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catena-Poly[[diaqua(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-*trans*-stilbene-4,4′-dicarboxylato-$\kappa^2O:O'$]

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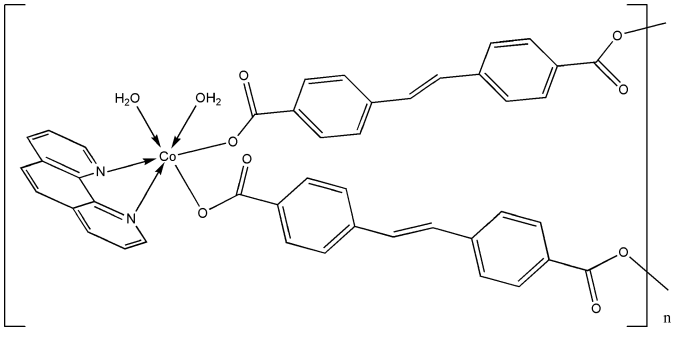
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.142; data-to-parameter ratio = 15.9.

In the title complex, $[Co(C_{16}H_{10}O_4)(C_{12}H_8N_2)(H_2O)_2]_n$, the Co^{II} ion exists in an octahedral geometry, coordinated by two N atoms of a 1,10-phenanthroline ligand, two carboxylate O atoms of two different *trans*-stilbene-4,4′-dicarboxylate ligands and two water molecules. The *trans*-stilbene-4,4′-dicarboxylate bridges give rise to a linear chain structure. These chains are further interconnected through intermolecular hydrogen bonds and π–π stacking interactions between one of the rings of the 1,10-phenanthroline ligand and a symmetry-related ring [centroid-to-centroid distance 3.6153 (8) Å], to form a three-dimensional supramolecular network.

Related literature

For other zinc and cadmium complexes, see Wang *et al.* (2004, 2006).



Experimental

Crystal data

$[Co(C_{16}H_{10}O_4)(C_{12}H_8N_2)H_2O)_2]$
M_r = 541.41
Triclinic, $P\overline{1}$
a = 7.5345 (15) Å
b = 9.2112 (18) Å
c = 18.524 (4) Å
α = 88.12 (3)°
β = 84.29 (3)°
γ = 76.38 (3)°
V = 1243.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 295 (2) K
0.36 × 0.24 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.811, T_{max} = 0.917
11895 measured reflections
5509 independent reflections
4338 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.142
S = 1.01
5509 reflections
346 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.069 (2)	Co1—N2	2.131 (2)
Co1—O4	2.105 (2)	Co1—N1	2.132 (3)
Co1—O1*W*	2.109 (2)	Co1—O2*W*	2.145 (2)
O2—Co1—O4	84.05 (8)	O1*W*—Co1—N1	171.27 (10)
O2—Co1—O1*W*	92.31 (10)	N2—Co1—N1	77.39 (10)
O4—Co1—O1*W*	87.44 (9)	O2—Co1—O2*W*	87.87 (8)
O2—Co1—N2	169.76 (9)	O4—Co1—O2*W*	169.94 (8)
O4—Co1—N2	100.04 (9)	O1*W*—Co1—O2*W*	86.90 (9)
O1*W*—Co1—N2	97.24 (10)	N2—Co1—O2*W*	88.93 (9)
O2—Co1—N1	93.57 (10)	N1—Co1—O2*W*	99.76 (9)
O4—Co1—N1	86.75 (9)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2*W*^{i}	0.85 (1)	1.900 (11)	2.749 (3)	177 (4)
O1*W*—H1*W*2···O3	0.85 (3)	1.83 (3)	2.653 (3)	164 (3)
O2*W*—H2*W*1···O3^{ii}	0.85 (1)	1.83 (3)	2.679 (3)	172 (3)
O2*W*—H2*W*2···O1	0.856 (10)	1.72 (3)	2.564 (3)	169 (4)
O2*W*—H2*W*2···O2	0.856 (10)	2.51 (4)	2.925 (3)	111 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *publCIF* (Westrip 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2367).

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supplementary materials

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catena-Poly[[diaqua(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-*trans*-stilbene-4,4'-dicarboxylato-$\kappa^2O:O'$]

H.-Y. Wang, S. Gao, L.-H. Huo and J.-G. Zhao

Comment

Many new complexes have been synthesized using polycarboxylates to combine with specific transition metal ions by introdcing neutral N-heterocyclic ligands (Wang *et al.*, 2004; Wang, Qin *et al.*, 2006). We report here the synthesis and structure of a new one-dimensional cobalt complex (Fig. 1).

The complex is an infinite one-dimensional chain polymer with a Co^{II} ion, two half of *trans*-stilbene-4,4'-dicarboxylato ligands, a 1,10-phenanthroline and two coordinated water molecules in the asymmetric unit. Each Co^{II} ion is in a distorted octahedral geometry. The [Co(1,10-phenanthroline)$(H_2O)_2$] units are connected by *trans*-stilbene-4,4'-dicarboxylato bridges with bis-dentate mode to form an one-dimensional zigzag chain structure. The chains are further interconnected through intermolecular hydrogen bonds and π–π stacking interactions between one of the rings of the 1,10-phenanthroline ligand (C7–C10/N2/C11) and symmetry-related ring at ($1 - x$, $2 - y$, $1 - z$), with a centroid-to-centroid distance of 3.6153 (8) Å into three-dimensional supramolecular network (Table 2 and Fig. 2). The structure contains voids of about 105.00 A^3 and there is no solvent molecules occupied.

Experimental

A mixture of $CoCl_2{\cdot}6H_2O$ (1 mmol), 1,10-phenanthroline (1 mmol), *trans*-stilbene-4,4'-dicarboxylic acid(1 mmol) and water (10 ml) was stirred for 15 min in air, then transferred and sealed in a 23 ml Parr teflon-lined stainless steel vessel, heated to 160 ° for 5 days, and then cooled to room temperature. The resulting red crystals were filtered, washed, and dried in air. Analysis calculated for $C_{28}H_{22}CoN_2O_6$: C 62.12, H 4.10, N 5.17%; found: C 62.14, H 4.13, N 5.15%.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) and were included in the refinement in the riding model approximation. The H atoms of hydroxyl groups were located in difference Fourier maps and refined with the O—H distance restrained to 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

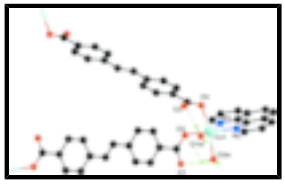

Fig. 1. Molecular structure of the title compound. Dashed lines indicate O—H···O hydrogen bonds.

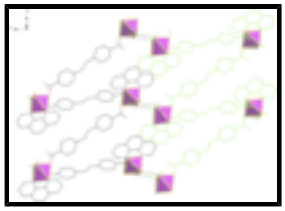

Fig. 2. The packing diagram of the title complex, with the hydrogen bonds denoted by dashed lines.

catena-Poly[[diaqua(1,10-phenanthroline-κ^2_N_,_N_')cobalt(II)]-μ-_trans_- stilbene-4,4'-dicarboxylato-κ^2_O_:_O_']

Crystal data

$[Co(C_{16}H_{10}O_4)(C_{12}H_8N_2)H_2O)_2]$	$Z = 2$
$M_r = 541.41$	$F_{000} = 558$
Triclinic, $P\overline{1}$	$D_x = 1.446$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.5345$ (15) Å	Cell parameters from 10169 reflections
$b = 9.2112$ (18) Å	$\theta = 3.1$–27.5°
$c = 18.524$ (4) Å	$\mu = 0.74$ mm^{-1}
$\alpha = 88.12$ (3)°	$T = 295$ (2) K
$\beta = 84.29$ (3)°	Prism, pink
$\gamma = 76.38$ (3)°	0.36 × 0.24 × 0.12 mm
$V = 1243.2$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5509 independent reflections
Radiation source: fine-focus sealed tube	4338 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 295$(2) K	$\theta_{min} = 3.1^\circ$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11 \rightarrow 11$
$T_{min} = 0.811$, $T_{max} = 0.917$	$l = -23 \rightarrow 24$
11895 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 1.1034P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
5509 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
346 parameters	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.43923 (5)	0.65500 (4)	0.628861 (19)	0.02933 (13)
O1W	0.6521 (3)	0.5294 (3)	0.55787 (12)	0.0440 (5)
H1W1	0.675 (5)	0.513 (5)	0.5126 (7)	0.066*
H1W2	0.744 (3)	0.549 (5)	0.5747 (17)	0.066*
O2W	0.2624 (3)	0.5328 (2)	0.58733 (10)	0.0347 (4)
H2W1	0.1490 (17)	0.559 (3)	0.6021 (18)	0.052*
H2W2	0.310 (4)	0.451 (2)	0.6084 (18)	0.052*
O1	0.3931 (3)	0.3052 (2)	0.66551 (12)	0.0458 (5)
O2	0.4849 (3)	0.4951 (2)	0.71028 (11)	0.0428 (5)
O3	0.9059 (3)	0.5857 (3)	0.63524 (11)	0.0441 (5)
O4	0.6409 (3)	0.7378 (2)	0.67405 (11)	0.0347 (4)
N1	0.2421 (3)	0.8101 (3)	0.69611 (13)	0.0368 (5)
N2	0.3447 (3)	0.8322 (3)	0.55504 (13)	0.0339 (5)
C1	0.1957 (5)	0.7976 (4)	0.76617 (18)	0.0500 (8)
H1A	0.2489	0.7107	0.7904	0.060*
C2	0.0693 (6)	0.9103 (5)	0.8053 (2)	0.0656 (12)
H2A	0.0391	0.8979	0.8547	0.079*
C3	−0.0089 (6)	1.0383 (5)	0.7706 (3)	0.0683 (12)
H3A	−0.0946	1.1129	0.7961	0.082*
C4	0.0386 (5)	1.0581 (4)	0.6969 (2)	0.0524 (9)
C5	−0.0311 (5)	1.1907 (4)	0.6553 (3)	0.0650 (12)
H5A	−0.1155	1.2703	0.6779	0.078*
C6	0.0238 (5)	1.2009 (4)	0.5847 (3)	0.0612 (11)
H6A	−0.0231	1.2882	0.5594	0.073*
C7	0.1512 (4)	1.0830 (3)	0.5473 (2)	0.0452 (8)
C8	0.2095 (5)	1.0866 (4)	0.4735 (2)	0.0523 (9)

H8A	0.1656	1.1712	0.4459	0.063*
C9	0.3301 (5)	0.9673 (4)	0.44203 (19)	0.0486 (8)
H9A	0.3696	0.9696	0.3929	0.058*
C10	0.3943 (5)	0.8406 (4)	0.48433 (16)	0.0417 (7)
H10A	0.4752	0.7587	0.4620	0.050*
C11	0.2226 (4)	0.9508 (3)	0.58613 (17)	0.0354 (6)
C12	0.1659 (4)	0.9390 (3)	0.66163 (17)	0.0378 (7)
C13	0.7921 (4)	0.6514 (3)	0.68497 (15)	0.0314 (6)
C14	0.8366 (4)	0.6222 (3)	0.76200 (15)	0.0348 (6)
C15	0.7248 (5)	0.7048 (4)	0.81696 (18)	0.0522 (9)
H15A	0.6250	0.7798	0.8056	0.063*
C16	0.7589 (6)	0.6776 (5)	0.88847 (19)	0.0627 (11)
H16A	0.6814	0.7347	0.9245	0.075*
C17	0.9054 (5)	0.5675 (5)	0.90771 (18)	0.0539 (9)
C18	1.0162 (5)	0.4823 (4)	0.85223 (19)	0.0515 (9)
H18A	1.1141	0.4057	0.8638	0.062*
C19	0.9832 (4)	0.5096 (4)	0.78023 (17)	0.0416 (7)
H19A	1.0596	0.4522	0.7440	0.050*
C20	0.9339 (6)	0.5462 (5)	0.9859 (2)	0.0654 (11)
H20A	0.8468	0.6061	1.0181	0.079*
C21	0.4532 (4)	0.3663 (3)	0.71367 (15)	0.0344 (6)
C22	0.4856 (4)	0.2819 (3)	0.78413 (15)	0.0351 (6)
C23	0.5623 (5)	0.3377 (4)	0.83860 (17)	0.0432 (7)
H23A	0.6004	0.4265	0.8314	0.052*
C24	0.5825 (5)	0.2607 (4)	0.90439 (17)	0.0478 (8)
H24A	0.6365	0.2978	0.9405	0.057*
C25	0.5232 (5)	0.1291 (4)	0.91687 (16)	0.0442 (8)
C26	0.4475 (6)	0.0748 (4)	0.86118 (18)	0.0525 (9)
H26A	0.4070	−0.0129	0.8685	0.063*
C27	0.4311 (5)	0.1479 (4)	0.79540 (18)	0.0471 (8)
H27A	0.3834	0.1078	0.7583	0.057*
C28	0.5413 (5)	0.0533 (4)	0.98769 (17)	0.0498 (8)
H28A	0.6174	0.0827	1.0180	0.060*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0294 (2)	0.0318 (2)	0.02577 (19)	−0.00472 (15)	−0.00555 (13)	0.00541 (14)
O1W	0.0322 (11)	0.0621 (15)	0.0343 (11)	−0.0023 (11)	−0.0047 (9)	−0.0101 (10)
O2W	0.0312 (10)	0.0420 (12)	0.0305 (10)	−0.0074 (9)	−0.0042 (8)	0.0039 (8)
O1	0.0629 (15)	0.0392 (12)	0.0369 (11)	−0.0127 (11)	−0.0139 (10)	0.0058 (9)
O2	0.0573 (14)	0.0435 (12)	0.0338 (11)	−0.0216 (11)	−0.0153 (10)	0.0154 (9)
O3	0.0327 (11)	0.0638 (15)	0.0332 (11)	−0.0054 (11)	−0.0050 (9)	−0.0014 (10)
O4	0.0352 (11)	0.0336 (11)	0.0355 (10)	−0.0065 (9)	−0.0097 (8)	0.0035 (8)
N1	0.0325 (12)	0.0403 (14)	0.0376 (13)	−0.0092 (11)	−0.0017 (10)	−0.0001 (10)
N2	0.0339 (12)	0.0353 (13)	0.0339 (12)	−0.0093 (11)	−0.0086 (10)	0.0062 (10)
C1	0.051 (2)	0.060 (2)	0.0406 (17)	−0.0186 (18)	0.0056 (15)	−0.0054 (15)
C2	0.066 (3)	0.083 (3)	0.051 (2)	−0.031 (2)	0.0185 (19)	−0.021 (2)

C3	0.052 (2)	0.069 (3)	0.079 (3)	−0.008 (2)	0.017 (2)	−0.035 (2)
C4	0.0349 (17)	0.050 (2)	0.072 (2)	−0.0099 (16)	0.0013 (16)	−0.0196 (18)
C5	0.045 (2)	0.038 (2)	0.109 (4)	0.0028 (17)	−0.012 (2)	−0.020 (2)
C6	0.049 (2)	0.0323 (18)	0.102 (3)	−0.0017 (16)	−0.024 (2)	0.0034 (19)
C7	0.0375 (16)	0.0291 (15)	0.072 (2)	−0.0081 (14)	−0.0220 (15)	0.0086 (14)
C8	0.056 (2)	0.0424 (19)	0.066 (2)	−0.0207 (18)	−0.0305 (18)	0.0263 (17)
C9	0.058 (2)	0.053 (2)	0.0422 (17)	−0.0248 (18)	−0.0189 (15)	0.0198 (15)
C10	0.0468 (17)	0.0473 (18)	0.0349 (15)	−0.0174 (15)	−0.0096 (13)	0.0085 (13)
C11	0.0281 (13)	0.0308 (14)	0.0488 (17)	−0.0072 (12)	−0.0120 (12)	0.0040 (12)
C12	0.0283 (14)	0.0363 (16)	0.0495 (17)	−0.0077 (13)	−0.0038 (12)	−0.0068 (13)
C13	0.0310 (14)	0.0336 (14)	0.0322 (14)	−0.0119 (12)	−0.0064 (11)	0.0043 (11)
C14	0.0354 (15)	0.0400 (16)	0.0317 (14)	−0.0129 (13)	−0.0083 (11)	0.0036 (11)
C15	0.055 (2)	0.056 (2)	0.0391 (17)	0.0019 (17)	−0.0096 (15)	−0.0065 (15)
C16	0.070 (3)	0.073 (3)	0.0359 (18)	0.004 (2)	−0.0074 (17)	−0.0105 (17)
C17	0.059 (2)	0.071 (2)	0.0336 (16)	−0.016 (2)	−0.0111 (15)	0.0014 (16)
C18	0.0441 (18)	0.062 (2)	0.0440 (18)	−0.0004 (17)	−0.0145 (14)	0.0094 (16)
C19	0.0380 (16)	0.0506 (19)	0.0343 (15)	−0.0061 (15)	−0.0054 (12)	0.0017 (13)
C20	0.067 (3)	0.087 (3)	0.0363 (18)	−0.002 (2)	−0.0122 (17)	−0.0025 (18)
C21	0.0336 (14)	0.0362 (15)	0.0302 (14)	−0.0033 (12)	−0.0019 (11)	0.0075 (11)
C22	0.0382 (15)	0.0323 (15)	0.0317 (14)	−0.0043 (13)	−0.0003 (11)	0.0079 (11)
C23	0.0530 (19)	0.0413 (17)	0.0370 (16)	−0.0155 (15)	−0.0057 (13)	0.0109 (13)
C24	0.064 (2)	0.049 (2)	0.0328 (15)	−0.0188 (18)	−0.0092 (14)	0.0073 (13)
C25	0.062 (2)	0.0352 (16)	0.0314 (15)	−0.0059 (15)	−0.0002 (14)	0.0073 (12)
C26	0.079 (3)	0.0394 (18)	0.0404 (17)	−0.0179 (18)	−0.0041 (17)	0.0093 (14)
C27	0.067 (2)	0.0377 (17)	0.0386 (16)	−0.0162 (17)	−0.0052 (15)	0.0043 (13)
C28	0.068 (2)	0.0435 (18)	0.0340 (16)	−0.0062 (17)	−0.0052 (15)	0.0090 (13)

Geometric parameters (Å, °)

Co1—O2	2.069 (2)	C8—H8A	0.9300
Co1—O4	2.105 (2)	C9—C10	1.400 (4)
Co1—O1W	2.109 (2)	C9—H9A	0.9300
Co1—N2	2.131 (2)	C10—H10A	0.9300
Co1—N1	2.132 (3)	C11—C12	1.430 (4)
Co1—O2W	2.145 (2)	C13—C14	1.499 (4)
O1W—H1W1	0.85 (1)	C14—C15	1.379 (5)
O1W—H1W2	0.85 (3)	C14—C19	1.386 (4)
O2W—H2W1	0.85 (1)	C15—C16	1.378 (5)
O2W—H2W2	0.856 (10)	C15—H15A	0.9300
O1—C21	1.246 (4)	C16—C17	1.379 (6)
O2—C21	1.263 (4)	C16—H16A	0.9300
O3—C13	1.259 (4)	C17—C18	1.393 (5)
O4—C13	1.257 (3)	C17—C20	1.485 (5)
N1—C1	1.319 (4)	C18—C19	1.385 (4)
N1—C12	1.360 (4)	C18—H18A	0.9300
N2—C10	1.331 (4)	C19—H19A	0.9300
N2—C11	1.354 (4)	C20—C20^{i}	1.290 (8)
C1—C2	1.399 (5)	C20—H20A	0.9300
C1—H1A	0.9300	C21—C22	1.508 (4)

C2—C3	1.360 (6)	C22—C23	1.381 (5)
C2—H2A	0.9300	C22—C27	1.394 (4)
C3—C4	1.394 (6)	C23—C24	1.393 (4)
C3—H3A	0.9300	C23—H23A	0.9300
C4—C12	1.406 (5)	C24—C25	1.392 (5)
C4—C5	1.440 (6)	C24—H24A	0.9300
C5—C6	1.340 (6)	C25—C26	1.388 (5)
C5—H5A	0.9300	C25—C28	1.469 (4)
C6—C7	1.417 (5)	C26—C27	1.375 (4)
C6—H6A	0.9300	C26—H26A	0.9300
C7—C8	1.394 (5)	C27—H27A	0.9300
C7—C11	1.415 (4)	C28—C28^{ii}	1.327 (7)
C8—C9	1.357 (5)	C28—H28A	0.9300
O2—Co1—O4	84.05 (8)	N2—C10—H10A	118.6
O2—Co1—O1W	92.31 (10)	C9—C10—H10A	118.6
O4—Co1—O1W	87.44 (9)	N2—C11—C7	122.9 (3)
O2—Co1—N2	169.76 (9)	N2—C11—C12	117.4 (3)
O4—Co1—N2	100.04 (9)	C7—C11—C12	119.7 (3)
O1W—Co1—N2	97.24 (10)	N1—C12—C4	123.2 (3)
O2—Co1—N1	93.57 (10)	N1—C12—C11	116.8 (3)
O4—Co1—N1	86.75 (9)	C4—C12—C11	120.0 (3)
O1W—Co1—N1	171.27 (10)	O4—C13—O3	123.8 (3)
N2—Co1—N1	77.39 (10)	O4—C13—C14	117.8 (3)
O2—Co1—O2W	87.87 (8)	O3—C13—C14	118.4 (3)
O4—Co1—O2W	169.94 (8)	C15—C14—C19	118.6 (3)
O1W—Co1—O2W	86.90 (9)	C15—C14—C13	119.6 (3)
N2—Co1—O2W	88.93 (9)	C19—C14—C13	121.8 (3)
N1—Co1—O2W	99.76 (9)	C16—C15—C14	120.9 (4)
Co1—O1W—H1W1	138 (3)	C16—C15—H15A	119.5
Co1—O1W—H1W2	100 (2)	C14—C15—H15A	119.5
H1W1—O1W—H1W2	110.2 (17)	C17—C16—C15	121.4 (4)
Co1—O2W—H2W1	117 (3)	C17—C16—H16A	119.3
Co1—O2W—H2W2	95 (2)	C15—C16—H16A	119.3
H2W1—O2W—H2W2	108.6 (16)	C16—C17—C18	117.5 (3)
C21—O2—Co1	129.21 (19)	C16—C17—C20	118.1 (4)
C13—O4—Co1	119.98 (18)	C18—C17—C20	124.3 (4)
C1—N1—C12	118.1 (3)	C19—C18—C17	121.3 (3)
C1—N1—Co1	127.6 (2)	C19—C18—H18A	119.4
C12—N1—Co1	114.2 (2)	C17—C18—H18A	119.4
C10—N2—C11	117.8 (3)	C18—C19—C14	120.2 (3)
C10—N2—Co1	128.1 (2)	C18—C19—H19A	119.9
C11—N2—Co1	114.14 (19)	C14—C19—H19A	119.9
N1—C1—C2	122.4 (4)	C20^{i}—C20—C17	127.2 (5)
N1—C1—H1A	118.8	C20^{i}—C20—H20A	116.4
C2—C1—H1A	118.8	C17—C20—H20A	116.4
C3—C2—C1	119.4 (4)	O1—C21—O2	126.3 (3)
C3—C2—H2A	120.3	O1—C21—C22	117.5 (3)
C1—C2—H2A	120.3	O2—C21—C22	116.2 (3)

C2—C3—C4	120.4 (4)	C23—C22—C27	119.4 (3)
C2—C3—H3A	119.8	C23—C22—C21	121.2 (3)
C4—C3—H3A	119.8	C27—C22—C21	119.3 (3)
C3—C4—C12	116.5 (4)	C22—C23—C24	119.9 (3)
C3—C4—C5	125.0 (4)	C22—C23—H23A	120.1
C12—C4—C5	118.5 (4)	C24—C23—H23A	120.1
C6—C5—C4	121.0 (4)	C25—C24—C23	121.0 (3)
C6—C5—H5A	119.5	C25—C24—H24A	119.5
C4—C5—H5A	119.5	C23—C24—H24A	119.5
C5—C6—C7	122.1 (4)	C26—C25—C24	118.0 (3)
C5—C6—H6A	119.0	C26—C25—C28	122.3 (3)
C7—C6—H6A	119.0	C24—C25—C28	119.6 (3)
C8—C7—C11	117.0 (3)	C27—C26—C25	121.4 (3)
C8—C7—C6	124.3 (3)	C27—C26—H26A	119.3
C11—C7—C6	118.7 (3)	C25—C26—H26A	119.3
C9—C8—C7	120.2 (3)	C26—C27—C22	120.2 (3)
C9—C8—H8A	119.9	C26—C27—H27A	119.9
C7—C8—H8A	119.9	C22—C27—H27A	119.9
C8—C9—C10	119.2 (3)	$C28^{ii}$—C28—C25	125.9 (5)
C8—C9—H9A	120.4	$C28^{ii}$—C28—H28A	117.1
C10—C9—H9A	120.4	C25—C28—H28A	117.1
N2—C10—C9	122.9 (3)		
O4—Co1—O2—C21	−157.9 (3)	C8—C7—C11—C12	−179.0 (3)
O1W—Co1—O2—C21	−70.7 (3)	C6—C7—C11—C12	−0.1 (4)
N2—Co1—O2—C21	88.0 (6)	C1—N1—C12—C4	−0.9 (4)
N1—Co1—O2—C21	115.8 (3)	Co1—N1—C12—C4	−177.4 (2)
O2W—Co1—O2—C21	16.1 (3)	C1—N1—C12—C11	178.4 (3)
O2—Co1—O4—C13	51.2 (2)	Co1—N1—C12—C11	1.9 (3)
O1W—Co1—O4—C13	−41.4 (2)	C3—C4—C12—N1	−0.4 (5)
N2—Co1—O4—C13	−138.3 (2)	C5—C4—C12—N1	178.9 (3)
N1—Co1—O4—C13	145.2 (2)	C3—C4—C12—C11	−179.7 (3)
O2W—Co1—O4—C13	14.5 (5)	C5—C4—C12—C11	−0.3 (5)
O2—Co1—N1—C1	6.0 (3)	N2—C11—C12—N1	1.0 (4)
O4—Co1—N1—C1	−77.8 (3)	C7—C11—C12—N1	−178.9 (3)
N2—Co1—N1—C1	−178.8 (3)	N2—C11—C12—C4	−179.7 (3)
O2W—Co1—N1—C1	94.5 (3)	C7—C11—C12—C4	0.4 (4)
O2—Co1—N1—C12	−177.9 (2)	Co1—O4—C13—O3	63.9 (3)
O4—Co1—N1—C12	98.3 (2)	Co1—O4—C13—C14	−114.4 (2)
N2—Co1—N1—C12	−2.8 (2)	O4—C13—C14—C15	−8.7 (4)
O2W—Co1—N1—C12	−89.5 (2)	O3—C13—C14—C15	172.8 (3)
O2—Co1—N2—C10	−150.0 (4)	O4—C13—C14—C19	168.4 (3)
O4—Co1—N2—C10	97.2 (3)	O3—C13—C14—C19	−10.0 (4)
O1W—Co1—N2—C10	8.5 (3)	C19—C14—C15—C16	0.8 (5)
N1—Co1—N2—C10	−178.5 (3)	C13—C14—C15—C16	178.1 (3)
O2W—Co1—N2—C10	−78.2 (3)	C14—C15—C16—C17	0.1 (7)
O2—Co1—N2—C11	31.8 (6)	C15—C16—C17—C18	−1.3 (6)
O4—Co1—N2—C11	−81.0 (2)	C15—C16—C17—C20	179.4 (4)
O1W—Co1—N2—C11	−169.68 (19)	C16—C17—C18—C19	1.6 (6)

N1—Co1—N2—C11	3.33 (19)	C20—C17—C18—C19	−179.1 (4)
O2W—Co1—N2—C11	103.58 (19)	C17—C18—C19—C14	−0.7 (6)
C12—N1—C1—C2	1.2 (5)	C15—C14—C19—C18	−0.5 (5)
Co1—N1—C1—C2	177.2 (3)	C13—C14—C19—C18	−177.7 (3)
N1—C1—C2—C3	−0.3 (6)	C16—C17—C20—C20^{i}	−177.1 (6)
C1—C2—C3—C4	−1.1 (6)	C18—C17—C20—C20^{i}	3.6 (9)
C2—C3—C4—C12	1.4 (6)	Co1—O2—C21—O1	3.4 (5)
C2—C3—C4—C5	−177.9 (4)	Co1—O2—C21—C22	−174.32 (19)
C3—C4—C5—C6	179.2 (4)	O1—C21—C22—C23	176.1 (3)
C12—C4—C5—C6	−0.1 (5)	O2—C21—C22—C23	−6.0 (4)
C4—C5—C6—C7	0.4 (6)	O1—C21—C22—C27	−6.3 (4)
C5—C6—C7—C8	178.5 (4)	O2—C21—C22—C27	171.6 (3)
C5—C6—C7—C11	−0.3 (5)	C27—C22—C23—C24	−0.7 (5)
C11—C7—C8—C9	−0.3 (5)	C21—C22—C23—C24	176.9 (3)
C6—C7—C8—C9	−179.0 (3)	C22—C23—C24—C25	−1.3 (6)
C7—C8—C9—C10	0.3 (5)	C23—C24—C25—C26	1.6 (6)
C11—N2—C10—C9	2.0 (4)	C23—C24—C25—C28	−178.1 (3)
Co1—N2—C10—C9	−176.2 (2)	C24—C25—C26—C27	0.0 (6)
C8—C9—C10—N2	−1.2 (5)	C28—C25—C26—C27	179.7 (4)
C10—N2—C11—C7	−1.9 (4)	C25—C26—C27—C22	−2.0 (6)
Co1—N2—C11—C7	176.5 (2)	C23—C22—C27—C26	2.3 (5)
C10—N2—C11—C12	178.1 (3)	C21—C22—C27—C26	−175.4 (3)
Co1—N2—C11—C12	−3.5 (3)	C26—C25—C28—C28^{ii}	−14.3 (7)
C8—C7—C11—N2	1.1 (4)	C24—C25—C28—C28^{ii}	165.4 (5)
C6—C7—C11—N2	180.0 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2W^{iii}	0.85 (1)	1.900 (11)	2.749 (3)	177 (4)
O1W—H1W2···O3	0.85 (3)	1.83 (3)	2.653 (3)	164 (3)
O2W—H2W1···O3^{iv}	0.85 (1)	1.83 (3)	2.679 (3)	172 (3)
O2W—H2W2···O1	0.856 (10)	1.72 (3)	2.564 (3)	169 (4)
O2W—H2W2···O2	0.856 (10)	2.51 (4)	2.925 (3)	111 (3)

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

Fig. 1

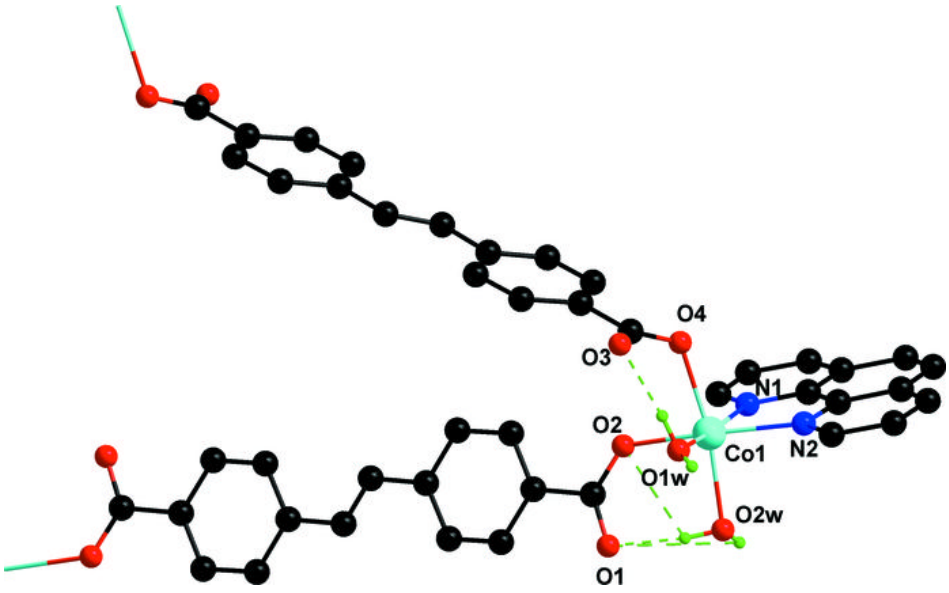
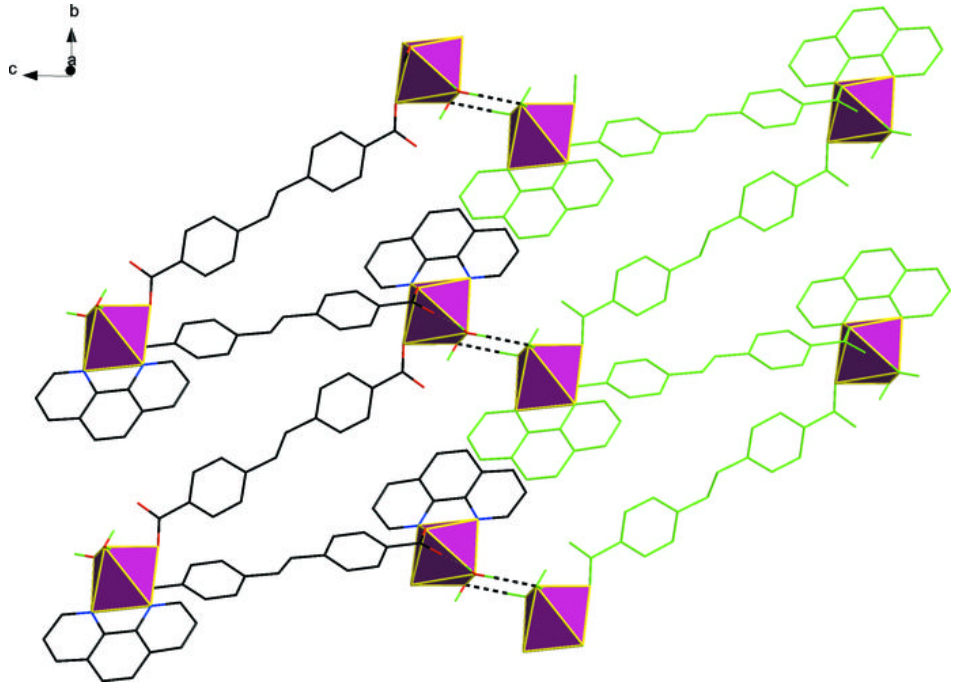
Fig. 2