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# *catena*-Poly[[bis(acetato-$\kappa^2O,O'$)-cobalt(II)]-$\mu$-4,4′-bis(benzimidazol-1-yl)-biphenyl-$\kappa^2N^3:N^{3'}$]

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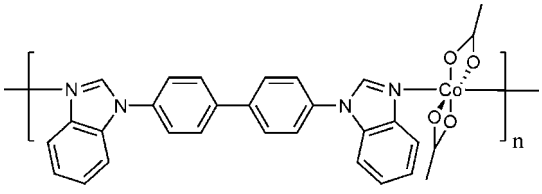
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.083; data-to-parameter ratio = 12.1.

In the title one-dimensional coordination polymer, $[Co(C_2H_3O_2)_2(C_{26}H_{18}N_4)]_n$, the $Co^{II}$ atom (site symmetry 2) is coordinated by two $O,O'$-bidentate acetate ions and two 4,4′-bis(benzimidazol-1-yl)biphenyl ligands in a distorted *cis*-$CoN_2O_4$ octahedral geometry. The bridging ligand, which is completed by crystallographic twofold symmetry, links the $Co^{II}$ atoms into $[10\bar{1}]$ chains. Within the ligand, the dihedral angle between the benzene and benzimidazole rings is 48.31 (8)°.

## Related literature

For background to benzimidazole-derived ligands in coordination polymers, see: Jin *et al.* (2006); Li *et al.* (2010); Su *et al.* (2003).




## Experimental

### Crystal data

$[Co(C_2H_3O_2)_2(C_{26}H_{18}N_4)]$
$M_r$ = 563.46
Orthorhombic, *Pbcn*
$a$ = 13.078 (3) Å
$b$ = 16.348 (3) Å
$c$ = 11.354 (2) Å
$V$ = 2427.5 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.75 mm$^{-1}$
$T$ = 293 K
0.25 × 0.22 × 0.18 mm

### Data collection

Rigaku CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.828, $T_{max}$ = 0.873
21778 measured reflections
2150 independent reflections
2101 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.083
$S$ = 1.10
2150 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co1—O1 | 2.0386 (16) | Co1—N1 | 2.0709 (16) |
| Co1—O2 | 2.4163 (18) | | |

Data collection: *CrystalClear* (Rigaku/MSC, 2005); 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5708).

## References

Jin, C. M., Lu, H., Wu, L. Y. & Huang, J. (2006). *Chem. Commun.* pp. 5039–5041.
Li, Z. X., Hu, T. L., Ma, H., Zeng, Y. F., Li, C. J., Tong, M. L. & Bu, X. H. (2010). *Cryst. Growth Des.* **10**, 1138–1144.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Su, C. Y., Cai, Y. P., Chen, C. L., Smith, M. D., Kaim, W. & zur Loye, H. C. (2003). *J. Am. Chem. Soc.* **125**, 8595–8613.

# supporting information

*Acta Cryst.* (2010). E**66**, m1638 [https://doi.org/10.1107/S160053681004715X]

## *catena*-Poly[[bis(acetato-$\kappa^2O,O'$)cobalt(II)]-$\mu$-4,4′-bis(benzimidazol-1-yl)biphenyl-$\kappa^2N^3:N^{3'}$]

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### S1. Comment

Benzoimidazole has been well used in crystal engineering, and a large number of benzoimidazole-containing flexible ligands have been extensively studied (Su *et al.*,2003; Jin *et al.*,2006). However, to our knowledge, the research on benzoimidazole ligands bearing rigid spacers is still less developed (Li *et al.*,2010).

Single-crystal X-ray diffraction analysis reveals that the title compound (**I**) crystallizes in the orthorhombic space group *Pbcn*. The geometry of the $Co^{II}$ ion is surrounded by two benzoiimidazole rings of distinct **L** ligands and two chelated acetate anions, which illustrates a slightly distorted octahedral coordination environment (Fig. 1). Notably, as shown in Fig. 2, the six-coordinated $Co^{II}$ center is bridged by the linear ligand **L** to form an infinite one-dimensional architecture.

### S2. Experimental

A mixture of $CH_3OH$ and $CHCl_3$ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of 4,4′-bis-(benzoimidazol-1-yl)terphenyl (**L**, 0.06 mmol) in $CHCl_3$ (6 ml). Then a solution of $Co(CH_3COO)_2$ (0.02 mmol) in $CH_3OH$ (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, purple blocks of (I) appeared at the boundary. Yield: ~25% (based on **L**).

### S3. Refinement

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$.

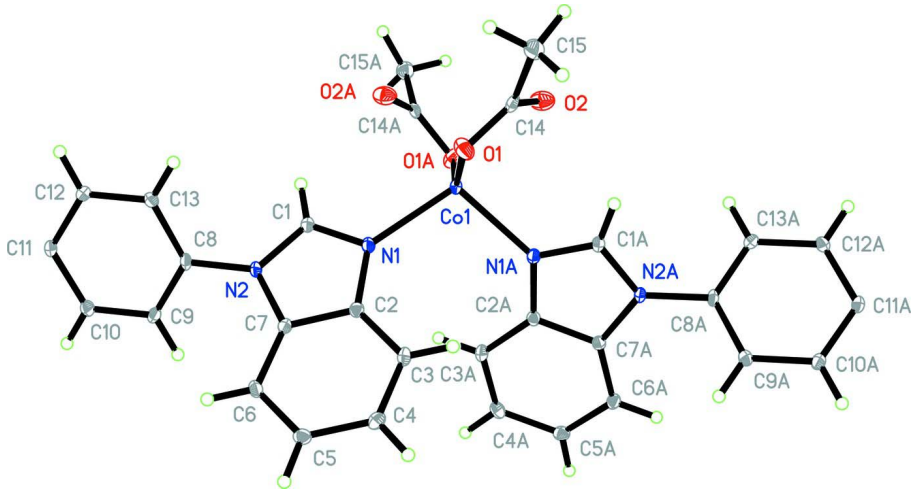


**Figure 1**

The molecular structure of (**I**). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

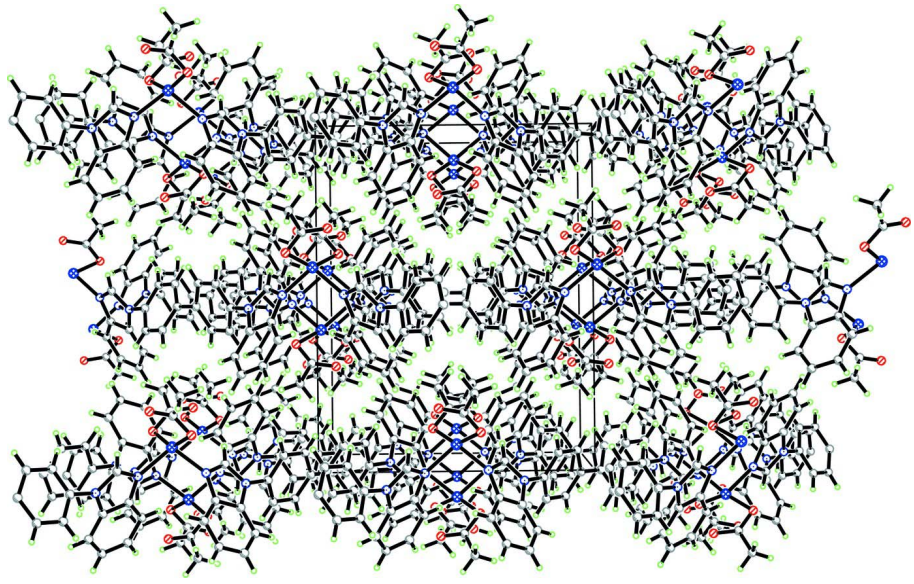

**Figure 2**

The crystal packing for (**I**).

***catena*-Poly[[bis(acetato-$\kappa^2O,O'$)cobalt(II)]-$\mu$- 4,4′-bis(benzimidazol-1-yl)biphenyl-$\kappa^2N^3:N^{3'}$]**

*Crystal data*

$[Co(C_2H_3O_2)_2(C_{26}H_{18}N_4)]$
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Orthorhombic, *Pbcn*
$a = 13.078\ (3)$ Å
$b = 16.348\ (3)$ Å
$c = 11.354\ (2)$ Å
$V = 2427.5\ (8)$ Å$^3$
$Z = 4$
$F(000) = 1164$
$D_x = 1.542$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6002 reflections
$\theta = 2.0–27.9°$
$\mu = 0.75$ mm$^{-1}$
$T = 293$ K
Block, purple
0.25 × 0.22 × 0.18 mm

*Data collection*

Rigaku CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.828, $T_{max}$ = 0.873
21778 measured reflections
2150 independent reflections
2101 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.7°
$h$ = −15→15
$k$ = −19→19
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.083
$S$ = 1.10
2150 reflections
178 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 2.7447P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 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 | 0.0000 | 0.40968 (2) | 0.2500 | 0.01345 (14) |
| O1 | 0.08394 (11) | 0.37040 (10) | 0.39033 (14) | 0.0268 (4) |
| C11 | 0.45996 (14) | 0.51680 (12) | −0.20359 (17) | 0.0138 (4) |
| C12 | 0.44299 (15) | 0.44856 (12) | −0.13277 (18) | 0.0160 (4) |
| H12 | 0.4800 | 0.4009 | −0.1461 | 0.019* |
| C7 | 0.23045 (15) | 0.58691 (12) | 0.15147 (17) | 0.0134 (4) |
| C3 | 0.11760 (15) | 0.61095 (13) | 0.31741 (17) | 0.0163 (4) |
| H3 | 0.0633 | 0.5956 | 0.3655 | 0.020* |
| N2 | 0.24267 (12) | 0.52419 (10) | 0.06971 (14) | 0.0140 (4) |
| N1 | 0.11225 (12) | 0.48650 (10) | 0.18429 (14) | 0.0148 (4) |
| C10 | 0.40024 (15) | 0.58655 (13) | −0.18495 (18) | 0.0171 (4) |
| H10 | 0.4096 | 0.6322 | −0.2327 | 0.021* |
| C13 | 0.37154 (15) | 0.45080 (12) | −0.04256 (18) | 0.0162 (4) |
| H13 | 0.3618 | 0.4054 | 0.0055 | 0.019* |
| C8 | 0.31481 (14) | 0.52118 (12) | −0.02460 (17) | 0.0144 (4) |
| C9 | 0.32729 (15) | 0.58878 (12) | −0.09655 (18) | 0.0164 (4) |

| | | | | |
|---|---|---|---|---|
| H9 | 0.2872 | 0.6351 | −0.0857 | 0.020* |
| C14 | 0.02557 (15) | 0.31459 (12) | 0.42490 (18) | 0.0163 (4) |
| O2 | −0.06065 (12) | 0.30382 (10) | 0.38106 (15) | 0.0292 (4) |
| C4 | 0.17056 (15) | 0.68295 (13) | 0.33635 (18) | 0.0184 (4) |
| H4 | 0.1517 | 0.7165 | 0.3989 | 0.022* |
| C1 | 0.17101 (15) | 0.46685 (12) | 0.09472 (17) | 0.0153 (4) |
| H1 | 0.1641 | 0.4184 | 0.0526 | 0.018* |
| C15 | 0.06315 (17) | 0.25921 (14) | 0.5229 (2) | 0.0249 (5) |
| H15A | 0.0636 | 0.2889 | 0.5958 | 0.037* |
| H15B | 0.1312 | 0.2408 | 0.5052 | 0.037* |
| H15C | 0.0185 | 0.2128 | 0.5297 | 0.037* |
| C2 | 0.14891 (15) | 0.56223 (12) | 0.22333 (17) | 0.0140 (4) |
| C6 | 0.28339 (15) | 0.65947 (12) | 0.16999 (17) | 0.0162 (4) |
| H6 | 0.3372 | 0.6753 | 0.1216 | 0.019* |
| C5 | 0.25205 (16) | 0.70673 (13) | 0.26368 (18) | 0.0176 (4) |
| H5 | 0.2858 | 0.7557 | 0.2792 | 0.021* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0112 (2) | 0.0150 (2) | 0.0141 (2) | 0.000 | 0.00353 (14) | 0.000 |
| O1 | 0.0208 (8) | 0.0286 (9) | 0.0311 (9) | −0.0010 (7) | 0.0001 (7) | 0.0116 (7) |
| C11 | 0.0112 (9) | 0.0182 (11) | 0.0121 (9) | −0.0018 (8) | 0.0014 (8) | −0.0006 (8) |
| C12 | 0.0148 (10) | 0.0151 (10) | 0.0182 (10) | 0.0020 (8) | 0.0026 (8) | −0.0013 (8) |
| C7 | 0.0132 (10) | 0.0144 (10) | 0.0126 (9) | 0.0016 (7) | 0.0007 (8) | 0.0005 (8) |
| C3 | 0.0146 (10) | 0.0214 (11) | 0.0131 (10) | 0.0008 (8) | 0.0029 (8) | 0.0006 (8) |
| N2 | 0.0134 (8) | 0.0153 (8) | 0.0133 (8) | −0.0009 (6) | 0.0049 (7) | −0.0002 (7) |
| N1 | 0.0145 (8) | 0.0154 (9) | 0.0146 (8) | −0.0018 (7) | 0.0037 (7) | −0.0016 (7) |
| C10 | 0.0173 (10) | 0.0173 (11) | 0.0167 (10) | 0.0001 (8) | 0.0041 (8) | 0.0032 (8) |
| C13 | 0.0176 (10) | 0.0144 (10) | 0.0166 (10) | −0.0023 (8) | 0.0035 (8) | 0.0012 (8) |
| C8 | 0.0109 (9) | 0.0189 (10) | 0.0135 (10) | −0.0017 (8) | 0.0042 (8) | −0.0012 (8) |
| C9 | 0.0141 (10) | 0.0166 (10) | 0.0184 (10) | 0.0031 (8) | 0.0036 (8) | 0.0001 (8) |
| C14 | 0.0138 (10) | 0.0187 (10) | 0.0165 (10) | 0.0023 (8) | 0.0040 (8) | −0.0055 (8) |
| O2 | 0.0279 (9) | 0.0226 (8) | 0.0372 (9) | −0.0004 (7) | −0.0079 (8) | −0.0027 (7) |
| C4 | 0.0200 (11) | 0.0197 (11) | 0.0154 (10) | 0.0025 (8) | 0.0005 (8) | −0.0043 (8) |
| C1 | 0.0139 (10) | 0.0159 (10) | 0.0162 (10) | −0.0007 (8) | 0.0038 (8) | −0.0009 (8) |
| C15 | 0.0237 (12) | 0.0244 (12) | 0.0265 (12) | 0.0012 (9) | 0.0015 (9) | 0.0031 (10) |
| C2 | 0.0126 (9) | 0.0151 (10) | 0.0144 (10) | 0.0010 (8) | 0.0004 (8) | 0.0007 (8) |
| C6 | 0.0129 (9) | 0.0176 (10) | 0.0180 (10) | −0.0015 (8) | 0.0020 (8) | 0.0019 (8) |
| C5 | 0.0162 (10) | 0.0147 (10) | 0.0220 (11) | −0.0014 (8) | −0.0022 (8) | −0.0016 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O1$^{i}$ | 2.0386 (16) | N1—C1 | 1.315 (3) |
| Co1—O1 | 2.0386 (16) | N1—C2 | 1.400 (3) |
| Co1—O2 | 2.4163 (18) | C10—C9 | 1.385 (3) |
| Co1—O2$^{i}$ | 2.4163 (18) | C10—H10 | 0.9300 |
| Co1—N1 | 2.0709 (16) | C13—C8 | 1.384 (3) |

| | | | |
|---|---|---|---|
| Co1—N1$^{i}$ | 2.0709 (16) | C13—H13 | 0.9300 |
| O1—C14 | 1.253 (3) | C8—C9 | 1.384 (3) |
| C11—C12 | 1.393 (3) | C9—H9 | 0.9300 |
| C11—C10 | 1.398 (3) | C14—O2 | 1.245 (3) |
| C11—C11$^{ii}$ | 1.486 (4) | C14—C15 | 1.516 (3) |
| C12—C13 | 1.387 (3) | C4—C5 | 1.403 (3) |
| C12—H12 | 0.9300 | C4—H4 | 0.9300 |
| C7—C6 | 1.390 (3) | C1—H1 | 0.9300 |
| C7—N2 | 1.392 (2) | C15—H15A | 0.9600 |
| C7—C2 | 1.402 (3) | C15—H15B | 0.9600 |
| C3—C4 | 1.383 (3) | C15—H15C | 0.9600 |
| C3—C2 | 1.394 (3) | C6—C5 | 1.377 (3) |
| C3—H3 | 0.9300 | C6—H6 | 0.9300 |
| N2—C1 | 1.356 (3) | C5—H5 | 0.9300 |
| N2—C8 | 1.428 (2) | | |

| | | | |
|---|---|---|---|
| O1$^{i}$—Co1—O1 | 143.29 (10) | C9—C8—C13 | 120.90 (18) |
| O1$^{i}$—Co1—N1 | 106.93 (7) | C9—C8—N2 | 119.55 (17) |
| O1—Co1—N1 | 95.21 (6) | C13—C8—N2 | 119.55 (17) |
| O1$^{i}$—Co1—N1$^{i}$ | 95.21 (6) | C8—C9—C10 | 119.21 (18) |
| O1—Co1—N1$^{i}$ | 106.93 (7) | C8—C9—H9 | 120.4 |
| N1—Co1—N1$^{i}$ | 105.34 (9) | C10—C9—H9 | 120.4 |
| C14—O1—Co1 | 98.41 (13) | O2—C14—O1 | 122.0 (2) |
| C12—C11—C10 | 118.47 (18) | O2—C14—C15 | 120.16 (19) |
| C12—C11—C11$^{ii}$ | 121.45 (13) | O1—C14—C15 | 117.86 (18) |
| C10—C11—C11$^{ii}$ | 120.07 (13) | C3—C4—C5 | 121.67 (19) |
| C13—C12—C11 | 120.84 (18) | C3—C4—H4 | 119.2 |
| C13—C12—H12 | 119.6 | C5—C4—H4 | 119.2 |
| C11—C12—H12 | 119.6 | N1—C1—N2 | 113.41 (18) |
| C6—C7—N2 | 132.25 (18) | N1—C1—H1 | 123.3 |
| C6—C7—C2 | 122.45 (18) | N2—C1—H1 | 123.3 |
| N2—C7—C2 | 105.27 (17) | C14—C15—H15A | 109.5 |
| C4—C3—C2 | 117.29 (18) | C14—C15—H15B | 109.5 |
| C4—C3—H3 | 121.4 | H15A—C15—H15B | 109.5 |
| C2—C3—H3 | 121.4 | C14—C15—H15C | 109.5 |
| C1—N2—C7 | 106.87 (16) | H15A—C15—H15C | 109.5 |
| C1—N2—C8 | 126.16 (17) | H15B—C15—H15C | 109.5 |
| C7—N2—C8 | 126.95 (16) | C3—C2—N1 | 130.35 (18) |
| C1—N1—C2 | 105.12 (16) | C3—C2—C7 | 120.32 (19) |
| C1—N1—Co1 | 123.02 (14) | N1—C2—C7 | 109.32 (17) |
| C2—N1—Co1 | 131.69 (13) | C5—C6—C7 | 116.59 (18) |
| C9—C10—C11 | 121.05 (19) | C5—C6—H6 | 121.7 |
| C9—C10—H10 | 119.5 | C7—C6—H6 | 121.7 |
| C11—C10—H10 | 119.5 | C6—C5—C4 | 121.67 (19) |
| C8—C13—C12 | 119.46 (18) | C6—C5—H5 | 119.2 |
| C8—C13—H13 | 120.3 | C4—C5—H5 | 119.2 |
| C12—C13—H13 | 120.3 | | |

| | | | |
|---|---|---|---|
| O1$^{i}$—Co1—O1—C14 | −43.39 (12) | C13—C8—C9—C10 | −2.3 (3) |
| N1—Co1—O1—C14 | −171.08 (13) | N2—C8—C9—C10 | 177.49 (18) |
| N1$^{i}$—Co1—O1—C14 | 81.14 (14) | C11—C10—C9—C8 | 1.1 (3) |
| C10—C11—C12—C13 | −2.7 (3) | Co1—O1—C14—O2 | −6.9 (2) |
| C11$^{ii}$—C11—C12—C13 | 176.7 (2) | Co1—O1—C14—C15 | 172.84 (15) |
| C6—C7—N2—C1 | 178.2 (2) | C2—C3—C4—C5 | 0.5 (3) |
| C2—C7—N2—C1 | 0.0 (2) | C2—N1—C1—N2 | −1.1 (2) |
| C6—C7—N2—C8 | −3.3 (3) | Co1—N1—C1—N2 | −176.94 (13) |
| C2—C7—N2—C8 | 178.53 (18) | C7—N2—C1—N1 | 0.7 (2) |
| O1$^{i}$—Co1—N1—C1 | −49.07 (17) | C8—N2—C1—N1 | −177.81 (17) |
| O1—Co1—N1—C1 | 101.29 (16) | C4—C3—C2—N1 | 178.6 (2) |
| N1$^{i}$—Co1—N1—C1 | −149.55 (18) | C4—C3—C2—C7 | −0.5 (3) |
| O1$^{i}$—Co1—N1—C2 | 136.34 (17) | C1—N1—C2—C3 | −178.1 (2) |
| O1—Co1—N1—C2 | −73.29 (18) | Co1—N1—C2—C3 | −2.8 (3) |
| N1$^{i}$—Co1—N1—C2 | 35.86 (15) | C1—N1—C2—C7 | 1.1 (2) |
| C12—C11—C10—C9 | 1.4 (3) | Co1—N1—C2—C7 | 176.39 (13) |
| C11$^{ii}$—C11—C10—C9 | −178.0 (2) | C6—C7—C2—C3 | 0.2 (3) |
| C11—C12—C13—C8 | 1.5 (3) | N2—C7—C2—C3 | 178.57 (17) |
| C12—C13—C8—C9 | 1.0 (3) | C6—C7—C2—N1 | −179.06 (18) |
| C12—C13—C8—N2 | −178.74 (17) | N2—C7—C2—N1 | −0.7 (2) |
| C1—N2—C8—C9 | 131.6 (2) | N2—C7—C6—C5 | −177.7 (2) |
| C7—N2—C8—C9 | −46.6 (3) | C2—C7—C6—C5 | 0.2 (3) |
| C1—N2—C8—C13 | −48.6 (3) | C7—C6—C5—C4 | −0.3 (3) |
| C7—N2—C8—C13 | 133.1 (2) | C3—C4—C5—C6 | −0.1 (3) |

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