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Tris(1,10-phenanthroline-κ^2N,N')cobalt(II) bis(2,4,5-tricarboxybenzoate) monohydrate

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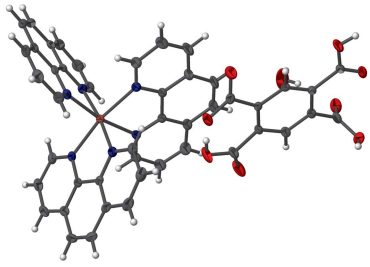
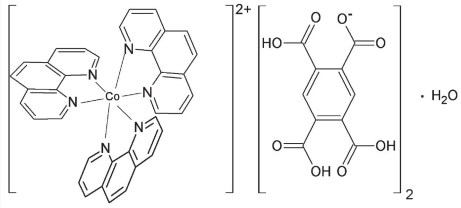
In the complex cation of the title salt, $[Co(C_{12}H_8N_2)_3](C_{10}H_5O_8)_2\cdot H_2O$, the Co^{II} cation is situated on a twofold rotation axis and is coordinated in a distorted octahedral manner by six N atoms from three chelating 1,10-phenanthroline (phen) ligands. In the crystal, the non-coordinating 2,4,5-tricarboxybenzoate anions interact with each other *via* O—H···O hydrogen bonds, generating a two-dimensional network parallel to (100). Adjacent sheets are connected by $_{water}O—H\cdots O_{carboxylate}$ hydrogen bonds, resulting in a three-dimensional network structure that surrounds the complex cations.

3D view



Chemical scheme



Structure description

Benzene-1,2,4,5-tetracarboxylic acid has been widely used to construct materials with metal–organic framework structures, because it not only possesses different coordination modes depending on the four carboxyl groups that can be completely or only partially deprotonated, but it can also act as a hydrogen-bond acceptor or donor. 1,10-Phenanthroline (phen) has also been well employed as a chelating ligand in coordination chemistry and in the assembly of metal–organic frameworks. Many cobalt complexes with benzene-1,2,4,5-tetracarboxylate acid and phen have been synthesized and reported, such as *catena*-[(μ_4-benzene-1,4-dicarboxylato-2,5-dicarboxylic acid)(μ_2-benzene-1,4-dicarboxylato-2,5-dicarboxylic acid)diaquabis(1,10-phenanthroline)dicobalt(II)] (Hu *et al.*, 2004), (μ_2-benzene-1,2,4,5-tetracarboxylato)hexaaquabis(1,10-phenanthroline)dicobalt(II) dihydrate (Qi *et al.*, 2005; Rogan *et al.*, 2006), (μ_2-benzene-1,2,4,5-tetracarboxylato)tetraaquabis(1,10-phenanthroline)dicobalt(II) (Shi *et al.*, 2009), triaqua(4,6-bis(methoxycarbonyl)isophthalato)(1,10-phenanthroline)cobalt(II) methanol solvate (Baruah *et al.*, 2007), (1,10-phenanthroline)triaqua(dihydrogen benzene-1,2,4,5-tetracarboxylato)cobalt(II) monohydrate (Bo *et al.*, 2007). However, reports of benzene-1,2,4,5-tetracarboxylate acting only as a counter-anion are rare, *e.g.* tris(1,10-phenan-

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.1159 (17)	Co1—N3	2.1412 (16)
Co1—N2	2.1251 (16)		
N1^{i}—Co1—N1	172.28 (9)	N1—Co1—N3	90.72 (6)
N1—Co1—N2^{i}	96.09 (6)	N1—Co1—N3^{i}	95.27 (6)
N1—Co1—N2	78.74 (6)		

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

throline)cobalt(II) 2,3,4-tricarboxybenzoate hemi(2,4-dicarboxybenzene-1,3-dicarboxylate) dimethylformamide solvate hexahydrate (Tao *et al.*, 2012) and bis[tetraaqua-(1,10-phenanthroline-*N*,*N*′)cobalt(II)] 1,2,4,5-benzenetetracarboxylate (Wang *et al.*, 2005). The title compound, tris(1,10-phenanthroline-κ^2N:*N*′)cobalt(II) bis(2,4,5-tricarboxybenzoate) monohydrate, was obtained unintentionally during an attempt to synthesize a mixed-ligand cobalt complex with multicarboxylate and phen ligands *via* a hydrothermal reaction.

The asymmetric unit of the title compound comprises one half of the complex $[Co(phen)_3]^{2+}$ cation, one benzene-1,2,4,5-tetracarboxylate anion and one half of a water molecule of crystallization (Fig. 1). The Co^{II} atom lies on a twofold rotation axis, which bisects the phen ligand containing atom N3; the water molecule of crystallization lies on the same rotation axis. In the complex cation, the Co^{II} atom is coordinated in a distorted octahedral manner by six N atoms from three chelating 1,10-phenanthroline (phen) ligands (Table 1). The N1—Co—N1^{i} [symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$] angle is nearly linear [172.28 (9) Å]. The *cis* bond angles around the Co^{II} atom range from 78.74 (6)–96.09 (6) Å. The planes of adjacent phen groups N1/N2/C1–C12 and N3/N3^{i}/C13–C18/C13^{i}–C18^{i} and the symmetry-related counterpart of N1/N2/C1–C12 make dihedral angles of 85.27 (5) and 71.71 (4)°, respectively. In the 2,4,5-tricarboxybenzoate anion, the dihedral angles between the least-squares planes of the benzene ring and the carboxy/carboxylate groups are 15.6 (3)° (C27/O5/O6), 4.7 (2)° (C26/O3/O4), 3.3 (3)° (C28/O3/O4) and 87.9 (3)° (C25/O1/O2). Thus, three of the appended groups are roughly coplanar with the central benzene plane, while the fourth is approximately normal to it (Fig. 1). Intramolecular O—H···O hydrogen bonding is observed for one of the three carboxylic groups to an adjacent carboxylate O atom (O7—H3···O6; Table 2).

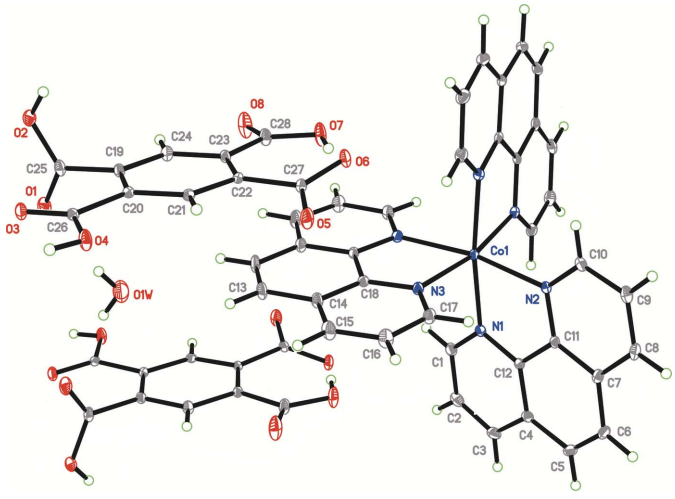


Figure 1
Expanded asymmetric unit of the title salt, showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are generated by the symmetry operation $-x+1, y, -z+\frac{1}{2}$.

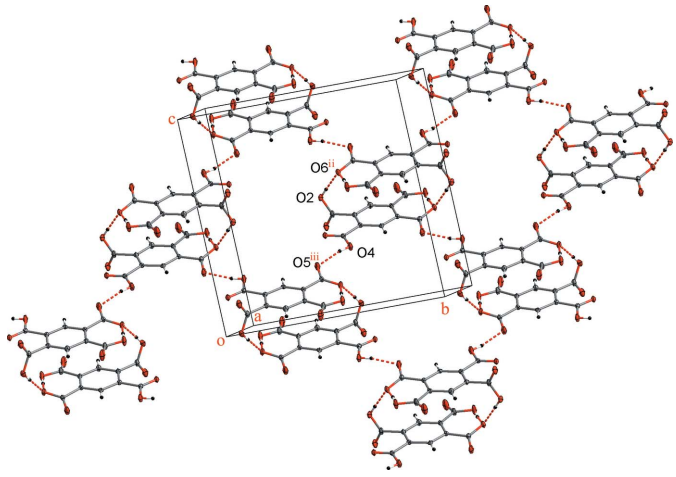


Figure 2
Supramolecular sheet, formed by O—H···O hydrogen bonds (shown as dashed lines) between benzene-1,2,4,5-tetracarboxylate anions. The complex cations and water molecules have been omitted for clarity. [Symmetry codes refer to Table 2.]

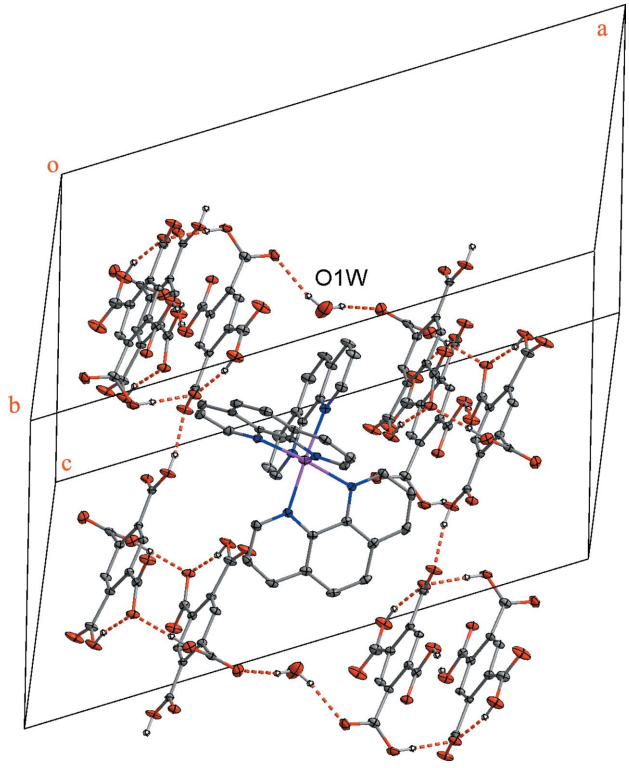


Figure 3
The packing of the title compound. All C-bound H atoms have been omitted for clarity and hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1	0.82	2.05	2.854 (2)	165
O2—H1···O6^{ii}	0.82	1.79	2.615 (2)	179
O4—H2···O5^{iii}	0.82	1.87	2.681 (2)	170
O7—H3···O6	0.82	1.64	2.443 (2)	164

Symmetry codes: (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

In the crystal, neighbouring benzene-1,2,4,5-tetracarboxylate anions interact through $_{\text{carboxyl}}$O—H···O$_{\text{carboxylate}}$ hydrogen bonds (O2—H1···O^{ii} and O4—H2···O5^{iii}) [symmetry codes as in Table 2] to build up an extended two-dimensional network extending parallel to (100) within which an $R_6^6(38)$ motif can be discerned (Fig. 2, Table 2). Adjacent sheets are interconnected by water–carboxylate hydrogen bonds O1W—H1WA···O1, resulting in a three-dimensional supramolecular structure with channels along [100] that are filled by $[Co(phen)_3]^{2+}$ complex cations (Fig. 3).

Synthesis and crystallization

0.1 mmol of $CoSO_4·7H_2O$, 0.3 mmol of 1,10-phenanthroline, 0.2 mmol of benzene-1,2,4,5-tetracarboxylic acid and 15 ml of water were mixed and placed in a thick Pyrex tube, which was sealed and heated to 393 K for 48 h. The tube was cooled to ambient temperature spontaneously, whereupon brown block-shaped crystals (51% yield, based on Co) suitable for X-ray analysis were obtained.

Refinement

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

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{12}H_8N_2)_3](C_{10}H_5O_8)_2·H_2O$
M_r	1123.84
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	173
a, b, c (Å)	24.014 (2), 14.1324 (8), 15.8922 (12)
β (°)	116.505 (8)
V (Å^3)	4826.6 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.44
Crystal size (mm)	0.32 × 0.25 × 0.15
Data collection	
Diffractometer	Rigaku Mercury CCD
Absorption correction	Multi-scan (*REQAB*; Jacobson, 1998)
T_{min}, T_{max}	0.760, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11427, 5584, 4395
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.692
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.102, 1.03
No. of reflections	5584
No. of parameters	362
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.42

Computer programs: *CrystalClear* (Rigaku, 2007), *SHELXS2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *XP* in *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

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full crystallographic data

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Tris(1,10-phenanthroline-κ^2N,N')cobalt(II) bis(2,4,5-tricarboxybenzoate) monohydrate

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Tris(1,10-phenanthroline-κ^2N,N')cobalt(II) bis(2,4,5-tricarboxybenzoate) monohydrate

Crystal data

$[Co(C_{12}H_8N_2)_3](C_{10}H_5O_8)_2\cdot H_2O$
M_r = 1123.84
Monoclinic, $C2/c$
a = 24.014 (2) Å
b = 14.1324 (8) Å
c = 15.8922 (12) Å
β = 116.505 (8)°
V = 4826.6 (7) Å^3
Z = 4
$F(000)$ = 2308
D_x = 1.547 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3101 reflections
θ = 3.9–29.3°
μ = 0.44 mm^{-1}
T = 173 K
Block, brown
0.32 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 28.5714 pixels mm^{-1}
Graphite Monochromator scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.760, T_{max} = 1.000
11427 measured reflections
5584 independent reflections
4395 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.5°, θ_{min} = 3.5°
h = −32→25
k = −19→17
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.102
S = 1.03
5584 reflections
362 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 4.8534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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. All H atoms bound to O atoms were located from a difference Fourier map and constrained to ride on their parent O atoms, with $U_{iso}(H) = 1.5U_{eq}(O)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	1.19153 (3)	0.2500	0.01770 (11)
N1	0.41551 (8)	1.20161 (11)	0.12526 (11)	0.0194 (4)
N2	0.52417 (8)	1.29112 (11)	0.17159 (11)	0.0193 (4)
N3	0.52863 (8)	1.07406 (11)	0.19354 (11)	0.0203 (4)
C17	0.55687 (11)	1.07451 (15)	0.13810 (15)	0.0266 (5)
H17A	0.5663	1.1326	0.1200	0.032*
O1	0.59618 (7)	0.47012 (11)	0.39051 (12)	0.0335 (4)
O1W	0.5000	0.58043 (19)	0.2500	0.0736 (10)
H1WA	0.5298	0.5471	0.2829	0.110*
O2	0.68365 (8)	0.46302 (10)	0.52099 (11)	0.0304 (4)
H1	0.7169	0.4901	0.5514	0.046*
O3	0.70717 (7)	0.44158 (9)	0.34916 (10)	0.0259 (3)
O4	0.74848 (8)	0.53589 (10)	0.27884 (11)	0.0328 (4)
H2	0.7578	0.4836	0.2665	0.049*
O5	0.73113 (8)	0.86923 (10)	0.28307 (12)	0.0361 (4)
O6	0.71041 (7)	0.94971 (9)	0.38479 (11)	0.0277 (4)
O7	0.64057 (8)	0.93373 (10)	0.45814 (13)	0.0406 (5)
H3	0.6583	0.9383	0.4245	0.061*
O8	0.60100 (10)	0.81840 (11)	0.50479 (14)	0.0500 (5)
C1	0.36137 (10)	1.15973 (15)	0.10432 (15)	0.0256 (5)
H1A	0.3574	1.1242	0.1506	0.031*
C2	0.31024 (11)	1.16662 (16)	0.01607 (16)	0.0302 (5)
H2A	0.2729	1.1369	0.0044	0.036*
C3	0.31572 (10)	1.21766 (15)	−0.05299 (15)	0.0287 (5)
H3A	0.2824	1.2215	−0.1126	0.034*
C4	0.37175 (10)	1.26408 (14)	−0.03349 (14)	0.0217 (4)
C5	0.38197 (11)	1.31980 (15)	−0.10107 (15)	0.0281 (5)
H5A	0.3498	1.3267	−0.1614	0.034*
C6	0.43679 (11)	1.36204 (14)	−0.07933 (14)	0.0263 (5)
H6A	0.4422	1.3966	−0.1250	0.032*
C7	0.48707 (10)	1.35460 (13)	0.01330 (14)	0.0220 (4)
C8	0.54479 (10)	1.40022 (14)	0.04180 (16)	0.0257 (5)
H8A	0.5523	1.4365	−0.0009	0.031*
C10	0.57776 (10)	1.33611 (14)	0.19553 (15)	0.0246 (5)
H10A	0.6086	1.3308	0.2571	0.030*
C12	0.42081 (9)	1.25390 (13)	0.05729 (13)	0.0178 (4)
C11	0.47898 (9)	1.30083 (13)	0.08158 (13)	0.0182 (4)
C19	0.66735 (9)	0.59724 (13)	0.41742 (14)	0.0191 (4)
C20	0.70134 (9)	0.60717 (13)	0.36600 (13)	0.0168 (4)
C21	0.71463 (9)	0.69806 (13)	0.34666 (13)	0.0172 (4)
H21A	0.7381	0.7048	0.3136	0.021*
C22	0.69446 (9)	0.78005 (13)	0.37449 (13)	0.0161 (4)
C23	0.66035 (9)	0.76940 (13)	0.42697 (13)	0.0185 (4)
C24	0.64829 (10)	0.67741 (14)	0.44699 (14)	0.0222 (4)
H24A	0.6263	0.6699	0.4821	0.027*

C25	0.64661 (11)	0.50314 (14)	0.43963 (15)	0.0236 (5)
C26	0.71991 (9)	0.51990 (13)	0.33138 (13)	0.0187 (4)
C27	0.71286 (10)	0.87263 (13)	0.34414 (14)	0.0205 (4)
C28	0.63172 (11)	0.84377 (15)	0.46626 (16)	0.0278 (5)
C9	0.58980 (11)	1.39097 (15)	0.13255 (16)	0.0281 (5)
H9A	0.6280	1.4210	0.1520	0.034*
C16	0.57307 (12)	0.99218 (16)	0.10572 (17)	0.0347 (6)
H16A	0.5928	0.9955	0.0670	0.042*
C15	0.55938 (12)	0.90636 (16)	0.13202 (17)	0.0354 (6)
H15A	0.5697	0.8508	0.1109	0.042*
C13	0.51427 (12)	0.81529 (14)	0.22173 (17)	0.0319 (5)
H13A	0.5239	0.7580	0.2026	0.038*
C18	0.51533 (9)	0.98834 (13)	0.21980 (13)	0.0184 (4)
C14	0.52980 (11)	0.90204 (14)	0.19094 (15)	0.0253 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0236 (2)	0.01387 (18)	0.01681 (19)	0.000	0.01004 (16)	0.000
N1	0.0205 (9)	0.0169 (8)	0.0206 (8)	−0.0012 (7)	0.0091 (7)	−0.0011 (7)
N2	0.0228 (9)	0.0135 (7)	0.0207 (8)	−0.0011 (7)	0.0089 (7)	−0.0014 (7)
N3	0.0273 (10)	0.0171 (8)	0.0202 (8)	−0.0015 (7)	0.0140 (8)	0.0005 (7)
C17	0.0371 (13)	0.0219 (10)	0.0299 (12)	−0.0014 (10)	0.0233 (11)	0.0016 (9)
O1	0.0300 (9)	0.0225 (8)	0.0474 (10)	−0.0075 (7)	0.0169 (8)	−0.0004 (7)
O1W	0.068 (2)	0.0336 (15)	0.078 (2)	0.000	−0.0035 (18)	0.000
O2	0.0412 (10)	0.0200 (7)	0.0310 (8)	−0.0084 (7)	0.0170 (8)	0.0034 (7)
O3	0.0368 (9)	0.0143 (7)	0.0308 (8)	0.0006 (6)	0.0189 (7)	0.0003 (6)
O4	0.0573 (11)	0.0171 (7)	0.0432 (10)	0.0036 (7)	0.0397 (9)	−0.0020 (7)
O5	0.0649 (12)	0.0198 (8)	0.0439 (10)	−0.0044 (8)	0.0425 (9)	0.0007 (7)
O6	0.0409 (10)	0.0137 (6)	0.0363 (9)	−0.0041 (7)	0.0242 (8)	−0.0034 (6)
O7	0.0658 (13)	0.0157 (7)	0.0660 (12)	0.0013 (8)	0.0526 (11)	−0.0034 (8)
O8	0.0835 (15)	0.0252 (9)	0.0814 (14)	0.0001 (9)	0.0728 (13)	−0.0049 (9)
C1	0.0283 (12)	0.0206 (10)	0.0282 (11)	−0.0044 (9)	0.0129 (10)	−0.0027 (9)
C2	0.0248 (12)	0.0280 (11)	0.0341 (12)	−0.0056 (10)	0.0099 (10)	−0.0079 (10)
C3	0.0251 (12)	0.0263 (11)	0.0254 (11)	0.0033 (10)	0.0028 (10)	−0.0056 (9)
C4	0.0268 (11)	0.0167 (9)	0.0195 (10)	0.0064 (9)	0.0084 (9)	−0.0039 (8)
C5	0.0395 (14)	0.0235 (10)	0.0173 (10)	0.0082 (10)	0.0092 (10)	0.0003 (9)
C6	0.0438 (14)	0.0188 (10)	0.0213 (10)	0.0081 (10)	0.0189 (10)	0.0047 (9)
C7	0.0331 (12)	0.0143 (9)	0.0258 (11)	0.0052 (9)	0.0196 (10)	0.0001 (8)
C8	0.0364 (13)	0.0163 (9)	0.0348 (12)	0.0034 (9)	0.0252 (11)	0.0043 (9)
C10	0.0265 (12)	0.0184 (9)	0.0279 (11)	−0.0047 (9)	0.0112 (10)	−0.0037 (9)
C12	0.0241 (11)	0.0130 (8)	0.0178 (9)	0.0023 (8)	0.0105 (8)	−0.0029 (8)
C11	0.0247 (11)	0.0116 (8)	0.0205 (10)	0.0029 (8)	0.0120 (9)	−0.0004 (8)
C19	0.0218 (11)	0.0153 (9)	0.0211 (10)	−0.0017 (8)	0.0104 (9)	−0.0003 (8)
C20	0.0193 (10)	0.0149 (9)	0.0156 (9)	0.0008 (8)	0.0074 (8)	−0.0007 (8)
C21	0.0208 (10)	0.0177 (9)	0.0145 (9)	−0.0005 (8)	0.0092 (8)	0.0006 (8)
C22	0.0193 (10)	0.0131 (8)	0.0146 (9)	−0.0001 (8)	0.0064 (8)	0.0008 (7)
C23	0.0230 (11)	0.0141 (9)	0.0199 (10)	0.0013 (8)	0.0108 (9)	−0.0013 (8)

C24	0.0291 (12)	0.0186 (10)	0.0273 (11)	0.0006 (9)	0.0201 (10)	0.0003 (8)
C25	0.0321 (13)	0.0149 (9)	0.0318 (12)	0.0002 (9)	0.0213 (10)	−0.0023 (9)
C26	0.0215 (11)	0.0168 (9)	0.0164 (9)	0.0022 (8)	0.0073 (8)	−0.0014 (8)
C27	0.0239 (11)	0.0153 (9)	0.0214 (10)	−0.0014 (8)	0.0093 (9)	0.0021 (8)
C28	0.0398 (14)	0.0185 (10)	0.0352 (12)	0.0026 (10)	0.0258 (11)	−0.0026 (9)
C9	0.0294 (12)	0.0206 (10)	0.0402 (13)	−0.0052 (10)	0.0208 (11)	−0.0021 (10)
C16	0.0525 (16)	0.0291 (12)	0.0422 (14)	0.0007 (11)	0.0390 (13)	−0.0011 (11)
C15	0.0532 (16)	0.0229 (11)	0.0457 (15)	0.0055 (11)	0.0362 (13)	−0.0051 (11)
C13	0.0496 (15)	0.0136 (9)	0.0422 (13)	0.0030 (10)	0.0291 (12)	−0.0021 (9)
C18	0.0209 (10)	0.0161 (9)	0.0187 (9)	0.0002 (8)	0.0095 (8)	−0.0005 (8)
C14	0.0342 (13)	0.0174 (10)	0.0305 (11)	0.0023 (9)	0.0198 (10)	−0.0004 (9)

Geometric parameters (Å, º)

Co1—N1^{i}	2.1158 (17)	C5—C6	1.343 (3)
Co1—N1	2.1159 (17)	C5—H5A	0.9300
Co1—N2^{i}	2.1251 (16)	C6—C7	1.432 (3)
Co1—N2	2.1251 (16)	C6—H6A	0.9300
Co1—N3	2.1412 (16)	C7—C11	1.407 (3)
Co1—N3^{i}	2.1412 (16)	C7—C8	1.408 (3)
N1—C1	1.329 (3)	C8—C9	1.369 (3)
N1—C12	1.361 (2)	C8—H8A	0.9300
N2—C10	1.330 (3)	C10—C9	1.395 (3)
N2—C11	1.363 (2)	C10—H10A	0.9300
N3—C17	1.330 (2)	C12—C11	1.435 (3)
N3—C18	1.365 (2)	C19—C24	1.380 (3)
C17—C16	1.396 (3)	C19—C20	1.396 (3)
C17—H17A	0.9300	C19—C25	1.516 (3)
O1—C25	1.204 (3)	C20—C21	1.391 (3)
O1W—H1WA	0.8199	C20—C26	1.497 (3)
O2—C25	1.326 (3)	C21—C22	1.401 (3)
O2—H1	0.8200	C21—H21A	0.9300
O3—C26	1.215 (2)	C22—C23	1.414 (3)
O4—C26	1.315 (2)	C22—C27	1.526 (3)
O4—H2	0.8203	C23—C24	1.399 (3)
O5—C27	1.232 (2)	C23—C28	1.533 (3)
O6—C27	1.281 (2)	C24—H24A	0.9300
O7—C28	1.305 (2)	C9—H9A	0.9300
O7—H3	0.8200	C16—C15	1.370 (3)
O8—C28	1.205 (3)	C16—H16A	0.9300
C1—C2	1.395 (3)	C15—C14	1.407 (3)
C1—H1A	0.9300	C15—H15A	0.9300
C2—C3	1.368 (3)	C13—C13^{i}	1.352 (4)
C2—H2A	0.9300	C13—C14	1.430 (3)
C3—C4	1.401 (3)	C13—H13A	0.9300
C3—H3A	0.9300	C18—C14	1.400 (3)
C4—C12	1.405 (3)	C18—C18^{i}	1.447 (4)
C4—C5	1.438 (3)		

N1^{i}—Co1—N1	172.28 (9)	C9—C10—H10A	118.5
N1^{i}—Co1—N2^{i}	78.74 (6)	N1—C12—C4	122.56 (19)
N1—Co1—N2^{i}	96.09 (6)	N1—C12—C11	117.53 (17)
N1^{i}—Co1—N2	96.09 (6)	C4—C12—C11	119.91 (18)
N1—Co1—N2	78.74 (6)	N2—C11—C7	122.98 (19)
N2^{i}—Co1—N2	97.05 (9)	N2—C11—C12	117.35 (17)
N1^{i}—Co1—N3	95.27 (6)	C7—C11—C12	119.67 (18)
N1—Co1—N3	90.72 (6)	C24—C19—C20	119.07 (18)
N2^{i}—Co1—N3	169.13 (6)	C24—C19—C25	116.58 (17)
N2—Co1—N3	92.57 (6)	C20—C19—C25	124.27 (17)
N1^{i}—Co1—N3^{i}	90.72 (6)	C21—C20—C19	118.30 (17)
N1—Co1—N3^{i}	95.27 (6)	C21—C20—C26	122.97 (17)
N2^{i}—Co1—N3^{i}	92.57 (6)	C19—C20—C26	118.69 (17)
N2—Co1—N3^{i}	169.13 (6)	C20—C21—C22	123.24 (17)
N3—Co1—N3^{i}	78.33 (8)	C20—C21—H21A	118.4
C1—N1—C12	118.09 (18)	C22—C21—H21A	118.4
C1—N1—Co1	128.81 (14)	C21—C22—C23	118.10 (16)
C12—N1—Co1	112.95 (13)	C21—C22—C27	114.80 (16)
C10—N2—C11	117.90 (17)	C23—C22—C27	127.10 (17)
C10—N2—Co1	129.17 (14)	C24—C23—C22	117.79 (17)
C11—N2—Co1	112.59 (13)	C24—C23—C28	111.63 (17)
C17—N3—C18	117.70 (17)	C22—C23—C28	130.58 (17)
C17—N3—Co1	128.89 (14)	C19—C24—C23	123.47 (18)
C18—N3—Co1	113.40 (12)	C19—C24—H24A	118.3
N3—C17—C16	123.26 (19)	C23—C24—H24A	118.3
N3—C17—H17A	118.4	O1—C25—O2	120.63 (19)
C16—C17—H17A	118.4	O1—C25—C19	121.9 (2)
C25—O2—H1	115.4	O2—C25—C19	117.07 (19)
C26—O4—H2	105.8	O3—C26—O4	124.13 (18)
C28—O7—H3	107.2	O3—C26—C20	121.18 (17)
N1—C1—C2	123.0 (2)	O4—C26—C20	114.65 (16)
N1—C1—H1A	118.5	O5—C27—O6	122.90 (18)
C2—C1—H1A	118.5	O5—C27—C22	118.08 (17)
C3—C2—C1	119.1 (2)	O6—C27—C22	118.99 (17)
C3—C2—H2A	120.4	O8—C28—O7	120.27 (19)
C1—C2—H2A	120.4	O8—C28—C23	119.38 (19)
C2—C3—C4	119.7 (2)	O7—C28—C23	120.35 (18)
C2—C3—H3A	120.1	C8—C9—C10	119.3 (2)
C4—C3—H3A	120.1	C8—C9—H9A	120.3
C3—C4—C12	117.49 (19)	C10—C9—H9A	120.3
C3—C4—C5	123.9 (2)	C15—C16—C17	118.78 (19)
C12—C4—C5	118.6 (2)	C15—C16—H16A	120.6
C6—C5—C4	121.7 (2)	C17—C16—H16A	120.6
C6—C5—H5A	119.1	C16—C15—C14	120.2 (2)
C4—C5—H5A	119.1	C16—C15—H15A	119.9
C5—C6—C7	120.81 (19)	C14—C15—H15A	119.9
C5—C6—H6A	119.6	C13^{i}—C13—C14	120.97 (12)

C7—C6—H6A	119.6	C13^{i}—C13—H13A	119.5
C11—C7—C8	117.01 (19)	C14—C13—H13A	119.5
C11—C7—C6	119.3 (2)	N3—C18—C14	123.14 (17)
C8—C7—C6	123.70 (19)	N3—C18—C18^{i}	117.43 (10)
C9—C8—C7	119.77 (19)	C14—C18—C18^{i}	119.43 (11)
C9—C8—H8A	120.1	C18—C14—C15	116.94 (19)
C7—C8—H8A	120.1	C18—C14—C13	119.60 (18)
N2—C10—C9	123.0 (2)	C15—C14—C13	123.46 (19)
N2—C10—H10A	118.5		

C18—N3—C17—C16	0.3 (3)	C20—C21—C22—C23	1.7 (3)
Co1—N3—C17—C16	−179.85 (18)	C20—C21—C22—C27	−178.64 (18)
C12—N1—C1—C2	0.4 (3)	C21—C22—C23—C24	−0.7 (3)
Co1—N1—C1—C2	−174.80 (15)	C27—C22—C23—C24	179.77 (18)
N1—C1—C2—C3	0.8 (3)	C21—C22—C23—C28	−179.3 (2)
C1—C2—C3—C4	−1.7 (3)	C27—C22—C23—C28	1.1 (4)
C2—C3—C4—C12	1.3 (3)	C20—C19—C24—C23	1.1 (3)
C2—C3—C4—C5	−179.6 (2)	C25—C19—C24—C23	−176.0 (2)
C3—C4—C5—C6	−179.19 (19)	C22—C23—C24—C19	−0.7 (3)
C12—C4—C5—C6	−0.2 (3)	C28—C23—C24—C19	178.2 (2)
C4—C5—C6—C7	−1.3 (3)	C24—C19—C25—O1	83.3 (3)
C5—C6—C7—C11	1.1 (3)	C20—C19—C25—O1	−93.5 (3)
C5—C6—C7—C8	−177.31 (19)	C24—C19—C25—O2	−89.7 (2)
C11—C7—C8—C9	0.0 (3)	C20—C19—C25—O2	93.5 (2)
C6—C7—C8—C9	178.45 (19)	C21—C20—C26—O3	−179.5 (2)
C11—N2—C10—C9	−1.1 (3)	C19—C20—C26—O3	−1.7 (3)
Co1—N2—C10—C9	171.70 (15)	C21—C20—C26—O4	−1.7 (3)
C1—N1—C12—C4	−0.7 (3)	C19—C20—C26—O4	176.08 (18)
Co1—N1—C12—C4	175.20 (14)	C21—C22—C27—O5	15.1 (3)
C1—N1—C12—C11	178.37 (17)	C23—C22—C27—O5	−165.3 (2)
Co1—N1—C12—C11	−5.7 (2)	C21—C22—C27—O6	−162.90 (19)
C3—C4—C12—N1	−0.1 (3)	C23—C22—C27—O6	16.7 (3)
C5—C4—C12—N1	−179.20 (18)	C24—C23—C28—O8	−3.1 (3)
C3—C4—C12—C11	−179.20 (17)	C22—C23—C28—O8	175.6 (2)
C5—C4—C12—C11	1.7 (3)	C24—C23—C28—O7	176.9 (2)
C10—N2—C11—C7	1.2 (3)	C22—C23—C28—O7	−4.4 (4)
Co1—N2—C11—C7	−172.78 (14)	C7—C8—C9—C10	0.1 (3)
C10—N2—C11—C12	−178.44 (17)	N2—C10—C9—C8	0.5 (3)
Co1—N2—C11—C12	7.6 (2)	N3—C17—C16—C15	0.0 (4)
C8—C7—C11—N2	−0.6 (3)	C17—C16—C15—C14	−0.3 (4)
C6—C7—C11—N2	−179.17 (17)	C17—N3—C18—C14	−0.2 (3)
C8—C7—C11—C12	178.97 (17)	Co1—N3—C18—C14	179.89 (17)
C6—C7—C11—C12	0.4 (3)	C17—N3—C18—C18^{i}	179.9 (2)
N1—C12—C11—N2	−1.3 (3)	Co1—N3—C18—C18^{i}	0.0 (3)
C4—C12—C11—N2	177.76 (16)	N3—C18—C14—C15	−0.1 (3)
N1—C12—C11—C7	179.04 (17)	C18^{i}—C18—C14—C15	179.8 (2)
C4—C12—C11—C7	−1.8 (3)	N3—C18—C14—C13	180.0 (2)
C24—C19—C20—C21	0.0 (3)	C18^{i}—C18—C14—C13	−0.2 (4)

C25—C19—C20—C21	176.80 (19)	C16—C15—C14—C18	0.3 (4)
C24—C19—C20—C26	−177.91 (18)	C16—C15—C14—C13	−179.7 (2)
C25—C19—C20—C26	−1.1 (3)	C13^{i}—C13—C14—C18	0.1 (4)
C19—C20—C21—C22	−1.4 (3)	C13^{i}—C13—C14—C15	−179.9 (3)
C26—C20—C21—C22	176.40 (18)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1	0.82	2.05	2.854 (2)	165
O2—H1···O6^{ii}	0.82	1.79	2.615 (2)	179
O4—H2···O5^{iii}	0.82	1.87	2.681 (2)	170
O7—H3···O6	0.82	1.64	2.443 (2)	164

Symmetry codes: (ii) −*x*+3/2, −*y*+3/2, −*z*+1; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2.