Acta Crystallographica Section E
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Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Poly[diaquadi-μ_3-malonato-μ-pyrazine-dinickel(II)]	Liu *et al.* (2005)	10.1107/S1600536805026358	GATWAA
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Liu *et al.* (2006)	10.1107/S1600536806038141	FONCUH03
Poly[[[μ_4-4,4′-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)-dipalladium(II)] dihydrate]	Li, Wang, Zhang & Yu (2007*e*)	10.1107/S1600536807039050	AFELAZ
Poly[diaqua-μ_3-malonato-μ-pyrazine-diiron(II)]	Li, Liu *et al.* (2007)	10.1107/S1600536807038743	AFELON
Poly[diaqua-di-μ_3-malonato-μ-pyrazine-dimanganese(II)]	Li, Wang, Zhang & Yu (2007*f*)	10.1107/S1600536807039773	VIJZAQ
Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*g*)	10.1107/S1600536807040275	VIKCIC
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Li, Wang, Zhang & Yu (2007*a*)	10.1107/S1600536807041657	DILGEL
catena-Poly[[(2,2′-bipyridine-κ^2N,N')iron(II)]-μ-5-carboxy-4-carboxylatoimidazol-1-ido-$\kappa^4N^3,O^4:N^1,O^5$]	Li, Wang, Zhang & Yu (2007*h*)	10.1107/S1600536807042122	XIKWAQ
Poly[[aqua(2,2′-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*b*)	10.1107/S1600536807046466	LEVZAO01
2-(Benzyliminomethyl)-6-methoxyphenol	Li, Wang, Zhang & Yu (2007*i*)	10.1107/S1600536807042134	SILDEX
Poly[aqua(2,2′-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]	Li, Wang, Zhang & Yu (2007*c*)	10.1107/S1600536807047575	SILXAN
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]iron(III)} bis(hexafluoridophosphate)	Liu, Dou, Li & Zhang (2007)	10.1107/S1600536807049665	TINRIS
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-manganese(III))	Liu, Dou, Niu & Zhang (2007*a*)	10.1107/S1600536807051008	GIMZAE
Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate	Li, Wang, Zhang & Yu (2007*d*)	10.1107/S1600536807048556	WIMZIC
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-chromium(III))	Liu, Dou, Niu & Zhang (2007*b*)	10.1107/S1600536807057996	HIQFIX
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluorido-phosphate)	Li, Wang *et al.* (2008)	10.1107/S1600536807061296	MIRNAD
μ-Oxido-bis({4,4′-dibromo-2,2′-ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-iron(III))	Meng *et al.* (2008*a*)	10.1107/S1600536807063143	MIRWUG
catena-Poly[[bis(1H-benzimidazole-κN^3)palladium(II)]-μ-benzene-1,4-dicarboxylato-$\kappa^2O^1:O^4$]	Meng *et al.* (2008*b*)	10.1107/S1600536807065051	XISCAE
Oxalatobis(propane-1,3-diamine)manganese(II) chloride monohydrate	Meng *et al.* (2008*e*)	10.1107/S1600536807065361	SISWIB
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluorido-phosphate)	Meng *et al.* (2008*c*)	10.1107/S1600536807066512	RISRIV
Bis[N-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganese(III) perchlorate monohydrate	Meng *et al.* (2008*d*)	10.1107/S1600536808000287	GISLEA
Diaquabis(pyridine-2-carboxylato-κ^2N,O)cobalt(II)	Huang (2008)	10.1107/S1600536808010507	WIZPOL
Tetra-μ-2,5-difluorobenzoato-bis[(2,2′-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]	Li, Zhang *et al.* (2008)	10.1107/S1600536808023507	BOFQIX
catena-Poly[[(2,2′-bipyridine-κ^2N,N')nickel(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]	Li, Yan *et al.* (2008)	10.1107/S1600536808028389	NOHYUF
catena-Poly[[aqua(2,2′-bipyridyl)cobalt(II)]-μ-5-nitroisophthlalato]	Liu *et al.* (2008)	10.1107/S1600536808038178	AFIREN
Diaquabis(pyridine-2-carboxylato-κ^2N,O)iron(II)	Xia & Sun (2009)	10.1107/S1600536809005765	RONFEG
catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]	Li *et al.* (2009)	10.1107/S1600536809008836	NOQNIR
1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one	Liu *et al.* (2009)	10.1107/S1600536809040227	PUGLOT

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catena-Poly[[aqua(2,2′-bipyridyl)-cobalt(II)]-μ-5-nitroisophthalato]

Ying Liu,* Qingpeng He, Xianxi Zhang, Zechun Xue and Chunyan Lv

College of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China
Correspondence e-mail: yllctu@yahoo.com.cn

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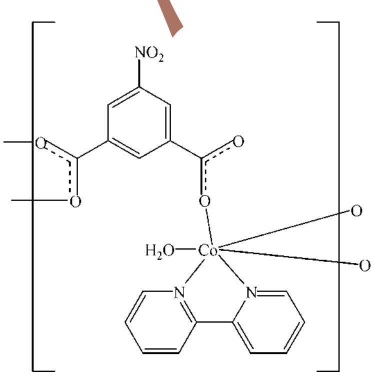
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.106; data-to-parameter ratio = 12.5.

Article retracted

In the crystal structure of the title compound, $[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]_n$, there are two symmetry-independent one-dimensional coordination polymers, which are approximately related by noncrystallographic inversion symmetry. Each zigzag chain is constructed from one Co^{II} ion, one *O*-monodentate 5-nitroisophthalate (ndc) dianion, one *N*,*N*′-bidentate 2,2′-bipyridyl ligand and one water molecule. A symmetry-generated *O*,*O*′-bidentate ndc dianion completes the cobalt coordination environment, which could be described as very distorted cis-CoN_2O_4 octahedral. The bridging ndc ligands result in parallel chains running along the *a* direction, and O—H···O hydrogen bonds arising from the water molecules complete the structure.

Related literature

For uses of carboxylic acids in materials science, see: Church & Halvorson (1959); and in biological systems, see: Okabe & Oya (2000).



Experimental

Crystal data

$[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]$
M_r = 442.24
Monoclinic, $P2_1/n$
a = 10.0125 (10) Å
b = 23.575 (2) Å
c = 15.403 (2) Å
β = 97.28 (1)°
V = 3606.3 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 (2) K
0.43 × 0.28 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.673, T_{max} = 0.825
18893 measured reflections
6672 independent reflections
5103 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 1.01
6672 reflections
535 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N2	2.065 (2)	Co2—N3	2.073 (2)
Co1—N1	2.075 (2)	Co2—N4	2.078 (3)
Co1—O2	2.0369 (19)	Co2—O12	2.031 (2)
Co1—O1*W*	2.102 (2)	Co2—O2*W*	2.089 (2)
Co1—O5^{i}	2.131 (2)	Co2—O10^{ii}	2.116 (2)
Co1—O6^{i}	2.257 (2)	Co2—O9^{ii}	2.294 (2)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O12^{i}	0.830 (10)	2.01 (2)	2.771 (3)	153 (3)
O2*W*—H4*W*···O2^{ii}	0.831 (10)	1.957 (17)	2.747 (3)	159 (3)
O1*W*—H2*W*···O9	0.830 (10)	2.05 (2)	2.763 (3)	143 (3)
O2*W*—H3*W*···O6	0.835 (10)	2.10 (3)	2.781 (3)	138 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2844).

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Article retracted

supporting information

Acta Cryst. (2008). E**64**, m1605–m1606 [doi:10.1107/S1600536808038178]

catena-Poly[[aqua(2,2′-bipyridyl)cobalt(II)]-μ-5-nitroisophthalato]

Ying Liu, Qingpeng He, Xianxi Zhang, Zechun Xue and Chunyan Lv

S1. Comment

In recent years, carboxylic acids have been widely used as polydentate ligands, which can coordinate to transition or rare earth ions yielding complexes with interesting properties that are useful in materials science (Church & Halvorson, 1959) and in biological systems (Okabe & Oya, 2000). The importance of transition metal dicarboxylate complexes motivated us to pursue synthetic strategies for these compounds, using 5-nitroisophthalic acid as a polydentate ligand. Here we report the synthesis and X-ray crystal structure analysis of the title compound, (I), (Fig. 1).

Compound (I) is constructed from two zigzag chains, each containing one Co^{II} atom, one O-monodentate 5-nitro-isophthalato (ndc) dianion, one N,N-bidentate 2,2′-bipyridyl ligand and one water molecule. A symmetry-generated, O,O-bidentate ndc dianion completes the cobalt coordination, which could be described as very distorted cis-CoN_2O_4 octahedral (Table 1). The bridging ndc ligands result in parallel chains running along the a direction (Fig. 2) and O—H···O hydrogen bonds arising from the water molecules (Table 2) complete the structure (Fig. 3).

S2. Experimental

A mixture of cobalt dichloride (0.5 mmol), 2,2′-bipyridine (0.5 mmol), and 5-nitroisophthalic acid (0.5 mmol) in H_2O (8 ml) and ethanol (8 ml) sealed in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for three days. Red blocks of (I) were obtained after cooling to room temperature with a yield of 27%. Anal. Calc. for $C_{18}H_{13}CoN_3O_7$: C 48.34, H 2.91, N 10.74%; Found: C 48.30, H 2.84, N 10.69%.

S3. Refinement

The H atoms of the water molecules were located from difference density maps and were refined with distance restraints of H···H = 1.38 (2) Å, O—H = 0.88 (2) Å, and with a fixed U_{iso} of 0.80 Å^2. All other H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Article retracted

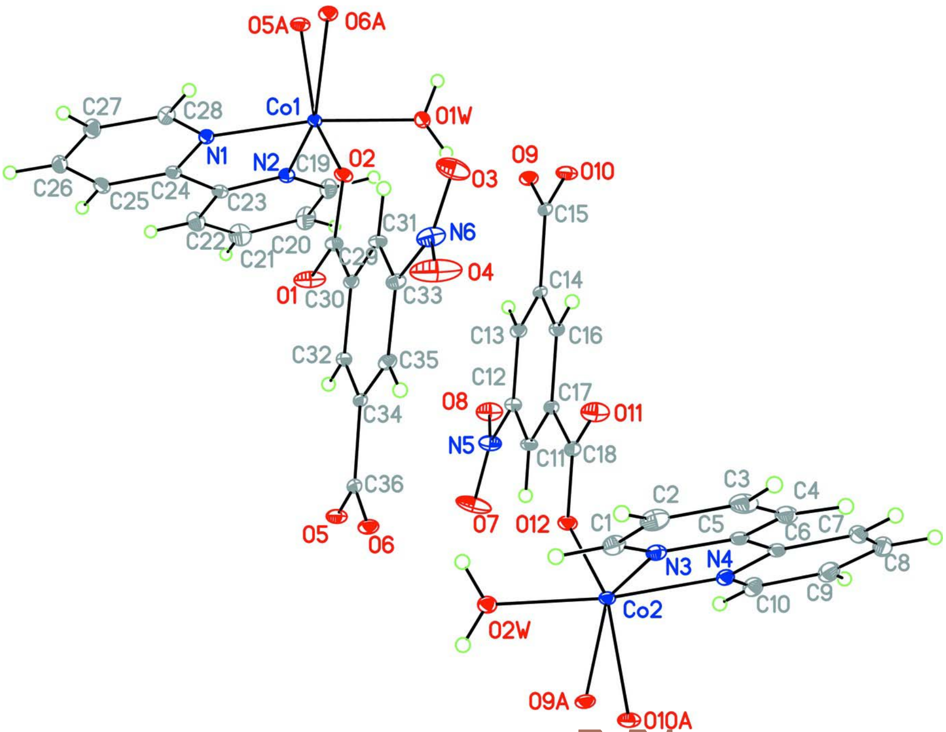

Figure 1

The asymmetric unit of (I), extended to show the Co coordination spheres, showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry codes: O5A, O6A; A = (1+x, y, z), O9A, O10A, A = (x-1, y, z).

Article retr

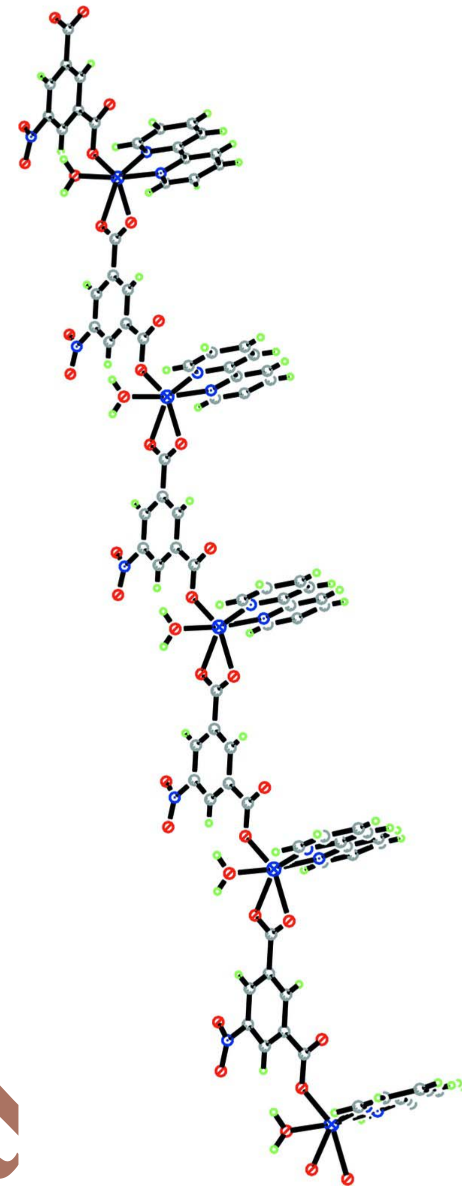

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Figure 2

Part of a one-dimensional polymeric chain in (I)

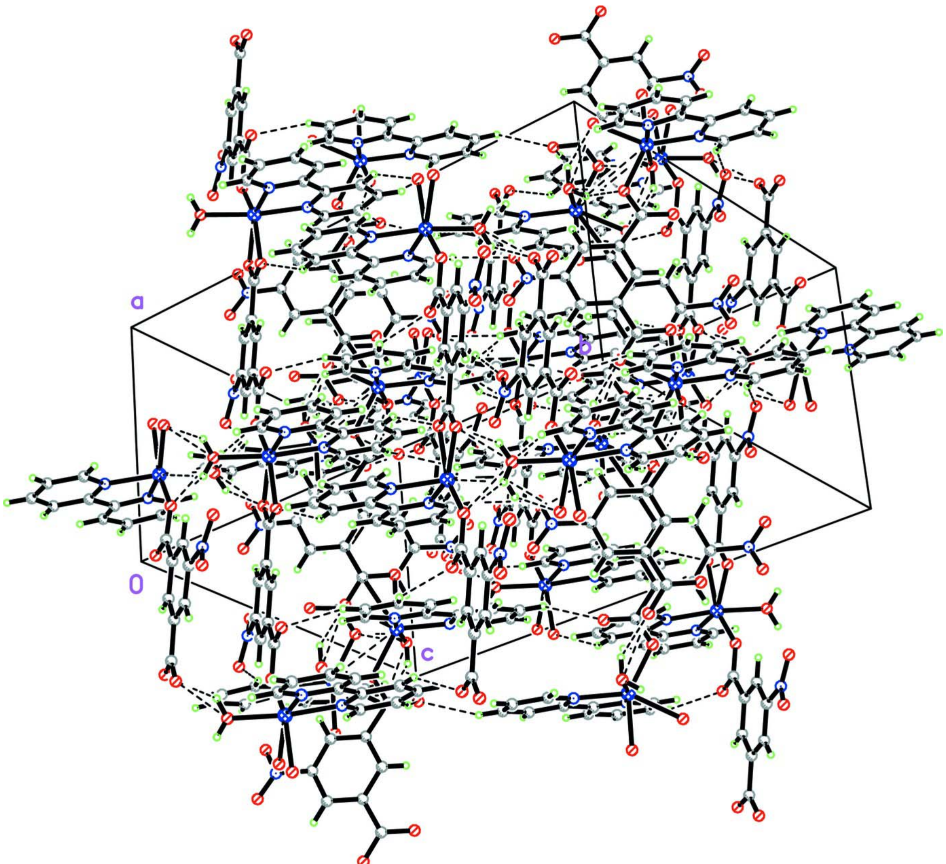

Figure 3

The packing diagram of (I) formed with the hydrogen bonds.

Article re

***catena*-Poly[[aqua(2,2′-bipyridyl)cobalt(II)]-*μ*-5-nitroisophthalato]**

Crystal data

$[Co(C_8H_3NO_6)(C_{10}H_8N_2)(H_2O)]$
$M_r = 442.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.0125$ (10) Å
$b = 23.575$ (2) Å
$c = 15.403$ (2) Å
$\beta = 97.28$ (1)°
$V = 3606.3$ (7) Å^3
$Z = 8$
$F(000) = 1800$
$D_x = 1.629$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6672 reflections
$\theta = 1.7$–25.5°
$\mu = 1.00$ mm^{-1}
$T = 293$ K
Block, red
0.43 × 0.28 × 0.20 mm

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)
$T_{min} = 0.673$, $T_{max} = 0.825$
18893 measured reflections
6672 independent reflections
5103 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.7°$
$h = -12 \rightarrow 10$
$k = -28 \rightarrow 22$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.106$
$S = 1.01$
6672 reflections
535 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 2.8058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.032$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ 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.

Article retracted

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

	x	y	z	U_{iso}*/U_{eq}
Co1	1.16169 (4)	0.154445 (14)	0.85573 (2)	0.02466 (11)
Co2	0.12374 (4)	0.354444 (15)	0.93350 (3)	0.02797 (12)
C1	0.0858 (3)	0.43912 (15)	0.7845 (2)	0.0469 (8)
H1	0.0715	0.4073	0.7489	0.056*
C2	0.0708 (4)	0.49272 (17)	0.7466 (3)	0.0555 (10)
H2	0.0482	0.4963	0.6864	0.067*
C3	0.0893 (4)	0.54031 (16)	0.7979 (3)	0.0570 (10)
H3	0.0810	0.5763	0.7731	0.068*
C4	0.1204 (3)	0.53368 (14)	0.8864 (3)	0.0474 (9)
H4	0.1307	0.5651	0.9231	0.057*
C5	0.1365 (3)	0.47893 (12)	0.9205 (2)	0.0363 (7)
C6	0.1704 (3)	0.46688 (12)	1.0143 (2)	0.0361 (7)
C7	0.1997 (3)	0.50925 (14)	1.0774 (3)	0.0490 (9)
H7	0.1978	0.5474	1.0616	0.059*
C8	0.2313 (3)	0.49307 (17)	1.1631 (3)	0.0557 (10)
H8	0.2506	0.5203	1.2067	0.067*
C9	0.2341 (4)	0.43613 (17)	1.1843 (3)	0.0559 (10)
H9	0.2569	0.4248	1.2421	0.067*
C10	0.2034 (3)	0.39623 (15)	1.1200 (2)	0.0468 (8)
H10	0.2049	0.3580	1.1351	0.056*
C11	0.5280 (3)	0.24937 (12)	1.02748 (19)	0.0320 (6)
H11	0.4449	0.2352	1.0380	0.038*
C12	0.6449 (3)	0.22104 (12)	1.05893 (19)	0.0321 (6)
C13	0.7703 (3)	0.24074 (12)	1.04616 (19)	0.0327 (7)

H13	0.8479	0.2213	1.0685	0.039*
C14	0.7776 (3)	0.29080 (11)	0.99863 (18)	0.0271 (6)
C15	0.9110 (3)	0.31378 (12)	0.9803 (2)	0.0312 (6)
C16	0.6606 (3)	0.31947 (12)	0.96577 (18)	0.0286 (6)
H16	0.6666	0.3527	0.9339	0.034*
C17	0.5354 (3)	0.29914 (12)	0.98002 (18)	0.0288 (6)
C18	0.4121 (3)	0.33266 (13)	0.9446 (2)	0.0325 (7)
C19	1.1953 (4)	0.07221 (15)	1.0079 (2)	0.0512 (9)
H19	1.2137	0.1044	1.0424	0.061*
C20	1.2036 (5)	0.01944 (18)	1.0474 (3)	0.0684 (12)
H20	1.2268	0.0164	1.1076	0.082*
C21	1.1774 (5)	−0.02879 (17)	0.9971 (3)	0.0688 (12)
H21	1.1813	−0.0645	1.0230	0.083*
C22	1.1455 (4)	−0.02303 (14)	0.9087 (2)	0.0526 (9)
H22	1.1289	−0.0547	0.8731	0.063*
C23	1.1386 (3)	0.03108 (12)	0.8732 (2)	0.0327 (7)
C24	1.1073 (3)	0.04138 (12)	0.7783 (2)	0.0314 (6)
C25	1.0794 (3)	−0.00192 (13)	0.7180 (2)	0.0411 (8)
H25	1.0787	−0.0396	0.7357	0.049*
C26	1.0526 (3)	0.01263 (15)	0.6307 (2)	0.0456 (8)
H26	1.0329	−0.0152	0.5883	0.055*
C27	1.0556 (3)	0.06936 (15)	0.6071 (2)	0.0459 (8)
H27	1.0365	0.0798	0.5486	0.055*
C28	1.0866 (3)	0.11017 (13)	0.6701 (2)	0.0381 (7)
H28	1.0889	0.1480	0.6532	0.046*
C29	0.8750 (3)	0.17566 (13)	0.8380 (2)	0.0336 (7)
C30	0.7500 (3)	0.20949 (12)	0.80607 (18)	0.0274 (6)
C31	0.7569 (3)	0.26263 (12)	0.76643 (19)	0.0314 (6)
H31	0.8396	0.2780	0.7575	0.038*
C32	0.6258 (3)	0.18764 (12)	0.81981 (19)	0.0297 (6)
H32	0.6210	0.1529	0.8477	0.036*
C33	0.6392 (3)	0.29172 (12)	0.7409 (2)	0.0347 (7)
C34	0.5084 (3)	0.21757 (12)	0.79203 (18)	0.0273 (6)
C35	0.5143 (3)	0.27061 (13)	0.75206 (19)	0.0332 (7)
H35	0.4363	0.2910	0.7336	0.040*
C36	0.3756 (3)	0.19401 (13)	0.8104 (2)	0.0331 (7)
H1W	1.243 (3)	0.2304 (11)	0.958 (3)	0.080*
H2W	1.126 (2)	0.2153 (14)	0.989 (3)	0.080*
H3W	0.164 (2)	0.2956 (15)	0.803 (3)	0.080*
H4W	0.042 (3)	0.2778 (10)	0.823 (3)	0.080*
N1	1.1134 (2)	0.09709 (10)	0.75443 (15)	0.0302 (5)
N2	1.1617 (3)	0.07823 (10)	0.92182 (16)	0.0349 (6)
N3	0.1199 (2)	0.43207 (10)	0.87001 (17)	0.0349 (6)
N4	0.1713 (2)	0.41090 (10)	1.03641 (17)	0.0361 (6)
N5	0.6352 (3)	0.16753 (12)	1.10790 (19)	0.0477 (7)
N6	0.6479 (3)	0.34937 (13)	0.7036 (2)	0.0578 (9)
O1	0.8634 (2)	0.12806 (12)	0.8691 (2)	0.0705 (9)
O2	0.98644 (19)	0.19824 (8)	0.82627 (15)	0.0379 (5)

Article retracted

O3	0.7556 (3)	0.37273 (12)	0.7088 (2)	0.0801 (10)
O4	0.5459 (3)	0.37066 (17)	0.6681 (3)	0.1342 (19)
O5	0.3733 (2)	0.14822 (9)	0.85254 (16)	0.0440 (6)
O6	0.26919 (19)	0.22039 (9)	0.78407 (15)	0.0422 (5)
O7	0.5264 (3)	0.14506 (14)	1.1063 (2)	0.0932 (12)
O8	0.7366 (3)	0.14819 (11)	1.14856 (19)	0.0642 (8)
O9	1.0167 (2)	0.28717 (9)	1.00726 (15)	0.0411 (5)
O10	0.9137 (2)	0.35927 (9)	0.93795 (16)	0.0442 (6)
O11	0.4241 (2)	0.37689 (11)	0.90426 (18)	0.0586 (7)
O12	0.30031 (19)	0.31194 (9)	0.96161 (15)	0.0409 (5)
O1W	1.1948 (2)	0.20370 (8)	0.97017 (15)	0.0371 (5)
O2W	0.0917 (2)	0.30554 (8)	0.81966 (16)	0.0374 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01864 (19)	0.02268 (19)	0.0325 (2)	0.00142 (14)	0.00270 (15)	0.00151 (15)
Co2	0.01822 (19)	0.0237 (2)	0.0425 (2)	0.00121 (14)	0.00602 (16)	0.00113 (16)
C1	0.0428 (19)	0.048 (2)	0.052 (2)	0.0030 (15)	0.0148 (16)	0.0066 (16)
C2	0.046 (2)	0.065 (3)	0.057 (2)	0.0082 (18)	0.0139 (18)	0.024 (2)
C3	0.043 (2)	0.042 (2)	0.090 (3)	0.0027 (16)	0.020 (2)	0.026 (2)
C4	0.0326 (18)	0.0322 (17)	0.080 (3)	0.0017 (14)	0.0173 (17)	0.0057 (17)
C5	0.0193 (14)	0.0299 (15)	0.062 (2)	−0.0004 (12)	0.0141 (14)	0.0001 (14)
C6	0.0188 (14)	0.0342 (16)	0.057 (2)	−0.0007 (12)	0.0101 (13)	−0.0045 (14)
C7	0.0352 (18)	0.0352 (18)	0.078 (3)	−0.0024 (14)	0.0127 (18)	−0.0098 (17)
C8	0.038 (2)	0.067 (3)	0.062 (3)	−0.0018 (17)	0.0042 (18)	−0.022 (2)
C9	0.043 (2)	0.073 (3)	0.052 (2)	0.0057 (18)	0.0078 (17)	−0.0072 (19)
C10	0.0398 (19)	0.051 (2)	0.050 (2)	0.0067 (16)	0.0065 (16)	0.0001 (17)
C11	0.0204 (14)	0.0411 (16)	0.0348 (17)	−0.0058 (12)	0.0051 (12)	0.0010 (13)
C12	0.0267 (15)	0.0373 (16)	0.0323 (16)	−0.0020 (12)	0.0039 (12)	0.0048 (12)
C13	0.0210 (14)	0.0419 (17)	0.0347 (17)	0.0023 (12)	0.0012 (12)	0.0005 (13)
C14	0.0194 (14)	0.0317 (14)	0.0313 (15)	−0.0005 (11)	0.0069 (11)	−0.0043 (12)
C15	0.0185 (14)	0.0359 (16)	0.0403 (17)	0.0013 (12)	0.0077 (12)	−0.0087 (13)
C16	0.0228 (14)	0.0299 (14)	0.0336 (16)	−0.0011 (11)	0.0054 (12)	−0.0007 (12)
C17	0.0194 (14)	0.0358 (16)	0.0310 (16)	0.0001 (11)	0.0023 (11)	−0.0047 (12)
C18	0.0209 (15)	0.0387 (17)	0.0373 (17)	0.0023 (12)	0.0010 (12)	−0.0054 (13)
C19	0.070 (3)	0.048 (2)	0.0355 (19)	0.0013 (18)	0.0076 (17)	0.0048 (15)
C20	0.102 (4)	0.065 (3)	0.038 (2)	0.005 (2)	0.009 (2)	0.0146 (19)
C21	0.096 (3)	0.046 (2)	0.063 (3)	0.002 (2)	0.008 (2)	0.030 (2)
C22	0.068 (3)	0.0338 (18)	0.056 (2)	−0.0038 (17)	0.0053 (19)	0.0100 (16)
C23	0.0258 (15)	0.0308 (15)	0.0415 (18)	−0.0007 (12)	0.0043 (12)	0.0044 (13)
C24	0.0230 (14)	0.0304 (15)	0.0408 (17)	−0.0015 (12)	0.0042 (12)	0.0016 (13)
C25	0.0343 (17)	0.0329 (16)	0.056 (2)	−0.0028 (13)	0.0052 (15)	−0.0044 (15)
C26	0.0389 (19)	0.051 (2)	0.046 (2)	−0.0031 (15)	0.0035 (15)	−0.0147 (16)
C27	0.045 (2)	0.055 (2)	0.0367 (18)	0.0019 (16)	−0.0003 (15)	−0.0041 (15)
C28	0.0405 (18)	0.0378 (17)	0.0353 (17)	0.0061 (14)	0.0027 (14)	0.0054 (13)
C29	0.0221 (15)	0.0413 (17)	0.0369 (17)	0.0018 (13)	0.0017 (12)	0.0045 (13)
C30	0.0185 (14)	0.0351 (15)	0.0285 (15)	0.0014 (11)	0.0021 (11)	−0.0006 (12)

Article retracted

C31	0.0192 (14)	0.0402 (16)	0.0351 (16)	−0.0014 (12)	0.0045 (12)	0.0051 (13)
C32	0.0256 (15)	0.0311 (15)	0.0328 (15)	−0.0014 (12)	0.0060 (12)	−0.0004 (12)
C33	0.0303 (16)	0.0368 (16)	0.0379 (17)	0.0033 (13)	0.0078 (13)	0.0108 (13)
C34	0.0193 (13)	0.0346 (15)	0.0284 (15)	−0.0007 (11)	0.0047 (11)	−0.0063 (12)
C35	0.0215 (14)	0.0439 (17)	0.0340 (16)	0.0086 (12)	0.0030 (12)	0.0023 (13)
C36	0.0240 (15)	0.0401 (17)	0.0361 (17)	−0.0022 (13)	0.0070 (12)	−0.0110 (13)
N1	0.0251 (12)	0.0298 (12)	0.0358 (14)	0.0034 (10)	0.0039 (10)	0.0004 (10)
N2	0.0335 (14)	0.0349 (14)	0.0369 (15)	−0.0008 (11)	0.0067 (11)	0.0042 (11)
N3	0.0247 (13)	0.0352 (14)	0.0458 (17)	0.0018 (10)	0.0085 (11)	0.0055 (11)
N4	0.0264 (13)	0.0343 (14)	0.0483 (16)	0.0041 (10)	0.0079 (11)	−0.0007 (11)
N5	0.0348 (16)	0.0546 (17)	0.0532 (18)	−0.0040 (14)	0.0034 (13)	0.0203 (14)
N6	0.0458 (19)	0.0573 (19)	0.073 (2)	0.0145 (16)	0.0191 (16)	0.0331 (16)
O1	0.0359 (14)	0.0722 (18)	0.105 (2)	0.0136 (13)	0.0152 (14)	0.0578 (17)
O2	0.0161 (10)	0.0346 (11)	0.0623 (14)	0.0004 (8)	0.0022 (9)	−0.0024 (10)
O3	0.065 (2)	0.0644 (18)	0.108 (2)	−0.0176 (15)	−0.0012 (17)	0.0410 (17)
O4	0.0504 (19)	0.129 (3)	0.228 (5)	0.039 (2)	0.036 (2)	0.134 (3)
O5	0.0274 (12)	0.0441 (13)	0.0621 (15)	−0.0034 (9)	0.0117 (10)	0.0051 (11)
O6	0.0187 (10)	0.0491 (13)	0.0594 (15)	0.0039 (9)	0.0073 (10)	−0.0021 (11)
O7	0.0504 (18)	0.100 (2)	0.123 (3)	−0.0321 (16)	−0.0136 (18)	0.068 (2)
O8	0.0439 (15)	0.0619 (17)	0.087 (2)	0.0111 (12)	0.0070 (14)	0.0357 (14)
O9	0.0185 (10)	0.0453 (12)	0.0603 (14)	0.0035 (9)	0.0079 (10)	−0.0007 (10)
O10	0.0276 (11)	0.0363 (12)	0.0711 (16)	−0.0028 (9)	0.0161 (11)	0.0094 (11)
O11	0.0374 (14)	0.0576 (16)	0.0799 (18)	0.0077 (11)	0.0040 (13)	0.0303 (14)
O12	0.0190 (10)	0.0378 (12)	0.0658 (15)	0.0009 (9)	0.0052 (10)	−0.0032 (10)
O1W	0.0303 (12)	0.0335 (11)	0.0465 (13)	0.0030 (9)	0.0009 (10)	−0.0036 (9)
O2W	0.0287 (11)	0.0335 (11)	0.0502 (13)	0.0025 (9)	0.0050 (10)	0.0004 (10)

Geometric parameters (Å, º)

Co1—N2	2.065 (2)	C19—C20	1.382 (5)
Co1—N1	2.075 (2)	C19—H19	0.9300
Co1—O2	2.0369 (19)	C20—C21	1.382 (6)
Co1—O1W	2.102 (2)	C20—H20	0.9300
Co1—O5^{i}	2.131 (2)	C21—C22	1.365 (5)
Co1—O6^{i}	2.257 (2)	C21—H21	0.9300
Co2—N3	2.073 (2)	C22—C23	1.386 (4)
Co2—N4	2.078 (3)	C22—H22	0.9300
Co2—O12	2.031 (2)	C23—N2	1.344 (4)
Co2—O2W	2.089 (2)	C23—C24	1.475 (4)
Co2—O10^{ii}	2.116 (2)	C24—N1	1.367 (4)
Co2—O9^{ii}	2.294 (2)	C24—C25	1.385 (4)
C1—N3	1.329 (4)	C25—C26	1.380 (5)
C1—C2	1.392 (5)	C25—H25	0.9300
C1—H1	0.9300	C26—C27	1.387 (5)
C2—C3	1.372 (6)	C26—H26	0.9300
C2—H2	0.9300	C27—C28	1.374 (4)
C3—C4	1.367 (6)	C27—H27	0.9300
C3—H3	0.9300	C28—N1	1.329 (4)

Article retracted

C4—C5	1.395 (4)	C28—H28	0.9300
C4—H4	0.9300	C29—O1	1.231 (4)
C5—N3	1.349 (4)	C29—O2	1.270 (3)
C5—C6	1.470 (5)	C29—C30	1.513 (4)
C6—N4	1.362 (4)	C30—C32	1.386 (4)
C6—C7	1.398 (5)	C30—C31	1.399 (4)
C7—C8	1.373 (5)	C31—C33	1.377 (4)
C7—H7	0.9300	C31—H31	0.9300
C8—C9	1.381 (5)	C32—C34	1.391 (4)
C8—H8	0.9300	C32—H32	0.9300
C9—C10	1.372 (5)	C33—C35	1.377 (4)
C9—H9	0.9300	C33—N6	1.482 (4)
C10—N4	1.332 (4)	C34—C35	1.398 (4)
C10—H10	0.9300	C34—C36	1.500 (4)
C11—C12	1.381 (4)	C35—H35	0.9300
C11—C17	1.389 (4)	C36—O6	1.256 (3)
C11—H11	0.9300	C36—O5	1.261 (4)
C12—C13	1.376 (4)	C36—Co1^{ii}	2.515 (3)
C12—N5	1.479 (4)	N5—O7	1.209 (4)
C13—C14	1.396 (4)	N5—O8	1.212 (3)
C13—H13	0.9300	N6—O3	1.204 (4)
C14—C16	1.390 (4)	N6—O4	1.205 (4)
C14—C15	1.501 (4)	O5—Co1^{ii}	2.131 (2)
C15—O9	1.255 (3)	O6—Co1^{ii}	2.257 (2)
C15—O10	1.257 (4)	O9—Co2^{i}	2.294 (2)
C16—C17	1.386 (4)	O10—Co2^{i}	2.116 (2)
C16—H16	0.9300	O1W—H1W	0.830 (10)
C17—C18	1.508 (4)	O1W—H2W	0.830 (10)
C18—O11	1.228 (4)	O2W—H3W	0.835 (10)
C18—O12	1.278 (3)	O2W—H4W	0.831 (10)
C19—N2	1.334 (4)		

O2—Co1—N2	119.80 (9)	C20—C19—H19	119.1
O2—Co1—N1	92.92 (9)	C19—C20—C21	119.9 (4)
N2—Co1—N1	77.83 (9)	C19—C20—H20	120.1
O2—Co1—O1W	86.94 (8)	C21—C20—H20	120.1
N2—Co1—O1W	94.42 (9)	C22—C21—C20	118.7 (3)
N1—Co1—O1W	171.00 (9)	C22—C21—H21	120.6
O2—Co1—O5^{i}	149.41 (9)	C20—C21—H21	120.6
N2—Co1—O5^{i}	90.78 (9)	C21—C22—C23	118.6 (3)
N1—Co1—O5^{i}	94.31 (9)	C21—C22—H22	120.7
O1W—Co1—O5^{i}	90.33 (9)	C23—C22—H22	120.7
O2—Co1—O6^{i}	89.58 (8)	N2—C23—C22	123.0 (3)
N2—Co1—O6^{i}	150.47 (9)	N2—C23—C24	114.6 (2)
N1—Co1—O6^{i}	99.27 (9)	C22—C23—C24	122.4 (3)
O1W—Co1—O6^{i}	89.73 (8)	N1—C24—C25	122.7 (3)
O5^{i}—Co1—O6^{i}	59.93 (8)	N1—C24—C23	114.4 (2)
O12—Co2—N3	119.99 (9)	C25—C24—C23	122.9 (3)

Article retracted

O12—Co2—N4	92.54 (9)
N3—Co2—N4	77.48 (10)
O12—Co2—O2W	86.76 (9)
N3—Co2—O2W	95.71 (9)
N4—Co2—O2W	171.71 (10)
O12—Co2—O10^{ii}	149.51 (9)
N3—Co2—O10^{ii}	90.50 (9)
N4—Co2—O10^{ii}	94.22 (9)
O2W—Co2—O10^{ii}	90.54 (9)
O12—Co2—O9^{ii}	90.11 (8)
N3—Co2—O9^{ii}	149.55 (8)
N4—Co2—O9^{ii}	98.13 (9)
O2W—Co2—O9^{ii}	90.14 (8)
O10^{ii}—Co2—O9^{ii}	59.50 (8)
N3—C1—C2	122.0 (4)
N3—C1—H1	119.0
C2—C1—H1	119.0
C3—C2—C1	120.1 (4)
C3—C2—H2	120.0
C1—C2—H2	120.0
C4—C3—C2	118.6 (3)
C4—C3—H3	120.7
C2—C3—H3	120.7
C3—C4—C5	118.8 (3)
C3—C4—H4	120.6
C5—C4—H4	120.6
N3—C5—C4	122.7 (3)
N3—C5—C6	113.9 (3)
C4—C5—C6	123.4 (3)
N4—C6—C7	121.6 (3)
N4—C6—C5	115.2 (3)
C7—C6—C5	123.2 (3)
C8—C7—C6	118.2 (3)
C8—C7—H7	120.9
C6—C7—H7	120.9
C7—C8—C9	119.5 (3)
C7—C8—H8	120.2
C9—C8—H8	120.3
C10—C9—C8	120.0 (4)
C10—C9—H9	120.0
C8—C9—H9	120.0
N4—C10—C9	121.6 (3)
N4—C10—H10	119.2
C9—C10—H10	119.2
C12—C11—C17	119.6 (3)
C12—C11—H11	120.2
C17—C11—H11	120.2
C13—C12—C11	122.3 (3)
C26—C25—C24	117.9 (3)
C26—C25—H25	121.0
C24—C25—H25	121.0
C25—C26—C27	119.2 (3)
C25—C26—H26	120.4
C27—C26—H26	120.4
C28—C27—C26	120.0 (3)
C28—C27—H27	120.0
C26—C27—H27	120.0
N1—C28—C27	121.8 (3)
N1—C28—H28	119.1
C27—C28—H28	119.1
O1—C29—O2	124.4 (3)
O1—C29—C30	119.5 (3)
O2—C29—C30	116.0 (3)
C32—C30—C31	119.6 (2)
C32—C30—C29	118.4 (3)
C31—C30—C29	121.9 (2)
C33—C31—C30	118.9 (3)
C33—C31—H31	120.6
C30—C31—H31	120.6
C30—C32—C34	120.3 (3)
C30—C32—H32	119.9
C34—C32—H32	119.9
C35—C33—C31	122.8 (3)
C35—C33—N6	118.6 (3)
C31—C33—N6	118.5 (3)
C32—C34—C35	120.5 (3)
C32—C34—C36	119.2 (3)
C35—C34—C36	120.2 (2)
C33—C35—C34	117.9 (3)
C33—C35—H35	121.0
C34—C35—H35	121.0
O6—C36—O5	121.3 (3)
O6—C36—C34	119.4 (3)
O5—C36—C34	119.3 (3)
O6—C36—Co1^{ii}	63.61 (16)
O5—C36—Co1^{ii}	57.85 (15)
C34—C36—Co1^{ii}	174.8 (2)
C28—N1—C24	118.4 (3)
C28—N1—Co1	125.6 (2)
C24—N1—Co1	115.95 (19)
C19—N2—C23	118.0 (3)
C19—N2—Co1	124.5 (2)
C23—N2—Co1	117.12 (19)
C1—N3—C5	117.8 (3)
C1—N3—Co2	124.4 (2)
C5—N3—Co2	117.2 (2)

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C13—C12—N5	118.7 (3)	C10—N4—C6	119.1 (3)
C11—C12—N5	119.0 (3)	C10—N4—Co2	125.1 (2)
C12—C13—C14	118.0 (3)	C6—N4—Co2	115.9 (2)
C12—C13—H13	121.0	O7—N5—O8	122.6 (3)
C14—C13—H13	121.0	O7—N5—C12	118.7 (3)
C16—C14—C13	120.3 (3)	O8—N5—C12	118.7 (3)
C16—C14—C15	119.0 (3)	O3—N6—O4	122.7 (3)
C13—C14—C15	120.7 (2)	O3—N6—C33	119.3 (3)
O9—C15—O10	121.7 (3)	O4—N6—C33	118.0 (3)
O9—C15—C14	119.4 (3)	C29—O2—Co1	120.23 (19)
O10—C15—C14	118.9 (2)	C36—O5—Co1^{ii}	92.08 (17)
C17—C16—C14	120.8 (3)	C36—O6—Co1^{ii}	86.49 (18)
C17—C16—H16	119.6	C15—O9—Co2^{i}	85.29 (18)
C14—C16—H16	119.6	C15—O10—Co2^{i}	93.31 (17)
C16—C17—C11	119.0 (3)	C18—O12—Co2	121.93 (19)
C16—C17—C18	118.5 (3)	Co1—O1W—H1W	105 (3)
C11—C17—C18	122.5 (3)	Co1—O1W—H2W	115 (3)
O11—C18—O12	124.9 (3)	H1W—O1W—H2W	111.4 (18)
O11—C18—C17	120.0 (3)	Co2—O2W—H3W	111 (3)
O12—C18—C17	115.1 (3)	Co2—O2W—H4W	114 (3)
N2—C19—C20	121.7 (3)	H3W—O2W—H4W	111.0 (17)
N2—C19—H19	119.1		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O12^{i}	0.83 (1)	2.01 (2)	2.771 (3)	153 (3)
O2*W*—H4*W*···O2^{ii}	0.83 (1)	1.96 (2)	2.747 (3)	159 (3)
O1*W*—H2*W*···O9	0.83 (1)	2.05 (2)	2.763 (3)	143 (3)
O2*W*—H3*W*···O6	0.84 (1)	2.10 (3)	2.781 (3)	138 (3)

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

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