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## Structure Reports

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## Aqua(2,2'-bipyridyl)(pyrazine-2,6-dicarboxylato)nickel(II) 1.25-hydrate

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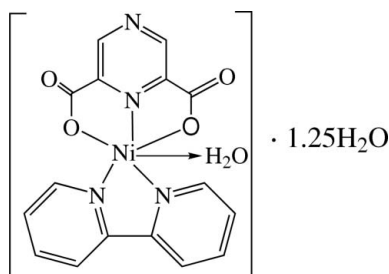
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Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å; disorder in solvent or counterion;  $R$  factor = 0.037;  $wR$  factor = 0.102; data-to-parameter ratio = 14.2.

The asymmetric unit of the title compound,  $[\text{Ni}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 1.25\text{H}_2\text{O}$ , contains two independent chemically identical  $\text{Ni}^{\text{II}}$  complex cations and two and a half solvent water molecules. The  $\text{Ni}^{\text{II}}$  ions are in slightly distorted coordination environments. In the crystal structure, intermolecular  $\text{O}-\text{H} \cdots \text{O}$  and weak  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds link cations and water molecules into a three-dimensional network. One of the three uncoordinated water molecules is half-occupied.

## Related literature

For related structures, see: Wang *et al.* (2006); Wang, Weng, *et al.* (2007); Wang, Zheng & Jin (2007); Wang, Zheng, *et al.* (2007, 2008); Wang, Mu *et al.* (2008).



## Experimental

## Crystal data

$[\text{Ni}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 1.25\text{H}_2\text{O}$

 $M_r = 421.5$ 

Monoclinic,  $P2_1/c$   
 $a = 10.7616$  (12) Å  
 $b = 14.8677$  (17) Å  
 $c = 21.933$  (2) Å

$\beta = 101.015$  (2)°  
 $V = 3444.6$  (7) Å<sup>3</sup>  
 $Z = 8$

Mo  $K\alpha$  radiation  
 $\mu = 1.17$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 $0.22 \times 0.10 \times 0.08$  mm

## Data collection

Bruker SMART CCD diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.796$ ,  $T_{\text{max}} = 0.871$

19122 measured reflections  
 7030 independent reflections  
 4740 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.102$   
 $S = 1.04$   
 7030 reflections

496 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Ni1—N1	1.986 (2)	Ni2—N5	1.986 (2)
Ni1—N3	2.047 (3)	Ni2—N8	2.044 (2)
Ni1—O5	2.059 (2)	Ni2—O10	2.068 (2)
Ni1—N4	2.067 (3)	Ni2—N7	2.072 (2)
Ni1—O3	2.143 (2)	Ni2—O6	2.125 (2)
Ni1—O1	2.184 (2)	Ni2—O8	2.175 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C32—H32 <sup>i</sup> ···O10	0.93	2.48	3.033 (4)	118
C31—H31 <sup>i</sup> ···O13 <sup>j</sup>	0.93	2.53	3.384 (11)	153
C29—H29 <sup>i</sup> ···O6 <sup>ii</sup>	0.93	2.53	3.318 (4)	143
C26—H26 <sup>i</sup> ···O6 <sup>ii</sup>	0.93	2.54	3.329 (4)	143
C14—H14 <sup>i</sup> ···O11 <sup>i</sup>	0.93	2.43	3.275 (5)	151
C9—H9 <sup>i</sup> ···O1 <sup>iii</sup>	0.93	2.47	3.281 (5)	146
C7—H7 <sup>i</sup> ···O5	0.93	2.50	3.000 (4)	114
O13—H13A <sup>i</sup> ···O13 <sup>iv</sup>	0.86	1.73	2.26 (2)	118
O12—H12B <sup>i</sup> ···O13	0.85	1.79	2.636 (12)	179
O12—H12A <sup>i</sup> ···O3	0.85	2.33	2.856 (4)	121
O11—H11B <sup>i</sup> ···O8	0.85	2.06	2.912 (3)	177
O11—H11A <sup>i</sup> ···O7 <sup>v</sup>	0.85	2.07	2.921 (4)	178
O10—H10B <sup>i</sup> ···O4 <sup>vi</sup>	0.86	1.85	2.699 (3)	170
O10—H10A <sup>i</sup> ···O2 <sup>vii</sup>	0.85	1.84	2.694 (3)	178
O5—H5B <sup>i</sup> ···O7 <sup>viii</sup>	0.85	1.85	2.686 (3)	169
O5—H5A <sup>i</sup> ···O9 <sup>ix</sup>	0.85	1.78	2.621 (3)	173

Symmetry codes: (i)  $-x + 1, -y + 1, -z$ ; (ii)  $-x + 2, -y + 1, -z$ ; (iii)  $-x + 1, -y, -z$ ; (iv)  $-x, -y, -z$ ; (v)  $x - 1, y, z$ ; (vi)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (vii)  $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (viii)  $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (ix)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH2711).

## References

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**supplementary materials**

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## Aqua(2,2'-bipyridyl)(pyrazine-2,6-dicarboxylato)nickel(II) 1.25-hydrate

F.-Q. Wang and Y.-F. Zhang

### Comment

In general, bridging multifunctional organic ligands with N- and O-donors have been proven to be good candidates as versatile coordination sites and as hydrogen-bond acceptors and donors. Pyrazine-2,6-dicarboxylic acid ( $H_2PZDC$ ) has two carboxylic groups and two pyrazine nitrogen atoms, and can be used as hydrogen-bond acceptor as well as hydrogen-bond donor, which assists in the generation of supramolecular structures. Because of the structural character, we have used this ligand in our previous work to construct 3d, 4f and 3d-4f complexes (Wang *et al.*, 2006; Wang, Weng, *et al.*, 2007; Wang, Zheng & Jin, 2007; Wang, Zheng, *et al.*, 2007; Wang, Zheng *et al.*, 2008; Wang, Mu *et al.*, 2008). Generally, when coordinated to transition metal ions, PZDC adopts tridentate (ONO) mode and is involved in various hydrogen-bonding interactions. In a continuation of our work, we report synthesis and structure of the title complex.

The asymmetric unit of the title compound is shown in Fig. 1. In the crystal structure, intermolecular O-H $\cdots$ O (Fig. 2) and weak C-H $\cdots$ O hydrogen bonds link cations and water molecules into a three-dimensional network.

### Experimental

A mixture of  $H_2PZDC$  (0.0204 g, 0.1 mmol),  $Ni(OAc)_2 \cdot 4H_2O$  (0.0249 g, 0.1 mmol), 2,2'-bipyridine (0.0156 g, 0.1 mmol), deionized water (5 ml) and isopropyl alcohol (1 ml) was sealed in a Teflon-lined stainless steel vessel (23 ml) and heated at 413K for 4 days under autogenous pressure and then cooled slowly to room temperature. The solution was filtered and allowed to stand for four weeks at room temperature. Green crystals were obtained. Anal. calcd. for  $C_{32}H_{29}Ni_2N_8O_{12.5}$ : C, 46.07; H, 3.38; N, 13.44. Found: C, 45.90; H, 3.49; N, 13.27%. IR (KBr pellet,  $cm^{-1}$ ): 3446br, 1663vs, 1630vs, 1475m, 1446 s, 1393m, 1339m, 1313w, 1192m, 1067m, 1024w, 791w, 766m, 749m.

### Refinement

All water H atoms were found in difference Fourier maps and were fixed during refinement at O–H distances of 0.85–0.86 Å, with  $U_{iso}(H) = 1.2 U_{eq}(O)$ . The H atoms of C–H and N–H groups were treated as riding, with C–H = 0.93 Å and N–H = 0.86 Å and  $U_{iso}(H) = 1.2 U_{eq}(C,N)$ .

### Figures

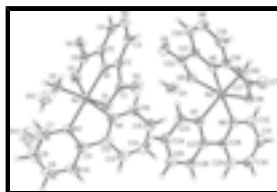


Fig. 1. The asymmetric unit of the title complex. Displacement ellipsoids are drawn at the 30% probability level.

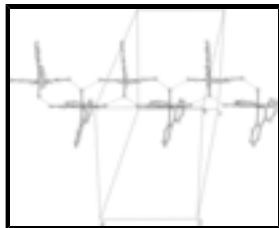


Fig. 2. Part of the crystal structure of the title compound. Dashed lines indicate the donor-acceptor separation of O-H...O hydrogen bonds. The solvent water molecules are not shown.

## Aqua(2,2'-bipyridyl)(pyrazine-2,6-dicarboxylato)nickel(II) 1.25-hydrate

### Crystal data

[Ni(C<sub>6</sub>H<sub>2</sub>N<sub>2</sub>O<sub>4</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)]·1.25H<sub>2</sub>O

$M_r = 421.5$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.7616$  (12) Å

$b = 14.8677$  (17) Å

$c = 21.933$  (2) Å

$\beta = 101.015$  (2)°

$V = 3444.6$  (7) Å<sup>3</sup>

$Z = 8$

$F_{000} = 1732$

$D_x = 1.626$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 5479 reflections

$\theta = 2.4$ – $26.1$ °

$\mu = 1.17$  mm<sup>-1</sup>

$T = 294$  (2) K

Block, green

$0.22 \times 0.1 \times 0.08$  mm

### Data collection

Bruker SMART CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294$ (2) K

$\varphi$  and  $\omega$  scans

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

$T_{\min} = 0.796$ ,  $T_{\max} = 0.871$

19122 measured reflections

7030 independent reflections

4740 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\text{max}} = 26.4$ °

$\theta_{\text{min}} = 1.7$ °

$h = -11 \rightarrow 13$

$k = -15 \rightarrow 18$

$l = -27 \rightarrow 27$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.102$

$S = 1.04$

7030 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 1.0664P]$

where  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\text{max}} = 0.31$  e Å<sup>-3</sup>

496 parameters

$$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$$

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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ni1	0.49882 (4)	0.13832 (3)	0.158117 (18)	0.04624 (12)	
Ni2	0.90485 (4)	0.54725 (3)	0.148920 (17)	0.04493 (12)	
O1	0.69996 (19)	0.12922 (15)	0.15470 (9)	0.0509 (5)	
O2	0.8901 (2)	0.17207 (17)	0.20621 (11)	0.0627 (6)	
O3	0.3425 (2)	0.17792 (16)	0.19965 (11)	0.0613 (6)	
O4	0.2998 (2)	0.24476 (17)	0.28546 (13)	0.0739 (7)	
O5	0.52042 (19)	0.01499 (15)	0.20153 (10)	0.0557 (6)	
H5A	0.4525	-0.0041	0.2114	0.067*	
H5B	0.5869	0.0128	0.2292	0.067*	
O6	1.10272 (19)	0.54558 (15)	0.15004 (9)	0.0504 (5)	
O7	1.2852 (2)	0.49209 (17)	0.20287 (10)	0.0633 (6)	
O8	0.73667 (19)	0.51540 (15)	0.18615 (10)	0.0556 (5)	
O9	0.6790 (2)	0.44246 (16)	0.26578 (12)	0.0682 (7)	
O10	0.91729 (19)	0.66902 (14)	0.19526 (9)	0.0529 (5)	
H10A	0.9788	0.6685	0.2263	0.063*	
H10B	0.8466	0.6873	0.2031	0.063*	
N1	0.5827 (2)	0.20244 (16)	0.23439 (11)	0.0444 (6)	
N2	0.6981 (3)	0.26952 (19)	0.34744 (12)	0.0604 (7)	
N3	0.4080 (3)	0.07653 (18)	0.07857 (12)	0.0550 (7)	
N4	0.4885 (2)	0.24284 (18)	0.09517 (12)	0.0519 (6)	
N5	0.9733 (2)	0.48052 (16)	0.22650 (11)	0.0442 (6)	
N6	1.0718 (3)	0.4020 (2)	0.33821 (12)	0.0604 (7)	
N7	0.8681 (2)	0.43822 (17)	0.08934 (11)	0.0461 (6)	
N8	0.8626 (2)	0.61198 (18)	0.06530 (11)	0.0489 (6)	
C1	0.7726 (3)	0.1651 (2)	0.19953 (14)	0.0473 (7)	
C2	0.7088 (3)	0.2040 (2)	0.24956 (13)	0.0438 (7)	
C3	0.7649 (3)	0.2362 (2)	0.30740 (14)	0.0534 (8)	
H3	0.8527	0.2345	0.3188	0.064*	
C4	0.5734 (4)	0.2687 (2)	0.32989 (16)	0.0594 (9)	
H4	0.5244	0.2930	0.3564	0.071*	

## supplementary materials

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C5	0.5125 (3)	0.2329 (2)	0.27347 (14)	0.0496 (7)
C6	0.3719 (3)	0.2181 (2)	0.25151 (18)	0.0577 (8)
C7	0.3595 (4)	-0.0066 (3)	0.07472 (19)	0.0750 (11)
H7	0.3617	-0.0396	0.1110	0.090*
C8	0.3065 (4)	-0.0447 (3)	0.0188 (2)	0.0921 (14)
H8	0.2738	-0.1027	0.0173	0.111*
C9	0.3022 (4)	0.0034 (3)	-0.0349 (2)	0.0946 (15)
H9	0.2684	-0.0219	-0.0733	0.114*
C10	0.3488 (4)	0.0897 (3)	-0.03107 (17)	0.0792 (12)
H10	0.3449	0.1240	-0.0668	0.095*
C11	0.4016 (3)	0.1253 (2)	0.02637 (15)	0.0570 (8)
C12	0.4508 (3)	0.2175 (2)	0.03524 (14)	0.0534 (8)
C13	0.4574 (3)	0.2769 (3)	-0.01248 (17)	0.0683 (10)
H13	0.4313	0.2588	-0.0535	0.082*
C14	0.5023 (4)	0.3625 (3)	0.00065 (19)	0.0726 (11)
H14	0.5083	0.4025	-0.0313	0.087*
C15	0.5384 (4)	0.3881 (3)	0.06166 (19)	0.0695 (10)
H15	0.5675	0.4461	0.0718	0.083*
C16	0.5307 (3)	0.3264 (2)	0.10734 (17)	0.0586 (8)
H16	0.5560	0.3437	0.1486	0.070*
C17	1.1696 (3)	0.5046 (2)	0.19481 (14)	0.0476 (7)
C18	1.0976 (3)	0.4675 (2)	0.24250 (13)	0.0453 (7)
C19	1.1455 (3)	0.4261 (2)	0.29852 (15)	0.0552 (8)
H19	1.2319	0.4146	0.3089	0.066*
C20	0.9481 (3)	0.4179 (2)	0.32100 (15)	0.0548 (8)
H20	0.8947	0.4032	0.3482	0.066*
C21	0.8961 (3)	0.4554 (2)	0.26393 (14)	0.0461 (7)
C22	0.7577 (3)	0.4730 (2)	0.23687 (16)	0.0504 (7)
C23	0.8701 (3)	0.3514 (2)	0.10518 (15)	0.0541 (8)
H23	0.8893	0.3365	0.1471	0.065*
C24	0.8451 (3)	0.2828 (2)	0.06233 (16)	0.0604 (9)
H24	0.8468	0.2230	0.0748	0.072*
C25	0.8175 (3)	0.3058 (2)	0.00035 (15)	0.0626 (9)
H25	0.8008	0.2611	-0.0298	0.075*
C26	0.8147 (3)	0.3947 (2)	-0.01701 (15)	0.0574 (8)
H26	0.7963	0.4106	-0.0588	0.069*
C27	0.8394 (3)	0.4604 (2)	0.02840 (14)	0.0468 (7)
C28	0.8390 (3)	0.5577 (2)	0.01516 (13)	0.0469 (7)
C29	0.8194 (3)	0.5928 (3)	-0.04470 (15)	0.0605 (9)
H29	0.7997	0.5548	-0.0788	0.073*
C30	0.8294 (3)	0.6840 (3)	-0.05311 (18)	0.0685 (10)
H30	0.8159	0.7084	-0.0929	0.082*
C31	0.8596 (3)	0.7385 (3)	-0.00193 (18)	0.0658 (10)
H31	0.8712	0.7999	-0.0066	0.079*
C32	0.8723 (3)	0.7013 (2)	0.05624 (17)	0.0585 (8)
H32	0.8882	0.7391	0.0907	0.070*
O11	0.4752 (3)	0.56707 (19)	0.13832 (11)	0.0797 (8)
H11A	0.4192	0.5445	0.1563	0.096*
H11B	0.5514	0.5504	0.1514	0.096*

O12	0.0915 (3)	0.1333 (3)	0.13827 (16)	0.1178 (12)	
H12A	0.1599	0.1044	0.1505	0.141*	
H12B	0.0622	0.1114	0.1026	0.141*	
O13	0.0028 (10)	0.0642 (8)	0.0279 (6)	0.235 (6)	0.50
H13A	0.0350	0.0114	0.0331	0.282*	0.50
H13B	-0.0776	0.0627	0.0204	0.282*	0.50

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0410 (2)	0.0513 (2)	0.0450 (2)	-0.00191 (17)	0.00470 (16)	-0.00111 (18)
Ni2	0.0391 (2)	0.0523 (2)	0.0422 (2)	0.00067 (17)	0.00479 (16)	-0.00043 (17)
O1	0.0459 (12)	0.0617 (14)	0.0452 (12)	-0.0003 (10)	0.0094 (10)	-0.0043 (10)
O2	0.0385 (13)	0.0865 (18)	0.0628 (14)	0.0001 (11)	0.0086 (10)	0.0134 (13)
O3	0.0426 (13)	0.0677 (15)	0.0741 (15)	-0.0030 (11)	0.0123 (11)	-0.0088 (13)
O4	0.0611 (16)	0.0648 (16)	0.107 (2)	-0.0064 (12)	0.0438 (15)	-0.0133 (14)
O5	0.0431 (12)	0.0632 (14)	0.0592 (13)	-0.0063 (10)	0.0061 (10)	0.0097 (11)
O6	0.0427 (12)	0.0635 (14)	0.0451 (11)	-0.0007 (10)	0.0092 (9)	0.0010 (10)
O7	0.0386 (13)	0.0897 (18)	0.0612 (14)	0.0015 (11)	0.0083 (10)	-0.0070 (13)
O8	0.0385 (12)	0.0664 (15)	0.0613 (14)	0.0016 (10)	0.0080 (10)	0.0019 (12)
O9	0.0531 (14)	0.0663 (16)	0.0934 (18)	0.0054 (11)	0.0350 (13)	0.0159 (13)
O10	0.0423 (12)	0.0601 (14)	0.0552 (12)	0.0041 (10)	0.0068 (10)	-0.0087 (10)
N1	0.0453 (15)	0.0449 (14)	0.0445 (13)	-0.0043 (11)	0.0122 (11)	0.0010 (11)
N2	0.074 (2)	0.0609 (18)	0.0449 (15)	-0.0132 (15)	0.0083 (14)	-0.0022 (13)
N3	0.0522 (16)	0.0561 (17)	0.0530 (16)	-0.0020 (13)	0.0004 (13)	-0.0071 (13)
N4	0.0491 (16)	0.0555 (17)	0.0501 (15)	0.0030 (12)	0.0071 (12)	0.0026 (12)
N5	0.0416 (14)	0.0484 (14)	0.0424 (13)	0.0000 (11)	0.0076 (11)	-0.0035 (11)
N6	0.065 (2)	0.0651 (19)	0.0488 (16)	0.0026 (14)	0.0050 (14)	0.0079 (14)
N7	0.0460 (14)	0.0533 (16)	0.0387 (13)	-0.0002 (11)	0.0072 (11)	0.0014 (11)
N8	0.0426 (14)	0.0539 (16)	0.0496 (15)	0.0022 (11)	0.0075 (12)	0.0024 (12)
C1	0.0461 (18)	0.0491 (18)	0.0470 (17)	0.0026 (14)	0.0095 (14)	0.0101 (14)
C2	0.0421 (17)	0.0447 (17)	0.0431 (16)	-0.0061 (13)	0.0046 (13)	0.0048 (13)
C3	0.057 (2)	0.0506 (19)	0.0494 (18)	-0.0080 (15)	0.0019 (15)	0.0025 (15)
C4	0.075 (3)	0.056 (2)	0.0527 (19)	-0.0087 (17)	0.0256 (18)	-0.0061 (16)
C5	0.054 (2)	0.0450 (17)	0.0525 (18)	-0.0047 (14)	0.0179 (15)	0.0016 (14)
C6	0.053 (2)	0.0485 (19)	0.076 (2)	-0.0003 (15)	0.0251 (18)	-0.0009 (17)
C7	0.076 (3)	0.065 (2)	0.076 (3)	-0.006 (2)	-0.006 (2)	-0.009 (2)
C8	0.100 (4)	0.066 (3)	0.096 (3)	-0.008 (2)	-0.017 (3)	-0.022 (3)
C9	0.104 (4)	0.096 (4)	0.072 (3)	0.008 (3)	-0.015 (2)	-0.036 (3)
C10	0.089 (3)	0.089 (3)	0.054 (2)	0.007 (2)	-0.001 (2)	-0.013 (2)
C11	0.0487 (19)	0.071 (2)	0.0497 (18)	0.0073 (16)	0.0052 (15)	-0.0071 (17)
C12	0.0469 (18)	0.067 (2)	0.0462 (17)	0.0096 (15)	0.0087 (14)	0.0018 (16)
C13	0.066 (2)	0.087 (3)	0.053 (2)	0.014 (2)	0.0145 (18)	0.0071 (19)
C14	0.071 (3)	0.075 (3)	0.076 (3)	0.011 (2)	0.024 (2)	0.025 (2)
C15	0.072 (3)	0.056 (2)	0.084 (3)	0.0040 (18)	0.021 (2)	0.011 (2)
C16	0.059 (2)	0.052 (2)	0.062 (2)	0.0026 (16)	0.0076 (17)	0.0027 (17)
C17	0.0385 (17)	0.0571 (19)	0.0473 (17)	-0.0020 (14)	0.0083 (13)	-0.0120 (15)
C18	0.0406 (17)	0.0494 (18)	0.0448 (16)	0.0029 (13)	0.0050 (13)	-0.0072 (13)

## supplementary materials

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C19	0.0495 (19)	0.060 (2)	0.0525 (19)	0.0075 (15)	0.0003 (15)	-0.0005 (16)
C20	0.060 (2)	0.057 (2)	0.0487 (18)	-0.0043 (16)	0.0140 (16)	0.0001 (15)
C21	0.0472 (17)	0.0454 (17)	0.0465 (16)	0.0006 (14)	0.0109 (14)	-0.0052 (14)
C22	0.0450 (18)	0.0493 (19)	0.0585 (19)	0.0033 (14)	0.0144 (15)	-0.0025 (15)
C23	0.058 (2)	0.057 (2)	0.0465 (17)	-0.0006 (16)	0.0093 (15)	0.0054 (15)
C24	0.064 (2)	0.055 (2)	0.062 (2)	-0.0036 (16)	0.0100 (17)	-0.0016 (17)
C25	0.076 (2)	0.062 (2)	0.0496 (19)	-0.0089 (18)	0.0109 (17)	-0.0112 (16)
C26	0.059 (2)	0.070 (2)	0.0437 (17)	-0.0057 (17)	0.0100 (15)	-0.0025 (16)
C27	0.0369 (16)	0.0585 (19)	0.0451 (16)	-0.0010 (13)	0.0085 (13)	-0.0002 (14)
C28	0.0374 (16)	0.061 (2)	0.0433 (16)	0.0036 (14)	0.0095 (13)	0.0022 (14)
C29	0.067 (2)	0.071 (2)	0.0465 (18)	0.0098 (18)	0.0168 (16)	0.0062 (16)
C30	0.069 (2)	0.076 (3)	0.064 (2)	0.014 (2)	0.0234 (19)	0.021 (2)
C31	0.061 (2)	0.057 (2)	0.080 (3)	0.0065 (17)	0.0164 (19)	0.018 (2)
C32	0.052 (2)	0.054 (2)	0.067 (2)	0.0039 (15)	0.0062 (16)	0.0003 (17)
O11	0.0726 (18)	0.099 (2)	0.0685 (16)	0.0126 (15)	0.0163 (13)	0.0101 (15)
O12	0.087 (2)	0.157 (3)	0.106 (2)	0.005 (2)	0.0110 (19)	0.023 (2)
O13	0.156 (9)	0.262 (15)	0.298 (16)	-0.084 (9)	0.074 (10)	-0.068 (12)

### *Geometric parameters (Å, °)*

Ni1—N1	1.986 (2)	C7—C8	1.373 (5)
Ni1—N3	2.047 (3)	C7—H7	0.9300
Ni1—O5	2.059 (2)	C8—C9	1.371 (6)
Ni1—N4	2.067 (3)	C8—H8	0.9300
Ni1—O3	2.143 (2)	C9—C10	1.374 (6)
Ni1—O1	2.184 (2)	C9—H9	0.9300
Ni2—N5	1.986 (2)	C10—C11	1.384 (5)
Ni2—N8	2.044 (2)	C10—H10	0.9300
Ni2—O10	2.068 (2)	C11—C12	1.470 (5)
Ni2—N7	2.072 (2)	C12—C13	1.381 (5)
Ni2—O6	2.125 (2)	C13—C14	1.373 (5)
Ni2—O8	2.175 (2)	C13—H13	0.9300
O1—C1	1.253 (4)	C14—C15	1.374 (5)
O2—C1	1.249 (4)	C14—H14	0.9300
O3—C6	1.270 (4)	C15—C16	1.372 (5)
O4—C6	1.238 (4)	C15—H15	0.9300
O5—H5A	0.8500	C16—H16	0.9300
O5—H5B	0.8460	C17—C18	1.519 (4)
O6—C17	1.258 (4)	C18—C19	1.383 (4)
O7—C17	1.237 (3)	C19—H19	0.9300
O8—C22	1.261 (4)	C20—C21	1.387 (4)
O9—C22	1.237 (4)	C20—H20	0.9300
O10—H10A	0.8543	C21—C22	1.517 (4)
O10—H10B	0.8555	C23—C24	1.377 (4)
N1—C5	1.326 (4)	C23—H23	0.9300
N1—C2	1.334 (4)	C24—C25	1.378 (5)
N2—C4	1.324 (4)	C24—H24	0.9300
N2—C3	1.332 (4)	C25—C26	1.375 (5)
N3—C7	1.339 (4)	C25—H25	0.9300

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N3—C11	1.346 (4)	C26—C27	1.384 (4)
N4—C16	1.332 (4)	C26—H26	0.9300
N4—C12	1.353 (4)	C27—C28	1.475 (4)
N5—C21	1.328 (4)	C28—C29	1.391 (4)
N5—C18	1.331 (4)	C29—C30	1.376 (5)
N6—C20	1.334 (4)	C29—H29	0.9300
N6—C19	1.334 (4)	C30—C31	1.372 (5)
N7—C23	1.337 (4)	C30—H30	0.9300
N7—C27	1.354 (4)	C31—C32	1.373 (5)
N8—C28	1.348 (4)	C31—H31	0.9300
N8—C32	1.350 (4)	C32—H32	0.9300
C1—C2	1.515 (4)	O11—H11A	0.8487
C2—C3	1.382 (4)	O11—H11B	0.8527
C3—H3	0.9300	O12—H12A	0.8501
C4—C5	1.390 (4)	O12—H12B	0.8505
C4—H4	0.9300	O13—H13A	0.8562
C5—C6	1.514 (5)	O13—H13B	0.8500
N1—Ni1—N3	177.78 (11)	C8—C7—H7	119.1
N1—Ni1—O5	92.57 (9)	C9—C8—C7	119.6 (4)
N3—Ni1—O5	89.30 (10)	C9—C8—H8	120.2
N1—Ni1—N4	99.17 (10)	C7—C8—H8	120.2
N3—Ni1—N4	79.18 (11)	C8—C9—C10	118.8 (4)
O5—Ni1—N4	164.84 (10)	C8—C9—H9	120.6
N1—Ni1—O3	77.15 (9)	C10—C9—H9	120.6
N3—Ni1—O3	101.53 (10)	C9—C10—C11	119.6 (4)
O5—Ni1—O3	94.39 (9)	C9—C10—H10	120.2
N4—Ni1—O3	97.53 (10)	C11—C10—H10	120.2
N1—Ni1—O1	76.38 (9)	N3—C11—C10	120.9 (4)
N3—Ni1—O1	104.94 (9)	N3—C11—C12	115.6 (3)
O5—Ni1—O1	86.31 (8)	C10—C11—C12	123.5 (3)
N4—Ni1—O1	87.17 (9)	N4—C12—C13	120.6 (3)
O3—Ni1—O1	153.53 (8)	N4—C12—C11	115.0 (3)
N5—Ni2—N8	170.60 (10)	C13—C12—C11	124.4 (3)
N5—Ni2—O10	92.16 (9)	C14—C13—C12	120.0 (4)
N8—Ni2—O10	90.64 (9)	C14—C13—H13	120.0
N5—Ni2—N7	98.30 (10)	C12—C13—H13	120.0
N8—Ni2—N7	79.60 (10)	C13—C14—C15	119.0 (4)
O10—Ni2—N7	168.92 (9)	C13—C14—H14	120.5
N5—Ni2—O6	77.14 (9)	C15—C14—H14	120.5
N8—Ni2—O6	93.80 (9)	C16—C15—C14	118.7 (4)
O10—Ni2—O6	91.94 (8)	C16—C15—H15	120.6
N7—Ni2—O6	93.92 (9)	C14—C15—H15	120.6
N5—Ni2—O8	76.62 (9)	N4—C16—C15	122.9 (3)
N8—Ni2—O8	112.40 (9)	N4—C16—H16	118.6
O10—Ni2—O8	89.23 (8)	C15—C16—H16	118.6
N7—Ni2—O8	89.66 (9)	O7—C17—O6	126.4 (3)
O6—Ni2—O8	153.76 (8)	O7—C17—C18	118.6 (3)
C1—O1—Ni1	114.87 (19)	O6—C17—C18	115.0 (3)
C6—O3—Ni1	115.4 (2)	N5—C18—C19	119.0 (3)

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## supplementary materials

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Ni1—O5—H5A	112.9	N5—C18—C17	112.6 (3)
Ni1—O5—H5B	111.8	C19—C18—C17	128.4 (3)
H5A—O5—H5B	117.0	N6—C19—C18	122.2 (3)
C17—O6—Ni2	115.92 (19)	N6—C19—H19	118.9
C22—O8—Ni2	114.71 (19)	C18—C19—H19	118.9
Ni2—O10—H10A	110.5	N6—C20—C21	122.3 (3)
Ni2—O10—H10B	113.6	N6—C20—H20	118.8
H10A—O10—H10B	115.2	C21—C20—H20	118.8
C5—N1—C2	120.7 (3)	N5—C21—C20	118.6 (3)
C5—N1—Ni1	119.0 (2)	N5—C21—C22	113.1 (3)
C2—N1—Ni1	119.7 (2)	C20—C21—C22	128.2 (3)
C4—N2—C3	116.7 (3)	O9—C22—O8	127.6 (3)
C7—N3—C11	119.2 (3)	O9—C22—C21	116.9 (3)
C7—N3—Ni1	125.8 (3)	O8—C22—C21	115.4 (3)
C11—N3—Ni1	115.0 (2)	N7—C23—C24	123.1 (3)
C16—N4—C12	118.8 (3)	N7—C23—H23	118.4
C16—N4—Ni1	126.5 (2)	C24—C23—H23	118.4
C12—N4—Ni1	114.0 (2)	C23—C24—C25	117.8 (3)
C21—N5—C18	120.8 (3)	C23—C24—H24	121.1
C21—N5—Ni2	119.8 (2)	C25—C24—H24	121.1
C18—N5—Ni2	119.2 (2)	C26—C25—C24	120.1 (3)
C20—N6—C19	117.0 (3)	C26—C25—H25	120.0
C23—N7—C27	118.8 (3)	C24—C25—H25	120.0
C23—N7—Ni2	126.9 (2)	C25—C26—C27	119.2 (3)
C27—N7—Ni2	114.3 (2)	C25—C26—H26	120.4
C28—N8—C32	118.5 (3)	C27—C26—H26	120.4
C28—N8—Ni2	115.2 (2)	N7—C27—C26	121.0 (3)
C32—N8—Ni2	125.8 (2)	N7—C27—C28	115.1 (3)
O2—C1—O1	126.4 (3)	C26—C27—C28	123.9 (3)
O2—C1—C2	118.2 (3)	N8—C28—C29	121.1 (3)
O1—C1—C2	115.4 (3)	N8—C28—C27	115.7 (3)
N1—C2—C3	118.7 (3)	C29—C28—C27	123.2 (3)
N1—C2—C1	113.1 (2)	C30—C29—C28	119.6 (3)
C3—C2—C1	128.2 (3)	C30—C29—H29	120.2
N2—C3—C2	122.6 (3)	C28—C29—H29	120.2
N2—C3—H3	118.7	C31—C30—C29	119.0 (3)
C2—C3—H3	118.7	C31—C30—H30	120.5
N2—C4—C5	122.8 (3)	C29—C30—H30	120.5
N2—C4—H4	118.6	C30—C31—C32	119.2 (3)
C5—C4—H4	118.6	C30—C31—H31	120.4
N1—C5—C4	118.4 (3)	C32—C31—H31	120.4
N1—C5—C6	113.8 (3)	N8—C32—C31	122.4 (3)
C4—C5—C6	127.6 (3)	N8—C32—H32	118.8
O4—C6—O3	127.7 (3)	C31—C32—H32	118.8
O4—C6—C5	117.7 (3)	H11A—O11—H11B	116.8
O3—C6—C5	114.6 (3)	H12A—O12—H12B	104.0
N3—C7—C8	121.8 (4)	H13A—O13—H13B	111.9
N3—C7—H7	119.1		
N1—Ni1—O1—C1	0.7 (2)	C2—N1—C5—C6	-174.5 (3)

N3—Ni1—O1—C1	178.8 (2)	Ni1—N1—C5—C6	-3.3 (3)
O5—Ni1—O1—C1	-92.9 (2)	N2—C4—C5—N1	-3.4 (5)
N4—Ni1—O1—C1	100.8 (2)	N2—C4—C5—C6	172.2 (3)
O3—Ni1—O1—C1	-0.4 (3)	Ni1—O3—C6—O4	-177.4 (3)
N1—Ni1—O3—C6	-2.6 (2)	Ni1—O3—C6—C5	1.7 (4)
N3—Ni1—O3—C6	179.2 (2)	N1—C5—C6—O4	-180.0 (3)
O5—Ni1—O3—C6	89.0 (2)	C4—C5—C6—O4	4.2 (5)
N4—Ni1—O3—C6	-100.3 (2)	N1—C5—C6—O3	0.9 (4)
O1—Ni1—O3—C6	-1.5 (4)	C4—C5—C6—O3	-174.9 (3)
N5—Ni2—O6—C17	1.5 (2)	C11—N3—C7—C8	1.9 (6)
N8—Ni2—O6—C17	-175.9 (2)	Ni1—N3—C7—C8	-176.1 (3)
O10—Ni2—O6—C17	93.3 (2)	N3—C7—C8—C9	-0.3 (7)
N7—Ni2—O6—C17	-96.1 (2)	C7—C8—C9—C10	-1.4 (7)
O8—Ni2—O6—C17	1.1 (3)	C8—C9—C10—C11	1.6 (7)
N5—Ni2—O8—C22	0.8 (2)	C7—N3—C11—C10	-1.8 (5)
N8—Ni2—O8—C22	178.0 (2)	Ni1—N3—C11—C10	176.5 (3)
O10—Ni2—O8—C22	-91.6 (2)	C7—N3—C11—C12	176.8 (3)
N7—Ni2—O8—C22	99.4 (2)	Ni1—N3—C11—C12	-5.0 (4)
O6—Ni2—O8—C22	1.2 (3)	C9—C10—C11—N3	0.0 (6)
O5—Ni1—N1—C5	-90.7 (2)	C9—C10—C11—C12	-178.4 (4)
N4—Ni1—N1—C5	98.9 (2)	C16—N4—C12—C13	0.8 (5)
O3—Ni1—N1—C5	3.2 (2)	Ni1—N4—C12—C13	-170.4 (2)
O1—Ni1—N1—C5	-176.3 (2)	C16—N4—C12—C11	-177.9 (3)
O5—Ni1—N1—C2	80.6 (2)	Ni1—N4—C12—C11	10.9 (3)
N4—Ni1—N1—C2	-89.8 (2)	N3—C11—C12—N4	-4.1 (4)
O3—Ni1—N1—C2	174.5 (2)	C10—C11—C12—N4	174.4 (3)
O1—Ni1—N1—C2	-5.0 (2)	N3—C11—C12—C13	177.3 (3)
O5—Ni1—N3—C7	16.3 (3)	C10—C11—C12—C13	-4.2 (5)
N4—Ni1—N3—C7	-173.6 (3)	N4—C12—C13—C14	0.0 (5)
O3—Ni1—N3—C7	-78.0 (3)	C11—C12—C13—C14	178.5 (3)
O1—Ni1—N3—C7	102.3 (3)	C12—C13—C14—C15	-1.1 (6)
O5—Ni1—N3—C11	-161.8 (2)	C13—C14—C15—C16	1.4 (6)
N4—Ni1—N3—C11	8.3 (2)	C12—N4—C16—C15	-0.4 (5)
O3—Ni1—N3—C11	103.9 (2)	Ni1—N4—C16—C15	169.5 (3)
O1—Ni1—N3—C11	-75.8 (2)	C14—C15—C16—N4	-0.7 (6)
N1—Ni1—N4—C16	0.7 (3)	Ni2—O6—C17—O7	176.5 (3)
N3—Ni1—N4—C16	179.2 (3)	Ni2—O6—C17—C18	-3.2 (3)
O5—Ni1—N4—C16	-139.6 (3)	C21—N5—C18—C19	0.9 (4)
O3—Ni1—N4—C16	78.8 (3)	Ni2—N5—C18—C19	175.9 (2)
O1—Ni1—N4—C16	-75.0 (3)	C21—N5—C18—C17	-177.4 (3)
N1—Ni1—N4—C12	171.0 (2)	Ni2—N5—C18—C17	-2.5 (3)
N3—Ni1—N4—C12	-10.5 (2)	O7—C17—C18—N5	-176.0 (3)
O5—Ni1—N4—C12	30.7 (5)	O6—C17—C18—N5	3.7 (4)
O3—Ni1—N4—C12	-110.8 (2)	O7—C17—C18—C19	5.8 (5)
O1—Ni1—N4—C12	95.3 (2)	O6—C17—C18—C19	-174.5 (3)
O10—Ni2—N5—C21	84.3 (2)	C20—N6—C19—C18	1.4 (5)
N7—Ni2—N5—C21	-92.1 (2)	N5—C18—C19—N6	-2.8 (5)
O6—Ni2—N5—C21	175.8 (2)	C17—C18—C19—N6	175.3 (3)
O8—Ni2—N5—C21	-4.4 (2)	C19—N6—C20—C21	1.7 (5)

## supplementary materials

O10—Ni2—N5—C18	-90.8 (2)	C18—N5—C21—C20	2.1 (4)
N7—Ni2—N5—C18	92.9 (2)	Ni2—N5—C21—C20	-172.9 (2)
O6—Ni2—N5—C18	0.7 (2)	C18—N5—C21—C22	-178.2 (3)
O8—Ni2—N5—C18	-179.5 (2)	Ni2—N5—C21—C22	6.9 (3)
N5—Ni2—N7—C23	10.9 (3)	N6—C20—C21—N5	-3.5 (5)
N8—Ni2—N7—C23	-178.4 (3)	N6—C20—C21—C22	176.8 (3)
O10—Ni2—N7—C23	-149.8 (4)	Ni2—O8—C22—O9	-175.5 (3)
O6—Ni2—N7—C23	88.4 (3)	Ni2—O8—C22—C21	2.4 (3)
O8—Ni2—N7—C23	-65.5 (3)	N5—C21—C22—O9	172.2 (3)
N5—Ni2—N7—C27	-169.2 (2)	C20—C21—C22—O9	-8.1 (5)
N8—Ni2—N7—C27	1.6 (2)	N5—C21—C22—O8	-5.9 (4)
O10—Ni2—N7—C27	30.2 (6)	C20—C21—C22—O8	173.9 (3)
O6—Ni2—N7—C27	-91.6 (2)	C27—N7—C23—C24	0.5 (5)
O8—Ni2—N7—C27	114.4 (2)	Ni2—N7—C23—C24	-179.6 (2)
O10—Ni2—N8—C28	-177.6 (2)	N7—C23—C24—C25	0.3 (5)
N7—Ni2—N8—C28	-2.9 (2)	C23—C24—C25—C26	-0.5 (5)
O6—Ni2—N8—C28	90.4 (2)	C24—C25—C26—C27	-0.2 (5)
O8—Ni2—N8—C28	-88.2 (2)	C23—N7—C27—C26	-1.1 (4)
O10—Ni2—N8—C32	11.3 (3)	Ni2—N7—C27—C26	178.9 (2)
N7—Ni2—N8—C32	-174.0 (3)	C23—N7—C27—C28	179.8 (3)
O6—Ni2—N8—C32	-80.7 (3)	Ni2—N7—C27—C28	-0.1 (3)
O8—Ni2—N8—C32	100.7 (3)	C25—C26—C27—N7	1.0 (5)
Ni1—O1—C1—O2	-176.4 (2)	C25—C26—C27—C28	179.9 (3)
Ni1—O1—C1—C2	3.1 (3)	C32—N8—C28—C29	-2.8 (4)
C5—N1—C2—C3	1.3 (4)	Ni2—N8—C28—C29	-174.6 (2)
Ni1—N1—C2—C3	-169.8 (2)	C32—N8—C28—C27	175.5 (3)
C5—N1—C2—C1	179.1 (3)	Ni2—N8—C28—C27	3.6 (3)
Ni1—N1—C2—C1	7.9 (3)	N7—C27—C28—N8	-2.3 (4)
O2—C1—C2—N1	172.5 (3)	C26—C27—C28—N8	178.7 (3)
O1—C1—C2—N1	-7.0 (4)	N7—C27—C28—C29	175.9 (3)
O2—C1—C2—C3	-10.0 (5)	C26—C27—C28—C29	-3.1 (5)
O1—C1—C2—C3	170.5 (3)	N8—C28—C29—C30	2.7 (5)
C4—N2—C3—C2	1.5 (5)	C27—C28—C29—C30	-175.4 (3)
N1—C2—C3—N2	-3.1 (5)	C28—C29—C30—C31	0.5 (5)
C1—C2—C3—N2	179.5 (3)	C29—C30—C31—C32	-3.4 (5)
C3—N2—C4—C5	1.7 (5)	C28—N8—C32—C31	-0.3 (5)
C2—N1—C5—C4	1.7 (4)	Ni2—N8—C32—C31	170.5 (3)
Ni1—N1—C5—C4	172.9 (2)	C30—C31—C32—N8	3.5 (5)

### Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C32—H32 $\cdots$ O10	0.93	2.48	3.033 (4)	118
C31—H31 $\cdots$ O13 <sup>i</sup>	0.93	2.53	3.384 (11)	153
C29—H29 $\cdots$ O6 <sup>ii</sup>	0.93	2.53	3.318 (4)	143
C26—H26 $\cdots$ O6 <sup>ii</sup>	0.93	2.54	3.329 (4)	143
C14—H14 $\cdots$ O11 <sup>i</sup>	0.93	2.43	3.275 (5)	151
C9—H9 $\cdots$ O1 <sup>iii</sup>	0.93	2.47	3.281 (5)	146

C7—H7…O5	0.93	2.50	3.000 (4)	114
O13—H13A…O13 <sup>iv</sup>	0.86	1.73	2.26 (2)	118
O12—H12B…O13	0.85	1.79	2.636 (12)	179
O12—H12A…O3	0.85	2.33	2.856 (4)	121
O11—H11B…O8	0.85	2.06	2.912 (3)	177
O11—H11A…O7 <sup>v</sup>	0.85	2.07	2.921 (4)	178
O10—H10B…O4 <sup>vi</sup>	0.86	1.85	2.699 (3)	170
O10—H10A…O2 <sup>vii</sup>	0.85	1.84	2.694 (3)	178
O5—H5B…O7 <sup>viii</sup>	0.85	1.85	2.686 (3)	169
O5—H5A…O9 <sup>ix</sup>	0.85	1.78	2.621 (3)	173

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $-x+2, -y+1, -z$ ; (iii)  $-x+1, -y, -z$ ; (iv)  $-x, -y, -z$ ; (v)  $x-1, y, z$ ; (vi)  $-x+1, y+1/2, -z+1/2$ ; (vii)  $-x+2, y+1/2, -z+1/2$ ; (viii)  $-x+2, y-1/2, -z+1/2$ ; (ix)  $-x+1, y-1/2, -z+1/2$ .

Fig. 1

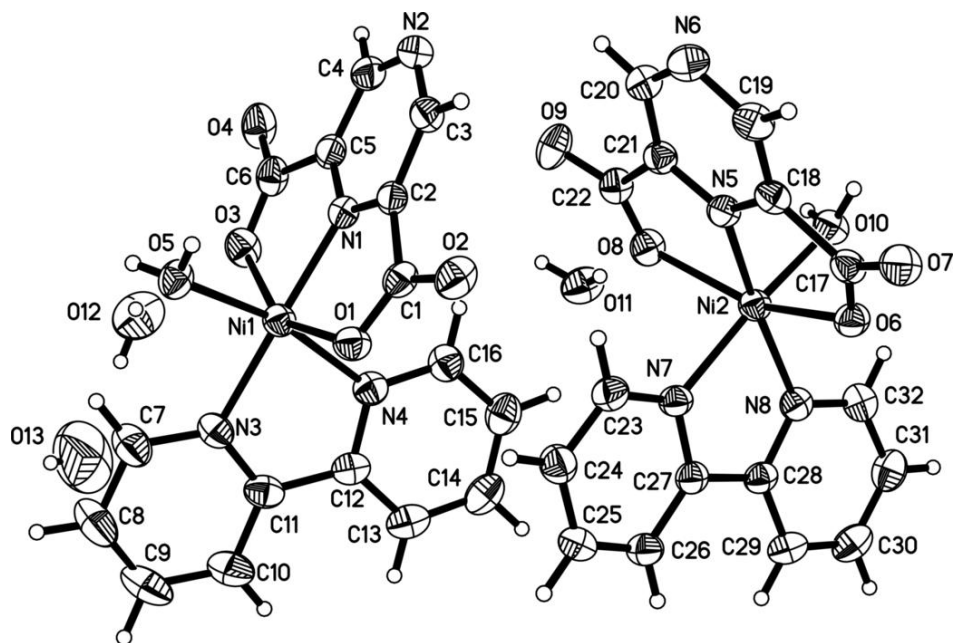


Fig. 2

