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catena-Poly[[(2,2-bipyridine)cobalt(II)]-μ-imidazole-4,5-dicarboxylato]

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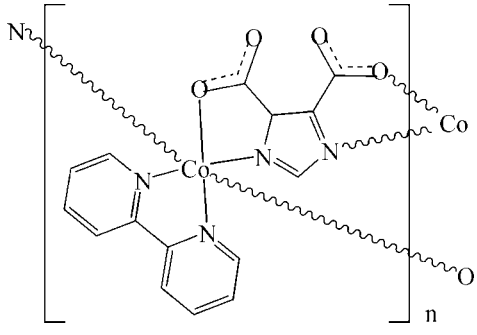
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.104; data-to-parameter ratio = 12.8.

In the title complex, $[Co(C_5HN_2O_4)(C_{10}H_8N_2)]_n$, the asymmetric unit contains two crystallographically independent monomer units with similar geometry. The Co^{II} cations are coordinated octahedrally by two carboxylate O atoms and by four N atoms, two of which belong to the 2,2-bipyridine ligand and two to different imidazole rings. The connectivity between the metal cations and the imidazole-4,5-carboxylate units gives rise to one-dimensional zigzag chains parallel to [010].

Related literature

For studies and reviews of inorganic–organic hybrid materials, see: Church & Halvorson (1959); Chung *et al.* (1971); Pocker & Fong (1980); Scapin *et al.* (1997); Okabe & Oya (2000); Serre *et al.* (2005).



Experimental

Crystal data

$[Co(C_5HN_2O_4)(C_{10}H_8N_2)]$
M_r = 368.19
Monoclinic, $P2_1/c$
a = 20.5002 (10) Å
b = 9.6500 (5) Å
c = 14.7623 (7) Å
β = 101.801 (1)°
V = 2858.7 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.23 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.887, T_{max} = 0.887
15047 measured reflections
5563 independent reflections
4855 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.104
S = 1.00
5563 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N2	2.091 (2)	Co2—N6	2.077 (2)
Co1—N1	2.117 (2)	Co2—N5	2.080 (2)
Co1—N4	2.132 (2)	Co2—N8	2.125 (2)
Co1—O3	2.1569 (18)	Co2—N7	2.205 (2)
Co1—O1	2.2067 (18)	Co2—O5	2.2071 (19)
Co1—N3	2.271 (2)	Co2—O7	2.2562 (19)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2118).

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supplementary materials

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catena-Poly[[(2,2-bipyridine)cobalt(II)]-μ-imidazole-4,5-dicarboxylato]

L.-J. Hao, Z.-M. Bao and T.-L. Yu

Comment

Hybrid organic-inorganic materials are important materials because of their application in catalysis, as optical materials, membranes, and in sorption (Church & Halvorson, 1959; Chung *et al.*, 1971), as well as in biological systems (Okabe & Oya, 2000; Serre *et al.*, 2005; Pocker & Fong, 1980; Scapin *et al.*, 1997). Herein, we report a new compound, *catena*-poly[(2,2-bipyridine)(imidazole-4,5-dicarboxylate)cobalt(II)], (I).

In the structure of compound (I), the asymmetric unit contains two crystallographically independent molecules with nearly the same geometry. As shown in Fig. 1, the Co^{II} cations exhibit a distorted octahedral coordination sphere, made up of two carboxylate oxygen atoms and four nitrogen atoms, two of which belong to the 2,2-bipyridine ligand and the other two to the imidazole ring. The Co—O and Co—N bond lengths are in the usual ranges with 2.1569 (18) to 2.2562 (19) and 2.077 (2) to 2.271 (2) Å, respectively. The two carboxylate groups of the imidazole-4,5-dicarboxylate ligand coordinate in a monodentate fashion to the Co^{II} ions, whereby the connectivity between the cations and the ligands gives rise to one-dimensional zigzag chains along [010] (Fig. 2). The 2,2-bipyridine ligands are situated in the space between the chains.

Experimental

All chemicals were purchased from Acros Co. Ltd. Compound (I) was obtained under hydrothermal conditions by reaction of cobalt sulfate (0.5 mmol), imidazole-4,5-dicarboxylic acid (0.5 mmol), 2,2-bipyridine (0.5 mmol) and KOH (1 mmol) in 20 ml distilled water. The mixture was heated in a 30 ml autoclave at 453 K for 3 d. Red crystals were obtained in a yield of approximately 25%. Analysis calculated for $C_{15}H_9N_4CoO_4$: C 48.96, H 2.47, N 15.23, Co 15.95%$_{wt}$; found: C 48.98, H 2.51, N 15.27, Co 16.08%$_{wt}$.

Refinement

All H atoms were positioned geometrically and refined as riding atoms with C—H= 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

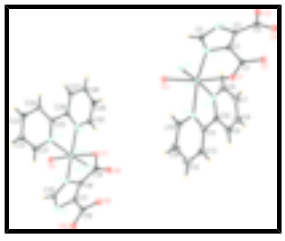


Fig. 1. The two crystallographically independent molecules in (I), showing 30% probability displacement ellipsoids. [Symmetry codes: (i) $-x + 1, y + 1/2, -z + 3/2$].

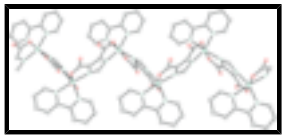


Fig. 2. A zigzag chain extending palallel to [010] in (I).

catena-Poly[[(2,2-bipyridine)cobalt(II)]-μ-imidazole-4,5-dicarboxylato]

Crystal data

$[Co(C_5HN_2O_4)(C_{10}H_8N_2)]$	F_{000} = 1488
M_r = 368.19	D_x = 1.711 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5547 reflections
a = 20.5002 (10) Å	θ = 2.3–26.1º
b = 9.6500 (5) Å	μ = 1.23 mm^{-1}
c = 14.7623 (7) Å	T = 293 (2) K
β = 101.801 (1)º	Cube, red
V = 2858.7 (2) Å^3	0.10 × 0.10 × 0.10 mm
Z = 8	

Data collection

Bruker APEX II CCD area-detector diffractometer	5563 independent reflections
Radiation source: fine-focus sealed tube	4855 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→20
T_{min} = 0.887, T_{max} = 0.887	k = −11→10
15047 measured reflections	l = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.9045P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
5563 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
433 parameters	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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	0.899411 (13)	−0.02479 (3)	0.214401 (19)	0.01403 (10)
Co2	0.597903 (14)	0.09584 (3)	0.81973 (2)	0.01626 (10)
N1	0.94287 (10)	−0.2240 (2)	0.23760 (13)	0.0241 (4)
O1	0.91439 (9)	−0.00358 (18)	0.07122 (12)	0.0264 (4)
O3	0.89860 (9)	−0.05143 (19)	0.35923 (12)	0.0292 (4)
O7	0.61837 (9)	0.0776 (2)	0.67573 (13)	0.0326 (4)
O5	0.56793 (9)	0.1364 (2)	0.95260 (13)	0.0325 (4)
N5	0.54592 (10)	0.2810 (2)	0.79047 (14)	0.0262 (5)
N2	0.98575 (11)	0.0964 (2)	0.23543 (14)	0.0244 (5)
N6	0.52456 (10)	−0.0428 (2)	0.75854 (14)	0.0258 (5)
N7	0.66335 (11)	−0.0778 (2)	0.87713 (15)	0.0276 (5)
N8	0.69413 (10)	0.1864 (2)	0.85720 (14)	0.0273 (5)
N3	0.84013 (11)	0.1734 (2)	0.17796 (15)	0.0292 (5)
N4	0.79750 (11)	−0.0866 (2)	0.17980 (15)	0.0274 (5)
C25	0.72862 (13)	−0.0456 (3)	0.90105 (17)	0.0268 (5)
C26	0.74592 (13)	0.1016 (3)	0.88752 (17)	0.0259 (5)
C27	0.81097 (13)	0.1492 (3)	0.90555 (18)	0.0316 (6)
H27	0.8461	0.0881	0.9249	0.038*
O8	0.58403 (10)	−0.0419 (2)	0.54499 (13)	0.0335 (4)
O4	0.94588 (10)	−0.1818 (2)	0.47970 (12)	0.0368 (5)
O6	0.49477 (10)	0.2666 (2)	1.00903 (12)	0.0345 (4)
O2	0.96716 (9)	0.13600 (19)	−0.01065 (11)	0.0286 (4)
C4	0.93289 (12)	−0.1533 (3)	0.39434 (17)	0.0262 (5)
C17	0.51348 (12)	0.3156 (3)	0.85967 (17)	0.0251 (5)
C20	0.47894 (12)	−0.1313 (3)	0.77887 (17)	0.0263 (5)
H20	0.4658	−0.1319	0.8355	0.032*
C24	0.77644 (13)	−0.1446 (3)	0.93791 (18)	0.0313 (6)
H24	0.8213	−0.1207	0.9542	0.038*
C1	0.95748 (12)	0.0865 (2)	0.06645 (17)	0.0234 (5)
C18	0.52989 (12)	−0.0767 (3)	0.67016 (17)	0.0241 (5)
C5	0.97688 (12)	−0.3213 (3)	0.20100 (16)	0.0245 (5)
H5	0.9747	−0.3305	0.1377	0.029*
C30	0.70633 (13)	0.3206 (3)	0.84595 (18)	0.0301 (6)

H30	0.6705	0.3795	0.8250	0.036*
C2	0.99722 (12)	0.1434 (3)	0.15254 (16)	0.0232 (5)
C3	0.95937 (12)	−0.2470 (2)	0.33094 (16)	0.0231 (5)
C28	0.82316 (14)	0.2885 (3)	0.89459 (19)	0.0339 (6)
H28	0.8665	0.3228	0.9075	0.041*
C16	0.52682 (12)	0.2342 (3)	0.94635 (17)	0.0270 (5)
C19	0.58001 (13)	−0.0072 (3)	0.62809 (18)	0.0270 (5)
C15	0.77793 (14)	−0.2154 (3)	0.19535 (19)	0.0326 (6)
H15	0.8103	−0.2803	0.2198	0.039*
C11	0.75122 (13)	0.0084 (3)	0.14536 (17)	0.0280 (6)
C10	0.77552 (13)	0.1525 (3)	0.13920 (17)	0.0282 (5)
C29	0.76973 (14)	0.3755 (3)	0.86409 (18)	0.0312 (6)
H29	0.7764	0.4696	0.8559	0.037*
C12	0.68375 (14)	−0.0266 (3)	0.1226 (2)	0.0392 (7)
H12	0.6522	0.0392	0.0968	0.047*
C6	0.86422 (15)	0.3021 (3)	0.1792 (2)	0.0358 (6)
H6	0.9087	0.3171	0.2063	0.043*
C22	0.68865 (14)	−0.3107 (3)	0.92572 (19)	0.0352 (6)
H22	0.6738	−0.4000	0.9337	0.042*
C9	0.73395 (15)	0.2603 (3)	0.10184 (19)	0.0369 (6)
H9	0.6893	0.2438	0.0761	0.044*
C23	0.75606 (14)	−0.2780 (3)	0.94960 (19)	0.0348 (6)
H23	0.7871	−0.3459	0.9733	0.042*
C14	0.71227 (14)	−0.2561 (3)	0.1769 (2)	0.0402 (7)
H14	0.7003	−0.3459	0.1896	0.048*
C21	0.64446 (14)	−0.2074 (3)	0.89001 (19)	0.0337 (6)
H21	0.5994	−0.2290	0.8741	0.040*
C8	0.75973 (17)	0.3918 (3)	0.1035 (2)	0.0445 (8)
H8A	0.7326	0.4655	0.0787	0.053*
C13	0.66438 (15)	−0.1595 (4)	0.1388 (2)	0.0464 (8)
H13	0.6196	−0.1842	0.1243	0.056*
C7	0.82565 (17)	0.4142 (3)	0.1418 (2)	0.0432 (7)
H7	0.8440	0.5024	0.1428	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01135 (17)	0.01285 (17)	0.01726 (17)	0.00016 (10)	0.00146 (12)	0.00298 (11)
Co2	0.01115 (17)	0.01302 (17)	0.02239 (18)	0.00011 (10)	−0.00177 (12)	−0.00095 (11)
N1	0.0253 (11)	0.0242 (11)	0.0222 (10)	0.0010 (8)	0.0032 (8)	0.0019 (8)
O1	0.0249 (9)	0.0274 (9)	0.0260 (9)	−0.0046 (7)	0.0033 (7)	−0.0023 (7)
O3	0.0312 (10)	0.0270 (9)	0.0299 (9)	0.0081 (8)	0.0076 (8)	0.0014 (8)
O7	0.0272 (10)	0.0338 (10)	0.0371 (10)	−0.0060 (8)	0.0073 (8)	−0.0015 (8)
O5	0.0315 (10)	0.0313 (10)	0.0326 (9)	0.0040 (8)	0.0015 (8)	0.0056 (8)
N5	0.0257 (11)	0.0272 (11)	0.0248 (10)	0.0004 (9)	0.0034 (8)	−0.0005 (9)
N2	0.0261 (11)	0.0242 (11)	0.0221 (10)	−0.0011 (8)	0.0031 (8)	0.0000 (8)
N6	0.0218 (11)	0.0278 (12)	0.0265 (10)	0.0006 (9)	0.0019 (8)	−0.0011 (9)
N7	0.0244 (11)	0.0260 (11)	0.0317 (11)	−0.0010 (9)	0.0041 (9)	0.0023 (9)

N8	0.0251 (11)	0.0271 (11)	0.0281 (11)	−0.0012 (9)	0.0017 (9)	−0.0004 (9)
N3	0.0285 (12)	0.0278 (12)	0.0320 (11)	0.0036 (9)	0.0074 (9)	0.0009 (9)
N4	0.0244 (11)	0.0313 (12)	0.0266 (11)	0.0001 (9)	0.0053 (9)	0.0014 (9)
C25	0.0252 (13)	0.0288 (14)	0.0251 (12)	−0.0005 (10)	0.0023 (10)	−0.0006 (10)
C26	0.0249 (13)	0.0283 (14)	0.0234 (12)	0.0009 (10)	0.0023 (10)	−0.0003 (10)
C27	0.0277 (14)	0.0314 (14)	0.0341 (14)	0.0005 (11)	0.0027 (11)	0.0048 (11)
O8	0.0340 (11)	0.0371 (11)	0.0316 (10)	−0.0005 (8)	0.0121 (8)	−0.0006 (8)
O4	0.0481 (12)	0.0397 (11)	0.0233 (9)	0.0145 (9)	0.0090 (8)	0.0014 (8)
O6	0.0380 (11)	0.0374 (11)	0.0288 (9)	0.0010 (9)	0.0089 (8)	0.0036 (8)
O2	0.0311 (10)	0.0309 (9)	0.0227 (8)	−0.0025 (8)	0.0033 (7)	−0.0005 (7)
C4	0.0253 (13)	0.0265 (13)	0.0264 (12)	0.0010 (10)	0.0046 (10)	0.0002 (10)
C17	0.0219 (12)	0.0266 (13)	0.0258 (12)	−0.0021 (10)	0.0024 (10)	−0.0006 (10)
C20	0.0237 (13)	0.0281 (13)	0.0267 (12)	−0.0020 (10)	0.0040 (10)	0.0000 (10)
C24	0.0256 (14)	0.0338 (15)	0.0324 (13)	0.0025 (11)	0.0010 (11)	−0.0001 (11)
C1	0.0220 (12)	0.0228 (12)	0.0255 (12)	0.0021 (10)	0.0049 (10)	0.0000 (9)
C18	0.0213 (12)	0.0244 (12)	0.0255 (12)	0.0039 (10)	0.0024 (10)	0.0006 (10)
C5	0.0270 (13)	0.0264 (13)	0.0197 (11)	0.0010 (10)	0.0039 (9)	0.0005 (10)
C30	0.0306 (14)	0.0248 (13)	0.0339 (13)	0.0008 (11)	0.0042 (11)	0.0029 (11)
C2	0.0222 (12)	0.0236 (12)	0.0230 (11)	0.0021 (10)	0.0027 (9)	0.0005 (10)
C3	0.0219 (12)	0.0232 (12)	0.0237 (11)	−0.0010 (10)	0.0039 (9)	0.0005 (10)
C28	0.0273 (14)	0.0386 (16)	0.0348 (14)	−0.0076 (12)	0.0037 (11)	0.0022 (12)
C16	0.0247 (13)	0.0261 (13)	0.0282 (12)	−0.0032 (10)	0.0005 (10)	0.0003 (10)
C19	0.0243 (13)	0.0261 (13)	0.0302 (13)	0.0041 (10)	0.0043 (10)	0.0012 (10)
C15	0.0315 (14)	0.0288 (14)	0.0362 (14)	−0.0030 (11)	0.0036 (11)	0.0004 (11)
C11	0.0249 (13)	0.0349 (14)	0.0230 (12)	0.0040 (11)	0.0021 (10)	−0.0011 (10)
C10	0.0267 (13)	0.0350 (14)	0.0240 (12)	0.0061 (11)	0.0077 (10)	0.0036 (11)
C29	0.0353 (15)	0.0261 (13)	0.0311 (13)	−0.0067 (11)	0.0045 (11)	0.0029 (11)
C12	0.0253 (14)	0.0472 (18)	0.0426 (16)	0.0040 (12)	0.0013 (12)	−0.0010 (13)
C6	0.0366 (16)	0.0295 (14)	0.0440 (16)	0.0029 (12)	0.0141 (13)	0.0015 (12)
C22	0.0387 (16)	0.0246 (13)	0.0412 (15)	−0.0010 (12)	0.0056 (12)	0.0045 (12)
C9	0.0328 (15)	0.0417 (17)	0.0364 (15)	0.0109 (13)	0.0072 (12)	0.0073 (13)
C23	0.0353 (15)	0.0281 (14)	0.0386 (15)	0.0085 (12)	0.0018 (12)	0.0047 (12)
C14	0.0359 (16)	0.0388 (16)	0.0448 (16)	−0.0091 (13)	0.0060 (13)	−0.0024 (13)
C21	0.0279 (14)	0.0326 (15)	0.0398 (15)	−0.0042 (11)	0.0051 (11)	0.0019 (12)
C8	0.0463 (19)	0.0386 (18)	0.0511 (18)	0.0192 (14)	0.0160 (15)	0.0123 (14)
C13	0.0246 (15)	0.056 (2)	0.0560 (19)	−0.0085 (14)	0.0023 (13)	−0.0086 (16)
C7	0.051 (2)	0.0271 (15)	0.0553 (19)	0.0068 (13)	0.0197 (16)	0.0043 (13)

Geometric parameters (Å, °)

Co1—N2	2.091 (2)	C4—C3	1.482 (3)
Co1—N1	2.117 (2)	C17—C18^{i}	1.380 (4)
Co1—N4	2.132 (2)	C17—C16	1.479 (3)
Co1—O3	2.1569 (18)	C20—N5^{iii}	1.345 (3)
Co1—O1	2.2067 (18)	C20—H20	0.9300
Co1—N3	2.271 (2)	C24—C23	1.375 (4)
Co2—N6	2.077 (2)	C24—H24	0.9300
Co2—N5	2.080 (2)	C1—C2	1.469 (3)

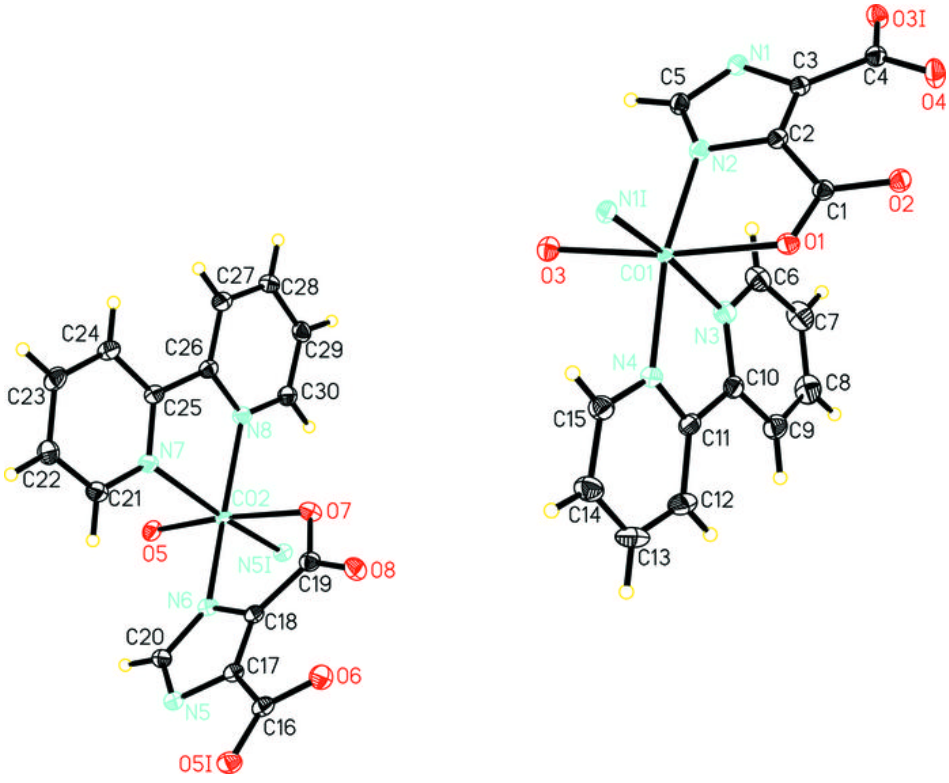
Co2—N8	2.125 (2)	C18—C17^{iii}	1.380 (4)
Co2—N7	2.205 (2)	C18—C19	1.467 (4)
Co2—O5	2.2071 (19)	C5—N2^{iv}	1.344 (3)
Co2—O7	2.2562 (19)	C5—H5	0.9300
N1—C5	1.347 (3)	C30—C29	1.378 (4)
N1—C3	1.368 (3)	C30—H30	0.9300
O1—C1	1.252 (3)	C2—C3^{ii}	1.371 (3)
O3—C4	1.257 (3)	C3—C2^{iv}	1.371 (3)
O7—C19	1.248 (3)	C28—C29	1.381 (4)
O5—C16	1.257 (3)	C28—H28	0.9300
N5—C20^{i}	1.345 (3)	C15—C14	1.375 (4)
N5—C17	1.369 (3)	C15—H15	0.9300
N2—C5^{ii}	1.344 (3)	C11—C12	1.396 (4)
N2—C2	1.370 (3)	C11—C10	1.486 (4)
N6—C20	1.345 (3)	C10—C9	1.386 (4)
N6—C18	1.371 (3)	C29—H29	0.9300
N7—C21	1.334 (3)	C12—C13	1.378 (4)
N7—C25	1.348 (3)	C12—H12	0.9300
N8—C30	1.335 (3)	C6—C7	1.386 (4)
N8—C26	1.343 (3)	C6—H6	0.9300
N3—C6	1.335 (4)	C22—C21	1.377 (4)
N3—C10	1.346 (3)	C22—C23	1.391 (4)
N4—C15	1.341 (3)	C22—H22	0.9300
N4—C11	1.342 (3)	C9—C8	1.373 (4)
C25—C24	1.397 (4)	C9—H9	0.9300
C25—C26	1.488 (4)	C23—H23	0.9300
C26—C27	1.384 (4)	C14—C13	1.387 (4)
C27—C28	1.383 (4)	C14—H14	0.9300
C27—H27	0.9300	C21—H21	0.9300
O8—C19	1.290 (3)	C8—C7	1.371 (5)
O4—C4	1.264 (3)	C8—H8A	0.9300
O6—C16	1.278 (3)	C13—H13	0.9300
O2—C1	1.286 (3)	C7—H7	0.9300
N2—Co1—N1	99.69 (8)	N5^{iii}—C20—H20	123.1
N2—Co1—N4	161.87 (8)	N6—C20—H20	123.1
N1—Co1—N4	98.29 (8)	C23—C24—C25	118.8 (3)
N2—Co1—O3	95.59 (8)	C23—C24—H24	120.6
N1—Co1—O3	79.61 (7)	C25—C24—H24	120.6
N4—Co1—O3	89.90 (7)	O1—C1—O2	123.1 (2)
N2—Co1—O1	79.10 (7)	O1—C1—C2	118.9 (2)
N1—Co1—O1	95.90 (7)	O2—C1—C2	117.9 (2)
N4—Co1—O1	96.78 (7)	N6—C18—C17^{iii}	108.2 (2)
O3—Co1—O1	172.46 (7)	N6—C18—C19	119.5 (2)
N2—Co1—N3	87.70 (8)	C17^{iii}—C18—C19	132.1 (2)
N1—Co1—N3	171.99 (8)	N2^{iv}—C5—N1	113.6 (2)
N4—Co1—N3	74.22 (8)	N2^{iv}—C5—H5	123.2

O3—Co1—N3	102.88 (7)	N1—C5—H5	123.2
O1—Co1—N3	82.39 (7)	N8—C30—C29	122.8 (3)
N6—Co2—N5	99.70 (8)	N8—C30—H30	118.6
N6—Co2—N8	158.35 (8)	C29—C30—H30	118.6
N5—Co2—N8	96.30 (8)	N2—C2—C3^{ii}	108.7 (2)
N6—Co2—N7	90.40 (8)	N2—C2—C1	118.9 (2)
N5—Co2—N7	168.06 (8)	C3^{ii}—C2—C1	131.8 (2)
N8—Co2—N7	75.70 (8)	N1—C3—C2^{iv}	108.8 (2)
N6—Co2—O5	101.08 (8)	N1—C3—C4	119.3 (2)
N5—Co2—O5	78.96 (7)	C2^{iv}—C3—C4	131.8 (2)
N8—Co2—O5	96.21 (8)	C29—C28—C27	118.6 (3)
N7—Co2—O5	92.93 (7)	C29—C28—H28	120.7
N6—Co2—O7	78.32 (7)	C27—C28—H28	120.7
N5—Co2—O7	93.30 (7)	O5—C16—O6	124.5 (2)
N8—Co2—O7	86.32 (7)	O5—C16—C17	117.7 (2)
N7—Co2—O7	94.99 (8)	O6—C16—C17	117.7 (2)
O5—Co2—O7	172.05 (7)	O7—C19—O8	123.4 (2)
C5—N1—C3	104.4 (2)	O7—C19—C18	118.5 (2)
C5—N1—Co1	143.46 (17)	O8—C19—C18	118.0 (2)
C3—N1—Co1	108.64 (16)	N4—C15—C14	123.1 (3)
C1—O1—Co1	110.88 (15)	N4—C15—H15	118.5
C4—O3—Co1	112.63 (16)	C14—C15—H15	118.5
C19—O7—Co2	111.41 (17)	N4—C11—C12	121.0 (3)
C16—O5—Co2	111.86 (16)	N4—C11—C10	116.2 (2)
C20^{i}—N5—C17	104.3 (2)	C12—C11—C10	122.6 (2)
C20^{i}—N5—Co2	142.80 (17)	N3—C10—C9	121.9 (3)
C17—N5—Co2	111.18 (16)	N3—C10—C11	115.3 (2)
C5^{ii}—N2—C2	104.5 (2)	C9—C10—C11	122.7 (2)
C5^{ii}—N2—Co1	141.16 (18)	C28—C29—C30	118.9 (3)
C2—N2—Co1	110.34 (15)	C28—C29—H29	120.6
C20—N6—C18	104.8 (2)	C30—C29—H29	120.6
C20—N6—Co2	141.90 (18)	C13—C12—C11	119.3 (3)
C18—N6—Co2	112.09 (17)	C13—C12—H12	120.3
C21—N7—C25	118.7 (2)	C11—C12—H12	120.3
C21—N7—Co2	126.56 (18)	N3—C6—C7	122.8 (3)
C25—N7—Co2	114.77 (17)	N3—C6—H6	118.6
C30—N8—C26	118.5 (2)	C7—C6—H6	118.6
C30—N8—Co2	123.64 (18)	C21—C22—C23	118.3 (3)
C26—N8—Co2	117.67 (17)	C21—C22—H22	120.8
C6—N3—C10	118.3 (2)	C23—C22—H22	120.8
C6—N3—Co1	126.98 (19)	C8—C9—C10	118.9 (3)
C10—N3—Co1	113.98 (17)	C8—C9—H9	120.5
C15—N4—C11	119.0 (2)	C10—C9—H9	120.5
C15—N4—Co1	122.09 (18)	C24—C23—C22	119.5 (3)
C11—N4—Co1	118.81 (18)	C24—C23—H23	120.3
N7—C25—C24	121.6 (2)	C22—C23—H23	120.3
N7—C25—C26	115.8 (2)	C15—C14—C13	118.1 (3)

C24—C25—C26	122.5 (2)	C15—C14—H14	120.9
N8—C26—C27	121.8 (2)	C13—C14—H14	120.9
N8—C26—C25	115.7 (2)	N7—C21—C22	123.1 (3)
C27—C26—C25	122.6 (2)	N7—C21—H21	118.5
C28—C27—C26	119.4 (3)	C22—C21—H21	118.5
C28—C27—H27	120.3	C7—C8—C9	119.7 (3)
C26—C27—H27	120.3	C7—C8—H8A	120.1
O3—C4—O4	124.5 (2)	C9—C8—H8A	120.1
O3—C4—C3	117.6 (2)	C12—C13—C14	119.4 (3)
O4—C4—C3	117.9 (2)	C12—C13—H13	120.3
N5—C17—C18^{i}	109.0 (2)	C14—C13—H13	120.3
N5—C17—C16	118.9 (2)	C8—C7—C6	118.4 (3)
C18^{i}—C17—C16	132.0 (2)	C8—C7—H7	120.8
N5^{iii}—C20—N6	113.7 (2)	C6—C7—H7	120.8

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

Fig. 1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C16
O5I

Fig. 2