

Retraction of articles by T. Liu *et al.*

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *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>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu & Xie (2007a) Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807026852 10.1107/S1600536807028255	EDUMAS EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNO₂</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu Wang, Wang & Xie (2007a) Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807027195 10.1107/S1600536807031224	ICSD 240891 WIHIED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxyacetato-κ²O:O')bis(I,10-phenanthroline-κ²N,N')-(2-pyridyloxyacetato-κO)neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonium (I/I)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(I,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(I,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamido-bis(I,10-phenanthroline)dicerium(III)-di-μ-anilinoacetamido]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')nickel(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')copper(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')cobalt(II)-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

addenda and errata

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
catena-Poly[μ (nitro- κO)(1,10-phenanthroline- $\kappa^2 N,N'$)manganese(II)]- μ -nitroato- $\kappa^2 O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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

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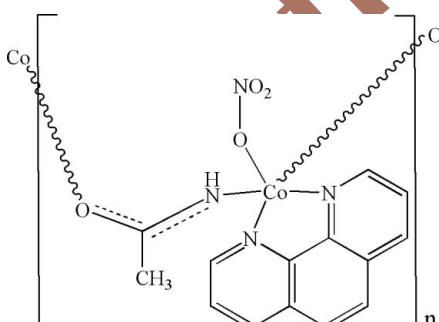
Received 17 November 2007; accepted 19 November 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.040; wR factor = 0.133; data-to-parameter ratio = 12.6.

In the crystal structure of the title compound, $[Co(C_2H_4NO)(NO_3)(C_{12}H_8N_2)]_n$, the Co^{II} atoms are linked by acetamide ligands to form a chain. Each Co^{II} atom is five-coordinated by two N atoms of a 1,10-phenanthroline ligand, one nitrate O atom, and one N atom and one O atom of an acetamide ligand within a trigonal-bipyramidal coordination geometry. In the crystal structure, the chains are linked by hydrogen bonds into a polymeric ribbon structure.

Related literature

For a related structure, see: Liu & Zhu (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Co(C_2H_4NO)(NO_3)(C_{12}H_8N_2)]$
 $M_r = 359.21$

Monoclinic, $P2_1/n$
 $a = 8.7208 (13)$ Å
 $b = 9.220 (2)$ Å
 $c = 16.9015 (16)$ Å
 $\beta = 101.821 (4)$ °

$V = 1330.2 (4)$ Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.32$ mm⁻¹

$T = 273 (2)$ K

$0.42 \times 0.24 \times 0.21$ mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.610$, $T_{\max} = 0.766$

8432 measured reflections
2643 independent reflections
2273 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.133$
 $S = 1.02$
2643 reflections
209 parameters

1 restraint
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.77$ e Å⁻³
 $\Delta\rho_{\min} = -0.67$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.938 (2)	Co1—N2	1.976 (3)
Co1—O4 ⁱ	2.325 (2)	Co1—N3	2.006 (2)
Co1—N1	2.015 (3)		
O1—Co1—O4 ⁱ	82.87 (9)	O4—Co1—N2 ⁱ	125.89 (5)
O1—Co1—N1	93.38 (11)	O4—Co1—N3 ⁱ	141.96 (6)
O1—Co1—N2	174.41 (11)	N1—Co1—N2	83.46 (11)
O1—Co1—N3	91.59 (11)	N1—Co1—N3	165.98 (11)
O4—Co1—N1 ⁱ	138.85 (4)	N2—Co1—N3	92.55 (10)

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

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

$D \cdots H$	$D—H$	$H \cdots A$	$D \cdots A$	$D—H \cdots A$
C9—H9 ⁱⁱ —O3 ⁱⁱ	0.93	2.51	3.334 (5)	148
C6—H6 ⁱⁱⁱ —O2 ⁱⁱⁱ	0.93	2.59	3.210 (5)	124

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

Data collection: *APEX2* (Bruker, 2005); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2496).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, m3144 [doi:10.1107/S1600536807060631]

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

T. Liu and J. Y. Zhu

Comment

The crystal structure of *catena*-poly[[(nitrato- κO) (1,10-phenanthroline- $\kappa^2 N,N'$)nickel(II)]- μ -acetamido- $\kappa^2 O:N$], (II), has previously been reported (Liu & Zhu, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The title compound, $[Co(NO_3)(C_2H_4NO)(C_{12}H_8N_2)]_n$, which are linked by acetamide ligands to form a chain. Each Co^{II} atom is five-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand, one nitrate O atom, and one N and one O atoms of acetamide within a bipyramidal coordination geometry (Table 1). The Co—O and Co—N bond are in the range [1.938 (2)–2.325 (2) Å] and [1.976 (3)–2.015 (3) Å], respectively (Table 1), as in (II).

In the crystal structure, no classic C—H···O hydrogen bonds (Fig. 2 and Table 2) seem to be effective in the stabilization of the structure, resulting in the formation of a polymeric ribbon structure, as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Cobalt (II) nitrate hexahydrate (291.8 mg, 1 mmol), phen (180.2 mg, 1 mmol), acetamide (59.1 mg, 1 mmol) and distilled water (8 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

The H atoms were positioned geometrically, with N—H = 0.86 Å (for NH), C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N)$, where $x = 1.2$ for aromatic and NH H atoms and $x = 1.5$ for methyl H atoms.

supplementary materials

Figures

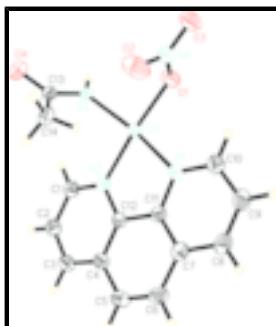


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

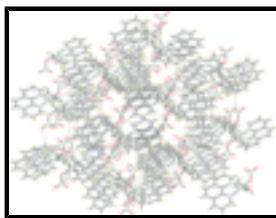


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

Crystal data

[Co(C₂H₄NO)(NO₃)(C₁₂H₈N₂)]

$M_r = 359.21$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.7208 (13)$ Å

$b = 9.220 (2)$ Å

$c = 16.9015 (16)$ Å

$\beta = 101.821 (4)^\circ$

$V = 1330.2 (4)$ Å³

$Z = 4$

$F_{000} = 732$

$D_x = 1.794 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5605 reflections

$\theta = 2.2\text{--}26.5^\circ$

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

$T = 273 (2)$ K

Prism, pink

$0.42 \times 0.24 \times 0.21$ mm

Data collection

Bruker APEXII area-detector
diffractometer

2643 independent reflections

Radiation source: fine-focus sealed tube

2273 reflections with $I > 2\sigma(I)$

Monochromator: graphite

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

$T = 273(2)$ K

$\theta_{\max} = 26.4^\circ$

φ and ω scans

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

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

$h = -10 \rightarrow 10$

$T_{\min} = 0.610, T_{\max} = 0.766$

$k = -11 \rightarrow 11$

8432 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
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.1002P)^2 + 0.5483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2643 reflections	$\Delta\rho_{\text{max}} = 0.77 \text{ e \AA}^{-3}$
209 parameters	$\Delta\rho_{\text{min}} = -0.67 \text{ e \AA}^{-3}$
1 restraint	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	0.66500 (4)	0.92784 (4)	0.80316 (2)	0.03317 (18)
O1	0.5482 (3)	1.0052 (3)	0.70200 (14)	0.0535 (6)
O2	0.3461 (4)	0.9007 (4)	0.7287 (2)	0.0839 (10)
O3	0.3289 (3)	1.0276 (4)	0.62188 (17)	0.0691 (8)
O4	0.6209 (3)	0.5051 (3)	0.74801 (16)	0.0533 (6)
N1	0.6077 (3)	1.0945 (3)	0.86858 (17)	0.0409 (6)
N2	0.7951 (3)	0.8672 (3)	0.90778 (15)	0.0395 (6)
N3	0.6876 (3)	0.7347 (3)	0.75214 (13)	0.0333 (5)
H3A	0.7415	0.7238	0.7153	0.040*
N4	0.4019 (3)	0.9773 (3)	0.68378 (16)	0.0452 (6)
C1	0.8958 (4)	0.7580 (3)	0.9239 (2)	0.0460 (7)
H1	0.9149	0.7011	0.8816	0.055*
C2	0.9727 (4)	0.7264 (4)	1.0013 (2)	0.0500 (8)
H2	1.0444	0.6507	1.0112	0.060*
C3	0.9418 (4)	0.8083 (4)	1.0634 (2)	0.0486 (8)
H3	0.9912	0.7868	1.1162	0.058*
C4	0.8364 (4)	0.9245 (3)	1.04827 (19)	0.0416 (7)

supplementary materials

C5	0.7957 (4)	1.0191 (4)	1.1082 (2)	0.0504 (8)
H5	0.8375	1.0011	1.1625	0.061*
C6	0.6979 (4)	1.1341 (4)	1.0883 (2)	0.0501 (8)
H6	0.6735	1.1922	1.1289	0.060*
C7	0.6328 (4)	1.1665 (4)	1.0065 (2)	0.0439 (7)
C8	0.5360 (4)	1.2872 (4)	0.9810 (2)	0.0528 (8)
H8	0.5089	1.3501	1.0189	0.063*
C9	0.4834 (4)	1.3110 (4)	0.9020 (2)	0.0543 (8)
H9	0.4234	1.3926	0.8843	0.065*
C10	0.5205 (4)	1.2104 (4)	0.8463 (2)	0.0500 (8)
H10	0.4820	1.2261	0.7915	0.060*
C11	0.6659 (4)	1.0733 (3)	0.94763 (19)	0.0369 (6)
C12	0.7671 (3)	0.9513 (3)	0.96847 (18)	0.0367 (6)
C13	0.6167 (3)	0.6286 (3)	0.77792 (17)	0.0338 (6)
C14	0.5446 (4)	0.6519 (3)	0.83138 (19)	0.0417 (7)
H14A	0.4401	0.6145	0.8155	0.062*
H14B	0.5404	0.7544	0.8404	0.062*
H14C	0.5966	0.6050	0.8802	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0397 (3)	0.0323 (3)	0.0261 (3)	0.00246 (14)	0.00342 (17)	0.00105 (13)
O1	0.0496 (13)	0.0638 (17)	0.0431 (12)	-0.0063 (12)	-0.0004 (10)	0.0131 (12)
O2	0.0657 (18)	0.127 (3)	0.0588 (18)	-0.0256 (18)	0.0113 (15)	0.0249 (19)
O3	0.0611 (15)	0.0756 (18)	0.0603 (17)	-0.0049 (15)	-0.0117 (13)	0.0176 (15)
O4	0.0513 (13)	0.0441 (13)	0.0650 (15)	-0.0039 (10)	0.0132 (12)	-0.0147 (12)
N1	0.0441 (13)	0.0378 (13)	0.0407 (14)	0.0014 (11)	0.0084 (11)	0.0054 (11)
N2	0.0449 (13)	0.0370 (13)	0.0361 (12)	0.0021 (11)	0.0070 (11)	-0.0014 (10)
N3	0.0414 (12)	0.0343 (12)	0.0258 (10)	-0.0032 (10)	0.0103 (9)	-0.0030 (9)
N4	0.0470 (14)	0.0451 (14)	0.0411 (14)	0.0001 (12)	0.0037 (12)	0.0015 (12)
C1	0.0523 (17)	0.0380 (16)	0.0463 (17)	0.0061 (13)	0.0068 (14)	-0.0034 (13)
C2	0.0537 (18)	0.0419 (17)	0.0506 (18)	0.0087 (14)	0.0014 (15)	0.0034 (15)
C3	0.0544 (18)	0.0463 (18)	0.0414 (16)	-0.0012 (15)	0.0012 (14)	0.0059 (14)
C4	0.0465 (16)	0.0427 (17)	0.0355 (15)	-0.0055 (13)	0.0079 (13)	0.0015 (12)
C5	0.0548 (19)	0.062 (2)	0.0354 (15)	0.0005 (17)	0.0118 (14)	-0.0014 (15)
C6	0.0589 (19)	0.054 (2)	0.0412 (16)	-0.0022 (16)	0.0193 (15)	-0.0087 (15)
C7	0.0434 (15)	0.0439 (16)	0.0469 (16)	-0.0041 (13)	0.0151 (14)	-0.0033 (14)
C8	0.0552 (19)	0.0430 (18)	0.064 (2)	0.0072 (15)	0.0210 (17)	-0.0056 (16)
C9	0.0531 (18)	0.0446 (18)	0.065 (2)	0.0118 (15)	0.0115 (16)	0.0010 (16)
C10	0.0508 (17)	0.0449 (18)	0.0524 (18)	0.0053 (15)	0.0061 (15)	0.0031 (15)
C11	0.0375 (14)	0.0353 (15)	0.0388 (15)	-0.0038 (11)	0.0098 (12)	0.0010 (11)
C12	0.0393 (14)	0.0345 (14)	0.0363 (15)	-0.0038 (11)	0.0077 (12)	0.0007 (11)
C13	0.0346 (13)	0.0304 (13)	0.0343 (14)	0.0020 (11)	0.0024 (11)	-0.0031 (11)
C14	0.0541 (17)	0.0336 (14)	0.0467 (16)	-0.0048 (13)	0.0324 (15)	-0.0056 (13)

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

Co1—O1	1.938 (2)	C3—C4	1.400 (5)
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Co1—O4 ⁱ	2.325 (2)	C3—H3	0.9300
Co1—N1	2.015 (3)	C4—C12	1.383 (4)
Co1—N2	1.976 (3)	C4—C5	1.436 (5)
Co1—N3	2.006 (2)	C5—C6	1.359 (6)
O1—N4	1.276 (4)	C5—H5	0.9300
O2—N4	1.210 (4)	C6—C7	1.414 (5)
O3—N4	1.201 (4)	C6—H6	0.9300
O4—C13	1.249 (4)	C7—C11	1.390 (4)
O4—Co1 ⁱⁱ	2.325 (2)	C7—C8	1.410 (5)
N1—C10	1.321 (4)	C8—C9	1.337 (5)
N1—C11	1.343 (4)	C8—H8	0.9300
N2—C1	1.328 (4)	C9—C10	1.406 (5)
N2—C12	1.348 (4)	C9—H9	0.9300
N3—C13	1.281 (4)	C10—H10	0.9300
N3—H3A	0.8600	C11—C12	1.428 (4)
C1—C2	1.373 (5)	C13—C14	1.221 (4)
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.363 (5)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
O1—Co1—O4 ⁱ	82.87 (9)	C3—C4—C5	125.7 (3)
O1—Co1—N1	93.38 (11)	C6—C5—C4	122.2 (3)
O1—Co1—N2	174.41 (11)	C6—C5—H5	118.9
O1—Co1—N3	91.59 (11)	C4—C5—H5	118.9
O4—Co1—N1 ⁱ	138.85 (4)	C5—C6—C7	120.9 (3)
O4—Co1—N2 ⁱ	125.89 (5)	C5—C6—H6	119.6
O4—Co1—N3 ⁱ	141.96 (6)	C7—C6—H6	119.6
N1—Co1—N2	83.46 (11)	C11—C7—C8	117.9 (3)
N1—Co1—N3	165.98 (11)	C11—C7—C6	117.9 (3)
N2—Co1—N3	92.55 (10)	C8—C7—C6	124.2 (3)
N4—O1—Co1	117.2 (2)	C9—C8—C7	119.8 (3)
C13—O4—Co1 ⁱⁱ	121.5 (2)	C9—C8—H8	120.1
C10—N1—C11	118.7 (3)	C7—C8—H8	120.1
C10—N1—Co1	130.8 (2)	C8—C9—C10	118.7 (3)
C11—N1—Co1	110.4 (2)	C8—C9—H9	120.6
C1—N2—C12	119.7 (3)	C10—C9—H9	120.6
C1—N2—Co1	129.3 (2)	N1—C10—C9	122.8 (3)
C12—N2—Co1	111.0 (2)	N1—C10—H10	118.6
C13—N3—Co1	115.79 (19)	C9—C10—H10	118.6
C13—N3—H3A	122.1	N1—C11—C7	122.0 (3)
Co1—N3—H3A	122.1	N1—C11—C12	116.7 (3)
O3—N4—O2	124.2 (3)	C7—C11—C12	121.3 (3)
O3—N4—O1	117.3 (3)	N2—C12—C4	121.9 (3)
O2—N4—O1	118.5 (3)	N2—C12—C11	117.7 (3)
N2—C1—C2	122.0 (3)	C4—C12—C11	120.4 (3)
N2—C1—H1	119.0	C14—C13—O4	121.5 (3)
C2—C1—H1	119.0	C14—C13—N3	118.4 (3)
C3—C2—C1	118.7 (3)	O4—C13—N3	120.1 (3)

supplementary materials

C3—C2—H2	120.6	C13—C14—H14A	109.5
C1—C2—H2	120.6	C13—C14—H14B	109.5
C2—C3—C4	120.6 (3)	H14A—C14—H14B	109.5
C2—C3—H3	119.7	C13—C14—H14C	109.5
C4—C3—H3	119.7	H14A—C14—H14C	109.5
C12—C4—C3	117.0 (3)	H14B—C14—H14C	109.5
C12—C4—C5	117.2 (3)		

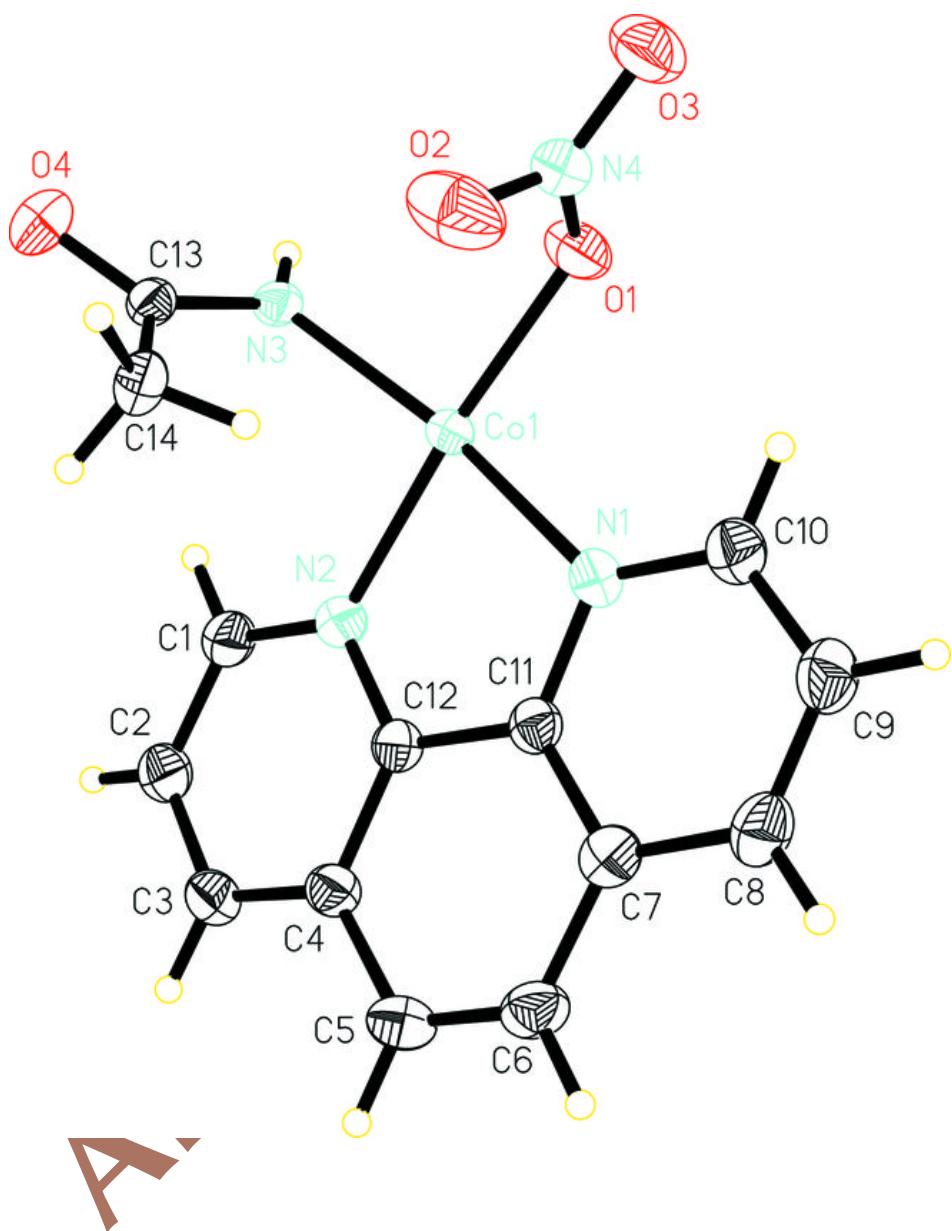
Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

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

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
C9—H9 \cdots O3 ⁱⁱⁱ	0.93	2.51	3.334 (5)	148
C6—H6 \cdots O2 ^{iv}	0.93	2.59	3.210 (5)	124

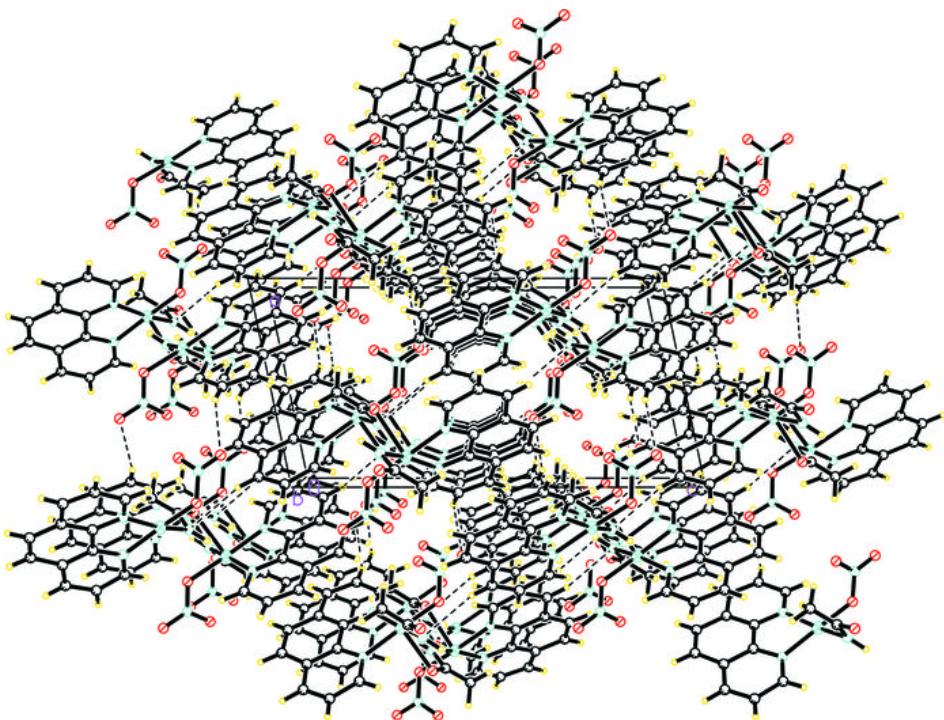
Symmetry codes: (iii) $-x+1/2, y+1/2, -z+3/2$; (iv) $-x+1, -y+2, -z+2$.

Fig. 1



supplementary materials

Fig. 2



Article re-