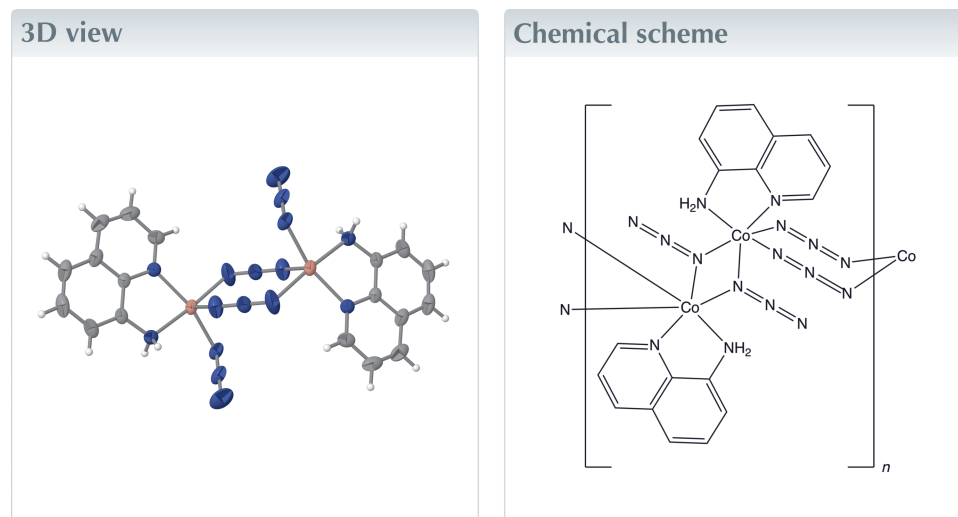


catena-Poly[[*(*(8-aminoquinoline)cobalt(II)]-di- μ -azido]

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The title coordination polymer, $[\text{Co}(\text{N}_3)_2(\text{C}_9\text{H}_8\text{N}_2)]_n$, was synthesized solvothermally. The Co^{II} atom exhibits a distorted octahedral $[\text{CoN}_6]$ coordination geometry with a bidentate 8-aminoquinoline ligand and four azide ligands. Bridging azide ligands result in chains extending along $[100]$. $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds join the chains to give an extended structure with sheets parallel to (002) .



Structure description

Pseudohalide and polynitrile compounds derived from transition-metal ions are of great interest from the perspective of their magnetic properties, rich molecular architectures and for their topologies (Atmani *et al.*, 2008; Benmansour *et al.*, 2008, 2010, 2012; Addala *et al.*, 2015; Setifi *et al.*, 2018, 2019; Dmitrienko *et al.*, 2020; Yuste *et al.*, 2009; Merabet *et al.*, 2022).

One of the pseudohalide ligands that has received much attention in the last decade is the azide $[\text{N}_3^-]$ ion, partly due to its ability to produce a wide variety of coordination compounds with different nuclearities ranging from simple mononuclear to polynuclear species. Different bonding modes are observed with the azide ion, which result in the formation of one-, two- and three-dimensional polymeric assemblies (Escuer *et al.*, 2006).

As a part of our continuing study of the structural and magnetic properties of transition-metal complexes containing both azide and polypyridyl units (Setifi, Ghazzali *et al.*, 2016; Setifi, Knaust *et al.*, 2016; Setifi, Moon *et al.*, 2016; Benamara *et al.*, 2021; Merabet *et al.*, 2023; Setifi, Setifi *et al.*, 2022, 2023), we report herein the crystal and molecular structure of a one-dimensional coordination polymer, (I), based on 8-aminoquinoline (8-aquin) as co-ligand and the azide anion as ligand with two different coordination modes.

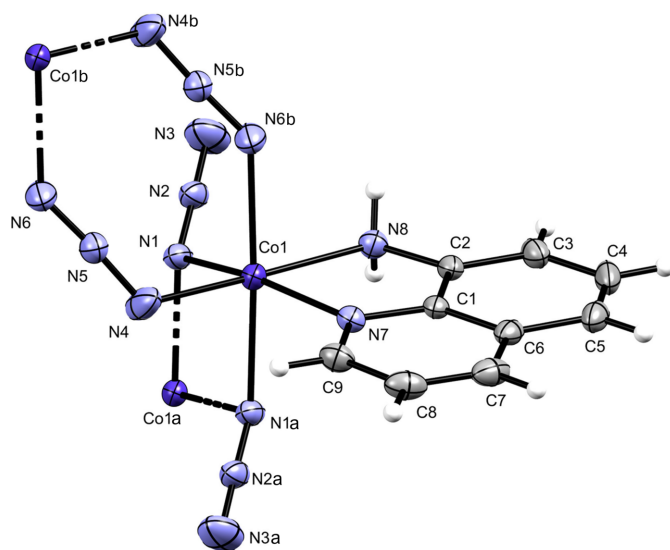


Figure 1
Representation of (the title compound showing the atom-labeling scheme. Non-H atom anisotropic displacement parameters are represented at the 50% probability level. Symmetry codes: (a) $-x, -y + 1, -z + 1$; (b) $-x + 1, -y + 1, -z + 1$.

The asymmetric unit of (I) is composed of a Co^{II} ion, a bidentate 8-amino ligand and two azide ligands. The distorted octahedral coordination sphere is completed by two additional azide ligands. One of the azide anions binds to two Co centers in a 1,3 bidentate mode, whereas the other one connects two Co centers in a 1,1 bidentate mode. The resulting coordination geometry and supramolecular association is shown in Fig. 1. Pertinent Co–N bond lengths are exhibited in Table 1.

The bridging ligands result in polymeric chains extending parallel to $[100]$, as shown in Fig. 2. The chains are composed of Co^{II} ions joined by alternating bis μ -(1,1- N_3) units and bis μ -(1,3- N_3) units with corresponding Co \cdots Co separations of 3.2817 (5) and 5.2427 (7) Å, respectively. The angle between the $(\text{N}_3)_2$ mean plane of the double *end-to-end* azide bridges and the plane defined by the Co^{II} and the bonded N_{azide} atom is 20.20 (14)°, corresponding to a flattened chair configuration for the eight-membered ring. For a flat bridge, an angle of 0°

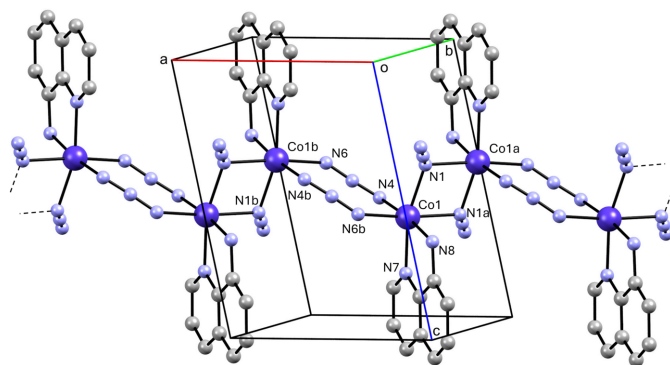


Figure 2
Partial packing diagram showing the polymeric chain parallel to $[100]$. H atoms are not shown. Symmetry codes: (a) $-x, -y + 1, -z + 1$; (b) $-x + 1, -y + 1, -z + 1$.

Table 1
Selected bond lengths (Å).

Co1–N1	2.1020 (13)	Co1–N8	2.1684 (13)
Co1–N7	2.1100 (12)	Co1–N6 ⁱ	2.1685 (15)
Co1–N4	2.1222 (17)	Co1–N1 ⁱⁱ	2.2047 (12)

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

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N8–H8A \cdots N3 ⁱⁱⁱ	0.84 (3)	2.46 (3)	3.218 (2)	151 (2)
N8–H8B \cdots N4 ⁱⁱ	0.88 (3)	2.73 (3)	3.502 (3)	148 (2)

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

would be observed. This angle compares to values of 8.2 (2) and 25.6 (1)° for the structurally similarly bridged polymorphic Fe^{II} complexes with a 5,5'-dimethyl-2,2'-bipyridine ligand (Setifi, Bernès *et al.*, 2022). In the 8-amino complexes of Mn^{II} and Co^{II} , the comparable angles are 20.3 (6)° and 25.5 (4)°, respectively (Benamara *et al.*, 2021).

$\text{N}\text{--}\text{H}\cdots\text{N}$ hydrogen-bonding interactions are observed in the extended structure (Table 2, Fig. 3). Within individual chains, $R_2^2(8)$ hydrogen-bonded rings are observed (Fig. 4). The polymeric chains are joined by hydrogen-bonding bridges involving the 8-amino substituent on the quinoline ligands and the terminal nitrogen atom of the μ -(1,1-azide) ligands of adjacent chains, resulting in sheets parallel to (002) containing $\text{N}\text{--}\text{H}\cdots\text{N}$ hydrogen-bond-derived $R_2^2(12)$ interchain rings, as seen in Figs. 3 and 5.

Synthesis and crystallization

The title compound was prepared solvothermally under autogenous pressure from a mixture of cobalt(II) sulfate heptahydrate (28 mg, 0.1 mmol), 8-aminoquinoline (14 mg,

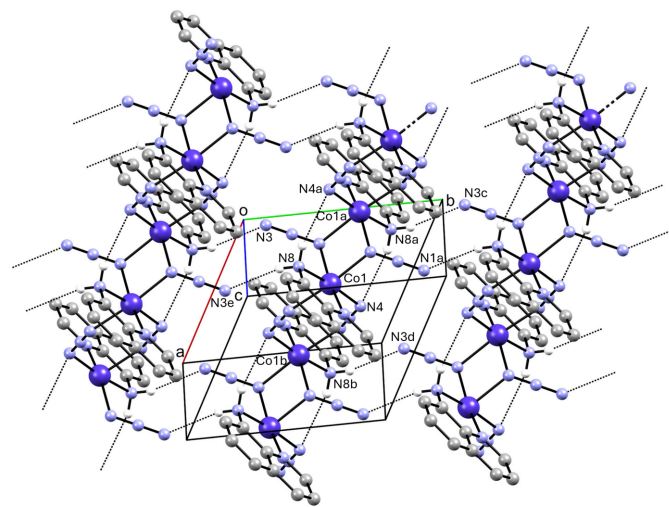
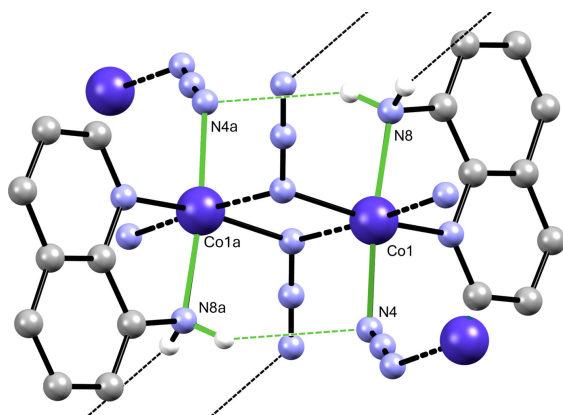


Figure 3
Partial packing diagram showing sheets parallel to (002) formed by $\text{N}\text{--}\text{H}\cdots\text{N}$ bonds. Only H atoms involved in the interactions are represented. Symmetry codes: (a) $-x, -y + 1, -z + 1$; (b) $-x + 1, -y + 1, -z + 1$; (c) $x, y + 1, z$; (d) $x + 1, y + 1, z$; (e) $-x, -y, -z + 1$.

**Figure 4**

View of the intrachain $R_2^2(8)$ N–H...N motif. Only H atoms involved in the hydrogen bonds are shown. Symmetry code: (a) $-x, -y + 1, -z + 1$.

0.1 mmol) and sodium azide (13 mg, 0.2 mmol) in a mixture of water and ethanol (3:1 v/v, 20 ml). This mixture was sealed in a Teflon-lined autoclave and held at 393 K for 2 days, and then cooled to ambient temperature at a rate of 10 K h^{-1} to give the product (yield 38%).

Refinement

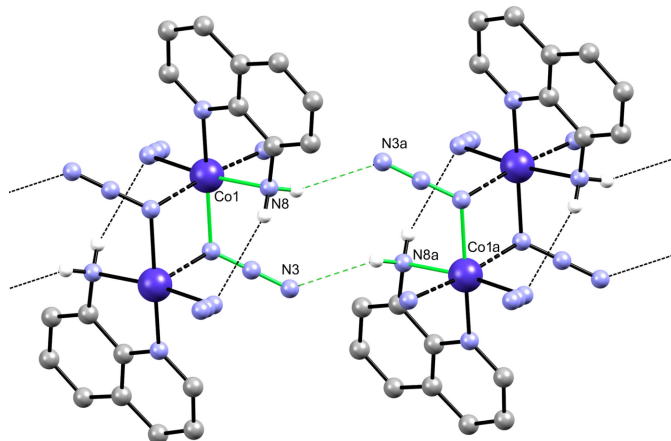
Crystal data, data collection and refinement details are summarized in Table 3.

Acknowledgements

The Service Commun de Diffraction X of the Université de Brest is thanked for the single-crystal X-ray crystallographic data collection and analysis.

Funding information

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**Figure 5**

View of the interchain $R_2^2(12)$ N–H...N motif. Only H atoms involved in hydrogen bonding are shown. Symmetry code: (a) $-x, -y, -z + 1$.

Table 3

Experimental details.

Crystal data	
Chemical formula	$[\text{Co}(\text{N}_3)_2(\text{C}_9\text{H}_8\text{N}_2)]$
M_r	287.16
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	301
a, b, c (Å)	7.3526 (10), 8.3354 (13), 10.4053 (17)
α, β, γ (°)	97.221 (6), 102.413 (6), 111.334 (5)
V (Å ³)	565.36 (15)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.51
Crystal size (mm)	$0.35 \times 0.30 \times 0.22$
Data collection	
Diffractometer	Xcalibur CCD Sapphire3
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2014)
T_{\min}, T_{\max}	0.769, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29909, 4356, 3882
R_{int}	0.033
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.773
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.088, 1.06
No. of reflections	4356
No. of parameters	171
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.72, -0.33

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *ShelXle* (Hübschle *et al.*, 2011) and *publCIF* (Westrip, 2010).

Recherche Scientifique); the Algerian DGRSDT (Direction Générale de la Recherche Scientifique et du Développement Technologique); PRFU project (grant No. B00L01UN190120230003).

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full crystallographic data

IUCrData (2024). **9**, x240849 [https://doi.org/10.1107/S2414314624008496]

catena-Poly[[[(8-aminoquinoline)cobalt(II)]-di- μ -azido]

Fatima Setifi, Zouaoui Setifi, David K. Geiger, Mohammed Hadi Al-Douh and Abderezak Addala

catena-Poly[[[(8-aminoquinoline)cobalt(II)]-di- μ -azido- $\kappa^4 N^1:N^3$]-[(8-aminoquinoline)cobalt(II)]-di- μ -azido- $\kappa^4 N^1:N^1$]

Crystal data

[Co(N₃)₂(C₉H₈N₂)]
M_r = 287.16
 Triclinic, *P* $\bar{1}$
a = 7.3526 (10) Å
b = 8.3354 (13) Å
c = 10.4053 (17) Å
 α = 97.221 (6)°
 β = 102.413 (6)°
 γ = 111.334 (5)°
V = 565.36 (15) Å³

Z = 2
F(000) = 290
D_x = 1.687 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 4847 reflections
 θ = 4.2–32.3°
 μ = 1.51 mm⁻¹
T = 301 K
 Block, purple
 0.35 × 0.30 × 0.22 mm

Data collection

Xcalibur CCD, Sapphire3
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.769, *T_{max}* = 1.000

29909 measured reflections
 4356 independent reflections
 3882 reflections with *I* > 2 σ (*I*)
R_{int} = 0.033
 θ_{\max} = 33.3°, θ_{\min} = 2.7°
h = -11→11
k = -12→12
l = -16→16

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[[*F*² > 2 σ (*F*²)] = 0.031
wR(*F*²) = 0.088
S = 1.06
 4356 reflections
 171 parameters
 0 restraints

Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.1945P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max}$ = 0.001
 $\Delta\rho_{\max}$ = 0.72 e Å⁻³
 $\Delta\rho_{\min}$ = -0.33 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.

Refinement. H atoms bonded to C were refined using a riding model, H atoms bonded to N were freely refined.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.19673 (3)	0.48517 (2)	0.59913 (2)	0.03117 (6)
N1	0.0070 (2)	0.37549 (18)	0.40029 (12)	0.0377 (3)
N2	-0.0569 (3)	0.21922 (19)	0.35544 (13)	0.0432 (3)
N3	-0.1176 (4)	0.0705 (2)	0.3110 (2)	0.0744 (6)
N4	0.4085 (3)	0.7020 (2)	0.5489 (2)	0.0668 (6)
N5	0.5181 (2)	0.68214 (18)	0.48714 (14)	0.0386 (3)
N6	0.6244 (3)	0.6686 (2)	0.42249 (18)	0.0515 (4)
N7	0.30637 (18)	0.58191 (15)	0.81040 (12)	0.0309 (2)
N8	0.0067 (2)	0.26670 (17)	0.66848 (13)	0.0351 (2)
H8A	0.023 (4)	0.175 (3)	0.642 (2)	0.057 (7)*
H8B	-0.122 (4)	0.246 (4)	0.635 (3)	0.069 (8)*
C1	0.2139 (2)	0.47062 (17)	0.88451 (13)	0.0291 (2)
C2	0.0569 (2)	0.30410 (18)	0.81392 (14)	0.0313 (2)
C3	-0.0357 (3)	0.1882 (2)	0.88582 (19)	0.0423 (3)
H3	-0.1379	0.0784	0.8402	0.051*
C4	0.0224 (3)	0.2336 (3)	1.0283 (2)	0.0528 (5)
H4	-0.0415	0.153	1.0754	0.063*
C5	0.1714 (3)	0.3946 (3)	1.09811 (17)	0.0485 (4)
H5	0.2072	0.4232	1.192	0.058*
C6	0.2705 (2)	0.5171 (2)	1.02765 (14)	0.0380 (3)
C7	0.4267 (3)	0.6859 (3)	1.09254 (17)	0.0472 (4)
H7	0.4694	0.7209	1.1863	0.057*
C8	0.5135 (3)	0.7961 (2)	1.01716 (19)	0.0477 (4)
H8	0.6143	0.9081	1.0587	0.057*
C9	0.4499 (2)	0.7397 (2)	0.87556 (17)	0.0399 (3)
H9	0.5114	0.8166	0.8252	0.048*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03912 (11)	0.03282 (10)	0.02878 (9)	0.01827 (8)	0.01518 (7)	0.01036 (7)
N1	0.0545 (7)	0.0401 (6)	0.0290 (5)	0.0302 (6)	0.0127 (5)	0.0079 (4)
N2	0.0667 (9)	0.0457 (7)	0.0283 (5)	0.0350 (7)	0.0140 (6)	0.0078 (5)
N3	0.1122 (18)	0.0450 (9)	0.0614 (11)	0.0375 (10)	0.0127 (11)	-0.0016 (8)
N4	0.0864 (13)	0.0440 (8)	0.0944 (14)	0.0265 (8)	0.0690 (12)	0.0229 (9)
N5	0.0422 (6)	0.0372 (6)	0.0418 (6)	0.0172 (5)	0.0174 (5)	0.0138 (5)
N6	0.0596 (9)	0.0660 (10)	0.0586 (9)	0.0427 (8)	0.0341 (8)	0.0322 (8)
N7	0.0330 (5)	0.0299 (5)	0.0327 (5)	0.0154 (4)	0.0094 (4)	0.0088 (4)
N8	0.0384 (6)	0.0306 (5)	0.0355 (6)	0.0125 (5)	0.0118 (5)	0.0065 (4)
C1	0.0347 (6)	0.0331 (6)	0.0295 (5)	0.0216 (5)	0.0125 (4)	0.0111 (4)
C2	0.0363 (6)	0.0321 (6)	0.0358 (6)	0.0195 (5)	0.0169 (5)	0.0137 (5)
C3	0.0457 (8)	0.0407 (7)	0.0561 (9)	0.0227 (6)	0.0275 (7)	0.0249 (7)
C4	0.0661 (11)	0.0702 (12)	0.0570 (10)	0.0443 (10)	0.0402 (9)	0.0426 (10)

C5	0.0646 (10)	0.0722 (12)	0.0359 (7)	0.0475 (10)	0.0247 (7)	0.0257 (8)
C6	0.0479 (8)	0.0513 (8)	0.0298 (6)	0.0352 (7)	0.0123 (5)	0.0115 (6)
C7	0.0541 (9)	0.0592 (10)	0.0331 (7)	0.0383 (8)	0.0005 (6)	-0.0009 (6)
C8	0.0439 (8)	0.0418 (8)	0.0489 (9)	0.0220 (7)	-0.0035 (7)	-0.0050 (7)
C9	0.0375 (7)	0.0325 (6)	0.0465 (8)	0.0138 (5)	0.0073 (6)	0.0065 (6)

Geometric parameters (Å, °)

Co1—N1	2.1020 (13)	N8—H8B	0.88 (3)
Co1—N7	2.1100 (12)	C1—C2	1.418 (2)
Co1—N4	2.1222 (17)	C1—C6	1.4186 (19)
Co1—N8	2.1684 (13)	C2—C3	1.371 (2)
Co1—N6 ⁱ	2.1685 (15)	C3—C4	1.411 (3)
Co1—N1 ⁱⁱ	2.2047 (12)	C3—H3	0.93
N1—N2	1.2012 (19)	C4—C5	1.368 (3)
N1—Co1 ⁱⁱ	2.2046 (12)	C4—H4	0.93
N2—N3	1.147 (2)	C5—C6	1.410 (3)
N4—N5	1.176 (2)	C5—H5	0.93
N5—N6	1.161 (2)	C6—C7	1.417 (3)
N6—Co1 ⁱ	2.1685 (15)	C7—C8	1.355 (3)
N7—C9	1.3273 (19)	C7—H7	0.93
N7—C1	1.3653 (18)	C8—C9	1.407 (2)
N8—C2	1.4427 (19)	C8—H8	0.93
N8—H8A	0.84 (3)	C9—H9	0.93
N1—Co1—N7	163.50 (5)	Co1—N8—H8B	110.0 (18)
N1—Co1—N4	94.66 (8)	H8A—N8—H8B	108 (2)
N7—Co1—N4	96.60 (7)	N7—C1—C2	117.90 (12)
N1—Co1—N8	90.80 (5)	N7—C1—C6	122.02 (13)
N7—Co1—N8	78.65 (5)	C2—C1—C6	120.08 (13)
N4—Co1—N8	173.93 (8)	C3—C2—C1	119.16 (14)
N1—Co1—N6 ⁱ	93.17 (6)	C3—C2—N8	123.91 (14)
N7—Co1—N6 ⁱ	98.59 (6)	C1—C2—N8	116.92 (12)
N4—Co1—N6 ⁱ	91.25 (7)	C2—C3—C4	120.74 (17)
N8—Co1—N6 ⁱ	85.77 (6)	C2—C3—H3	119.6
N1—Co1—N1 ⁱⁱ	80.75 (5)	C4—C3—H3	119.6
N7—Co1—N1 ⁱⁱ	87.21 (4)	C5—C4—C3	120.97 (16)
N4—Co1—N1 ⁱⁱ	90.05 (7)	C5—C4—H4	119.5
N8—Co1—N1 ⁱⁱ	93.47 (5)	C3—C4—H4	119.5
N6 ⁱ —Co1—N1 ⁱⁱ	173.87 (6)	C4—C5—C6	119.92 (15)
N2—N1—Co1	119.76 (10)	C4—C5—H5	120.0
N2—N1—Co1 ⁱⁱ	122.01 (12)	C6—C5—H5	120.0
Co1—N1—Co1 ⁱⁱ	99.25 (5)	C5—C6—C7	123.32 (15)
N3—N2—N1	179.1 (2)	C5—C6—C1	119.12 (16)
N5—N4—Co1	121.28 (13)	C7—C6—C1	117.56 (15)
N6—N5—N4	176.53 (18)	C8—C7—C6	119.57 (15)
N5—N6—Co1 ⁱ	137.61 (13)	C8—C7—H7	120.2
C9—N7—C1	118.25 (13)	C6—C7—H7	120.2

C9—N7—Co1	126.30 (11)	C7—C8—C9	119.45 (16)
C1—N7—Co1	115.42 (9)	C7—C8—H8	120.3
C2—N8—Co1	111.12 (9)	C9—C8—H8	120.3
C2—N8—H8A	108.7 (17)	N7—C9—C8	123.12 (16)
Co1—N8—H8A	109.8 (17)	N7—C9—H9	118.4
C2—N8—H8B	109.3 (18)	C8—C9—H9	118.4
C9—N7—C1—C2	178.36 (12)	C3—C4—C5—C6	-0.6 (3)
Co1—N7—C1—C2	0.21 (14)	C4—C5—C6—C7	-179.72 (15)
C9—N7—C1—C6	-1.73 (19)	C4—C5—C6—C1	-0.1 (2)
Co1—N7—C1—C6	-179.88 (9)	N7—C1—C6—C5	-178.82 (12)
N7—C1—C2—C3	178.61 (12)	C2—C1—C6—C5	1.10 (19)
C6—C1—C2—C3	-1.30 (19)	N7—C1—C6—C7	0.79 (19)
N7—C1—C2—N8	-0.50 (17)	C2—C1—C6—C7	-179.29 (12)
C6—C1—C2—N8	179.58 (12)	C5—C6—C7—C8	-179.68 (15)
Co1—N8—C2—C3	-178.54 (11)	C1—C6—C7—C8	0.7 (2)
Co1—N8—C2—C1	0.52 (15)	C6—C7—C8—C9	-1.3 (2)
C1—C2—C3—C4	0.6 (2)	C1—N7—C9—C8	1.2 (2)
N8—C2—C3—C4	179.60 (14)	Co1—N7—C9—C8	179.11 (11)
C2—C3—C4—C5	0.4 (3)	C7—C8—C9—N7	0.3 (2)

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N8—H8A \cdots N3 ⁱⁱⁱ	0.84 (3)	2.46 (3)	3.218 (2)	151 (2)
N8—H8B \cdots N4 ⁱⁱ	0.88 (3)	2.73 (3)	3.502 (3)	148 (2)

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