

Retraction of articles by H. Zhong *et al.*

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Received 20 November 2009; accepted 15 December 2009

A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ²N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinolinol-κ²N,O)bis(8-quinolinolato-κ²N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METOQM
<i>(8-Quinolinol-κ²N,O)-bis(8-quinolinolato-κ²N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chlorodibis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITCP001
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ²O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ²N,N')tetrakis(nitrato-κ²O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ²N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ²N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ²O,O')bis(μ-anilinoacetato-κ²O,O')bis(1,10-phenanthroline-κ²N,N')samarium(III)]-μ-anilinoacetato-κ²O,O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-neodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaqua copper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

addenda and errata

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra- μ -anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di- μ -anilinoacetato]	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[{(acetato- κ O)}(1,10-phenanthroline- κ^2 N,N')cobalt(II)]- μ -acetato- κ^2 O:O']	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[{(acetato- κ O)}(1,10-phenanthroline- κ^2 N,N')copper(II)]- μ -acetato- κ^2 O:O']	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEQ
catena-Poly[[{(acetato- κ O)}(1,10-phenanthroline- κ^2 N,N')nickel(II)]- μ -acetato- κ^2 O:O']	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra- μ -anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di- μ -anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime- κ^2 N,N')bis(1,10-phenanthroline- κ^2 N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[{(1,10-phenanthroline- κ^2 N,N')praseodymium(III)]-di- μ -phenoxyacetato- κ^4 O:O'-[(1,10-phenanthroline- κ^2 N,N')-praseodymium(III)]-di- μ -phenoxyacetato- κ^4 O:O'-di- μ -phenoxyacetato- κ^3 O,O':O; κ^3 O:O,O']	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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catena-Poly[[acetato- κ O](1,10-phenanthroline- κ^2 N,N')cobalt(II)]- μ -acetato- κ^2 O:O']

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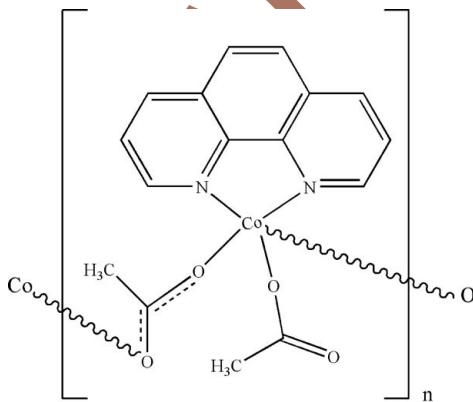
Received 26 October 2007; accepted 26 October 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.005$ Å;
R factor = 0.042; wR factor = 0.127; data-to-parameter ratio = 13.2.

The title compound, $[Co(C_2H_3O_2)_2(C_{12}H_8N_2)]_n$, is a polymeric complex involving bridging of Co^{II} ions by single *syn-anti* acetate ligands. Each Co atom is five-coordinated by two 1,10-phenanthroline N atoms and three O atoms of acetate ligands within a bipyramidal coordination geometry. In the crystal structure, C—H···O hydrogen bonds result in the formation of a polymeric ribbon structure.

Related literature

For related literature, see: Desiraju (1995, 1997); Braga *et al.* (1998); Wu *et al.* (2003); Pan & Xu (2004); Liu *et al.* (2004); Li *et al.* (2005); McCann *et al.* (1995, 1996); Wai *et al.* (1990); Yaghi *et al.* (1996); Min & Lee (2002); Maira *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Co(C_2H_3O_2)_2(C_{12}H_8N_2)]$
 $M_r = 357.22$
Monoclinic, $P2_1/n$

$a = 8.6864$ (17) Å
 $b = 9.183$ (2) Å
 $c = 17.0024$ (11) Å

$\beta = 101.897$ (4)°
 $V = 1327.1$ (4) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 1.32$ mm⁻¹
 $T = 273$ (2) K
 $0.41 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $R_{\text{int}} = 0.017$
 $T_{\min} = 0.617$, $T_{\max} = 0.774$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
2 restraints
 $wR(F^2) = 0.127$
H-atom parameters constrained
 $S = 1.02$
 $\Delta\rho_{\max} = 0.69$ e Å⁻³
2779 reflections
 $\Delta\rho_{\min} = -0.51$ e Å⁻³
210 parameters

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.999 (2)	Co1—N1	2.008 (3)
Co1—O2	1.941 (2)	Co1—N2	1.984 (2)
Co1—O3 ⁱ	2.320 (2)		
O1—Co1—O2	91.00 (10)	O2—Co1—N1	93.96 (11)
O1—Co1—O3 ⁱ	86.94 (9)	O2—Co1—N2	174.47 (10)
O2—Co1—O3 ⁱ	82.25 (9)	O3—Co1—N1 ⁱ	138.62 (4)
O1—Co1—N1	165.97 (10)	O3—Co1—N2 ⁱ	125.59 (5)
O1—Co1—N2	93.00 (9)	N1—Co1—N2	83.03 (10)

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C2—H2···O4 ⁱⁱ	0.93	2.51	3.327 (4)	147
C10—H10···O2 ⁱⁱⁱ	0.93	2.36	3.263 (4)	164

Symmetry codes: (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$; (iii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

We thank the Science and Technology Program of Jinggangshan University for financial support of this work (grant No. 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2355).

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Article retracted

supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2895-m2896 [doi:10.1107/S1600536807053494]

catena-Poly[[(acetato- κO)(1,10-phenanthroline- $\kappa^2 N,N'$)cobalt(II)]- μ -acetato- $\kappa^2 O:O'$]

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Aromatic polycyclic compounds, such as phenanthroline, quinoline and benzimidazole, are one of the most important classes of biological ligands and the coordinations of metal-aromatic polycyclic compounds are of critical importance in biological systems, organic materials and coordination chemistry (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). As a bidentate flexible ligand, carboxyl groups compounds are also good ligands with excellent coordination capabilities to generate mono-, bi- or trinuclear complexes, which are commonly used as precursors for the formation of supramolecular architectures (McCann *et al.*, 1996; McCann *et al.*, 1995; Wai *et al.*, 1990; Yaghi *et al.*, 1996; Min & Lee 2002; Maira *et al.*, 2001). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It has an inversion centre midway between the two Co^{II} ions, which are bridged by two bidentate and two monodentate carboxyl groups. Each Co atom is five-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and three O atoms of acetate ligands. The Co—O and Co—N bonds are in the range of [1.941 (2)–2.320 (2) Å] and [1.984 (2)–2.008 (3) Å], respectively (Table 1).

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 2, Fig. 2) result in the formation of a polymeric ribbon structure.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Cobalt (II) nitrate hexahydrate (291.1 mg, 1 mmol), phen (180.2 mg, 1 mmol), acetic acid (120.1 mg, 2 mmol), ammonia (4 ml, 0.5 mol/l) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small pink crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H atoms.

supplementary materials

Figures

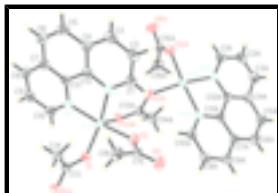


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

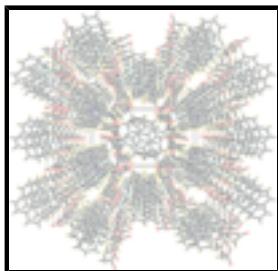


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[acetato- κ O)(1,10-phenanthroline- κ^2N,N')cobalt(II)]- μ - acetato- $\kappa^2O:O'$]

Crystal data

$[Co(C_2H_3O_2)_2(C_{12}H_8N_2)]$

$F_{000} = 732$

$M_r = 357.22$

$D_x = 1.788 \text{ Mg m}^{-3}$

Monoclinic, $P2_1/n$

Mo $K\alpha$ radiation

Hall symbol: -p 2yn

$\lambda = 0.71073 \text{ \AA}$

$a = 8.6864 (17) \text{ \AA}$

Cell parameters from 5524 reflections

$b = 9.183 (2) \text{ \AA}$

$\theta = 2.3\text{--}28.0^\circ$

$c = 17.0024 (11) \text{ \AA}$

$\mu = 1.32 \text{ mm}^{-1}$

$\beta = 101.897 (4)^\circ$

$T = 273 (2) \text{ K}$

$V = 1327.1 (4) \text{ \AA}^3$

Prism, pink

$Z = 4$

$0.41 \times 0.24 \times 0.20 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

2779 independent reflections

Radiation source: fine-focus sealed tube

2349 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.017$

$T = 273(2) \text{ K}$

$\theta_{\max} = 27.0^\circ$

φ and ω scans

$\theta_{\min} = 2.5^\circ$

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$h = -11 \rightarrow 11$

$T_{\min} = 0.617, T_{\max} = 0.774$

$k = -11 \rightarrow 11$

8683 measured reflections

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0915P)^2 + 0.5483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2779 reflections	$\Delta\rho_{\text{max}} = 0.69 \text{ e \AA}^{-3}$
210 parameters	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$
2 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.66505 (4)	0.92788 (4)	0.803184 (19)	0.03316 (17)
O1	0.6876 (3)	0.7352 (2)	0.75202 (12)	0.0458 (5)
O2	0.5483 (3)	1.0049 (3)	0.70205 (13)	0.0530 (6)
O3	0.6215 (3)	0.5047 (2)	0.74862 (15)	0.0528 (6)
O4	0.3286 (3)	1.0280 (4)	0.62132 (17)	0.0706 (8)
N1	0.6077 (3)	1.0939 (3)	0.86847 (16)	0.0412 (5)
N2	0.7957 (3)	0.8671 (3)	0.90793 (14)	0.0393 (5)
C1	0.5195 (4)	1.2113 (4)	0.8471 (2)	0.0489 (7)
H1	0.4800	1.2274	0.7927	0.059*
C2	0.4838 (4)	1.3105 (4)	0.9017 (2)	0.0546 (8)
H2	0.4234	1.3922	0.8837	0.065*
C3	0.5366 (4)	1.2887 (4)	0.9811 (2)	0.0531 (8)
H3	0.5101	1.3531	1.0184	0.064*
C4	0.6330 (3)	1.1659 (3)	1.00699 (18)	0.0424 (6)
C5	0.6983 (4)	1.1338 (4)	1.0880 (2)	0.0515 (8)
H5	0.6746	1.1926	1.1284	0.062*
C6	0.7946 (4)	1.0188 (4)	1.10743 (19)	0.0495 (7)

supplementary materials

H6	0.8355	0.9995	1.1614	0.059*
C7	0.8360 (4)	0.9255 (3)	1.04817 (18)	0.0416 (6)
C8	0.9430 (4)	0.8077 (4)	1.06368 (18)	0.0474 (7)
H8	0.9931	0.7862	1.1162	0.057*
C9	0.9723 (4)	0.7262 (4)	1.0018 (2)	0.0505 (7)
H9	1.0434	0.6493	1.0117	0.061*
C10	0.8957 (4)	0.7581 (3)	0.92380 (19)	0.0466 (7)
H10	0.9154	0.7011	0.8817	0.056*
C11	0.7671 (3)	0.9514 (3)	0.96843 (17)	0.0370 (6)
C12	0.6651 (3)	1.0725 (3)	0.94750 (18)	0.0367 (6)
C13	0.6166 (3)	0.6284 (3)	0.77790 (16)	0.0339 (5)
C14	0.5457 (4)	0.6525 (3)	0.83168 (19)	0.0441 (7)
H14A	0.4484	0.5995	0.8215	0.066*
H14B	0.5243	0.7549	0.8336	0.066*
H14C	0.6088	0.6222	0.8822	0.066*
C15	0.4032 (3)	0.9782 (3)	0.68379 (16)	0.0366 (6)
C16	0.3456 (4)	0.9001 (5)	0.7293 (2)	0.0565 (9)
H16A	0.2335	0.9124	0.7181	0.085*
H16B	0.3881	0.9271	0.7840	0.085*
H16C	0.3705	0.8001	0.7212	0.085*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0395 (2)	0.0320 (2)	0.0266 (2)	0.00247 (13)	0.00361 (16)	0.00086 (13)
O1	0.0559 (12)	0.0429 (11)	0.0393 (10)	-0.0051 (10)	0.0115 (9)	-0.0023 (9)
O2	0.0501 (12)	0.0604 (16)	0.0443 (12)	-0.0060 (11)	-0.0001 (10)	0.0126 (11)
O3	0.0516 (12)	0.0417 (12)	0.0654 (14)	-0.0049 (10)	0.0127 (11)	-0.0152 (11)
O4	0.0609 (15)	0.0780 (18)	0.0622 (16)	-0.0064 (14)	-0.0117 (13)	0.0198 (15)
N1	0.0439 (12)	0.0375 (12)	0.0420 (13)	0.0019 (10)	0.0083 (11)	0.0042 (10)
N2	0.0454 (12)	0.0359 (12)	0.0359 (11)	0.0016 (10)	0.0066 (10)	-0.0015 (10)
C1	0.0508 (16)	0.0449 (17)	0.0500 (16)	0.0058 (14)	0.0078 (14)	0.0047 (14)
C2	0.0521 (17)	0.0441 (17)	0.067 (2)	0.0122 (14)	0.0108 (16)	0.0045 (16)
C3	0.0532 (17)	0.0442 (18)	0.065 (2)	0.0079 (14)	0.0206 (16)	-0.0054 (15)
C4	0.0434 (14)	0.0413 (15)	0.0456 (15)	-0.0025 (12)	0.0161 (12)	-0.0028 (12)
C5	0.0588 (18)	0.0550 (19)	0.0451 (16)	-0.0029 (16)	0.0206 (15)	-0.0098 (14)
C6	0.0535 (17)	0.0598 (19)	0.0356 (14)	0.0007 (15)	0.0100 (13)	-0.0008 (14)
C7	0.0453 (15)	0.0425 (16)	0.0366 (14)	-0.0051 (12)	0.0077 (12)	0.0027 (11)
C8	0.0528 (16)	0.0476 (17)	0.0387 (14)	0.0008 (14)	0.0025 (13)	0.0067 (13)
C9	0.0538 (17)	0.0405 (16)	0.0538 (17)	0.0087 (13)	0.0032 (14)	0.0043 (14)
C10	0.0517 (16)	0.0391 (15)	0.0471 (16)	0.0065 (13)	0.0059 (13)	-0.0051 (13)
C11	0.0411 (14)	0.0334 (13)	0.0373 (14)	-0.0032 (11)	0.0097 (11)	0.0001 (11)
C12	0.0376 (13)	0.0348 (14)	0.0385 (14)	-0.0030 (10)	0.0097 (11)	0.0024 (11)
C13	0.0343 (12)	0.0321 (13)	0.0344 (13)	0.0004 (10)	0.0048 (10)	-0.0030 (11)
C14	0.0571 (17)	0.0342 (14)	0.0520 (16)	-0.0042 (12)	0.0368 (15)	-0.0044 (12)
C15	0.0378 (13)	0.0356 (13)	0.0338 (13)	-0.0001 (11)	0.0012 (11)	0.0002 (11)
C16	0.0439 (16)	0.088 (3)	0.0378 (16)	-0.0182 (16)	0.0085 (13)	0.0191 (17)

Geometric parameters (\AA , $^\circ$)

Co1—O1	1.999 (2)	C4—C5	1.408 (5)
Co1—O2	1.941 (2)	C5—C6	1.346 (5)
Co1—O3 ⁱ	2.320 (2)	C5—H5	0.9300
Co1—N1	2.008 (3)	C6—C7	1.424 (5)
Co1—N2	1.984 (2)	C6—H6	0.9300
O1—C13	1.283 (4)	C7—C11	1.385 (4)
O2—C15	1.259 (4)	C7—C8	1.415 (5)
O3—C13	1.245 (4)	C8—C9	1.357 (5)
O3—Co1 ⁱⁱ	2.320 (2)	C8—H8	0.9300
O4—C15	1.214 (4)	C9—C10	1.387 (5)
N1—C1	1.329 (4)	C9—H9	0.9300
N1—C12	1.348 (4)	C10—H10	0.9300
N2—C10	1.316 (4)	C11—C12	1.421 (4)
N2—C11	1.351 (4)	C13—C14	1.223 (4)
C1—C2	1.381 (5)	C14—H14A	0.9600
C1—H1	0.9300	C14—H14B	0.9600
C2—C3	1.348 (5)	C14—H14C	0.9600
C2—H2	0.9300	C15—C16	1.234 (4)
C3—C4	1.419 (5)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C12	1.398 (4)	C16—H16C	0.9600
O1—Co1—O2	91.00 (10)	C11—C7—C8	116.6 (3)
O1—Co1—O3 ⁱ	86.94 (9)	C11—C7—C6	118.0 (3)
O2—Co1—O3 ⁱ	82.25 (9)	C8—C7—C6	125.4 (3)
O1—Co1—N1	165.97 (10)	C9—C8—C7	119.9 (3)
O1—Co1—N2	93.00 (9)	C9—C8—H8	120.1
O2—Co1—N1	93.96 (11)	C7—C8—H8	120.1
O2—Co1—N2	174.47 (10)	C8—C9—C10	119.7 (3)
O3—Co1—N1 ⁱ	138.62 (4)	C8—C9—H9	120.2
O3—Co1—N2 ⁱ	125.59 (5)	C10—C9—H9	120.2
N1—Co1—N2	83.03 (10)	N2—C10—C9	121.5 (3)
C13—O1—Co1	115.45 (18)	N2—C10—H10	119.2
C15—O2—Co1	117.46 (19)	C9—C10—H10	119.2
C13—O3—Co1 ⁱⁱ	121.71 (18)	N2—C11—C7	122.5 (3)
C1—N1—C12	117.7 (3)	N2—C11—C12	117.4 (3)
C1—N1—Co1	131.2 (2)	C7—C11—C12	120.0 (3)
C12—N1—Co1	110.95 (19)	N1—C12—C4	123.0 (3)
C10—N2—C11	119.8 (3)	N1—C12—C11	116.6 (3)
C10—N2—Co1	129.0 (2)	C4—C12—C11	120.4 (3)
C11—N2—Co1	111.18 (19)	C14—C13—O3	121.9 (3)
N1—C1—C2	123.3 (3)	C14—C13—O1	118.0 (3)
N1—C1—H1	118.4	O3—C13—O1	120.1 (3)
C2—C1—H1	118.4	C13—C14—H14A	109.5
C3—C2—C1	119.8 (3)	C13—C14—H14B	109.5

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C3—C2—H2	120.1	H14A—C14—H14B	109.5
C1—C2—H2	120.1	C13—C14—H14C	109.5
C2—C3—C4	119.1 (3)	H14A—C14—H14C	109.5
C2—C3—H3	120.5	H14B—C14—H14C	109.5
C4—C3—H3	120.5	O4—C15—C16	123.8 (3)
C12—C4—C5	118.6 (3)	O4—C15—O2	118.0 (3)
C12—C4—C3	117.1 (3)	C16—C15—O2	118.3 (3)
C5—C4—C3	124.3 (3)	C15—C16—H16A	109.5
C6—C5—C4	120.7 (3)	C15—C16—H16B	109.5
C6—C5—H5	119.7	H16A—C16—H16B	109.5
C4—C5—H5	119.7	C15—C16—H16C	109.5
C5—C6—C7	122.2 (3)	H16A—C16—H16C	109.5
C5—C6—H6	118.9	H16B—C16—H16C	109.5
C7—C6—H6	118.9		

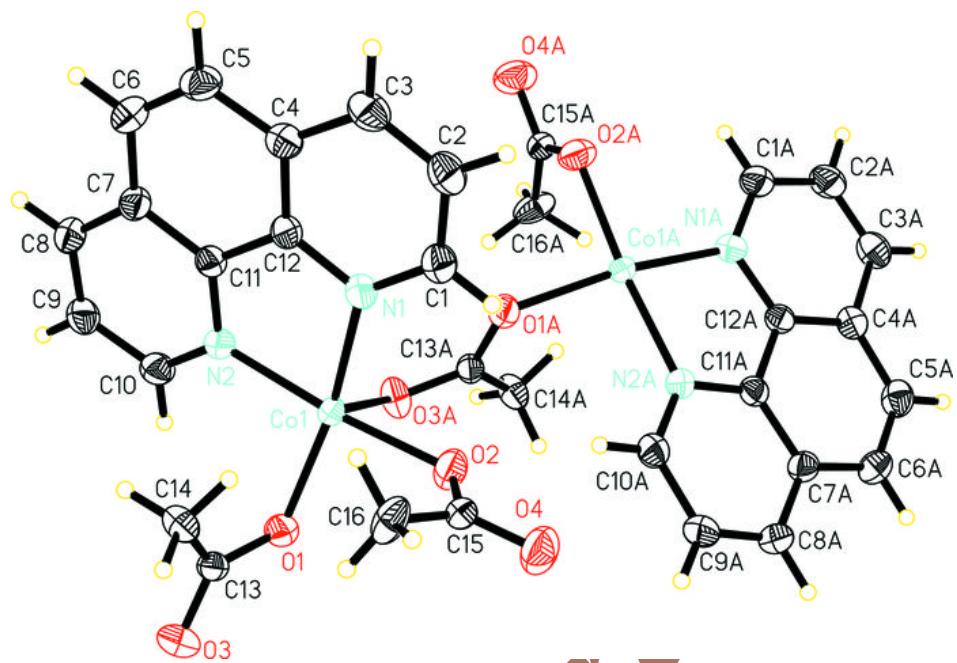
Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D—\text{H}\cdots A$	$D—\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D—\text{H}\cdots A$
C2—H2 \cdots O4 ⁱⁱⁱ	0.93	2.51	3.327 (4)	147
C10—H10 \cdots O2 ⁱⁱ	0.93	2.36	3.263 (4)	164

Symmetry codes: (iii) $-x+1/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

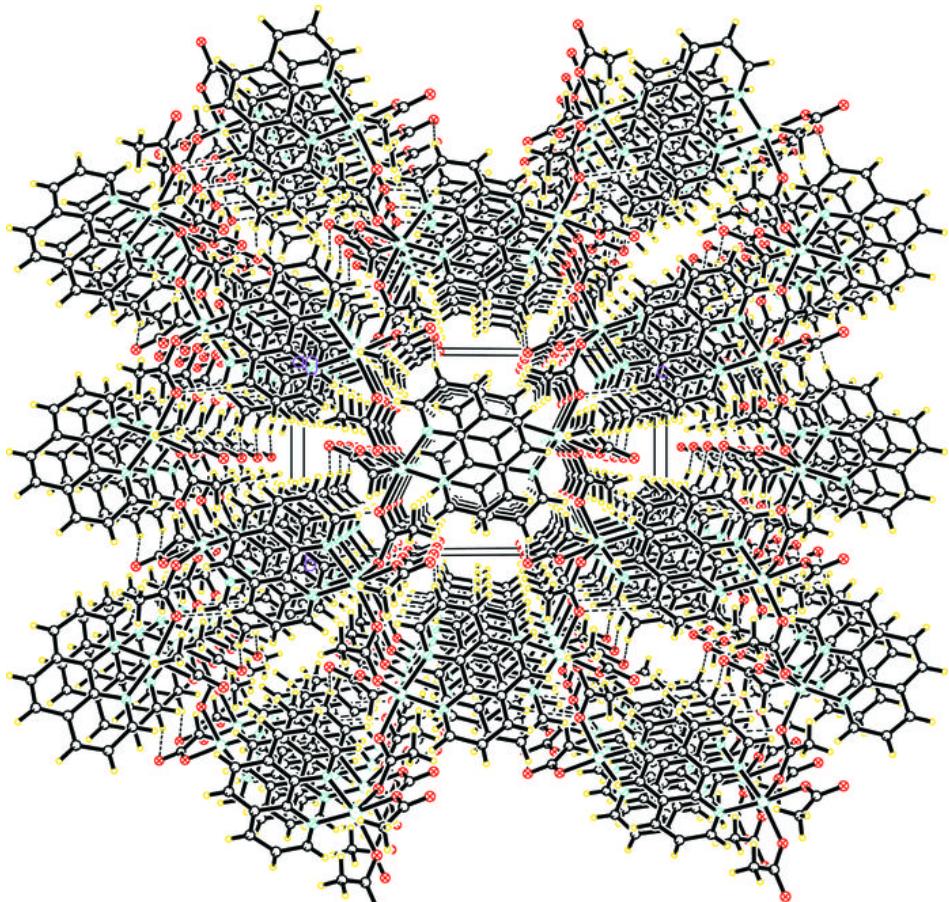
Fig. 1



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supplementary materials

Fig. 2



Article