

Crystal structure of bis(2-[(pyridin-2-yl)methylidene]amino}benzoato- κ^3N,N',O)cobalt(II) N,N -dimethylformamide sesquisolvate

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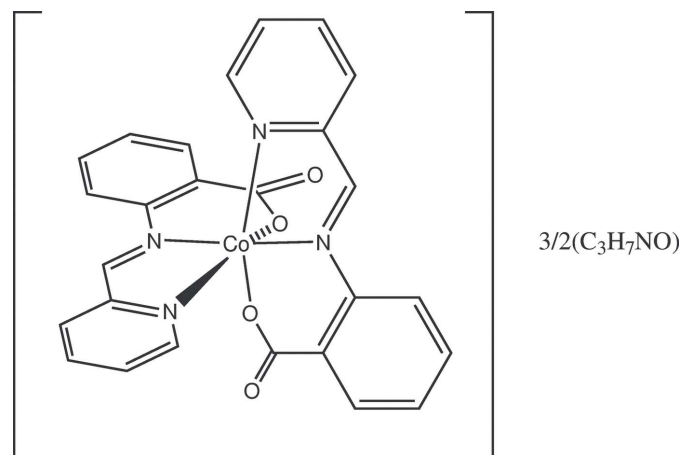
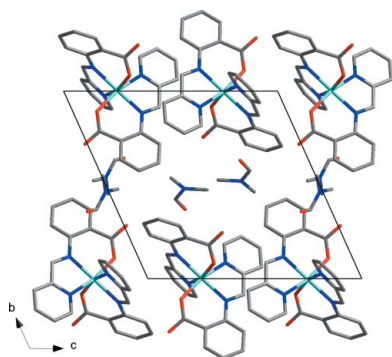
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The title compound, [Co(C₁₃H₉N₂O₂)₂] \cdot 1.5C₃H₇NO, is formed as a neutral Co^{II} complex with dimethylformamide (DMF) solvent molecules. The Co^{II} atom has a distorted O₂N₄ octahedral coordination sphere defined by two tridentate anionic Schiff base ligands with the O atoms being *cis*. The coordination sphere around the Co^{II} atom is geometrically different from that reported for the co-crystal [Co(C₁₃H₉N₂O₂)₂] \cdot AA \cdot H₂O (AA is anthranilic acid). One of the DMF solvent molecules was modelled as being disordered about a crystallographic inversion centre with half-occupancy. The crystal structure is made up from alternating layers of complex molecules and DMF molecules parallel to (010). C–H \cdots O hydrogen-bonding interactions between the complex molecules and the solvent molecules consolidate the crystal packing.

1. Chemical context

Metal complexes containing Schiff bases are the most fundamental chelating systems in coordination chemistry. Their interesting chemical and physical properties and their wide-ranging applications in numerous scientific areas have been explored widely (Vigato *et al.*, 2012). During the last few years, we have investigated the chemistry of 3d metal complexes of Schiff base ligands with the aim of preparing mono- and heterometallic polynuclear compounds.



Recently, we have investigated the coordination behaviour of the tridentate carboxylate Schiff base ligand 2-*N*-(2'-pyridylimine)benzoic acid (HL), which results from the condensation between pyridine-2-carbaldehyde and anthranilic acid (AA) and reported the cation–anion complex CrL₂NO₃ \cdot H₂O (Buvaylo *et al.*, 2014a) and co-crystals of ML₂

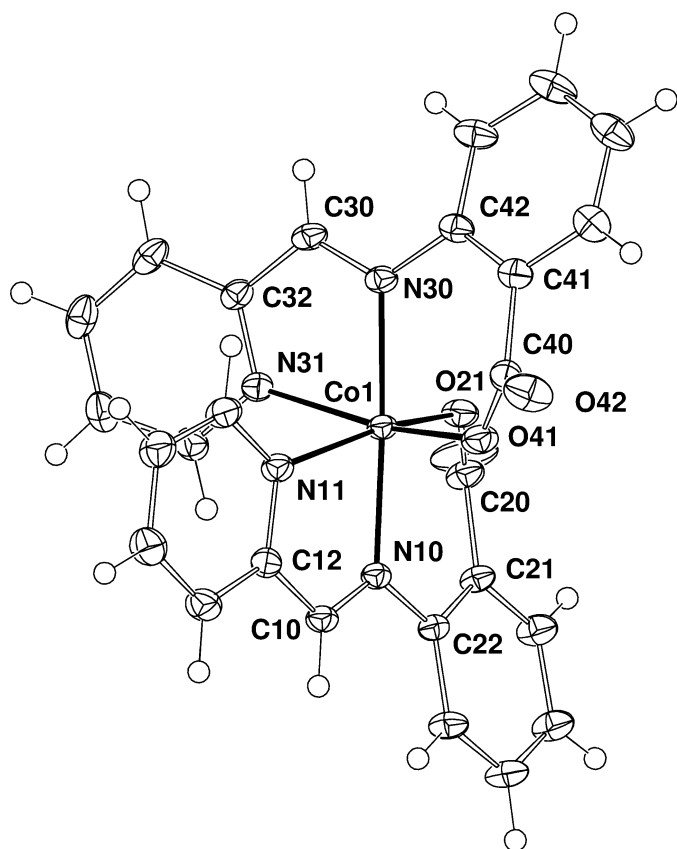


Figure 1
The molecular structure of the title complex, showing the atom-numbering scheme. Non-H atoms are shown as displacement ellipsoids at the 50% probability level.

($M = \text{Co}, \text{Ni}, \text{Zn}$) and anthranilic acid (Buvaylo *et al.*, 2014b). The respective compounds were prepared by *in situ* Schiff base synthesis. ML_2 molecules of the isotypic $\text{CoL}_2 \cdot \text{AA} \cdot \text{H}_2\text{O}$ and $\text{NiL}_2 \cdot \text{AA} \cdot \text{H}_2\text{O}$ co-crystals retained the intramolecular distances $M-(\text{N},\text{O})$ as found in the structure of the ‘native’ Schiff base metal complex $\text{NiL}_2 \cdot \text{H}_2\text{O}$ (Mukhopadhyay & Pal, 2005). The crystal packing of the co-crystals was described as an insertion of the organic molecules between the layers of ML_2 complexes as they occur in the reported $\text{NiL}_2 \cdot \text{H}_2\text{O}$ structure.

The title compound, $[\text{Co}(\text{C}_{13}\text{H}_9\text{N}_2\text{O}_2)_2] \cdot 1.5\text{C}_3\text{H}_7\text{NO}$, was prepared similarly to the co-crystals (Buvaylo *et al.*, 2014b) but using additional $[\text{Cd}(\text{CH}_3\text{COO})_2] \cdot 2\text{H}_2\text{O}$ in an attempt to prepare a heterometallic compound with HL. The obtained crystals, however, did not appear to contain anthranilic acid molecules or cadmium.

2. Structural commentary

The asymmetric unit of the title compound consists of one neutral CoL_2 molecule and 1.5 dimethylformamide (DMF) solvent molecules, of which one is fully ordered, the other being disordered about a crystallographic inversion centre. The CoL_2 molecule has no crystallographically imposed symmetry. The ligand molecules are deprotonated at the carboxylato oxygen atom and coordinate to the Co^{II} atom

Table 1
Selected bond lengths (\AA).

Co1—O41	2.0072 (12)	Co1—N10	2.1189 (13)
Co1—O21	2.0181 (13)	Co1—N31	2.1358 (14)
Co1—N30	2.1057 (13)	Co1—N11	2.1498 (14)

Table 2
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C10—H10 \cdots O42 ⁱ	0.95	2.46	3.393 (2)	169
C102—H10E \cdots O42 ⁱⁱ	0.98	2.46	3.369 (3)	154
C16—H16 \cdots O101	0.95	2.41	3.326 (3)	163
C201—H20C \cdots O22 ⁱⁱⁱ	0.98	1.97	2.819 (10)	143
C23—H23 \cdots O42 ⁱ	0.95	2.60	3.454 (2)	150
C30—H30 \cdots O22 ^{iv}	0.95	2.42	3.344 (3)	163
C36—H36 \cdots O201 ^v	0.95	2.54	3.235 (13)	130

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

through the azomethine, pyridine-N and carboxylato-O atoms in such a way that the metal atom is octahedrally surrounded by two anionic ligands with *cis* O atoms (Fig. 1, Table 1). The octahedral geometry is severely distorted: the $\text{Co}-(\text{N},\text{O})$ distances fall in the range 2.0072 (12)–2.1498 (14) \AA , the *trans* angles at the Co^{II} ion lie in the range 161.53 (6)–177.35 (5), the *cis* angles vary from 77.91 (5) to 103.70 (5) $^\circ$. Surprisingly, the coordination geometry around the Co^{II} ion is markedly different from that of $\text{CoL}_2 \cdot \text{AA} \cdot \text{H}_2\text{O}$ (Buvaylo *et al.*, 2014b) where the $\text{Co}-(\text{N},\text{O})$ distances range from 1.990 (2) to 2.088 (18) \AA , and the *trans* and *cis* angles at the Co^{II} ion vary from 167.96 (6) to 176.95 (7) and from 80.93 (7) to 98.81 (7) $^\circ$, respectively. The reason for such a discrepancy could be the absence of classical hydrogen bonds in the title compound in

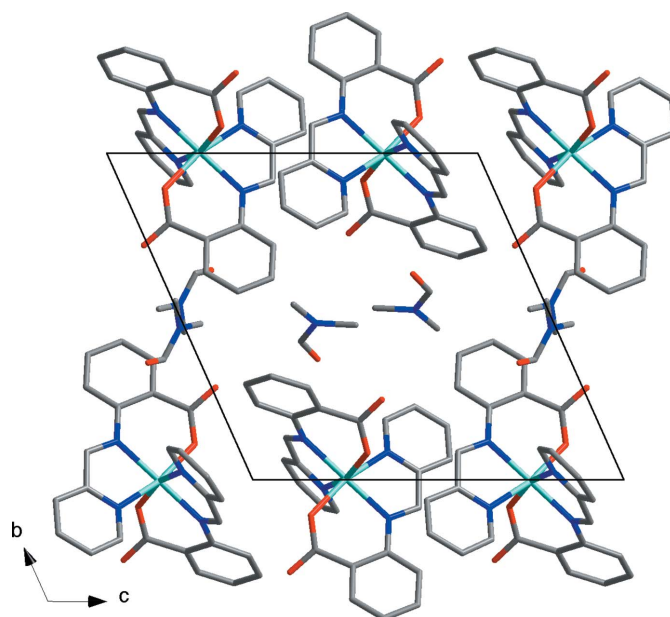


Figure 2
Packing diagram showing alternating layers of $[\text{CoL}_2]$ and DMF molecules. CH hydrogens have been omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Co(C ₁₃ H ₉ N ₂ O ₂) ₂] \cdot 1.5C ₃ H ₇ NO
<i>M_r</i>	619.02
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.4361 (6), 13.2603 (10), 13.8664 (10)
α , β , γ (°)	110.061 (7), 103.559 (6), 101.430 (6)
<i>V</i> (Å ³)	1348.9 (2)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.69
Crystal size (mm)	0.40 \times 0.30 \times 0.18
Data collection	
Diffractometer	Oxford Diffraction Xcalibur
Absorption correction	Analytical [<i>CrysAlis PRO</i> (Agilent, 2011) using an expres- sion derived by Clark & Reid (1995)]
<i>T_{min}</i> , <i>T_{max}</i>	0.821, 0.898
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	33209, 10748, 8599
<i>R_{int}</i>	0.036
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.787
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.127, 1.05
No. of reflections	10748
No. of parameters	410
No. of restraints	35
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.74, -0.54

Computer programs: *CrysAlis PRO* (Agilent, 2011), *SIR92* (Altomare *et al.*, 1994), *SHELXL97* (Sheldrick, 2008), *ORTEPII* (Johnson, 1976), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

contrast to the co-crystal CoL₂·AA·H₂O. A metal site with mixed (Co/Cd) occupancy for the title compound was ruled out by the refinement.

3. Supramolecular features

The crystal lattice is built of alternating layers of complex CoL₂ molecules and DMF molecules parallel to (010) (Fig. 2). Neighbouring CoL₂ molecules within a layer are related by an inversion centre with Co...Co separations of 6.8713 (6) and 6.9985 (6) Å. Weak C—H...O hydrogen-bonding interactions between the complex molecules and the solvent molecules lead to a consolidation of the crystal packing.

4. Synthesis and crystallization

The Schiff base ligand HL was prepared by refluxing pyridine-2-carbaldehyde (0.38 ml, 4 mmol) with anthranilic acid (0.55 g, 4 mmol) in 20 ml methanol for half an hour. The resultant yellow solution was left in open air overnight and used without further purification.

To a stirred DMF solution (5 ml) of Cd(CH₃COO)₂·2H₂O (0.53 g, 2 mmol) in a 50 ml conic flask, HL (0.21 g, 4 mmol) in methanol from the previous preparation was added. The

solution was magnetically stirred at 323 K for 20 minutes and a yellow precipitate of a Cd complex formed. Co(CH₃COO)₂·4H₂O (0.25 g, 1 mmol) in DMF (10 ml) was added to the reaction mixture after a week. The mixture was stirred magnetically at 323 K for an hour, however, the yellow precipitate did not dissolve and was filtered off. The resulting red-brown solution was left to evaporate at room temperature. Red-brown block-like crystals of the title compound formed the next day. They were collected by filter-suction, washed with dry isopropanol and finally dried *in vacuo* (yield: 23% based on cobalt salt). Analysis for C₂₆H₁₈CoN₄O₄·1.5C₃H₇NO calculated (%) C: 59.18 H: 4.64 N: 12.45 Co: 9.52. Found (%) C: 59.33 H: 4.49 N: 12.41 Co: 9.76. Spectroscopic data (IR, KBr) are available as an additional Figure in the supporting information.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The refinement of the metal occupancy as part Co and part Cd gave 100% Co. One solvent DMF molecule was modelled as being disordered about a crystallographic inversion centre with resulting half-occupancy and with geometries restrained to ideal values. All hydrogen atoms were placed at calculated positions and refined by use of the riding-model approximation, with *U*_{iso}(H) = 1.2*U*_{eq} of the parent C atom.

Acknowledgements

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supporting information

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Crystal structure of bis(2-[(pyridin-2-yl)methylidene]amino)benzoato- κ^3N,N',O)cobalt(II) *N,N*-dimethylformamide sesquisolvate

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP11* (Johnson, 1976) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis(2-[(pyridin-2-yl)methylidene]amino)benzoato- κ^3N,N',O)cobalt(II) *N,N*-dimethylformamide sesquisolvate

Crystal data

[Co(C₁₃H₉N₂O₂)₂] \cdot 1.5C₃H₇NO

$M_r = 619.02$

Triclinic, *P1*

Hall symbol: -P 1

$a = 8.4361$ (6) Å

$b = 13.2603$ (10) Å

$c = 13.8664$ (10) Å

$\alpha = 110.061$ (7)°

$\beta = 103.559$ (6)°

$\gamma = 101.430$ (6)°

$V = 1348.9$ (2) Å³

$Z = 2$

$F(000) = 642$

$D_x = 1.524$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 10672 reflections

$\theta = 2.8$ – 34.5 °

$\mu = 0.69$ mm⁻¹

$T = 100$ K

Block, red-brown

$0.40 \times 0.30 \times 0.18$ mm

Data collection

Oxford Diffraction Xcalibur
diffractometer

Graphite monochromator

Detector resolution: 16.0009 pixels mm⁻¹

ω scans

Absorption correction: analytical

[*CrysAlis PRO* (Agilent, 2011) using an

expression derived by Clark & Reid (1995)]

$T_{\min} = 0.821$, $T_{\max} = 0.898$

33209 measured reflections

10748 independent reflections

8599 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 34$ °, $\theta_{\min} = 2.8$ °

$h = -12 \rightarrow 13$

$k = -20 \rightarrow 19$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.127$

$S = 1.05$

10748 reflections

410 parameters

35 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.4745P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.006$
 $\Delta\rho_{\max} = 0.74 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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. One solvent dmf molecule was modelled as being disordered about a crystallographic inversion centre. The geometries were restrained to ideal values.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.50566 (3)	0.996180 (17)	0.747260 (16)	0.01696 (6)	
N11	0.28320 (17)	0.91486 (12)	0.60369 (11)	0.0197 (2)	
C12	0.2706 (2)	0.97508 (14)	0.54251 (12)	0.0194 (3)	
C13	0.1383 (2)	0.93697 (15)	0.44446 (14)	0.0255 (3)	
H13	0.1345	0.9792	0.4012	0.031*	
C14	0.0121 (2)	0.83562 (17)	0.41152 (15)	0.0307 (4)	
H14	-0.0801	0.8077	0.3453	0.037*	
C15	0.0221 (2)	0.77579 (16)	0.47596 (15)	0.0289 (4)	
H15	-0.0645	0.7073	0.4556	0.035*	
C16	0.1607 (2)	0.81754 (15)	0.57109 (14)	0.0245 (3)	
H16	0.1687	0.7755	0.6144	0.029*	
C10	0.4017 (2)	1.08481 (13)	0.58651 (12)	0.0192 (3)	
H10	0.4017	1.131	0.5472	0.023*	
N10	0.51714 (16)	1.11742 (11)	0.67961 (10)	0.0170 (2)	
C21	0.7536 (2)	1.26504 (14)	0.83458 (12)	0.0205 (3)	
C22	0.65025 (19)	1.22222 (13)	0.72478 (12)	0.0174 (3)	
C23	0.6816 (2)	1.28292 (14)	0.66229 (13)	0.0240 (3)	
H23	0.6106	1.2552	0.5888	0.029*	
C24	0.8144 (2)	1.38261 (15)	0.70634 (14)	0.0277 (3)	
H24	0.833	1.4234	0.6634	0.033*	
C25	0.9208 (2)	1.42328 (16)	0.81350 (15)	0.0285 (4)	
H25	1.0149	1.4901	0.8431	0.034*	
C26	0.8883 (2)	1.36573 (15)	0.87639 (14)	0.0269 (3)	
H26	0.9591	1.3952	0.9501	0.032*	
C20	0.7319 (2)	1.21453 (15)	0.91605 (13)	0.0240 (3)	
O21	0.69029 (16)	1.10880 (10)	0.88645 (9)	0.0232 (2)	
O22	0.7636 (3)	1.28251 (13)	1.01092 (11)	0.0475 (4)	
N31	0.31332 (17)	1.02612 (12)	0.82016 (11)	0.0203 (2)	
C32	0.2642 (2)	0.94913 (14)	0.85884 (12)	0.0197 (3)	
C33	0.1204 (2)	0.93994 (16)	0.89184 (13)	0.0257 (3)	

H33	0.0913	0.8875	0.9222	0.031*	
C34	0.0202 (2)	1.00887 (17)	0.87943 (13)	0.0284 (4)	
H34	-0.0811	1.0023	0.8986	0.034*	
C35	0.0694 (2)	1.08726 (17)	0.83884 (13)	0.0270 (3)	
H35	0.0025	1.1352	0.8296	0.032*	
C36	0.2188 (2)	1.09467 (16)	0.81177 (13)	0.0245 (3)	
H36	0.255	1.1504	0.7864	0.029*	
C30	0.3667 (2)	0.87175 (14)	0.85948 (12)	0.0205 (3)	
H30	0.3484	0.821	0.8931	0.025*	
N30	0.48205 (17)	0.87471 (11)	0.81309 (10)	0.0181 (2)	
C41	0.6719 (2)	0.78101 (13)	0.73476 (12)	0.0207 (3)	
C42	0.5915 (2)	0.80600 (13)	0.81452 (12)	0.0199 (3)	
C43	0.6270 (2)	0.76728 (15)	0.89722 (14)	0.0271 (3)	
H43	0.5707	0.7825	0.9501	0.033*	
C44	0.7429 (3)	0.70727 (16)	0.90256 (15)	0.0329 (4)	
H44	0.7668	0.6823	0.9594	0.039*	
C45	0.8246 (3)	0.68328 (15)	0.82488 (15)	0.0313 (4)	
H45	0.9061	0.6434	0.8293	0.038*	
C46	0.7858 (2)	0.71809 (14)	0.74084 (14)	0.0261 (3)	
H46	0.838	0.6987	0.6861	0.031*	
C40	0.6515 (2)	0.81957 (14)	0.64211 (13)	0.0214 (3)	
O41	0.63573 (16)	0.91724 (11)	0.65820 (10)	0.0244 (2)	
O42	0.6581 (2)	0.75447 (12)	0.55549 (10)	0.0344 (3)	
C101	0.2797 (3)	0.5260 (2)	0.53693 (17)	0.0462 (6)	
H10A	0.1781	0.5472	0.5112	0.069*	
H10B	0.2719	0.4523	0.4839	0.069*	
H10C	0.3825	0.5826	0.5457	0.069*	
C102	0.4048 (3)	0.4635 (2)	0.6791 (2)	0.0492 (6)	
H10D	0.5229	0.5046	0.6912	0.074*	
H10E	0.3748	0.3864	0.6245	0.074*	
H10F	0.3947	0.4615	0.7475	0.074*	
N101	0.2892 (2)	0.52022 (14)	0.64083 (13)	0.0314 (3)	
C103	0.2097 (2)	0.57619 (16)	0.70349 (15)	0.0292 (4)	
H103	0.2267	0.5737	0.7728	0.035*	
O101	0.1172 (2)	0.63017 (13)	0.68000 (13)	0.0384 (3)	
C201	0.6583 (8)	0.4774 (8)	1.0471 (4)	0.074 (2)	0.5
H20A	0.6872	0.5372	1.1196	0.11*	0.5
H20B	0.7402	0.4981	1.0122	0.11*	0.5
H20C	0.6635	0.4067	1.0537	0.11*	0.5
C202	0.4086 (11)	0.5472 (7)	1.0070 (9)	0.094 (3)	0.5
H20D	0.4843	0.62	1.0193	0.141*	0.5
H20E	0.3758	0.5541	1.0718	0.141*	0.5
H20F	0.3056	0.5245	0.9445	0.141*	0.5
N201	0.4968 (10)	0.4635 (6)	0.9856 (6)	0.0754 (17)	0.5
C203	0.4235 (7)	0.3681 (6)	0.9046 (5)	0.0535 (12)	0.5
H203	0.4778	0.312	0.8829	0.064*	0.5
O201	0.2772 (15)	0.3581 (9)	0.8592 (9)	0.211 (4)	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01868 (10)	0.01863 (11)	0.01563 (10)	0.00464 (7)	0.00591 (7)	0.00978 (8)
N11	0.0208 (6)	0.0218 (6)	0.0165 (5)	0.0045 (5)	0.0054 (5)	0.0092 (5)
C12	0.0192 (6)	0.0232 (7)	0.0163 (6)	0.0063 (5)	0.0056 (5)	0.0091 (5)
C13	0.0258 (8)	0.0286 (8)	0.0208 (7)	0.0062 (6)	0.0038 (6)	0.0123 (6)
C14	0.0247 (8)	0.0347 (10)	0.0249 (8)	0.0029 (7)	-0.0012 (6)	0.0127 (7)
C15	0.0231 (8)	0.0294 (9)	0.0267 (8)	-0.0005 (6)	0.0024 (6)	0.0112 (7)
C16	0.0243 (7)	0.0252 (8)	0.0224 (7)	0.0019 (6)	0.0055 (6)	0.0124 (6)
C10	0.0223 (7)	0.0213 (7)	0.0171 (6)	0.0071 (5)	0.0075 (5)	0.0107 (5)
N10	0.0191 (6)	0.0183 (6)	0.0157 (5)	0.0061 (5)	0.0067 (4)	0.0084 (5)
C21	0.0247 (7)	0.0207 (7)	0.0176 (6)	0.0041 (6)	0.0087 (5)	0.0102 (5)
C22	0.0207 (6)	0.0172 (6)	0.0170 (6)	0.0059 (5)	0.0082 (5)	0.0087 (5)
C23	0.0317 (8)	0.0237 (8)	0.0182 (7)	0.0058 (6)	0.0082 (6)	0.0120 (6)
C24	0.0372 (9)	0.0241 (8)	0.0243 (8)	0.0040 (7)	0.0110 (7)	0.0149 (7)
C25	0.0335 (9)	0.0239 (8)	0.0271 (8)	0.0017 (7)	0.0096 (7)	0.0133 (7)
C26	0.0305 (8)	0.0235 (8)	0.0213 (7)	-0.0004 (6)	0.0046 (6)	0.0102 (6)
C20	0.0273 (8)	0.0249 (8)	0.0182 (7)	0.0017 (6)	0.0070 (6)	0.0108 (6)
O21	0.0260 (6)	0.0228 (6)	0.0201 (5)	0.0040 (4)	0.0039 (4)	0.0123 (4)
O22	0.0860 (13)	0.0276 (7)	0.0186 (6)	-0.0018 (8)	0.0160 (7)	0.0088 (5)
N31	0.0203 (6)	0.0258 (7)	0.0176 (6)	0.0068 (5)	0.0067 (5)	0.0118 (5)
C32	0.0200 (7)	0.0224 (7)	0.0140 (6)	0.0021 (5)	0.0055 (5)	0.0068 (5)
C33	0.0246 (8)	0.0298 (8)	0.0192 (7)	0.0005 (6)	0.0102 (6)	0.0082 (6)
C34	0.0200 (7)	0.0399 (10)	0.0181 (7)	0.0039 (7)	0.0076 (6)	0.0056 (7)
C35	0.0238 (8)	0.0385 (10)	0.0179 (7)	0.0132 (7)	0.0063 (6)	0.0089 (7)
C36	0.0252 (8)	0.0333 (9)	0.0208 (7)	0.0130 (7)	0.0092 (6)	0.0143 (7)
C30	0.0245 (7)	0.0208 (7)	0.0145 (6)	0.0023 (6)	0.0056 (5)	0.0086 (5)
N30	0.0202 (6)	0.0179 (6)	0.0139 (5)	0.0025 (5)	0.0033 (4)	0.0071 (4)
C41	0.0233 (7)	0.0172 (7)	0.0171 (6)	0.0034 (5)	0.0027 (5)	0.0060 (5)
C42	0.0233 (7)	0.0165 (6)	0.0158 (6)	0.0035 (5)	0.0019 (5)	0.0063 (5)
C43	0.0380 (9)	0.0236 (8)	0.0184 (7)	0.0082 (7)	0.0044 (6)	0.0108 (6)
C44	0.0454 (11)	0.0269 (9)	0.0228 (8)	0.0134 (8)	0.0002 (7)	0.0121 (7)
C45	0.0380 (10)	0.0210 (8)	0.0285 (8)	0.0120 (7)	0.0002 (7)	0.0082 (7)
C46	0.0278 (8)	0.0207 (7)	0.0236 (7)	0.0071 (6)	0.0033 (6)	0.0056 (6)
C40	0.0207 (7)	0.0247 (8)	0.0191 (7)	0.0066 (6)	0.0062 (5)	0.0098 (6)
O41	0.0304 (6)	0.0269 (6)	0.0244 (6)	0.0114 (5)	0.0145 (5)	0.0153 (5)
O42	0.0531 (9)	0.0341 (7)	0.0206 (6)	0.0208 (7)	0.0145 (6)	0.0107 (5)
C101	0.0517 (13)	0.0484 (13)	0.0279 (9)	0.0014 (11)	0.0207 (10)	0.0063 (9)
C102	0.0334 (11)	0.0434 (13)	0.0490 (13)	0.0134 (10)	0.0020 (10)	0.0004 (11)
N101	0.0294 (8)	0.0303 (8)	0.0251 (7)	0.0033 (6)	0.0089 (6)	0.0035 (6)
C103	0.0306 (9)	0.0291 (9)	0.0251 (8)	0.0031 (7)	0.0119 (7)	0.0094 (7)
O101	0.0432 (8)	0.0358 (8)	0.0400 (8)	0.0142 (7)	0.0170 (7)	0.0165 (7)
C201	0.036 (3)	0.148 (6)	0.030 (2)	0.033 (3)	0.004 (2)	0.031 (3)
C202	0.055 (4)	0.078 (5)	0.136 (6)	0.025 (4)	0.035 (5)	0.024 (5)
N201	0.049 (2)	0.115 (4)	0.071 (3)	0.016 (4)	0.020 (3)	0.053 (4)
C203	0.043 (3)	0.079 (4)	0.056 (3)	0.033 (3)	0.019 (2)	0.039 (3)
O201	0.227 (7)	0.144 (6)	0.183 (7)	0.017 (6)	0.015 (6)	0.032 (6)

Geometric parameters (Å, °)

Co1—O41	2.0072 (12)	C35—C36	1.392 (2)
Co1—O21	2.0181 (13)	C35—H35	0.9500
Co1—N30	2.1057 (13)	C36—H36	0.9500
Co1—N10	2.1189 (13)	C30—N30	1.288 (2)
Co1—N31	2.1358 (14)	C30—H30	0.9500
Co1—N11	2.1498 (14)	N30—C42	1.421 (2)
N11—C16	1.338 (2)	C41—C46	1.398 (2)
N11—C16	1.338 (2)	C41—C42	1.409 (2)
N11—C12	1.351 (2)	C41—C40	1.524 (2)
C12—C13	1.394 (2)	C42—C43	1.404 (2)
C12—C10	1.466 (2)	C43—C44	1.382 (3)
C13—C14	1.390 (3)	C43—H43	0.9500
C13—H13	0.9500	C44—C45	1.392 (3)
C14—C15	1.383 (3)	C44—H44	0.9500
C14—H14	0.9500	C45—C46	1.389 (3)
C15—C16	1.390 (2)	C45—H45	0.9500
C15—H15	0.9500	C46—H46	0.9500
C16—H16	0.9500	C40—O42	1.237 (2)
C10—N10	1.289 (2)	C40—O41	1.276 (2)
C10—H10	0.9500	C101—N101	1.453 (3)
N10—C22	1.428 (2)	C101—H10A	0.9800
C21—C26	1.403 (2)	C101—H10B	0.9800
C21—C22	1.410 (2)	C101—H10C	0.9800
C21—C20	1.525 (2)	C102—N101	1.456 (3)
C22—C23	1.404 (2)	C102—H10D	0.9800
C23—C24	1.384 (2)	C102—H10E	0.9800
C23—H23	0.9500	C102—H10F	0.9800
C24—C25	1.392 (3)	N101—C103	1.336 (2)
C24—H24	0.9500	C103—O101	1.221 (2)
C25—C26	1.380 (2)	C103—H103	0.9500
C25—H25	0.9500	C201—N201	1.366 (9)
C26—H26	0.9500	C201—H20A	0.9800
C20—O22	1.241 (2)	C201—H20B	0.9800
C20—O21	1.265 (2)	C201—H20C	0.9800
N31—C36	1.339 (2)	C202—N201	1.442 (10)
N31—C32	1.347 (2)	C202—H20D	0.9800
C32—C33	1.391 (2)	C202—H20E	0.9800
C32—C30	1.468 (2)	C202—H20F	0.9800
C33—C34	1.387 (3)	N201—C203	1.278 (9)
C33—H33	0.9500	C203—O201	1.204 (11)
C34—C35	1.382 (3)	C203—H203	0.9500
C34—H34	0.9500		
O41—Co1—O21	103.70 (5)	C33—C32—C30	121.74 (15)
O41—Co1—N30	89.97 (5)	C34—C33—C32	118.64 (16)
O21—Co1—N30	90.57 (5)	C34—C33—H33	120.7

O41—Co1—N10	91.81 (5)	C32—C33—H33	120.7
O21—Co1—N10	90.92 (5)	C35—C34—C33	119.31 (15)
N30—Co1—N10	177.35 (5)	C35—C34—H34	120.3
O41—Co1—N31	161.53 (6)	C33—C34—H34	120.3
O21—Co1—N31	90.55 (5)	C34—C35—C36	118.72 (17)
N30—Co1—N31	78.03 (5)	C34—C35—H35	120.6
N10—Co1—N31	99.76 (5)	C36—C35—H35	120.6
O41—Co1—N11	87.74 (5)	N31—C36—C35	122.40 (16)
O21—Co1—N11	164.36 (5)	N31—C36—H36	118.8
N30—Co1—N11	100.20 (5)	C35—C36—H36	118.8
N10—Co1—N11	77.91 (5)	N30—C30—C32	118.03 (14)
N31—Co1—N11	80.75 (5)	N30—C30—H30	121.0
C16—N11—C12	118.76 (14)	C32—C30—H30	121.0
C16—N11—Co1	128.75 (11)	C30—N30—C42	121.33 (14)
C12—N11—Co1	112.47 (10)	C30—N30—Co1	114.82 (11)
N11—C12—C13	122.22 (15)	C42—N30—Co1	123.70 (10)
N11—C12—C10	116.19 (13)	C46—C41—C42	118.51 (15)
C13—C12—C10	121.57 (15)	C46—C41—C40	115.46 (15)
C14—C13—C12	118.33 (16)	C42—C41—C40	126.01 (15)
C14—C13—H13	120.8	C43—C42—C41	119.54 (16)
C12—C13—H13	120.8	C43—C42—N30	120.99 (15)
C15—C14—C13	119.39 (16)	C41—C42—N30	119.40 (14)
C15—C14—H14	120.3	C44—C43—C42	120.71 (17)
C13—C14—H14	120.3	C44—C43—H43	119.6
C14—C15—C16	118.94 (17)	C42—C43—H43	119.6
C14—C15—H15	120.5	C43—C44—C45	120.18 (17)
C16—C15—H15	120.5	C43—C44—H44	119.9
N11—C16—C15	122.28 (16)	C45—C44—H44	119.9
N11—C16—H16	118.9	C46—C45—C44	119.41 (17)
C15—C16—H16	118.9	C46—C45—H45	120.3
N10—C10—C12	118.75 (14)	C44—C45—H45	120.3
N10—C10—H10	120.6	C45—C46—C41	121.60 (17)
C12—C10—H10	120.6	C45—C46—H46	119.2
C10—N10—C22	120.97 (13)	C41—C46—H46	119.2
C10—N10—Co1	114.38 (11)	O42—C40—O41	123.49 (15)
C22—N10—Co1	124.31 (10)	O42—C40—C41	116.99 (15)
C26—C21—C22	118.32 (14)	O41—C40—C41	119.46 (14)
C26—C21—C20	115.13 (14)	C40—O41—Co1	127.35 (11)
C22—C21—C20	126.52 (14)	N101—C101—H10A	109.5
C23—C22—C21	119.32 (14)	N101—C101—H10B	109.5
C23—C22—N10	121.59 (14)	H10A—C101—H10B	109.5
C21—C22—N10	119.08 (13)	N101—C101—H10C	109.5
C24—C23—C22	120.89 (15)	H10A—C101—H10C	109.5
C24—C23—H23	119.6	H10B—C101—H10C	109.5
C22—C23—H23	119.6	N101—C102—H10D	109.5
C23—C24—C25	120.10 (15)	N101—C102—H10E	109.5
C23—C24—H24	120.0	H10D—C102—H10E	109.5
C25—C24—H24	120.0	N101—C102—H10F	109.5

C26—C25—C24	119.40 (17)	H10D—C102—H10F	109.5
C26—C25—H25	120.3	H10E—C102—H10F	109.5
C24—C25—H25	120.3	C103—N101—C101	120.47 (19)
C25—C26—C21	121.91 (16)	C103—N101—C102	121.65 (18)
C25—C26—H26	119.0	C101—N101—C102	117.44 (19)
C21—C26—H26	119.0	O101—C103—N101	126.04 (18)
O22—C20—O21	123.53 (15)	O101—C103—H103	117.0
O22—C20—C21	116.35 (15)	N101—C103—H103	117.0
O21—C20—C21	120.06 (14)	C203—N201—C201	115.3 (7)
C20—O21—Co1	124.57 (11)	C203—N201—C202	120.1 (8)
C36—N31—C32	118.68 (14)	C201—N201—C202	124.6 (7)
C36—N31—Co1	127.42 (11)	O201—C203—N201	111.9 (8)
C32—N31—Co1	112.43 (11)	O201—C203—H203	124.1
N31—C32—C33	122.15 (16)	N201—C203—H203	124.1
N31—C32—C30	116.05 (13)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C10—H10 \cdots O42 ⁱ	0.95	2.46	3.393 (2)	169
C102—H10E \cdots O42 ⁱⁱ	0.98	2.46	3.369 (3)	154
C16—H16 \cdots O101	0.95	2.41	3.326 (3)	163
C201—H20C \cdots O22 ⁱⁱⁱ	0.98	1.97	2.819 (10)	143
C23—H23 \cdots O42 ⁱ	0.95	2.60	3.454 (2)	150
C30—H30 \cdots O22 ^{iv}	0.95	2.42	3.344 (3)	163
C36—H36 \cdots O201 ^v	0.95	2.54	3.235 (13)	130

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