

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

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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-Quinololinol-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	METQIM
<i>(8-Quinololinol-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>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITPCOO1
<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)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

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

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

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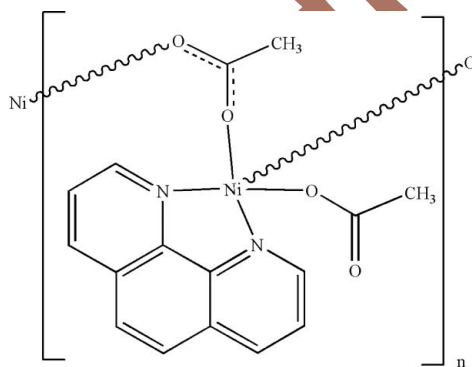
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.040; wR factor = 0.119; data-to-parameter ratio = 12.2.

In the polymeric title complex, $[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)]_n$, Ni^{II} ions are bridged by single *syn-anti* acetate ligands. Each Ni atom is five-coordinated by two 1,10-phenanthroline N atoms and three O atoms of acetate ligands in a distorted square-pyramidal coordination geometry. In the crystal structure, $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds result in the formation of a polymeric ribbon structure.

Related literature

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



Experimental

Crystal data

$[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)]$
 $M_r = 357.00$
Monoclinic, $P2_1/n$
 $a = 8.6901$ (16) Å
 $b = 9.2108$ (11) Å
 $c = 16.9013$ (12) Å
 $\beta = 102.009$ (2)°

$V = 1323.2$ (3) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.49$ mm⁻¹
 $T = 273$ (2) K
 $0.41 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.634$, $T_{\text{max}} = 0.750$
8148 measured reflections
2565 independent reflections
2201 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.119$
 $S = 0.99$
2565 reflections
210 parameters
2 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	2.004 (2)	Ni1—N1	2.005 (3)
Ni1—O2	1.933 (2)	Ni1—N2	1.976 (2)
Ni1—O4 ⁱ	2.319 (2)		
O1—Ni1—O2	91.46 (10)	O2—Ni1—N1	93.55 (11)
O1—Ni1—O4 ⁱ	87.15 (9)	O2—Ni1—N2	174.38 (11)
O2—Ni1—O4 ⁱ	82.54 (9)	O4—Ni1—N1 ⁱ	138.82 (4)
O1—Ni1—N1	166.01 (10)	O4—Ni1—N2 ⁱ	125.88 (5)
O1—Ni1—N2	92.61 (10)	N1—Ni1—N2	83.38 (10)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}3^{\text{ii}}$	0.93	2.51	3.332 (5)	149
$\text{C}10-\text{H}10\cdots\text{O}2^{\text{iii}}$	0.93	2.35	3.259 (4)	163

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2379).

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supplementary materials

Article retracted

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***catena*-Poly[[*(acetato-κO)*(1,10-phenanthroline- κ^2N,N')nickel(II)]- μ -*acetato-κ²O:O'*]**

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

Comment

The crystal structure of *catena*-Poly[[*(acetato-κO)*(1,10-phenanthroline- κ^2N,N')cobalt(II)]- μ -*acetato-κ²O:O'*], (II), has previously been reported (Zhong *et al.*, 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). It is a polymeric complex involving bridging of Ni^{II} ions by single *syn-anti* acetate ligands. Each Ni atom is five-coordinated by two 1,10-phenanthroline (phen) N atoms and three O atoms of acetate ligands in a distorted square-pyramidal coordination geometry. The Ni—O and Ni—N bonds are in the range of [1.933 (2)–2.319 (2) Å] and [1.976 (2)–2.005 (3) Å], respectively (Table 1), as in (II).

In the crystal structure, C—H \cdots O hydrogen bonds (Table 2, Fig. 2) result 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. Nickel (II) nitrate hexahydrate (295.6 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 green 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 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 $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms.

Figures

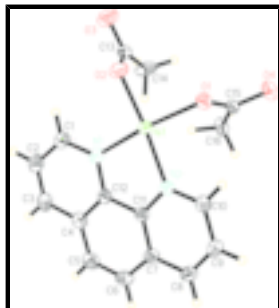


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

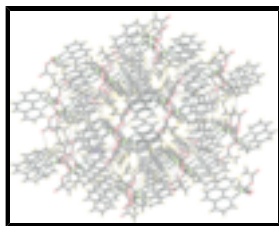


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

Crystal data

[Ni(C₂H₃O₂)₂(C₁₂H₈N₂)]

$M_r = 357.00$

Monoclinic, $P2_1/n$

Hall symbol: -p 2yn

$a = 8.6901$ (16) Å

$b = 9.2108$ (11) Å

$c = 16.9013$ (12) Å

$\beta = 102.009$ (2)°

$V = 1323.2$ (3) Å³

$Z = 4$

$F_{000} = 736$

$D_x = 1.792$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5583 reflections

$\theta = 2.3$ – 27.2 °

$\mu = 1.49$ mm⁻¹

$T = 273$ (2) K

Prism, green

$0.41 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

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

$T_{\min} = 0.634$, $T_{\max} = 0.750$

8148 measured reflections

2565 independent reflections

2201 reflections with $I > 2\sigma(I)$

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

$\theta_{\text{max}} = 26.3$ °

$\theta_{\text{min}} = 2.5$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -21 \rightarrow 21$

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
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2 + 1.1936P]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
2565 reflections	$(\Delta/\sigma)_{\max} = 0.001$
210 parameters	$\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.66500 (4)	0.92790 (4)	0.80317 (2)	0.03410 (17)
O1	0.6879 (3)	0.7349 (2)	0.75205 (12)	0.0429 (5)
O2	0.5482 (3)	1.0050 (3)	0.70200 (13)	0.0513 (6)
O3	0.3284 (3)	1.0286 (4)	0.62163 (17)	0.0680 (8)
O4	0.6213 (3)	0.5048 (3)	0.74825 (15)	0.0504 (6)
N1	0.6078 (3)	1.0936 (3)	0.86839 (16)	0.0389 (6)
N2	0.7958 (3)	0.8672 (3)	0.90797 (14)	0.0374 (5)
C1	0.5196 (4)	1.2113 (4)	0.8470 (2)	0.0470 (7)
H1	0.4802	1.2276	0.7922	0.056*
C2	0.4836 (4)	1.3104 (4)	0.9017 (2)	0.0524 (8)
H2	0.4229	1.3916	0.8836	0.063*
C3	0.5369 (4)	1.2885 (4)	0.9811 (2)	0.0504 (8)
H3	0.5113	1.3529	1.0188	0.060*
C4	0.6327 (4)	1.1660 (4)	1.00686 (19)	0.0409 (7)
C5	0.6983 (4)	1.1338 (4)	1.0880 (2)	0.0486 (8)
H5	0.6750	1.1926	1.1287	0.058*
C6	0.7948 (4)	1.0185 (4)	1.10778 (19)	0.0474 (8)

supplementary materials

H6	0.8355	0.9993	1.1621	0.057*
C7	0.8364 (4)	0.9251 (3)	1.04826 (19)	0.0396 (7)
C8	0.9429 (4)	0.8077 (4)	1.06368 (19)	0.0454 (7)
H8	0.9932	0.7865	1.1165	0.055*
C9	0.9724 (4)	0.7257 (4)	1.0018 (2)	0.0478 (8)
H9	1.0433	0.6489	1.0118	0.057*
C10	0.8956 (4)	0.7578 (4)	0.92392 (19)	0.0442 (7)
H10	0.9146	0.7009	0.8815	0.053*
C11	0.7674 (3)	0.9513 (3)	0.96839 (17)	0.0346 (6)
C12	0.6652 (3)	1.0726 (3)	0.94744 (18)	0.0345 (6)
C13	0.4031 (3)	0.9781 (3)	0.68378 (16)	0.0338 (6)
C14	0.3459 (4)	0.9000 (5)	0.7292 (2)	0.0539 (10)
H14A	0.2383	0.9274	0.7266	0.081*
H14B	0.4044	0.9112	0.7837	0.081*
H14C	0.3502	0.8006	0.7128	0.081*
C15	0.6165 (3)	0.6289 (3)	0.77794 (17)	0.0318 (6)
C16	0.5458 (4)	0.6523 (3)	0.83168 (19)	0.0408 (7)
H16A	0.4439	0.6077	0.8183	0.061*
H16B	0.5341	0.7551	0.8376	0.061*
H16C	0.6038	0.6125	0.8815	0.061*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0405 (2)	0.0333 (2)	0.0270 (2)	0.00251 (14)	0.00368 (16)	0.00088 (13)
O1	0.0530 (12)	0.0407 (12)	0.0356 (10)	-0.0038 (10)	0.0102 (9)	-0.0024 (9)
O2	0.0493 (13)	0.0601 (16)	0.0404 (12)	-0.0058 (11)	-0.0002 (10)	0.0118 (11)
O3	0.0587 (15)	0.0760 (18)	0.0595 (16)	-0.0063 (14)	-0.0102 (13)	0.0185 (15)
O4	0.0505 (13)	0.0402 (13)	0.0611 (14)	-0.0044 (10)	0.0132 (11)	-0.0145 (11)
N1	0.0410 (13)	0.0357 (13)	0.0397 (13)	0.0024 (10)	0.0077 (11)	0.0044 (10)
N2	0.0437 (13)	0.0343 (13)	0.0337 (12)	0.0025 (11)	0.0067 (10)	-0.0015 (10)
C1	0.0494 (17)	0.0427 (17)	0.0473 (17)	0.0057 (14)	0.0067 (14)	0.0059 (15)
C2	0.0504 (18)	0.0424 (18)	0.064 (2)	0.0127 (15)	0.0110 (16)	0.0045 (16)
C3	0.0515 (18)	0.0421 (18)	0.061 (2)	0.0077 (15)	0.0201 (16)	-0.0044 (16)
C4	0.0409 (15)	0.0408 (16)	0.0438 (15)	-0.0033 (13)	0.0155 (13)	-0.0034 (13)
C5	0.0562 (19)	0.053 (2)	0.0404 (16)	-0.0026 (16)	0.0185 (15)	-0.0092 (15)
C6	0.0526 (18)	0.057 (2)	0.0325 (15)	-0.0004 (16)	0.0093 (14)	-0.0018 (14)
C7	0.0442 (16)	0.0404 (16)	0.0340 (14)	-0.0041 (12)	0.0076 (13)	0.0027 (12)
C8	0.0500 (17)	0.0468 (18)	0.0364 (15)	0.0005 (14)	0.0019 (13)	0.0068 (13)
C9	0.0511 (18)	0.0390 (17)	0.0498 (17)	0.0088 (14)	0.0023 (14)	0.0032 (14)
C10	0.0496 (17)	0.0378 (16)	0.0434 (16)	0.0067 (13)	0.0055 (14)	-0.0038 (13)
C11	0.0388 (14)	0.0322 (14)	0.0332 (14)	-0.0040 (11)	0.0087 (12)	-0.0006 (11)
C12	0.0360 (14)	0.0329 (14)	0.0355 (14)	-0.0030 (11)	0.0092 (12)	0.0021 (11)
C13	0.0340 (13)	0.0343 (13)	0.0300 (13)	0.0001 (12)	-0.0005 (11)	-0.0001 (11)
C14	0.0401 (16)	0.088 (3)	0.0335 (16)	-0.0182 (17)	0.0074 (13)	0.0195 (17)
C15	0.0320 (12)	0.0298 (13)	0.0322 (13)	0.0007 (11)	0.0036 (11)	-0.0024 (11)
C16	0.0542 (17)	0.0318 (14)	0.0473 (16)	-0.0047 (13)	0.0355 (15)	-0.0054 (13)

Geometric parameters (Å, °)

Ni1—O1	2.004 (2)	C4—C5	1.403 (5)
Ni1—O2	1.933 (2)	C5—C6	1.352 (5)
Ni1—O4 ⁱ	2.319 (2)	C5—H5	0.9300
Ni1—N1	2.005 (3)	C6—C7	1.426 (5)
Ni1—N2	1.976 (2)	C6—H6	0.9300
O1—C15	1.282 (4)	C7—C11	1.379 (4)
O2—C13	1.259 (4)	C7—C8	1.412 (5)
O3—C13	1.207 (4)	C8—C9	1.357 (5)
O4—C15	1.253 (4)	C8—H8	0.9300
O4—Ni1 ⁱⁱ	2.319 (2)	C9—C10	1.379 (5)
N1—C1	1.333 (4)	C9—H9	0.9300
N1—C12	1.339 (4)	C10—H10	0.9300
N2—C10	1.320 (4)	C11—C12	1.426 (4)
N2—C11	1.344 (4)	C13—C14	1.230 (4)
C1—C2	1.381 (5)	C14—H14A	0.9600
C1—H1	0.9300	C14—H14B	0.9600
C2—C3	1.341 (5)	C14—H14C	0.9600
C2—H2	0.9300	C15—C16	1.217 (4)
C3—C4	1.416 (5)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C12	1.395 (4)	C16—H16C	0.9600
O1—Ni1—O2	91.46 (10)	C11—C7—C8	116.7 (3)
O1—Ni1—O4 ⁱ	87.15 (9)	C11—C7—C6	117.6 (3)
O2—Ni1—O4 ⁱ	82.54 (9)	C8—C7—C6	125.8 (3)
O1—Ni1—N1	166.01 (10)	C9—C8—C7	120.4 (3)
O1—Ni1—N2	92.61 (10)	C9—C8—H8	119.8
O2—Ni1—N1	93.55 (11)	C7—C8—H8	119.8
O2—Ni1—N2	174.38 (11)	C8—C9—C10	119.0 (3)
O4—Ni1—N1 ⁱ	138.82 (4)	C8—C9—H9	120.5
O4—Ni1—N2 ⁱ	125.88 (5)	C10—C9—H9	120.5
N1—Ni1—N2	83.38 (10)	N2—C10—C9	121.7 (3)
C15—O1—Ni1	115.48 (18)	N2—C10—H10	119.1
C13—O2—Ni1	117.3 (2)	C9—C10—H10	119.1
C15—O4—Ni1 ⁱⁱ	121.65 (19)	N2—C11—C7	122.1 (3)
C1—N1—C12	117.5 (3)	N2—C11—C12	117.8 (3)
C1—N1—Ni1	131.6 (2)	C7—C11—C12	120.1 (3)
C12—N1—Ni1	110.76 (19)	N1—C12—C4	122.7 (3)
C10—N2—C11	120.1 (3)	N1—C12—C11	116.4 (3)
C10—N2—Ni1	129.0 (2)	C4—C12—C11	120.9 (3)
C11—N2—Ni1	110.8 (2)	O3—C13—C14	123.7 (3)
N1—C1—C2	123.6 (3)	O3—C13—O2	117.9 (3)
N1—C1—H1	118.2	C14—C13—O2	118.5 (3)
C2—C1—H1	118.2	C13—C14—H14A	109.5
C3—C2—C1	119.5 (3)	C13—C14—H14B	109.5

supplementary materials

C3—C2—H2	120.3	H14A—C14—H14B	109.5
C1—C2—H2	120.3	C13—C14—H14C	109.5
C2—C3—C4	119.0 (3)	H14A—C14—H14C	109.5
C2—C3—H3	120.5	H14B—C14—H14C	109.5
C4—C3—H3	120.5	C16—C15—O4	121.6 (3)
C12—C4—C5	118.1 (3)	C16—C15—O1	118.4 (3)
C12—C4—C3	117.7 (3)	O4—C15—O1	120.0 (3)
C5—C4—C3	124.2 (3)	C15—C16—H16A	109.5
C6—C5—C4	120.8 (3)	C15—C16—H16B	109.5
C6—C5—H5	119.6	H16A—C16—H16B	109.5
C4—C5—H5	119.6	C15—C16—H16C	109.5
C5—C6—C7	122.3 (3)	H16A—C16—H16C	109.5
C5—C6—H6	118.8	H16B—C16—H16C	109.5
C7—C6—H6	118.8		

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

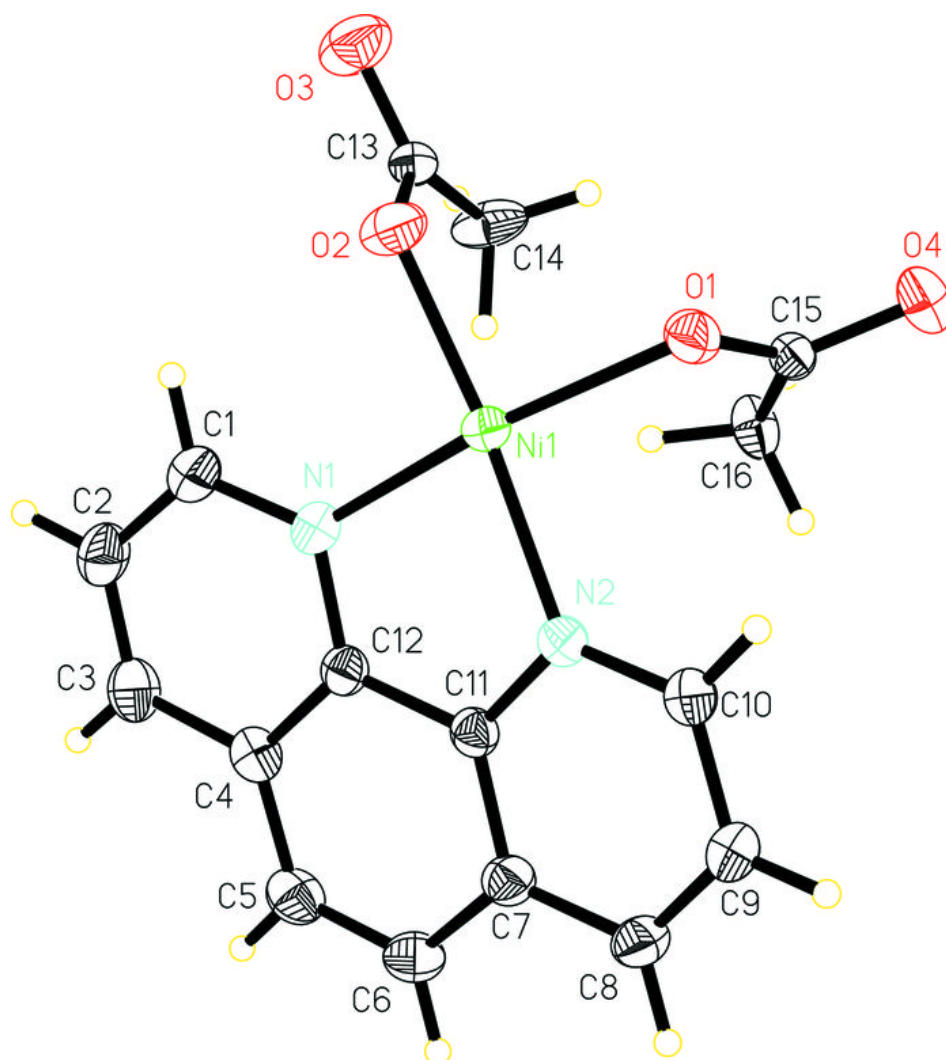
Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O3 ⁱⁱⁱ	0.93	2.51	3.332 (5)	149
C10—H10 \cdots O2 ⁱⁱ	0.93	2.35	3.259 (4)	163

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

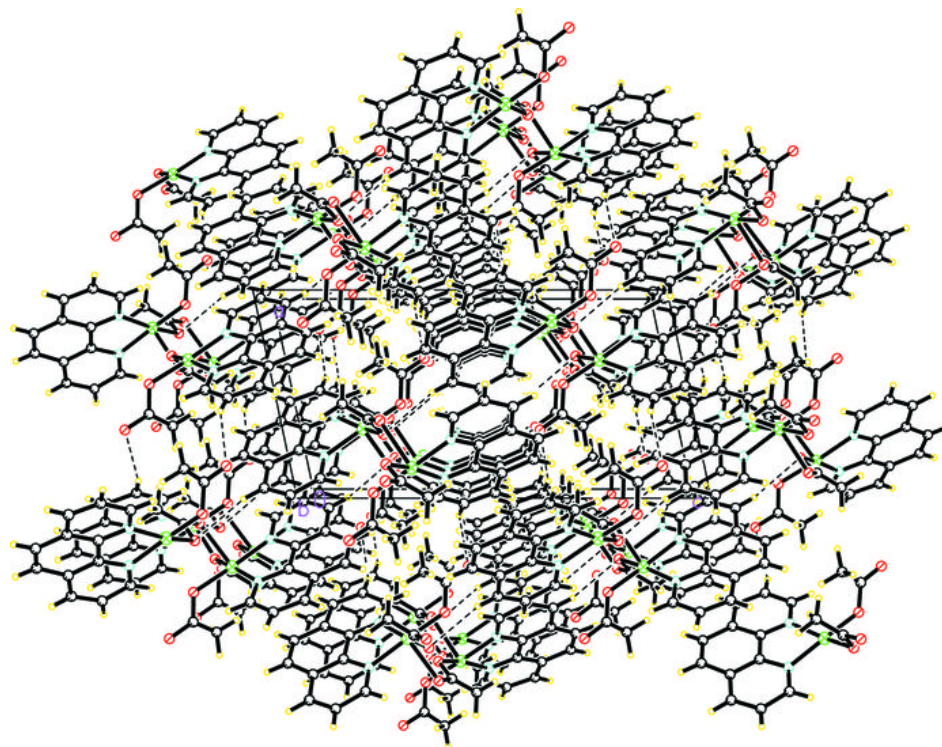
Article retracted

Fig. 1



Arc

Fig. 2



Article re