Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[(2,2′-bipyridine)nickel(II)]-*μ*-imidazole-4,5-dicarboxylato]

Lu-Jiang Hao* and Tong-Li Yu

College of Food and Biological Engineering, Shandong Institute of Light Industry, Jinan 250353, People's Republic of China
Correspondence e-mail: lujianghao001@yahoo.com.cn

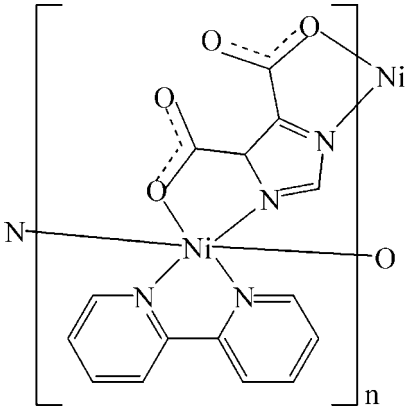
Received 15 July 2007; accepted 14 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.066; data-to-parameter ratio = 13.0.

The title compound, $[Ni(C_5HN_2O_4)(C_{10}H_8N_2)]_n$, is isotypic with its Co^{II} and Zn^{II} analogues. The asymmetric unit contains two crystallographically independent monomer units with similar geometry. The Ni^{II} cations have a distorted octahedral environment formed by two carboxylate O atoms and by four N atoms, two of which belong to the 2,2′-bipyridine ligands and two to different imidazole rings. One imidazole-4,5-carboxylate ligand is connected to two Ni^{II} cations, which results in the formation of one-dimensional zigzag chains parallel to [010].

Related literature

For the isotypic Co^{II} and Zn^{II} structures, see: Hao *et al.* (2007); Li *et al.* (2007).



Experimental

Crystal data

$[Ni(C_5HN_2O_4)(C_{10}H_8N_2)]$
M_r = 367.97
Monoclinic, $P2_1/c$
a = 20.424 (2) Å
b = 9.6712 (10) Å
c = 14.751 (1) Å
β = 101.798 (1)°
V = 2852.1 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.39 mm^{-1}
T = 293 (2) K
0.15 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.819, T_{max} = 0.819
15248 measured reflections
5614 independent reflections
4906 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.066
S = 1.00
5614 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N7^{i}	2.0869 (16)	Ni2—N4^{ii}	2.0775 (17)
Ni1—N6	2.1188 (17)	Ni2—N3	2.0840 (17)
Ni1—N5	2.1235 (17)	Ni2—N1	2.1167 (17)
Ni1—N8	2.2721 (17)	Ni2—N2	2.2040 (17)
Ni1—O8	2.1543 (14)	Ni2—O1	2.2060 (15)
Ni1—O6^{i}	2.2052 (14)	Ni2—O4^{ii}	2.2562 (15)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank Shandong Institute of Light Industry for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2133).

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supplementary materials

Acta Cryst. (2007). E**63**, m2374 [**doi:10.1107/S1600536807040330**]

catena-Poly[[(2,2'-bipyridine)nickel(II)]-μ-imidazole-4,5-dicarboxylato]

L.-J. Hao and T.-L. Yu

Comment

In connection with our strucure determination of *catena*-poly[[(2,2'-bipyridine)cobalt(II)]-μ-imidazole-4,5-dicarboxylato] (Hao *et al.*, 2007), we report here the isotypic structure of the Ni^{II} compound. The Zn^{II} analogue (Li *et al.*, 2007) crystallizes also isotypically.

In the title compound, (I), two crystallographically independent monomer units are present in the asymmetric unit. The Ni^{II} cations have a distorted octahedral coordination sphere formed by two carboxylate O atoms and by four N atoms, two of which belong to the 2,2'-bipyridine ligand and the other two to the imidazole ring (Fig. 1). The Ni—O and Ni—N bond lengths are in the range of 2.1543 (14)–2.2562 (15) and 2.0775 (17)–2.2721 (17) Å, respectively, and are similar to the *M*—O and *M*—N bond lengths (*M* = Co, Zn) observed in the corresponding isotypic structures. The two carboxylate groups of the imidazole-4,5-dicarboxylate ligand coordinate in a monodentate fashion with the Ni^{II} cations, whereby the connectivity between the cations and the ligands gives rise to one-dimensional zigzag chains along [010] (Fig. 2). The 2,2'-bipyridine ligands are situated in the space between the chains.

Experimental

All chemicals were purchased from Acros Co. Ltd. The title compound was obtained from the hydrothermal reaction (30 ml autoclave at 452 K for 3 d) of $NiCl_2{\cdot}6H_2O$ (0.5 mmol), imidazole-4,5-dicarboxylic acid (0.5 mmol), 2,2'-bipyridine (0.5 mmol) and KOH (1 mmol) in 20 ml distilled water. Green crystals were obtained in a yield of approximately 22%. Analysis calculated for $C_{15}H_9N_4NiO_4$: C 48.96, H 2.47, N 15.23%; Found: C 48.88, H 2.47, N 15.16%.

Refinement

The H atoms were positioned geometrically and refined as riding atoms with C—H= 0.93 Å and U_{iso}(H)= 1.2U_{eq}(C).

Figures

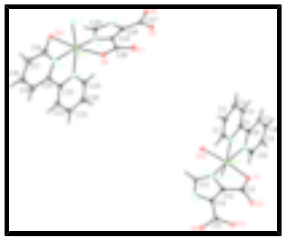

Fig. 1. The two independent molecules in (I), displayed with anisotropic displacement ellipsoids at the 30% probability level for all non-H atoms. H atoms are given as spheres of arbitrary radius. [Symmetry code: (i) $-x + 1, y + 1/2, -z + 3/2$.]

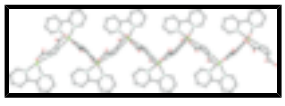

Fig. 2. A zigzag chain extending parallel to [010] in (I). H atoms have been omitted for clarity.

catena-Poly[[(2,2'-bipyridine)nickel(II)]-μ-imidazole-4,5-dicarboxylato]

Crystal data

$[Ni(C_5HN_2O_4)(C_{10}H_8N_2)]$	F_{000} = 1496
M_r = 367.97	D_x = 1.714 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5614 reflections
a = 20.424 (2) Å	θ = 2.3–26.1º
b = 9.6712 (10) Å	μ = 1.39 mm^{-1}
c = 14.7510 (10) Å	T = 293 (2) K
β = 101.7980 (10)º	Cube, green
V = 2852.1 (4) Å^3	0.15 × 0.15 × 0.15 mm
Z = 8	

Data collection

Bruker APEXII CCD area-detector diffractometer	5614 independent reflections
Radiation source: fine-focus sealed tube	4906 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −25→20
T_{min} = 0.819, T_{max} = 0.819	k = −11→10
15248 measured reflections	l = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.066	$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 1.5005P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.039
5614 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
433 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.70626 (11)	0.3208 (2)	0.84600 (14)	0.0280 (5)
H1	0.6703	0.3795	0.8250	0.034*
C2	0.76975 (11)	0.3757 (2)	0.86436 (14)	0.0292 (5)
H2	0.7765	0.4696	0.8565	0.035*
C3	0.82307 (11)	0.2885 (2)	0.89466 (15)	0.0313 (5)
H3	0.8665	0.3227	0.9076	0.038*
C4	0.81098 (10)	0.1489 (2)	0.90560 (14)	0.0295 (5)
H4	0.8464	0.0881	0.9250	0.035*
C5	0.74584 (10)	0.1011 (2)	0.88736 (13)	0.0236 (4)
C6	0.72867 (10)	−0.0457 (2)	0.90085 (13)	0.0243 (4)
C7	0.77634 (11)	−0.1445 (2)	0.93791 (14)	0.0290 (5)
H7	0.8213	−0.1206	0.9544	0.035*
C8	0.75597 (11)	−0.2782 (2)	0.94981 (15)	0.0327 (5)
H8	0.7872	−0.3458	0.9738	0.039*
C9	0.68885 (11)	−0.3107 (2)	0.92581 (16)	0.0330 (5)
H9	0.6739	−0.4000	0.9335	0.040*
C10	0.64444 (11)	−0.2073 (2)	0.89007 (15)	0.0311 (5)
H10	0.5992	−0.2288	0.8743	0.037*
C11	0.52685 (10)	0.2341 (2)	0.94608 (14)	0.0250 (4)
C12	0.51350 (9)	0.3154 (2)	0.85976 (13)	0.0226 (4)
C13	0.52113 (10)	0.3687 (2)	0.72120 (14)	0.0240 (4)
H13	0.5344	0.3682	0.6645	0.029*
C14	0.47021 (10)	0.4233 (2)	0.82990 (13)	0.0218 (4)
C15	0.41987 (10)	0.4930 (2)	0.87196 (14)	0.0249 (4)
C16	0.86416 (12)	1.3021 (2)	0.17951 (16)	0.0336 (5)
H16	0.9088	1.3170	0.2069	0.040*
C17	0.82576 (13)	1.4144 (2)	0.14208 (18)	0.0409 (6)
H17	0.8443	1.5024	0.1434	0.049*
C18	0.75971 (13)	1.3921 (3)	0.10311 (18)	0.0425 (6)
H18	0.7325	1.4654	0.0779	0.051*
C19	0.73392 (12)	1.2599 (2)	0.10156 (15)	0.0349 (5)
H19	0.6892	1.2432	0.0754	0.042*
C20	0.77551 (10)	1.1524 (2)	0.13943 (13)	0.0259 (4)

C21	0.75113 (10)	1.0085 (2)	0.14528 (14)	0.0256 (4)
C22	0.68389 (11)	0.9734 (3)	0.12219 (16)	0.0369 (5)
H22	0.6522	1.0388	0.0959	0.044*
C23	0.66441 (12)	0.8402 (3)	0.13871 (18)	0.0436 (6)
H23	0.6195	0.8156	0.1241	0.052*
C24	0.95914 (9)	0.7532 (2)	0.33096 (13)	0.0207 (4)
C25	0.77823 (11)	0.7847 (2)	0.19550 (15)	0.0298 (5)
H25	0.8108	0.7201	0.2199	0.036*
C26	0.93275 (10)	0.8466 (2)	0.39410 (13)	0.0237 (4)
C27	1.04263 (9)	0.5862 (2)	0.43335 (13)	0.0213 (4)
C28	1.00285 (9)	0.6432 (2)	0.34751 (13)	0.0212 (4)
C29	0.97693 (10)	0.6785 (2)	0.20109 (13)	0.0228 (4)
H29	0.9748	0.6693	0.1378	0.027*
C30	0.71208 (11)	0.7442 (3)	0.17694 (16)	0.0383 (6)
H30	0.7000	0.6547	0.1898	0.046*
N1	0.69405 (8)	0.18621 (18)	0.85704 (11)	0.0246 (4)
N2	0.66336 (8)	−0.07771 (18)	0.87706 (12)	0.0253 (4)
N3	0.54579 (8)	0.28113 (17)	0.79038 (11)	0.0235 (4)
N4	0.47564 (8)	0.45708 (17)	0.74142 (11)	0.0231 (4)
N5	0.79758 (8)	0.91347 (18)	0.17983 (11)	0.0246 (4)
N6	0.94283 (8)	0.77605 (17)	0.23760 (11)	0.0219 (4)
N7	1.01414 (8)	0.59611 (17)	0.26445 (11)	0.0220 (4)
N8	0.84001 (8)	1.17327 (18)	0.17805 (12)	0.0269 (4)
Ni1	0.899423 (11)	0.97523 (2)	0.214416 (15)	0.01502 (7)
Ni2	0.597902 (11)	0.09584 (2)	0.819724 (16)	0.01727 (7)
O1	0.56785 (7)	0.13633 (15)	0.95264 (10)	0.0299 (3)
O2	0.49461 (7)	0.26686 (16)	1.00906 (10)	0.0322 (3)
O3	0.41600 (7)	0.45809 (16)	0.95508 (10)	0.0306 (3)
O4	0.38170 (7)	0.57763 (15)	0.82446 (10)	0.0296 (3)
O5	1.03289 (7)	0.63626 (15)	0.51070 (9)	0.0262 (3)
O6	1.08547 (7)	0.49642 (14)	0.42874 (9)	0.0237 (3)
O7	0.94594 (8)	0.81809 (16)	0.47985 (10)	0.0344 (4)
O8	0.89858 (7)	0.94843 (15)	0.35916 (9)	0.0270 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0278 (11)	0.0235 (11)	0.0318 (11)	0.0002 (9)	0.0040 (9)	0.0035 (9)
C2	0.0332 (12)	0.0245 (11)	0.0292 (11)	−0.0064 (9)	0.0051 (9)	0.0023 (9)
C3	0.0241 (11)	0.0357 (13)	0.0328 (11)	−0.0075 (9)	0.0028 (9)	0.0031 (10)
C4	0.0241 (11)	0.0297 (12)	0.0328 (11)	0.0003 (9)	0.0013 (9)	0.0048 (9)
C5	0.0223 (10)	0.0255 (11)	0.0218 (10)	0.0007 (8)	0.0019 (8)	−0.0001 (8)
C6	0.0221 (10)	0.0263 (11)	0.0232 (10)	−0.0004 (8)	0.0020 (8)	−0.0010 (8)
C7	0.0229 (11)	0.0315 (12)	0.0303 (11)	0.0022 (9)	0.0003 (8)	−0.0005 (9)
C8	0.0333 (12)	0.0264 (12)	0.0359 (12)	0.0079 (10)	0.0010 (10)	0.0044 (10)
C9	0.0357 (13)	0.0224 (11)	0.0398 (13)	−0.0014 (9)	0.0054 (10)	0.0046 (9)
C10	0.0262 (11)	0.0296 (12)	0.0368 (12)	−0.0039 (9)	0.0045 (9)	0.0025 (10)
C11	0.0220 (10)	0.0249 (11)	0.0260 (10)	−0.0036 (9)	−0.0001 (8)	0.0002 (9)

C12	0.0190 (10)	0.0241 (11)	0.0237 (10)	−0.0020 (8)	0.0019 (8)	−0.0006 (8)
C13	0.0216 (10)	0.0264 (11)	0.0237 (10)	0.0017 (8)	0.0038 (8)	0.0000 (8)
C14	0.0187 (10)	0.0222 (10)	0.0234 (10)	−0.0032 (8)	0.0017 (8)	−0.0004 (8)
C15	0.0218 (10)	0.0242 (11)	0.0284 (11)	−0.0039 (8)	0.0044 (8)	−0.0014 (9)
C16	0.0342 (13)	0.0281 (12)	0.0414 (13)	0.0024 (10)	0.0145 (10)	0.0002 (10)
C17	0.0481 (16)	0.0254 (12)	0.0533 (15)	0.0066 (11)	0.0202 (12)	0.0045 (11)
C18	0.0441 (15)	0.0357 (14)	0.0500 (15)	0.0196 (11)	0.0154 (12)	0.0124 (11)
C19	0.0306 (12)	0.0398 (14)	0.0345 (12)	0.0107 (10)	0.0067 (10)	0.0073 (10)
C20	0.0244 (11)	0.0321 (12)	0.0223 (10)	0.0060 (9)	0.0074 (8)	0.0028 (9)
C21	0.0225 (11)	0.0325 (12)	0.0212 (10)	0.0036 (9)	0.0028 (8)	−0.0007 (8)
C22	0.0225 (11)	0.0456 (15)	0.0402 (13)	0.0042 (10)	0.0008 (10)	−0.0012 (11)
C23	0.0224 (12)	0.0523 (16)	0.0536 (15)	−0.0079 (11)	0.0019 (11)	−0.0087 (13)
C24	0.0189 (10)	0.0216 (10)	0.0211 (9)	−0.0006 (8)	0.0028 (8)	0.0008 (8)
C25	0.0278 (11)	0.0269 (12)	0.0335 (12)	−0.0030 (9)	0.0034 (9)	0.0001 (9)
C26	0.0228 (10)	0.0242 (11)	0.0237 (10)	0.0014 (8)	0.0039 (8)	−0.0001 (8)
C27	0.0196 (10)	0.0213 (10)	0.0228 (10)	−0.0026 (8)	0.0039 (8)	0.0000 (8)
C28	0.0202 (10)	0.0217 (10)	0.0211 (9)	−0.0013 (8)	0.0027 (8)	−0.0008 (8)
C29	0.0247 (10)	0.0247 (11)	0.0183 (9)	0.0004 (8)	0.0030 (8)	0.0000 (8)
C30	0.0339 (13)	0.0375 (14)	0.0430 (13)	−0.0103 (11)	0.0064 (10)	−0.0029 (11)
N1	0.0220 (9)	0.0239 (9)	0.0263 (9)	−0.0012 (7)	0.0013 (7)	0.0002 (7)
N2	0.0215 (9)	0.0238 (9)	0.0297 (9)	−0.0012 (7)	0.0033 (7)	0.0019 (7)
N3	0.0213 (9)	0.0253 (9)	0.0230 (8)	0.0009 (7)	0.0027 (7)	−0.0006 (7)
N4	0.0193 (8)	0.0249 (9)	0.0241 (8)	−0.0006 (7)	0.0018 (7)	0.0010 (7)
N5	0.0213 (9)	0.0282 (10)	0.0243 (9)	0.0004 (7)	0.0046 (7)	0.0010 (7)
N6	0.0229 (9)	0.0225 (9)	0.0198 (8)	0.0008 (7)	0.0029 (7)	0.0020 (7)
N7	0.0230 (9)	0.0221 (9)	0.0201 (8)	0.0014 (7)	0.0028 (7)	−0.0004 (7)
N8	0.0253 (9)	0.0261 (10)	0.0300 (9)	0.0032 (7)	0.0073 (7)	0.0010 (8)
Ni1	0.01218 (12)	0.01396 (13)	0.01827 (12)	0.00018 (9)	0.00154 (9)	0.00298 (9)
Ni2	0.01201 (12)	0.01406 (13)	0.02351 (13)	0.00011 (9)	−0.00159 (9)	−0.00094 (9)
O1	0.0289 (8)	0.0294 (8)	0.0297 (8)	0.0042 (7)	0.0017 (6)	0.0053 (6)
O2	0.0350 (9)	0.0362 (9)	0.0261 (8)	0.0005 (7)	0.0081 (7)	0.0033 (7)
O3	0.0313 (8)	0.0339 (9)	0.0290 (8)	−0.0002 (7)	0.0117 (6)	0.0004 (7)
O4	0.0233 (8)	0.0314 (8)	0.0345 (8)	0.0059 (6)	0.0067 (6)	0.0015 (7)
O5	0.0282 (8)	0.0299 (8)	0.0197 (7)	0.0023 (6)	0.0027 (6)	0.0006 (6)
O6	0.0213 (7)	0.0253 (8)	0.0237 (7)	0.0044 (6)	0.0026 (6)	0.0023 (6)
O7	0.0453 (10)	0.0375 (9)	0.0213 (7)	0.0138 (7)	0.0086 (7)	0.0016 (6)
O8	0.0298 (8)	0.0255 (8)	0.0262 (7)	0.0078 (6)	0.0071 (6)	0.0017 (6)

Geometric parameters (Å, °)

C1—N1	1.341 (3)	C18—H18	0.9300
C1—C2	1.376 (3)	C19—C20	1.386 (3)
C1—H1	0.9300	C19—H19	0.9300
C2—C3	1.378 (3)	C20—N8	1.339 (3)
C2—H2	0.9300	C20—C21	1.487 (3)
C3—C4	1.388 (3)	C21—N5	1.344 (3)
C3—H3	0.9300	C21—C22	1.388 (3)
C4—C5	1.382 (3)	C22—C23	1.385 (3)
C4—H4	0.9300	C22—H22	0.9300

C5—N1	1.343 (3)	C23—C30	1.380 (3)
C5—C6	1.486 (3)	C23—H23	0.9300
C6—N2	1.344 (3)	C24—N6	1.367 (2)
C6—C7	1.393 (3)	C24—C28	1.378 (3)
C7—C8	1.381 (3)	C24—C26	1.477 (3)
C7—H7	0.9300	C25—N5	1.341 (3)
C8—C9	1.380 (3)	C25—C30	1.379 (3)
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.380 (3)	C26—O8	1.255 (2)
C9—H9	0.9300	C26—O7	1.269 (2)
C10—N2	1.337 (3)	C27—O6	1.244 (2)
C10—H10	0.9300	C27—O5	1.292 (2)
C11—O1	1.253 (2)	C27—C28	1.465 (3)
C11—O2	1.283 (2)	C28—N7	1.370 (2)
C11—C12	1.474 (3)	C29—N7	1.340 (2)
C12—N3	1.367 (3)	C29—N6	1.348 (3)
C12—C14	1.380 (3)	C29—H29	0.9300
C13—N4	1.340 (3)	C30—H30	0.9300
C13—N3	1.343 (3)	Ni1—N7^{i}	2.0869 (16)
C13—H13	0.9300	Ni1—N6	2.1188 (17)
C14—N4	1.372 (3)	Ni1—N5	2.1235 (17)
C14—C15	1.469 (3)	Ni1—N8	2.2721 (17)
C15—O4	1.243 (2)	Ni1—O8	2.1543 (14)
C15—O3	1.290 (2)	Ni1—O6^{i}	2.2052 (14)
C16—N8	1.338 (3)	Ni2—N4^{ii}	2.0775 (17)
C16—C17	1.387 (3)	Ni2—N3	2.0840 (17)
C16—H16	0.9300	Ni2—N1	2.1167 (17)
C17—C18	1.371 (4)	Ni2—N2	2.2040 (17)
C17—H17	0.9300	Ni2—O1	2.2060 (15)
C18—C19	1.381 (3)	Ni2—O4^{ii}	2.2562 (15)
N1—C1—C2	122.8 (2)	C30—C25—H25	118.6
N1—C1—H1	118.6	O8—C26—O7	124.56 (19)
C2—C1—H1	118.6	O8—C26—C24	117.73 (17)
C1—C2—C3	118.6 (2)	O7—C26—C24	117.72 (18)
C1—C2—H2	120.7	O6—C27—O5	123.16 (17)
C3—C2—H2	120.7	O6—C27—C28	119.16 (17)
C2—C3—C4	119.1 (2)	O5—C27—C28	117.63 (17)
C2—C3—H3	120.5	N7—C28—C24	108.64 (16)
C4—C3—H3	120.5	N7—C28—C27	118.86 (17)
C5—C4—C3	119.3 (2)	C24—C28—C27	131.94 (18)
C5—C4—H4	120.3	N7—C29—N6	113.77 (17)
C3—C4—H4	120.3	N7—C29—H29	123.1
N1—C5—C4	121.45 (19)	N6—C29—H29	123.1
N1—C5—C6	116.03 (17)	C23—C30—C25	118.0 (2)
C4—C5—C6	122.51 (19)	C23—C30—H30	121.0
N2—C6—C7	121.41 (19)	C25—C30—H30	121.0
N2—C6—C5	115.71 (18)	C5—N1—C1	118.79 (18)
C7—C6—C5	122.86 (19)	C5—N1—Ni2	117.35 (14)

C8—C7—C6	119.2 (2)	C1—N1—Ni2	123.69 (14)
C8—C7—H7	120.4	C10—N2—C6	118.62 (18)
C6—C7—H7	120.4	C10—N2—Ni2	126.76 (14)
C7—C8—C9	119.3 (2)	C6—N2—Ni2	114.62 (13)
C7—C8—H8	120.3	C13—N3—C12	104.63 (16)
C9—C8—H8	120.3	C13—N3—Ni2	142.82 (14)
C10—C9—C8	118.3 (2)	C12—N3—Ni2	110.93 (13)
C10—C9—H9	120.9	C13—N4—C14	104.74 (16)
C8—C9—H9	120.9	C13—N4—Ni2^{iii}	141.99 (14)
N2—C10—C9	123.2 (2)	C14—N4—Ni2^{iii}	112.03 (13)
N2—C10—H10	118.4	C25—N5—C21	119.34 (18)
C9—C10—H10	118.4	C25—N5—Ni1	121.91 (14)
O1—C11—O2	124.32 (19)	C21—N5—Ni1	118.67 (14)
O1—C11—C12	118.16 (18)	C29—N6—C24	104.46 (16)
O2—C11—C12	117.50 (18)	C29—N6—Ni1	143.59 (13)
N3—C12—C14	108.67 (17)	C24—N6—Ni1	108.51 (13)
N3—C12—C11	119.01 (18)	C29—N7—C28	104.53 (16)
C14—C12—C11	132.26 (19)	C29—N7—Ni1^{iv}	141.18 (14)
N4—C13—N3	113.74 (18)	C28—N7—Ni1^{iv}	110.15 (12)
N4—C13—H13	123.1	C16—N8—C20	118.33 (18)
N3—C13—H13	123.1	C16—N8—Ni1	127.12 (15)
N4—C14—C12	108.22 (17)	C20—N8—Ni1	113.87 (14)
N4—C14—C15	119.50 (17)	N7^{i}—Ni1—N6	99.90 (6)
C12—C14—C15	132.07 (19)	N7^{i}—Ni1—N5	161.90 (6)
O4—C15—O3	123.69 (19)	N6—Ni1—N5	98.05 (6)
O4—C15—C14	118.47 (18)	N7^{i}—Ni1—O8	95.58 (6)
O3—C15—C14	117.78 (18)	N6—Ni1—O8	79.55 (6)
N8—C16—C17	123.1 (2)	N5—Ni1—O8	89.91 (6)
N8—C16—H16	118.4	N7^{i}—Ni1—O6^{i}	79.12 (6)
C17—C16—H16	118.4	N6—Ni1—O6^{i}	95.92 (6)
C18—C17—C16	118.1 (2)	N5—Ni1—O6^{i}	96.78 (6)
C18—C17—H17	120.9	O8—Ni1—O6^{i}	172.42 (5)
C16—C17—H17	120.9	N7^{i}—Ni1—N8	87.57 (6)
C17—C18—C19	119.5 (2)	N6—Ni1—N8	171.93 (6)
C17—C18—H18	120.3	N5—Ni1—N8	74.38 (6)
C19—C18—H18	120.3	O8—Ni1—N8	102.90 (6)
C18—C19—C20	119.2 (2)	O6^{i}—Ni1—N8	82.42 (6)
C18—C19—H19	120.4	N4^{ii}—Ni2—N3	99.91 (6)
C20—C19—H19	120.4	N4^{ii}—Ni2—N1	158.35 (7)
N8—C20—C19	121.8 (2)	N3—Ni2—N1	96.10 (7)
N8—C20—C21	115.37 (18)	N4^{ii}—Ni2—N2	90.15 (6)
C19—C20—C21	122.7 (2)	N3—Ni2—N2	168.11 (6)
N5—C21—C22	120.8 (2)	N1—Ni2—N2	75.93 (6)
N5—C21—C20	116.31 (18)	N4^{ii}—Ni2—O1	101.11 (6)
C22—C21—C20	122.7 (2)	N3—Ni2—O1	78.98 (6)

C23—C22—C21	119.3 (2)	N1—Ni2—O1	96.17 (6)
C23—C22—H22	120.3	N2—Ni2—O1	92.94 (6)
C21—C22—H22	120.3	N4^{ii}—Ni2—O4^{ii}	78.28 (6)
C30—C23—C22	119.6 (2)	N3—Ni2—O4^{ii}	93.22 (6)
C30—C23—H23	120.2	N1—Ni2—O4^{ii}	86.39 (6)
C22—C23—H23	120.2	N2—Ni2—O4^{ii}	95.04 (6)
N6—C24—C28	108.60 (17)	O1—Ni2—O4^{ii}	171.99 (5)
N6—C24—C26	119.41 (17)	C11—O1—Ni2	111.60 (12)
C28—C24—C26	131.89 (18)	C15—O4—Ni2^{iii}	111.54 (13)
N5—C25—C30	122.8 (2)	C27—O6—Ni1^{iv}	110.79 (12)
N5—C25—H25	118.6	C26—O8—Ni1	112.64 (12)

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

Fig. 1

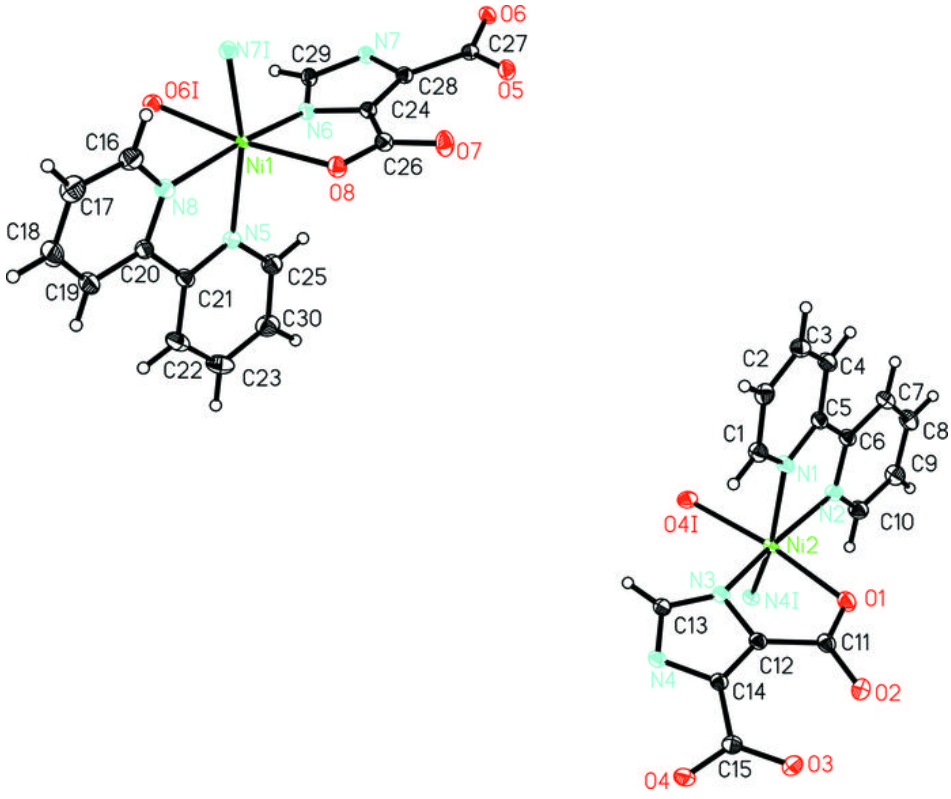
O6
C27
N7I
C29
N7
O5
C28
O6I
C24
N6
C16
Ni1
O7
C26
O8
N8
C17
C18
N5
C20
C25
C19
C21
C30
C22
C23
C3
C2
C4
C7
C5
C8
C1
C6
C9
N1
N2
C10
O4I
Ni2
N3
N4I
O1
C13
C11
C12
N4
C14
O2
O4
C15
O3

Fig. 2