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ISSN 2414-3146

Poly[[μ_3-2-(benzotriazol-1-yl)acetato-$\kappa^3O:O':N^3$]-chlorido(ethanol-κO)cobalt(II)]

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Received 6 June 2024
Accepted 27 June 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

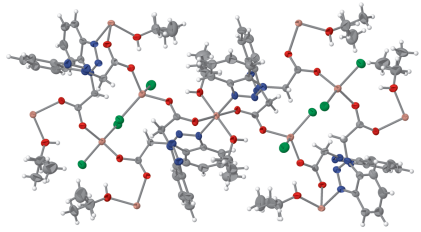
Keywords: 2-(benzotriazol-1-yl) acetic acid; cobalt; coordination polymers; crystal structure.

CCDC reference: 2366143

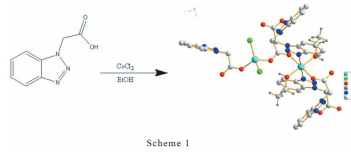
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]_n$, the Co^{II} atoms adopt octahedral *trans*-CoN_2O_4 and tetrahedral $CoCl_2O_2$ coordination geometries (site symmetries $\overline{1}$ and *m*, respectively). The bridging μ_3-*O*:*O*:*N* 2-(benzotriazol-1-yl)acetato ligands connect the octahedral cobalt nodes into (010) sheets and the $CoCl_2$ fragments link the sheets into a tri-periodic network. The structure displays O—H···O hydrogen bonding and the ethanol molecule is disordered over two orientations.

3D view



Chemical scheme



Scheme 1

Structure description

As a ligand with multiple coordination sites, benzotriazole is a good linker in the generation of metal–organic frameworks (MOFs) as it can bridge different metal cations to afford coordination polymers that exhibit structural diversity and facile accessibility of functionalized new magnetic materials (Bai *et al.*, 2008; Shao *et al.*, 2008; Müller-Buschbaum & Mokaddem, 2006). Functional groups such as carboxylate, hydroxy and pyridyl can be added to the benzotriazole core, increasing its coordination possibilities (Stoumpos *et al.*, 2008; Zhang *et al.*, 2007; Hu *et al.*, 2008; Hang & Ye, 2008). 1*H*-Benzotriazole-1-acetic acid (Hbtaa), a flexible ligand, containing a carboxylate group (when deprotonated) and a triazole unit has been used to construct MOFs (Zheng *et al.*, 2010; Zeng, 2013). As part of our work in this area, we now report the synthesis and crystal structure of the title coordination polymer, $[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]_n$, where $C_8H_6N_3O_2^-$ (L^-) is the 2-benzotriazol-1-yl)acetate anion.

Single-crystal structural analysis reveals that the asymmetric unit consists of two Co^{II} cations (one with site symmetry *m* and one with site symmetry $\overline{1}$), one L^- ligand, two chloride ions (both site symmetry *m*) and one disordered ethanol molecule (Fig. 1). Co1 is four-coordinated by two L^- ligands in O-monodentate mode and two μ^1-chloride ions in a tetrahedral coordination geometry, whereas Co2 is six-coordinated by four L^- ligands

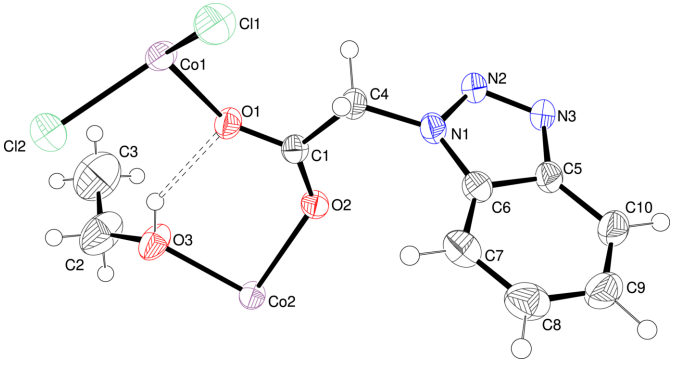


Figure 1
The asymmetric unit of the title compound showing 50% displacement ellipsoids. Only one orientation of the disordered ethanol molecule is shown.

(two in N-monodentate mode and two in O-monodentate mode) and two ethanol molecules. In the extended structure, the μ^3-*O*,*O*,*N* bridging L^- ligand links the Co2 nodes into (010) sheets (Fig. 2) and the $Co1Cl_2$ fragments link the sheets into a tri-periodic network (Fig. 3). An O—H···O hydrogen bond (Table 1) occurs.

Synthesis and crystallization

$CoCl_2$ (1.00 mmol) and 2-(benzotriazol-1-yl) acetic acid (1.00 mmol) were mixed in 10.0 ml of ethanol with stirring for about 30 min at room temperature. Blue block-shaped crystals of the title compound were collected by filtration in 40% yield. Analysis (%) calculated (Found) for $C_{10}H_{12}O_3N_3ClCo$: C, 37.94 (37.72); H, 3.82 (3.89); N, 13.27 (13.32).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.86 (1)	2.01 (2)	2.734 (3)	141 (2)

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]$
M_r	316.61
Crystal system, space group	Orthorhombic, *Pnma*
Temperature (K)	223
a, *b*, *c* (Å)	9.681 (2), 18.411 (4), 13.163 (3)
V (Å^3)	2346.1 (9)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	1.69
Crystal size (mm)	0.25 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.745, 0.859
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13580, 3058, 2337
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.672
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.120, 1.09
No. of reflections	3058
No. of parameters	184
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, −0.38

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXD1997* and *SHELXL* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

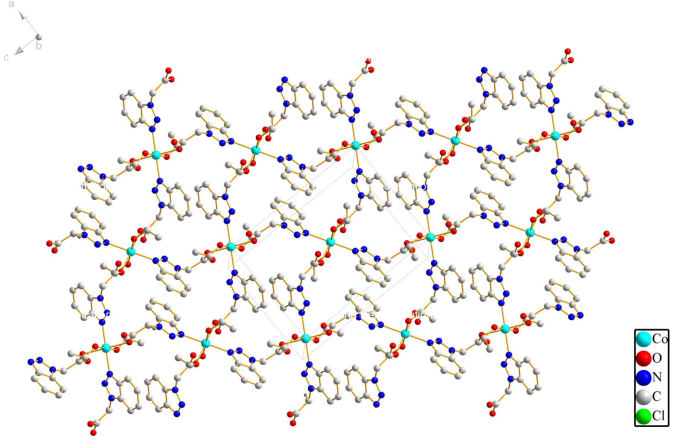


Figure 2
Part of a (010) sheet in the title compound.

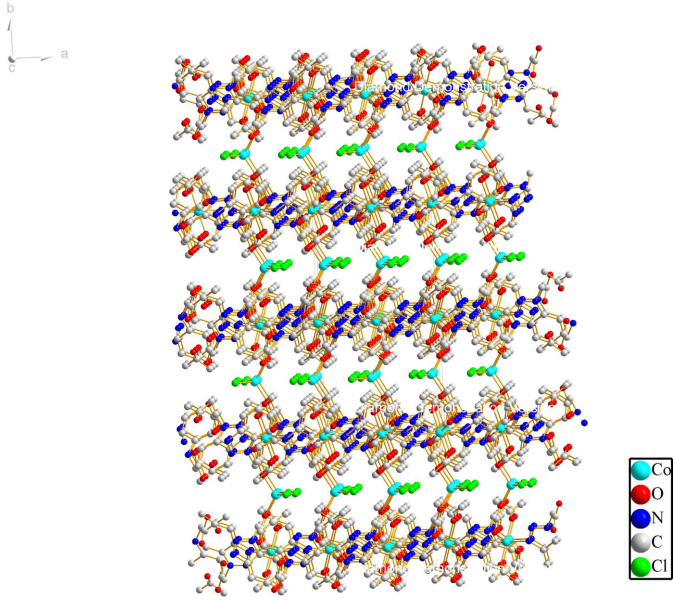


Figure 3
The three-dimensional network in the title compound.

Funding information

Funding for this research was provided by: the Program for Public Welfare Sciedtific Research Institute in Fujian Province (grant No. 2020R1022003); the Project for Youth Innovation Team in Fujian Academy of Agricultural Sciences (grant No. STIT 2021011-3); Collaborative innovation project in Fujian Province (grant No. XTCXGC2021020).

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full crystallographic data

IUCrData (2024). **9**, x240630 [https://doi.org/10.1107/S2414314624006308]

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Crystal data

$[Co(C_8H_6N_3O_2)Cl(C_2H_6O)]$
M_r = 316.61
Orthorhombic, *Pnma*
a = 9.681 (2) Å
b = 18.411 (4) Å
c = 13.163 (3) Å
V = 2346.1 (9) Å^3
Z = 8
$F(000)$ = 1288
D_x = 1.793 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 39979 reflections
θ = 2.6–27.6°
μ = 1.69 mm^{-1}
T = 223 K
Block, blue
0.25 × 0.15 × 0.09 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.745, T_{max} = 0.859
13580 measured reflections
3058 independent reflections
2337 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.5°, θ_{min} = 1.9°
h = −12→13
k = −23→24
l = −11→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.09
3058 reflections
184 parameters
3 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 2.3224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.43288 (6)	0.2500	0.34271 (4)	0.03019 (17)	

Co2	0.5000	0.5000	0.5000	0.02529 (16)	
Cl1	0.34331 (13)	0.2500	0.18726 (8)	0.0404 (3)	
Cl2	0.27129 (14)	0.2500	0.46492 (10)	0.0472 (3)	
O1	0.5318 (2)	0.33968 (11)	0.37700 (15)	0.0296 (4)	
O2	0.5907 (2)	0.45529 (11)	0.36795 (15)	0.0288 (4)	
O3	0.4442 (3)	0.40048 (12)	0.55516 (16)	0.0404 (6)	
H3	0.448 (4)	0.3656 (8)	0.5120 (12)	0.061*	
N1	0.6491 (2)	0.44636 (13)	0.16425 (17)	0.0279 (5)	
N2	0.7812 (3)	0.44389 (13)	0.13833 (18)	0.0303 (5)	
N3	0.8091 (3)	0.50073 (13)	0.08376 (18)	0.0296 (5)	
C1	0.5701 (3)	0.39542 (15)	0.3296 (2)	0.0245 (6)	
C2	0.4659 (6)	0.3692 (2)	0.6509 (3)	0.0657 (13)	
H2AA	0.4721	0.4093	0.6986	0.079*	0.507 (11)
H2AB	0.3817	0.3432	0.6674	0.079*	0.507 (11)
H2BC	0.5343	0.3314	0.6415	0.079*	0.493 (11)
H2BD	0.5090	0.4063	0.6925	0.079*	0.493 (11)
C3	0.5741 (13)	0.3227 (7)	0.6741 (10)	0.095 (4)	0.507 (11)
H3A	0.6599	0.3487	0.6695	0.143*	0.507 (11)
H3B	0.5747	0.2829	0.6270	0.143*	0.507 (11)
H3C	0.5626	0.3045	0.7419	0.143*	0.507 (11)
C4	0.5894 (3)	0.38538 (16)	0.2171 (2)	0.0303 (6)	
H4A	0.6480	0.3433	0.2062	0.036*	
H4B	0.5002	0.3748	0.1870	0.036*	
C5	0.6926 (3)	0.54205 (16)	0.0755 (2)	0.0297 (6)	
C6	0.5883 (3)	0.50689 (16)	0.1263 (2)	0.0303 (6)	
C7	0.4538 (3)	0.5326 (2)	0.1284 (3)	0.0388 (7)	
H7	0.3835	0.5079	0.1619	0.047*	
C8	0.4311 (4)	0.5955 (2)	0.0789 (3)	0.0464 (9)	
H8	0.3422	0.6146	0.0776	0.056*	
C9	0.5380 (4)	0.6334 (2)	0.0290 (3)	0.0446 (8)	
H9	0.5181	0.6775	−0.0022	0.053*	
C10	0.6678 (4)	0.60771 (17)	0.0254 (2)	0.0389 (7)	
H10	0.7376	0.6324	−0.0087	0.047*	
C3A	0.3657 (10)	0.3405 (5)	0.7065 (6)	0.061 (3)	0.493 (11)
H3AA	0.3169	0.3050	0.6670	0.092*	0.493 (11)
H3AB	0.3030	0.3781	0.7272	0.092*	0.493 (11)
H3AC	0.4047	0.3178	0.7655	0.092*	0.493 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0432 (4)	0.0220 (3)	0.0254 (3)	0.000	0.0007 (2)	0.000
Co2	0.0336 (3)	0.0231 (3)	0.0191 (3)	−0.0040 (2)	−0.0011 (2)	−0.0030 (2)
Cl1	0.0500 (7)	0.0401 (6)	0.0310 (6)	0.000	−0.0062 (5)	0.000
Cl2	0.0544 (7)	0.0450 (7)	0.0423 (6)	0.000	0.0154 (6)	0.000
O1	0.0409 (11)	0.0250 (10)	0.0230 (10)	−0.0056 (9)	0.0008 (9)	0.0008 (8)
O2	0.0389 (11)	0.0259 (10)	0.0217 (9)	−0.0043 (8)	0.0033 (8)	−0.0050 (8)
O3	0.0704 (16)	0.0263 (11)	0.0245 (11)	−0.0106 (11)	−0.0037 (11)	−0.0014 (9)

N1	0.0327 (12)	0.0291 (12)	0.0220 (11)	−0.0024 (10)	0.0040 (10)	0.0015 (9)
N2	0.0369 (13)	0.0287 (12)	0.0252 (12)	0.0001 (11)	0.0060 (10)	0.0035 (10)
N3	0.0351 (13)	0.0273 (12)	0.0265 (12)	−0.0005 (10)	0.0046 (11)	0.0059 (10)
C1	0.0249 (13)	0.0263 (14)	0.0223 (13)	0.0001 (11)	−0.0018 (11)	0.0015 (10)
C2	0.112 (4)	0.047 (2)	0.038 (2)	−0.001 (2)	−0.014 (2)	0.0075 (18)
C3	0.111 (10)	0.079 (8)	0.096 (9)	0.013 (7)	−0.004 (7)	0.027 (6)
C4	0.0430 (16)	0.0242 (13)	0.0238 (13)	−0.0065 (12)	0.0059 (12)	−0.0004 (11)
C5	0.0386 (16)	0.0295 (14)	0.0210 (13)	−0.0006 (12)	0.0021 (12)	0.0013 (11)
C6	0.0385 (15)	0.0307 (15)	0.0217 (13)	0.0012 (12)	0.0007 (12)	−0.0015 (11)
C7	0.0369 (16)	0.0463 (19)	0.0332 (17)	0.0021 (15)	0.0027 (14)	−0.0039 (15)
C8	0.047 (2)	0.054 (2)	0.0388 (19)	0.0146 (17)	−0.0046 (16)	−0.0047 (16)
C9	0.062 (2)	0.0367 (18)	0.0351 (18)	0.0117 (16)	−0.0053 (16)	0.0043 (15)
C10	0.055 (2)	0.0334 (16)	0.0281 (15)	0.0023 (15)	0.0004 (15)	0.0046 (13)
C3A	0.082 (6)	0.069 (6)	0.033 (4)	−0.019 (5)	0.003 (4)	0.007 (4)

Geometric parameters (Å, º)

Co1—Cl1	2.2223 (13)	C2—H2BC	0.9700
Co1—Cl2	2.2439 (14)	C2—H2BD	0.9700
Co1—O1^{i}	1.961 (2)	C2—C3	1.387 (12)
Co1—O1	1.961 (2)	C2—C3A	1.324 (9)
Co2—O2	2.114 (2)	C3—H3A	0.9600
Co2—O2^{ii}	2.114 (2)	C3—H3B	0.9600
Co2—O3^{ii}	2.043 (2)	C3—H3C	0.9600
Co2—O3	2.043 (2)	C4—H4A	0.9700
Co2—N3^{iii}	2.152 (3)	C4—H4B	0.9700
Co2—N3^{iv}	2.152 (3)	C5—C6	1.373 (4)
O1—C1	1.257 (3)	C5—C10	1.397 (4)
O2—C1	1.228 (3)	C6—C7	1.386 (5)
O3—H3	0.859 (9)	C7—H7	0.9300
O3—C2	1.401 (4)	C7—C8	1.347 (5)
N1—N2	1.324 (3)	C8—H8	0.9300
N1—C4	1.441 (4)	C8—C9	1.410 (5)
N1—C6	1.356 (4)	C9—H9	0.9300
N2—N3	1.298 (3)	C9—C10	1.344 (5)
N3—Co2^{v}	2.152 (2)	C10—H10	0.9300
N3—C5	1.365 (4)	C3A—H3AA	0.9600
C1—C4	1.505 (4)	C3A—H3AB	0.9600
C2—H2AA	0.9700	C3A—H3AC	0.9600
C2—H2AB	0.9700		

Cl1—Co1—Cl2	112.83 (6)	C3—C2—O3	124.4 (7)
O1—Co1—Cl1	113.73 (6)	C3—C2—H2AA	106.2
O1^{i}—Co1—Cl1	113.73 (6)	C3—C2—H2AB	106.2
O1—Co1—Cl2	100.10 (7)	C3A—C2—O3	123.4 (6)
O1^{i}—Co1—Cl2	100.10 (7)	C3A—C2—H2BC	106.5
O1—Co1—O1^{i}	114.66 (13)	C3A—C2—H2BD	106.5
O2^{ii}—Co2—O2	180.0	C2—C3—H3A	109.5

O2^{ii}—Co2—N3^{iii}	93.56 (9)	C2—C3—H3B	109.5
O2—Co2—N3^{iii}	86.44 (9)	C2—C3—H3C	109.5
O2^{ii}—Co2—N3^{iv}	86.44 (9)	H3A—C3—H3B	109.5
O2—Co2—N3^{iv}	93.56 (9)	H3A—C3—H3C	109.5
O3—Co2—O2	93.03 (8)	H3B—C3—H3C	109.5
O3^{ii}—Co2—O2^{ii}	93.03 (8)	N1—C4—C1	115.4 (2)
O3^{ii}—Co2—O2	86.97 (8)	N1—C4—H4A	108.4
O3—Co2—O2^{ii}	86.97 (8)	N1—C4—H4B	108.4
O3^{ii}—Co2—O3	180.0	C1—C4—H4A	108.4
O3—Co2—N3^{iii}	87.74 (10)	C1—C4—H4B	108.4
O3—Co2—N3^{iv}	92.26 (10)	H4A—C4—H4B	107.5
O3^{ii}—Co2—N3^{iii}	92.25 (10)	N3—C5—C6	107.8 (2)
O3^{ii}—Co2—N3^{iv}	87.75 (10)	N3—C5—C10	131.4 (3)
N3^{iii}—Co2—N3^{iv}	180.0	C6—C5—C10	120.8 (3)
C1—O1—Co1	135.83 (19)	N1—C6—C5	104.4 (3)
C1—O2—Co2	128.27 (18)	N1—C6—C7	133.0 (3)
Co2—O3—H3	115.0 (14)	C5—C6—C7	122.6 (3)
C2—O3—Co2	130.4 (2)	C6—C7—H7	122.0
C2—O3—H3	106.3 (14)	C8—C7—C6	115.9 (3)
N2—N1—C4	119.0 (2)	C8—C7—H7	122.0
N2—N1—C6	110.6 (2)	C7—C8—H8	119.0
C6—N1—C4	130.1 (3)	C7—C8—C9	122.1 (3)
N3—N2—N1	108.4 (2)	C9—C8—H8	119.0
N2—N3—Co2^{v}	117.20 (19)	C8—C9—H9	119.0
N2—N3—C5	108.8 (2)	C10—C9—C8	121.9 (3)
C5—N3—Co2^{v}	132.23 (19)	C10—C9—H9	119.0
O1—C1—C4	115.1 (2)	C5—C10—H10	121.7
O2—C1—O1	125.2 (3)	C9—C10—C5	116.6 (3)
O2—C1—C4	119.6 (2)	C9—C10—H10	121.7
O3—C2—H2AA	106.2	C2—C3A—H3AA	109.5
O3—C2—H2AB	106.2	C2—C3A—H3AB	109.5
O3—C2—H2BC	106.5	C2—C3A—H3AC	109.5
O3—C2—H2BD	106.5	H3AA—C3A—H3AB	109.5
H2AA—C2—H2AB	106.4	H3AA—C3A—H3AC	109.5
H2BC—C2—H2BD	106.5	H3AB—C3A—H3AC	109.5

Co1—O1—C1—O2	154.9 (2)	N2—N3—C5—C10	−179.9 (3)
Co1—O1—C1—C4	−24.5 (4)	N3—C5—C6—N1	1.1 (3)
Co2—O2—C1—O1	−27.3 (4)	N3—C5—C6—C7	−176.7 (3)
Co2—O2—C1—C4	152.1 (2)	N3—C5—C10—C9	177.7 (3)
Co2—O3—C2—C3	−96.0 (8)	C4—N1—N2—N3	174.0 (2)
Co2—O3—C2—C3A	127.9 (6)	C4—N1—C6—C5	−174.1 (3)
Co2^{v}—N3—C5—C6	162.5 (2)	C4—N1—C6—C7	3.3 (5)
Co2^{v}—N3—C5—C10	−16.0 (5)	C5—C6—C7—C8	−1.3 (5)
O1—C1—C4—N1	−172.8 (3)	C6—N1—N2—N3	−0.5 (3)
O2—C1—C4—N1	7.8 (4)	C6—N1—C4—C1	−84.3 (4)
N1—N2—N3—Co2^{v}	−165.54 (18)	C6—C5—C10—C9	−0.7 (5)
N1—N2—N3—C5	1.1 (3)	C6—C7—C8—C9	−0.8 (5)

N1—C6—C7—C8	−178.3 (3)	C7—C8—C9—C10	2.1 (6)
N2—N1—C4—C1	102.4 (3)	C8—C9—C10—C5	−1.3 (5)
N2—N1—C6—C5	−0.4 (3)	C10—C5—C6—N1	179.8 (3)
N2—N1—C6—C7	177.0 (3)	C10—C5—C6—C7	2.0 (5)
N2—N3—C5—C6	−1.4 (3)		

Symmetry codes: (i) x, $-y+1/2$, z; (ii) $-x+1$, $-y+1$, $-z+1$; (iii) $x-1/2$, y, $-z+1/2$; (iv) $-x+3/2$, $-y+1$, $z+1/2$; (v) $-x+3/2$, $-y+1$, $z-1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.86 (1)	2.01 (2)	2.734 (3)	141 (2)