



Orientational disorder in the one-dimensional coordination polymer *catena*-poly[[bis(acetylacetonato- κ^2O,O')cobalt(II)]- μ -1,4-diazabicyclo[2.2.2]octane- $\kappa^2N^1:N^4$]

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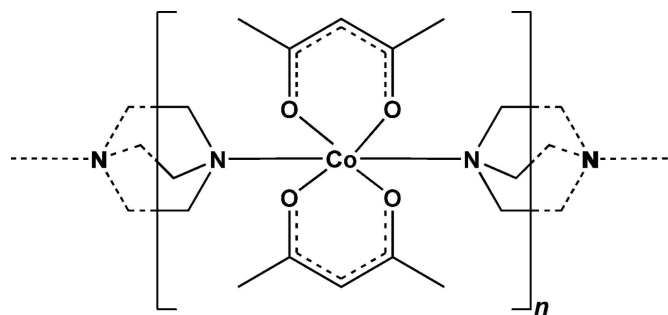
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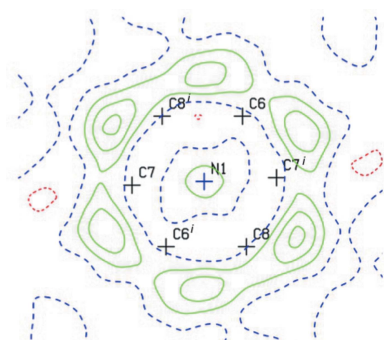
The title compound, $[\text{Co}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_6\text{H}_{12}\text{N}_2)]_n$, was obtained as a one-dimensional coordination polymer from bis(acetylacetonato)diaquacobalt(II), $[\text{Co}(\text{acac})_2(\text{OH}_2)_2]$, and 1,4-diazabicyclo[2.2.2]octane (DABCO), a diamine with good bridging ability and rod-like spacer function. In the chain complex that extends along the *c* axis, the Co^{II} atom is six-coordinated, the O-donor atoms of the chelating acac ligands occupying the equatorial positions and the bridging DABCO ligands being in *trans*-axial positions. In the crystal structure, the DABCO ligand is conformationally disordered in a 50:50 manner as a result of its location across a crystallographic mirror plane. The metal–metal distance is very close to that in a related compound exhibiting weak antiferromagnetic exchange between the Co^{II} ions, and the title compound can thus be useful for obtaining more information about the contribution of different bridges to the magnetic coupling between paramagnetic ions.

1. Chemical context

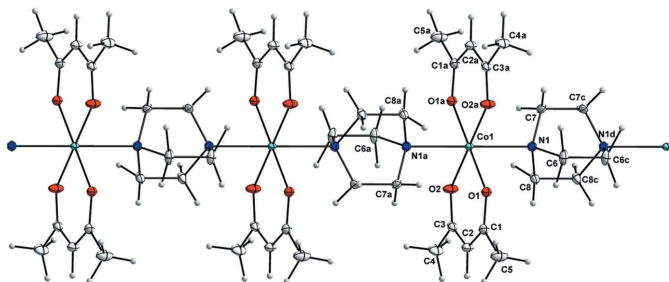
Self-assembly of coordination polymers from simple building blocks is of considerable interest due to their diverse architectures and potential applications in catalysis and advanced materials, such as magnetic, optic and electronic materials.



In this paper, two simple building blocks, namely 1,4-diazabicyclo[2.2.2]octane (DABCO), a diamine with good bridging ability and rod-like spacer function, and the unsaturated square-planar metal complex bis(acetylacetonato- κ^2O,O')cobalt(II), $[\text{Co}(\text{acac})_2]$, have been chosen to design a one-dimensional coordination polymer in which the paramagnetic Co^{II} ions are separated by a distance of 7.2328 (7) Å. This metal–metal distance is very close to the distance of 7.267 (3) Å reported by Ma *et al.* (2001) for the



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Figure 1

A section of the coordination polymer of (I). Only one of the 50:50 DABCO disorder forms and one orientation of the disordered acac methyl groups are shown. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles. [Symmetry codes: (a) $-x, -y, -z$; (c) $x, y, -z + 1$; (d) $-x, -y, -z + 1$.]

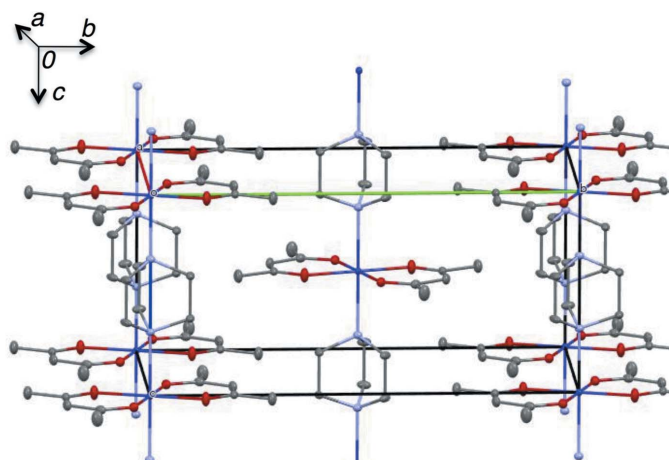
structurally related $[\text{Co}(\text{acac})_2(\text{pyrazine})]_n$ compound which exhibits weak antiferromagnetic exchange between the Co^{II} ions.

Within this context, the title compound *catena*-poly[[bis(acetylacetonato- $\kappa^2 O, O'$)cobalt(II)]- μ -1,4-diazabicyclo[2.2.2]octane- $\kappa^2 N^1: N^4$], $[\text{Co}(\text{acac})_2(\text{DABCO})]_n$, (I), can serve for a comparative investigation of the magnetic behaviour of analogous compounds and, thus, allow more information about the contribution of different bridges to the magnetic coupling between paramagnetic ions to be obtained.

2. Structural commentary

In the crystalline state, the title compound, (I), represents a one-dimensional coordination polymer self-assembled from bis(acetylacetonato)cobalt(II) units as metal–complex connectors and 1,4-diazabicyclo[2.2.2]octane (DABCO) as linkers.

The acetylacetonate (acac) ligand, which is the deprotonated form of acetylacetonone (pentane-2,4-dione, acacH), is a well-known mononegative O, O' -chelating donor agent and its metal coordination chemistry is well documented [for reviews


Figure 2

The molecular packing of the coordination polymer chains.

on the coordination chemistry of acac ligands, see: Aromí *et al.* (2008); Bray *et al.* (2007); Vigato *et al.* (2009)]. For DABCO, the bridging coordination behaviour is most exploited for the generation of coordination polymers and metal–organic frameworks (MOFs), with Zn^{2+} being the most common metal ion used in these structures [for representative examples, see: Furukawa *et al.* (2009); Uemura *et al.* (2007)].

The complex crystallizes in the orthorhombic $Pnmm$ space group with the metal atom on a special position with site symmetry \dots/m . The Co^{II} atom shows an octahedral environment defined by four equatorial acac O atoms on a mirror plane, with bond lengths ranging from 2.0299 (10) to 2.0411 (10) Å, and with two N atoms of bridging DABCO groups on a twofold rotation axis in the axial positions at distances of 2.3071 (12) Å (Fig. 1).

3. Supramolecular features

The centrosymmetric DABCO ligand is bonded to two $[\text{Co}(\text{acac})_2]$ units, which gives rise to the formation of chains extending along the c axis (Fig. 2). The individual chains run parallel in the crystal and do not interact with each other. This polymer is essentially a one-dimensional coordination polymer, the only structural motif that is present being based on the Co^{II} coordination requirements.

4. Database survey

Although some polymeric complexes of the form $[\text{Co}(\text{acac})_2(\mu\text{-diamine})]_n$ [diamine = $\text{NH}_2\text{-R-NH}_2$, with $R = \text{C}_y\text{H}_{2y+1}$ ($y = 6, 11, 12$; Fine, 1973), piperazine (Pellacani *et al.*, 1973), 2,5-dimethylpyrazine (Blake & Hatfield, 1978), and 1,2-bis(4-pyridyl)ethane and *trans*-1,2-bis(4-pyridyl)ethylene (Atienza *et al.*, 2008)] have been synthesized over the years, their structures were elucidated only on the basis of spectroscopic and magnetic analyses. $[\text{Co}(\text{acac})_2(\mu\text{-diamine})]_n$ complexes similar in structure to the title compound, with square-planar $[\text{Co}(\text{acac})_2]$ units connected by bridging diamine ligands into infinite linear chains, were retrieved from the Cambridge Structural Database (CSD, Version 5.36 of November 2014; Groom & Allen, 2014), *viz.* $[\text{Co}(\text{acac})_2(\mu\text{-}1,3\text{-bis}(\text{pyridin-}4\text{-yl})\text{propane})]_n$ (Lennartson & Håkansson, 2009), $[\text{Co}(\text{acac})_2(\text{pyrazine})]_n$ and $[\text{Co}(\text{acac})_2(4,4'\text{-bipyridine})]_n$ (Ma *et al.*, 2001).

5. Synthesis and crystallization

$[\text{Co}(\text{acac})_2(\text{H}_2\text{O})_2]$ was prepared by precipitation of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ with aqueous ammonia, followed by solubilization and complexation with acetylacetonone. Elemental analysis calculated for $[\text{Co}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]$ (%): C 40.96, H 6.14; found: C 40.94, H 6.19.

$[\text{Co}(\text{acac})_2(\text{H}_2\text{O})_2]$ (293 mg, 1 mmol) and 1,4-diazabicyclo[2.2.2]octane (DABCO) (112 mg, 1 mmol) were stirred in CH_3OH (15 ml) at 333 K for 1 h. The pink precipitate which formed was collected by filtration and redissolved in dimethyl sulfoxide (DMSO, 5 ml). Elemental analysis calculated for

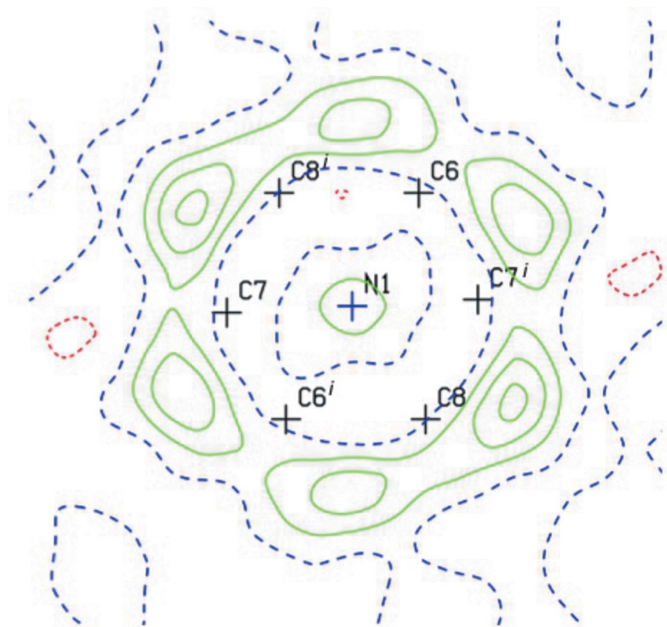


Figure 3
Difference-density Fourier synthesis in the ab plane through three DABCO C atoms before assignment of the DABCO H-atom positions; contour lines are drawn at $0.2 \text{ e } \text{Å}^{-3}$ intervals.

[Co(acac)₂(DABCO)] (%): C 52.04, H 7.05, N 7.59; found: C 51.63, H 7.39, N 7.41. Layering the solution of the complex in DMSO with CH₃OH at 293 K gave pale-pink crystals suitable for X-ray single-crystal analysis.

Elemental analyses were carried out on a Heraeus CHNO Rapid apparatus (Institute of Inorganic Chemistry, RWTH Aachen University).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Space filling more symmetric than atom positions leads to pronounced orientational disorder (Herberich *et al.*, 1993) for the DABCO ligand over two positions due to mirror symmetry. As a result, the site occupancies of the C atoms are constrained to 0.5. In principle, the same should be true for the associated H atoms, their alternative positions for the different C positions overlap very closely, thus forming the hexagon of local residual electron-density maxima about the C-atom scaffold shown in Fig. 3. These maxima can be freely refined as H atoms with reasonable C–H geometry and displacement parameters.

H atoms attached to C atoms were calculated, introduced in their idealized positions and treated as riding, with C–H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ otherwise. For consistency, we opted to calculate the positions of the DABCO H atoms and fix them in their idealized positions. Due to the fact that the acac ligand lies on a mirror plane, the acac methyl groups are therefore equally disordered over two orientations.

Table 1
Experimental details.

Crystal data	
Chemical formula	[Co(C ₅ H ₇ O ₂) ₂ (C ₆ H ₁₂ N ₂)]
M_r	369.32
Crystal system, space group	Orthorhombic, $Pnmm$
Temperature (K)	100
a, b, c (Å)	7.7468 (3), 15.1573 (4), 7.2328 (7)
V (Å ³)	849.28 (9)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.03
Crystal size (mm)	0.48 × 0.10 × 0.04
Data collection	
Diffractometer	Stoe IPDS 2T
Absorption correction	Multi-scan (MULABS in PLATON; Spek, 2003)
$T_{\text{min}}, T_{\text{max}}$	0.637, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11457, 1045, 944
R_{int}	0.045
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.020, 0.055, 1.09
No. of reflections	1045
No. of parameters	81
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.25, -0.39

Computer programs: X-AREA (Stoe & Cie, 2002), X-RED (Stoe & Cie, 2002), SHELXS2013 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), DIAMOND (Brandenburg, 1999), Mercury (Macrae *et al.*, 2006), PLATON (Spek, 2009) and publCIF (Westrip, 2010).

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Florina Dumitru, Ulli Englert and Beatrice Braun

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 1999) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

catena-Poly[[bis(acetylacetonato- κ^2O,O')cobalt(II)]- μ -1,4-diazabicyclo[2.2.2]octane- $\kappa^2N^1:N^4$]

Crystal data

[Co(C₅H₇O₂)₂(C₆H₁₂N₂)₂]

$M_r = 369.32$

Orthorhombic, *Pnmm*

$a = 7.7468$ (3) Å

$b = 15.1573$ (4) Å

$c = 7.2328$ (7) Å

$V = 849.28$ (9) Å³

$Z = 2$

$F(000) = 390$

$D_x = 1.444$ Mg m⁻³

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

Cell parameters from 16455 reflections

$\theta = 3.8$ – 29.5°

$\mu = 1.03$ mm⁻¹

$T = 100$ K

Elongated plate, pale pink

$0.48 \times 0.10 \times 0.04$ mm

Data collection

Stoe IPDS 2T
diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4
mm long-fine focus

Plane graphite monochromator

Detector resolution: 6.67 pixels mm⁻¹

rotation method scans

Absorption correction: multi-scan
(MULABS in *PLATON*; Spek, 2003)

$T_{\min} = 0.637$, $T_{\max} = 0.960$

11457 measured reflections

1045 independent reflections

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

$R_{\text{int}} = 0.045$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.8^\circ$

$h = -10 \rightarrow 10$

$k = -19 \rightarrow 19$

$l = -8 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.055$

$S = 1.09$

1045 reflections

81 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.25$ e Å⁻³

$\Delta\rho_{\min} = -0.39$ e Å⁻³

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.0000	0.0000	0.0000	0.00790 (10)	
O1	0.24789 (12)	0.04561 (6)	0.0000	0.0122 (2)	
O2	-0.08057 (13)	0.12744 (7)	0.0000	0.0173 (2)	
N1	0.0000	0.0000	0.31898 (17)	0.0106 (3)	
C1	0.29942 (18)	0.12455 (10)	0.0000	0.0134 (3)	
C2	0.19083 (19)	0.19922 (9)	0.0000	0.0148 (3)	
H2	0.2442	0.2557	0.0000	0.018*	
C3	0.01048 (18)	0.19635 (10)	0.0000	0.0127 (3)	
C4	-0.0887 (2)	0.28217 (9)	0.0000	0.0196 (3)	
H4A	-0.1733	0.2817	0.1008	0.029*	0.5
H4B	-0.1488	0.2891	-0.1184	0.029*	0.5
H4C	-0.0085	0.3314	0.0176	0.029*	0.5
C5	0.49196 (18)	0.13858 (12)	0.0000	0.0228 (3)	
H5A	0.5190	0.1944	-0.0619	0.034*	0.5
H5B	0.5481	0.0899	-0.0659	0.034*	0.5
H5C	0.5340	0.1405	0.1277	0.034*	0.5
C6	0.1745 (3)	-0.02067 (16)	0.3932 (3)	0.0167 (4)	0.5
H6A	0.2582	0.0237	0.3477	0.020*	0.5
H6B	0.2115	-0.0793	0.3477	0.020*	0.5
C7	-0.1237 (3)	-0.06034 (13)	0.3934 (3)	0.0155 (4)	0.5
H7A	-0.0975	-0.1206	0.3484	0.019*	0.5
H7B	-0.2402	-0.0442	0.3484	0.019*	0.5
C8	-0.0438 (3)	0.09127 (13)	0.3934 (3)	0.0142 (4)	0.5
H8A	-0.1589	0.1093	0.3477	0.017*	0.5
H8B	0.0420	0.1345	0.3477	0.017*	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01008 (15)	0.00601 (15)	0.00760 (15)	-0.00078 (8)	0.000	0.000
O1	0.0133 (5)	0.0109 (5)	0.0122 (5)	-0.0013 (4)	0.000	0.000
O2	0.0147 (5)	0.0089 (5)	0.0282 (6)	-0.0001 (4)	0.000	0.000
N1	0.0122 (6)	0.0114 (6)	0.0081 (5)	0.0000 (4)	0.000	0.000
C1	0.0158 (7)	0.0143 (7)	0.0102 (6)	-0.0041 (5)	0.000	0.000
C2	0.0195 (7)	0.0093 (6)	0.0156 (6)	-0.0036 (5)	0.000	0.000
C3	0.0202 (7)	0.0089 (7)	0.0089 (6)	0.0004 (5)	0.000	0.000
C4	0.0238 (8)	0.0106 (6)	0.0243 (8)	0.0022 (5)	0.000	0.000
C5	0.0151 (7)	0.0177 (8)	0.0355 (9)	-0.0031 (5)	0.000	0.000
C6	0.0143 (9)	0.0269 (10)	0.0090 (9)	0.0046 (8)	0.0003 (8)	0.0007 (8)

C7	0.0219 (10)	0.0169 (9)	0.0079 (9)	-0.0109 (8)	0.0005 (8)	-0.0015 (7)
C8	0.0252 (10)	0.0099 (9)	0.0075 (9)	0.0030 (7)	-0.0007 (8)	0.0006 (7)

Geometric parameters (Å, °)

Co1—O2 ⁱ	2.0299 (10)	C2—H2	0.9500
Co1—O2	2.0299 (10)	C3—C4	1.511 (2)
Co1—O1	2.0410 (10)	C4—H4A	0.9800
Co1—O1 ⁱ	2.0411 (10)	C4—H4B	0.9800
Co1—N1	2.3071 (12)	C4—H4C	0.9800
Co1—N1 ⁱ	2.3071 (12)	C5—H5A	0.9800
O1—C1	1.2612 (18)	C5—H5B	0.9800
O2—C3	1.2603 (18)	C5—H5C	0.9800
N1—C7 ⁱⁱ	1.4299 (19)	C6—C6 ⁱⁱⁱ	1.545 (4)
N1—C7	1.4299 (19)	C6—H6A	0.9900
N1—C6	1.488 (2)	C6—H6B	0.9900
N1—C6 ⁱⁱ	1.488 (2)	C7—C7 ⁱⁱⁱ	1.542 (4)
N1—C8	1.523 (2)	C7—H7A	0.9900
N1—C8 ⁱⁱ	1.523 (2)	C7—H7B	0.9900
C1—C2	1.410 (2)	C8—C8 ⁱⁱⁱ	1.541 (4)
C1—C5	1.5067 (19)	C8—H8A	0.9900
C2—C3	1.398 (2)	C8—H8B	0.9900
O2 ⁱ —Co1—O2	180.0	O1—C1—C5	116.56 (13)
O2 ⁱ —Co1—O1	91.89 (4)	C2—C1—C5	118.50 (14)
O2—Co1—O1	88.11 (4)	C3—C2—C1	124.83 (14)
O2 ⁱ —Co1—O1 ⁱ	88.11 (4)	C3—C2—H2	117.6
O2—Co1—O1 ⁱ	91.89 (4)	C1—C2—H2	117.6
O1—Co1—O1 ⁱ	180.0	O2—C3—C2	125.82 (14)
O2 ⁱ —Co1—N1	90.0	O2—C3—C4	115.39 (13)
O2—Co1—N1	90.0	C2—C3—C4	118.79 (14)
O1—Co1—N1	90.0	C3—C4—H4A	109.5
O1 ⁱ —Co1—N1	90.0	C3—C4—H4B	109.5
O2 ⁱ —Co1—N1 ⁱ	90.0	H4A—C4—H4B	109.5
O2—Co1—N1 ⁱ	90.0	C3—C4—H4C	109.5
O1—Co1—N1 ⁱ	90.0	H4A—C4—H4C	109.5
O1 ⁱ —Co1—N1 ⁱ	90.0	H4B—C4—H4C	109.5
N1—Co1—N1 ⁱ	180.0	C1—C5—H5A	109.5
C1—O1—Co1	128.25 (9)	C1—C5—H5B	109.5
C3—O2—Co1	128.06 (9)	H5A—C5—H5B	109.5
C7 ⁱⁱ —N1—C7	135.78 (17)	C1—C5—H5C	109.5
C7 ⁱⁱ —N1—C6	52.41 (12)	H5A—C5—H5C	109.5
C7—N1—C6	109.78 (13)	H5B—C5—H5C	109.5
C7 ⁱⁱ —N1—C6 ⁱⁱ	109.78 (13)	N1—C6—C6 ⁱⁱⁱ	111.15 (9)
C7—N1—C6 ⁱⁱ	52.41 (12)	N1—C6—H6A	109.4
C6—N1—C6 ⁱⁱ	137.70 (17)	C6 ⁱⁱⁱ —C6—H6A	109.4
C7 ⁱⁱ —N1—C8	55.60 (12)	N1—C6—H6B	109.4
C7—N1—C8	107.38 (12)	C6 ⁱⁱⁱ —C6—H6B	109.4

C6—N1—C8	105.43 (13)	H6A—C6—H6B	108.0
C6 ⁱⁱ —N1—C8	58.58 (12)	N1—C7—C7 ⁱⁱⁱ	112.11 (9)
C7 ⁱⁱ —N1—C8 ⁱⁱ	107.38 (12)	N1—C7—H7A	109.2
C7—N1—C8 ⁱⁱ	55.60 (12)	C7 ⁱⁱⁱ —C7—H7A	109.2
C6—N1—C8 ⁱⁱ	58.58 (12)	N1—C7—H7B	109.2
C6 ⁱⁱ —N1—C8 ⁱⁱ	105.43 (13)	C7 ⁱⁱⁱ —C7—H7B	109.2
C8—N1—C8 ⁱⁱ	138.58 (17)	H7A—C7—H7B	107.9
C7 ⁱⁱ —N1—Co1	112.11 (9)	N1—C8—C8 ⁱⁱⁱ	110.71 (8)
C7—N1—Co1	112.11 (9)	N1—C8—H8A	109.5
C6—N1—Co1	111.15 (9)	C8 ⁱⁱⁱ —C8—H8A	109.5
C6 ⁱⁱ —N1—Co1	111.15 (9)	N1—C8—H8B	109.5
C8—N1—Co1	110.71 (8)	C8 ⁱⁱⁱ —C8—H8B	109.5
C8 ⁱⁱ —N1—Co1	110.71 (8)	H8A—C8—H8B	108.1
O1—C1—C2	124.93 (13)		
Co1—O1—C1—C2	0.0	Co1—N1—C6—C6 ⁱⁱⁱ	179.998 (1)
Co1—O1—C1—C5	180.0	C7 ⁱⁱ —N1—C7—C7 ⁱⁱⁱ	-0.002 (1)
O1—C1—C2—C3	0.0	C6—N1—C7—C7 ⁱⁱⁱ	55.94 (12)
C5—C1—C2—C3	180.0	C6 ⁱⁱ —N1—C7—C7 ⁱⁱⁱ	-79.70 (11)
Co1—O2—C3—C2	0.0	C8—N1—C7—C7 ⁱⁱⁱ	-58.19 (11)
Co1—O2—C3—C4	180.0	C8 ⁱⁱ —N1—C7—C7 ⁱⁱⁱ	79.37 (10)
C1—C2—C3—O2	0.0	Co1—N1—C7—C7 ⁱⁱⁱ	179.998 (1)
C1—C2—C3—C4	180.0	C7 ⁱⁱ —N1—C8—C8 ⁱⁱⁱ	-76.77 (11)
C7 ⁱⁱ —N1—C6—C6 ⁱⁱⁱ	77.79 (11)	C7—N1—C8—C8 ⁱⁱⁱ	57.32 (11)
C7—N1—C6—C6 ⁱⁱⁱ	-55.39 (11)	C6—N1—C8—C8 ⁱⁱⁱ	-59.70 (11)
C6 ⁱⁱ —N1—C6—C6 ⁱⁱⁱ	-0.002 (1)	C6 ⁱⁱ —N1—C8—C8 ⁱⁱⁱ	77.23 (10)
C8—N1—C6—C6 ⁱⁱⁱ	59.99 (10)	C8 ⁱⁱ —N1—C8—C8 ⁱⁱⁱ	0.000 (1)
C8 ⁱⁱ —N1—C6—C6 ⁱⁱⁱ	-77.99 (10)	Co1—N1—C8—C8 ⁱⁱⁱ	180.000 (1)

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