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A new supramolecular cobalt(II) complex based on 1,10-phenanthroline and 4-nitrophthalate ligands

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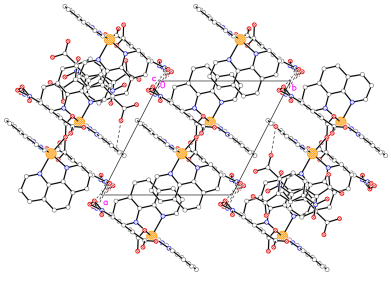
The title compound, bis(μ-2-carboxy-4-nitrobenzoato-κ^2O^1:$O^{1'}$)bis[bis(1,10-phenanthroline-κ^2N,N')cobalt(II)] bis(2-carboxy-4-nitrobenzoate) tetrahydrate, $[Co_2(C_8H_4NO_6)_2(C_{12}H_8N_2)_4](C_8H_4NO_6)_2\cdot 4H_2O$, comprises a centrosymmetric dinuclear cobalt(II) complex dication, two hydrogen 4-nitrophthalate anions and four water molecules of crystallization. The two Co^{II} atoms are linked by two μ-hydrogen 4-nitrophthalato ligands, generating a centrosymmetric dinuclear unit. Each cobalt(II) centre adopts a distorted octahedral coordination geometry defined by four N atoms from two chelating 1,10-phenanthroline ligands and two O atoms from two symmetry-related bridging hydrogen 4-nitrophthalate ligands. In the crystal, O—H···O and C—H···O hydrogen bonds link the ionic components into a three-dimensional supramolecular framework, which is further reinforced by aromatic π–π stacking interactions between neighbouring phenanthroline and hydrogen 4-nitrophthalate rings, with centroid-to-centroid separations ranging from 3.501 (5) to 3.687 (4) Å. Hirshfeld surface analysis shows that O···H/H···O contacts make the largest contribution (38.1%) to the crystal packing, confirming the dominant role of hydrogen bonding in consolidating the crystal structure.

1. Chemical context

Mixed-ligand cobalt(II) complexes containing aromatic N-donor and polycarboxylate ligands continue to attract attention because of their structural diversity and supramolecular assembly patterns (Sammes & Yahioglu, 1994; Bencini & Lippolis, 2010). In particular, 1,10-phenanthroline commonly forms stable chelating coordination environments, whereas nitrophthalate ligands exhibit versatile coordination modes and hydrogen-bonding capabilities. As part of our ongoing studies of cobalt(II) complexes containing mixed N- and O-donor ligands, the title dinuclear complex incorporating 1,10-phenanthroline and hydrogen 4-nitrophthalate ligands was synthesized and characterized by single-crystal X-ray diffraction analysis.



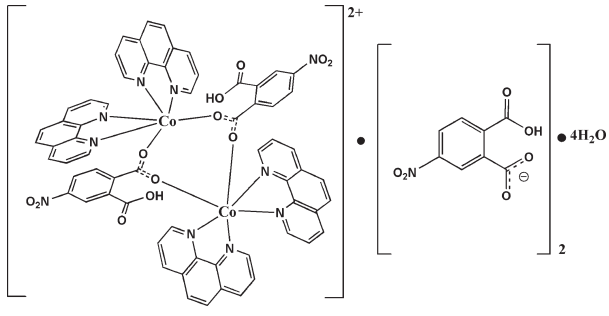


Table 1
Selected geometric parameters (Å, °).

Co1—O5	2.070 (4)	O6—C8	1.273 (6)
Co1—N5	2.126 (4)	O5—C8	1.254 (6)
Co1—N3	2.126 (4)	O4—C7	1.237 (7)
Co1—N4	2.137 (5)	O3—C7	1.326 (7)
Co1—N2	2.169 (4)		
O5—Co1—O6^{i}	91.94 (13)	O6^{i}—Co1—N2	166.84 (15)
N5—Co1—N3	173.52 (16)	N3—Co1—N2	77.25 (16)
O5—Co1—N4	171.16 (16)	O5—C8—O6	124.9 (5)
N5—Co1—N4	77.74 (18)	O4—C7—O3	122.5 (7)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The complex crystallizes in the triclinic space group $P\overline{1}$. The asymmetric unit comprises one Co^{II} atom, two chelating 1,10-phenanthroline ligands, one μ_2-bridging hydrogen 4-nitrophthalate ligand, one uncoordinated hydrogen 4-nitrophthalate anion and two solvent oxygen atoms (O1*W* and O2*W*) corresponding to highly disordered water molecules. The complete centrosymmetric dinuclear complex dication is generated by inversion symmetry.

Each Co^{II} centre adopts a distorted octahedral CoN_4O_2 coordination geometry defined by four nitrogen atoms from two chelating 1,10-phenanthroline ligands and two oxygen atoms from two symmetry-related hydrogen 4-nitrophthalate ligands. The Co—O bond length is 2.070 (4) Å, while the Co—N bond distances range from 2.126 (4) to 2.169 (4) Å (Table 1). The *cis* angle O5—Co1—O6^{i} is 91.94 (13)°, while the *trans* angles N3—Co1—N5 and O5—Co1—N4 are 173.52 (16) and 171.16 (16)°, respectively, indicating only a slight distortion from an ideal octahedral geometry.

The coordinated hydrogen 4-nitrophthalate ligand adopts a μ_2-κO:$\kappa O'$ bridging coordination mode, linking two symmetry-related cobalt(II) centres into a centrosymmetric dinuclear complex dication with an intramolecular Co···Co separation of 4.795 (2) Å. Within the coordinated carboxylate group, the C—O bond distances [1.254 (6) and 1.273 (6) Å] are consistent with electron delocalization, whereas the uncoordinated carboxylic group exhibits unequal C—O bond lengths [1.237 (7) and 1.326 (7) Å], confirming its protonated nature.

The coordinated 1,10-phenanthroline ligands are essentially planar and provide extended aromatic surfaces that participate in significant intermolecular π–π stacking interactions, which, together with the hydrogen-bonding network, contribute to the cohesion of the crystal packing and the formation of a three-dimensional supramolecular architecture.

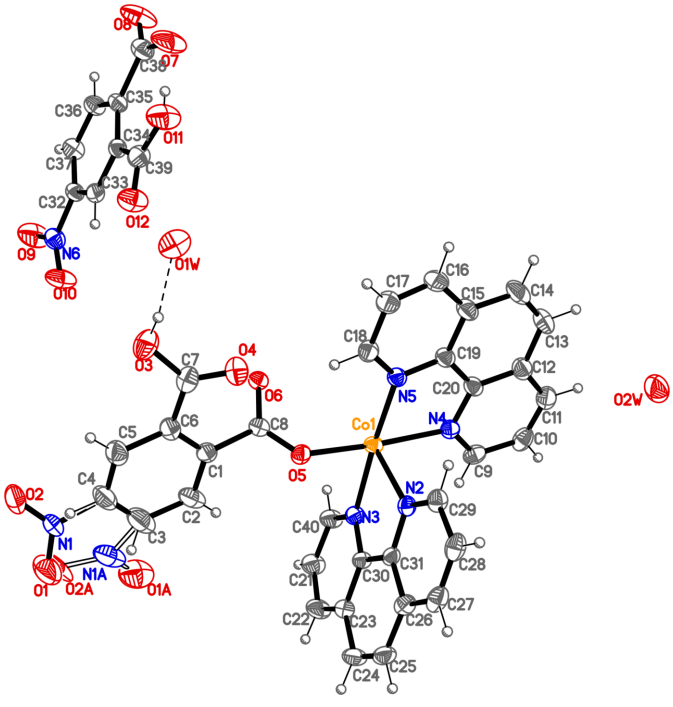


Figure 1
The asymmetric unit of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1*W*	0.82	1.78	2.549 (8)	155
O11—H11*A*···O7	0.82	1.58	2.400 (8)	178
C18—H18···O4	0.93	2.50	3.397 (8)	162
C9—H9···O12^{i}	0.93	2.58	3.462 (8)	158
C40—H40···O6^{i}	0.93	2.54	3.079 (6)	117
C21—H21···O7^{ii}	0.93	2.42	3.329 (8)	165
C4—H4$^{b\cdots O2A}$b	0.93	2.00	2.49 (2)	112

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

3. Supramolecular features

The crystal packing is governed by a combination of classical O—H···O and weak C—H···O hydrogen bonds (Table 2), together with significant aromatic π–π stacking interactions (Fig. 2). The uncoordinated hydrogen 4-nitrophthalate anions act as both hydrogen-bond donors and acceptors, whereas the solvent water oxygen atoms serve as hydrogen-bond accep-

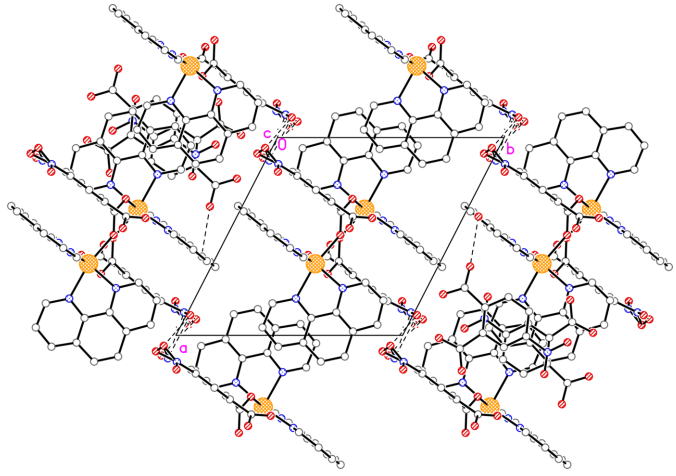


Figure 2
Crystal packing of the title compound viewed along the [001] direction.

tors. Collectively, these interactions link the centrosymmetric dinuclear complex dications, hydrogen 4-nitrophthalate anions and solvent species into a three-dimensional supramolecular architecture.

Several significant π–π stacking interactions are observed between the aromatic rings of the coordinated 1,10-phenanthroline ligands and the hydrogen 4-nitrophthalate ligands. The shortest interaction occurs between the pyridine ring of one 1,10-phenanthroline ligand (N4/C9–C12/C20; *Cg*5) and the benzene ring of a hydrogen 4-nitrophthalate ligand (C1–C6; *Cg*7), with a centroid-to-centroid distance of 3.500 (5) Å, an interplanar angle of 0.6° and a slippage of 1.03 Å, indicating an almost ideal face-to-face arrangement. Additional significant contacts are observed: *Cg*3···*Cg*3^{i} [3.600 (4) Å, 0.0°, 1.19 Å], *Cg*7···*Cg*8^{i} [3.609 (5) Å, 1.4°, 1.42 Å] and *Cg*9···*Cg*10^{i} [3.687 (4) Å, 2.7°, 1.18 Å] [*Cg*3, *Cg*7, *Cg*8, *Cg*9 and *Cg*10 are the centroids of the N2/C26–C29/C31, C1–C6, C12–C15/C19/C20, C23–C26/C30/C31 and C32–C37 rings, respectively; symmetry code: (i) $-x+2, -y+1, -z+1$]. These geometrical parameters indicate efficient overlap of the aromatic π systems and contribute significantly to the cohesion of the crystal packing.

4. Hirshfeld surface analysis

Hirshfeld surface analysis and the corresponding two-dimensional fingerprint plots were generated using *CrystalExplorer21.5* (Spackman *et al.*, 2021) to investigate the intermolecular interactions responsible for the crystal packing. The Hirshfeld surface mapped over d_{norm} and the associated fingerprint plots are shown in Figs. 3 and 4, respectively.

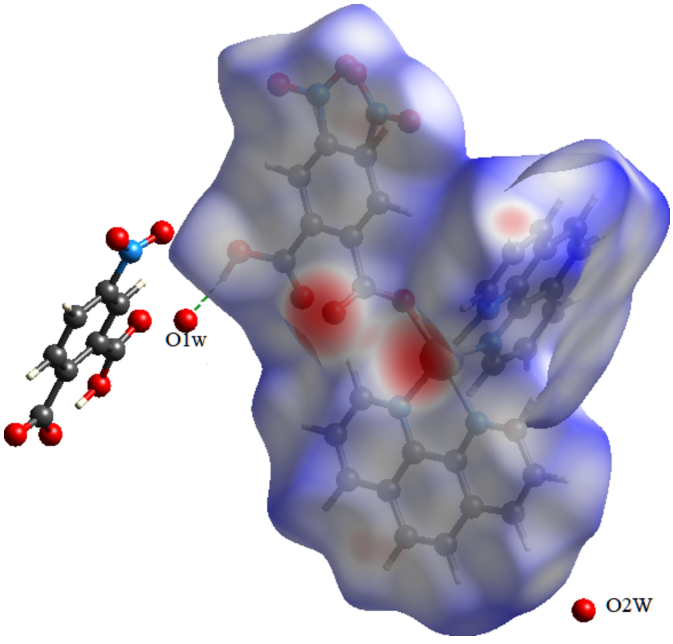


Figure 3
Hirshfeld surface mapped over d_{norm} showing short intermolecular O···H/H···O contacts as red regions.

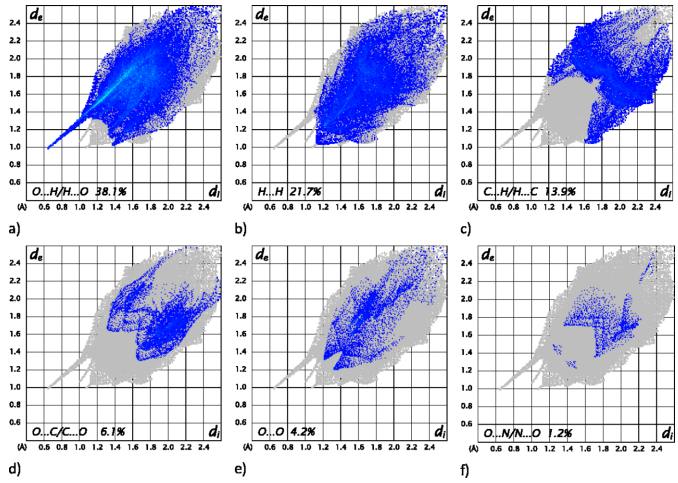


Figure 4
Two-dimensional fingerprint plots showing the percentage contributions of (*a*) O···H/H···O, (*b*) H···H, (*c*) C···H/H···C, (*d*) O···C/C···O, (*e*) O···O and (*f*) O···N/N···O contacts.

The O···H/H···O contacts make the largest contribution to the Hirshfeld surface (38.1%), confirming that hydrogen bonding involving the carboxylate, carboxylic acid and nitro oxygen atoms plays the dominant role in consolidating the crystal structure. H···H contacts account for 21.7% of the surface, reflecting the contribution of van der Waals interactions, whereas C···H/H···C contacts contribute 13.9%, indicating numerous weak intermolecular C···H contacts within the crystal packing. Smaller contributions arise from O···C/C···O (6.1%), O···O (4.2%) and O···N/N···O (1.2%) contacts.

The Hirshfeld surface analysis is consistent with the crystallographic study, demonstrating that the crystal packing is governed primarily by classical hydrogen bonding, supplemented by weak intermolecular contacts and significant aromatic π–π stacking interactions, which together generate the observed three-dimensional supramolecular architecture.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 2025.3.1, update of February 2026; Groom *et al.*, 2016) revealed several cobalt(II) complexes containing the 4-nitrophthalate ligand. Representative examples include HOJHOF (Li *et al.*, 2014), JUYREC and JUYRIG (Wang *et al.*, 2015*a*), and LUDJUR (Yin & Li, 2015), in which the 4-nitrophthalate ligand adopts various bridging coordination modes and gives rise to one-dimensional or higher-dimensional coordination architectures.

A separate search for cobalt(II) complexes containing both 1,10-phenanthroline and aromatic polycarboxylate ligands identified several structurally related dinuclear complexes, including AJIYID (Wang *et al.*, 2015*b*) and HUBCOY and HUBCUE (Wang *et al.*, 2015*c*). In these compounds, the Co^{II} centres exhibit distorted octahedral coordination geometries defined by nitrogen atoms from chelating 1,10-phenanthroline ligands and oxygen atoms from bridging carboxylate groups.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Co_2(C_8H_4NO_6)_2(C_{12}H_8N_2)_4]$-$(C_8H_4NO_6)_2{\cdot}4H_2O$
M_r	1743.16
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	273
a, b, c (Å)	12.0908 (9), 13.2379 (15), 14.0783 (14)
α, β, γ (°)	111.315 (10), 92.136 (7), 114.312 (9)
V (Å^3)	1866.1 (4)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.32
Crystal size (mm)	0.2 × 0.1 × 0.05
Data collection	
Diffractometer	XCalibur
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.931, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13202, 7530, 3848
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.072, 0.192, 0.99
No. of reflections	7530
No. of parameters	578
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.35

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*) and *CrystalExplorer21.5* (Spackman *et al.*, 2021).

The title compound displays structural features characteristic of both families, combining a centrosymmetric dinuclear cobalt(II) core bridged by hydrogen 4-nitrophthalate ligands with chelating 1,10-phenanthroline ligands. A search of the current version of the CSD revealed no previously reported cobalt(II) complex containing both 1,10-phenanthroline and 4-nitrophthalate ligands. To the best of our knowledge, the present structure therefore represents the first crystallographically characterized example of this type.

6. Synthesis and crystallization

The title compound was synthesized from cobalt(II) chloride hexahydrate, 4-nitrophthalic acid and 1,10-phenanthroline using a molar ratio of 1:1:0.5. 4-Nitrophthalic acid (1.00 mmol, 0.211 g) was dissolved in *N,N*-dimethylformamide (DMF), 1,10-phenanthroline (0.50 mmol, 0.090 g) in ethanol, and cobalt(II) chloride hexahydrate (1.00 mmol, 0.238 g) in distilled water. The solutions of 4-nitrophthalic acid and cobalt(II) chloride hexahydrate were mixed and stirred magnetically for 20 min, after which the 1,10-phenanthroline solution was added dropwise. The resulting reaction mixture was stirred at 333 ± 0.5 K for a further 20 min. The clear solution was then left to stand at room temperature in a loosely covered vessel at pH ≃ 6.0. After 12 days, bright-red prismatic crystals suitable for single-crystal X-ray diffraction analysis were obtained. The crystals were collected by filtration and dried in air.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms of the carboxylic acid groups were located in difference-Fourier maps and subsequently refined using a riding model with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O). The nitro group of the coordinated hydrogen 4-nitrophthalate ligand is disordered over two orientations and was refined using a split-atom model with refined site-occupancy factors of 0.51 (1) and 0.49 (1). Similarity restraints were applied to the N—O bond distances and anisotropic displacement parameters of the disordered atoms. Two solvent oxygen atoms (O1*W* and O2*W*), assigned to water molecules of crystallization, were located in difference-Fourier maps and refined anisotropically. The corresponding hydrogen atoms could not be identified reliably in difference-Fourier maps and were therefore not included in the refinement.

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supporting information

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A new supramolecular cobalt(II) complex based on 1,10-phenanthroline and 4-nitrophthalate ligands

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Computing details

Bis(*μ*-2-carboxy-4-nitrobenzoato-*κ*^{2}*O*^{1}:*O*$^{1'}$)bis[bis(1,10-phenanthroline-*κ*^{2}*N*,*N*′)cobalt(II)] bis(2-carboxy-4-nitrobenzoate) tetrahydrate

Crystal data

$[Co_2(C_8H_4NO_6)_2(C_{12}H_8N_2)_4](C_8H_4NO_6)_2\cdot 4H_2O$
M_r = 1743.16
Triclinic, $P\overline{1}$
a = 12.0908 (9) Å
b = 13.2379 (15) Å
c = 14.0783 (14) Å
α = 111.315 (10)°
β = 92.136 (7)°
γ = 114.312 (9)°
V = 1866.1 (4) Å^3
Z = 1
$F(000)$ = 890
D_x = 1.551 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1481 reflections
θ = 3.5–76.0°
μ = 4.32 mm^{-1}
T = 273 K
Prism, red
0.2 × 0.1 × 0.05 mm

Data collection

XCalibur diffractometer
ω scans
Absorption correction: multi-scan (CrysAlisPro; Agilent, 2014)
T_{min} = 0.931, T_{max} = 1.000
13202 measured reflections
7530 independent reflections
3848 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 76.0°, θ_{min} = 3.5°
h = −9→15
k = −16→14
l = −16→17
3 standard reflections every 100 reflections
intensity decay: 2.6%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.192
S = 0.99
7530 reflections
578 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.63780 (7)	0.45259 (8)	0.58202 (7)	0.0501 (2)	
O6	0.5074 (3)	0.5019 (3)	0.4000 (3)	0.0529 (8)	
O5	0.6897 (3)	0.5301 (3)	0.4768 (3)	0.0573 (9)	
O4	0.5934 (4)	0.4004 (4)	0.2137 (3)	0.0831 (13)	
N5	0.5321 (4)	0.2729 (4)	0.4639 (3)	0.0549 (11)	
N4	0.5800 (4)	0.3470 (4)	0.6715 (3)	0.0549 (11)	
N3	0.7613 (4)	0.6286 (4)	0.6985 (3)	0.0572 (11)	
N2	0.8139 (4)	0.4459 (4)	0.5925 (3)	0.0535 (10)	
N6	0.0849 (5)	0.6768 (5)	0.2091 (4)	0.0727 (14)	
O12	0.1791 (4)	0.3410 (4)	0.0291 (4)	0.0993 (16)	
O3	0.5422 (5)	0.4770 (5)	0.1104 (3)	0.1009 (16)	
H3	0.502126	0.404406	0.071380	0.151*	
C32	0.0050 (5)	0.5470 (5)	0.1446 (4)	0.0575 (13)	
C34	−0.0120 (5)	0.3480 (5)	0.0469 (4)	0.0541 (13)	
O11	0.0133 (5)	0.1661 (4)	−0.0429 (4)	0.121 (2)	
H11A	−0.062094	0.139988	−0.047965	0.182*	
C29	0.8381 (5)	0.3532 (6)	0.5451 (5)	0.0650 (15)	
H29	0.771860	0.277347	0.504139	0.078*	
C31	0.9116 (4)	0.5571 (5)	0.6515 (4)	0.0507 (12)	
O10	0.1954 (4)	0.7124 (4)	0.2352 (4)	0.1085 (18)	
C8	0.6257 (5)	0.5512 (5)	0.4216 (4)	0.0533 (12)	
C35	−0.1421 (5)	0.2998 (5)	0.0286 (4)	0.0580 (13)	
C33	0.0596 (5)	0.4727 (5)	0.1059 (4)	0.0587 (13)	
H33	0.145924	0.506035	0.119276	0.070*	
C30	0.8836 (4)	0.6554 (5)	0.7057 (4)	0.0543 (13)	
C20	0.5052 (5)	0.2269 (5)	0.6125 (5)	0.0603 (14)	
O8	−0.3482 (5)	0.1418 (5)	−0.0361 (5)	0.138 (2)	
C18	0.5107 (5)	0.2382 (5)	0.3611 (4)	0.0650 (15)	
H18	0.548094	0.295772	0.334311	0.078*	
C19	0.4786 (5)	0.1873 (5)	0.5010 (4)	0.0594 (13)	
C7	0.6005 (6)	0.4889 (7)	0.1984 (5)	0.0717 (17)	
O9	0.0352 (5)	0.7429 (4)	0.2350 (5)	0.130 (2)	
C23	0.9800 (5)	0.7720 (5)	0.7650 (5)	0.0673 (15)	
C26	1.0366 (5)	0.5777 (6)	0.6641 (5)	0.0653 (15)	
C37	−0.1213 (5)	0.5033 (6)	0.1252 (5)	0.0715 (17)	
H37	−0.157196	0.555220	0.150060	0.086*	
C36	−0.1936 (5)	0.3802 (5)	0.0679 (5)	0.0683 (16)	
H36	−0.279661	0.349082	0.054714	0.082*	
C39	0.0671 (6)	0.2821 (6)	0.0091 (5)	0.0730 (17)	

C9	0.6056 (5)	0.3854 (6)	0.7739 (5)	0.0685 (16)	
H9	0.656358	0.467758	0.815176	0.082*	
O7	−0.2078 (5)	0.0856 (4)	−0.0594 (5)	0.134 (2)	
C25	1.1324 (5)	0.6983 (7)	0.7233 (5)	0.0771 (18)	
H25	1.214947	0.712587	0.729719	0.093*	
C10	0.5582 (6)	0.3052 (7)	0.8228 (5)	0.0783 (19)	
H10	0.578271	0.334874	0.895220	0.094*	
C40	0.7333 (5)	0.7166 (5)	0.7505 (5)	0.0701 (17)	
H40	0.649847	0.698499	0.746163	0.084*	
C28	0.9600 (6)	0.3637 (7)	0.5538 (5)	0.0770 (18)	
H28	0.973335	0.296045	0.521427	0.092*	
C38	−0.2404 (7)	0.1660 (6)	−0.0278 (5)	0.0808 (19)	
C17	0.4331 (6)	0.1173 (6)	0.2923 (5)	0.0811 (19)	
H17	0.421146	0.095545	0.220702	0.097*	
C27	1.0572 (6)	0.4764 (7)	0.6112 (5)	0.0772 (19)	
H27	1.138242	0.486258	0.615381	0.093*	
C15	0.3986 (6)	0.0643 (5)	0.4358 (6)	0.0768 (18)	
C24	1.1069 (5)	0.7926 (7)	0.7706 (5)	0.085 (2)	
H24	1.171526	0.870970	0.806768	0.102*	
C12	0.4542 (6)	0.1423 (6)	0.6554 (6)	0.0753 (17)	
C16	0.3757 (6)	0.0321 (6)	0.3275 (5)	0.086 (2)	
H16	0.321369	−0.047351	0.281117	0.104*	
C11	0.4843 (6)	0.1861 (7)	0.7649 (6)	0.0806 (19)	
H11	0.453254	0.132920	0.796878	0.097*	
C22	0.9462 (6)	0.8645 (6)	0.8177 (5)	0.086 (2)	
H22	1.007077	0.944291	0.856043	0.104*	
C21	0.8231 (6)	0.8357 (6)	0.8119 (6)	0.085 (2)	
H21	0.799544	0.895001	0.848520	0.102*	
C14	0.3459 (7)	−0.0191 (6)	0.4830 (6)	0.098 (2)	
H14	0.291867	−0.100385	0.440788	0.117*	
C13	0.3730 (7)	0.0181 (6)	0.5869 (6)	0.089 (2)	
H13	0.338160	−0.038425	0.615184	0.106*	
C1	0.6950 (5)	0.6438 (5)	0.3808 (5)	0.0634 (15)	
C2	0.7699 (6)	0.7631 (6)	0.4538 (7)	0.093 (2)	
H2	0.782074	0.780983	0.524832	0.112*	
C4	0.8068 (7)	0.8263 (8)	0.3159 (9)	0.105 (3)	
H4	0.844534	0.888375	0.293977	0.126*	0.402 (7)
C5	0.7353 (6)	0.7117 (7)	0.2422 (6)	0.086 (2)	
H5	0.725177	0.695380	0.171541	0.103*	
C6	0.6763 (5)	0.6172 (6)	0.2756 (5)	0.0659 (15)	
N1	0.8655 (10)	0.9355 (10)	0.3002 (11)	0.105 (4)	0.598 (7)
O1	0.947 (2)	1.0306 (18)	0.3634 (16)	0.228 (13)	0.598 (7)
O2	0.8274 (10)	0.9203 (8)	0.2134 (8)	0.119 (4)	0.598 (7)
O1A	0.8979 (19)	1.0175 (17)	0.5584 (17)	0.154 (9)	0.402 (7)
N1A	0.8839 (17)	0.9840 (18)	0.467 (2)	0.125 (9)	0.402 (7)
O2A	0.919 (2)	1.0523 (18)	0.414 (2)	0.137 (12)	0.402 (7)
C3	0.8262 (8)	0.8554 (8)	0.4204 (10)	0.122 (3)	
H3A	0.876183	0.935342	0.468435	0.147*	0.598 (7)

O1W	0.3637 (5)	0.2669 (5)	−0.0019 (3)	0.1107 (18)
O2W	0.3993 (5)	0.0657 (6)	0.9609 (4)	0.153 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0440 (4)	0.0457 (4)	0.0549 (5)	0.0204 (3)	0.0095 (3)	0.0152 (4)
O6	0.0457 (19)	0.053 (2)	0.060 (2)	0.0243 (16)	0.0158 (16)	0.0210 (17)
O5	0.0468 (19)	0.070 (2)	0.068 (2)	0.0323 (18)	0.0182 (17)	0.035 (2)
O4	0.109 (4)	0.083 (3)	0.075 (3)	0.054 (3)	0.036 (3)	0.037 (3)
N5	0.054 (2)	0.048 (2)	0.060 (3)	0.024 (2)	0.010 (2)	0.019 (2)
N4	0.048 (2)	0.062 (3)	0.063 (3)	0.028 (2)	0.018 (2)	0.029 (2)
N3	0.057 (3)	0.050 (2)	0.059 (3)	0.026 (2)	0.007 (2)	0.017 (2)
N2	0.059 (3)	0.053 (3)	0.058 (3)	0.031 (2)	0.016 (2)	0.025 (2)
N6	0.083 (4)	0.055 (3)	0.075 (3)	0.031 (3)	0.019 (3)	0.021 (3)
O12	0.067 (3)	0.085 (3)	0.132 (4)	0.040 (3)	0.020 (3)	0.024 (3)
O3	0.136 (4)	0.116 (4)	0.069 (3)	0.075 (4)	0.022 (3)	0.037 (3)
C32	0.063 (3)	0.047 (3)	0.056 (3)	0.021 (3)	0.014 (3)	0.019 (3)
C34	0.060 (3)	0.051 (3)	0.053 (3)	0.027 (3)	0.013 (2)	0.022 (3)
O11	0.110 (4)	0.074 (3)	0.145 (5)	0.055 (3)	0.004 (4)	−0.005 (3)
C29	0.067 (4)	0.072 (4)	0.073 (4)	0.042 (3)	0.025 (3)	0.035 (3)
C31	0.044 (3)	0.063 (3)	0.055 (3)	0.027 (2)	0.013 (2)	0.032 (3)
O10	0.074 (3)	0.063 (3)	0.132 (5)	0.017 (2)	0.002 (3)	0.000 (3)
C8	0.050 (3)	0.050 (3)	0.056 (3)	0.024 (2)	0.017 (2)	0.016 (2)
C35	0.059 (3)	0.049 (3)	0.055 (3)	0.016 (3)	0.017 (3)	0.020 (3)
C33	0.062 (3)	0.055 (3)	0.058 (3)	0.025 (3)	0.011 (3)	0.024 (3)
C30	0.044 (3)	0.058 (3)	0.058 (3)	0.020 (2)	0.009 (2)	0.025 (3)
C20	0.054 (3)	0.048 (3)	0.079 (4)	0.025 (3)	0.016 (3)	0.026 (3)
O8	0.069 (3)	0.081 (4)	0.193 (6)	0.004 (3)	0.037 (4)	0.017 (4)
C18	0.078 (4)	0.058 (3)	0.057 (3)	0.034 (3)	0.009 (3)	0.020 (3)
C19	0.062 (3)	0.049 (3)	0.062 (3)	0.024 (3)	0.011 (3)	0.019 (3)
C7	0.083 (4)	0.101 (5)	0.062 (4)	0.059 (4)	0.039 (3)	0.044 (4)
O9	0.114 (4)	0.061 (3)	0.181 (6)	0.050 (3)	0.018 (4)	0.004 (3)
C23	0.057 (3)	0.062 (4)	0.075 (4)	0.020 (3)	0.006 (3)	0.030 (3)
C26	0.054 (3)	0.093 (5)	0.062 (3)	0.035 (3)	0.023 (3)	0.042 (3)
C37	0.068 (4)	0.066 (4)	0.084 (4)	0.037 (3)	0.027 (3)	0.027 (3)
C36	0.052 (3)	0.066 (4)	0.086 (4)	0.026 (3)	0.022 (3)	0.032 (3)
C39	0.084 (5)	0.064 (4)	0.070 (4)	0.041 (4)	0.010 (3)	0.019 (3)
C9	0.057 (3)	0.082 (4)	0.064 (4)	0.037 (3)	0.011 (3)	0.021 (3)
O7	0.101 (4)	0.053 (3)	0.181 (6)	0.026 (3)	−0.002 (4)	−0.006 (3)
C25	0.043 (3)	0.103 (5)	0.086 (5)	0.025 (3)	0.012 (3)	0.050 (4)
C10	0.081 (4)	0.118 (6)	0.064 (4)	0.057 (4)	0.026 (3)	0.052 (4)
C40	0.061 (3)	0.047 (3)	0.082 (4)	0.026 (3)	0.005 (3)	0.006 (3)
C28	0.097 (5)	0.099 (5)	0.078 (4)	0.071 (4)	0.038 (4)	0.048 (4)
C38	0.087 (5)	0.061 (4)	0.080 (5)	0.026 (4)	0.020 (4)	0.024 (3)
C17	0.099 (5)	0.059 (4)	0.064 (4)	0.033 (4)	−0.002 (4)	0.008 (3)
C27	0.074 (4)	0.122 (6)	0.083 (5)	0.067 (4)	0.040 (4)	0.063 (5)
C15	0.077 (4)	0.049 (3)	0.093 (5)	0.022 (3)	0.012 (4)	0.025 (3)

C24	0.051 (3)	0.084 (5)	0.090 (5)	0.004 (3)	0.001 (3)	0.037 (4)
C12	0.070 (4)	0.073 (4)	0.092 (5)	0.032 (3)	0.024 (4)	0.043 (4)
C16	0.094 (5)	0.049 (4)	0.080 (5)	0.021 (3)	−0.009 (4)	0.006 (3)
C11	0.083 (5)	0.088 (5)	0.088 (5)	0.044 (4)	0.023 (4)	0.048 (4)
C22	0.080 (4)	0.053 (4)	0.085 (5)	0.011 (3)	−0.001 (4)	0.009 (3)
C21	0.081 (4)	0.052 (4)	0.102 (5)	0.031 (3)	0.003 (4)	0.011 (4)
C14	0.106 (6)	0.045 (4)	0.116 (7)	0.020 (4)	0.016 (5)	0.023 (4)
C13	0.101 (5)	0.063 (4)	0.103 (6)	0.027 (4)	0.032 (4)	0.046 (4)
C1	0.048 (3)	0.068 (4)	0.085 (4)	0.031 (3)	0.017 (3)	0.038 (3)
C2	0.065 (4)	0.063 (4)	0.122 (6)	0.012 (3)	0.013 (4)	0.028 (4)
C4	0.067 (5)	0.085 (6)	0.179 (9)	0.025 (4)	0.035 (6)	0.081 (7)
C5	0.070 (4)	0.100 (6)	0.115 (6)	0.042 (4)	0.037 (4)	0.067 (5)
C6	0.056 (3)	0.070 (4)	0.092 (5)	0.037 (3)	0.030 (3)	0.044 (4)
N1	0.086 (7)	0.081 (8)	0.123 (10)	−0.004 (6)	−0.005 (7)	0.068 (8)
O1	0.23 (2)	0.153 (15)	0.138 (14)	−0.074 (13)	−0.068 (14)	0.089 (12)
O2	0.141 (9)	0.092 (7)	0.120 (8)	0.025 (6)	0.020 (6)	0.072 (6)
O1A	0.141 (16)	0.096 (13)	0.19 (2)	0.059 (11)	0.008 (16)	0.012 (14)
N1A	0.068 (10)	0.073 (13)	0.20 (3)	0.021 (9)	0.017 (15)	0.038 (16)
O2A	0.087 (10)	0.063 (10)	0.28 (4)	0.027 (9)	0.078 (17)	0.101 (17)
C3	0.092 (6)	0.074 (6)	0.190 (11)	0.026 (5)	0.031 (7)	0.059 (7)
O1W	0.107 (4)	0.131 (5)	0.097 (4)	0.071 (4)	0.023 (3)	0.030 (3)
O2W	0.098 (4)	0.147 (6)	0.254 (8)	0.048 (4)	0.053 (5)	0.132 (6)

Geometric parameters (Å, º)

Co1—O5	2.070 (4)	C26—C27	1.406 (9)
Co1—O6^{i}	2.073 (3)	C26—C25	1.422 (9)
Co1—N5	2.126 (4)	C37—C36	1.374 (8)
Co1—N3	2.126 (4)	C37—H37	0.9300
Co1—N4	2.137 (5)	C36—H36	0.9300
Co1—N2	2.169 (4)	C9—C10	1.410 (8)
O6—C8	1.273 (6)	C9—H9	0.9300
O5—C8	1.254 (6)	O7—C38	1.225 (8)
O4—C7	1.237 (7)	C25—C24	1.351 (9)
N5—C18	1.328 (7)	C25—H25	0.9300
N5—C19	1.351 (7)	C10—C11	1.342 (9)
N4—C9	1.319 (7)	C10—H10	0.9300
N4—C20	1.355 (7)	C40—C21	1.393 (8)
N3—C40	1.316 (6)	C40—H40	0.9300
N3—C30	1.361 (6)	C28—C27	1.368 (9)
N2—C29	1.324 (7)	C28—H28	0.9300
N2—C31	1.363 (6)	C17—C16	1.336 (9)
N6—O10	1.210 (6)	C17—H17	0.9300
N6—O9	1.215 (6)	C27—H27	0.9300
N6—C32	1.464 (7)	C15—C16	1.407 (9)
O12—C39	1.209 (7)	C15—C14	1.432 (9)
O3—C7	1.326 (7)	C24—H24	0.9300
O3—H3	0.8200	C12—C11	1.407 (9)

C32—C33	1.367 (7)	C12—C13	1.430 (9)
C32—C37	1.367 (7)	C16—H16	0.9300
C34—C33	1.392 (7)	C11—H11	0.9300
C34—C35	1.404 (7)	C22—C21	1.366 (9)
C34—C39	1.532 (7)	C22—H22	0.9300
O11—C39	1.281 (7)	C21—H21	0.9300
O11—H11A	0.8200	C14—C13	1.342 (9)
C29—C28	1.418 (8)	C14—H14	0.9300
C29—H29	0.9300	C13—H13	0.9300
C31—C26	1.412 (7)	C1—C6	1.378 (8)
C31—C30	1.432 (7)	C1—C2	1.394 (9)
C8—C1	1.496 (8)	C2—C3	1.391 (11)
C35—C36	1.403 (7)	C2—H2	0.9300
C35—C38	1.534 (8)	C4—C5	1.354 (11)
C33—H33	0.9300	C4—C3	1.363 (13)
C30—C23	1.395 (8)	C4—N1	1.428 (12)
C20—C12	1.398 (8)	C4—H4	0.9300
C20—C19	1.437 (8)	C5—C6	1.418 (8)
O8—C38	1.197 (8)	C5—H5	0.9300
C18—C17	1.396 (8)	N1—O2	1.204 (13)
C18—H18	0.9300	N1—O1	1.20 (2)
C19—C15	1.407 (8)	O1A—N1A	1.18 (3)
C7—C6	1.485 (9)	N1A—O2A	1.32 (3)
C23—C22	1.411 (9)	N1A—C3	1.41 (2)
C23—C24	1.437 (8)	C3—H3A	0.9300

O5—Co1—O6^{i}	91.94 (13)	O12—C39—O11	121.6 (6)
O5—Co1—N5	94.13 (16)	O12—C39—C34	119.1 (6)
O6^{i}—Co1—N5	96.86 (15)	O11—C39—C34	119.3 (6)
O5—Co1—N3	85.40 (17)	N4—C9—C10	121.9 (6)
O6^{i}—Co1—N3	89.61 (15)	N4—C9—H9	119.0
N5—Co1—N3	173.52 (16)	C10—C9—H9	119.0
O5—Co1—N4	171.16 (16)	C24—C25—C26	121.8 (6)
O6^{i}—Co1—N4	92.48 (15)	C24—C25—H25	119.1
N5—Co1—N4	77.74 (18)	C26—C25—H25	119.1
N3—Co1—N4	102.28 (17)	C11—C10—C9	120.1 (6)
O5—Co1—N2	87.92 (15)	C11—C10—H10	120.0
O6^{i}—Co1—N2	166.84 (15)	C9—C10—H10	120.0
N5—Co1—N2	96.27 (16)	N3—C40—C21	122.9 (6)
N3—Co1—N2	77.25 (16)	N3—C40—H40	118.5
N4—Co1—N2	89.51 (16)	C21—C40—H40	118.5
C8—O6—Co1^{i}	140.8 (3)	C27—C28—C29	118.0 (6)
C8—O5—Co1	128.7 (3)	C27—C28—H28	121.0
C18—N5—C19	118.3 (5)	C29—C28—H28	121.0
C18—N5—Co1	127.5 (4)	O8—C38—O7	121.0 (7)
C19—N5—Co1	114.1 (4)	O8—C38—C35	119.0 (6)
C9—N4—C20	118.3 (5)	O7—C38—C35	119.9 (6)
C9—N4—Co1	128.1 (4)	C16—C17—C18	121.2 (7)

C20—N4—Co1	113.6 (4)	C16—C17—H17	119.4
C40—N3—C30	118.3 (5)	C18—C17—H17	119.4
C40—N3—Co1	127.0 (4)	C28—C27—C26	121.0 (6)
C30—N3—Co1	113.9 (3)	C28—C27—H27	119.5
C29—N2—C31	118.0 (5)	C26—C27—H27	119.5
C29—N2—Co1	129.2 (4)	C19—C15—C16	116.9 (6)
C31—N2—Co1	112.6 (3)	C19—C15—C14	118.6 (6)
O10—N6—O9	123.5 (6)	C16—C15—C14	124.5 (6)
O10—N6—C32	118.9 (5)	C25—C24—C23	120.1 (6)
O9—N6—C32	117.6 (5)	C25—C24—H24	120.0
C7—O3—H3	109.5	C23—C24—H24	120.0
C33—C32—C37	121.9 (5)	C20—C12—C11	117.3 (6)
C33—C32—N6	118.7 (5)	C20—C12—C13	118.8 (6)
C37—C32—N6	119.4 (5)	C11—C12—C13	123.9 (7)
C33—C34—C35	118.3 (5)	C17—C16—C15	119.1 (6)
C33—C34—C39	112.7 (5)	C17—C16—H16	120.4
C35—C34—C39	129.0 (5)	C15—C16—H16	120.4
C39—O11—H11A	109.5	C10—C11—C12	119.5 (7)
N2—C29—C28	123.3 (6)	C10—C11—H11	120.3
N2—C29—H29	118.4	C12—C11—H11	120.3
C28—C29—H29	118.4	C21—C22—C23	119.4 (6)
N2—C31—C26	123.2 (5)	C21—C22—H22	120.3
N2—C31—C30	117.3 (4)	C23—C22—H22	120.3
C26—C31—C30	119.4 (5)	C22—C21—C40	119.4 (6)
O5—C8—O6	124.9 (5)	C22—C21—H21	120.3
O5—C8—C1	116.9 (5)	C40—C21—H21	120.3
O6—C8—C1	118.2 (5)	C13—C14—C15	121.1 (7)
C36—C35—C34	118.4 (5)	C13—C14—H14	119.5
C36—C35—C38	113.2 (5)	C15—C14—H14	119.5
C34—C35—C38	128.3 (5)	C14—C13—C12	121.7 (7)
C32—C33—C34	121.0 (5)	C14—C13—H13	119.1
C32—C33—H33	119.5	C12—C13—H13	119.1
C34—C33—H33	119.5	C6—C1—C2	120.2 (7)
N3—C30—C23	122.9 (5)	C6—C1—C8	122.0 (6)
N3—C30—C31	117.2 (5)	C2—C1—C8	117.4 (6)
C23—C30—C31	119.9 (5)	C3—C2—C1	119.9 (9)
N4—C20—C12	122.9 (6)	C3—C2—H2	120.0
N4—C20—C19	117.3 (5)	C1—C2—H2	120.0
C12—C20—C19	119.8 (6)	C5—C4—C3	123.4 (9)
N5—C18—C17	121.4 (6)	C5—C4—N1	127.5 (11)
N5—C18—H18	119.3	C3—C4—N1	109.0 (10)
C17—C18—H18	119.3	C5—C4—H4	118.3
N5—C19—C15	122.9 (6)	C3—C4—H4	118.3
N5—C19—C20	117.1 (5)	C4—C5—C6	118.4 (8)
C15—C19—C20	120.0 (6)	C4—C5—H5	120.8
O4—C7—O3	122.5 (7)	C6—C5—H5	120.8
O4—C7—C6	123.2 (6)	C1—C6—C5	119.4 (7)
O3—C7—C6	114.3 (6)	C1—C6—C7	119.6 (6)

C30—C23—C22	117.1 (5)	C5—C6—C7	120.9 (7)
C30—C23—C24	119.6 (6)	O2—N1—O1	123.0 (14)
C22—C23—C24	123.2 (6)	O2—N1—C4	111.8 (11)
C27—C26—C31	116.5 (6)	O1—N1—C4	125.0 (13)
C27—C26—C25	124.5 (6)	O1A—N1A—O2A	127 (2)
C31—C26—C25	118.9 (6)	O1A—N1A—C3	108 (3)
C32—C37—C36	117.8 (5)	O2A—N1A—C3	124 (2)
C32—C37—H37	121.1	C4—C3—C2	118.7 (9)
C36—C37—H37	121.1	C4—C3—N1A	103.8 (15)
C37—C36—C35	122.4 (5)	C2—C3—N1A	136.2 (16)
C37—C36—H36	118.8	C4—C3—H3A	120.7
C35—C36—H36	118.8	C2—C3—H3A	120.7

O10—N6—C32—C33	−7.4 (9)	Co1—N3—C40—C21	−168.4 (5)
O9—N6—C32—C33	173.6 (6)	N2—C29—C28—C27	−2.3 (9)
O10—N6—C32—C37	172.2 (6)	C36—C35—C38—O8	1.9 (10)
O9—N6—C32—C37	−6.8 (9)	C34—C35—C38—O8	179.9 (7)
C31—N2—C29—C28	0.7 (8)	C36—C35—C38—O7	−174.8 (7)
Co1—N2—C29—C28	175.7 (4)	C34—C35—C38—O7	3.3 (11)
C29—N2—C31—C26	0.2 (8)	N5—C18—C17—C16	1.2 (10)
Co1—N2—C31—C26	−175.6 (4)	C29—C28—C27—C26	2.9 (9)
C29—N2—C31—C30	−177.5 (5)	C31—C26—C27—C28	−2.1 (9)
Co1—N2—C31—C30	6.7 (6)	C25—C26—C27—C28	−178.5 (6)
Co1—O5—C8—O6	−18.6 (7)	N5—C19—C15—C16	0.1 (9)
Co1—O5—C8—C1	159.8 (4)	C20—C19—C15—C16	179.4 (6)
Co1^{i}—O6—C8—O5	119.9 (5)	N5—C19—C15—C14	−179.6 (6)
Co1^{i}—O6—C8—C1	−58.5 (8)	C20—C19—C15—C14	−0.3 (9)
C33—C34—C35—C36	1.9 (8)	C26—C25—C24—C23	2.3 (10)
C39—C34—C35—C36	−177.0 (6)	C30—C23—C24—C25	−3.6 (10)
C33—C34—C35—C38	−176.1 (6)	C22—C23—C24—C25	175.9 (7)
C39—C34—C35—C38	5.0 (10)	N4—C20—C12—C11	−0.6 (9)
C37—C32—C33—C34	−1.6 (9)	C19—C20—C12—C11	179.5 (5)
N6—C32—C33—C34	178.0 (5)	N4—C20—C12—C13	178.0 (6)
C35—C34—C33—C32	−0.5 (8)	C19—C20—C12—C13	−1.9 (9)
C39—C34—C33—C32	178.6 (5)	C18—C17—C16—C15	−2.9 (11)
C40—N3—C30—C23	−0.5 (9)	C19—C15—C16—C17	2.2 (10)
Co1—N3—C30—C23	169.7 (5)	C14—C15—C16—C17	−178.1 (7)
C40—N3—C30—C31	177.7 (5)	C9—C10—C11—C12	−0.3 (10)
Co1—N3—C30—C31	−12.1 (6)	C20—C12—C11—C10	0.7 (10)
N2—C31—C30—N3	3.5 (7)	C13—C12—C11—C10	−177.8 (7)
C26—C31—C30—N3	−174.3 (5)	C30—C23—C22—C21	2.5 (10)
N2—C31—C30—C23	−178.3 (5)	C24—C23—C22—C21	−177.1 (7)
C26—C31—C30—C23	3.9 (8)	C23—C22—C21—C40	−2.6 (11)
C9—N4—C20—C12	0.1 (8)	N3—C40—C21—C22	1.2 (12)
Co1—N4—C20—C12	−178.2 (4)	C19—C15—C14—C13	−1.0 (11)
C9—N4—C20—C19	179.9 (5)	C16—C15—C14—C13	179.3 (7)
Co1—N4—C20—C19	1.7 (6)	C15—C14—C13—C12	0.8 (12)
C19—N5—C18—C17	1.2 (8)	C20—C12—C13—C14	0.7 (11)

Co1—N5—C18—C17	−176.2 (4)	C11—C12—C13—C14	179.2 (7)
C18—N5—C19—C15	−1.8 (8)	O5—C8—C1—C6	123.9 (5)
Co1—N5—C19—C15	175.9 (5)	O6—C8—C1—C6	−57.6 (7)
C18—N5—C19—C20	178.9 (5)	O5—C8—C1—C2	−63.1 (7)
Co1—N5—C19—C20	−3.4 (6)	O6—C8—C1—C2	115.3 (6)
N4—C20—C19—N5	1.2 (7)	C6—C1—C2—C3	−0.3 (10)
C12—C20—C19—N5	−179.0 (5)	C8—C1—C2—C3	−173.4 (6)
N4—C20—C19—C15	−178.2 (5)	C3—C4—C5—C6	0.8 (13)
C12—C20—C19—C15	1.7 (8)	N1—C4—C5—C6	−174.3 (9)
N3—C30—C23—C22	−0.9 (9)	C2—C1—C6—C5	1.0 (8)
C31—C30—C23—C22	−179.1 (5)	C8—C1—C6—C5	173.8 (5)
N3—C30—C23—C24	178.6 (5)	C2—C1—C6—C7	177.5 (5)
C31—C30—C23—C24	0.5 (9)	C8—C1—C6—C7	−9.7 (8)
N2—C31—C26—C27	0.5 (8)	C4—C5—C6—C1	−1.2 (9)
C30—C31—C26—C27	178.1 (5)	C4—C5—C6—C7	−177.8 (6)
N2—C31—C26—C25	177.1 (5)	O4—C7—C6—C1	−29.9 (9)
C30—C31—C26—C25	−5.2 (8)	O3—C7—C6—C1	151.2 (5)
C33—C32—C37—C36	2.1 (9)	O4—C7—C6—C5	146.6 (6)
N6—C32—C37—C36	−177.4 (6)	O3—C7—C6—C5	−32.3 (8)
C32—C37—C36—C35	−0.6 (10)	C5—C4—N1—O2	12.5 (18)
C34—C35—C36—C37	−1.4 (9)	C3—C4—N1—O2	−163.2 (12)
C38—C35—C36—C37	176.9 (6)	C5—C4—N1—O1	−164.2 (19)
C33—C34—C39—O12	−2.5 (9)	C3—C4—N1—O1	20 (2)
C35—C34—C39—O12	176.5 (6)	C5—C4—C3—C2	−0.1 (14)
C33—C34—C39—O11	177.4 (6)	N1—C4—C3—C2	175.8 (8)
C35—C34—C39—O11	−3.6 (10)	C5—C4—C3—N1A	−169.0 (11)
C20—N4—C9—C10	0.4 (8)	C1—C2—C3—C4	−0.2 (13)
Co1—N4—C9—C10	178.4 (4)	C1—C2—C3—N1A	164.1 (15)
C27—C26—C25—C24	178.5 (6)	O1A—N1A—C3—C4	176.0 (18)
C31—C26—C25—C24	2.2 (10)	O2A—N1A—C3—C4	−6 (2)
N4—C9—C10—C11	−0.3 (9)	O1A—N1A—C3—C2	10 (3)
C30—N3—C40—C21	0.4 (10)	O2A—N1A—C3—C2	−172.0 (15)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1*W*	0.82	1.78	2.549 (8)	155
O11—H11*A*···O7	0.82	1.58	2.400 (8)	178
C18—H18···O4	0.93	2.50	3.397 (8)	162
C9—H9···O12^{i}	0.93	2.58	3.462 (8)	158
C40—H40···O6^{i}	0.93	2.54	3.079 (6)	117
C21—H21···O7^{ii}	0.93	2.42	3.329 (8)	165
C4—H4$^{b\cdots O24}$b	0.93	2.00	2.49 (2)	112

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1, *y*+1, *z*+1.