IUCrData

ISSN 2414-3146

catena-Poly[[[bis(pyridin-2-yl-κN)amine]zinc(II)]-μ_2-(2*E*,4*E*)-hexa-2,4-dienedioato-$\kappa^4O^1,O^{1'}:O^6,O^{6'}$] monohydrate]

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Received 1 April 2016
Accepted 15 April 2016

Edited by A. J. Lough, University of Toronto, Canada

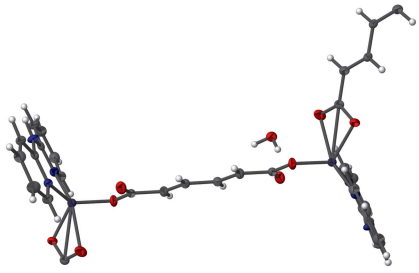
Keywords: crystal structure; Zn–MOF; muconate; di(pyridin-2-yl)amine; hydrogen bonds.

CCDC reference: 1474269

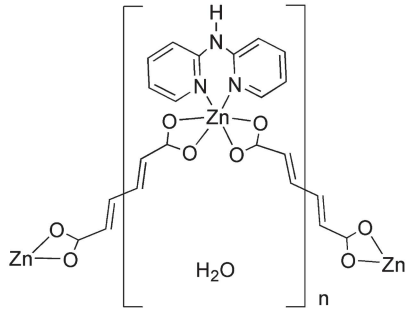
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $\{[Zn(C_6H_4O_4)(C_{10}H_9N_3)]\cdot H_2O\}_n$, the di(pyridin-2-yl)-amine (dpa) ligands chelate the Zn^{II} ions, forming $[Zn(dpa)]^{2+}$ units which are connected by two independent bridging muconate [(2*E*,4*E*)-hexa-2,4-dienedioate] ligands to form chains. A crystallographic inversion centre is located at the mid-point of the central C—C bond of each muconate ligand. The carboxylate groups of the muconate ligands bridge the Zn^{II} ions in asymmetric chelating modes. The Zn^{II} ion is coordinated by four O atoms of two chelating carboxylate groups and two pyridyl N atoms in a distorted octahedral coordination environment. In the crystal, N—H···O and O—H···O hydrogen bonds connect chains and solvent water molecules, forming a two-dimensional network parallel to (101).

3D view



Chemical scheme



Structure description

Metal–organic frameworks (MOFs), constructed from metal ions and polytopic bridging ligands, have been used for selective gas sorption, heterogeneous catalysis, separation, sensors, drug delivery and biological imaging. Dicarboxylates have provided structures of various dimensionalities with different coordination modes and pore sizes. Rigid aromatic dicarboxylates (Sumida *et al.*, 2012) have been used for the synthesis of MOFs, and flexible cyclohexanedicarboxylates (Lee *et al.* 2011; Kim *et al.* 2011) have also been used. One particular group of flexible dicarboxylates, α,ω-alkane-dicarboxylates, has been shown to be particularly suitable as ligands in MOFs of various topologies. Though less frequently employed in MOFs than aromatic dicarboxylates, recently a systematic investigation of MOFs containing these α,ω-alkane (or alkene)-dicarboxylate has been

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

D—H···A	D—H	H···A	D···A	D—H···A
N22—H22N···O1W^{i}	0.88	1.97	2.835 (3)	168
O1W—H1WB···O12	0.93 (1)	1.88 (1)	2.791 (3)	165 (3)
O1W—H1WA···O13^{ii}	0.93 (1)	1.89 (1)	2.816 (3)	172 (3)

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

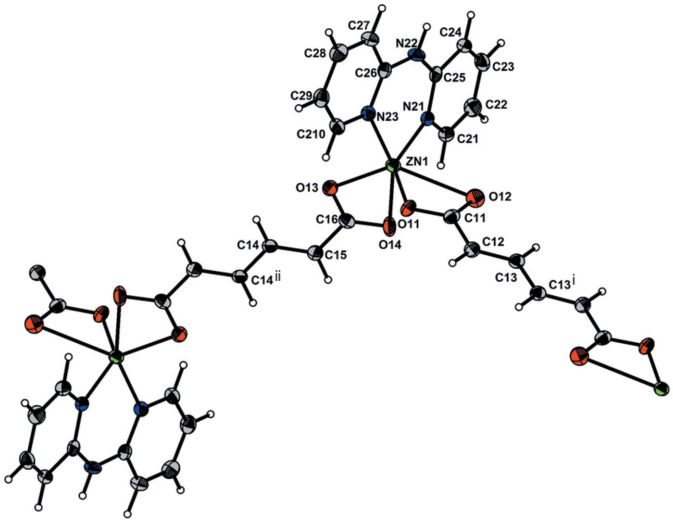


Figure 1
A fragment of the one-dimensional structure of the title compound showing displacement ellipsoids at the 50% probability level [symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, -y, -z$].

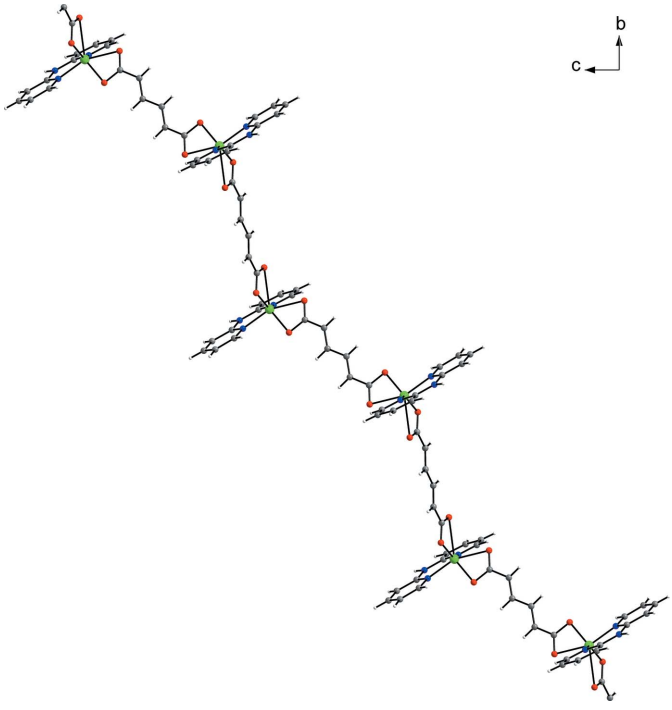


Figure 2
The one-dimensional structure of the title compound. Solvent water molecules are omitted for clarity.

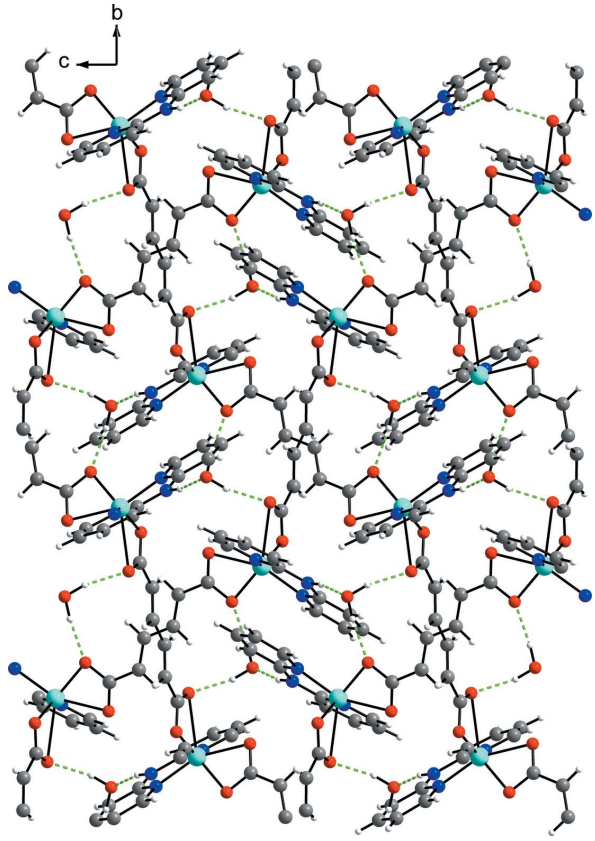


Figure 3
Part of the crystal structure showing a hydrogen-bonded layer parallel to (101). Hydrogen bonds are shown as green dotted lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_6H_4O_4)(C_{10}H_9N_3)]\cdot H_2O$
M_r	394.68
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	170
a, b, c (Å)	8.9885 (13), 15.430 (2), 11.4182 (16)
β (°)	91.806 (2)
V (Å^3)	1582.8 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.59
Crystal size (mm)	0.20 × 0.08 × 0.08
Data collection	
Diffractometer	Bruker APEX CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8674, 3089, 2391
R_{int}	0.074
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.083, 0.91
No. of reflections	3089
No. of parameters	232
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.82, −0.51

Computer programs: *SMART* and *SAINT* (Bruker, 1997), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2013* (Sheldrick, 2015).

reported (Hyun *et al.* 2013; Hwang *et al.*, 2012, 2013; Lee *et al.* 2014). We report herein the crystal structure of the title compound.

A fragment of the one-dimensional title compound, in which 2,2′-dipyridylamine ligands chelate Zn^{II} ions to form $[Zn(C_{10}H_9N_3)]^{2+}$ units, is shown in Fig. 1. The units are connected by two independent bridging muconate ligands, forming chains along [011] (Fig. 2). The carboxylate groups of the muconate ligands bridge Zn^{II} ions in asymmetric chelating modes. A crystallographic inversion centre is located at the mid-point of the central C—-C bond of each muconate ligand. The Zn^{II} ion is coordinated by four O atoms of two chelating carboxyaltes and two pyridyl N atoms in a distorted octahedral coordination environment.

In the crystal, N—H···O and O—H···O hydrogen bonds (Table 1) connect the chains and solvent water molecules, forming a two-dimensional network parallel to (101) (Fig. 3).

Synthesis and crystallization

Muconic acid (0.1 mmol, 14.2 mg) and $Zn(NO_3)_2{\cdot}6H_2O$ (0.1 mmol, 30.4 mg) were dissolved in 4 ml H_2O and carefully layered with a 4 ml acetonitrile solution of 2,2′-dipyridylaime (0.2 mmol, 34.2 mg). Suitable crystals of the title compound were obtained in a few weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

Financial support from Kwangwoon University in the year 2016 is gratefully acknowledged.

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full crystallographic data

IUCrData (2016). **1**, x160636 [doi:10.1107/S2414314616006362]

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Crystal data

$[Zn(C_6H_4O_4)(C_{10}H_9N_3)]\cdot H_2O$
M_r = 394.68
Monoclinic, $P2_1/n$
a = 8.9885 (13) Å
b = 15.430 (2) Å
c = 11.4182 (16) Å
β = 91.806 (2)°
V = 1582.8 (4) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.656 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2966 reflections
θ = 2.2–26.2°
μ = 1.59 mm^{-1}
T = 170 K
Rod, colorless
0.20 × 0.08 × 0.08 mm

Data collection

Bruker APEX CCD diffractometer
φ and ω scans
8674 measured reflections
3089 independent reflections
2391 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 26.0°, θ_{min} = 2.2°
h = −11→10
k = −17→19
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.083
S = 0.91
3089 reflections
232 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.23460 (3)	0.17315 (2)	0.36458 (3)	0.01835 (11)
O11	0.4060 (2)	0.23845 (11)	0.43746 (16)	0.0230 (4)
O12	0.2405 (2)	0.34027 (13)	0.39400 (17)	0.0275 (5)
O13	0.3294 (2)	0.08005 (12)	0.25952 (15)	0.0220 (4)
O14	0.3079 (2)	0.20738 (12)	0.17690 (17)	0.0271 (5)
N21	0.0120 (2)	0.19005 (13)	0.34368 (18)	0.0171 (5)
N22	−0.0519 (2)	0.12860 (14)	0.52676 (18)	0.0202 (5)
H22N	−0.1257	0.1249	0.5754	0.024*
N23	0.2028 (2)	0.09561 (14)	0.50930 (18)	0.0186 (5)
C11	0.3651 (3)	0.31814 (17)	0.4334 (2)	0.0203 (6)
C12	0.4757 (3)	0.38258 (17)	0.4777 (2)	0.0210 (6)
H12	0.5701	0.3626	0.5062	0.025*
C13	0.4478 (3)	0.46740 (16)	0.4790 (2)	0.0189 (6)
H13	0.3528	0.4863	0.4505	0.023*
C14	0.4636 (3)	0.01539 (17)	0.0515 (2)	0.0183 (6)
H14	0.4374	−0.0258	0.1092	0.022*
C15	0.4311 (3)	0.09863 (18)	0.0699 (2)	0.0214 (6)
H15	0.4604	0.1398	0.0133	0.026*
C16	0.3517 (3)	0.13086 (18)	0.1738 (2)	0.0190 (6)
C21	−0.0364 (3)	0.22925 (18)	0.2433 (2)	0.0227 (6)
H21	0.0344	0.2430	0.1862	0.027*
C22	−0.1815 (3)	0.24981 (18)	0.2204 (3)	0.0278 (7)
H22	−0.2112	0.2756	0.1478	0.033*
C23	−0.2856 (3)	0.23254 (18)	0.3048 (2)	0.0242 (6)
H23	−0.3873	0.2472	0.2912	0.029*
C24	−0.2399 (3)	0.19425 (17)	0.4073 (2)	0.0201 (6)
H24	−0.3090	0.1831	0.4667	0.024*
C25	−0.0897 (3)	0.17159 (16)	0.4240 (2)	0.0180 (6)
C26	0.0778 (3)	0.09022 (16)	0.5689 (2)	0.0173 (6)
C27	0.0723 (3)	0.04551 (18)	0.6760 (2)	0.0228 (6)
H27	−0.0181	0.0420	0.7166	0.027*
C28	0.1984 (3)	0.00719 (18)	0.7208 (2)	0.0255 (7)
H28	0.1970	−0.0226	0.7935	0.031*
C29	0.3296 (3)	0.01208 (18)	0.6589 (2)	0.0242 (6)
H29	0.4182	−0.0152	0.6876	0.029*
C210	0.3272 (3)	0.05701 (17)	0.5565 (2)	0.0227 (6)
H210	0.4172	0.0618	0.5156	0.027*
O1W	0.2013 (2)	0.40671 (13)	0.16781 (17)	0.0265 (5)
H1WA	0.197 (3)	0.4654 (5)	0.186 (2)	0.040*
H1WB	0.204 (3)	0.3763 (17)	0.2381 (14)	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01736 (17)	0.01915 (19)	0.01871 (18)	−0.00168 (13)	0.00328 (12)	−0.00258 (14)

O11	0.0260 (11)	0.0143 (10)	0.0287 (11)	−0.0055 (8)	0.0006 (8)	−0.0032 (8)
O12	0.0220 (11)	0.0287 (12)	0.0314 (11)	−0.0029 (9)	−0.0040 (9)	−0.0058 (9)
O13	0.0299 (11)	0.0186 (10)	0.0180 (10)	−0.0006 (8)	0.0080 (8)	−0.0018 (8)
O14	0.0357 (12)	0.0176 (11)	0.0284 (11)	0.0087 (9)	0.0061 (9)	−0.0021 (9)
N21	0.0192 (12)	0.0143 (12)	0.0180 (12)	−0.0003 (9)	0.0028 (9)	−0.0014 (9)
N22	0.0177 (12)	0.0263 (14)	0.0168 (12)	0.0004 (10)	0.0057 (9)	0.0050 (10)
N23	0.0182 (12)	0.0177 (12)	0.0200 (12)	0.0000 (9)	0.0009 (9)	−0.0011 (10)
C11	0.0259 (15)	0.0195 (15)	0.0158 (14)	−0.0055 (12)	0.0051 (11)	−0.0025 (12)
C12	0.0195 (14)	0.0193 (15)	0.0241 (15)	−0.0027 (12)	0.0006 (11)	−0.0029 (12)
C13	0.0182 (14)	0.0204 (15)	0.0182 (14)	−0.0023 (12)	0.0007 (11)	−0.0015 (12)
C14	0.0162 (13)	0.0191 (15)	0.0196 (14)	−0.0027 (11)	0.0033 (11)	0.0002 (12)
C15	0.0240 (15)	0.0202 (15)	0.0203 (15)	−0.0002 (12)	0.0055 (11)	0.0003 (12)
C16	0.0157 (13)	0.0235 (16)	0.0178 (15)	−0.0009 (12)	0.0001 (11)	−0.0028 (12)
C21	0.0259 (16)	0.0203 (15)	0.0223 (15)	0.0004 (12)	0.0069 (12)	0.0022 (12)
C22	0.0324 (17)	0.0268 (17)	0.0244 (16)	0.0056 (13)	0.0015 (13)	0.0066 (13)
C23	0.0201 (15)	0.0238 (16)	0.0288 (17)	0.0054 (12)	−0.0004 (12)	−0.0002 (13)
C24	0.0197 (14)	0.0191 (15)	0.0217 (14)	0.0000 (11)	0.0056 (11)	0.0000 (12)
C25	0.0226 (14)	0.0122 (13)	0.0193 (14)	−0.0002 (11)	0.0003 (11)	−0.0039 (11)
C26	0.0204 (14)	0.0142 (14)	0.0174 (14)	−0.0020 (11)	−0.0013 (11)	−0.0048 (11)
C27	0.0202 (14)	0.0274 (16)	0.0212 (15)	−0.0007 (12)	0.0055 (11)	0.0006 (12)
C28	0.0325 (17)	0.0252 (16)	0.0189 (15)	−0.0006 (13)	−0.0013 (12)	0.0042 (13)
C29	0.0237 (15)	0.0223 (16)	0.0264 (16)	0.0039 (13)	−0.0045 (12)	0.0016 (13)
C210	0.0174 (14)	0.0215 (16)	0.0292 (16)	0.0022 (11)	0.0025 (12)	−0.0015 (12)
O1W	0.0296 (11)	0.0208 (11)	0.0296 (12)	0.0023 (9)	0.0080 (9)	−0.0014 (9)

Geometric parameters (Å, º)

Zn1—O11	2.0000 (18)	C14—C14^{ii}	1.444 (5)
Zn1—N21	2.024 (2)	C14—H14	0.9500
Zn1—N23	2.067 (2)	C15—C16	1.489 (4)
Zn1—O13	2.0719 (18)	C15—H15	0.9500
Zn1—O14	2.3225 (19)	C21—C22	1.359 (4)
Zn1—C16	2.535 (3)	C21—H21	0.9500
O11—C11	1.284 (3)	C22—C23	1.390 (4)
O12—C11	1.242 (3)	C22—H22	0.9500
O13—C16	1.275 (3)	C23—C24	1.363 (4)
O14—C16	1.246 (3)	C23—H23	0.9500
N21—C25	1.346 (3)	C24—C25	1.402 (4)
N21—C21	1.356 (3)	C24—H24	0.9500
N22—C26	1.381 (3)	C26—C27	1.406 (4)
N22—C25	1.381 (3)	C27—C28	1.364 (4)
N22—H22N	0.8800	C27—H27	0.9500
N23—C26	1.335 (3)	C28—C29	1.396 (4)
N23—C210	1.362 (3)	C28—H28	0.9500
C11—C12	1.484 (3)	C29—C210	1.358 (4)
C12—C13	1.333 (4)	C29—H29	0.9500
C12—H12	0.9500	C210—H210	0.9500
C13—C13^{i}	1.447 (5)	O1W—H1WA	0.929 (2)

C13—H13	0.9500	O1W—H1WB	0.930 (2)
C14—C15	1.335 (4)		

O11—Zn1—N21	136.85 (8)	C14—C15—H15	118.0
O11—Zn1—N23	94.76 (8)	C16—C15—H15	118.0
N21—Zn1—N23	90.45 (8)	O14—C16—O13	120.2 (2)
O11—Zn1—O13	105.36 (7)	O14—C16—C15	120.0 (2)
N21—Zn1—O13	116.36 (8)	O13—C16—C15	119.8 (2)
N23—Zn1—O13	97.54 (8)	O14—C16—Zn1	65.86 (14)
O11—Zn1—O14	91.85 (7)	O13—C16—Zn1	54.45 (13)
N21—Zn1—O14	99.78 (8)	C15—C16—Zn1	173.3 (2)
N23—Zn1—O14	156.86 (8)	N21—C21—C22	123.2 (3)
O13—Zn1—O14	59.32 (7)	N21—C21—H21	118.4
O11—Zn1—C16	98.74 (8)	C22—C21—H21	118.4
N21—Zn1—C16	111.57 (8)	C21—C22—C23	119.0 (3)
N23—Zn1—C16	127.56 (9)	C21—C22—H22	120.5
O13—Zn1—C16	30.05 (8)	C23—C22—H22	120.5
O14—Zn1—C16	29.31 (7)	C24—C23—C22	119.2 (3)
C11—O11—Zn1	104.57 (17)	C24—C23—H23	120.4
C16—O13—Zn1	95.50 (16)	C22—C23—H23	120.4
C16—O14—Zn1	84.84 (16)	C23—C24—C25	119.2 (3)
C25—N21—C21	117.6 (2)	C23—C24—H24	120.4
C25—N21—Zn1	125.63 (18)	C25—C24—H24	120.4
C21—N21—Zn1	116.55 (18)	N21—C25—N22	121.8 (2)
C26—N22—C25	133.2 (2)	N21—C25—C24	121.8 (2)
C26—N22—H22N	113.4	N22—C25—C24	116.4 (2)
C25—N22—H22N	113.4	N23—C26—N22	120.7 (2)
C26—N23—C210	117.7 (2)	N23—C26—C27	121.8 (2)
C26—N23—Zn1	125.69 (18)	N22—C26—C27	117.5 (2)
C210—N23—Zn1	115.92 (18)	C28—C27—C26	119.2 (2)
O12—C11—O11	122.0 (2)	C28—C27—H27	120.4
O12—C11—C12	121.8 (2)	C26—C27—H27	120.4
O11—C11—C12	116.2 (2)	C27—C28—C29	119.5 (3)
C13—C12—C11	122.5 (2)	C27—C28—H28	120.3
C13—C12—H12	118.7	C29—C28—H28	120.3
C11—C12—H12	118.7	C210—C29—C28	118.2 (3)
C12—C13—C13^{i}	124.5 (3)	C210—C29—H29	120.9
C12—C13—H13	117.8	C28—C29—H29	120.9
C13^{i}—C13—H13	117.8	C29—C210—N23	123.7 (3)
C15—C14—C14^{ii}	123.5 (3)	C29—C210—H210	118.2
C15—C14—H14	118.3	N23—C210—H210	118.2
C14^{ii}—C14—H14	118.3	H1WA—O1W—H1WB	107 (3)
C14—C15—C16	124.0 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N22—H22*N*···O1*W*^{iii}	0.88	1.97	2.835 (3)	168
O1*W*—H1*WB*···O12	0.93 (1)	1.88 (1)	2.791 (3)	165 (3)
O1*W*—H1*WA*···O13^{iv}	0.93 (1)	1.89 (1)	2.816 (3)	172 (3)

Symmetry codes: (iii) $x-1/2, -y+1/2, z+1/2$; (iv) $-x+1/2, y+1/2, -z+1/2$.