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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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

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Table 1 (continued)

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

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

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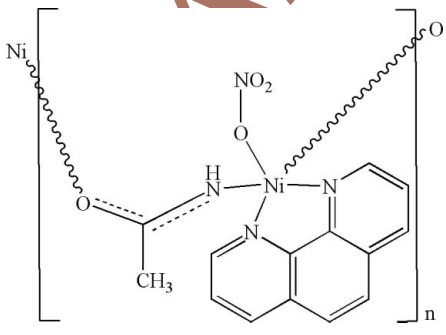
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.123; data-to-parameter ratio = 12.7.

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

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); Wu *et al.* (2003); Pan & Xu (2004); Liu *et al.* (2004); Li *et al.* (2005); Harrop *et al.* (2003); Qi, Ma *et al.* (2003); Qi, Qiu *et al.* (2003); Rauko *et al.* (2001); Foster *et al.* (1999); Zhou *et al.* (1999). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Ni(C_2H_4NO)(NO_3)(C_{12}H_8N_2)]$
M_r = 358.99
Monoclinic, $P2_1/n$
a = 8.7113 (11) Å
b = 9.2019 (14) Å
c = 16.9102 (16) Å
β = 102.104 (6)°
V = 1325.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 273 (2) K
0.40 × 0.25 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.584, T_{max} = 0.751
8403 measured reflections
2653 independent reflections
2273 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.123
S = 1.01
2653 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.933 (2)	Ni1—N2	1.971 (2)
Ni1—O4^{i}	2.329 (2)	Ni1—N3	2.003 (2)
Ni1—N1	2.010 (2)		
O1—Ni1—O4^{i}	82.63 (9)	O4—Ni1—N2^{i}	125.85 (4)
O1—Ni1—N1	93.54 (10)	O4—Ni1—N3^{i}	141.92 (5)
O1—Ni1—N2	174.49 (10)	N1—Ni1—N2	83.31 (10)
O1—Ni1—N3	91.54 (10)	N1—Ni1—N3	165.94 (10)
O4—Ni1—N1^{i}	138.78 (4)	N2—Ni1—N3	92.56 (9)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{ii}	0.93	2.50	3.323 (4)	148
C5—H5···O2^{iii}	0.93	2.60	3.215 (4)	125

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: AT2467).

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Article retracted

supplementary materials

Article retracted

Acta Cryst. (2007). E**63**, m2977-m2978 [**doi:10.1107/S1600536807056504**]

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

T. Liu and J.-Y. Zhu

Article retracted

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, 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, acyl groups compounds are also a good ligand with excellent coordination capability to generate mono-, bi- or trinuclear complexes, which are commonly used as precursors for the formation of supramolecular architectures (Harrop *et al.*, 2003; Qi, Ma *et al.*, 2003; Qi, Qiu *et al.*, 2003; Rauko *et al.*, 2001; Foster *et al.*, 1999; Zhou *et al.*, 1999). 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). The title compound, $[Ni_2(NO_3)_2(C_2H_4NO)_2(C_{12}H_8N_2)_2]_n$, which are bridged by two bidentate acetamido groups with an inversion centre between the two Ni^{II} ions. Each Ni atom is five-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand, one O atom of NO_3^- and one N and one O atoms of acetamido ligands (Table 1). The Ni—O bond lengths are in the range 1.933 (2) to 2.329 (2) Å. The Ni—N bond lengths are in the range 1.971 (2) to 2.010 (2) Å.

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.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Nickel (II) nitrate hexahydrate (290.8 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 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 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 imino H atoms, and $x = 1.5$ for methyl H atoms.

Figures

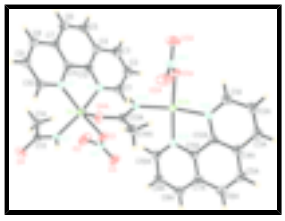

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2$, $y + 1/2$, $-z + 1/2$].

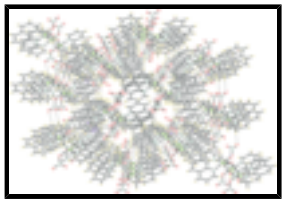

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Article retracted

catena-Poly[[(nitrato-κ*O*)(1,10-phenanthroline- κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]

Crystal data

$[Ni(C_2H_4NO)(NO_3)(C_{12}H_8N_2)]$	F_{000} = 736
M_r = 358.99	D_x = 1.799 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5602 reflections
a = 8.7113 (11) Å	θ = 2.2–27.5°
b = 9.2019 (14) Å	μ = 1.49 mm^{-1}
c = 16.9102 (16) Å	T = 273 (2) K
β = 102.104 (6)°	Prism, green
V = 1325.4 (3) Å^3	0.40 × 0.25 × 0.20 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	2653 independent reflections
Radiation source: fine-focus sealed tube	2273 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 273(2) K	θ_{max} = 26.5°
φ and ω scans	θ_{min} = 2.5°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→10
T_{min} = 0.584, T_{max} = 0.751	k = −11→11
8403 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.123$

$S = 1.01$

2653 reflections

209 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0915P)^2 + 0.5483P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.72$ e Å^{-3}

$\Delta\rho_{min} = -0.61$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.66504 (4)	0.92789 (4)	0.803171 (18)	0.03382 (16)
O1	0.5482 (3)	1.0052 (3)	0.70208 (12)	0.0503 (5)
O2	0.3465 (3)	0.9000 (4)	0.72889 (18)	0.0803 (9)
O3	0.3287 (3)	1.0276 (3)	0.62167 (16)	0.0662 (7)
O4	0.6208 (2)	0.5051 (2)	0.74830 (14)	0.0499 (5)
N1	0.6079 (3)	1.0940 (3)	0.86863 (15)	0.0383 (5)
N2	0.7950 (3)	0.8670 (3)	0.90780 (13)	0.0365 (5)
N3	0.6878 (3)	0.7348 (2)	0.75215 (12)	0.0306 (4)
H3A	0.7418	0.7239	0.7154	0.037*
N4	0.4024 (3)	0.9773 (3)	0.68400 (15)	0.0432 (5)
C1	0.5205 (4)	1.2104 (3)	0.8465 (2)	0.0473 (7)
H1	0.4819	1.2262	0.7916	0.057*
C2	0.4830 (4)	1.3112 (4)	0.9018 (2)	0.0507 (7)
H2	0.4224	1.3926	0.8839	0.061*
C3	0.5365 (4)	1.2877 (4)	0.9809 (2)	0.0507 (7)
H3	0.5101	1.3511	1.0188	0.061*
C4	0.6330 (3)	1.1665 (3)	1.00661 (18)	0.0412 (6)
C5	0.6981 (4)	1.1344 (4)	1.08803 (18)	0.0473 (7)
H5	0.6737	1.1926	1.1286	0.057*
C6	0.7960 (4)	1.0193 (4)	1.10811 (18)	0.0471 (7)
H6	0.8382	1.0012	1.1624	0.057*
C7	0.8363 (4)	0.9252 (3)	1.04826 (18)	0.0392 (6)

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C8	0.9426 (4)	0.8077 (3)	1.06353 (18)	0.0458 (7)
H8	0.9926	0.7861	1.1164	0.055*
C9	0.9724 (4)	0.7260 (4)	1.00158 (19)	0.0475 (7)
H9	1.0437	0.6496	1.0116	0.057*
C10	0.8958 (4)	0.7578 (3)	0.92384 (19)	0.0440 (7)
H10	0.9152	0.7011	0.8815	0.053*
C11	0.7672 (3)	0.9512 (3)	0.96844 (17)	0.0342 (5)
C12	0.6655 (3)	1.0728 (3)	0.94748 (17)	0.0345 (6)
C13	0.6164 (3)	0.6283 (3)	0.77801 (15)	0.0318 (5)
C14	0.5451 (3)	0.6523 (3)	0.83137 (18)	0.0402 (6)
H14A	0.4509	0.5950	0.8223	0.060*
H14B	0.5184	0.7535	0.8311	0.060*
H14C	0.6099	0.6272	0.8828	0.060*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0402 (2)	0.0328 (2)	0.0268 (2)	0.00247 (13)	0.00345 (15)	0.00109 (12)
O1	0.0468 (11)	0.0589 (15)	0.0406 (11)	−0.0053 (10)	−0.0012 (9)	0.0129 (10)
O2	0.0612 (16)	0.123 (3)	0.0568 (16)	−0.0217 (16)	0.0122 (13)	0.0270 (17)
O3	0.0586 (14)	0.0730 (16)	0.0565 (15)	−0.0050 (13)	−0.0119 (12)	0.0174 (14)
O4	0.0491 (12)	0.0397 (12)	0.0611 (13)	−0.0040 (9)	0.0118 (10)	−0.0149 (10)
N1	0.0407 (12)	0.0358 (12)	0.0381 (12)	0.0003 (10)	0.0076 (10)	0.0046 (10)
N2	0.0416 (11)	0.0331 (11)	0.0338 (11)	0.0020 (10)	0.0057 (9)	−0.0012 (9)
N3	0.0389 (10)	0.0301 (10)	0.0241 (9)	−0.0035 (9)	0.0094 (8)	−0.0030 (8)
N4	0.0445 (13)	0.0420 (13)	0.0404 (12)	0.0002 (11)	0.0031 (11)	0.0008 (11)
C1	0.0482 (15)	0.0421 (16)	0.0492 (16)	0.0060 (13)	0.0048 (13)	0.0042 (14)
C2	0.0505 (16)	0.0422 (16)	0.0593 (19)	0.0120 (13)	0.0117 (14)	0.0027 (14)
C3	0.0517 (17)	0.0417 (16)	0.0623 (19)	0.0074 (13)	0.0206 (15)	−0.0058 (14)
C4	0.0421 (14)	0.0404 (14)	0.0440 (14)	−0.0034 (12)	0.0157 (12)	−0.0036 (12)
C5	0.0546 (17)	0.0525 (18)	0.0384 (14)	−0.0026 (15)	0.0182 (13)	−0.0088 (13)
C6	0.0522 (16)	0.0567 (18)	0.0330 (14)	0.0000 (15)	0.0103 (13)	−0.0016 (13)
C7	0.0439 (14)	0.0406 (15)	0.0330 (13)	−0.0042 (11)	0.0079 (12)	0.0025 (11)
C8	0.0513 (16)	0.0444 (16)	0.0385 (14)	0.0007 (13)	0.0017 (12)	0.0063 (13)
C9	0.0517 (16)	0.0387 (15)	0.0479 (16)	0.0088 (13)	0.0008 (13)	0.0038 (13)
C10	0.0506 (15)	0.0361 (14)	0.0433 (15)	0.0063 (12)	0.0052 (13)	−0.0045 (12)
C11	0.0375 (13)	0.0319 (13)	0.0334 (13)	−0.0029 (10)	0.0076 (11)	0.0008 (10)
C12	0.0359 (13)	0.0323 (13)	0.0363 (13)	−0.0031 (10)	0.0095 (11)	0.0016 (10)
C13	0.0319 (11)	0.0303 (12)	0.0312 (12)	0.0021 (10)	0.0020 (10)	−0.0028 (10)
C14	0.0523 (15)	0.0325 (13)	0.0456 (14)	−0.0044 (12)	0.0328 (13)	−0.0053 (11)

Geometric parameters (Å, °)

Ni1—O1	1.933 (2)	C3—C4	1.409 (5)
Ni1—O4^{i}	2.329 (2)	C3—H3	0.9300
Ni1—N1	2.010 (2)	C4—C12	1.394 (4)
Ni1—N2	1.971 (2)	C4—C5	1.406 (4)
Ni1—N3	2.003 (2)	C5—C6	1.357 (5)

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O1—N4	1.269 (3)	C5—H5	0.9300
O2—N4	1.214 (4)	C6—C7	1.431 (4)
O3—N4	1.206 (4)	C6—H6	0.9300
O4—C13	1.244 (3)	C7—C11	1.378 (4)
O4—Ni1^{ii}	2.329 (2)	C7—C8	1.412 (4)
N1—C1	1.322 (4)	C8—C9	1.358 (5)
N1—C12	1.337 (4)	C8—H8	0.9300
N2—C10	1.325 (4)	C9—C10	1.375 (4)
N2—C11	1.346 (4)	C9—H9	0.9300
N3—C13	1.286 (4)	C10—H10	0.9300
N3—H3A	0.8600	C11—C12	1.426 (4)
C1—C2	1.404 (5)	C13—C14	1.218 (4)
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.339 (5)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
O1—Ni1—O4^{i}	82.63 (9)	C5—C4—C3	124.1 (3)
O1—Ni1—N1	93.54 (10)	C6—C5—C4	120.8 (3)
O1—Ni1—N2	174.49 (10)	C6—C5—H5	119.6
O1—Ni1—N3	91.54 (10)	C4—C5—H5	119.6
O4—Ni1—N1^{i}	138.78 (4)	C5—C6—C7	122.0 (3)
O4—Ni1—N2^{i}	125.85 (4)	C5—C6—H6	119.0
O4—Ni1—N3^{i}	141.92 (5)	C7—C6—H6	119.0
N1—Ni1—N2	83.31 (10)	C11—C7—C8	116.5 (3)
N1—Ni1—N3	165.94 (10)	C11—C7—C6	117.8 (3)
N2—Ni1—N3	92.56 (9)	C8—C7—C6	125.7 (3)
N4—O1—Ni1	116.96 (18)	C9—C8—C7	120.5 (3)
C13—O4—Ni1^{ii}	121.59 (18)	C9—C8—H8	119.8
C1—N1—C12	118.3 (3)	C7—C8—H8	119.8
C1—N1—Ni1	130.9 (2)	C8—C9—C10	119.1 (3)
C12—N1—Ni1	110.71 (18)	C8—C9—H9	120.4
C10—N2—C11	119.8 (2)	C10—C9—H9	120.4
C10—N2—Ni1	129.1 (2)	N2—C10—C9	121.7 (3)
C11—N2—Ni1	111.07 (18)	N2—C10—H10	119.2
C13—N3—Ni1	115.54 (17)	C9—C10—H10	119.2
C13—N3—H3A	122.2	N2—C11—C7	122.3 (3)
Ni1—N3—H3A	122.2	N2—C11—C12	117.6 (2)
O3—N4—O2	124.1 (3)	C7—C11—C12	120.0 (3)
O3—N4—O1	117.1 (3)	N1—C12—C4	122.4 (3)
O2—N4—O1	118.7 (3)	N1—C12—C11	116.5 (2)
N1—C1—C2	123.1 (3)	C4—C12—C11	121.1 (3)
N1—C1—H1	118.4	C14—C13—O4	121.9 (3)
C2—C1—H1	118.4	C14—C13—N3	118.1 (3)
C3—C2—C1	118.6 (3)	O4—C13—N3	120.0 (2)
C3—C2—H2	120.7	C13—C14—H14A	109.5
C1—C2—H2	120.7	C13—C14—H14B	109.5
C2—C3—C4	119.7 (3)	H14A—C14—H14B	109.5
C2—C3—H3	120.1	C13—C14—H14C	109.5

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C4—C3—H3	120.1	H14A—C14—H14C	109.5
C12—C4—C5	118.1 (3)	H14B—C14—H14C	109.5
C12—C4—C3	117.8 (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 (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{iii}	0.93	2.50	3.323 (4)	148
C5—H5···O2^{iv}	0.93	2.60	3.215 (4)	125

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

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Fig. 1

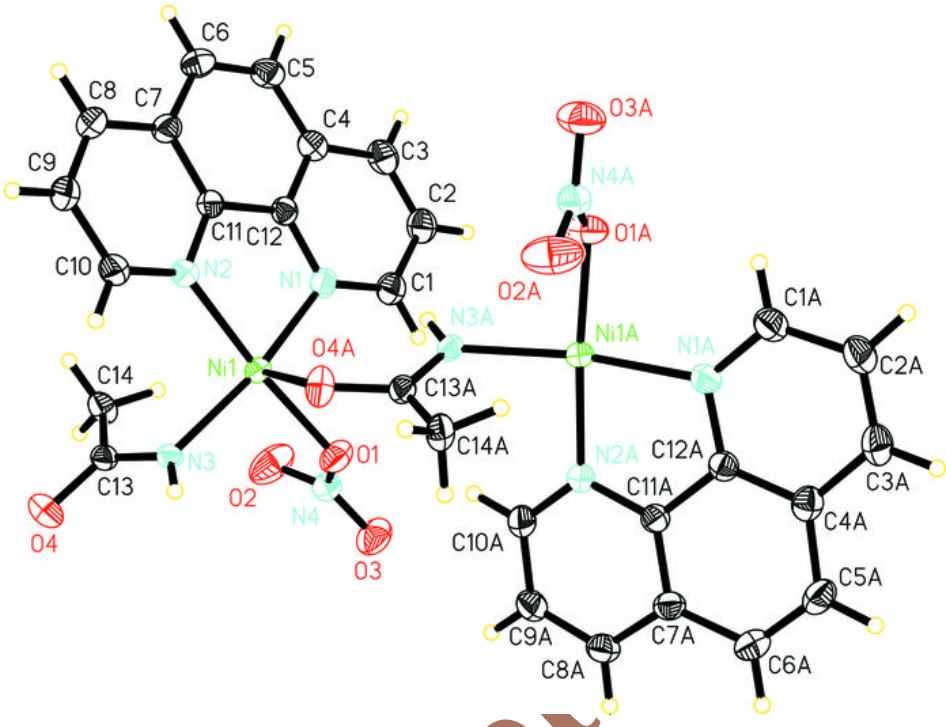

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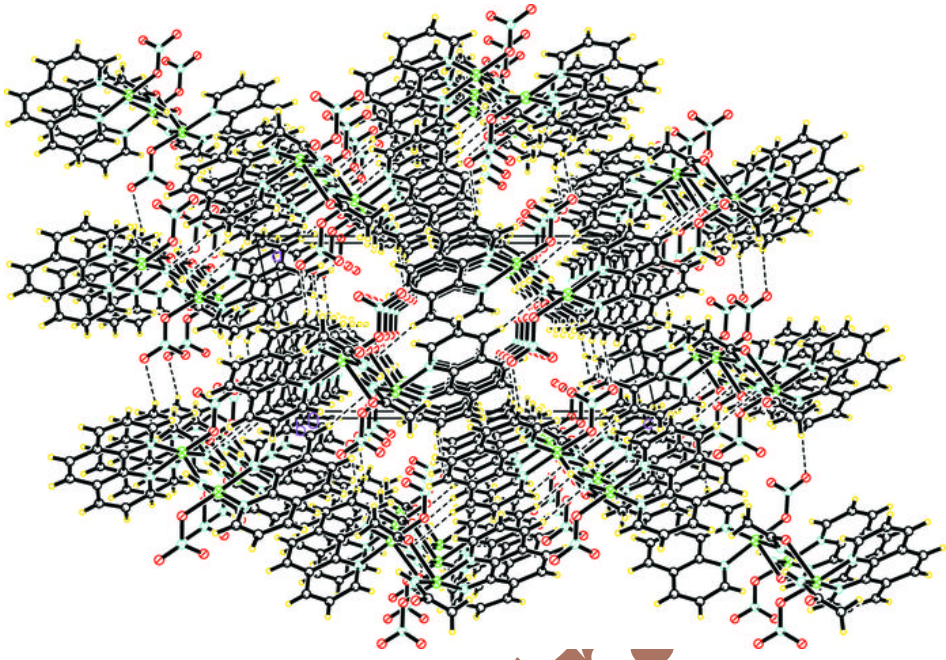
Fig. 2



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