

catena-Poly[[[bis[aquanickel(II)]bis(μ -pyridine-2,6-dicarboxylato *N*-oxide)]- μ -1,2-di-4-pyridylethane] tetrahydrate]

Ming-Hua Yang

Department of Chemistry, Lishui University, Lishui 323000, People's Republic of China

Correspondence e-mail: zjlsyxh@126.com

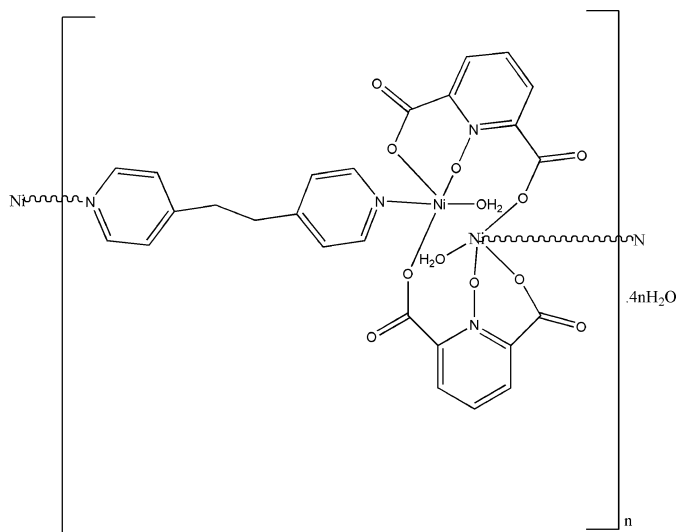
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.028; wR factor = 0.063; data-to-parameter ratio = 14.3.

In the title compound, $[\text{Ni}_2(\text{C}_7\text{H}_3\text{NO}_5)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$, two Ni^{II} ions, two tridentate pyridine-2,6-dicarboxylate *N*-oxide ligands and two coordinated water molecules form centrosymmetric dinuclear units, which are further bridged by centrosymmetric 1,2-di-4-pyridylethane ligands into polymeric chains along [210]. Each Ni^{II} ion has a distorted square-pyramidal environment, with the basal plane formed by three O [$\text{Ni}-\text{O} = 1.9290(16)$ – $1.9588(10)$ Å] and one N [$\text{Ni}-\text{N} = 1.9828(18)$ Å] atoms and the apical position occupied by the water molecule [$\text{Ni}-\text{O} = 2.2643(11)$ Å]. The water molecules are involved in the formation of $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds.

Related literature

For related literature, see: Laine *et al.* (1995*a,b*); Lin *et al.* (2006); Nathan *et al.* (1985). For a related structure, see: Wen *et al.* (2005).



Experimental

Crystal data

$[\text{Ni}_2(\text{C}_7\text{H}_3\text{NO}_5)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$	$\beta = 104.282(2)^\circ$
$M_r = 771.96$	$\gamma = 100.255(2)^\circ$
Triclinic, $P\bar{1}$	$V = 804.4(2) \text{ \AA}^3$
$a = 8.2803(16) \text{ \AA}$	$Z = 1$
$b = 10.3542(15) \text{ \AA}$	Mo $K\alpha$ radiation
$c = 11.1326(16) \text{ \AA}$	$\mu = 1.25 \text{ mm}^{-1}$
$\alpha = 113.727(2)^\circ$	$T = 298(2) \text{ K}$
	$0.25 \times 0.19 \times 0.16 \text{ mm}$

Data collection

Bruker APEXII area-detector diffractometer	4146 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2850 independent reflections
$T_{\text{min}} = 0.745$, $T_{\text{max}} = 0.825$	2180 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	199 parameters
$wR(F^2) = 0.063$	H-atom parameters constrained
$S = 0.83$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
2850 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1W}-\text{H1W} \cdots \text{O3W}^i$	0.85	1.99	2.8144 (15)	162
$\text{O1W}-\text{H2W} \cdots \text{O2}^i$	0.86	1.98	2.824 (2)	168
$\text{O3W}-\text{H6W} \cdots \text{O5}^i$	0.85	1.94	2.7791 (13)	170
$\text{O3W}-\text{H5W} \cdots \text{O2W}$	0.86	2.44	2.8527 (13)	110
$\text{O2W}-\text{H3W} \cdots \text{O2}$	0.84	2.15	2.976 (2)	167
$\text{O2W}-\text{H4W} \cdots \text{O3W}^{ii}$	0.84	1.97	2.7985 (14)	169

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEPIII (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2458).

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supplementary materials

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catena-Poly[[[bis[aquanickel(II)]bis(μ -pyridine-2,6-dicarboxylato *N*-oxide)]- μ -1,2-di-4-pyridylethane] tetrahydrate]

M.-H. Yang

Comment

The complexation of metal ions by dicarboxylate acid (pyridine-2,6-dicarboxylic acid) has been extensively studied (Laine *et al.*, 1995*a,b*). Owing to the unique ability of the ligand to form stable chelates with various coordination modes and its biological activity, many crystal structures have been determined. Pyridine-2,6-dicarboxylic acid *N*-oxide (pydco), has limited steric hindrance and weak stacking interactions and can offer possibilities to form complicated coordination polymers through polycarboxylate ligands. However, the coordination chemistry and structural properties of metal polymers containing pydco ligands have seldom been documented to date (Nathan *et al.*, 1985; Lin *et al.*, 2006; Wen *et al.*, 2005). In this paper, we report the synthesis and crystal structure of the title compound, (I).

In (I) (Fig. 1), each Ni^{II} atom is coordinated by three oxygen atoms from the carboxylato groups and one *N*-oxide entity from two pydco anions and one N atom from bridging 1,2-di-4-pyridylethane (bpa) ligand to form the basal plane, and further it coordinated by one apical oxygen atom from one water molecule to form a quasi-square pyramidal environment. Each carboxylato group is coordinated to the Ni atom in a monodentate fashion and the two carboxyl groups are out of coplanarity with the correspondingly linking pyridine rings, with the dihedral angles between them being *ca* 46° and 39°, respectively. They are very different from those in the free H₂pydco, in which the carboxyl groups are found to be essentially coplanar with the pyridine rings. Owing to the monodentate coordination modes of carboxylate groups, a binuclear [Ni₂(pydco)₂] unit was formed. Finally, bpa ligands connect the dimeric units into polymeric zigzag chain.

The crystalline water molecules contribute to intermolecular O—H...O hydrogen bonds (Table 1), which stabilize the crystal packing.

Experimental

Ni(AC)₂ (25 mg, 0.07 mmol), H₂pydco (31 mg, 0.15 mmol), bpa (19 mg, 0.09 mmol) were added in a solvent of acetonitrile, the mixture was heated for two hours under reflux. during the process stirring and influx were required. The resultant was kept at room temperature for six weeks, when single crystals were obtained.

Refinement

C-bound H atoms were geometrically positioned (C—H 0.93-0.97 Å). The O-bound H atoms were located on a Fourier difference map with O—H 0.84-0.86 °. All H atoms were refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}$ of the parent atom.

Figures

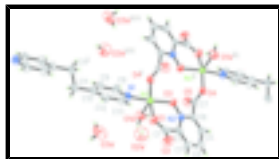


Fig. 1. A portion of the crystal structure of (I) showing the atomic numbering scheme and 40% probability displacement ellipsoids [symmetry codes: (i) $-x, -y, 2 - z$; (ii) $-x, -y, 1 - z'$ (iii) $-x, 1 - y, 1 - z$].

catena-Poly[[[bis[aquanickel(II)]bis(μ -pyridine-2,6-dicarboxylato N-oxide)]- μ -1,2-di-4-pyridylethane] tetrahydrate]

Crystal data

$[\text{Ni}_2(\text{C}_7\text{H}_3\text{NO}_5)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$

$M_r = 771.96$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.2803\ (16)\ \text{\AA}$

$b = 10.3542\ (15)\ \text{\AA}$

$c = 11.1326\ (16)\ \text{\AA}$

$\alpha = 113.727\ (2)^\circ$

$\beta = 104.282\ (2)^\circ$

$\gamma = 100.255\ (2)^\circ$

$V = 804.4\ (2)\ \text{\AA}^3$

$Z = 1$

$F_{000} = 398$

$D_x = 1.594\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2850 reflections

$\theta = 2.1\text{--}25.2^\circ$

$\mu = 1.25\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, green

$0.25 \times 0.19 \times 0.16\ \text{mm}$

Data collection

Bruker APEXII area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

φ and ω scans

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

$T_{\min} = 0.745, T_{\max} = 0.825$

4146 measured reflections

2850 independent reflections

2180 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.2^\circ$

$\theta_{\min} = 2.1^\circ$

$h = -9 \rightarrow 9$

$k = -12 \rightarrow 12$

$l = -13 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.063$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.19P]$

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

$S = 0.83$	$(\Delta/\sigma)_{\max} < 0.001$
2850 reflections	$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$
199 parameters	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
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	0.19610 (4)	0.10188 (3)	0.85792 (3)	0.03124 (11)
O1	0.0912 (2)	0.1451 (2)	0.70832 (19)	0.0473 (5)
O2	-0.1257 (2)	0.1548 (2)	0.5550 (2)	0.0600 (6)
O3	-0.03449 (19)	0.0177 (2)	0.85274 (17)	0.0433 (4)
N1	0.4335 (2)	0.2138 (2)	0.8837 (2)	0.0376 (5)
N2	-0.1753 (2)	-0.0555 (2)	0.7358 (2)	0.0354 (5)
C1	-0.0673 (3)	0.1028 (3)	0.6318 (3)	0.0401 (6)
C2	-0.2011 (3)	-0.0227 (3)	0.6272 (3)	0.0368 (6)
C3	-0.3544 (3)	-0.1043 (3)	0.5128 (3)	0.0489 (7)
H3	-0.3736	-0.0847	0.4369	0.059*
C4	-0.4795 (4)	-0.2144 (3)	0.5092 (3)	0.0570 (8)
H4	-0.5824	-0.2686	0.4315	0.068*
C5	-0.4508 (3)	-0.2433 (3)	0.6215 (3)	0.0492 (7)
H5	-0.5343	-0.3172	0.6205	0.059*
C6	-0.2980 (3)	-0.1624 (3)	0.7350 (3)	0.0366 (6)
C8	0.5711 (3)	0.1727 (3)	0.9306 (3)	0.0490 (7)
H8	0.5514	0.0953	0.9529	0.059*
C9	0.7394 (3)	0.2397 (3)	0.9470 (3)	0.0507 (7)
H9	0.8307	0.2077	0.9798	0.061*
C10	0.7726 (3)	0.3553 (3)	0.9144 (3)	0.0436 (6)
C11	0.9551 (3)	0.4316 (3)	0.9304 (3)	0.0518 (7)
H11A	1.0234	0.3635	0.9215	0.062*
H11B	0.9488	0.4587	0.8559	0.062*
C12	0.6307 (3)	0.3995 (3)	0.8690 (3)	0.0479 (7)
H12	0.6474	0.4782	0.8482	0.058*
C13	0.46548 (10)	0.32671 (9)	0.85477 (8)	0.0442 (7)
H13	0.3722	0.3577	0.8236	0.053*

supplementary materials

O1W	0.22201 (10)	-0.11885 (9)	0.72089 (8)	0.0584 (5)
H1W	0.1610	-0.1939	0.7212	0.088*
H2W	0.2045	-0.1367	0.6357	0.088*
O2W	0.15515 (10)	0.41900 (9)	0.61420 (8)	0.0944 (8)
H3W	0.0828	0.3364	0.5887	0.142*
H4W	0.1122	0.489	0.6354	0.142*
O3W	0.03080 (10)	0.37588 (9)	0.33371 (8)	0.0875 (7)
H6W	0.0820	0.3592	0.2741	0.131*
H5W	0.1116	0.4510	0.4044	0.131*
C7	-0.25478 (10)	-0.18425 (9)	0.86469 (8)	0.0374 (6)
O4	-0.28538 (10)	-0.09359 (9)	0.96606 (8)	0.0401 (4)
O5	-0.19822 (10)	-0.28825 (9)	0.85957 (8)	0.0540 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02697 (17)	0.0386 (2)	0.03728 (19)	0.00914 (13)	0.01384 (14)	0.02526 (16)
O1	0.0408 (10)	0.0605 (12)	0.0545 (12)	0.0133 (9)	0.0172 (9)	0.0406 (11)
O2	0.0654 (13)	0.0709 (14)	0.0579 (13)	0.0196 (11)	0.0122 (10)	0.0495 (12)
O3	0.0302 (9)	0.0632 (12)	0.0351 (10)	0.0041 (8)	0.0070 (8)	0.0286 (9)
N1	0.0335 (11)	0.0434 (13)	0.0472 (13)	0.0122 (10)	0.0175 (10)	0.0297 (11)
N2	0.0296 (11)	0.0454 (13)	0.0341 (12)	0.0114 (10)	0.0107 (10)	0.0218 (11)
C1	0.0484 (16)	0.0430 (16)	0.0361 (15)	0.0176 (13)	0.0183 (13)	0.0219 (13)
C2	0.0388 (14)	0.0456 (16)	0.0335 (14)	0.0180 (12)	0.0152 (12)	0.0221 (13)
C3	0.0471 (16)	0.0630 (19)	0.0386 (16)	0.0170 (15)	0.0102 (14)	0.0285 (15)
C4	0.0403 (16)	0.073 (2)	0.0413 (17)	0.0064 (15)	0.0009 (14)	0.0243 (16)
C5	0.0403 (15)	0.0570 (19)	0.0440 (17)	0.0067 (13)	0.0102 (13)	0.0241 (15)
C6	0.0319 (13)	0.0431 (16)	0.0374 (15)	0.0096 (12)	0.0129 (12)	0.0219 (13)
C8	0.0419 (15)	0.0528 (18)	0.070 (2)	0.0182 (13)	0.0246 (15)	0.0413 (16)
C9	0.0376 (15)	0.0531 (18)	0.070 (2)	0.0172 (13)	0.0220 (14)	0.0340 (16)
C10	0.0384 (14)	0.0430 (16)	0.0456 (16)	0.0072 (12)	0.0191 (13)	0.0172 (14)
C11	0.0420 (16)	0.0497 (18)	0.0549 (18)	0.0048 (13)	0.0224 (14)	0.0172 (14)
C12	0.0497 (16)	0.0403 (16)	0.0560 (18)	0.0061 (13)	0.0202 (14)	0.0270 (15)
C13	0.0400 (15)	0.0445 (16)	0.0553 (17)	0.0127 (13)	0.0167 (13)	0.0305 (15)
O1W	0.0732 (13)	0.0580 (13)	0.0531 (12)	0.0221 (11)	0.0286 (11)	0.0301 (11)
O2W	0.1038 (19)	0.0682 (16)	0.113 (2)	0.0268 (14)	0.0349 (16)	0.0454 (15)
O3W	0.127 (2)	0.0742 (16)	0.0925 (17)	0.0440 (15)	0.0679 (16)	0.0463 (14)
C7	0.0256 (13)	0.0449 (17)	0.0418 (16)	0.0028 (12)	0.0102 (12)	0.0249 (14)
O4	0.0350 (9)	0.0520 (11)	0.0420 (10)	0.0147 (8)	0.0165 (8)	0.0278 (9)
O5	0.0675 (13)	0.0502 (12)	0.0608 (13)	0.0252 (10)	0.0269 (11)	0.0360 (11)

Geometric parameters (\AA , $^\circ$)

Ni1—O3	1.9290 (16)	C8—C9	1.373 (3)
Ni1—O1	1.9373 (16)	C8—H8	0.9300
Ni1—O4 ⁱ	1.9588 (10)	C9—C10	1.386 (3)
Ni1—N1	1.9828 (18)	C9—H9	0.9300
Ni1—O1W	2.2643 (11)	C10—C12	1.390 (3)

O1—C1	1.258 (3)	C10—C11	1.506 (3)
O2—C1	1.230 (3)	C11—C11 ⁱⁱ	1.501 (5)
O3—N2	1.331 (2)	C11—H11A	0.9700
N1—C13	1.3332 (19)	C11—H11B	0.9700
N1—C8	1.345 (3)	C12—C13	1.376 (3)
N2—C6	1.358 (3)	C12—H12	0.9300
N2—C2	1.361 (3)	C13—H13	0.9300
C1—C2	1.525 (3)	O1W—H1W	0.85
C2—C3	1.379 (3)	O1W—H2W	0.86
C3—C4	1.377 (4)	O2W—H3W	0.84
C3—H3	0.9300	O2W—H4W	0.84
C4—C5	1.375 (3)	O3W—H6W	0.85
C4—H4	0.9300	O3W—H5W	0.86
C5—C6	1.371 (3)	C7—O5	1.2351 (14)
C5—H5	0.9300	C7—O4	1.2618 (12)
C6—C7	1.517 (3)	O4—Ni1 ⁱ	1.9588 (10)
O3—Ni1—O1	89.83 (7)	N2—C6—C5	120.3 (2)
O3—Ni1—O4 ⁱ	86.14 (5)	N2—C6—C7	116.2 (2)
O1—Ni1—O4 ⁱ	167.38 (6)	C5—C6—C7	123.6 (3)
O3—Ni1—N1	172.23 (8)	N1—C8—C9	123.1 (2)
O1—Ni1—N1	90.76 (7)	N1—C8—H8	118.5
O4 ⁱ —Ni1—N1	91.65 (6)	C9—C8—H8	118.5
O3—Ni1—O1W	94.95 (6)	C8—C9—C10	119.7 (2)
O1—Ni1—O1W	97.00 (6)	C8—C9—H9	120.2
O4 ⁱ —Ni1—O1W	95.30 (6)	C10—C9—H9	120.2
N1—Ni1—O1W	92.67 (6)	C9—C10—C12	117.0 (2)
C1—O1—Ni1	129.11 (16)	C9—C10—C11	121.5 (2)
N2—O3—Ni1	123.58 (13)	C12—C10—C11	121.5 (2)
C13—N1—C8	117.39 (17)	C11 ⁱⁱ —C11—C10	111.5 (3)
C13—N1—Ni1	123.82 (12)	C11 ⁱⁱ —C11—H11A	109.3
C8—N1—Ni1	118.78 (15)	C10—C11—H11A	109.3
O3—N2—C6	114.80 (18)	C11 ⁱⁱ —C11—H11B	109.3
O3—N2—C2	123.49 (19)	C10—C11—H11B	109.3
C6—N2—C2	121.6 (2)	H11A—C11—H11B	108.0
O2—C1—O1	124.3 (2)	C13—C12—C10	120.0 (2)
O2—C1—C2	115.3 (2)	C13—C12—H12	120.0
O1—C1—C2	120.5 (2)	C10—C12—H12	120.0
N2—C2—C3	118.2 (2)	N1—C13—C12	122.78 (15)
N2—C2—C1	121.5 (2)	N1—C13—H13	118.6
C3—C2—C1	120.3 (2)	C12—C13—H13	118.6
C4—C3—C2	121.1 (2)	Ni1—O1W—H1W	115.3
C4—C3—H3	119.5	Ni1—O1W—H2W	114.2
C2—C3—H3	119.5	H1W—O1W—H2W	108.3
C5—C4—C3	119.4 (3)	H3W—O2W—H4W	113.1
C5—C4—H4	120.3	H6W—O3W—H5W	99.6
C3—C4—H4	120.3	O5—C7—O4	127.3 (1)
C6—C5—C4	119.5 (2)	O5—C7—C6	117.9 (2)

supplementary materials

C6—C5—H5	120.3	O4—C7—C6	114.9 (2)
C4—C5—H5	120.3	C7—O4—Ni ⁱ	114.7 (1)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O3W ⁱⁱⁱ	0.85	1.99	2.8144 (15)	162
O1W—H2W \cdots O2 ⁱⁱⁱ	0.86	1.98	2.824 (2)	168
O3W—H6W \cdots O5 ⁱⁱⁱ	0.85	1.94	2.7791 (13)	170
O3W—H5W \cdots O2W	0.86	2.44	2.8527 (13)	110
O2W—H3W \cdots O2	0.84	2.15	2.976 (2)	167
O2W—H4W \cdots O3W ^{iv}	0.84	1.97	2.7985 (14)	169

Symmetry codes: (iii) $-x, -y, -z+1$; (iv) $-x, -y+1, -z+1$.

Fig. 1

