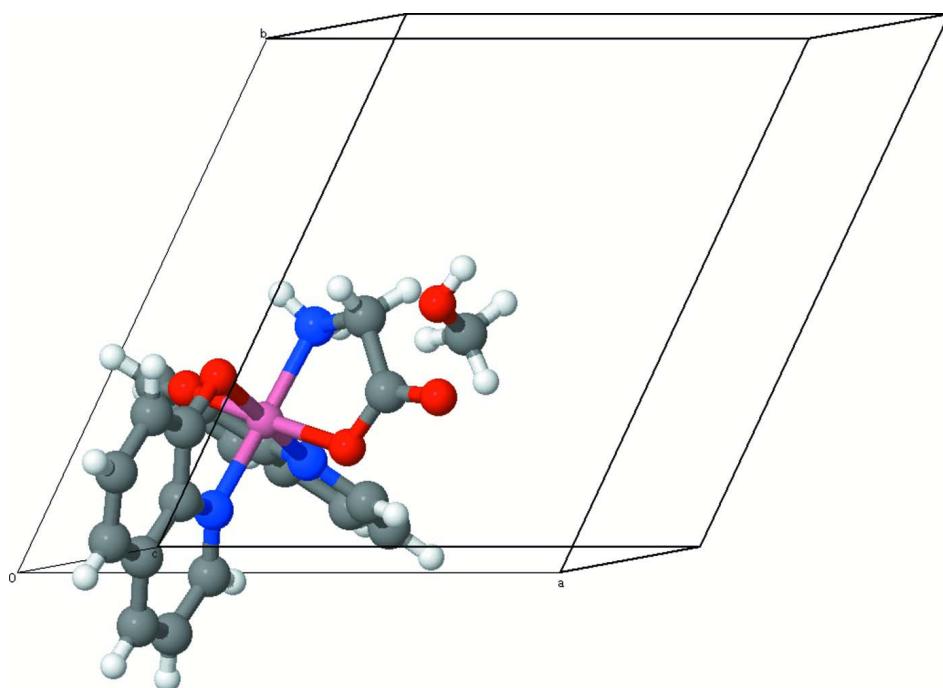
**Figure 3**
Interactive view of the complex.

**(Aminoacetato-$\kappa^2O,N$)bis(quinolin-8-olato- $\kappa^2O,N$)cobalt(III) methanol solvate**

*Crystal data*

| | |
|---|---|
| $[Co(C_2H_4NO_2)(C_9H_6NO)_2]\cdot CH_4O$ | $Z = 2$ |
| $M_r = 453.33$ | $F(000) = 468$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.522$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.8377$ (4) Å | Cell parameters from 7882 reflections |
| $b = 10.6526$ (4) Å | $\theta = 2.4$–28.2° |
| $c = 10.7369$ (4) Å | $\mu = 0.91$ mm$^{-1}$ |
| $\alpha = 82.047$ (1)° | $T = 273$ K |
| $\beta = 76.289$ (1)° | Block, purple |
| $\gamma = 64.941$ (1)° | $0.20 \times 0.15 \times 0.12$ mm |
| $V = 989.32$ (7) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11346 measured reflections |
| | 3486 independent reflections |
| Radiation source: fine-focus sealed tube | 3261 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.017$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.1°$, $\theta_{min} = 2.0°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -9 \rightarrow 11$ |
| | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.840$, $T_{max} = 0.899$ | $l = -12 \rightarrow 12$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.094$ | |
| $S = 1.00$ | H atoms treated by a mixture of independent and constrained refinement |
| 3486 reflections | |
| 281 parameters | $w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.17P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} = 0.001$ |
| | $\Delta\rho_{max} = 0.28$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |

*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.

**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 | 0.21615 (2) | 0.26369 (2) | 0.46144 (2) | 0.03237 (12) |
| O1 | 0.36577 (14) | 0.20861 (13) | 0.56554 (12) | 0.0381 (3) |
| O2 | 0.46440 (17) | 0.29619 (16) | 0.67761 (14) | 0.0553 (4) |
| O3 | 0.05933 (15) | 0.33761 (13) | 0.60596 (13) | 0.0418 (3) |
| O4 | 0.06935 (14) | 0.32742 (13) | 0.35430 (13) | 0.0421 (3) |
| O5 | 0.4828 (3) | 0.4912 (3) | 0.2562 (2) | 0.1083 (9) |
| H5 | 0.4933 | 0.5573 | 0.2770 | 0.162* |
| N1 | 0.18775 (16) | 0.09298 (15) | 0.50938 (14) | 0.0348 (3) |
| N2 | 0.36569 (17) | 0.19377 (15) | 0.30857 (14) | 0.0349 (3) |
| N3 | 0.23374 (19) | 0.43960 (16) | 0.43835 (17) | 0.0397 (4) |
| C1 | 0.0225 (2) | 0.23999 (19) | 0.67578 (17) | 0.0391 (4) |
| C2 | −0.0769 (2) | 0.2598 (2) | 0.7924 (2) | 0.0539 (5) |
| H2 | −0.1231 | 0.3465 | 0.8279 | 0.065* |
| C3 | −0.1088 (3) | 0.1483 (3) | 0.8583 (2) | 0.0683 (7) |
| H3 | −0.1735 | 0.1626 | 0.9386 | 0.082* |
| C4 | −0.0487 (3) | 0.0206 (3) | 0.8091 (2) | 0.0656 (6) |
| H4 | −0.0744 | −0.0498 | 0.8543 | 0.079* |
| C5 | 0.0530 (2) | −0.0043 (2) | 0.6888 (2) | 0.0460 (5) |
| C6 | 0.1205 (2) | −0.1297 (2) | 0.6232 (2) | 0.0528 (5) |
| H6 | 0.0999 | −0.2057 | 0.6600 | 0.063* |
| C7 | 0.2144 (2) | −0.1391 (2) | 0.5076 (2) | 0.0504 (5) |
| H7 | 0.2567 | −0.2210 | 0.4642 | 0.060* |
| C8 | 0.2488 (2) | −0.02614 (18) | 0.45221 (19) | 0.0413 (4) |
| H8 | 0.3162 | −0.0354 | 0.3735 | 0.050* |

| C9 | 0.08930 (19) | 0.10617 (18) | 0.62504 (17) | 0.0364 (4) |
| C10 | 0.1360 (2) | 0.30635 (18) | 0.23300 (19) | 0.0422 (4) |
| C11 | 0.0622 (3) | 0.3473 (2) | 0.1301 (2) | 0.0590 (6) |
| H11 | −0.0435 | 0.3965 | 0.1439 | 0.071* |
| C12 | 0.1463 (4) | 0.3150 (3) | 0.0052 (2) | 0.0690 (7) |
| H12 | 0.0939 | 0.3445 | −0.0622 | 0.083* |
| C13 | 0.3015 (4) | 0.2421 (3) | −0.0224 (2) | 0.0657 (7) |
| H13 | 0.3530 | 0.2230 | −0.1068 | 0.079* |
| C14 | 0.3826 (3) | 0.1964 (2) | 0.07908 (19) | 0.0500 (5) |
| C15 | 0.5417 (3) | 0.1158 (2) | 0.0668 (2) | 0.0576 (5) |
| H15 | 0.6026 | 0.0903 | −0.0139 | 0.069* |
| C16 | 0.6059 (2) | 0.0755 (2) | 0.1726 (2) | 0.0558 (5) |
| H16 | 0.7101 | 0.0205 | 0.1645 | 0.067* |
| C17 | 0.5149 (2) | 0.1171 (2) | 0.29365 (19) | 0.0438 (4) |
| H17 | 0.5602 | 0.0904 | 0.3653 | 0.053* |
| C18 | 0.2987 (2) | 0.23139 (18) | 0.20409 (18) | 0.0393 (4) |
| C19 | 0.3819 (2) | 0.31043 (19) | 0.60261 (16) | 0.0392 (4) |
| C20 | 0.2899 (2) | 0.45316 (19) | 0.5487 (2) | 0.0452 (4) |
| H20A | 0.2040 | 0.5039 | 0.6144 | 0.054* |
| H20B | 0.3538 | 0.5047 | 0.5221 | 0.054* |
| C21 | 0.5849 (6) | 0.4394 (5) | 0.1517 (4) | 0.1377 (19) |
| H21A | 0.5343 | 0.4321 | 0.0885 | 0.207* |
| H21B | 0.6579 | 0.3490 | 0.1722 | 0.207* |
| H21C | 0.6367 | 0.4993 | 0.1183 | 0.207* |
| H22 | 0.143 (3) | 0.502 (3) | 0.436 (2) | 0.060 (7)* |
| H21 | 0.295 (3) | 0.444 (2) | 0.369 (2) | 0.048 (6)* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| --- | --- | --- | --- | --- | --- | --- |
| Co1 | 0.02705 (16) | 0.02604 (16) | 0.04380 (17) | −0.01193 (11) | −0.00651 (10) | 0.00211 (10) |
| O1 | 0.0359 (7) | 0.0324 (7) | 0.0464 (7) | −0.0132 (5) | −0.0107 (5) | −0.0006 (5) |
| O2 | 0.0585 (9) | 0.0602 (9) | 0.0529 (8) | −0.0229 (7) | −0.0185 (7) | −0.0116 (7) |
| O3 | 0.0365 (7) | 0.0317 (6) | 0.0529 (7) | −0.0144 (5) | 0.0006 (5) | −0.0027 (5) |
| O4 | 0.0315 (6) | 0.0366 (7) | 0.0594 (8) | −0.0142 (5) | −0.0147 (6) | 0.0056 (6) |
| O5 | 0.1061 (17) | 0.1167 (19) | 0.1255 (19) | −0.0846 (16) | 0.0328 (15) | −0.0453 (15) |
| N1 | 0.0294 (7) | 0.0310 (7) | 0.0468 (8) | −0.0139 (6) | −0.0126 (6) | 0.0036 (6) |
| N2 | 0.0330 (8) | 0.0318 (7) | 0.0431 (8) | −0.0165 (6) | −0.0089 (6) | 0.0020 (6) |
| N3 | 0.0316 (8) | 0.0305 (8) | 0.0567 (10) | −0.0144 (7) | −0.0078 (7) | 0.0035 (7) |
| C1 | 0.0321 (9) | 0.0415 (10) | 0.0468 (10) | −0.0187 (7) | −0.0087 (7) | 0.0023 (8) |
| C2 | 0.0489 (12) | 0.0610 (13) | 0.0523 (11) | −0.0273 (10) | 0.0013 (9) | −0.0072 (10) |
| C3 | 0.0685 (15) | 0.0868 (18) | 0.0532 (12) | −0.0460 (14) | 0.0061 (11) | 0.0020 (12) |
| C4 | 0.0710 (15) | 0.0741 (16) | 0.0641 (14) | −0.0506 (13) | −0.0070 (12) | 0.0173 (12) |
| C5 | 0.0414 (10) | 0.0463 (11) | 0.0589 (11) | −0.0272 (9) | −0.0163 (9) | 0.0131 (9) |
| C6 | 0.0506 (11) | 0.0379 (10) | 0.0813 (15) | −0.0285 (9) | −0.0242 (11) | 0.0152 (9) |
| C7 | 0.0458 (11) | 0.0330 (9) | 0.0788 (14) | −0.0189 (8) | −0.0193 (10) | −0.0011 (9) |
| C8 | 0.0377 (9) | 0.0336 (9) | 0.0547 (11) | −0.0146 (7) | −0.0135 (8) | −0.0003 (8) |
| C9 | 0.0310 (9) | 0.0374 (9) | 0.0461 (9) | −0.0185 (7) | −0.0135 (7) | 0.0070 (7) |

| | | | | | |
|---|---|---|---|---|---|
| C10 | 0.0461 (10) | 0.0310 (9) | 0.0590 (12) | −0.0226 (8) | −0.0218 (9) | 0.0108 (8) |
| C11 | 0.0656 (14) | 0.0484 (12) | 0.0783 (15) | −0.0302 (11) | −0.0415 (12) | 0.0196 (11) |
| C12 | 0.101 (2) | 0.0613 (15) | 0.0661 (15) | −0.0430 (15) | −0.0491 (15) | 0.0208 (12) |
| C13 | 0.104 (2) | 0.0626 (14) | 0.0471 (12) | −0.0481 (15) | −0.0239 (12) | 0.0099 (10) |
| C14 | 0.0691 (14) | 0.0482 (12) | 0.0451 (10) | −0.0369 (11) | −0.0115 (10) | 0.0026 (9) |
| C15 | 0.0618 (14) | 0.0653 (14) | 0.0516 (12) | −0.0374 (11) | 0.0071 (10) | −0.0148 (10) |
| C16 | 0.0408 (11) | 0.0627 (13) | 0.0630 (13) | −0.0224 (10) | 0.0013 (9) | −0.0159 (10) |
| C17 | 0.0340 (9) | 0.0455 (10) | 0.0523 (10) | −0.0160 (8) | −0.0078 (8) | −0.0051 (8) |
| C18 | 0.0472 (10) | 0.0330 (9) | 0.0463 (10) | −0.0241 (8) | −0.0143 (8) | 0.0062 (7) |
| C19 | 0.0337 (9) | 0.0423 (10) | 0.0383 (9) | −0.0145 (8) | 0.0010 (7) | −0.0084 (7) |
| C20 | 0.0412 (10) | 0.0362 (9) | 0.0614 (12) | −0.0182 (8) | −0.0087 (9) | −0.0070 (8) |
| C21 | 0.197 (5) | 0.142 (4) | 0.116 (3) | −0.129 (4) | 0.030 (3) | −0.047 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O1 | 1.9045 (12) | C5—C6 | 1.417 (3) |
| Co1—O3 | 1.8926 (13) | C6—C7 | 1.348 (3) |
| Co1—O4 | 1.9002 (13) | C6—H6 | 0.9300 |
| Co1—N1 | 1.9373 (14) | C7—C8 | 1.403 (3) |
| Co1—N2 | 1.9179 (15) | C7—H7 | 0.9300 |
| Co1—N3 | 1.9309 (15) | C8—H8 | 0.9300 |
| O1—C19 | 1.287 (2) | C10—C11 | 1.384 (3) |
| O2—C19 | 1.225 (2) | C10—C18 | 1.431 (3) |
| O3—C1 | 1.323 (2) | C11—C12 | 1.400 (4) |
| O4—C10 | 1.314 (2) | C11—H11 | 0.9300 |
| O5—C21 | 1.319 (4) | C12—C13 | 1.367 (4) |
| O5—H5 | 0.8200 | C12—H12 | 0.9300 |
| N1—C8 | 1.320 (2) | C13—C14 | 1.413 (3) |
| N1—C9 | 1.365 (2) | C13—H13 | 0.9300 |
| N2—C17 | 1.326 (2) | C14—C18 | 1.405 (3) |
| N2—C18 | 1.362 (2) | C14—C15 | 1.413 (3) |
| N3—C20 | 1.468 (3) | C15—C16 | 1.361 (3) |
| N3—H22 | 0.86 (3) | C15—H15 | 0.9300 |
| N3—H21 | 0.85 (2) | C16—C17 | 1.399 (3) |
| C1—C2 | 1.374 (3) | C16—H16 | 0.9300 |
| C1—C9 | 1.419 (3) | C17—H17 | 0.9300 |
| C2—C3 | 1.410 (3) | C19—C20 | 1.518 (3) |
| C2—H2 | 0.9300 | C20—H20A | 0.9700 |
| C3—C4 | 1.359 (4) | C20—H20B | 0.9700 |
| C3—H3 | 0.9300 | C21—H21A | 0.9600 |
| C4—C5 | 1.414 (3) | C21—H21B | 0.9600 |
| C4—H4 | 0.9300 | C21—H21C | 0.9600 |
| C5—C9 | 1.414 (2) | | |
| | | | |
| O3—Co1—O4 | 90.60 (6) | C6—C7—H7 | 119.8 |
| O3—Co1—O1 | 89.93 (6) | C8—C7—H7 | 119.8 |
| O4—Co1—O1 | 176.81 (5) | N1—C8—C7 | 121.45 (18) |
| O3—Co1—N2 | 176.47 (5) | N1—C8—H8 | 119.3 |

| | | | |
|---|---|---|---|
| O4—Co1—N2 | 85.88 (6) | C7—C8—H8 | 119.3 |
| O1—Co1—N2 | 93.56 (6) | N1—C9—C5 | 122.64 (17) |
| O3—Co1—N3 | 87.07 (7) | N1—C9—C1 | 115.27 (15) |
| O4—Co1—N3 | 91.14 (6) | C5—C9—C1 | 122.07 (17) |
| O1—Co1—N3 | 85.75 (6) | O4—C10—C11 | 125.8 (2) |
| N2—Co1—N3 | 92.71 (7) | O4—C10—C18 | 117.56 (16) |
| O3—Co1—N1 | 85.82 (6) | C11—C10—C18 | 116.6 (2) |
| O4—Co1—N1 | 92.39 (6) | C10—C11—C12 | 120.2 (2) |
| O1—Co1—N1 | 90.79 (6) | C10—C11—H11 | 119.9 |
| N2—Co1—N1 | 94.60 (6) | C12—C11—H11 | 119.9 |
| N3—Co1—N1 | 172.09 (7) | C13—C12—C11 | 123.2 (2) |
| C19—O1—Co1 | 113.96 (11) | C13—C12—H12 | 118.4 |
| C1—O3—Co1 | 111.40 (11) | C11—C12—H12 | 118.4 |
| C10—O4—Co1 | 111.26 (11) | C12—C13—C14 | 119.0 (2) |
| C21—O5—H5 | 109.5 | C12—C13—H13 | 120.5 |
| C8—N1—C9 | 119.18 (15) | C14—C13—H13 | 120.5 |
| C8—N1—Co1 | 131.33 (13) | C18—C14—C13 | 117.7 (2) |
| C9—N1—Co1 | 109.46 (12) | C18—C14—C15 | 116.45 (19) |
| C17—N2—C18 | 119.37 (17) | C13—C14—C15 | 125.8 (2) |
| C17—N2—Co1 | 129.99 (13) | C16—C15—C14 | 120.2 (2) |
| C18—N2—Co1 | 110.63 (12) | C16—C15—H15 | 119.9 |
| C20—N3—Co1 | 107.24 (11) | C14—C15—H15 | 119.9 |
| C20—N3—H22 | 111.7 (16) | C15—C16—C17 | 119.9 (2) |
| Co1—N3—H22 | 106.0 (17) | C15—C16—H16 | 120.1 |
| C20—N3—H21 | 110.4 (15) | C17—C16—H16 | 120.1 |
| Co1—N3—H21 | 111.4 (15) | N2—C17—C16 | 121.50 (18) |
| H22—N3—H21 | 110 (2) | N2—C17—H17 | 119.3 |
| O3—C1—C2 | 124.64 (18) | C16—C17—H17 | 119.3 |
| O3—C1—C9 | 117.25 (15) | N2—C18—C14 | 122.54 (18) |
| C2—C1—C9 | 118.10 (17) | N2—C18—C10 | 114.32 (17) |
| C1—C2—C3 | 119.9 (2) | C14—C18—C10 | 123.13 (18) |
| C1—C2—H2 | 120.1 | O2—C19—O1 | 123.35 (17) |
| C3—C2—H2 | 120.1 | O2—C19—C20 | 120.82 (17) |
| C4—C3—C2 | 122.5 (2) | O1—C19—C20 | 115.83 (15) |
| C4—C3—H3 | 118.7 | N3—C20—C19 | 109.90 (15) |
| C2—C3—H3 | 118.7 | N3—C20—H20A | 109.7 |
| C3—C4—C5 | 119.62 (19) | C19—C20—H20A | 109.7 |
| C3—C4—H4 | 120.2 | N3—C20—H20B | 109.7 |
| C5—C4—H4 | 120.2 | C19—C20—H20B | 109.7 |
| C4—C5—C9 | 117.7 (2) | H20A—C20—H20B | 108.2 |
| C4—C5—C6 | 126.22 (19) | O5—C21—H21A | 109.5 |
| C9—C5—C6 | 116.04 (18) | O5—C21—H21B | 109.5 |
| C7—C6—C5 | 120.19 (17) | H21A—C21—H21B | 109.5 |
| C7—C6—H6 | 119.9 | O5—C21—H21C | 109.5 |
| C5—C6—H6 | 119.9 | H21A—C21—H21C | 109.5 |
| C6—C7—C8 | 120.45 (19) | H21B—C21—H21C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5···O2ⁱ | 0.82 | 1.92 | 2.743 (3) | 175 |
| N3—H21···O5 | 0.85 (2) | 2.17 (3) | 2.950 (3) | 153 (2) |
| N3—H22···O3ⁱⁱ | 0.86 (3) | 2.10 (3) | 2.952 (2) | 169 (2) |

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