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Poly[(μ_3-benzene-1,3-dicarboxylato-$\kappa^4O,O':O'':O'''$)(μ_4-benzene-1,3-dicarboxylato-$\kappa^5O,O':O':O'':O'''$)(μ_2-1,3-di-4-pyridylpropane-$\kappa^2N:N'$)dicobalt(II)]

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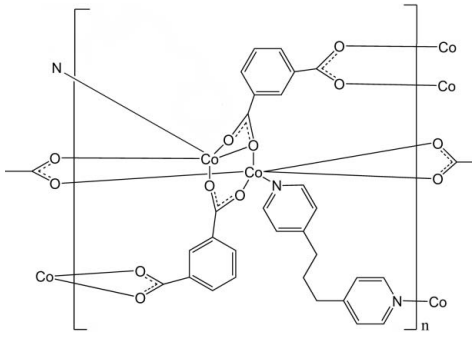
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.076; data-to-parameter ratio = 17.3.

The hydro(solvo)thermal reaction of zinc nitrate with benzene-1,3-dicarboxylic acid and 1,3-di-4-pyridylpropane in water and ethanol gave the title complex, $[Co_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]_n$. The complex exhibits a twofold interpenetrated three-dimensional structure, which is built up from distorted square-pyramidal CoO_4N and octahedral CoO_5N units, and bridging benzene-1,3-dicarboxylate and 1,3-di-4-pyridylpropane ligands.

Related literature

For related literature, see: Chen *et al.* (2006); Kitagawa *et al.* (2004).



Experimental

Crystal data

$[Co_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]$
M_r = 644.35
Triclinic, $P\overline{1}$
a = 9.3705 (6) Å
b = 9.9598 (7) Å
c = 15.031 (1) Å
α = 81.334 (2)°
β = 72.739 (2)°
γ = 76.015 (1)°
V = 1295.22 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.34 mm^{-1}
T = 295 (2) K
0.20 × 0.05 × 0.03 mm

Data collection

Bruker Kappa-APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.793, T_{max} = 0.969
15494 measured reflections
6411 independent reflections
4026 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.076
S = 0.81
6411 reflections
370 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0283 (16)	Co2—O2	1.9884 (18)
Co1—O6	2.0371 (16)	Co2—O5	2.0036 (16)
Co1—O3^{i}	2.1202 (16)	Co2—N1	2.038 (2)
Co1—N2^{ii}	2.125 (2)	Co2—O8^{iii}	2.0476 (17)
Co1—O4^{i}	2.1747 (17)	Co2—O7^{iii}	2.3408 (18)
Co1—O8^{iii}	2.355 (2)		
O1—Co1—O6	113.69 (7)	N2^{ii}—Co1—O8^{iii}	167.81 (7)
O1—Co1—O3^{i}	151.03 (7)	O4^{i}—Co1—O8^{iii}	99.74 (7)
O6—Co1—O3^{i}	95.02 (7)	O2—Co2—O5	106.63 (8)
O1—Co1—N2^{ii}	91.35 (7)	O2—Co2—N1	92.31 (8)
O6—Co1—N2^{ii}	87.65 (7)	O5—Co2—N1	98.57 (7)
O3^{i}—Co1—N2^{ii}	93.69 (7)	O2—Co2—O8^{iii}	106.80 (7)
O1—Co1—O4^{i}	90.17 (6)	O5—Co2—O8^{iii}	100.11 (7)
O6—Co1—O4^{i}	156.14 (7)	N1—Co2—O8^{iii}	148.00 (8)
O3^{i}—Co1—O4^{i}	61.15 (6)	O2—Co2—O7^{iii}	94.08 (8)
N2^{ii}—Co1—O4^{i}	92.41 (8)	O5—Co2—O7^{iii}	154.82 (8)
O1—Co1—O8^{iii}	89.58 (7)	N1—Co2—O7^{iii}	94.67 (7)
O6—Co1—O8^{iii}	80.86 (6)	O8^{iii}—Co2—O7^{iii}	59.32 (7)
O3^{i}—Co1—O8^{iii}	91.36 (7)		

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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: HY2073).

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supplementary materials

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Poly[(μ_3-benzene-1,3-dicarboxylato-$\kappa^4O,O':O'':O'''$)(μ_4-benzene-1,3-dicarboxylato-$\kappa^5O,O':O':O'':O'''$)(μ_2-1,3-di-4-pyridylpropane-$\kappa^2N:N'$)dicobalt(II)]

T.-H. Tsao and C.-H. Lin

Comment

The synthesis of coordination polymers, the so-called metal–organic framework, has been a subject of intense research owing to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism and luminescence. A large number of these materials have been synthesized by hydro(solvo)thermal reactions with mixed organic pyridines and carboxylic acids (Kitagawa *et al.*, 2004). They commonly adopt three-dimensional framework structures *via* employing metal ions as nodes and rigid or flexible organic ligands as linkers. As a further study of such complexes, we report the title compound (Fig. 1), which is isostructural with $[CoZn(C_8H_4O_4)_2(C_{13}H_{14}N_2)]_n$ (Chen *et al.*, 2006) and has a parallel twofold interpenetrated three-dimensional structure (Fig. 2). All the geometric parameters are within normal ranges (Table 1). The two Co^{II} atoms are five- and six-coordinated, respectively, by one N atom of the 1,3-di-4-pyridylpropane ligand and four or five O atoms of the carboxylate ligands, giving distorted square pyramidal and octahedral geometries.

Experimental

The hydro(solvo)thermal reaction was carried out at 423 K for 2 d in a 23 ml Teflon-lined acid digestion bomb followed by slowly cooling to room temperature at 6 K h^{-1}. A single-phase product consisting of transparent purple crystals was obtained from a mixture of 1,3-di-4-pyridylpropane (0.086 g, 0.43 mmol), $Co(NO_3)\cdot 6H_2O$ (0.044 g, 0.15 mmol), benzene-1,3-dicarboxylic acid (0.073 g, 0.43 mmol), H_2O (5 ml) and ethanol (5 ml). Powder X-ray diffraction measurements were performed to confirm the phase purity before all chemical and physical analyses. Thermal analyses, using a Perkin–Elmer TGA7 thermal analyzer, were performed on powder samples under flowing oxygen with a heating rate of 10 K min^{-1}. A total weight loss of 67.8% was observed from 623 to 773 K.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å (CH), 0.97Å (CH_2) and U_{iso}(H) = 1.2U_{eq}(C).

Figures

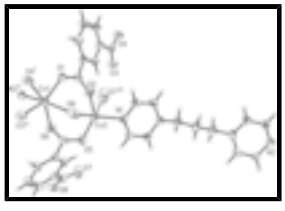

Fig. 1. The asymmetric unit of the title compound, together with symmetry-related atoms to complete the Co coordination. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, y+1, z$; (ii) $x, y+1, z-1$; (iii) $x+1, y, z$; (iv) $x, y+1, z$.]

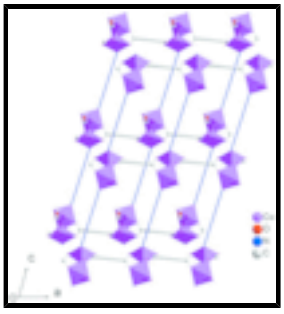

Fig. 2. View of the structure along the b direction. The organic linkers are represented by rods.

Poly[[(μ$_3$-benzene-1,3-dicarboxylato-κ^4*O*,*O*':*O*'':*O*''')(μ$_4$– benzene-1,3-dicarboxylato-κ^5*O*,*O*':*O*':*O*'':*O*''')(μ$_2$-1,3-di-4- pyridylpropane-κ^2*N*:*N*')dicobalt(II)]

Crystal data

$[Co_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]$	$Z = 2$
$M_r = 644.35$	$F_{000} = 656$
Triclinic, $P\overline{1}$	$D_x = 1.652$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.3705$ (6) Å	Cell parameters from 3042 reflections
$b = 9.9598$ (7) Å	$\theta = 2.4$–$25.5°$
$c = 15.031$ (1) Å	$\mu = 1.34$ mm^{-1}
$\alpha = 81.334$ (2)°	$T = 295$ (2) K
$\beta = 72.739$ (2)°	Tabular, purple
$\gamma = 76.015$ (1)°	0.20 × 0.05 × 0.03 mm
$V = 1295.22$ (15) Å^3	

Data collection

Bruker Kappa-APEXII CCD area-detector diffractometer	6411 independent reflections
Radiation source: fine-focus sealed tube	4026 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.055$
$T = 295(2)$ K	$\theta_{max} = 28.3°$
φ and ω scans	$\theta_{min} = 1.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.793$, $T_{max} = 0.969$	$k = -13 \rightarrow 13$
15494 measured reflections	$l = -20 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained

$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.81$	$(\Delta/\sigma)_{max} = 0.013$
6411 reflections	$\Delta\rho_{max} = 0.56$ e Å^{-3}
370 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.75864 (4)	0.08878 (3)	0.20151 (2)	0.02702 (10)
Co2	0.68764 (4)	−0.12244 (3)	0.39787 (3)	0.03015 (10)
O1	0.88439 (18)	−0.10487 (16)	0.17578 (12)	0.0341 (4)
O2	0.7618 (2)	−0.23941 (17)	0.29052 (13)	0.0406 (5)
O3	0.74129 (19)	−0.69493 (17)	0.20116 (13)	0.0392 (5)
O4	0.95949 (19)	−0.82411 (17)	0.13263 (14)	0.0430 (5)
O5	0.46794 (18)	−0.03594 (17)	0.40657 (13)	0.0376 (5)
O6	0.53562 (18)	0.09259 (18)	0.27191 (12)	0.0347 (4)
O7	−0.0666 (2)	−0.1274 (2)	0.40799 (15)	0.0548 (6)
O8	−0.21808 (18)	0.04965 (18)	0.35554 (14)	0.0407 (5)
N1	0.6565 (2)	−0.2897 (2)	0.49237 (14)	0.0274 (5)
N2	0.6932 (2)	−0.8902 (2)	1.07549 (15)	0.0324 (5)
C1	0.8557 (3)	−0.2205 (2)	0.21317 (19)	0.0280 (6)
C2	0.9401 (3)	−0.3475 (2)	0.16182 (18)	0.0292 (6)
C3	1.0840 (3)	−0.3529 (3)	0.1012 (2)	0.0420 (7)
H3A	1.1272	−0.2749	0.0877	0.050*
C4	1.1645 (3)	−0.4750 (3)	0.0602 (2)	0.0524 (9)
H4A	1.2622	−0.4790	0.0202	0.063*
C5	1.0996 (3)	−0.5902 (3)	0.0787 (2)	0.0440 (8)
H5A	1.1546	−0.6723	0.0522	0.053*
C6	0.9530 (3)	−0.5839 (2)	0.13643 (19)	0.0324 (6)
C7	0.8744 (3)	−0.4627 (2)	0.17912 (18)	0.0312 (6)
H7A	0.7770	−0.4590	0.2196	0.037*
C8	0.8807 (3)	−0.7078 (3)	0.15697 (19)	0.0324 (6)
C9	0.4390 (3)	0.0523 (2)	0.34116 (18)	0.0264 (6)
C10	0.2745 (2)	0.1136 (2)	0.34641 (17)	0.0255 (5)
C11	0.1654 (3)	0.0318 (2)	0.37069 (17)	0.0286 (6)
H11A	0.1922	−0.0618	0.3899	0.034*
C12	0.0172 (3)	0.0886 (3)	0.36648 (18)	0.0292 (6)
C13	−0.0260 (3)	0.2304 (3)	0.3471 (2)	0.0390 (7)
H13A	−0.1269	0.2700	0.3477	0.047*
C14	0.0800 (3)	0.3136 (3)	0.3270 (2)	0.0408 (7)
H14A	0.0497	0.4094	0.3168	0.049*
C15	0.2300 (3)	0.2547 (3)	0.32221 (18)	0.0323 (6)
H15A	0.3029	0.3097	0.3026	0.039*
C16	−0.0932 (3)	−0.0037 (3)	0.37848 (19)	0.0353 (6)
C17	0.7692 (3)	−0.4039 (3)	0.48892 (19)	0.0378 (7)

H17A	0.8648	−0.4000	0.4479	0.045*
C18	0.7500 (3)	−0.5251 (3)	0.54273 (19)	0.0382 (7)
H18A	0.8312	−0.6013	0.5376	0.046*
C19	0.6089 (3)	−0.5346 (2)	0.60521 (18)	0.0293 (6)
C20	0.4945 (3)	−0.4157 (3)	0.60964 (18)	0.0322 (6)
H20A	0.3989	−0.4158	0.6516	0.039*
C21	0.5211 (3)	−0.2984 (2)	0.55279 (18)	0.0287 (6)
H21A	0.4414	−0.2212	0.5563	0.034*
C22	0.5777 (3)	−0.6648 (3)	0.66473 (19)	0.0370 (7)
H22A	0.6350	−0.7437	0.6293	0.044*
H22B	0.4700	−0.6649	0.6772	0.044*
C23	0.6170 (3)	−0.6850 (3)	0.75696 (19)	0.0438 (7)
H23A	0.5701	−0.6020	0.7899	0.053*
H23B	0.7268	−0.6989	0.7454	0.053*
C24	0.5616 (3)	−0.8100 (3)	0.81811 (19)	0.0406 (7)
H24A	0.4511	−0.7928	0.8322	0.049*
H24B	0.6028	−0.8911	0.7828	0.049*
C25	0.6061 (3)	−0.8414 (3)	0.90826 (19)	0.0327 (6)
C26	0.7264 (3)	−0.9455 (3)	0.92081 (19)	0.0361 (6)
H26A	0.7812	−1.0021	0.8728	0.043*
C27	0.7672 (3)	−0.9672 (3)	1.00318 (19)	0.0342 (6)
H27A	0.8497	−1.0384	1.0090	0.041*
C28	0.5746 (3)	−0.7884 (3)	1.06415 (19)	0.0418 (7)
H28A	0.5206	−0.7336	1.1132	0.050*
C29	0.5304 (3)	−0.7624 (3)	0.9834 (2)	0.0439 (7)
H29A	0.4480	−0.6904	0.9787	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02627 (19)	0.01979 (17)	0.0341 (2)	−0.00850 (14)	−0.00425 (15)	−0.00160 (15)
Co2	0.02764 (19)	0.02552 (19)	0.0367 (2)	−0.00947 (15)	−0.00748 (16)	0.00301 (16)
O1	0.0393 (10)	0.0190 (9)	0.0402 (11)	−0.0095 (8)	−0.0035 (9)	−0.0001 (8)
O2	0.0496 (12)	0.0305 (10)	0.0379 (12)	−0.0191 (9)	0.0035 (9)	−0.0045 (9)
O3	0.0361 (11)	0.0299 (10)	0.0491 (13)	−0.0161 (8)	0.0030 (9)	−0.0106 (9)
O4	0.0358 (10)	0.0205 (9)	0.0683 (15)	−0.0093 (8)	−0.0027 (10)	−0.0084 (9)
O5	0.0311 (10)	0.0358 (10)	0.0451 (12)	−0.0100 (8)	−0.0143 (9)	0.0119 (9)
O6	0.0239 (9)	0.0437 (11)	0.0354 (11)	−0.0108 (8)	−0.0053 (8)	0.0006 (9)
O7	0.0596 (14)	0.0549 (14)	0.0656 (16)	−0.0377 (11)	−0.0321 (12)	0.0200 (12)
O8	0.0211 (9)	0.0406 (11)	0.0657 (14)	−0.0079 (8)	−0.0117 (9)	−0.0187 (10)
N1	0.0262 (11)	0.0264 (11)	0.0293 (12)	−0.0057 (9)	−0.0080 (9)	−0.0008 (9)
N2	0.0336 (12)	0.0261 (11)	0.0349 (14)	−0.0078 (9)	−0.0054 (10)	0.0001 (10)
C1	0.0258 (13)	0.0235 (13)	0.0367 (16)	−0.0076 (11)	−0.0094 (12)	−0.0029 (12)
C2	0.0312 (14)	0.0209 (12)	0.0346 (16)	−0.0062 (11)	−0.0070 (12)	−0.0019 (11)
C3	0.0377 (16)	0.0267 (14)	0.059 (2)	−0.0161 (12)	−0.0017 (14)	−0.0038 (14)
C4	0.0335 (16)	0.0307 (15)	0.079 (2)	−0.0131 (13)	0.0137 (15)	−0.0110 (16)
C5	0.0349 (15)	0.0265 (14)	0.062 (2)	−0.0081 (12)	0.0039 (14)	−0.0104 (14)
C6	0.0329 (14)	0.0219 (13)	0.0411 (17)	−0.0112 (11)	−0.0045 (12)	−0.0011 (12)

C7	0.0304 (14)	0.0230 (13)	0.0371 (16)	−0.0097 (11)	−0.0019 (12)	−0.0010 (12)
C8	0.0368 (15)	0.0239 (13)	0.0361 (16)	−0.0108 (12)	−0.0058 (13)	−0.0028 (12)
C9	0.0262 (13)	0.0245 (13)	0.0347 (16)	−0.0111 (11)	−0.0110 (12)	−0.0061 (12)
C10	0.0218 (12)	0.0293 (13)	0.0274 (14)	−0.0086 (10)	−0.0065 (10)	−0.0031 (11)
C11	0.0272 (13)	0.0293 (13)	0.0306 (15)	−0.0101 (11)	−0.0070 (11)	−0.0014 (11)
C12	0.0229 (13)	0.0348 (14)	0.0327 (15)	−0.0119 (11)	−0.0047 (11)	−0.0074 (12)
C13	0.0263 (14)	0.0403 (16)	0.057 (2)	−0.0014 (12)	−0.0196 (13)	−0.0155 (14)
C14	0.0374 (16)	0.0265 (14)	0.066 (2)	−0.0041 (12)	−0.0248 (15)	−0.0086 (14)
C15	0.0319 (14)	0.0308 (14)	0.0411 (17)	−0.0140 (11)	−0.0153 (12)	−0.0005 (12)
C16	0.0280 (14)	0.0481 (18)	0.0336 (17)	−0.0178 (13)	−0.0033 (12)	−0.0092 (14)
C17	0.0252 (14)	0.0390 (16)	0.0398 (17)	−0.0017 (12)	−0.0014 (12)	0.0022 (13)
C18	0.0336 (15)	0.0297 (14)	0.0442 (18)	0.0028 (12)	−0.0080 (13)	−0.0017 (13)
C19	0.0366 (15)	0.0257 (13)	0.0286 (15)	−0.0110 (11)	−0.0107 (12)	−0.0006 (11)
C20	0.0293 (14)	0.0324 (14)	0.0305 (16)	−0.0067 (11)	−0.0015 (11)	−0.0024 (12)
C21	0.0265 (13)	0.0263 (13)	0.0326 (15)	−0.0026 (11)	−0.0077 (11)	−0.0057 (11)
C22	0.0485 (17)	0.0281 (14)	0.0366 (17)	−0.0130 (12)	−0.0136 (14)	0.0026 (12)
C23	0.0577 (19)	0.0420 (17)	0.0397 (18)	−0.0227 (14)	−0.0202 (15)	0.0064 (14)
C24	0.0532 (18)	0.0361 (16)	0.0382 (17)	−0.0174 (13)	−0.0174 (14)	0.0026 (13)
C25	0.0394 (15)	0.0286 (14)	0.0322 (16)	−0.0152 (12)	−0.0101 (13)	0.0048 (12)
C26	0.0442 (16)	0.0283 (14)	0.0329 (17)	−0.0087 (12)	−0.0041 (13)	−0.0044 (12)
C27	0.0330 (15)	0.0267 (14)	0.0395 (18)	−0.0029 (11)	−0.0074 (13)	−0.0028 (12)
C28	0.0432 (17)	0.0393 (16)	0.0323 (17)	0.0062 (13)	−0.0055 (13)	−0.0046 (13)
C29	0.0401 (17)	0.0405 (17)	0.0426 (19)	0.0050 (13)	−0.0113 (14)	0.0006 (14)

Geometric parameters (Å, °)

Co1—O1	2.0283 (16)	C7—H7A	0.9300
Co1—O6	2.0371 (16)	C8—Co1^{iv}	2.474 (2)
Co1—O3^{i}	2.1202 (16)	C9—C10	1.498 (3)
Co1—N2^{ii}	2.125 (2)	C10—C15	1.391 (3)
Co1—O4^{i}	2.1747 (17)	C10—C11	1.390 (3)
Co1—O8^{iii}	2.355 (2)	C11—C12	1.383 (3)
Co2—O2	1.9884 (18)	C11—H11A	0.9300
Co2—O5	2.0036 (16)	C12—C13	1.383 (3)
Co2—N1	2.038 (2)	C12—C16	1.498 (3)
Co2—O8^{iii}	2.0476 (17)	C13—C14	1.382 (3)
Co2—O7^{iii}	2.3408 (18)	C13—H13A	0.9300
O1—C1	1.257 (3)	C14—C15	1.371 (3)
O2—C1	1.253 (3)	C14—H14A	0.9300
O3—C8	1.263 (3)	C15—H15A	0.9300
O3—Co1^{iv}	2.1202 (16)	C17—C18	1.367 (3)
O4—C8	1.255 (3)	C17—H17A	0.9300
O4—Co1^{iv}	2.1747 (17)	C18—C19	1.391 (3)
O5—C9	1.263 (3)	C18—H18A	0.9300
O6—C9	1.247 (3)	C19—C20	1.387 (3)
O7—C16	1.237 (3)	C19—C22	1.499 (3)
O7—Co2^{v}	2.3408 (18)	C20—C21	1.368 (3)

O8—C16	1.286 (3)	C20—H20A	0.9300
O8—Co2^{v}	2.0476 (17)	C21—H21A	0.9300
O8—Co1^{v}	2.355 (2)	C22—C23	1.511 (4)
N1—C21	1.337 (3)	C22—H22A	0.9700
N1—C17	1.347 (3)	C22—H22B	0.9700
N2—C27	1.340 (3)	C23—C24	1.533 (3)
N2—C28	1.345 (3)	C23—H23A	0.9700
N2—Co1^{vi}	2.125 (2)	C23—H23B	0.9700
C1—C2	1.506 (3)	C24—C25	1.501 (4)
C2—C3	1.380 (3)	C24—H24A	0.9700
C2—C7	1.385 (3)	C24—H24B	0.9700
C3—C4	1.390 (3)	C25—C26	1.373 (3)
C3—H3A	0.9300	C25—C29	1.386 (4)
C4—C5	1.381 (3)	C26—C27	1.373 (4)
C4—H4A	0.9300	C26—H26A	0.9300
C5—C6	1.382 (3)	C27—H27A	0.9300
C5—H5A	0.9300	C28—C29	1.365 (4)
C6—C7	1.391 (3)	C28—H28A	0.9300
C6—C8	1.497 (3)	C29—H29A	0.9300
O1—Co1—O6	113.69 (7)	C6—C8—Co1^{iv}	176.4 (2)
O1—Co1—O3^{i}	151.03 (7)	O6—C9—O5	125.7 (2)
O6—Co1—O3^{i}	95.02 (7)	O6—C9—C10	116.8 (2)
O1—Co1—N2^{ii}	91.35 (7)	O5—C9—C10	117.5 (2)
O6—Co1—N2^{ii}	87.65 (7)	C15—C10—C11	118.8 (2)
O3^{i}—Co1—N2^{ii}	93.69 (7)	C15—C10—C9	119.5 (2)
O1—Co1—O4^{i}	90.17 (6)	C11—C10—C9	121.7 (2)
O6—Co1—O4^{i}	156.14 (7)	C12—C11—C10	120.5 (2)
O3^{i}—Co1—O4^{i}	61.15 (6)	C12—C11—H11A	119.7
N2^{ii}—Co1—O4^{i}	92.41 (8)	C10—C11—H11A	119.7
O1—Co1—O8^{iii}	89.58 (7)	C11—C12—C13	119.4 (2)
O6—Co1—O8^{iii}	80.86 (6)	C11—C12—C16	120.2 (2)
O3^{i}—Co1—O8^{iii}	91.36 (7)	C13—C12—C16	120.4 (2)
N2^{ii}—Co1—O8^{iii}	167.81 (7)	C14—C13—C12	120.3 (2)
O4^{i}—Co1—O8^{iii}	99.74 (7)	C14—C13—H13A	119.9
O1—Co1—C8^{i}	120.49 (8)	C12—C13—H13A	119.9
O6—Co1—C8^{i}	125.71 (8)	C15—C14—C13	119.9 (2)
O3^{i}—Co1—C8^{i}	30.69 (7)	C15—C14—H14A	120.1
N2^{ii}—Co1—C8^{i}	94.06 (8)	C13—C14—H14A	120.1
O4^{i}—Co1—C8^{i}	30.47 (7)	C14—C15—C10	120.7 (2)
O8^{iii}—Co1—C8^{i}	95.93 (7)	C14—C15—H15A	119.7
O2—Co2—O5	106.63 (8)	C10—C15—H15A	119.7
O2—Co2—N1	92.31 (8)	O7—C16—O8	120.1 (2)
O5—Co2—N1	98.57 (7)	O7—C16—C12	122.3 (2)
O2—Co2—O8^{iii}	106.80 (7)	O8—C16—C12	117.6 (2)

O5—Co2—O8^{iii}	100.11 (7)	N1—C17—C18	123.2 (2)
N1—Co2—O8^{iii}	148.00 (8)	N1—C17—H17A	118.4
O2—Co2—O7^{iii}	94.08 (8)	C18—C17—H17A	118.4
O5—Co2—O7^{iii}	154.82 (8)	C17—C18—C19	120.1 (2)
N1—Co2—O7^{iii}	94.67 (7)	C17—C18—H18A	120.0
O8^{iii}—Co2—O7^{iii}	59.32 (7)	C19—C18—H18A	120.0
C1—O1—Co1	129.32 (16)	C20—C19—C18	116.3 (2)
C1—O2—Co2	128.46 (16)	C20—C19—C22	120.4 (2)
C8—O3—Co1^{iv}	90.33 (14)	C18—C19—C22	123.2 (2)
C8—O4—Co1^{iv}	88.07 (15)	C21—C20—C19	120.5 (2)
C9—O5—Co2	117.62 (16)	C21—C20—H20A	119.7
C9—O6—Co1	149.34 (17)	C19—C20—H20A	119.7
C16—O7—Co2^{v}	84.13 (15)	N1—C21—C20	123.1 (2)
C16—O8—Co2^{v}	96.22 (16)	N1—C21—H21A	118.5
C16—O8—Co1^{v}	125.14 (16)	C20—C21—H21A	118.5
Co2^{v}—O8—Co1^{v}	98.83 (7)	C19—C22—C23	115.4 (2)
C21—N1—C17	116.8 (2)	C19—C22—H22A	108.4
C21—N1—Co2	122.43 (16)	C23—C22—H22A	108.4
C17—N1—Co2	120.33 (17)	C19—C22—H22B	108.4
C27—N2—C28	116.7 (2)	C23—C22—H22B	108.4
C27—N2—Co1^{vi}	124.54 (17)	H22A—C22—H22B	107.5
C28—N2—Co1^{vi}	118.67 (18)	C22—C23—C24	111.4 (2)
O1—C1—O2	125.2 (2)	C22—C23—H23A	109.3
O1—C1—C2	118.1 (2)	C24—C23—H23A	109.3
O2—C1—C2	116.7 (2)	C22—C23—H23B	109.3
C3—C2—C7	119.6 (2)	C24—C23—H23B	109.3
C3—C2—C1	121.1 (2)	H23A—C23—H23B	108.0
C7—C2—C1	119.2 (2)	C25—C24—C23	114.1 (2)
C2—C3—C4	120.0 (2)	C25—C24—H24A	108.7
C2—C3—H3A	120.0	C23—C24—H24A	108.7
C4—C3—H3A	120.0	C25—C24—H24B	108.7
C5—C4—C3	120.2 (3)	C23—C24—H24B	108.7
C5—C4—H4A	119.9	H24A—C24—H24B	107.6
C3—C4—H4A	119.9	C26—C25—C29	115.7 (2)
C4—C5—C6	120.2 (2)	C26—C25—C24	122.8 (3)
C4—C5—H5A	119.9	C29—C25—C24	121.4 (2)
C6—C5—H5A	119.9	C25—C26—C27	121.0 (2)
C5—C6—C7	119.5 (2)	C25—C26—H26A	119.5
C5—C6—C8	120.8 (2)	C27—C26—H26A	119.5
C7—C6—C8	119.6 (2)	N2—C27—C26	122.8 (2)
C2—C7—C6	120.5 (2)	N2—C27—H27A	118.6
C2—C7—H7A	119.7	C26—C27—H27A	118.6
C6—C7—H7A	119.7	N2—C28—C29	122.6 (3)
O4—C8—O3	120.4 (2)	N2—C28—H28A	118.7
O4—C8—C6	120.1 (2)	C29—C28—H28A	118.7
O3—C8—C6	119.5 (2)	C28—C29—C25	121.2 (2)

O4—C8—Co1^{iv}	61.46 (13)	C28—C29—H29A	119.4
O3—C8—Co1^{iv}	58.97 (12)	C25—C29—H29A	119.4

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, *y*+1, *z*−1; (iii) *x*+1, *y*, *z*; (iv) *x*, *y*−1, *z*; (v) *x*−1, *y*, *z*; (vi) *x*, *y*−1, *z*+1.

Fig. 1

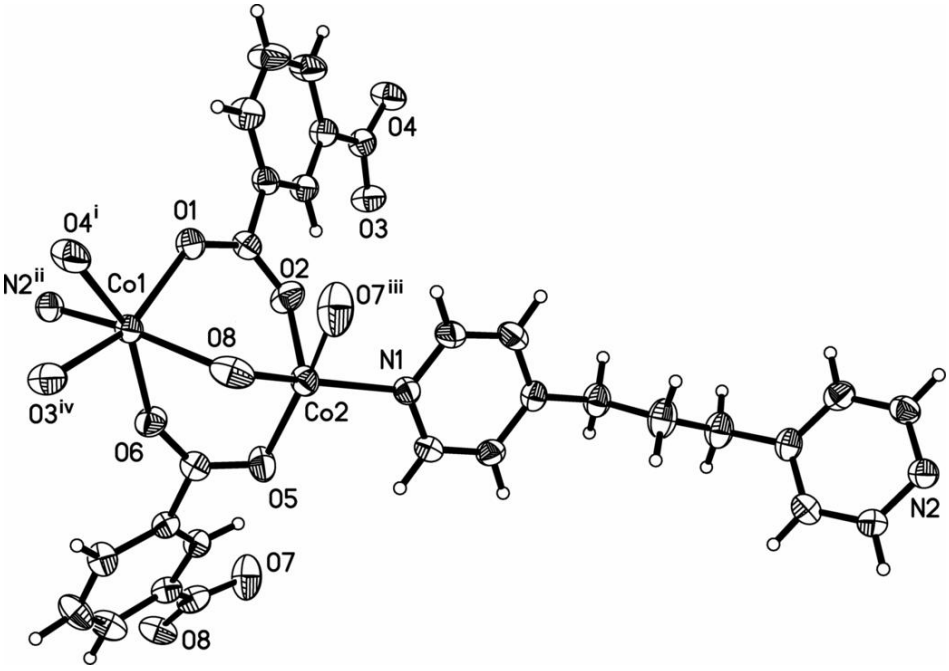

Fig. 2