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Poly[aqua[μ_3-5-(2-carboxylatophenyl)-1*H*-tetrazolato]zinc(II)]

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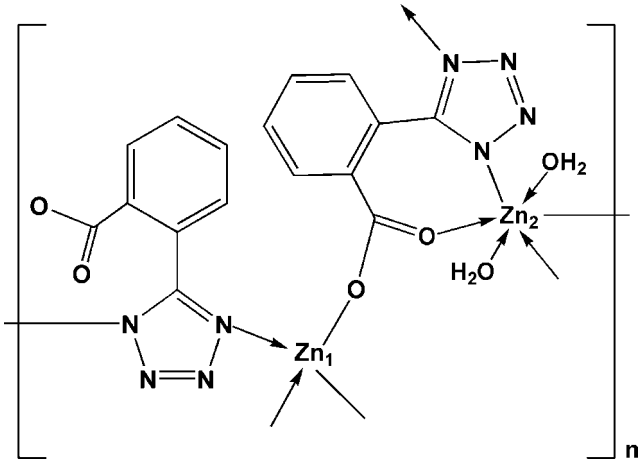
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.112; data-to-parameter ratio = 14.8.

The title coordination polymer, $[Zn(C_8H_4N_4O_2)(H_2O)]_n$, was prepared by the hydrothermal reaction of zinc nitrate and 2-(1*H*-tetrazol-5-yl)benzoic acid. Two types of coordinated zinc cations exist in the structure. One is tetrahedrally coordinated by two O and two N from two ligands, the other is octahedrally coordinated by two N and two O from two ligands at equatorial sites and by two O atoms of water molecules at axial sites, resulting in a two-dimensional framework. The crystal structure is stabilized by intramolecular O—H···O and O—H···N hydrogen bonds.

Related literature

For the chemistry of tetrazoles, see: Xiong *et al.* (2002); Xue *et al.* (2002); Dunica *et al.* (1991); Wang *et al.* (2005); Wittenberger *et al.* (1993); Hu *et al.* (2007). For the crystal structure of a related compound, see: Li *et al.* (2005).



Experimental

Crystal data

$[Zn(C_8H_4N_4O_2)(H_2O)]$
M_r = 271.56
Monoclinic, $C2/c$
a = 19.696 (8) Å
b = 7.1340 (18) Å
c = 14.932 (6) Å
β = 114.39 (2)°
V = 1910.9 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.57 mm^{-1}
T = 293 (2) K
0.07 × 0.07 × 0.06 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.835, T_{max} = 0.860
9320 measured reflections
2173 independent reflections
1623 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.112
S = 1.08
2173 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O1^{i}	0.82	2.08	2.804 (4)	147
O1W—H2W···N3^{ii}	0.79	2.25	2.976 (5)	155

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *PRPKAPPA* (Ferguson, 1999).

This work was supported by a Start-up Grant from Southeast University to ZRQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2210).

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supporting information

Acta Cryst. (2008). E**64**, m808 [doi:10.1107/S1600536808013688]

Poly[aqua[μ_3-5-(2-carboxylatophenyl)-1*H*-tetrazolato]zinc(II)]

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S1. Comment

Coordination frameworks have received much attention over the past decade because of their potential applications. Multifunctional organic ligands are necessary to construct such frameworks. 2-(1*H*-Tetrazol-5-yl)benzoic acid is a ligand with two functional groups, a carboxylate group and a tetrazole ring. Tetrazole compounds have a wide range of applications in coordination chemistry, medicinal chemistry and material science (Hu, *et al.*, 2007; Xiong, *et al.*, 2002; Xue, *et al.*, 2002; Wang, *et al.*, 2005; Dunica, *et al.*, 1991; Wittenberger & Donner, 1993). We report here the crystal structure of the title compound, which was obtained by the hydrothermal reaction of zinc nitrate and 2-(1*H*-tetrazol-5-yl)benzoic acid.

In the structure of the title compound, two types of coordinated zinc cations exist (Fig. 1). Zn1 is tetrahedrally coordinated by two O and two N from two ligands, while Zn2 is octahedrally coordinated, with two N and two O from two ligands at equatorial sites and two O atoms of H_2O molecules at axial sites, resulting in a two-dimensional framework (Fig 2). Bond lengths and angles in the compound are within normal ranges (Li *et al.*, 2005). The crystal structure is stabilized by intramolecular O—H···O and O—H···N hydrogen bonds (Table 1).

S2. Experimental

A mixture of $Zn(NO_3)_2$ (0.2 mmol) and 2-(1*H*-tetrazol-5-yl)benzoic acid (0.2 mmol) in H_2O (4 ml) was heated in Pyrex tube at 100°C for two days. After slowly cooling down to room temperature over a period of 12 h, colourless crystals of the title compound suitable for diffraction were isolated.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on their parent atoms, with C—H = 0.93 Å, O—H = 0.81Å and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O).

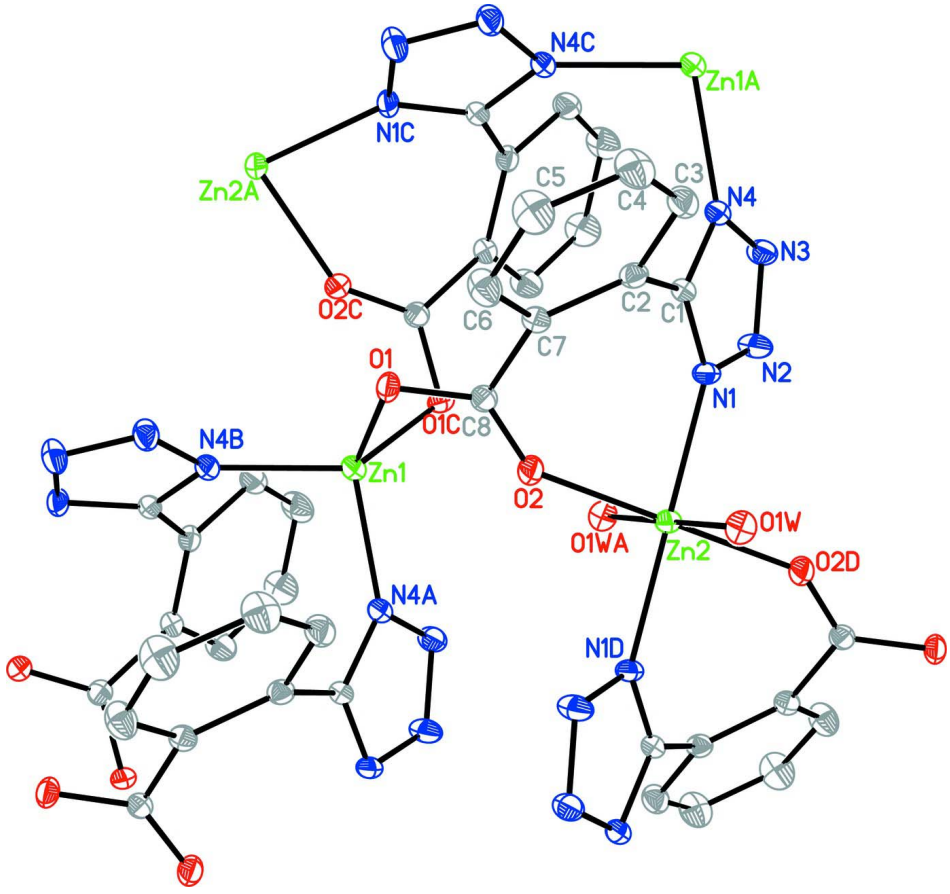

Figure 1

A partial packing diagram of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are omitted for clarity. [Symmetry codes: (A) 2-x, -y, 1-z; (B) x, y-1, z; (C) 2-x, y-1, 1/2-z; (D) 2-x, y, 1/2-z].

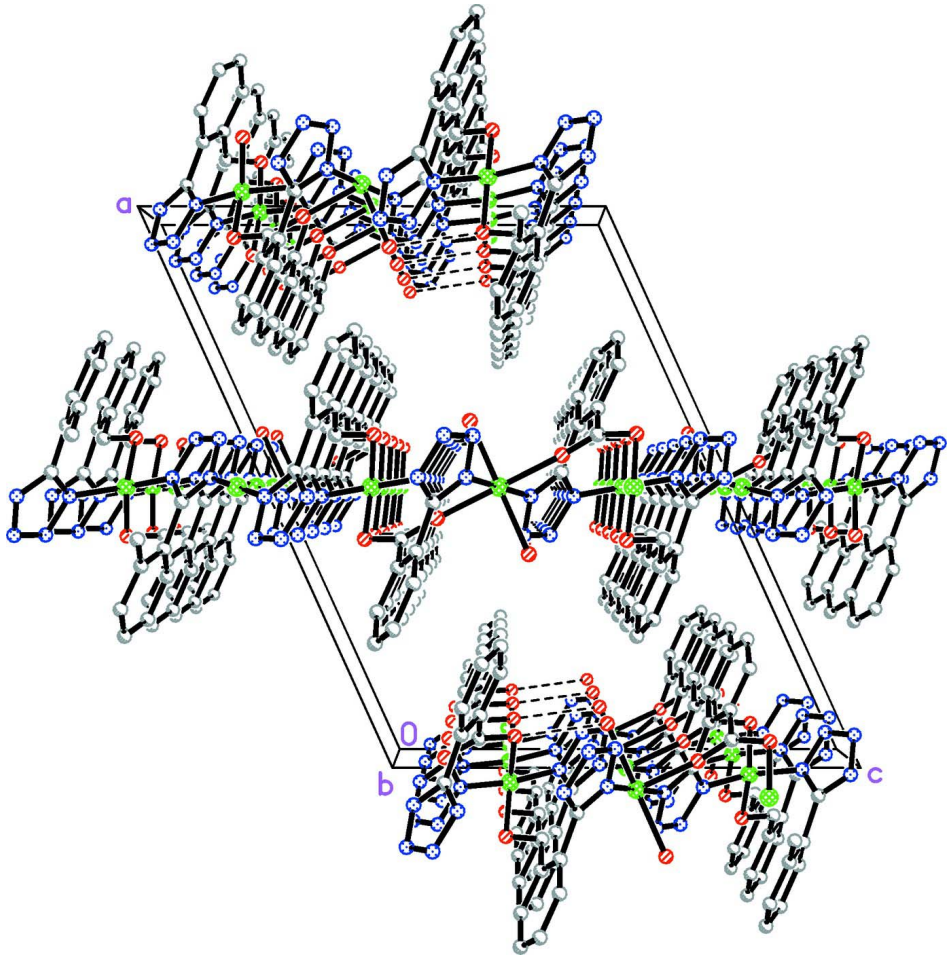

Figure 2

Packing diagram of the title compound, showing the structure along the *b* axis. H atoms are omitted for clarity.

Poly[aqua[μ_3-5-(2-carboxylatophenyl)-1*H*-tetrazolato]zinc(II)]

Crystal data

$[Zn(C_8H_4N_4O_2)(H_2O)]$
M_r = 271.56
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 19.696 (8) Å
b = 7.1340 (18) Å
c = 14.932 (6) Å
β = 114.39 (2)°
V = 1910.9 (12) Å^3
Z = 8
F(000) = 1088.0
D_x = 1.888 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1979 reflections
θ = 3.1–27.5°
μ = 2.57 mm^{-1}
T = 293 K
Block, colourless
0.07 × 0.07 × 0.06 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.835, T_{max} = 0.860
9320 measured reflections

2173 independent reflections
1623 reflections with $I > 2\sigma(I)$
$R_{int} = 0.085$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -25 \rightarrow 25$
$k = -9 \rightarrow 9$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.112$
$S = 1.08$
2173 reflections
147 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2 + 0.0509P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-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^ > σ(*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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	1.0000	−0.31787 (9)	0.2500	0.0245 (2)
Zn2	1.0000	0.0000	0.5000	0.0242 (2)
C1	0.9761 (2)	0.3503 (5)	0.3649 (3)	0.0202 (8)
C2	0.8990 (2)	0.3170 (6)	0.2905 (3)	0.0213 (8)
C3	0.8527 (2)	0.4731 (6)	0.2629 (3)	0.0289 (10)
H3	0.8693	0.5859	0.2959	0.035*
C4	0.7821 (3)	0.4630 (6)	0.1866 (4)	0.0383 (12)
H4	0.7514	0.5681	0.1693	0.046*
C5	0.7577 (3)	0.2978 (7)	0.1370 (4)	0.0410 (12)
H5	0.7104	0.2910	0.0858	0.049*
C6	0.8032 (3)	0.1407 (6)	0.1630 (3)	0.0339 (11)
H6	0.7864	0.0299	0.1279	0.041*
C7	0.8733 (2)	0.1459 (6)	0.2405 (3)	0.0222 (9)
C8	0.9165 (2)	−0.0327 (5)	0.2671 (3)	0.0217 (9)
N1	1.0151 (2)	0.2573 (5)	0.4466 (2)	0.0241 (8)
N2	1.0788 (2)	0.3533 (5)	0.4939 (3)	0.0295 (9)
N3	1.0792 (2)	0.4999 (5)	0.4424 (3)	0.0280 (8)
N4	1.01491 (19)	0.5018 (4)	0.3598 (2)	0.0220 (7)
O1	0.91662 (17)	−0.1326 (4)	0.1958 (2)	0.0270 (7)
O2	0.94994 (17)	−0.0846 (4)	0.3536 (2)	0.0314 (7)

O1W	0.89412 (16)	0.0990 (4)	0.4984 (2)	0.0322 (7)
H1W	0.8913	0.0681	0.5497	0.048*
H2W	0.8872	0.2061	0.5035	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0335 (4)	0.0167 (3)	0.0215 (4)	0.000	0.0097 (3)	0.000
Zn2	0.0341 (4)	0.0186 (4)	0.0186 (4)	−0.0009 (3)	0.0097 (3)	0.0027 (3)
C1	0.026 (2)	0.0153 (19)	0.021 (2)	−0.0018 (17)	0.0104 (17)	0.0000 (16)
C2	0.021 (2)	0.022 (2)	0.0183 (19)	−0.0016 (17)	0.0057 (17)	0.0025 (16)
C3	0.032 (2)	0.023 (2)	0.030 (2)	0.0042 (19)	0.011 (2)	0.0001 (18)
C4	0.031 (3)	0.033 (3)	0.045 (3)	0.013 (2)	0.009 (2)	0.003 (2)
C5	0.026 (2)	0.043 (3)	0.039 (3)	0.004 (2)	−0.002 (2)	−0.001 (2)
C6	0.029 (2)	0.029 (2)	0.035 (3)	0.001 (2)	0.004 (2)	−0.004 (2)
C7	0.024 (2)	0.019 (2)	0.022 (2)	0.0019 (17)	0.0094 (18)	0.0021 (16)
C8	0.023 (2)	0.021 (2)	0.021 (2)	−0.0050 (16)	0.0088 (18)	−0.0013 (16)
N1	0.032 (2)	0.0186 (17)	0.0189 (17)	−0.0044 (15)	0.0083 (16)	0.0033 (14)
N2	0.029 (2)	0.0235 (19)	0.030 (2)	−0.0030 (16)	0.0062 (17)	0.0079 (16)
N3	0.031 (2)	0.0223 (19)	0.0235 (19)	−0.0053 (15)	0.0041 (17)	0.0025 (14)
N4	0.0271 (18)	0.0168 (17)	0.0210 (18)	−0.0020 (14)	0.0088 (15)	0.0001 (13)
O1	0.0390 (18)	0.0226 (15)	0.0179 (14)	0.0056 (13)	0.0101 (13)	−0.0029 (12)
O2	0.048 (2)	0.0232 (16)	0.0191 (15)	0.0050 (14)	0.0100 (15)	−0.0004 (12)
O1W	0.0385 (18)	0.0309 (17)	0.0284 (17)	0.0003 (15)	0.0150 (15)	−0.0012 (14)

Geometric parameters (Å, º)

Zn1—O1^{i}	2.000 (3)	C3—H3	0.9300
Zn1—O1	2.000 (3)	C4—C5	1.369 (6)
Zn1—N4^{ii}	2.008 (3)	C4—H4	0.9300
Zn1—N4^{iii}	2.008 (3)	C5—C6	1.387 (6)
Zn2—N1	2.072 (3)	C5—H5	0.9300
Zn2—N1^{iv}	2.072 (3)	C6—C7	1.389 (6)
Zn2—O2^{iv}	2.082 (3)	C6—H6	0.9300
Zn2—O2	2.082 (3)	C7—C8	1.491 (5)
Zn2—O1W^{iv}	2.193 (3)	C8—O2	1.240 (5)
Zn2—O1W	2.193 (3)	C8—O1	1.281 (5)
C1—N1	1.321 (5)	N1—N2	1.345 (5)
C1—N4	1.343 (5)	N2—N3	1.300 (4)
C1—C2	1.484 (5)	N3—N4	1.353 (5)
C2—C3	1.390 (5)	N4—Zn1^{v}	2.008 (3)
C2—C7	1.411 (5)	O1W—H1W	0.8200
C3—C4	1.389 (6)	O1W—H2W	0.7851
O1^{i}—Zn1—O1	97.27 (17)	C2—C3—H3	119.5
O1^{i}—Zn1—N4^{ii}	124.90 (13)	C5—C4—C3	119.8 (4)
O1—Zn1—N4^{ii}	105.93 (12)	C5—C4—H4	120.1
O1^{i}—Zn1—N4^{iii}	105.93 (12)	C3—C4—H4	120.1

O1—Zn1—N4^{iii}	124.90 (13)	C4—C5—C6	120.2 (4)
N4^{ii}—Zn1—N4^{iii}	100.34 (19)	C4—C5—H5	119.9
N1—Zn2—N1^{iv}	180.000 (1)	C6—C5—H5	119.9
N1—Zn2—O2^{iv}	93.81 (13)	C5—C6—C7	121.1 (4)
N1^{iv}—Zn2—O2^{iv}	86.19 (13)	C5—C6—H6	119.4
N1—Zn2—O2	86.19 (13)	C7—C6—H6	119.4
N1^{iv}—Zn2—O2	93.81 (13)	C6—C7—C2	118.7 (4)
O2^{iv}—Zn2—O2	180.000 (1)	C6—C7—C8	117.4 (4)
N1—Zn2—O1W^{iv}	90.11 (13)	C2—C7—C8	123.9 (3)
N1^{iv}—Zn2—O1W^{iv}	89.89 (13)	O2—C8—O1	121.1 (4)
O2^{iv}—Zn2—O1W^{iv}	92.66 (12)	O2—C8—C7	122.1 (4)
O2—Zn2—O1W^{iv}	87.34 (12)	O1—C8—C7	116.8 (4)
N1—Zn2—O1W	89.89 (13)	C1—N1—N2	106.9 (3)
N1^{iv}—Zn2—O1W	90.11 (13)	C1—N1—Zn2	132.8 (3)
O2^{iv}—Zn2—O1W	87.34 (12)	N2—N1—Zn2	120.0 (3)
O2—Zn2—O1W	92.66 (12)	N3—N2—N1	109.3 (3)
O1W^{iv}—Zn2—O1W	180.000 (1)	N2—N3—N4	108.4 (3)
N1—C1—N4	109.2 (4)	C1—N4—N3	106.3 (3)
N1—C1—C2	129.5 (4)	C1—N4—Zn1^{v}	131.8 (3)
N4—C1—C2	121.1 (3)	N3—N4—Zn1^{v}	121.1 (3)
C3—C2—C7	119.2 (4)	C8—O1—Zn1	108.4 (3)
C3—C2—C1	115.9 (4)	C8—O2—Zn2	145.6 (3)
C7—C2—C1	124.5 (4)	Zn2—O1W—H1W	109.5
C4—C3—C2	120.9 (4)	Zn2—O1W—H2W	121.0
C4—C3—H3	119.5	H1W—O1W—H2W	95.2

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O1^{vi}	0.82	2.08	2.804 (4)	147
O1*W*—H2*W*···N3^{vii}	0.79	2.25	2.976 (5)	155

Symmetry codes: (vi) *x*, −*y*, *z*+1/2; (vii) −*x*+2, −*y*+1, −*z*+1.