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catena-Poly[[tetraaqua(μ-4,4′-bipyridine-κ^2N:N')zinc(II)] fumarate tetrahydrate]

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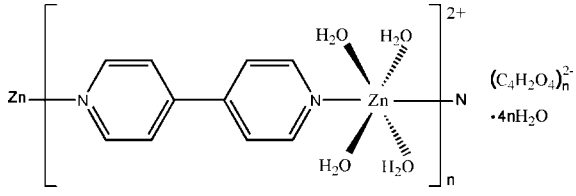
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 14.2.

In the title compound, $\{[Zn(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O\}_n$, the Zn^{II} atom is coordinated by two N atoms from two μ-4,4′-bipyridine ligands and four water molecules in a distorted octahedral geometry. The coordination unit is extended through the Zn—N bond, leading to a one-dimensional cationic chain. A twofold rotation axis passes through the Zn atom and along the axis of the 4,4′-bipyridine ligand. Each uncoordinated water molecule acts as both hydrogen-bond donor and acceptor. A three-dimensional network is constructed through hydrogen bonds involving water molecules and fumarate dianions.

Related literature

For related literature, see: Lu *et al.* (2006); Moulton & Zaworotko (2001); Nordell *et al.* (2003); Wagner *et al.* (2002); Wen *et al.* (2005); Yaghi *et al.* (1997); Zaworotko (2001); Zhou *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O$
M_r = 479.74
Monoclinic, $C2/c$
a = 17.094 (5) Å
b = 11.394 (3) Å
c = 13.082 (6) Å
β = 126.652 (2)°
V = 2044.3 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 293 (2) K
0.39 × 0.28 × 0.26 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.626, T_{max} = 0.712
7538 measured reflections
1907 independent reflections
1724 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.09
1907 reflections
134 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	2.0697 (18)	Zn1—N1	2.146 (3)
Zn1—N2^{i}	2.133 (3)	Zn1—O1	2.186 (2)
O2^{ii}—Zn1—O2	179.01 (9)	O2—Zn1—O1	88.01 (7)
O2—Zn1—N2^{i}	89.50 (4)	N2^{i}—Zn1—O1	89.21 (4)
O2—Zn1—N1	90.50 (4)	N1—Zn1—O1	90.79 (4)
O2—Zn1—O1^{ii}	91.97 (7)	O1^{ii}—Zn1—O1	178.43 (8)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···O3^{iii}	0.83	1.93	2.757 (2)	173
O1—H2W···O4^{iv}	0.83	2.01	2.835 (3)	172
O2—H3W···O3	0.83	1.91	2.732 (2)	172
O2—H4W···O6^{v}	0.82	1.83	2.623 (3)	162
O3—H5W···O5	0.83	1.88	2.707 (3)	173
O3—H6W···O4^{iv}	0.82	2.10	2.911 (3)	172
O4—H7W···O6^{v}	0.83	2.00	2.832 (3)	175
O4—H8W···O5	0.83	1.99	2.811 (3)	169

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: HY2122).

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supporting information

Acta Cryst. (2008). E**64**, m662–m663 [doi:10.1107/S1600536808009227]

catena-Poly[[tetraaqua(*μ*-4,4′-bipyridine-*κ*^{2}*N*:*N*′)zinc(II)] fumarate tetrahydrate]

Yong Tian, Ya-Pan Wu, Dong-Sheng Li, Hui Wang and Ji-Wu Wang

S1. Comment

Coordination polymer networks represent a result of applying supramolecular concepts to the design of new functional solids and are well exemplified by compounds in which transition metal centers (nodes) are connected by linear bidentate organic ligands (spacer groups) such as 4,4′-bipyridine (Lu *et al.*, 2006; Nordell *et al.*, 2003; Wagner *et al.*, 2002; Wen *et al.*, 2005; Yaghi *et al.*, 1997; Zhou *et al.*, 2007). These supramolecular structures are of interest as they provide opportunity for generating open framework compounds with controllable cavity sizes and they therefore have the potential to exhibit porosity and/or encapsulate guest molecules (Moulton & Zaworotko, 2001; Zaworotko, 2001).

The title compound consists of one $[Zn(C_{10}H_8N_2)(H_2O)_4]^{2+}$ cation, one fumarate dianion and four lattice water molecules (Fig. 1). Each Zn^{II} atom is six-coordinated in an octahedral geometry with four O atoms of four water molecules in the equatorial plane and two N atoms from two *μ*-4,4′-bipyridine ligands in the axial sites, resulting a one-dimensional cationic chain along the *b*-axis. The two pyridyl rings of 4,4′-bipyridine present a torsion angle of 10.0 (2)°.

Each lattice water molecule acts as both hydrogen-bond donor and acceptor. In the crystal structure, the cationic chains are arranged parallel to the *bc* plane with the fumarate dianions and lattice water molecules located between the sheets composed of the chains. A three-dimensional supramolecular network is formed by hydrogen-bonding interactions involving the water molecules and fumarate dianions (Fig. 2).

S2. Experimental

A mixture of $Zn(NO_3)_2.6H_2O$ (0.030 g, 0.1 mmol), 4,4′-bipyridine (0.016 g, 0.1 mmol), mercaptosuccinic acid (0.015 g, 0.1 mmol), NaOH (0.008 g, 0.2 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave and heated at 433 K for 72 h under autogenous pressure. After slowly cooling to room temperature, yellow block-like crystals of the title compound suitable for X-ray analysis were obtained from the reaction mixture by filtration.

S3. Refinement

H atoms of the water molecules were located in a difference Fourier map and fixed in the refinements with $U_{iso}(H) = 1.5U_{eq}(O)$. The remaining H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$

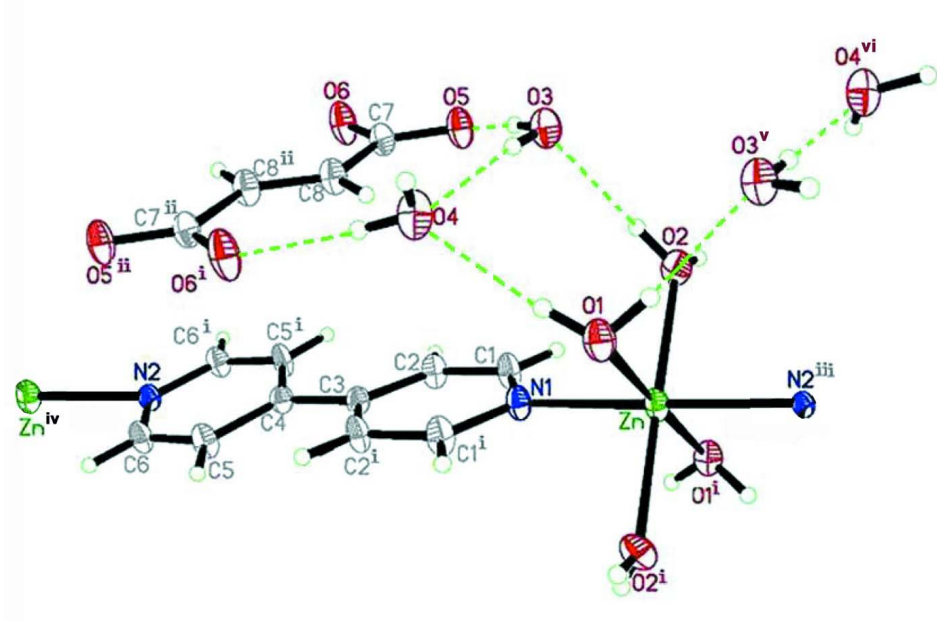

Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1 - *x*, *y*, 3/2 - *z*; (ii) 1/2 - *x*, 3/2 - *y*, 1 - *z*; (iii) *x*, -1 + *y*, *z*; (iv) *x*, 1 + *y*, *z*; (v) 1/2 - *x*, 1/2 - *y*, 1 - *z*; (vi) 1/2 - *x*, -1/2 + *y*, 3/2 - *z*.]

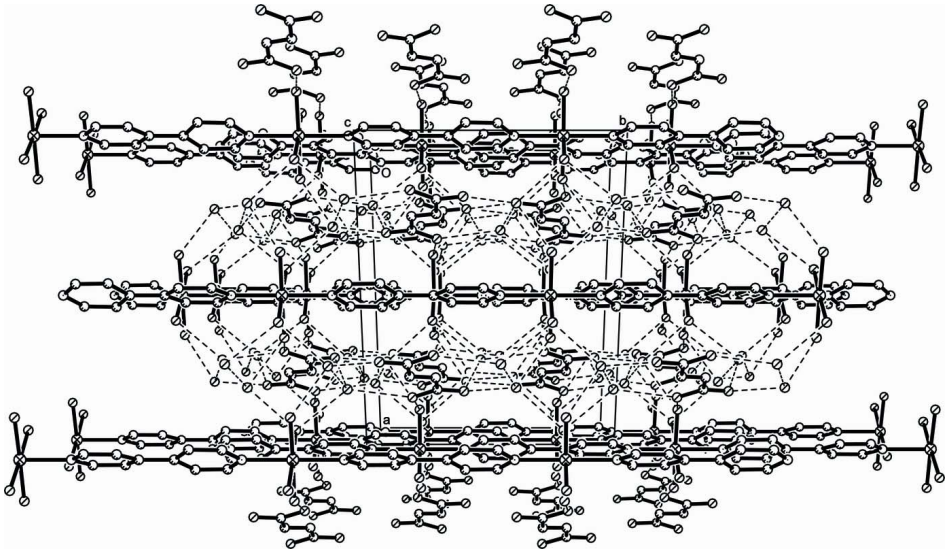

Figure 2

A view of the three-dimensional network in the title compound, viewed down the *a* axis.

catena-Poly[[tetraaqua(*μ*-4,4′-bipyridine- $\kappa^2N:N'$)zinc(II)] fumarate tetrahydrate]

Crystal data

$[Zn(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O$
M_r = 479.74
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.094 (5) Å
b = 11.394 (3) Å

c = 13.082 (6) Å
β = 126.652 (2)°
V = 2044.3 (12) Å^3
Z = 4
F(000) = 1000
D_x = 1.559 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 3920 reflections
θ = 2.3–28.2°
μ = 1.27 mm^{-1}
T = 293 K
Block, colorless
0.39 × 0.28 × 0.26 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.626, T_{max} = 0.712

7538 measured reflections
1907 independent reflections
1724 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −20→20
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.09
1907 reflections
134 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
$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 0.2551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.27603 (3)	0.7500	0.02705 (18)
O1	0.41826 (14)	0.27340 (13)	0.54278 (17)	0.0358 (4)
H1W	0.3814	0.2172	0.5259	0.054*
H2W	0.3864	0.3328	0.5041	0.054*
O2	0.36784 (13)	0.27446 (13)	0.72328 (17)	0.0358 (4)
H3W	0.3232	0.3120	0.6610	0.054*
H4W	0.3621	0.2706	0.7812	0.054*
O3	0.21520 (12)	0.40439 (15)	0.53213 (15)	0.0396 (4)
H5W	0.2070	0.4658	0.5581	0.059*
H6W	0.2331	0.4167	0.4872	0.059*
O4	0.29343 (13)	0.53785 (16)	0.89255 (16)	0.0454 (5)
H7W	0.3041	0.4667	0.8933	0.068*
H8W	0.2635	0.5646	0.8191	0.068*
O5	0.19945 (14)	0.59997 (17)	0.63613 (17)	0.0437 (4)
O6	0.17990 (18)	0.79445 (17)	0.6206 (2)	0.0499 (5)
N1	0.5000	0.4644 (2)	0.7500	0.0305 (6)
N2	0.5000	1.0888 (2)	0.7500	0.0281 (6)

C1	0.47776 (19)	0.5262 (2)	0.8170 (2)	0.0375 (6)
H1A	0.4613	0.4854	0.8633	0.045*
C2	0.47816 (19)	0.6469 (2)	0.8206 (2)	0.0352 (5)
H2A	0.4638	0.6856	0.8702	0.042*
C3	0.5000	0.7114 (3)	0.7500	0.0288 (7)
C4	0.5000	0.8413 (3)	0.7500	0.0286 (7)
C5	0.5361 (2)	0.9065 (2)	0.6958 (3)	0.0378 (6)
H5	0.5612	0.8681	0.6584	0.045*
C6	0.53453 (18)	1.0269 (2)	0.6974 (2)	0.0358 (5)
H6	0.5587	1.0677	0.6601	0.043*
C7	0.20633 (18)	0.6996 (2)	0.6001 (2)	0.0330 (5)
C8	0.24700 (18)	0.7029 (2)	0.5263 (2)	0.0355 (5)
H8	0.2699	0.6328	0.5167	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0401 (3)	0.0197 (3)	0.0348 (3)	0.000	0.0296 (2)	0.000
O1	0.0500 (10)	0.0311 (10)	0.0364 (9)	−0.0015 (6)	0.0313 (8)	0.0004 (6)
O2	0.0455 (10)	0.0390 (11)	0.0419 (10)	0.0077 (7)	0.0362 (8)	0.0091 (7)
O3	0.0540 (10)	0.0334 (9)	0.0408 (9)	−0.0009 (7)	0.0334 (8)	−0.0006 (7)
O4	0.0691 (12)	0.0338 (10)	0.0394 (10)	0.0009 (8)	0.0357 (9)	0.0017 (7)
O5	0.0722 (12)	0.0362 (10)	0.0497 (10)	−0.0015 (9)	0.0509 (10)	0.0025 (8)
O6	0.0879 (15)	0.0365 (10)	0.0668 (13)	−0.0006 (9)	0.0685 (13)	0.0000 (9)
N1	0.0468 (15)	0.0214 (13)	0.0374 (14)	0.000	0.0327 (13)	0.000
N2	0.0357 (13)	0.0213 (13)	0.0346 (14)	0.000	0.0250 (12)	0.000
C1	0.0596 (15)	0.0256 (12)	0.0471 (14)	−0.0003 (11)	0.0424 (13)	0.0025 (11)
C2	0.0574 (14)	0.0249 (11)	0.0435 (13)	0.0034 (10)	0.0410 (12)	−0.0010 (10)
C3	0.0341 (16)	0.0228 (17)	0.0319 (16)	0.000	0.0211 (14)	0.000
C4	0.0354 (15)	0.0247 (16)	0.0308 (15)	0.000	0.0224 (13)	0.000
C5	0.0595 (15)	0.0249 (12)	0.0547 (15)	0.0010 (11)	0.0480 (13)	−0.0029 (11)
C6	0.0528 (13)	0.0271 (12)	0.0489 (14)	0.0000 (10)	0.0418 (12)	0.0019 (10)
C7	0.0462 (13)	0.0339 (12)	0.0312 (11)	−0.0023 (10)	0.0297 (11)	−0.0014 (10)
C8	0.0528 (14)	0.0326 (11)	0.0401 (13)	0.0016 (10)	0.0381 (12)	−0.0007 (10)

Geometric parameters (Å, º)

Zn1—O2^{i}	2.0697 (18)	N2—C6	1.344 (3)
Zn1—O2	2.0697 (18)	N2—C6^{i}	1.344 (3)
Zn1—N2^{ii}	2.133 (3)	N2—Zn1^{iii}	2.133 (3)
Zn1—N1	2.146 (3)	C1—C2	1.376 (3)
Zn1—O1^{i}	2.186 (2)	C1—H1A	0.9300
Zn1—O1	2.186 (2)	C2—C3	1.394 (3)
O1—H1W	0.8300	C2—H2A	0.9300
O1—H2W	0.8259	C3—C2^{i}	1.394 (3)
O2—H3W	0.8283	C3—C4	1.480 (5)
O2—H4W	0.8210	C4—C5	1.400 (3)
O3—H5W	0.8263	C4—C5^{i}	1.400 (3)

O3—H6W	0.8200	C5—C6	1.372 (4)
O4—H7W	0.8299	C5—H5	0.9300
O4—H8W	0.8315	C6—H6	0.9300
O5—C7	1.261 (3)	C7—C8	1.490 (3)
O6—C7	1.261 (3)	C8—C8^{iv}	1.312 (5)
N1—C1^{i}	1.345 (3)	C8—H8	0.9300
N1—C1	1.345 (3)		

O2^{i}—Zn1—O2	179.01 (9)	C6—N2—Zn1^{iii}	121.70 (14)
O2^{i}—Zn1—N2^{ii}	89.50 (4)	C6^{i}—N2—Zn1^{iii}	121.70 (14)
O2—Zn1—N2^{ii}	89.50 (4)	N1—C1—C2	123.2 (2)
O2^{i}—Zn1—N1	90.50 (4)	N1—C1—H1A	118.4
O2—Zn1—N1	90.50 (4)	C2—C1—H1A	118.4
N2^{ii}—Zn1—N1	179.999 (1)	C1—C2—C3	120.1 (2)
O2^{i}—Zn1—O1^{i}	88.01 (7)	C1—C2—H2A	119.9
O2—Zn1—O1^{i}	91.97 (7)	C3—C2—H2A	119.9
N2^{ii}—Zn1—O1^{i}	89.21 (4)	C2^{i}—C3—C2	116.4 (3)
N1—Zn1—O1^{i}	90.79 (4)	C2^{i}—C3—C4	121.79 (14)
O2^{i}—Zn1—O1	91.98 (7)	C2—C3—C4	121.79 (14)
O2—Zn1—O1	88.01 (7)	C5—C4—C5^{i}	115.9 (3)
N2^{ii}—Zn1—O1	89.21 (4)	C5—C4—C3	122.05 (15)
N1—Zn1—O1	90.79 (4)	C5^{i}—C4—C3	122.05 (15)
O1^{i}—Zn1—O1	178.43 (8)	C6—C5—C4	120.3 (2)
Zn1—O1—H1W	99.4	C6—C5—H5	119.9
Zn1—O1—H2W	116.6	C4—C5—H5	119.9
H1W—O1—H2W	110.6	N2—C6—C5	123.5 (2)
Zn1—O2—H3W	115.7	N2—C6—H6	118.3
Zn1—O2—H4W	124.3	C5—C6—H6	118.3
H3W—O2—H4W	112.8	O6—C7—O5	124.5 (2)
H5W—O3—H6W	112.2	O6—C7—C8	118.8 (2)
H7W—O4—H8W	110.5	O5—C7—C8	116.7 (2)
C1^{i}—N1—C1	116.8 (3)	C8^{iv}—C8—C7	124.9 (3)
C1^{i}—N1—Zn1	121.60 (14)	C8^{iv}—C8—H8	117.5
C1—N1—Zn1	121.60 (14)	C7—C8—H8	117.5
C6—N2—C6^{i}	116.6 (3)		

O2^{i}—Zn1—N1—C1^{i}	45.69 (14)	C1—C2—C3—C4	179.23 (18)
O2—Zn1—N1—C1^{i}	−134.31 (14)	C2^{i}—C3—C4—C5	−10.02 (17)
O1^{i}—Zn1—N1—C1^{i}	133.71 (14)	C2—C3—C4—C5	169.98 (17)
O1—Zn1—N1—C1^{i}	−46.29 (14)	C2^{i}—C3—C4—C5^{i}	169.97 (17)
O2^{i}—Zn1—N1—C1	−134.31 (14)	C2—C3—C4—C5^{i}	−10.02 (17)
O2—Zn1—N1—C1	45.69 (14)	C5^{i}—C4—C5—C6	−0.19 (18)
O1^{i}—Zn1—N1—C1	−46.29 (15)	C3—C4—C5—C6	179.81 (18)
O1—Zn1—N1—C1	133.70 (15)	C6^{i}—N2—C6—C5	−0.21 (19)
C1^{i}—N1—C1—C2	−0.83 (19)	Zn1^{iii}—N2—C6—C5	179.80 (19)
Zn1—N1—C1—C2	179.17 (19)	C4—C5—C6—N2	0.4 (4)

N1—C1—C2—C3	1.6 (4)	O6—C7—C8—C8^{iv}	−3.9 (5)
C1—C2—C3—C2^{i}	−0.77 (18)	O5—C7—C8—C8^{iv}	174.9 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···O3^{v}	0.83	1.93	2.757 (2)	173
O1—H2*W*···O4^{vi}	0.83	2.01	2.835 (3)	172
O2—H3*W*···O3	0.83	1.91	2.732 (2)	172
O2—H4*W*···O6^{vii}	0.82	1.83	2.623 (3)	162
O3—H5*W*···O5	0.83	1.88	2.707 (3)	173
O3—H6*W*···O4^{vi}	0.82	2.10	2.911 (3)	172
O4—H7*W*···O6^{vii}	0.83	2.00	2.832 (3)	175
O4—H8*W*···O5	0.83	1.99	2.811 (3)	169

Symmetry codes: (v) −*x*+1/2, −*y*+1/2, −*z*+1; (vi) *x*, −*y*+1, *z*−1/2; (vii) −*x*+1/2, *y*−1/2, −*z*+3/2.