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fac-Triaqua(2,2′-bipyridine-κ^2N,N')(nitrato-κO)-cobalt(II) chloride

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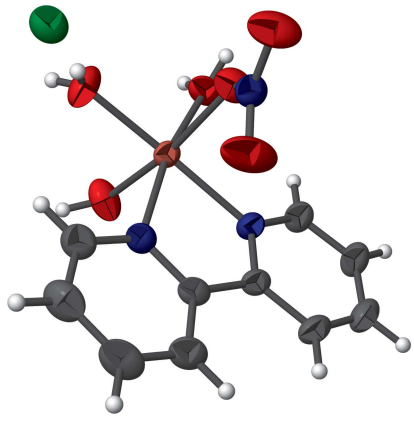
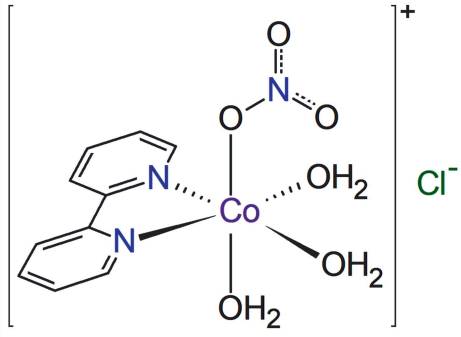
The asymmetric unit of the title complex, $[Co(NO_3)(C_{10}H_8N_2)(H_2O)_3]Cl$, consists of a chloride anion and a complex cation, which is built on a monodentate nitrate anion, three water molecules and one bidentate 2,2′-bipyridine molecule, coordinated to a Co^{II} cation, in a distorted octahedral geometry. The water molecules are arranged in a *facial* geometry, and serve as donors for hydrogen bonding. Acceptor sites in the crystal are chloride ions and one O atom of the coordinating nitrate ion. A three-dimensional framework is formed, based on O—H···O and O—H···Cl contacts.

3D view



Chemical scheme



Structure description

As a component of several enzymes, vitamins, proteins and nucleic acids, pyridine derivatives have a main role in many biological systems. Some complexes containing 2,2′-bipyridine (bipy) have been reported to present antibacterial activity (El-Hamid *et al.*, 2017; Lu *et al.*, 2015; Segura *et al.*, 2014), including cobalt complexes (Buriez *et al.*, 2006; Gu *et al.*, 2017). It can be expected that the combination of the high bactericidal activity of bipy and a cobalt cation may lead to a compound of interest. In this dynamic, we have initiated the study of the interaction between $[Na_3Co(NO_2)_6]$, dimethylammonium chloride and bipy. The complex reported herein results from a redox process over the cobalt complex used as starting material, when the reaction is carried out in acetone and in a non-controlled atmosphere: the nitrite anion NO_2^- behaves as a reducing agent to reduce Co^{III} to Co^{II}, and is in turn oxidized to form nitrate ions NO_3^-. A stable cation complex $[Co(bipy)(OH_2)_3(NO_3)]^+$ is then formed, which crystallizes as a chloride salt in presence of $[NH_2Me_2]^+Cl^-$.

The asymmetric unit of the title compound (Fig. 1) consists of a chloride anion and a complex cation containing a chelating 2,2′-bipyridine molecule, a monocoordinating

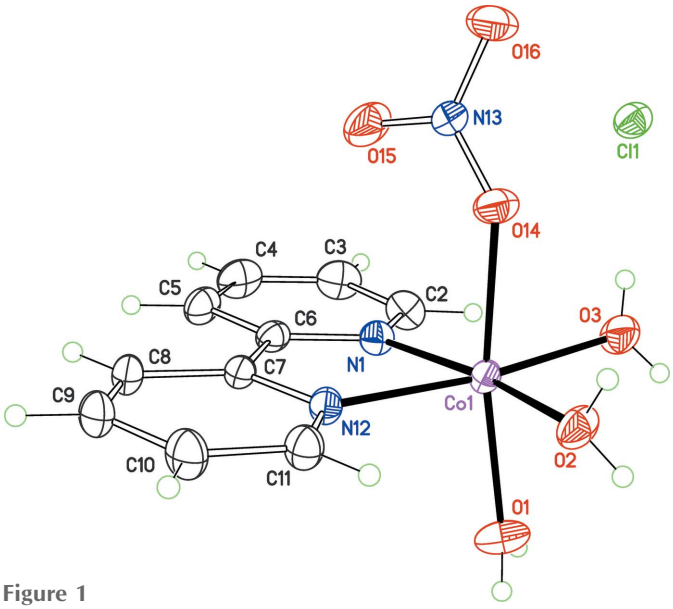


Figure 1
The structure of the complex cation and the anion in the title compound, with displacement ellipsoids for non-H atoms at the 30% probability level.

nitrate anion and three water molecules to complete the octahedral coordination sphere around the cobalt cation. Coordination bond lengths are in the small range 2.0300 (16)–2.1769 (15) Å, indicating that the ligand field should be small enough to stabilize a high spin $3d^7$ metal configuration, reflected in the limited Jahn–Teller tetragonal distortion. Using the octahedral symmetry measure defined by Alvarez *et al.* (2002), $S(O_h) = 5.39\Delta^2 - 0.33|\Delta|$, where Δ is the difference between long and short distances, we compute $S(O_h) = 0.07$ for the cation, close to the measure expected for an ideal octahedral field, $S(O_h) = 0$. The coordinating water molecules have a *facial* geometry, with the longest Co—OH_2 bond displayed by the axial water molecule O1 (Abboud *et al.*, 1996; Johnson *et al.*, 2015). The nitrate ion is placed *trans* to this water molecule, forming an angle O1—Co1—O14 of 170.47 (7)°. The equatorial plane includes the chelating bipy ligand and two water molecules, at normal distances (Xiao, 2006; Gong *et al.*, 2012). The planarity of this $[CoO_2N_2]$ core is confirmed by the sum of the four *cis* angles, 360.0 (3)°. The distortion from the octahedral symmetry results essentially from the bipy bite angle, N1—Co1—N12 = 77.37 (6)°. The metal is displaced by 0.04 Å from the equatorial mean plane. A similar arrangement was observed with other cations $[M(\text{bipy})(OH_2)_3(NO_3)]^+$ using different transition metals, *M* = Mn (Zhang *et al.*, 2002), *M* = Ni (Walmsley *et al.*, 1989; Rujiwatra *et al.*, 2012), *M* = Cu (Mathews & Manohar, 1991) and *M* = Zn (Harrowfield *et al.*, 2017).

Coordinating water molecules are oriented in such a way that all O—H groups serve as donors to form weak hydrogen bonds with chloride ions and atom O16 of the nitrate ion (Table 1). Each complex cation is then directly linked to four neighbours through intermolecular O—H···O bonds, and the supramolecular structure is extended to a three-dimensional framework through $R_4^2(8)$ ring motifs based on O—H···Cl bonds (Fig. 2). The relative orientation of the cations in the crystal resulting from this supramolecular structure does not prevent π–π interactions between bipy ligands: two cations related by inversion have their bipy parts placed parallel, with a separation between the mean planes of 3.375 Å.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···Cl1^{i}	0.85 (4)	2.33 (4)	3.1560 (19)	166 (4)
O1—H12···O16^{ii}	0.73 (3)	2.13 (3)	2.825 (2)	160 (4)
O2—H21···Cl1^{iii}	0.81 (4)	2.39 (4)	3.1833 (18)	167 (3)
O2—H22···Cl1^{ii}	0.74 (4)	2.37 (4)	3.1088 (16)	177 (4)
O3—H31···Cl1	0.74 (4)	2.36 (4)	3.100 (2)	176 (3)
O3—H32···O16^{i}	0.77 (4)	1.98 (4)	2.745 (2)	178 (4)

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

Synthesis and crystallization

All chemicals were purchased from Aldrich Company and used as received. Sodium hexanitrocobaltate(III) $[Na_3Co(NO_2)_6]$ (125 mg, 0.309 mmol), dimethylammonium chloride (25 mg, 0.309 mmol) and 2,2′-bipyridine (48 mg, 0.309 mmol) were mixed together at room temperature in slightly hydrated acetone. The resulting solution was stirred for about two h at 303 K. After a week of slow evaporation at room temperature, orange crystals suitable for X-ray crystallographic analysis were obtained.

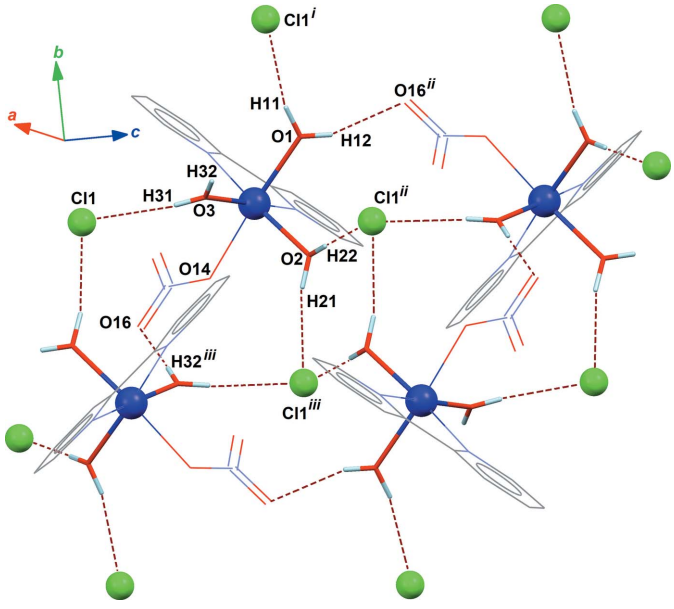


Figure 2
Part of the crystal structure of the title compound showing four cations and ten chloride forming hydrogen bonds (dashed lines). H atoms belonging to the bipy ligands have been omitted for clarity. The asymmetric unit contains the upper-left cation and Cl1. Symmetry codes: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (iii) $-x, -\frac{1}{2}+y, \frac{1}{2}-z$.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Intensities were collected at high resolution [$(\sin\theta)/\lambda$ = 0.92 Å^{-1}; d = 0.54 Å].

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(NO_3)(C_{10}H_8N_2)(H_2O)_3]Cl$
M_r	366.62
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	11.5309 (5), 8.9688 (3), 14.7820 (6)
β (°)	111.915 (3)
V (Å^3)	1418.26 (10)
Z	4
Radiation type	Ag $K\alpha$, λ = 0.56083 Å
μ (mm^{-1})	0.74
Crystal size (mm)	0.60 × 0.60 × 0.60
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Multi-scan (*X-AREA* and *X-RED32*; Stoe & Cie, 2015)
T_{min}, T_{max}	0.321, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	139350, 9203, 5851
R_{int}	0.068
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.918
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.140, 1.10
No. of reflections	9203
No. of parameters	214
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.28, −0.58

Computer programs: *X-AREA* (Stoe & Cie, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2018). **3**, x180866 [https://doi.org/10.1107/S2414314618008660]

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Crystal data

$[Co(NO_3)(C_{10}H_8N_2)(H_2O)_3]Cl$
M_r = 366.62
Monoclinic, $P2_1/c$
a = 11.5309 (5) Å
b = 8.9688 (3) Å
c = 14.7820 (6) Å
β = 111.915 (3)°
V = 1418.26 (10) Å^3
Z = 4
$F(000)$ = 748
D_x = 1.717 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56083 Å
Cell parameters from 86540 reflections
θ = 2.1–34.9°
μ = 0.74 mm^{-1}
T = 295 K
Prism, orange
0.60 × 0.60 × 0.60 mm

Data collection

Stoe Stadivari diffractometer
Radiation source: Sealed X-ray tube, Axo Astix-f Microfocus source
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (X-AREA and X-RED32; Stoe & Cie, 2015)
T_{min} = 0.321, T_{max} = 1.000
139350 measured reflections
9203 independent reflections
5851 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 31.0°, θ_{min} = 2.1°
h = −21→21
k = −16→16
l = −27→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.140
S = 1.10
9203 reflections
214 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 1.4068P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Special details

Refinement. H atoms of the bipy ligand were placed in calculated positions and refined as riding to their carrier C atoms, with U_{iso} = 1.2 U_{eq}(carrier C). In contrast, water H atoms were refined with free coordinates and free U_{iso} displacement parameters. O—H bond lengths converged to acceptable values in the range 0.73 (3)–0.85 (4) Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.18156 (2)	0.28540 (3)	0.38779 (2)	0.02773 (6)
Cl1	−0.05849 (5)	0.28742 (6)	0.06897 (4)	0.04189 (11)
N1	0.27083 (15)	0.43391 (18)	0.32300 (11)	0.0324 (3)
C2	0.2127 (2)	0.5247 (2)	0.24833 (16)	0.0422 (4)
H2A	0.126113	0.532237	0.226040	0.051*
C3	0.2760 (3)	0.6083 (3)	0.20253 (18)	0.0491 (5)
H3A	0.233048	0.669023	0.149601	0.059*
C4	0.4047 (3)	0.5986 (3)	0.23788 (19)	0.0508 (5)
H4A	0.449930	0.654775	0.209499	0.061*
C5	0.4665 (2)	0.5053 (2)	0.31573 (17)	0.0409 (4)
H5A	0.553186	0.497382	0.339837	0.049*
C6	0.39652 (17)	0.4238 (2)	0.35692 (13)	0.0309 (3)
C7	0.45350 (15)	0.3213 (2)	0.44012 (13)	0.0299 (3)
C8	0.58164 (17)	0.2946 (2)	0.48387 (16)	0.0384 (4)
H8A	0.636987	0.342089	0.460973	0.046*
C9	0.62560 (19)	0.1968 (3)	0.56154 (17)	0.0448 (5)
H9A	0.710634	0.176436	0.590586	0.054*
C10	0.5423 (2)	0.1298 (3)	0.59550 (17)	0.0451 (5)
H10A	0.570169	0.065224	0.648497	0.054*
C11	0.41622 (18)	0.1607 (2)	0.54913 (15)	0.0381 (4)
H11A	0.359795	0.115400	0.571893	0.046*
N12	0.37249 (13)	0.25299 (18)	0.47297 (11)	0.0305 (3)
N13	0.21743 (15)	0.08151 (19)	0.22784 (12)	0.0339 (3)
O14	0.18036 (16)	0.09312 (18)	0.29758 (11)	0.0418 (3)
O15	0.2944 (2)	0.1667 (2)	0.21857 (19)	0.0689 (6)
O16	0.1752 (2)	−0.0228 (2)	0.16916 (13)	0.0560 (5)
O1	0.1557 (2)	0.4565 (2)	0.47721 (14)	0.0501 (4)
H11	0.120 (4)	0.539 (5)	0.455 (3)	0.077 (11)*
H12	0.167 (3)	0.453 (4)	0.529 (2)	0.054 (9)*
O2	0.12743 (16)	0.13141 (19)	0.46916 (13)	0.0415 (3)
H21	0.107 (3)	0.048 (4)	0.450 (2)	0.056 (9)*
H22	0.085 (3)	0.153 (4)	0.494 (3)	0.070 (11)*
O3	0.00497 (15)	0.3211 (2)	0.29102 (13)	0.0484 (4)
H31	−0.011 (3)	0.309 (4)	0.238 (3)	0.053 (9)*
H32	−0.047 (3)	0.363 (4)	0.301 (3)	0.067 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02527 (9)	0.03019 (11)	0.02956 (10)	0.00029 (8)	0.01235 (7)	0.00041 (8)
Cl1	0.0487 (3)	0.0382 (2)	0.0462 (2)	−0.00178 (19)	0.0263 (2)	−0.00160 (19)
N1	0.0344 (7)	0.0314 (6)	0.0322 (6)	−0.0008 (5)	0.0135 (5)	0.0019 (5)
C2	0.0462 (10)	0.0392 (9)	0.0380 (9)	−0.0015 (8)	0.0120 (8)	0.0065 (8)
C3	0.0668 (15)	0.0416 (11)	0.0417 (10)	−0.0021 (10)	0.0233 (10)	0.0088 (8)
C4	0.0696 (15)	0.0440 (11)	0.0518 (12)	−0.0087 (11)	0.0376 (12)	0.0051 (9)

C5	0.0426 (9)	0.0408 (9)	0.0484 (10)	−0.0071 (8)	0.0276 (9)	−0.0009 (8)
C6	0.0350 (7)	0.0298 (7)	0.0327 (7)	−0.0044 (6)	0.0181 (6)	−0.0032 (6)
C7	0.0265 (6)	0.0320 (7)	0.0333 (7)	−0.0028 (5)	0.0136 (6)	−0.0051 (6)
C8	0.0246 (6)	0.0460 (10)	0.0456 (10)	−0.0023 (7)	0.0141 (6)	−0.0072 (8)
C9	0.0270 (7)	0.0536 (12)	0.0483 (11)	0.0070 (8)	0.0076 (7)	−0.0035 (9)
C10	0.0354 (9)	0.0503 (12)	0.0426 (10)	0.0078 (8)	0.0065 (8)	0.0089 (9)
C11	0.0331 (8)	0.0432 (10)	0.0369 (8)	0.0022 (7)	0.0120 (7)	0.0070 (7)
N12	0.0257 (5)	0.0348 (6)	0.0310 (6)	−0.0006 (5)	0.0107 (5)	0.0015 (5)
N13	0.0329 (7)	0.0353 (7)	0.0362 (7)	0.0012 (5)	0.0159 (6)	−0.0047 (6)
O14	0.0543 (9)	0.0399 (7)	0.0392 (7)	−0.0043 (6)	0.0267 (7)	−0.0068 (6)
O15	0.0752 (13)	0.0606 (11)	0.0999 (17)	−0.0284 (10)	0.0662 (13)	−0.0288 (11)
O16	0.0763 (12)	0.0543 (10)	0.0487 (9)	−0.0240 (9)	0.0363 (9)	−0.0226 (8)
O1	0.0793 (13)	0.0393 (8)	0.0397 (8)	0.0133 (8)	0.0316 (8)	0.0000 (6)
O2	0.0482 (8)	0.0363 (7)	0.0526 (9)	−0.0060 (6)	0.0336 (7)	−0.0005 (6)
O3	0.0321 (7)	0.0713 (12)	0.0386 (8)	0.0144 (7)	0.0096 (6)	−0.0044 (8)

Geometric parameters (Å, º)

Co1—O3	2.0300 (16)	C7—C8	1.395 (2)
Co1—O2	2.0746 (15)	C8—C9	1.382 (3)
Co1—N12	2.1090 (15)	C8—H8A	0.9300
Co1—O1	2.1177 (16)	C9—C10	1.377 (3)
Co1—N1	2.1183 (15)	C9—H9A	0.9300
Co1—O14	2.1769 (15)	C10—C11	1.384 (3)
N1—C2	1.333 (3)	C10—H10A	0.9300
N1—C6	1.348 (2)	C11—N12	1.335 (2)
C2—C3	1.386 (3)	C11—H11A	0.9300
C2—H2A	0.9300	N13—O15	1.217 (2)
C3—C4	1.380 (4)	N13—O16	1.245 (2)
C3—H3A	0.9300	N13—O14	1.259 (2)
C4—C5	1.386 (4)	O1—H11	0.85 (4)
C4—H4A	0.9300	O1—H12	0.73 (3)
C5—C6	1.387 (3)	O2—H21	0.81 (4)
C5—H5A	0.9300	O2—H22	0.74 (4)
C6—C7	1.479 (3)	O3—H31	0.74 (4)
C7—N12	1.350 (2)	O3—H32	0.77 (4)
O3—Co1—O2	94.24 (8)	C5—C6—C7	122.82 (18)
O3—Co1—N12	172.53 (7)	N12—C7—C8	120.71 (18)
O2—Co1—N12	92.01 (7)	N12—C7—C6	115.41 (15)
O3—Co1—O1	89.28 (8)	C8—C7—C6	123.88 (16)
O2—Co1—O1	88.72 (7)	C9—C8—C7	119.40 (19)
N12—Co1—O1	94.94 (8)	C9—C8—H8A	120.3
O3—Co1—N1	96.37 (7)	C7—C8—H8A	120.3
O2—Co1—N1	169.37 (7)	C10—C9—C8	119.36 (18)
N12—Co1—N1	77.37 (6)	C10—C9—H9A	120.3
O1—Co1—N1	91.83 (7)	C8—C9—H9A	120.3
O3—Co1—O14	85.30 (7)	C9—C10—C11	118.6 (2)

O2—Co1—O14	83.87 (6)	C9—C10—H10A	120.7
N12—Co1—O14	91.32 (6)	C11—C10—H10A	120.7
O1—Co1—O14	170.47 (7)	N12—C11—C10	122.52 (19)
N1—Co1—O14	96.56 (6)	N12—C11—H11A	118.7
C2—N1—C6	119.15 (17)	C10—C11—H11A	118.7
C2—N1—Co1	125.40 (14)	C11—N12—C7	119.36 (16)
C6—N1—Co1	115.22 (12)	C11—N12—Co1	124.77 (13)
N1—C2—C3	122.8 (2)	C7—N12—Co1	115.53 (12)
N1—C2—H2A	118.6	O15—N13—O16	120.34 (18)
C3—C2—H2A	118.6	O15—N13—O14	121.67 (18)
C4—C3—C2	118.0 (2)	O16—N13—O14	117.96 (17)
C4—C3—H3A	121.0	N13—O14—Co1	129.84 (13)
C2—C3—H3A	121.0	Co1—O1—H11	124 (3)
C3—C4—C5	120.0 (2)	Co1—O1—H12	128 (3)
C3—C4—H4A	120.0	H11—O1—H12	108 (4)
C5—C4—H4A	120.0	Co1—O2—H21	122 (2)
C4—C5—C6	118.7 (2)	Co1—O2—H22	121 (3)
C4—C5—H5A	120.7	H21—O2—H22	105 (4)
C6—C5—H5A	120.7	Co1—O3—H31	121 (3)
N1—C6—C5	121.50 (18)	Co1—O3—H32	126 (3)
N1—C6—C7	115.68 (14)	H31—O3—H32	112 (4)
C6—N1—C2—C3	1.0 (3)	C5—C6—C7—C8	−1.2 (3)
Co1—N1—C2—C3	−173.21 (18)	N12—C7—C8—C9	0.1 (3)
N1—C2—C3—C4	−1.5 (4)	C6—C7—C8—C9	179.84 (19)
C2—C3—C4—C5	1.2 (4)	C7—C8—C9—C10	−1.3 (3)
C3—C4—C5—C6	−0.5 (4)	C8—C9—C10—C11	1.3 (4)
C2—N1—C6—C5	−0.2 (3)	C9—C10—C11—N12	−0.1 (4)
Co1—N1—C6—C5	174.59 (15)	C10—C11—N12—C7	−1.0 (3)
C2—N1—C6—C7	179.69 (17)	C10—C11—N12—Co1	172.08 (18)
Co1—N1—C6—C7	−5.5 (2)	C8—C7—N12—C11	1.0 (3)
C4—C5—C6—N1	−0.1 (3)	C6—C7—N12—C11	−178.73 (17)
C4—C5—C6—C7	−179.96 (19)	C8—C7—N12—Co1	−172.70 (14)
N1—C6—C7—N12	−1.3 (2)	C6—C7—N12—Co1	7.5 (2)
C5—C6—C7—N12	178.58 (18)	O15—N13—O14—Co1	22.7 (3)
N1—C6—C7—C8	178.93 (17)	O16—N13—O14—Co1	−159.05 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···O2	0.93	2.54	3.101 (3)	119
O1—H11···Cl1^{i}	0.85 (4)	2.33 (4)	3.1560 (19)	166 (4)
O1—H12···O16^{ii}	0.73 (3)	2.13 (3)	2.825 (2)	160 (4)
O2—H21···Cl1^{iii}	0.81 (4)	2.39 (4)	3.1833 (18)	167 (3)
O2—H22···Cl1^{ii}	0.74 (4)	2.37 (4)	3.1088 (16)	177 (4)

O3—H31···Cl1	0.74 (4)	2.36 (4)	3.100 (2)	176 (3)
O3—H32···O16^{i}	0.77 (4)	1.98 (4)	2.745 (2)	178 (4)

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