A binuclear cobalt(II) complex of an NO$_3$-donor Schiff base derived from 3-carboxylsalicylaldehyde and 2-nitroaniline

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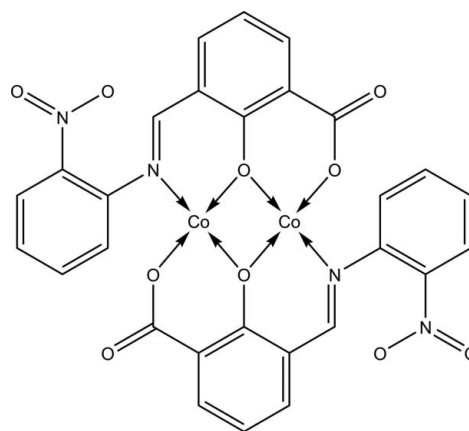Correspondence e-mail: zhw@henu.edu.cn

In the crystal structure of the centrosymmetric title complex, bis{μ-3-[(2-nitrophenyl)iminomethyl]-2-oxidobenzoato}dicobalt(II), [Co$_2$(C$_{14}$H$_8$N$_2$O$_5$)$_2$], in which the ligand is 3-[(2-nitrophenyl)iminomethyl]-2-oxidobenzoate, a Schiff base synthesized from 2-nitroaniline with 3-carboxylsalicylaldehyde, the two cobalt(II) ions in the molecular unit are bridged by two phenolate O atoms of the ligands. Each metal centre has a distorted square-planar geometry. In the crystal structure, molecules are linked by Co$\cdots$O interactions involving the nitro O atoms, forming a two-dimensional network. There are also C—H$\cdots$O and π–π stacking interactions [centroid–centroid distances of 3.5004 (2), 3.6671 (2) and 3.6677 (2) Å] between adjacent benzene rings of the two-dimensional networks, leading to the formation of a three-dimensional framework.

Related literature

For binuclear cobalt(II) complexes of Schiff base ligands, see: Adams *et al.* (2002); Tone *et al.* (2007). For the design of molecular solids, see: Zheng *et al.* (2003). For bond-valence parameters, see: Brown & Altermatt (1985). For luminescence emission, see: Li *et al.* (2008).

Experimental

Crystal data

[Co$_2$(C$_{14}$H$_8$N$_2$O$_5$)$_2$]
M_r = 686.31
Monoclinic, $P2_1/c$
a = 8.3398 (6) Å
b = 11.0454 (8) Å
c = 13.3681 (9) Å
β = 99.6040 (10)°

V = 1214.16 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 296 (2) K
0.21 × 0.16 × 0.11 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.752, T_{max} = 0.858

6134 measured reflections
2132 independent reflections
1536 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.00
2132 reflections

199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O3	1.936 (3)	Co1—O2^i	1.874 (3)
Co1—N1	1.947 (4)	Co1—O3^i	1.929 (3)
Co1$\cdots$O4	2.807 (4)	Co1$\cdots$O5^{ii}	2.867 (5)
O3—Co1—N1	92.51 (14)	O2^i—Co1—N1	95.83 (14)
O2^i—Co1—O3	171.54 (13)	O3^i—Co1—N1	170.41 (14)
O3—Co1—O3^i	78.42 (11)	O2^i—Co1—O3^i	93.33 (12)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots$O5^{iii}	0.93	2.55	3.295 (6)	138
C12—H12$\cdots$O1^{iv}	0.93	2.58	3.230 (7)	128

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

metal-organic compounds

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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supporting information

A binuclear cobalt(II) complex of an NO₃-donor Schiff base derived from 3-carboxylsalicylaldehyde and 2-nitroaniline

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S1. Comment

Weak intermolecular forces, such as hydrogen bonding, π—π stacking, dipole—dipole attractions, and van der Waals interactions, have been studied in depth and can be used in the design of molecular solids with specific supramolecular structures and functions (Zheng *et al.*, 2003). Numerous binuclear cobalt(II) complexes of Schiff bases have been studied (Tone *et al.*, 2007). To the best of our knowledge, 2-NA (2-nitroaniline) Schiff bases have not been reported up to now. As a result of our interest in the design of organic systems suitable for the assembly of supramolecular compounds, we have synthesized the Schiff base ligand H₂CSNA, from the condensation reaction of 3-carboxylsalicylaldehyde with 2-nitroaniline, and its binuclear cobalt(II) complex, [Co₂(CSNA)₂], (I) [where CSNA^{2-} = 3-[(2-nitrophenyl)iminomethyl]-2-oxidobenzoate dianion].

Complex (I), a 2-NA Schiff base cobalt(II) complex, consists of centrosymmetric binuclear molecular units of [Co₂(CSNA)₂], as shown in Fig. 1. Selected bond distances and angles are given in Table 1. Each molecular unit contains two CSNA^{2-} anions and two Co^{2+} ions. The two CSNA^{2-} anions act as N1,O2,O3 tridentate ligands to chelate two Co^{2+} ions with the phenolate O-atoms (O3 and O3^{i}: (i) = -x + 2, -y, -z + 1) as bridging atoms. The distance between the two metal centres is found to be 2.9950 (11) Å. These coordination bonds, forming a basal plane, are of normal strength with average bond length of Co—O 1.914 (3) Å, and Co—N 1.947 (4) Å.

The distances of the nitro group O-atoms O4 and O5^{i} [symmetry code: (i) -x + 2, -y, -z + 1] to atom Co1 are 2.8066 (44) Å and 2.8667 (44) Å, respectively. Calculated by the formula of s = exp[(r$_{o}$-r)/B], (r = bond length, s = bond value) (Brown & Altermatt, 1985), the two bond values are 0.049 and 0.042. Hence, only weak interactions exist between atoms O4 and Co1, and Co1 and O5^{i} (Tabel 1). Thus every binuclear cobalt unit interacts with four adjacent ones through four nitro groups, forming a two-dimensional network (Fig. 2). The conformation of the ligand has changed obviously after coordination. It can be deduced that the free ligand might be a planar molecule because all the nonhydrogen atoms are in a conjugated system. In order to fulfil the intramolecular axial interaction of the nitro group, distortion has occurred between the two benzene rings of the ligand. In the binuclear molecular unit, the dihedral angle between the two benzene rings is 64.31 (13)°.

In the crystal structure there are C—H···O(nitro) interactions (Table 2), and relatively strong π···π stacking interactions [the distances between the centroids of the adjacent benzene rings are 3.5004 (2) Å, 3.6671 (2) Å and 3.6677 (2) Å] leading to the formation of a three-dimensional framework (Fig. 3).

The emission spectra of ethanol solutions of H₂CSNA and complex (I) were measured at rt. As seen in Fig. 4, the results show that H₂CSNA, exhibits two emissions at 394 nm and 466 nm (v_{ex} = 351 nm). Measurement of the complex revealed two emissions at 394 nm and 468 nm (v_{ex} = 351 nm). The similarity of the emissions bands of complex (I) and H₂CSNA indicates that the luminescence emission of complex (I) may be assigned to the intraligand emission of the H₂CSNA

ligand (Li *et al.*, 2008).

In summary, an unprecedented 2-nitroaniline Schiff base complex, [Co₂(CSNA)₂], has been synthesized and structurally characterized. This successful synthesis provides a feasible and effective synthetic method for searching and exploring other novel 2-nitroaniline Schiff base complexes.

S2. Experimental

0.166 g (1.0 mmol) of 3-carboxylsalicylaldehyde and 0.138 g (1.0 mmol) of 2-nitroaniline were dissolved in 10 ml of methanol. The mixture was stirred at 60°C, and gradually a yellow precipitate (H₂CSNA) was formed. 1 h later, 10 ml of a methanol solution of 0.08 g (2.0 mmol) NaOH, and 10 ml of a methanol solution of 0.285 g (1.2 mmol) CoCl₂.6H₂O were added to the H₂CSNA solution, sequentially. After sirring for 1 h at 60°C the solution was allowed to cool to rt and then filtered. The filtrate was left to slowly evaporate at rt. After 10 d, blue crystals, suitable for X-ray structural analysis, were formed. FT/IR data for compound (I): 1634 cm^{-1}(s, C=N), 1601 cm^{-1} (s, benzene ring), 1579 cm^{-1} (s, v_{as}(COO)), 1549 cm^{-1} (s, v_{as}(NO₂)), 1360 cm^{-1} (s, v_s(COO)), 1299 cm^{-1} (s, v_s(NO₂)).

S3. Refinement

All the H-atoms were included in calculated positions, with C—H distances constrained to 0.93 Å, and refined in the riding-model approximation, with U_{iso}(H) = 1.2 U_{eq}(parent C-atom).
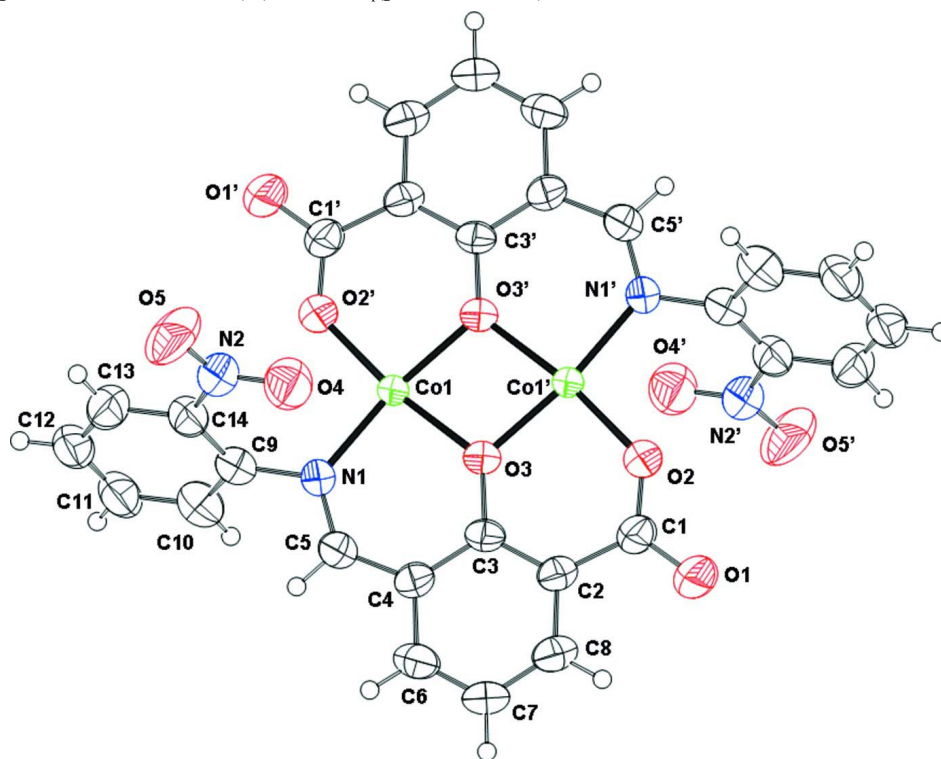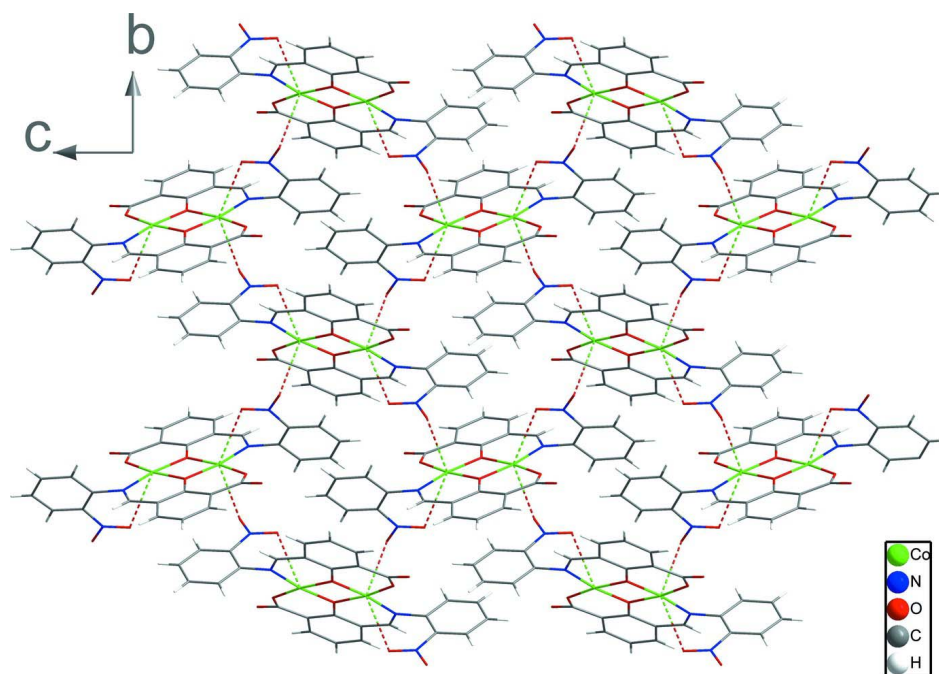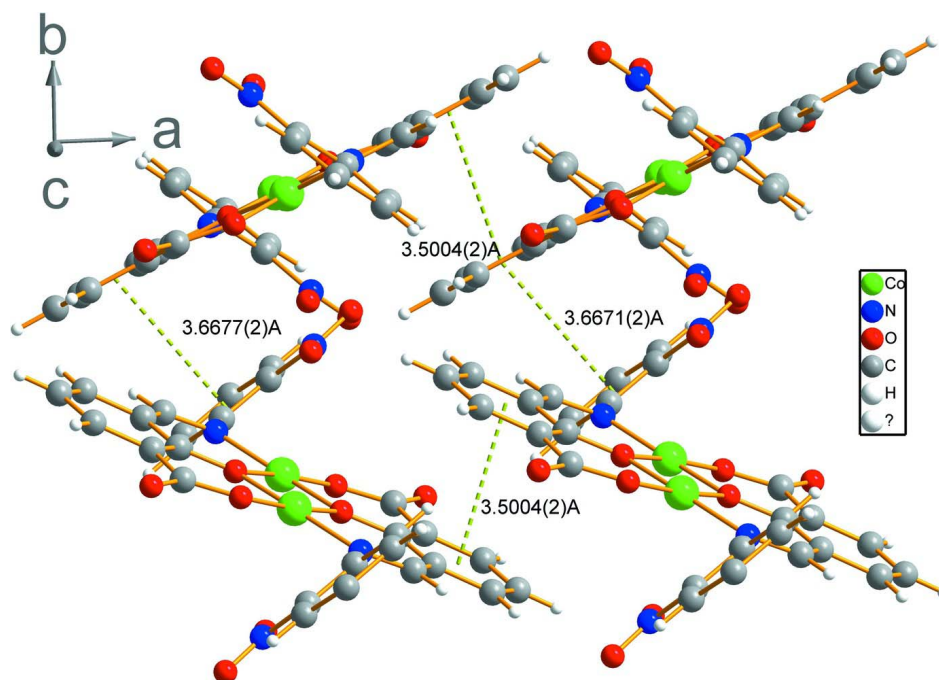

Figure 1
A view of the molecular structure of compound (I), showing the atom-labeling scheme. Atoms labeled (′) are generated by the symmetry code -*x* + 2, -*y*, -*z* + 1.

Figure 2

View along the *a*-axis of the two-dimensional network of complex (I).

Figure 3

A view down the c axis of the *π*—*π* stacking interactions between the two-dimensional networks in compound (I).
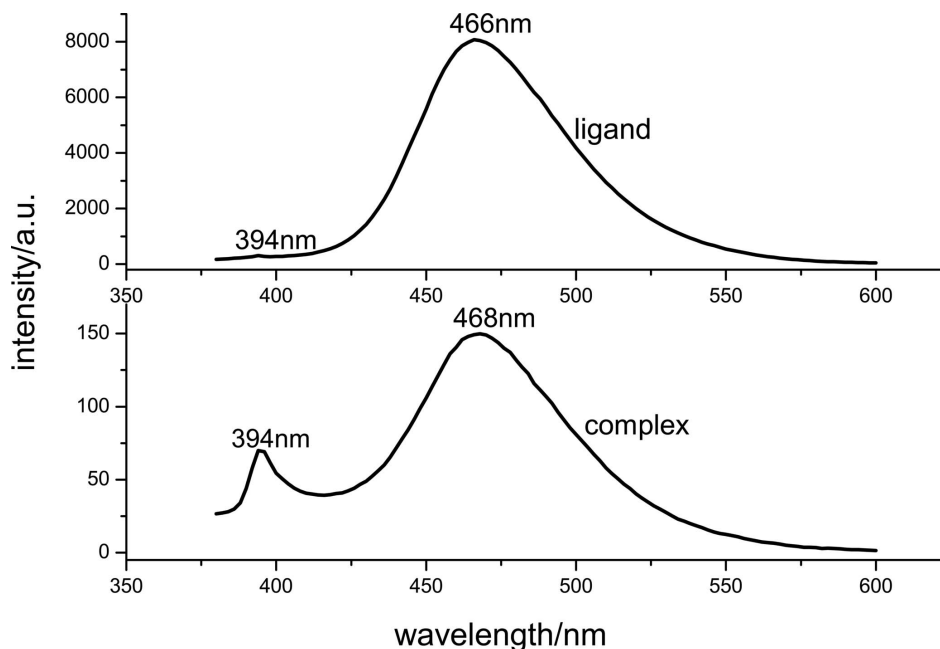
Figure 4

Emission spectra of the ligand and complex (I) in ethanol solution, $\lambda_{ex} = 351$ nm.

bis{μ-3-[(2-nitrophenyl)iminomethyl]-2-oxidobenzoato}dicopper(II)

Crystal data

[Co₂(C₁₄H₈N₂O₅)₂]	$F(000) = 692$
$M_r = 686.31$	$D_x = 1.877$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1063 reflections
$a = 8.3398$ (6) Å	$\theta = 3.1–22.1°$
$b = 11.0454$ (8) Å	$\mu = 1.44$ mm⁻¹
$c = 13.3681$ (9) Å	$T = 296$ K
$\beta = 99.604$ (1)°	Block, colourless
$V = 1214.16$ (15) Å³	$0.21 \times 0.16 \times 0.11$ mm
$Z = 2$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	6134 measured reflections
	2132 independent reflections
Radiation source: fine-focus sealed tube	1536 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.045$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan	$h = -9 \rightarrow 9$
(*SADABS*; Bruker, 2005)	$k = -11 \rightarrow 13$
$T_{min} = 0.752$, $T_{max} = 0.858$	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	2132 reflections
Least-squares matrix: full	199 parameters
$R[F^2 > 2\sigma(F^2)] = 0.045$	0 restraints
$wR(F^2) = 0.123$	Primary atom site location: structure-invariant
$S = 1.00$	direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.98614 (6)	0.01580 (5)	0.38763 (4)	0.0353 (2)
O1	0.6445 (5)	0.0607 (5)	0.7562 (3)	0.0940 (18)
O2	0.8752 (4)	0.0241 (3)	0.7042 (2)	0.0581 (11)
O3	0.8641 (3)	0.0427 (3)	0.4968 (2)	0.0452 (10)
O4	1.0672 (5)	0.2394 (4)	0.3097 (3)	0.0765 (17)
O5	1.1737 (5)	0.2946 (4)	0.1830 (4)	0.101 (2)
N1	0.8176 (4)	0.0891 (3)	0.2876 (3)	0.0456 (12)
N2	1.0763 (5)	0.2359 (4)	0.2183 (3)	0.0615 (17)
C1	0.7269 (6)	0.0597 (5)	0.6879 (4)	0.0515 (17)
C2	0.6501 (5)	0.1047 (4)	0.5856 (3)	0.0430 (16)
C3	0.7180 (5)	0.0937 (3)	0.4962 (3)	0.0390 (14)
C4	0.6304 (5)	0.1389 (4)	0.4043 (3)	0.0433 (16)
C5	0.6823 (6)	0.1325 (4)	0.3083 (4)	0.0501 (17)
C6	0.4790 (5)	0.1957 (4)	0.4036 (4)	0.0541 (19)
C7	0.4134 (6)	0.2066 (4)	0.4893 (4)	0.0529 (19)
C8	0.4995 (5)	0.1602 (4)	0.5784 (4)	0.0502 (17)
C9	0.8350 (6)	0.0974 (4)	0.1838 (4)	0.0529 (17)
C10	0.7265 (7)	0.0345 (5)	0.1114 (4)	0.0668 (19)
C11	0.7394 (7)	0.0423 (5)	0.0094 (4)	0.069 (2)
C12	0.8596 (7)	0.1094 (5)	−0.0233 (4)	0.065 (2)
C13	0.9691 (7)	0.1698 (5)	0.0476 (4)	0.071 (2)
C14	0.9579 (6)	0.1648 (4)	0.1501 (4)	0.0540 (17)
H5	0.61030	0.16330	0.25350	0.0600*
H6	0.42290	0.22650	0.34290	0.0650*
H7	0.31340	0.24430	0.48820	0.0640*
H8	0.45370	0.16660	0.63700	0.0600*
H10	0.64530	−0.01270	0.13150	0.0800*
H11	0.66480	0.00110	−0.03810	0.0830*
H12	0.86670	0.11380	−0.09190	0.0780*
H13	1.05180	0.21470	0.02670	0.0850*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0287 (3)	0.0470 (4)	0.0303 (3)	0.0063 (3)	0.0052 (2)	0.0036 (3)
O1	0.062 (3)	0.174 (4)	0.049 (2)	0.029 (3)	0.018 (2)	−0.001 (3)
O2	0.048 (2)	0.083 (2)	0.0446 (19)	0.0159 (17)	0.0113 (15)	0.0061 (17)
O3	0.0358 (17)	0.0562 (18)	0.0441 (18)	0.0091 (14)	0.0080 (13)	0.0063 (15)
O4	0.072 (3)	0.091 (3)	0.065 (3)	−0.014 (2)	0.007 (2)	−0.004 (2)
O5	0.084 (3)	0.125 (4)	0.107 (4)	−0.035 (3)	0.052 (3)	0.003 (3)
N1	0.040 (2)	0.059 (2)	0.038 (2)	0.0039 (18)	0.0074 (16)	0.0094 (18)
N2	0.055 (3)	0.075 (3)	0.056 (3)	0.000 (2)	0.014 (2)	0.009 (2)
C1	0.046 (3)	0.067 (3)	0.043 (3)	0.005 (2)	0.012 (2)	−0.006 (2)
C2	0.035 (2)	0.047 (3)	0.048 (3)	−0.002 (2)	0.010 (2)	−0.005 (2)
C3	0.030 (2)	0.038 (2)	0.048 (3)	−0.0018 (18)	0.0033 (19)	−0.001 (2)
C4	0.036 (2)	0.046 (3)	0.049 (3)	−0.004 (2)	0.010 (2)	0.000 (2)
C5	0.040 (3)	0.060 (3)	0.049 (3)	0.003 (2)	0.004 (2)	0.010 (2)
C6	0.037 (3)	0.053 (3)	0.070 (4)	0.004 (2)	0.002 (2)	0.012 (3)
C7	0.033 (3)	0.059 (3)	0.067 (4)	0.006 (2)	0.009 (2)	−0.002 (3)
C8	0.037 (3)	0.057 (3)	0.058 (3)	−0.002 (2)	0.012 (2)	−0.012 (2)
C9	0.043 (3)	0.063 (3)	0.051 (3)	0.006 (2)	0.003 (2)	0.007 (2)
C10	0.060 (3)	0.076 (4)	0.060 (3)	0.001 (3)	−0.003 (3)	0.001 (3)
C11	0.067 (4)	0.084 (4)	0.050 (3)	0.014 (3)	−0.005 (3)	0.003 (3)
C12	0.066 (4)	0.083 (4)	0.045 (3)	0.022 (3)	0.004 (3)	−0.001 (3)
C13	0.071 (4)	0.083 (4)	0.064 (4)	0.023 (3)	0.027 (3)	0.016 (3)
C14	0.054 (3)	0.059 (3)	0.048 (3)	0.011 (2)	0.006 (2)	0.006 (2)

Geometric parameters (Å, º)

Co1—O3	1.936 (3)	C4—C6	1.409 (6)
Co1—N1	1.947 (4)	C6—C7	1.355 (7)
Co1—O2[i]	1.874 (3)	C7—C8	1.383 (7)
Co1—O3[i]	1.929 (3)	C9—C10	1.395 (7)
O1—C1	1.231 (7)	C9—C14	1.401 (7)
O2—C1	1.281 (6)	C10—C11	1.388 (8)
O3—C3	1.341 (5)	C11—C12	1.375 (8)
O4—N2	1.237 (6)	C12—C13	1.374 (8)
O5—N2	1.196 (6)	C13—C14	1.390 (7)
N1—C5	1.298 (6)	C5—H5	0.9300
N1—C9	1.422 (7)	C6—H6	0.9300
N2—C14	1.457 (6)	C7—H7	0.9300
C1—C2	1.495 (7)	C8—H8	0.9300
C2—C3	1.411 (6)	C10—H10	0.9300
C2—C8	1.386 (6)	C11—H11	0.9300
C3—C4	1.412 (6)	C12—H12	0.9300
C4—C5	1.423 (7)	C13—H13	0.9300
Co1···O4	2.807 (4)	C3···C8[ix]	3.398 (6)
Co1···N2	3.488 (4)	C3···C13[iv]	3.347 (7)

Co1···O5ⁱⁱ	2.867 (5)	C4···C8ⁱˣ	3.496 (6)
Co1···N2ⁱⁱ	3.404 (4)	C4···C2ⁱˣ	3.583 (6)
Co1···C13ⁱⁱ	3.923 (6)	C4···C12ⁱᵛ	3.421 (7)
O1···C11ⁱⁱⁱ	3.351 (7)	C5···O4	3.417 (7)
O1···C12ⁱⁱⁱ	3.230 (7)	C6···C2ⁱˣ	3.499 (6)
O2···N2ⁱ	3.057 (5)	C6···C1ⁱˣ	3.421 (7)
O2···C9ⁱ	2.946 (6)	C7···C2ⁱˣ	3.596 (6)
O2···C14ⁱ	3.030 (6)	C7···C3ⁱˣ	3.509 (6)
O2···O3	2.766 (4)	C8···C3ⁱˣ	3.398 (6)
O2···N2ⁱᵛ	3.126 (5)	C8···O5ˣ	3.295 (6)
O2···O4ⁱ	2.961 (6)	C8···C4ⁱˣ	3.496 (6)
O2···N1ⁱ	2.836 (5)	C11···C13ˣⁱ	3.549 (8)
O3···O2	2.766 (4)	C11···O1ˣⁱⁱ	3.351 (7)
O3···O3ⁱ	2.444 (4)	C12···C4ᵛⁱⁱⁱ	3.421 (7)
O3···N1	2.806 (5)	C12···O1ˣⁱⁱ	3.230 (7)
O3···C13ⁱᵛ	3.334 (6)	C12···C3ᵛⁱⁱⁱ	3.510 (7)
O3···C5	2.891 (6)	C12···C13ˣⁱ	3.437 (8)
O4···Co1	2.807 (4)	C12···C12ˣⁱ	3.351 (8)
O4···N1	2.640 (5)	C13···C11ˣⁱ	3.549 (8)
O4···C5	3.417 (7)	C13···Co1ᵛⁱ	3.923 (6)
O4···O2ⁱ	2.961 (6)	C13···C3ᵛⁱⁱⁱ	3.347 (7)
O5···C8ᵛ	3.295 (6)	C13···C12ˣⁱ	3.437 (8)
O5···Co1ᵛⁱ	2.867 (5)	C13···O3ᵛⁱⁱⁱ	3.334 (6)
O1···H11ⁱⁱⁱ	2.8100	C14···O2ⁱ	3.030 (6)
O1···H8	2.3700	C1···H12ⁱⁱⁱ	3.0400
O1···H12ⁱⁱⁱ	2.5800	C5···H10	2.8300
O2···H12ⁱⁱⁱ	2.9100	C8···H5ⁱᵛ	3.0700
O4···H7ᵛⁱⁱ	2.8800	C10···H5	2.6800
O4···H12ⁱᵛ	2.8100	H5···C10	2.6800
O5···H13	2.3400	H5···H6	2.2300
O5···H6ᵛⁱⁱ	2.8200	H5···H10	2.5900
O5···H8ᵛ	2.5500	H5···C8ᵛⁱⁱⁱ	3.0700
N1···O3	2.806 (5)	H6···O5ˣⁱⁱⁱ	2.8200
N1···O4	2.640 (5)	H6···H5	2.2300
N1···N2	2.968 (5)	H7···O4ˣⁱⁱⁱ	2.8800
N1···C3	3.040 (6)	H7···H13ˣ	2.3700
N1···O2ⁱ	2.836 (5)	H8···O1	2.3700
N2···Co1	3.488 (4)	H8···O5ˣ	2.5500
N2···N1	2.968 (5)	H10···C5	2.8300
N2···Co1ᵛⁱ	3.404 (4)	H10···H5	2.5900
N2···O2ⁱ	3.057 (5)	H11···O1ˣⁱⁱ	2.8100
N2···O2ᵛⁱⁱⁱ	3.126 (5)	H12···O1ˣⁱⁱ	2.5800
C1···C6ⁱˣ	3.421 (7)	H12···O2ˣⁱⁱ	2.9100
C2···C6ⁱˣ	3.499 (6)	H12···C1ˣⁱⁱ	3.0400
C2···C4ⁱˣ	3.583 (6)	H12···O4ᵛⁱⁱⁱ	2.8100
C2···C7ⁱˣ	3.596 (6)	H13···O5	2.3400
C3···C12ⁱᵛ	3.510 (7)	H13···H7ᵛ	2.3700
C3···C7ⁱˣ	3.509 (6)		

O3—Co1—N1	92.51 (14)	C4—C6—C7	121.5 (5)
O2ⁱ—Co1—O3	171.54 (13)	C6—C7—C8	118.1 (4)
O3—Co1—O3ⁱ	78.42 (11)	C2—C8—C7	123.9 (5)
O2ⁱ—Co1—N1	95.83 (14)	N1—C9—C10	119.0 (4)
O3ⁱ—Co1—N1	170.41 (14)	N1—C9—C14	123.2 (4)
O2ⁱ—Co1—O3ⁱ	93.33 (12)	C10—C9—C14	117.8 (5)
Co1ⁱ—O2—C1	130.1 (3)	C9—C10—C11	120.2 (5)
Co1—O3—C3	130.6 (2)	C10—C11—C12	121.7 (5)
Co1—O3—Co1ⁱ	101.58 (12)	C11—C12—C13	118.6 (5)
Co1ⁱ—O3—C3	127.7 (2)	C12—C13—C14	121.0 (5)
Co1—N1—C5	124.1 (3)	N2—C14—C9	122.8 (5)
Co1—N1—C9	121.2 (3)	N2—C14—C13	116.5 (4)
C5—N1—C9	114.7 (4)	C9—C14—C13	120.8 (5)
O4—N2—O5	122.0 (5)	N1—C5—H5	116.00
O4—N2—C14	119.2 (4)	C4—C5—H5	116.00
O5—N2—C14	118.6 (4)	C4—C6—H6	119.00
O1—C1—O2	121.3 (5)	C7—C6—H6	119.00
O1—C1—C2	117.9 (5)	C6—C7—H7	121.00
O2—C1—C2	120.8 (4)	C8—C7—H7	121.00
C1—C2—C3	125.1 (4)	C2—C8—H8	118.00
C1—C2—C8	117.1 (4)	C7—C8—H8	118.00
C3—C2—C8	117.8 (4)	C9—C10—H10	120.00
O3—C3—C2	121.6 (4)	C11—C10—H10	120.00
O3—C3—C4	119.4 (4)	C10—C11—H11	119.00
C2—C3—C4	119.0 (4)	C12—C11—H11	119.00
C3—C4—C5	125.2 (4)	C11—C12—H12	121.00
C3—C4—C6	119.8 (4)	C13—C12—H12	121.00
C5—C4—C6	115.1 (4)	C12—C13—H13	120.00
N1—C5—C4	128.1 (5)	C14—C13—H13	120.00
N1—Co1—O3—C3	0.1 (3)	O2—C1—C2—C3	11.4 (7)
N1—Co1—O3—Co1ⁱ	−176.86 (15)	O2—C1—C2—C8	−169.5 (4)
O3ⁱ—Co1—O3—C3	176.9 (4)	C1—C2—C3—O3	−1.7 (6)
O3ⁱ—Co1—O3—Co1ⁱ	−0.02 (14)	C1—C2—C3—C4	179.0 (4)
O3—Co1—N1—C5	−0.5 (4)	C8—C2—C3—O3	179.1 (4)
O3—Co1—N1—C9	−179.7 (3)	C8—C2—C3—C4	−0.2 (6)
O2ⁱ—Co1—N1—C5	178.1 (4)	C1—C2—C8—C7	179.9 (4)
O2ⁱ—Co1—N1—C9	−1.2 (3)	C3—C2—C8—C7	−0.9 (7)
N1—Co1—O2ⁱ—C1ⁱ	168.2 (4)	O3—C3—C4—C5	1.8 (6)
O3—Co1—O3ⁱ—Co1ⁱ	0.02 (14)	O3—C3—C4—C6	−178.2 (4)
O3—Co1—O3ⁱ—C3ⁱ	177.1 (3)	C2—C3—C4—C5	−179.0 (4)
Co1ⁱ—O2—C1—O1	166.4 (4)	C2—C3—C4—C6	1.1 (6)
Co1ⁱ—O2—C1—C2	−15.3 (7)	C3—C4—C5—N1	−2.4 (8)
Co1—O3—C3—C2	−179.9 (3)	C6—C4—C5—N1	177.6 (4)
Co1—O3—C3—C4	−0.7 (5)	C3—C4—C6—C7	−1.0 (7)
Co1ⁱ—O3—C3—C2	−3.7 (5)	C5—C4—C6—C7	179.0 (4)
Co1ⁱ—O3—C3—C4	175.5 (3)	C4—C6—C7—C8	0.0 (7)

Co1—N1—C5—C4	1.6 (7)	C6—C7—C8—C2	1.0 (7)
C9—N1—C5—C4	−179.1 (4)	N1—C9—C10—C11	179.2 (5)
Co1—N1—C9—C10	116.1 (4)	C14—C9—C10—C11	−1.7 (8)
Co1—N1—C9—C14	−63.1 (5)	N1—C9—C14—N2	−2.0 (7)
C5—N1—C9—C10	−63.3 (6)	N1—C9—C14—C13	−180.0 (4)
C5—N1—C9—C14	117.6 (5)	C10—C9—C14—N2	178.8 (5)
O4—N2—C14—C9	−1.4 (7)	C10—C9—C14—C13	0.9 (7)
O4—N2—C14—C13	176.6 (5)	C9—C10—C11—C12	1.2 (9)
O5—N2—C14—C9	−177.2 (5)	C10—C11—C12—C13	0.0 (9)
O5—N2—C14—C13	0.8 (7)	C11—C12—C13—C14	−0.8 (8)
O1—C1—C2—C3	−170.3 (5)	C12—C13—C14—N2	−177.7 (5)
O1—C1—C2—C8	8.9 (7)	C12—C13—C14—C9	0.4 (8)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) −*x*+2, *y*−1/2, −*z*+1/2; (iii) *x*, *y*, *z*+1; (iv) *x*, −*y*+1/2, *z*+1/2; (v) *x*+1, −*y*+1/2, *z*−1/2; (vi) −*x*+2, *y*+1/2, −*z*+1/2; (vii) *x*+1, *y*, *z*; (viii) *x*, −*y*+1/2, *z*−1/2; (ix) −*x*+1, −*y*, −*z*+1; (x) *x*−1, −*y*+1/2, *z*+1/2; (xi) −*x*+2, −*y*, −*z*; (xii) *x*, *y*, *z*−1; (xiii) *x*−1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1	0.93	2.37	2.713 (7)	102
C8—H8···O5[x]	0.93	2.55	3.295 (6)	138
C12—H12···O1[xii]	0.93	2.58	3.230 (7)	128
C13—H13···O5	0.93	2.34	2.657 (7)	100

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