# Bis(μ-N,N′-di-4-pyridylpyridine-2,6-diamine)bis[dimethacrylatocobalt(II)] dihydrate

## Liang-Gui Wang[a]* and Ai-Hua Peng[b]

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The Co$^{II}$ ion in the title complex, [Co$_2$(C$_4$H$_5$O$_2$)$_4$(C$_{15}$H$_{13}$N$_5$)$_2$]·2H$_2$O, has a distorted square-planar coordination formed by the bridging bidentate N,N′-di-4-pyridylpyridine-2,6-diamine (dapmp) ligands and two monodentate carboxylate groups from methacrylates. Two dapmp ligands bridge two Co atoms, forming a dinuclear complex arranged around an inversion centre. N—H···O and O—H···O hydrogen bonds involving the solvent water molecule result in the formation of a three-dimensional network. The aliphatic moiety of one of the methacrylate groups is disordered over two positions with fixed occupancies of 0.67 and 0.33.

## Related literature

For related literature, see: Liu *et al.* (2008); Patra *et al.* (2004); Thorsten *et al.* (2004); Burchell *et al.* (2006).
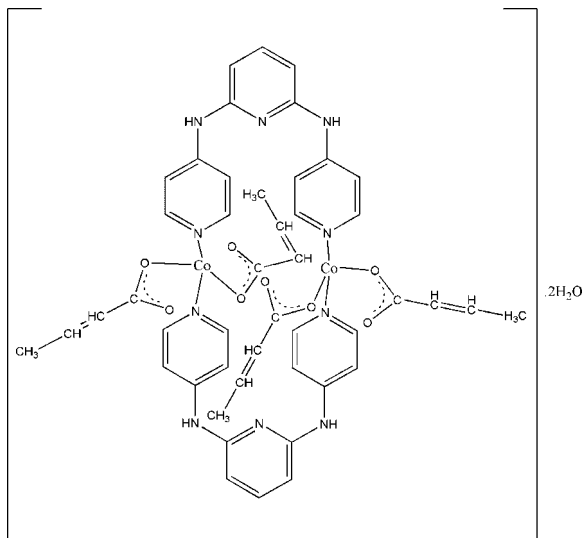


## Experimental

### Crystal data

[Co$_2$(C$_4$H$_5$O$_2$)$_4$(C$_{15}$H$_{13}$N$_5$)$_2$]·2H$_2$O$_2$
$M_r$ = 1020.82
Monoclinic, $C2/c$
$a$ = 16.852 (3) Å
$b$ = 17.425 (3) Å
$c$ = 16.206 (2) Å
$\beta$ = 91.848 (2)°
$V$ = 4756.6 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.77 mm$^{-1}$
$T$ = 298 (2) K
0.28 × 0.20 × 0.16 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.814, $T_{max}$ = 0.887
11993 measured reflections
4289 independent reflections
3333 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.113
$S$ = 1.00
4289 reflections
319 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
| --- | --- | --- | --- | --- |
| N2—H2···O4$^i$ | 0.86 | 1.99 | 2.831 (4) | 167 |
| N4—H4···O5$^{ii}$ | 0.86 | 1.98 | 2.840 (3) | 174 |
| O5—H5$B$···O2 | 0.86 | 1.89 | 2.737 (3) | 170 |
| O5—H5$C$···O2$^{iii}$ | 0.86 | 2.10 | 2.917 (3) | 158 |

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$; (iii) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

## References

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**supplementary materials**

## Bis(*μ*-*N*,*N*'-di-4-pyridylpyridine-2,6-diamine)bis[dimethacrylatocobalt(II)] dihydrate

## L.-G. Wang and A.-H. Peng

### Comment

Bridging bis(amidopyridine) ligands have been widely explored in coordination chemistry for building various novel structural architectures and functional solid materials. Besides their diverse coordination modes, amide groups of ligands have proved to be useful in self-assembly, since they give predictable patterns of hydrogen bonding that can add extra dimensionality and helicity to the supramolecular structures (Burchell, *et al.*, 2006; Patra *et al.*, 2004). The 2,4-di(2-aminopyridine)-6-methypyrimidine (dapmp) ligand is a versatile ligand like but with more diversity than terpyridine (tpy). The modified title ligand and its complexes have been reported (Thorsten *et al.*, 2004). In this paper, we report here the synthesis and crystal structure of the title compound (I).

The Co(II) atom in the title complex, has a square coordination formed by two N atoms of two bridging dapmp ligands and two O atoms of two monodentate carboxylate groups from methacrylates. The bridging dapmp ligands bridge two Co atoms forming a dinuclear complex arranged around inversion center (Fig.1). The average Co—N bond length of 2.006 Å is close to the values observed in related complexes (Liu *et al.*, 2008).

The occurence of N-H···O and O-H···O hydrogen bondings involving the solvent water molecule results in the formation of a three dimensionnal network (Table 1).

### Experimental

dapmp (0.05 g, 0.18 mmol), Co(CH3COO)2 (0.035 g, 0.16 mmol), methacrylic acid (0.032 g, 0.15 mmol) and NaOH (1*M*, 0.5 mL) were added distilled water(15 mL), the mixture was heated for fifty hours under reflux. during the process stirring and influx were required. The resultant was kept at room temperature, two weeks later some single crystals of the size suitable for X-Ray diffraction measurement.

### Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.98 Å (methyl) or 0.97 Å (methylene) and N—H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}(C$ or N). 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 and H···H= 1.38 (2)Å) with $U_{iso}(H) = 1.5U_{eq}(O)$. In the last stage of refinement, they were treated as riding on their parent O atom.

The C atoms of one of the methacrylate group are disordered. The ratio of the occupancy factors of each component was determined to be 0.33/0.67. The two components were refined using the tools available in SHELXL-97 (PART and SAME instructions). Each corresponding C atoms were anisotropically refined using EADP restraints.
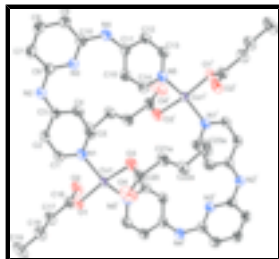
# supplementary materials

**Figures**



Fig. 1. The structure of the dinuclear complex showing the atom-labeling scheme.Displacement ellipsoids are shown at the 30% probability level. H atoms and solvent water molecule have been omitted for clarity. Only one component of the disordered methacrylate is represented. [Symmetric codes: (i) 1/2-x, 1/2-y, 2-z].

**Bis(μ-N,N'-di-4-pyridylpyridine-2,6-diamine)bis[dimethacrylatocobalt(II)] dihydrate**

*Crystal data*

$[Co_2(C_4H_5O_2)_4(C_{15}H_{13}N_5)_2] \cdot 2H_2O$

$M_r = 1020.82$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 16.852\ (3)$ Å

$b = 17.425\ (3)$ Å

$c = 16.206\ (2)$ Å

$\beta = 91.848\ (2)°$

$V = 4756.6\ (12)$ Å$^3$

$Z = 4$

$F_{000} = 2120$

$D_x = 1.425$ Mg m$^{-3}$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 4289 reflections

$\theta = 1.7–25.2°$

$\mu = 0.77$ mm$^{-1}$

$T = 298\ (2)$ K

Block, pink

$0.28 \times 0.20 \times 0.16$ mm

*Data collection*

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)$ K

φ and ω scan

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.814$, $T_{max} = 0.887$

11993 measured reflections

4289 independent reflections

3333 reflections with $I > 2\sigma(I)$

$R_{int} = 0.021$

$\theta_{max} = 25.2°$

$\theta_{min} = 1.7°$

$h = -20 \rightarrow 19$

$k = -20 \rightarrow 13$

$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.113$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 1.1663P]$
where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.00$

$(\Delta/\sigma)_{max} = 0.003$

4289 reflections

$\Delta\rho_{max} = 0.67$ e Å$^{-3}$

319 parameters

$\Delta\rho_{min} = -0.25$ e Å$^{-3}$

5 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|------|------|------|------|------|------|
| Co1 | 0.235159 (18) | 0.431425 (16) | 0.937768 (18) | 0.05265 (14) | |
| N1 | 0.20029 (13) | 0.45034 (12) | 1.05235 (13) | 0.0639 (5) | |
| N2 | 0.10374 (13) | 0.46526 (12) | 1.28525 (13) | 0.0653 (5) | |
| H2 | 0.0961 | 0.5113 | 1.3023 | 0.078* | |
| N3 | 0.08770 (11) | 0.33476 (11) | 1.31525 (12) | 0.0558 (5) | |
| N4 | 0.07043 (12) | 0.20360 (11) | 1.34321 (13) | 0.0643 (5) | |
| H4 | 0.0504 | 0.1709 | 1.3764 | 0.077* | |
| N5 | 0.19558 (12) | 0.10578 (11) | 1.15108 (12) | 0.0605 (5) | |
| O1 | 0.25618 (10) | 0.53794 (9) | 0.91709 (11) | 0.0603 (4) | |
| O2 | 0.37530 (12) | 0.52113 (10) | 0.97624 (14) | 0.0822 (6) | |
| O3 | 0.18484 (15) | 0.32931 (12) | 0.93913 (15) | 0.0935 (7) | |
| O4 | 0.1035 (2) | 0.38372 (17) | 0.8496 (2) | 0.1382 (11) | |
| O5 | 0.50106 (12) | 0.59087 (12) | 1.05678 (14) | 0.0931 (7) | |
| H5B | 0.4648 | 0.5637 | 1.0324 | 0.140* | |
| H5C | 0.5423 | 0.5617 | 1.0600 | 0.140* | |
| C1 | 0.16847 (16) | 0.51510 (13) | 1.08051 (16) | 0.0622 (6) | |
| H1 | 0.1669 | 0.5578 | 1.0460 | 0.075* | |
| C2 | 0.13828 (16) | 0.52194 (14) | 1.15691 (16) | 0.0637 (6) | |
| H2A | 0.1165 | 0.5684 | 1.1732 | 0.076* | |
| C3 | 0.13977 (14) | 0.45961 (14) | 1.21099 (15) | 0.0565 (6) | |
| C4 | 0.17974 (16) | 0.39479 (15) | 1.18482 (17) | 0.0673 (7) | |
| H4A | 0.1881 | 0.3536 | 1.2205 | 0.081* | |
| C5 | 0.20654 (17) | 0.39206 (15) | 1.10674 (18) | 0.0745 (8) | |
| H5 | 0.2308 | 0.3471 | 1.0897 | 0.089* | |
| C6 | 0.07752 (14) | 0.40755 (14) | 1.33749 (15) | 0.0545 (5) | |
| C7 | 0.03970 (16) | 0.42917 (15) | 1.40823 (16) | 0.0649 (7) | |

| | | | | | |
|---|---|---|---|---|---|
| H7 | 0.0346 | 0.4806 | 1.4223 | 0.078* | |
| C8 | 0.00997 (16) | 0.37248 (16) | 1.45714 (16) | 0.0690 (7) | |
| H8 | −0.0163 | 0.3852 | 1.5049 | 0.083* | |
| C9 | 0.01910 (15) | 0.29651 (15) | 1.43540 (16) | 0.0643 (6) | |
| H9 | −0.0008 | 0.2573 | 1.4677 | 0.077* | |
| C10 | 0.05876 (13) | 0.28040 (14) | 1.36400 (15) | 0.0554 (6) | |
| C11 | 0.10900 (13) | 0.17245 (13) | 1.27789 (15) | 0.0550 (6) | |
| C12 | 0.13584 (16) | 0.09731 (14) | 1.28272 (17) | 0.0652 (7) | |
| H12 | 0.1252 | 0.0675 | 1.3286 | 0.078* | |
| C13 | 0.17805 (16) | 0.06716 (13) | 1.21981 (17) | 0.0650 (7) | |
| H13 | 0.1957 | 0.0168 | 1.2249 | 0.078* | |
| C14 | 0.16509 (16) | 0.17700 (14) | 1.14514 (15) | 0.0643 (6) | |
| H14 | 0.1737 | 0.2046 | 1.0971 | 0.077* | |
| C15 | 0.12263 (15) | 0.21124 (14) | 1.20446 (15) | 0.0613 (6) | |
| H15 | 0.1026 | 0.2605 | 1.1962 | 0.074* | |
| C16 | 0.32418 (15) | 0.56277 (13) | 0.94107 (16) | 0.0592 (6) | |
| C17 | 0.34147 (17) | 0.64439 (15) | 0.92618 (19) | 0.0729 (7) | |
| H17 | 0.3916 | 0.6623 | 0.9425 | 0.087* | |
| C18 | 0.29301 (18) | 0.69284 (16) | 0.8925 (2) | 0.0808 (8) | |
| H18 | 0.2430 | 0.6747 | 0.8763 | 0.097* | |
| C19 | 0.3099 (3) | 0.77605 (18) | 0.8772 (3) | 0.1243 (15) | |
| H19A | 0.3629 | 0.7879 | 0.8966 | 0.186* | |
| H19B | 0.2728 | 0.8071 | 0.9060 | 0.186* | |
| H19C | 0.3049 | 0.7864 | 0.8190 | 0.186* | |
| C20 | 0.1275 (2) | 0.32774 (18) | 0.8840 (2) | 0.0810 (9) | |
| C21A | 0.1154 (8) | 0.2382 (5) | 0.8948 (7) | 0.0857 (13) | 0.33 |
| H21A | 0.1329 | 0.2140 | 0.9432 | 0.103* | 0.33 |
| C22A | 0.0812 (6) | 0.1992 (5) | 0.8364 (7) | 0.0802 (12) | 0.33 |
| H22A | 0.0648 | 0.2209 | 0.7862 | 0.096* | 0.33 |
| C23A | 0.070 (6) | 0.1110 (16) | 0.857 (5) | 0.134 (4) | 0.33 |
| H23A | 0.1120 | 0.0940 | 0.8936 | 0.201* | 0.33 |
| H23B | 0.0701 | 0.0816 | 0.8068 | 0.201* | 0.33 |
| H23C | 0.0197 | 0.1038 | 0.8829 | 0.201* | 0.33 |
| C21B | 0.0859 (3) | 0.2565 (2) | 0.8567 (3) | 0.0857 (13) | 0.67 |
| H21B | 0.0453 | 0.2601 | 0.8166 | 0.103* | 0.67 |
| C22B | 0.1039 (3) | 0.1905 (2) | 0.8862 (3) | 0.0802 (12) | 0.67 |
| H22B | 0.1384 | 0.1870 | 0.9321 | 0.096* | 0.67 |
| C23B | 0.069 (3) | 0.1154 (8) | 0.846 (2) | 0.134 (4) | 0.67 |
| H23D | 0.0147 | 0.1243 | 0.8282 | 0.201* | 0.67 |
| H23E | 0.0705 | 0.0748 | 0.8863 | 0.201* | 0.67 |
| H23F | 0.0995 | 0.1012 | 0.7998 | 0.201* | 0.67 |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0661 (2) | 0.03338 (19) | 0.0593 (2) | −0.00546 (13) | 0.01459 (15) | −0.00101 (13) |
| N1 | 0.0783 (14) | 0.0434 (11) | 0.0706 (13) | 0.0006 (10) | 0.0128 (11) | 0.0045 (10) |
| N2 | 0.0872 (15) | 0.0476 (11) | 0.0614 (13) | 0.0011 (11) | 0.0100 (11) | −0.0024 (10) |

| | | | | | |
|---|---|---|---|---|---|
| N3 | 0.0622 (11) | 0.0488 (11) | 0.0566 (11) | −0.0004 (9) | 0.0051 (9) | −0.0009 (9) |
| N4 | 0.0753 (13) | 0.0483 (11) | 0.0704 (13) | −0.0017 (10) | 0.0186 (11) | 0.0029 (10) |
| N5 | 0.0723 (13) | 0.0426 (11) | 0.0673 (13) | −0.0016 (10) | 0.0106 (10) | 0.0014 (9) |
| O1 | 0.0619 (9) | 0.0440 (9) | 0.0750 (11) | −0.0025 (8) | 0.0048 (8) | 0.0018 (8) |
| O2 | 0.0795 (12) | 0.0498 (10) | 0.1157 (16) | 0.0080 (9) | −0.0190 (11) | 0.0010 (10) |
| O3 | 0.1185 (18) | 0.0611 (12) | 0.1031 (16) | −0.0207 (12) | 0.0382 (14) | −0.0023 (11) |
| O4 | 0.167 (3) | 0.101 (2) | 0.147 (3) | −0.010 (2) | 0.012 (2) | 0.0440 (19) |
| O5 | 0.0819 (13) | 0.0755 (13) | 0.1209 (18) | 0.0158 (11) | −0.0102 (12) | −0.0395 (12) |
| C1 | 0.0803 (16) | 0.0408 (12) | 0.0657 (15) | −0.0017 (12) | 0.0067 (13) | 0.0037 (11) |
| C2 | 0.0817 (17) | 0.0406 (13) | 0.0691 (16) | 0.0003 (12) | 0.0066 (13) | −0.0038 (11) |
| C3 | 0.0655 (14) | 0.0438 (12) | 0.0603 (14) | −0.0024 (11) | 0.0003 (11) | −0.0003 (11) |
| C4 | 0.0770 (16) | 0.0540 (14) | 0.0719 (17) | 0.0105 (13) | 0.0158 (13) | 0.0161 (13) |
| C5 | 0.0934 (19) | 0.0492 (15) | 0.0823 (19) | 0.0154 (14) | 0.0272 (15) | 0.0130 (13) |
| C6 | 0.0586 (13) | 0.0484 (13) | 0.0563 (13) | 0.0010 (11) | 0.0003 (11) | −0.0022 (11) |
| C7 | 0.0734 (16) | 0.0564 (15) | 0.0652 (16) | 0.0010 (12) | 0.0090 (13) | −0.0109 (12) |
| C8 | 0.0767 (16) | 0.0668 (17) | 0.0643 (15) | 0.0012 (14) | 0.0155 (13) | −0.0107 (13) |
| C9 | 0.0698 (15) | 0.0609 (15) | 0.0630 (15) | −0.0033 (12) | 0.0121 (12) | −0.0024 (12) |
| C10 | 0.0543 (13) | 0.0509 (13) | 0.0609 (14) | −0.0012 (11) | 0.0034 (11) | −0.0013 (11) |
| C11 | 0.0554 (13) | 0.0474 (13) | 0.0623 (14) | −0.0022 (10) | 0.0048 (11) | −0.0044 (11) |
| C12 | 0.0809 (17) | 0.0457 (13) | 0.0701 (16) | 0.0002 (12) | 0.0180 (13) | 0.0065 (12) |
| C13 | 0.0754 (16) | 0.0425 (13) | 0.0778 (17) | 0.0025 (12) | 0.0124 (14) | 0.0043 (12) |
| C14 | 0.0870 (18) | 0.0494 (13) | 0.0566 (14) | 0.0046 (13) | 0.0055 (13) | 0.0022 (11) |
| C15 | 0.0759 (16) | 0.0484 (13) | 0.0594 (14) | 0.0088 (12) | −0.0011 (12) | −0.0004 (11) |
| C16 | 0.0629 (15) | 0.0444 (13) | 0.0707 (16) | 0.0016 (12) | 0.0080 (12) | −0.0010 (11) |
| C17 | 0.0677 (16) | 0.0481 (14) | 0.102 (2) | −0.0056 (13) | −0.0045 (15) | 0.0045 (14) |
| C18 | 0.0806 (18) | 0.0525 (16) | 0.108 (2) | −0.0039 (14) | −0.0137 (16) | 0.0082 (15) |
| C19 | 0.140 (3) | 0.0547 (18) | 0.176 (4) | −0.008 (2) | −0.038 (3) | 0.029 (2) |
| C20 | 0.103 (2) | 0.0555 (17) | 0.086 (2) | −0.0206 (17) | 0.0293 (19) | −0.0119 (16) |
| C21A | 0.115 (4) | 0.055 (3) | 0.085 (4) | −0.020 (3) | −0.010 (3) | 0.008 (2) |
| C22A | 0.101 (3) | 0.054 (2) | 0.086 (3) | −0.003 (2) | 0.001 (3) | 0.009 (3) |
| C23A | 0.163 (4) | 0.066 (3) | 0.173 (12) | −0.041 (3) | 0.025 (5) | −0.019 (4) |
| C21B | 0.115 (4) | 0.055 (3) | 0.085 (4) | −0.020 (3) | −0.010 (3) | 0.008 (2) |
| C22B | 0.101 (3) | 0.054 (2) | 0.086 (3) | −0.003 (2) | 0.001 (3) | 0.009 (3) |
| C23B | 0.163 (4) | 0.066 (3) | 0.173 (12) | −0.041 (3) | 0.025 (5) | −0.019 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Co1—O1 | 1.9210 (17) | C8—H8 | 0.9300 |
| Co1—O3 | 1.972 (2) | C9—C10 | 1.383 (3) |
| Co1—N5[i] | 1.991 (2) | C9—H9 | 0.9300 |
| Co1—N1 | 1.993 (2) | C11—C12 | 1.387 (3) |
| N1—C1 | 1.336 (3) | C11—C15 | 1.394 (3) |
| N1—C5 | 1.347 (3) | C12—C13 | 1.367 (4) |
| N2—C3 | 1.369 (3) | C12—H12 | 0.9300 |
| N2—C6 | 1.395 (3) | C13—H13 | 0.9300 |
| N2—H2 | 0.8600 | C14—C15 | 1.355 (3) |
| N3—C6 | 1.331 (3) | C14—H14 | 0.9300 |
| N3—C10 | 1.336 (3) | C15—H15 | 0.9300 |
| N4—C11 | 1.372 (3) | C16—C17 | 1.473 (3) |

| | | | |
|---|---|---|---|
| N4—C10 | 1.395 (3) | C17—C18 | 1.284 (4) |
| N4—H4 | 0.8600 | C17—H17 | 0.9300 |
| N5—C13 | 1.342 (3) | C18—C19 | 1.500 (4) |
| N5—C14 | 1.346 (3) | C18—H18 | 0.9300 |
| N5—Co1$^i$ | 1.991 (2) | C19—H19A | 0.9600 |
| O1—C16 | 1.274 (3) | C19—H19B | 0.9600 |
| O2—C16 | 1.250 (3) | C19—H19C | 0.9600 |
| O3—C20 | 1.295 (4) | C20—C21B | 1.485 (5) |
| O4—C20 | 1.188 (4) | C20—C21A | 1.583 (10) |
| O5—H5B | 0.8591 | C21A—C22A | 1.287 (12) |
| O5—H5C | 0.8618 | C21A—H21A | 0.9300 |
| C1—C2 | 1.359 (4) | C22A—C23A | 1.59 (2) |
| C1—H1 | 0.9300 | C22A—H22A | 0.9300 |
| C2—C3 | 1.395 (3) | C23A—H23A | 0.9600 |
| C2—H2A | 0.9300 | C23A—H23B | 0.9600 |
| C3—C4 | 1.388 (3) | C23A—H23C | 0.9600 |
| C4—C5 | 1.358 (4) | C21B—C22B | 1.279 (6) |
| C4—H4A | 0.9300 | C21B—H21B | 0.9300 |
| C5—H5 | 0.9300 | C22B—C23B | 1.568 (18) |
| C6—C7 | 1.382 (4) | C22B—H22B | 0.9300 |
| C7—C8 | 1.371 (4) | C23B—H23D | 0.9600 |
| C7—H7 | 0.9300 | C23B—H23E | 0.9600 |
| C8—C9 | 1.380 (4) | C23B—H23F | 0.9600 |
| O1—Co1—O3 | 162.90 (10) | N4—C11—C15 | 124.2 (2) |
| O1—Co1—N5$^i$ | 94.17 (8) | C12—C11—C15 | 116.3 (2) |
| O3—Co1—N5$^i$ | 88.66 (8) | C13—C12—C11 | 119.8 (2) |
| O1—Co1—N1 | 93.69 (8) | C13—C12—H12 | 120.1 |
| O3—Co1—N1 | 89.94 (9) | C11—C12—H12 | 120.1 |
| N5$^i$—Co1—N1 | 157.66 (9) | N5—C13—C12 | 124.1 (2) |
| C1—N1—C5 | 115.9 (2) | N5—C13—H13 | 118.0 |
| C1—N1—Co1 | 126.27 (18) | C12—C13—H13 | 118.0 |
| C5—N1—Co1 | 117.78 (18) | N5—C14—C15 | 124.4 (2) |
| C3—N2—C6 | 129.8 (2) | N5—C14—H14 | 117.8 |
| C3—N2—H2 | 115.1 | C15—C14—H14 | 117.8 |
| C6—N2—H2 | 115.1 | C14—C15—C11 | 119.8 (2) |
| C6—N3—C10 | 117.6 (2) | C14—C15—H15 | 120.1 |
| C11—N4—C10 | 129.8 (2) | C11—C15—H15 | 120.1 |
| C11—N4—H4 | 115.1 | O2—C16—O1 | 122.8 (2) |
| C10—N4—H4 | 115.1 | O2—C16—C17 | 119.9 (2) |
| C13—N5—C14 | 115.4 (2) | O1—C16—C17 | 117.3 (2) |
| C13—N5—Co1$^i$ | 125.92 (17) | C18—C17—C16 | 125.3 (3) |
| C14—N5—Co1$^i$ | 118.68 (16) | C18—C17—H17 | 117.3 |
| C16—O1—Co1 | 116.37 (15) | C16—C17—H17 | 117.3 |
| C20—O3—Co1 | 108.8 (2) | C17—C18—C19 | 125.8 (3) |
| H5B—O5—H5C | 105.3 | C17—C18—H18 | 117.1 |
| N1—C1—C2 | 123.5 (2) | C19—C18—H18 | 117.1 |
| N1—C1—H1 | 118.3 | C18—C19—H19A | 109.5 |

| | | | |
|---|---|---|---|
| C2—C1—H1 | 118.3 | C18—C19—H19B | 109.5 |
| C1—C2—C3 | 120.3 (2) | H19A—C19—H19B | 109.5 |
| C1—C2—H2A | 119.9 | C18—C19—H19C | 109.5 |
| C3—C2—H2A | 119.9 | H19A—C19—H19C | 109.5 |
| N2—C3—C4 | 124.1 (2) | H19B—C19—H19C | 109.5 |
| N2—C3—C2 | 119.8 (2) | O4—C20—O3 | 122.8 (3) |
| C4—C3—C2 | 116.1 (2) | O4—C20—C21B | 113.3 (4) |
| C5—C4—C3 | 119.5 (2) | O3—C20—C21B | 123.9 (4) |
| C5—C4—H4A | 120.3 | O4—C20—C21A | 144.8 (5) |
| C3—C4—H4A | 120.3 | O3—C20—C21A | 92.3 (5) |
| N1—C5—C4 | 124.2 (2) | C21B—C20—C21A | 31.7 (4) |
| N1—C5—H5 | 117.9 | C22A—C21A—C20 | 119.7 (9) |
| C4—C5—H5 | 117.9 | C22A—C21A—H21A | 120.1 |
| N3—C6—C7 | 123.5 (2) | C20—C21A—H21A | 120.1 |
| N3—C6—N2 | 118.4 (2) | C21A—C22A—C23A | 114 (3) |
| C7—C6—N2 | 118.1 (2) | C21A—C22A—H22A | 122.8 |
| C8—C7—C6 | 118.0 (2) | C23A—C22A—H22A | 122.8 |
| C8—C7—H7 | 121.0 | C22B—C21B—C20 | 122.4 (5) |
| C6—C7—H7 | 121.0 | C22B—C21B—H21B | 118.8 |
| C7—C8—C9 | 119.8 (2) | C20—C21B—H21B | 118.8 |
| C7—C8—H8 | 120.1 | C21B—C22B—C23B | 121.0 (15) |
| C9—C8—H8 | 120.1 | C21B—C22B—H22B | 119.5 |
| C8—C9—C10 | 118.0 (2) | C23B—C22B—H22B | 119.5 |
| C8—C9—H9 | 121.0 | C22B—C23B—H23D | 109.5 |
| C10—C9—H9 | 121.0 | C22B—C23B—H23E | 109.5 |
| N3—C10—C9 | 123.1 (2) | H23D—C23B—H23E | 109.5 |
| N3—C10—N4 | 118.7 (2) | C22B—C23B—H23F | 109.5 |
| C9—C10—N4 | 118.2 (2) | H23D—C23B—H23F | 109.5 |
| N4—C11—C12 | 119.5 (2) | H23E—C23B—H23F | 109.5 |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O4[ii] | 0.86 | 1.99 | 2.831 (4) | 167 |
| N4—H4···O5[iii] | 0.86 | 1.98 | 2.840 (3) | 174 |
| O5—H5B···O2 | 0.86 | 1.89 | 2.737 (3) | 170 |
| O5—H5C···O2[iv] | 0.86 | 2.10 | 2.917 (3) | 158 |

Symmetry codes: (ii) *x*, −*y*+1, *z*+1/2; (iii) −*x*+1/2, *y*−1/2, −*z*+5/2; (iv) −*x*+1, −*y*+1, −*z*+2.

**Fig. 1**