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catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-μ-pyrazine-2-carboxylato]

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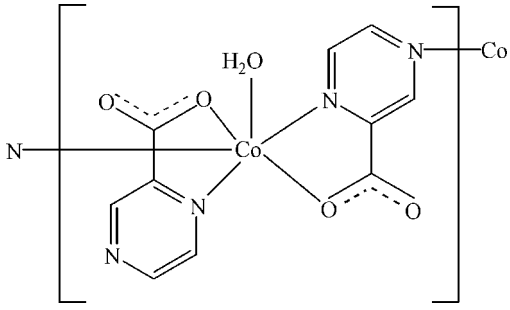
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.055; data-to-parameter ratio = 11.6.

The title compound, $[Co(C_5H_3N_2O_2)_2(H_2O)]_n$, prepared by hydrothermal synthesis, is isostructural with its Fe^{II} and Ni^{II} analogues. The asymmetric unit contains two bidendate pyrazine-2-carboxylate anions bonded to Co^{II} in the equatorial plane through one N and one O atom. The Co^{II} atoms are linked into chains by the second N atom of one of the pyrazine-2-carboxylate anions bonding to an axial site of a neighbouring Co^{II} atom. The slightly distorted octahedral coordination around Co^{II} is completed by a water molecule, which forms hydrogen bonds to link the chains into a three-dimensional structure. The refined Flack parameter of 0.452 (15) indicates inversion twinning.

Related literature

For the isostructural Fe^{II} and Ni^{II} analogues, see: Hao & Liu (2007); Hao *et al.* (2007).



Experimental

Crystal data

$[Co(C_5H_3N_2O_2)_2(H_2O)]$
M_r = 323.13
Orthorhombic, $P2_12_12_1$
a = 8.0121 (10) Å
b = 9.5327 (10) Å
c = 15.023 (2) Å
V = 1147.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.52 mm^{-1}
T = 298 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
5916 measured reflections
2198 independent reflections
2064 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.055
S = 1.04
2198 reflections
190 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), with 907 Friedel pairs
Flack parameter: 0.452 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H52···O2^{i}	0.82 (1)	1.88 (1)	2.697 (3)	172 (3)
O5—H51···O3^{ii}	0.82 (1)	2.00 (1)	2.814 (3)	172 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: BI2194).

References

Bruker (2001). *SMART*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hao, L.-J. & Liu, T.-T. (2007). *Acta Cryst.* E**63**, m169–m171.
Hao, L.-J., Mu, C.-H. & Liu, T.-T. (2007). *Acta Cryst.* E**63**, m281–m283.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, m1882 [**doi:10.1107/S1600536807027961**]

catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-μ-pyrazine-2-carboxylato]

Y.-X. Gao, L.-B. Wang, Y.-L. Niu and L.-J. Hao

Comment

The title compound, $[Co(C_5H_3N_2O_2)_2(H_2O)]_n$, is isostructural with its Fe^{II} and Ni^{II} analogues (Hao & Liu, 2007; Hao, Mu & Liu, 2007).

The Co^{II} atom is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octahedral coordination is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Fig. 1). The Co—N and Co—O bond lengths are in the range 2.057 (2)–2.104 (2) and 2.0384 (17)–2.0723 (18) Å, respectively.

One pyrazine-2-carboxylate ligand coordinates to a neighboring Co^{II} atom *via* its second N atom, leading to a polymeric structure with zigzag chains extending parallel to the *b* axis (Fig. 2). Hydrogen bonding between the water molecules stabilizes the structure.

Experimental

All chemicals were used as purchased from Jinan Henghua Sci & Tec Co. Ltd. A mixture of $NiCl_2·6H_2O$ (0.5 mmol), KOH (0.5 mmol), 2-pyrazine carboxylic acid (0.5 mmol), EtOH (8 ml) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was heated to 413 K for 2 d. On cooling to room temperature, red crystals were obtained in a yield of 36%. Elemental analysis calculated: C 37.15, H 3.10, N 17.34, Co 18.27%; found: C 37.12, H 3.12, N 17.38, Co 18.19%.

Refinement

H atoms on C atoms were placed geometrically and refined as riding with C—H = 0.93 Å and U_{iso}(H)= 1.2U_{eq}(C). The H atoms of the water molecule were located from difference Fourier maps and were refined with distance restraints of O—H = 0.82 (1) Å and H···H = 1.35 (1) Å. The refined Flack parameter (Flack, 1983) from 907 Friedel pairs is 0.452 (15), indicating inversion twinning.

Figures

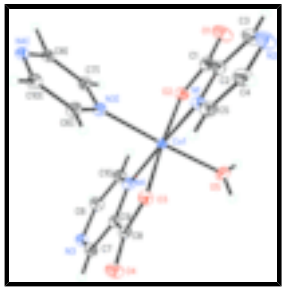

Fig. 1. The asymmetric unit of the title compound expanded to show the complete coordination sphere of Co^{II}. Displacement ellipsoids are shown at 30% probability for non-H atoms. Symmetry code (i): $1-x, y+1/2, -z+1/2$.

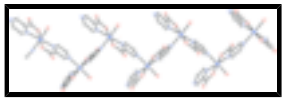

Fig. 2. View of the $[Co(C_5H_3N_2O_2)_2(H_2O)]_n$ coordination polymer.

catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-μ-pyrazine-2-carboxylato]

Crystal data

$[Co(C_5H_3N_2O_2)_2(H_2O)]$	F_{000} = 652
M_r = 323.13	D_x = 1.871 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2198 reflections
a = 8.0121 (10) Å	θ = 2.5–26.0º
b = 9.5327 (10) Å	μ = 1.52 mm^{-1}
c = 15.023 (2) Å	T = 298 (2) K
V = 1147.4 (2) Å^3	Block, red
Z = 4	0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2064 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.026
Monochromator: graphite	θ_{max} = 26.0º
T = 298(2) K	θ_{min} = 2.5º
ω scans	h = −8→9
Absorption correction: none	k = −11→10
5916 measured reflections	l = −18→9
2198 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.024	$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.055	$(\Delta/\sigma)_{max} < 0.001$
S = 1.04	$\Delta\rho_{max}$ = 0.80 e Å^{-3}
2198 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
190 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), with 907 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.452 (15)
Secondary atom site location: difference Fourier map	

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	0.42683 (4)	0.36583 (3)	0.409285 (19)	0.01727 (9)
C1	0.6433 (3)	0.5285 (3)	0.51916 (18)	0.0279 (6)
C2	0.4620 (3)	0.5736 (3)	0.54104 (17)	0.0279 (6)
C3	0.4253 (4)	0.6652 (3)	0.60858 (18)	0.0388 (7)
H3A	0.5122	0.7030	0.6419	0.047*
C4	0.1419 (3)	0.6488 (3)	0.57852 (19)	0.0363 (6)
H4A	0.0320	0.6742	0.5902	0.044*
C5	0.1760 (3)	0.5570 (3)	0.51064 (18)	0.0311 (6)
H5A	0.0890	0.5208	0.4767	0.037*
C6	0.6842 (3)	0.0674 (3)	0.23679 (18)	0.0291 (6)
H6A	0.7913	0.0407	0.2200	0.035*
C7	0.3951 (3)	0.0422 (3)	0.22755 (17)	0.0251 (6)
H7A	0.3024	−0.0040	0.2046	0.030*
C8	0.1943 (3)	0.1916 (3)	0.31693 (16)	0.0229 (5)
C9	0.3723 (3)	0.1454 (3)	0.28905 (15)	0.0226 (5)
C10	0.6630 (3)	0.1690 (3)	0.29927 (18)	0.0274 (6)
H10A	0.7555	0.2117	0.3249	0.033*
N1	0.3349 (3)	0.5187 (2)	0.49264 (13)	0.0254 (5)
N2	0.2661 (3)	0.7025 (3)	0.62837 (17)	0.0447 (7)
N3	0.5503 (3)	0.0048 (2)	0.19881 (13)	0.0253 (5)
N4	0.5061 (3)	0.2085 (2)	0.32447 (14)	0.0239 (5)
O1	0.7625 (2)	0.5798 (3)	0.55879 (15)	0.0487 (6)
O2	0.6535 (2)	0.43497 (18)	0.45923 (11)	0.0270 (4)
O3	0.1939 (2)	0.29727 (18)	0.36884 (11)	0.0268 (4)
O4	0.0688 (2)	0.13059 (19)	0.29097 (11)	0.0356 (4)
O5	0.4188 (3)	0.23496 (19)	0.51651 (12)	0.0333 (4)
H51	0.501 (2)	0.219 (3)	0.5471 (17)	0.041 (10)*
H52	0.344 (3)	0.179 (3)	0.527 (2)	0.067 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Co1	0.01816 (14)	0.01545 (14)	0.01821 (14)	0.00010 (13)	0.00071 (13)	−0.00059 (13)
C1	0.0271 (13)	0.0267 (14)	0.0297 (14)	0.0013 (11)	−0.0016 (11)	0.0032 (11)
C2	0.0294 (16)	0.0273 (13)	0.0271 (13)	−0.0015 (11)	−0.0007 (11)	0.0022 (11)
C3	0.0341 (15)	0.0380 (16)	0.0443 (18)	−0.0030 (14)	−0.0049 (14)	−0.0150 (12)
C4	0.0303 (13)	0.0336 (15)	0.0449 (16)	0.0038 (12)	0.0041 (12)	−0.0077 (14)
C5	0.0264 (14)	0.0285 (14)	0.0384 (16)	−0.0029 (11)	−0.0033 (12)	0.0001 (11)
C6	0.0240 (14)	0.0298 (14)	0.0333 (15)	0.0011 (11)	−0.0001 (11)	−0.0042 (12)
C7	0.0265 (15)	0.0234 (12)	0.0253 (12)	0.0009 (10)	−0.0018 (11)	−0.0023 (10)
C8	0.0221 (13)	0.0243 (12)	0.0222 (13)	0.0001 (10)	0.0014 (10)	0.0025 (10)
C9	0.0263 (12)	0.0220 (12)	0.0196 (11)	−0.0010 (11)	−0.0008 (9)	0.0026 (10)
C10	0.0229 (13)	0.0283 (15)	0.0309 (14)	0.0003 (11)	−0.0014 (11)	−0.0033 (11)
N1	0.0261 (11)	0.0218 (11)	0.0281 (11)	−0.0007 (9)	−0.0004 (9)	−0.0001 (9)
N2	0.0410 (15)	0.0440 (15)	0.0492 (15)	0.0038 (12)	0.0048 (12)	−0.0184 (12)
N3	0.0282 (12)	0.0228 (10)	0.0248 (10)	−0.0014 (10)	−0.0011 (9)	−0.0007 (8)
N4	0.0246 (11)	0.0221 (11)	0.0251 (12)	0.0006 (9)	0.0011 (9)	0.0032 (9)
O1	0.0305 (11)	0.0535 (13)	0.0620 (14)	−0.0047 (10)	−0.0088 (10)	−0.0188 (11)
O2	0.0270 (9)	0.0237 (9)	0.0303 (10)	0.0020 (8)	−0.0022 (8)	−0.0017 (8)
O3	0.0246 (9)	0.0272 (10)	0.0285 (9)	0.0015 (8)	0.0031 (7)	−0.0033 (8)
O4	0.0255 (9)	0.0383 (10)	0.0432 (10)	−0.0059 (11)	0.0014 (9)	−0.0096 (9)
O5	0.0331 (10)	0.0326 (10)	0.0341 (10)	−0.0102 (10)	−0.0081 (10)	0.0126 (8)

Geometric parameters (Å, °)

Co1—O5	2.0384 (17)	C5—H5A	0.930
Co1—N1	2.057 (2)	C6—N3	1.354 (3)
Co1—N4	2.068 (2)	C6—C10	1.359 (4)
Co1—O3	2.0687 (17)	C6—H6A	0.930
Co1—O2	2.0723 (18)	C7—C9	1.362 (4)
Co1—N3^{i}	2.104 (2)	C7—N3	1.364 (3)
C1—O1	1.227 (3)	C7—H7A	0.930
C1—O2	1.270 (3)	C8—O4	1.226 (3)
C1—C2	1.550 (4)	C8—O3	1.274 (3)
C2—N1	1.357 (3)	C8—C9	1.550 (3)
C2—C3	1.371 (4)	C9—N4	1.339 (3)
C3—N2	1.357 (4)	C10—N4	1.366 (3)
C3—H3A	0.930	C10—H10A	0.930
C4—N2	1.346 (4)	N3—Co1^{ii}	2.104 (2)
C4—C5	1.371 (4)	O5—H51	0.82 (1)
C4—H4A	0.930	O5—H52	0.82 (1)
C5—N1	1.352 (3)		
O5—Co1—N1	86.63 (8)	N3—C6—C10	120.4 (2)
O5—Co1—N4	93.02 (8)	N3—C6—H6A	119.8
N1—Co1—N4	176.88 (9)	C10—C6—H6A	119.8
O5—Co1—O3	90.59 (8)	C9—C7—N3	121.7 (2)
N1—Co1—O3	94.56 (8)	C9—C7—H7A	119.1
N4—Co1—O3	82.34 (7)	N3—C7—H7A	119.1
O5—Co1—O2	86.35 (8)	O4—C8—O3	124.6 (2)
N1—Co1—O2	82.42 (8)	O4—C8—C9	122.3 (2)

N4—Co1—O2	100.65 (8)	O3—C8—C9	113.1 (2)
O3—Co1—O2	175.81 (7)	N4—C9—C7	119.1 (2)
O5—Co1—N3^{i}	176.49 (9)	N4—C9—C8	120.1 (2)
N1—Co1—N3^{i}	93.15 (8)	C7—C9—C8	120.8 (2)
N4—Co1—N3^{i}	87.39 (8)	C6—C10—N4	120.2 (2)
O3—Co1—N3^{i}	92.92 (8)	C6—C10—H10A	119.9
O2—Co1—N3^{i}	90.15 (8)	N4—C10—H10A	119.9
O1—C1—O2	125.0 (3)	C5—N1—C2	119.7 (2)
O1—C1—C2	121.0 (2)	C5—N1—Co1	130.57 (18)
O2—C1—C2	113.9 (2)	C2—N1—Co1	109.32 (17)
N1—C2—C3	118.8 (2)	C4—N2—C3	118.3 (2)
N1—C2—C1	118.9 (2)	C6—N3—C7	118.3 (2)
C3—C2—C1	122.3 (2)	C6—N3—Co1^{ii}	122.25 (17)
N2—C3—C2	122.0 (3)	C7—N3—Co1^{ii}	119.24 (16)
N2—C3—H3A	119.0	C9—N4—C10	120.2 (2)
C2—C3—H3A	119.0	C9—N4—Co1	108.97 (16)
N2—C4—C5	120.6 (3)	C10—N4—Co1	130.79 (17)
N2—C4—H4A	119.7	C1—O2—Co1	115.09 (16)
C5—C4—H4A	119.7	C8—O3—Co1	115.28 (15)
N1—C5—C4	120.6 (3)	Co1—O5—H51	122.1 (19)
N1—C5—H5A	119.7	Co1—O5—H52	125 (2)
C4—C5—H5A	119.7	H51—O5—H52	111.4 (17)
O1—C1—C2—N1	177.0 (2)	C10—C6—N3—C7	−2.7 (4)
O2—C1—C2—N1	−4.0 (3)	C10—C6—N3—Co1^{ii}	172.10 (19)
O1—C1—C2—C3	−4.1 (4)	C9—C7—N3—C6	3.8 (4)
O2—C1—C2—C3	174.8 (2)	C9—C7—N3—Co1^{ii}	−171.17 (18)
N1—C2—C3—N2	0.0 (4)	C7—C9—N4—C10	−0.3 (4)
C1—C2—C3—N2	−178.9 (3)	C8—C9—N4—C10	−179.3 (2)
N2—C4—C5—N1	0.1 (4)	C7—C9—N4—Co1	176.90 (18)
N3—C7—C9—N4	−2.3 (4)	C8—C9—N4—Co1	−2.1 (3)
N3—C7—C9—C8	176.6 (2)	C6—C10—N4—C9	1.3 (4)
O4—C8—C9—N4	−174.9 (2)	C6—C10—N4—Co1	−175.16 (18)
O3—C8—C9—N4	4.9 (3)	O5—Co1—N4—C9	89.80 (17)
O4—C8—C9—C7	6.2 (4)	O3—Co1—N4—C9	−0.39 (16)
O3—C8—C9—C7	−174.1 (2)	O2—Co1—N4—C9	176.64 (16)
N3—C6—C10—N4	0.2 (4)	N3^{i}—Co1—N4—C9	−93.69 (16)
C4—C5—N1—C2	−1.3 (4)	O5—Co1—N4—C10	−93.4 (2)
C4—C5—N1—Co1	170.45 (19)	O3—Co1—N4—C10	176.4 (2)
C3—C2—N1—C5	1.3 (4)	O2—Co1—N4—C10	−6.6 (2)
C1—C2—N1—C5	−179.9 (2)	N3^{i}—Co1—N4—C10	83.1 (2)
C3—C2—N1—Co1	−172.1 (2)	O1—C1—O2—Co1	177.7 (2)
C1—C2—N1—Co1	6.8 (3)	C2—C1—O2—Co1	−1.2 (3)
O5—Co1—N1—C5	−91.2 (2)	O5—Co1—O2—C1	−83.30 (18)
O3—Co1—N1—C5	−0.9 (2)	N1—Co1—O2—C1	3.78 (18)
O2—Co1—N1—C5	−178.0 (2)	N4—Co1—O2—C1	−175.68 (18)
N3^{i}—Co1—N1—C5	92.3 (2)	N3^{i}—Co1—O2—C1	96.94 (18)

O5—Co1—N1—C2	81.21 (17)	O4—C8—O3—Co1	174.82 (19)
O3—Co1—N1—C2	171.53 (16)	C9—C8—O3—Co1	−4.9 (3)
O2—Co1—N1—C2	−5.55 (16)	O5—Co1—O3—C8	−89.72 (18)
N3^{i}—Co1—N1—C2	−95.29 (16)	N1—Co1—O3—C8	−176.38 (17)
C5—C4—N2—C3	1.1 (5)	N4—Co1—O3—C8	3.24 (17)
C2—C3—N2—C4	−1.2 (4)	N3^{i}—Co1—O3—C8	90.22 (18)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H52···O2^{iii}	0.82 (1)	1.88 (1)	2.697 (3)	172 (3)
O5—H51···O3^{iv}	0.82 (1)	2.00 (1)	2.814 (3)	172 (3)

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

Fig. 1

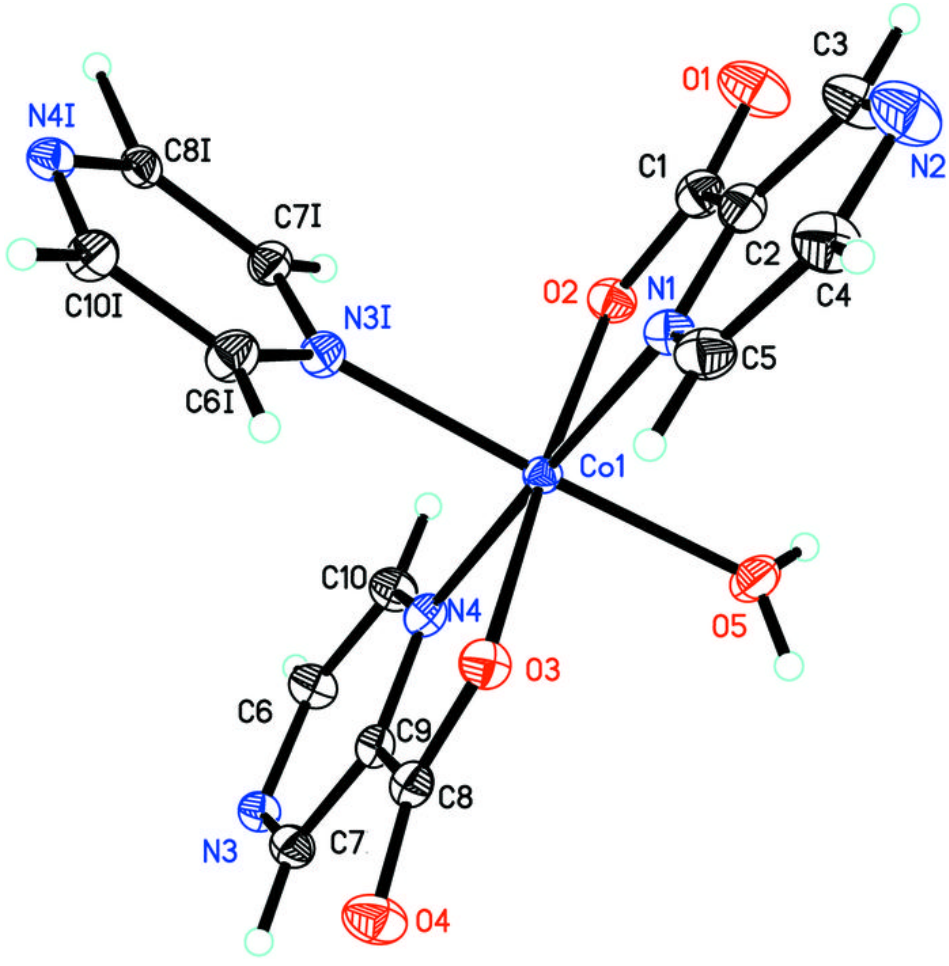
C3
O1
N4I
C8I
C1
N2
C7I
C2
O2
N1
C4
C10I
N3I
C5
C6I
Co1
C10
N4
O5
O3
C6
C9
C8
N3
C7
O4

Fig. 2