

Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. 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>Poly[diacquadi-μ_3-malonato-μ-pyrazine-dinickel(II)] catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]</i>	Liu <i>et al.</i> (2005) Liu <i>et al.</i> (2006)	10.1107/S1600536805026358 10.1107/S1600536806038141	GATWAA FONCUH03
<i>Poly[[[μ_4-4,4'-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)-dipalladium(II)] dihydrate]</i>	Li, Wang, Zhang & Yu (2007e)	10.1107/S1600536807039050	AFELAZ
<i>Poly[diacqua-μ_3-malonato-μ-pyrazine-diiron(II)]</i>	Li, Liu <i>et al.</i> (2007)	10.1107/S1600536807038743	AFELON
<i>Poly[diacqua-di-μ_3-malonato-μ-pyrazine-dimanganese(II)]</i>	Li, Wang, Zhang & Yu (2007f)	10.1107/S1600536807039773	VIJZAO
<i>Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]</i>	Li, Wang, Zhang & Yu (2007g)	10.1107/S1600536807040275	VIKIC
<i>catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]</i>	Li, Wang, Zhang & Yu (2007a)	10.1107/S1600536807041657	DILGEL
<i>catena-Poly[[[2,2'-bipyridine-κ^2N,N']iron(II)]-μ-5-carboxy-4-carboxylatoimidazol-1-ido-κ^4N³,O⁴:N¹,O²]</i>	Li, Wang, Zhang & Yu (2007h)	10.1107/S1600536807042122	XIKWAO
<i>Poly[[aqua(2,2'-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]</i>	Li, Wang, Zhang & Yu (2007b)	10.1107/S1600536807046466	LEVZAO01
<i>2-(Benzyliminomethyl)-6-methoxyphenol</i>	Li, Wang, Zhang & Yu (2007i)	10.1107/S1600536807042134	SILDEX
<i>Poly[aqua(2,2'-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]</i>	Li, Wang, Zhang & Yu (2007c)	10.1107/S1600536807047575	SILXAN
<i>μ-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]iron(III)] bis(hexafluoridophosphate)</i>	Liu, Dou, Li & Zhang (2007)	10.1107/S1600536807049665	TINRIS
<i>μ-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-manganese(III)]</i>	Liu, Dou, Niu & Zhang (2007a)	10.1107/S1600536807051008	GIMZAE
<i>Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate</i>	Li, Wang, Zhang & Yu (2007d)	10.1107/S1600536807048556	WIMZIC
<i>μ-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-chromium(III)]</i>	Liu, Dou, Niu & Zhang (2007b)	10.1107/S1600536807057996	HIQFIX
<i>μ-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]chromium(III)] bis(hexafluoridophosphate)</i>	Li, Wang <i>et al.</i> (2008)	10.1107/S1600536807061296	MIRNAD
<i>μ-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-iron(III)]</i>	Meng <i>et al.</i> (2008a)	10.1107/S1600536807063143	MIRWUG
<i>catena-Poly[[bis(1H-benzimidazole-κN³)palladium(II)]-μ-benzene-1,4-dicarboxylato-κ^2O¹:O²]</i>	Meng <i>et al.</i> (2008b)	10.1107/S1600536807065051	XISCAE
<i>Oxalato-bis(propene-1,3-diamine)manganese(II) chloride monohydrate</i>	Meng <i>et al.</i> (2008e)	10.1107/S1600536807065361	SISWIB
<i>μ-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]manganese(III)] bis(hexafluoridophosphate)</i>	Meng <i>et al.</i> (2008c)	10.1107/S1600536807066512	RISRIV
<i>Bis[N-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N''manganese(III)] perchlorate monohydrate</i>	Meng <i>et al.</i> (2008d)	10.1107/S1600536808000287	GISLEA
<i>Diaquabis(pyridine-2-carboxylato-κ^2N,O)cobalt(II)</i>	Huang (2008)	10.1107/S1600536808010507	WIZPOL
<i>Tetra-μ-2,5-difluorobenzoato-bis[(2,2'-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]</i>	Li, Zhang <i>et al.</i> (2008)	10.1107/S1600536808023507	BOFQIX
<i>catena-Poly[[[2,2'-bipyridine-κ^2N,N']nickel(II)]-μ-oxalato-κ^4O¹,O²:O¹,O²]</i>	Li, Yan <i>et al.</i> (2008)	10.1107/S1600536808028389	NOHYUF
<i>catena-Poly[[aqua(2,2'-bipyridyl)cobalt(II)]-μ-5-nitrosophthalalato]</i>	Liu <i>et al.</i> (2008)	10.1107/S1600536808038178	AFIREN
<i>Diaquabis(pyridine-2-carboxylato-κ^2N,O)iron(II)</i>	Xia & Sun (2009)	10.1107/S1600536809005765	RONFEG
<i>catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]</i>	Li <i>et al.</i> (2009)	10.1107/S1600536809008836	NOQNIR
<i>1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one</i>	Liu <i>et al.</i> (2009)	10.1107/S1600536809040227	PUGLOT

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catena-Poly[[*(2,2'*-bipyridine- κ^2N,N')-nickel(II)]- μ -oxalato- $\kappa^4O^1,O^2:O^1',O^2'$]

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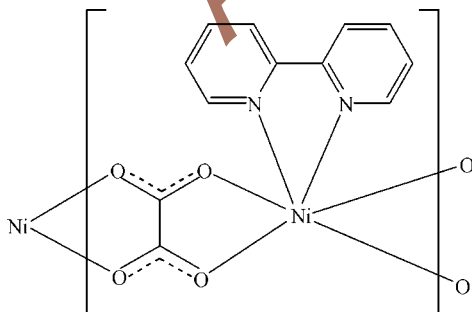
Received 4 August 2008; accepted 4 September 2008

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.010$ Å; R factor = 0.048; wR factor = 0.155; data-to-parameter ratio = 12.2.

The title compound, $[Ni(C_2O_4)(C_{10}H_8N_2)]_n$, is isostructural with its Mn^{II} , Fe^{II} , Cu^{II} and Zn^{II} analogues. Each Ni^{II} atom is chelated by two oxalate ligands and one 2,2'-bipyridine, forming a slightly distorted octahedral geometry. Oxalate acts as a bridge to link neighbouring pairs of Ni^{II} cations, forming a one-dimensional wave-like chain. The crystal showed partial inversion twinning.

Related literature

For related literature, see: Hong & Do (1997); Eddaoudi *et al.* (2001); Liang *et al.* (2004); Shi *et al.* (2005). For the isostructural Mn^{II} , Fe^{II} , Cu^{II} and Zn^{II} complexes, see: Li *et al.* (2006); Deguenon *et al.* (1990); Fun *et al.* (1999); Luo *et al.* (2001); Yu *et al.* (2006); Lin *et al.* (2006).



Experimental

Crystal data

$[Ni(C_2O_4)(C_{10}H_8N_2)]$	$V = 1240.7 (3) \text{ \AA}^3$
$M_r = 302.91$	$Z = 4$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 9.6486 (14) \text{ \AA}$	$\mu = 1.57 \text{ mm}^{-1}$
$b = 9.2627 (14) \text{ \AA}$	$T = 296 (2) \text{ K}$
$c = 13.883 (2) \text{ \AA}$	$0.12 \times 0.10 \times 0.06 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer	6146 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	2114 independent reflections
$T_{\min} = 0.834$, $T_{\max} = 0.912$	1810 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.154$	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
$S = 1.00$	$\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$
2114 reflections	Absolute structure: Flack (1983),
173 parameters	971 Friedel pairs
1 restraint	Flack parameter: 0.20 (3)

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: CF2213).

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supporting information

Acta Cryst. (2008). E64, m1258 [doi:10.1107/S1600536808028389]

catena-Poly[[*(2,2'*-bipyridine- κ^2N,N')nickel(II)]- μ -oxalato- $\kappa^4O^1,O^2:O^1',O^2'$]

Sheng Li, Xing-Lian Yan, Shou-Bin Wang and Yuan-Fang Ma

S1. Comment

The design of coordination compounds has attracted long-lasting research interest not only because of their appealing structural and topological novelty but also due to their unusual optical, electronic, magnetic and catalytic properties, and their further potential medical value derived from their antiviral properties and the inhibition of angiogenesis. To date, much of the work has been focused on coordination polymers with organic acid ligands (Hong *et al.* 1997; Eddaoudi *et al.* 2001; Liang *et al.* 2004; Shi *et al.* 2005).

Here we report the synthesis and X-ray crystal structure analysis of the title compound, (I), with a bridging oxalate ligand. It is isostructural with its Mn^{II}, Fe^{II}, Cu^{II}, and Zn^{II} analogues (Li *et al.*, 2006; Deguenon *et al.*, 1990; Fun *et al.*, 1999; Luo *et al.*, 2001; Yu *et al.*, 2006; Lin *et al.*, 2006).

As shown in Fig. 1, the Ni(II) atom is chelated by two oxalates and one 2,2'-bipyridine, forming a slightly distorted octahedral geometry. Oxalate acts as a bridge to link neighboring pairs of Ni(II) cations, forming a one-dimensional wave-like chain (Fig. 2). The Ni—N and Ni—O bond lengths are in the ranges 2.239 (5)–2.243 (5) and 2.161 (4)–2.166 (4) Å, respectively.

S2. Experimental

A mixture of nickel(II) nitrate hexahydrate (0.1 mmol), oxalic acid (0.2 mmol), 2,2'-bipyridine (0.1 mmol), and water (16 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 473 K for three days. Green crystals were obtained after cooling to room temperature, with a yield of 6%. Anal. Calc. for C₁₂H₈N₂NiO₄: C 47.54, H 2.64, N 9.24%; Found: C 47.51, H 2.58, N 9.16%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

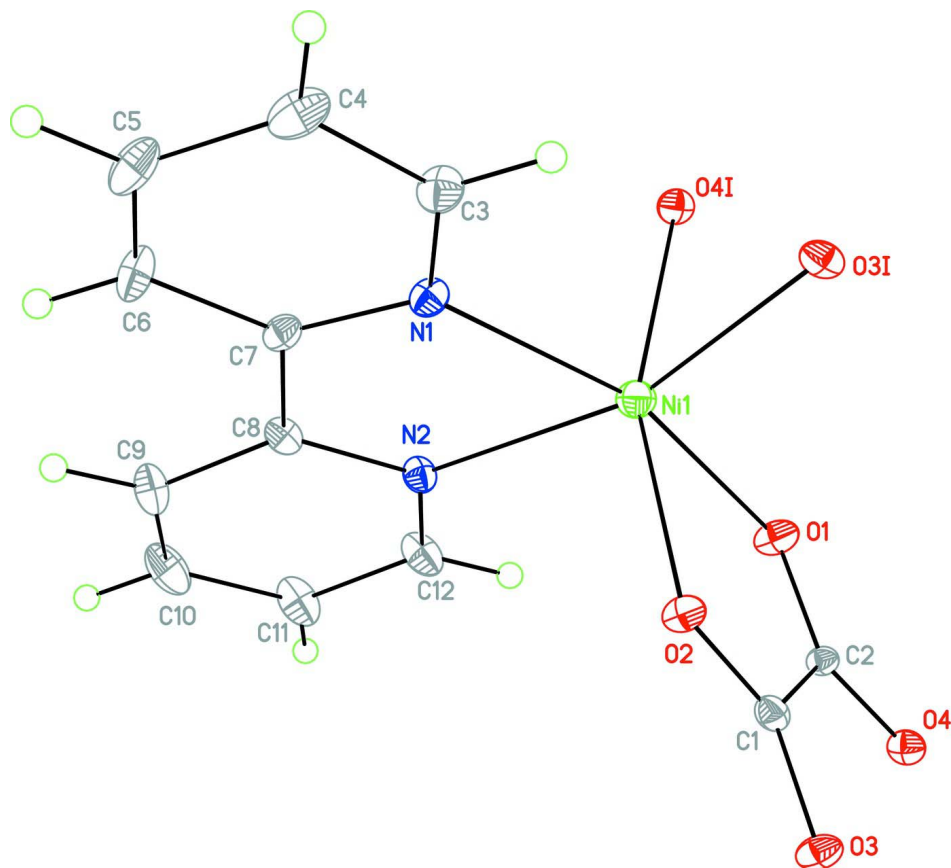


Figure 1

The coordination of the Ni atom in the title structure, drawn with 30% probability displacement ellipsoids. [Symmetry code: (I) 1/2+x, 1/2-y, z.]

Article

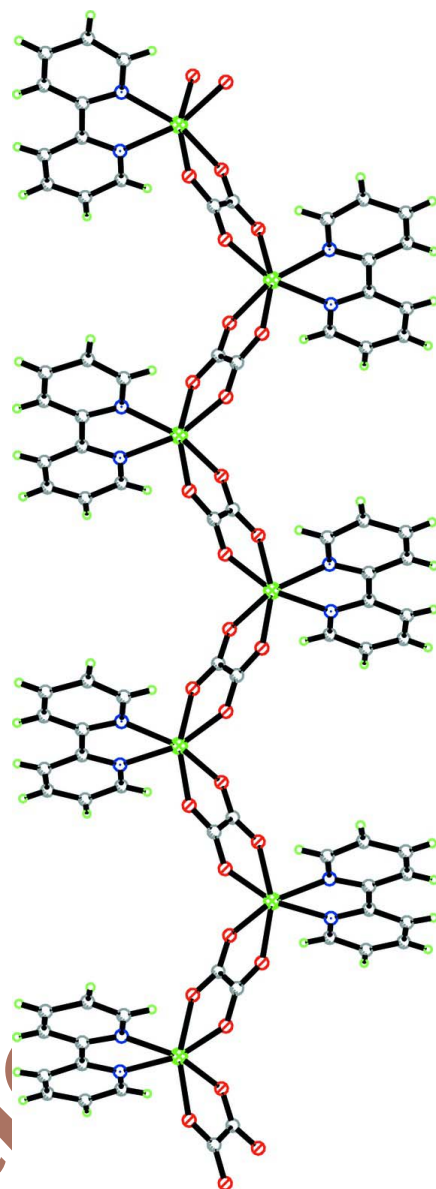


Figure 2

The chain of the title compound, viewed along the [010] direction.

catena-Poly[[*(2,2'*-bipyridine- κ^2N,N')nickel(II)]- μ -oxalato- $\kappa^4O^1,O^2:O^1',O^2'$]

Crystal data

[Ni(C₂O₄)(C₁₀H₈N₂)]

$M_r = 302.91$

Orthorhombic, *Pna*2₁

Hall symbol: P 2c -2n

$a = 9.6486$ (14) Å

$b = 9.2627$ (14) Å

$c = 13.883$ (2) Å

$V = 1240.7$ (3) Å³

$Z = 4$

$F(000) = 616$

$D_x = 1.622$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1779 reflections

$\theta = 2.6$ – 21.5°

$\mu = 1.57$ mm⁻¹

$T = 296$ K

Block, green

$0.12 \times 0.10 \times 0.06$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)
 $T_{\min} = 0.834$, $T_{\max} = 0.912$

6146 measured reflections
2114 independent reflections
1810 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\max} = 25.1^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -11 \rightarrow 5$
 $k = -11 \rightarrow 11$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.154$
 $S = 1.00$
2114 reflections
173 parameters
1 restraint
Primary atom site location: structure-invariant
direct methods
Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.118P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.44 \text{ e } \text{\AA}^{-3}$
Absolute structure: Flack (1983), 971 Friedel
pairs
Absolute structure parameter: 0.20 (3)

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	0.88396 (7)	1.09402 (7)	0.25107 (8)	0.04352 (14)
O1	1.0093 (4)	1.2363 (5)	0.1613 (3)	0.0503 (11)
O2	1.0673 (4)	1.1297 (4)	0.3368 (3)	0.0415 (9)
O3	0.7686 (4)	1.2511 (5)	0.3347 (3)	0.0452 (10)
O4	0.7033 (4)	1.1389 (4)	0.1640 (3)	0.0416 (9)
N1	0.8006 (5)	0.9059 (5)	0.3352 (4)	0.0401 (11)
N2	0.9510 (5)	0.8925 (5)	0.1747 (4)	0.0395 (11)
C1	1.1555 (6)	1.2124 (6)	0.3004 (4)	0.0380 (12)
C2	1.1199 (4)	1.2745 (6)	0.1993 (4)	0.0305 (12)
C3	0.7196 (8)	0.9174 (8)	0.4115 (5)	0.0535 (17)
H3	0.6964	1.0099	0.4320	0.064*
C4	0.6668 (8)	0.8030 (10)	0.4630 (5)	0.070 (2)
H4	0.6106	0.8163	0.5168	0.084*
C5	0.7033 (9)	0.6629 (9)	0.4291 (6)	0.073 (2)
H5	0.6728	0.5809	0.4613	0.087*

C6	0.7820 (8)	0.6507 (7)	0.3504 (6)	0.0633 (19)
H6	0.8054	0.5598	0.3269	0.076*
C7	0.8286 (6)	0.7736 (6)	0.3038 (4)	0.0405 (13)
C8	0.9159 (6)	0.7661 (7)	0.2154 (4)	0.0408 (13)
C9	0.9646 (9)	0.6356 (7)	0.1766 (6)	0.0627 (19)
H9	0.9447	0.5484	0.2067	0.075*
C10	1.0418 (10)	0.6383 (10)	0.0936 (7)	0.081 (3)
H10	1.0713	0.5519	0.0663	0.097*
C11	1.0758 (8)	0.7647 (9)	0.0510 (5)	0.066 (2)
H11	1.1292	0.7669	-0.0048	0.080*
C12	1.0277 (8)	0.8924 (8)	0.0937 (5)	0.0601 (19)
H12	1.0495	0.9802	0.0651	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0387 (2)	0.0456 (2)	0.0463 (2)	0.0000 (2)	-0.0004 (3)	0.0045 (3)
O1	0.042 (2)	0.065 (3)	0.044 (3)	-0.012 (2)	-0.0101 (19)	0.022 (2)
O2	0.0384 (19)	0.052 (2)	0.034 (2)	-0.0078 (19)	-0.0056 (16)	0.0150 (18)
O3	0.039 (2)	0.061 (2)	0.036 (2)	0.0098 (19)	-0.0144 (18)	-0.0128 (19)
O4	0.042 (2)	0.048 (2)	0.035 (2)	-0.0017 (18)	-0.0036 (17)	-0.0095 (18)
N1	0.043 (3)	0.045 (3)	0.032 (2)	-0.0063 (18)	0.006 (2)	-0.0005 (19)
N2	0.045 (3)	0.038 (2)	0.036 (3)	0.0049 (19)	0.008 (2)	0.002 (2)
C1	0.038 (3)	0.036 (3)	0.040 (3)	0.007 (3)	-0.004 (3)	0.004 (3)
C2	0.028 (3)	0.034 (3)	0.029 (3)	-0.002 (2)	-0.0031 (19)	0.005 (2)
C3	0.062 (4)	0.058 (4)	0.041 (4)	-0.005 (3)	0.016 (3)	0.005 (3)
C4	0.068 (4)	0.098 (6)	0.043 (4)	-0.024 (5)	0.015 (4)	0.011 (4)
C5	0.087 (5)	0.071 (5)	0.060 (4)	-0.034 (4)	0.011 (4)	0.021 (4)
C6	0.088 (5)	0.039 (3)	0.063 (4)	-0.022 (3)	0.004 (4)	-0.002 (3)
C7	0.040 (3)	0.045 (3)	0.037 (3)	-0.008 (3)	0.000 (3)	0.005 (2)
C8	0.045 (3)	0.046 (3)	0.031 (3)	0.008 (3)	0.000 (3)	-0.005 (2)
C9	0.089 (5)	0.041 (3)	0.058 (4)	0.012 (3)	-0.002 (4)	0.005 (3)
C10	0.096 (7)	0.073 (5)	0.073 (5)	0.040 (5)	0.009 (5)	-0.017 (5)
C11	0.091 (5)	0.070 (5)	0.037 (4)	0.028 (4)	0.012 (4)	0.003 (3)
C12	0.069 (5)	0.064 (4)	0.047 (4)	0.023 (3)	0.014 (3)	0.012 (3)

Geometric parameters (Å, °)

Ni1—O4	2.162 (4)	C3—C4	1.376 (10)
Ni1—O2	2.157 (4)	C3—H3	0.930
Ni1—O1	2.180 (4)	C4—C5	1.425 (13)
Ni1—O3	2.169 (4)	C4—H4	0.930
Ni1—N2	2.242 (5)	C5—C6	1.335 (12)
Ni1—N1	2.246 (5)	C5—H5	0.930
O1—C2	1.242 (6)	C6—C7	1.385 (9)
O2—C1	1.251 (7)	C6—H6	0.930
O3—C1 ⁱ	1.238 (6)	C7—C8	1.491 (8)
O4—C2 ⁱ	1.237 (6)	C8—C9	1.404 (9)

N1—C3	1.322 (8)	C9—C10	1.372 (12)
N1—C7	1.328 (7)	C9—H9	0.930
N2—C8	1.343 (8)	C10—C11	1.353 (13)
N2—C12	1.346 (9)	C10—H10	0.930
C1—O3 ⁱⁱ	1.238 (6)	C11—C12	1.402 (10)
C1—C2	1.554 (6)	C11—H11	0.930
C2—O4 ⁱⁱ	1.237 (6)	C12—H12	0.930
O4—Ni1—O2	160.07 (14)	N1—C3—C4	125.0 (7)
O4—Ni1—O1	90.65 (14)	N1—C3—H3	117.5
O2—Ni1—O1	76.55 (13)	C4—C3—H3	117.5
O4—Ni1—O3	75.90 (14)	C3—C4—C5	115.9 (7)
O2—Ni1—O3	91.31 (15)	C3—C4—H4	122.0
O1—Ni1—O3	100.66 (17)	C5—C4—H4	122.0
O4—Ni1—N2	97.39 (17)	C6—C5—C4	119.3 (7)
O2—Ni1—N2	98.72 (18)	C6—C5—H5	120.4
O1—Ni1—N2	94.20 (18)	C4—C5—H5	120.4
O3—Ni1—N2	163.69 (17)	C5—C6—C7	119.8 (7)
O4—Ni1—N1	98.71 (17)	C5—C6—H6	120.1
O2—Ni1—N1	97.23 (17)	C7—C6—H6	120.1
O1—Ni1—N1	164.72 (18)	N1—C7—C6	122.7 (6)
O3—Ni1—N1	93.35 (18)	N1—C7—C8	115.3 (5)
N2—Ni1—N1	72.74 (17)	C6—C7—C8	122.0 (6)
C2—O1—Ni1	114.0 (3)	N2—C8—C9	120.3 (6)
C1—O2—Ni1	115.4 (4)	N2—C8—C7	116.6 (5)
C1 ⁱ —O3—Ni1	115.4 (3)	C9—C8—C7	123.0 (6)
C2 ⁱ —O4—Ni1	115.3 (3)	C8—C9—C10	119.2 (7)
C3—N1—C7	117.2 (5)	C8—C9—H9	120.4
C3—N1—Ni1	124.5 (4)	C10—C9—H9	120.4
C7—N1—Ni1	118.2 (4)	C11—C10—C9	121.0 (7)
C8—N2—C12	119.3 (5)	C11—C10—H10	119.5
C8—N2—Ni1	117.0 (4)	C9—C10—H10	119.5
C12—N2—Ni1	123.7 (4)	C10—C11—C12	117.7 (7)
O2—C1—O3 ⁱⁱⁱ	127.7 (5)	C10—C11—H11	121.2
O2—C1—C2	116.2 (5)	C12—C11—H11	121.2
O3 ⁱⁱ —C1—C2	116.2 (5)	N2—C12—C11	122.4 (7)
O4 ⁱⁱ —C2—O1	125.1 (5)	N2—C12—H12	118.8
O4 ⁱⁱ —C2—C1	117.0 (4)	C11—C12—H12	118.8
O1—C2—C1	117.8 (4)		
O4—Ni1—O1—C2	162.4 (4)	O1—Ni1—N2—C12	-7.8 (6)
O2—Ni1—O1—C2	-2.1 (4)	O3—Ni1—N2—C12	147.8 (6)
O3—Ni1—O1—C2	86.7 (4)	N1—Ni1—N2—C12	-179.8 (6)
N2—Ni1—O1—C2	-100.1 (4)	Ni1—O2—C1—O3 ⁱⁱⁱ	-179.5 (5)
N1—Ni1—O1—C2	-69.5 (8)	Ni1—O2—C1—C2	-0.7 (6)
O4—Ni1—O2—C1	-49.9 (7)	Ni1—O1—C2—O4 ⁱⁱ	-175.8 (5)
O1—Ni1—O2—C1	1.4 (4)	Ni1—O1—C2—C1	2.5 (6)
O3—Ni1—O2—C1	-99.2 (4)	O2—C1—C2—O4 ⁱⁱ	177.1 (6)

N2—Ni1—O2—C1	93.7 (4)	O3 ⁱⁱ —C1—C2—O4 ⁱⁱ	-3.9 (7)
N1—Ni1—O2—C1	167.2 (4)	O2—C1—C2—O1	-1.3 (7)
O4—Ni1—O3—C1 ⁱ	3.6 (4)	O3 ⁱⁱ —C1—C2—O1	177.7 (6)
O2—Ni1—O3—C1 ⁱ	168.2 (4)	C7—N1—C3—C4	2.7 (11)
O1—Ni1—O3—C1 ⁱ	91.6 (4)	Ni1—N1—C3—C4	179.3 (6)
N2—Ni1—O3—C1 ⁱ	-63.7 (8)	N1—C3—C4—C5	-0.5 (11)
N1—Ni1—O3—C1 ⁱ	-94.5 (4)	C3—C4—C5—C6	-1.4 (12)
O2—Ni1—O4—C2 ⁱ	-52.8 (7)	C4—C5—C6—C7	1.0 (12)
O1—Ni1—O4—C2 ⁱ	-102.2 (4)	C3—N1—C7—C6	-3.1 (9)
O3—Ni1—O4—C2 ⁱ	-1.3 (4)	Ni1—N1—C7—C6	-179.9 (5)
N2—Ni1—O4—C2 ⁱ	163.5 (4)	C3—N1—C7—C8	177.8 (6)
N1—Ni1—O4—C2 ⁱ	89.9 (4)	Ni1—N1—C7—C8	0.9 (6)
O4—Ni1—N1—C3	-80.8 (6)	C5—C6—C7—N1	1.3 (11)
O2—Ni1—N1—C3	87.1 (6)	C5—C6—C7—C8	-179.6 (7)
O1—Ni1—N1—C3	152.0 (6)	C12—N2—C8—C9	3.2 (9)
O3—Ni1—N1—C3	-4.6 (6)	Ni1—N2—C8—C9	-174.3 (5)
N2—Ni1—N1—C3	-175.9 (6)	C12—N2—C8—C7	-178.8 (6)
O4—Ni1—N1—C7	95.7 (4)	Ni1—N2—C8—C7	3.6 (7)
O2—Ni1—N1—C7	-96.3 (4)	N1—C7—C8—N2	-3.0 (7)
O1—Ni1—N1—C7	-31.5 (9)	C6—C7—C8—N2	177.8 (6)
O3—Ni1—N1—C7	171.9 (4)	N1—C7—C8—C9	174.9 (6)
N2—Ni1—N1—C7	0.6 (4)	C6—C7—C8—C9	-4.3 (9)
O4—Ni1—N2—C8	-99.2 (5)	N2—C8—C9—C10	-3.7 (11)
O2—Ni1—N2—C8	92.6 (4)	C7—C8—C9—C10	178.5 (7)
O1—Ni1—N2—C8	169.6 (4)	C8—C9—C10—C11	2.4 (13)
O3—Ni1—N2—C8	-34.7 (9)	C9—C10—C11—C12	-0.9 (13)
N1—Ni1—N2—C8	-2.3 (4)	C8—N2—C12—C11	-1.7 (11)
O4—Ni1—N2—C12	83.4 (6)	Ni1—N2—C12—C11	175.7 (6)
O2—Ni1—N2—C12	-84.9 (6)	C10—C11—C12—N2	0.4 (12)

Symmetry codes: (i) $x-1/2, -y+5/2, z$; (ii) $x+1/2, -y+5/2, z$.