Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[hexaaquazinc(II) bis[[triaquazincate(II)]-μ-(5-carboxylato-*m*-phenylenedioxy)diacetato-κ^2O^1:O^5] heptahydrate]

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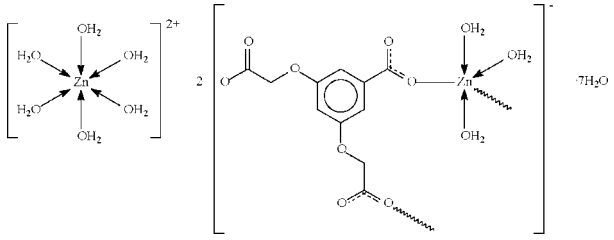
Received 10 August 2007; accepted 13 August 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.030; wR factor = 0.082; data-to-parameter ratio = 14.2.

The reaction of zinc cations and (5-carboxy-*m*-phenylenedioxy)diacetate anions in water yields the title salt, $\{[Zn(H_2O)_6][Zn(C_{11}H_7O_8)(H_2O)_3]_2\cdot 7H_2O\}_n$. The cation has the Zn atom surrounded octahedrally by six water molecules. The anion exists as a linear carboxylate-bridged chain, as it uses the carboxy and one of the two oxyacetate arms of the trianion to connect the triaquazincate species. The Zn atoms in the two independent polyanionic chains exist in trigonal–bipyramidal geometries. The cation and anions are linked by extensive hydrogen bonds into a three-dimensional network structure.

Related literature

There is currently only one other structure report of a metal (5-carboxy-*m*-phenylenedioxy)diacetate, namely a cadmium–sodium compound (Wen & Ng, 2007).



Experimental

Crystal data

$[Zn(H_2O)_6][Zn(C_{11}H_7O_8)(H_2O)_3]_2\cdot 7H_2O$
M_r = 1072.75
Triclinic, $P\overline{1}$
a = 7.2044 (1) Å
b = 11.2959 (1) Å
c = 13.6932 (2) Å
α = 70.872 (1)°
β = 76.436 (1)°
γ = 74.589 (1)°
V = 1001.59 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.90 mm^{-1}
T = 295 (2) K
0.53 × 0.13 × 0.06 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.796, T_{max} = 1.000
(expected range = 0.710–0.892)
14916 measured reflections
7671 independent reflections
7353 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.082
S = 1.04
7671 reflections
542 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Absolute structure: Flack (1983), with 3182 Friedel pairs
Flack parameter: 0.150 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O10	0.85	1.90	2.742 (3)	170
O1W—H1B···O7^{i}	0.85	1.89	2.711 (3)	162
O2W—H2A···O13W^{ii}	0.85	1.94	2.769 (4)	165
O2W—H2B···O14W^{iii}	0.85	1.74	2.591 (4)	173
O3W—H3A···O13W	0.84	1.91	2.747 (4)	176
O3W—H3B···O15^{iv}	0.84	1.89	2.722 (3)	171
O4W—H4A···O15^{v}	0.85	1.91	2.726 (3)	161
O4W—H4B···O2	0.85	1.95	2.765 (3)	163
O5W—H5A···O17W	0.85	1.84	2.651 (4)	159
O5W—H5B···O15W^{vi}	0.86	1.93	2.756 (4)	163
O6W—H6A···O7^{vii}	0.84	1.95	2.767 (4)	164
O6W—H6B···O15W	0.84	1.92	2.737 (4)	162
O7W—H7A···O5^{i}	0.87	1.90	2.726 (4)	161
O7W—H7B···O16	0.85	2.12	2.868 (4)	147
O8W—H8A···O1^{viii}	0.86	2.06	2.893 (3)	163
O8W—H8B···O19W^{ix}	0.85	1.93	2.694 (4)	151
O9W—H9A···O2W^{viii}	0.85	2.01	2.825 (4)	162
O9W—H9B···O18W	0.85	1.96	2.768 (5)	161
O10W—H10B···O18W	0.85	1.99	2.739 (4)	146
O11W—H11A···O3^{vii}	0.85	2.27	3.029 (4)	148
O11W—H11A···O3^{vii}	0.85	2.27	3.029 (4)	148
O12W—H12A···O19W^{ix}	0.85	2.00	2.740 (3)	144
O12W—H12B···O9	0.85	1.95	2.788 (3)	171
O13W—H13A···O7^{i}	0.86	2.09	2.814 (3)	142
O13W—H13B···O10^{vi}	0.86	2.07	2.849 (3)	150
O14W—H14A···O12^{x}	0.85	1.96	2.782 (4)	164
O14W—H14B···O16^{v}	0.85	1.84	2.678 (4)	168
O15W—H15A···O2^{ii}	0.84	2.30	2.914 (3)	131
O15W—H15B···O15^{v}	0.84	1.93	2.759 (4)	169
O16W—H16B···O6W^{vi}	0.86	2.17	2.937 (5)	149
O17W—H17A···O8^{viii}	0.85	1.86	2.693 (4)	170
O17W—H17B···O4	0.85	2.01	2.845 (4)	168
O18W—H18A···O8W^{ii}	0.87	2.15	2.975 (4)	156
O18W—H18B···O3W^{xi}	0.86	1.91	2.769 (4)	173
O19W—H19A···O11	0.85	2.10	2.915 (4)	164
O19W—H19B···O8^{vii}	0.85	1.95	2.759 (4)	159

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

  doi:10.1107/S1600536807040093

The authors thank the Foundation of the Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces (grant No. 0506) and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2477).

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supplementary materials

Acta Cryst. (2007). E**63**, m2378-m2379 [**doi:10.1107/S1600536807040093**]

catena-Poly[hexaaquazinc(II) bis[[triaquazincate(II)]-μ-(5-carboxylato-*m*-phenylenedioxy)diacetato-$\kappa^2O^1:O^5$] heptahydrate]

Y.-H. Wen and S. W. Ng

Comment

The reaction of zinc cations and (5-carboxy-*m*-phenylenedioxy)diacetate anions in water yields the salt, $[Zn(H_2O)_6]^{2+}$ $2[Zn(C_{11}H_7O_8)(H_2O)_3]^{-}\cdot 7H_2O$. The cation has the zinc atom surrounded octahedrally by six water molecules. The anion exists as a linear, carboxylate-bridged chain as it uses the carboxy and one of the two oxyacetate arms of the trianion to connect the triaquazinc species. The zinc atom in the two independent polyanionic chains exists in trigonal-bipyramidal geometries. The cation and anions are linked by extensive hydrogen bonds into a three-dimensional network structure.

Experimental

(5-Carboxy-*m*-phenylenedioxy)diacetic acid (0.282 g, 1 mol) and zinc nitrate hexahydrate (0.298 g, 1 mmol) were mixed in 20 ml e thanol-water (1:1, *v*/*v*) solution. The pH value was adjusted to 7 by sodium carbonate solution. The filtered solution was set aside for the growth of crystals after a week.

Refinement

The water were placed in chemically sensible positions on the basis of hydrogen bonds but they were not refined. Their temperature factors tied to those of the oxygen atoms by a factor of 1.5. The carbon-bound H-atoms were generated geometrically (C—H 0.93 to 0.97 Å); they were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

Figures

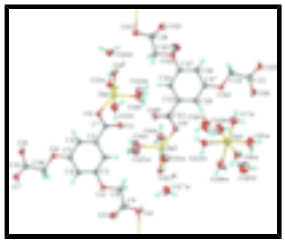


Fig. 1. Thermal ellipsoid plot depicting the coordination geometries the zinc atoms of $[Zn(H_2O)_6]^{2+}2[Zn(C_{11}H_7O_8)(H_2O)_3]^{-}\cdot 7H_2O$; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. The lattice water molecules are not shown. [Translational code: (i) $x-1, y, z$; (ii) $1+x, y-1, z$.]

catena-Poly[hexaaquazinc(II) bis[[triaquazincate(II)]-μ-(5-carboxylato-*m*-phenylenedioxy)diacetato- $\kappa^2O^1:O^5$] heptahydrate]

Crystal data

$[Zn(H_2O)_6][Zn(C_{11}H_7O_8)(H_2O)_3]_2\cdot 7H_2O$ $Z = 1$

M_r = 1072.75	F_{000} = 554
Triclinic, $P\overline{1}$	D_x = 1.779 Mg m^{-3}
Hall symbol: P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.2044 (1) Å	Cell parameters from 9439 reflections
b = 11.2959 (1) Å	θ = 2.8–27.5º
c = 13.6932 (2) Å	μ = 1.90 mm^{-1}
α = 70.872 (1)º	T = 295 (2) K
β = 76.436 (1)º	Prism, colourless
γ = 74.589 (1)º	0.53 × 0.13 × 0.06 mm
V = 1001.59 (2) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	7671 independent reflections
Radiation source: fine-focus sealed tube	7353 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.016
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→9
T_{min} = 0.796, T_{max} = 1.000	k = −14→14
14916 measured reflections	l = −17→17

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.082	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
7671 reflections	$\Delta\rho_{min}$ = −0.61 e Å^{-3}
542 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), with 3182 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.150 (6)
Secondary atom site location: difference Fourier map	

Special details

Experimental. A somewhat long crystal was used in the measurements as attempts to cut the larger ones ended up shattering the crystal. The growth of crystals could not be easily reproduced either.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.50020 (4)	0.49999 (3)	0.50000 (2)	0.02494 (9)
Zn2	1.09107 (4)	−0.01775 (3)	0.75462 (2)	0.02540 (9)
Zn3	0.83895 (6)	−0.22965 (4)	1.16257 (3)	0.03107 (9)
O1	0.6895 (3)	0.4346 (2)	0.38485 (17)	0.0275 (5)
O2	0.8194 (3)	0.2799 (2)	0.51287 (16)	0.0291 (5)
O3	1.1508 (4)	−0.07046 (19)	0.32384 (17)	0.0303 (5)
O4	1.2618 (4)	−0.3575 (2)	0.5234 (2)	0.0387 (6)
O5	1.3998 (4)	−0.2917 (2)	0.3622 (2)	0.0428 (7)
O6	1.0672 (4)	0.3287 (2)	0.06085 (16)	0.0298 (5)
O7	1.1763 (4)	0.3157 (2)	−0.20182 (18)	0.0332 (5)
O8	1.0586 (5)	0.4765 (2)	−0.1298 (2)	0.0483 (8)
O9	0.9041 (3)	0.05406 (19)	0.86500 (17)	0.0273 (5)
O10	0.7751 (4)	0.2131 (2)	0.73999 (16)	0.0305 (5)
O11	0.4494 (4)	0.55586 (19)	0.93352 (17)	0.0276 (5)
O12	0.3162 (4)	0.8365 (2)	0.73159 (19)	0.0320 (5)
O13	0.1907 (4)	0.7768 (2)	0.8983 (2)	0.0422 (6)
O14	0.5828 (4)	0.1589 (2)	1.19514 (16)	0.0293 (5)
O15	0.4309 (4)	0.1582 (2)	1.45986 (17)	0.0312 (5)
O16	0.5407 (5)	0.0034 (2)	1.3813 (2)	0.0493 (8)
O1W	0.4777 (4)	0.3952 (2)	0.65198 (18)	0.0347 (6)
H1A	0.5676	0.3326	0.6757	0.052*
H1B	0.3717	0.3875	0.6949	0.052*
O2W	0.7069 (4)	0.5919 (2)	0.5134 (2)	0.0326 (6)
H2A	0.7899	0.5459	0.5527	0.049*
H2B	0.6719	0.6667	0.5218	0.049*
O3W	0.3050 (4)	0.4050 (2)	0.4675 (2)	0.0353 (6)
H3A	0.2063	0.4105	0.5141	0.053*
H3B	0.3398	0.3315	0.4584	0.053*
O4W	1.1147 (4)	0.0933 (3)	0.60334 (19)	0.0406 (6)
H4A	1.2257	0.0959	0.5653	0.061*
H4B	1.0259	0.1397	0.5683	0.061*
O5W	0.8840 (4)	−0.1083 (3)	0.7440 (3)	0.0451 (7)
H5A	0.9317	−0.1700	0.7174	0.068*
H5B	0.7843	−0.0621	0.7160	0.068*
O6W	1.2974 (4)	0.0640 (3)	0.7922 (2)	0.0358 (6)
H6A	1.2680	0.1351	0.8051	0.054*
H6B	1.4065	0.0546	0.7534	0.054*
O7W	0.5925 (4)	−0.1146 (3)	1.2179 (2)	0.0450 (7)
H7A	0.5077	−0.1567	1.2609	0.068*
H7B	0.6092	−0.0632	1.2471	0.068*
O8W	0.6677 (4)	−0.3664 (2)	1.18827 (19)	0.0334 (5)
H8A	0.6994	−0.4246	1.2439	0.050*
H8B	0.7241	−0.3993	1.1389	0.050*
O9W	0.9205 (5)	−0.3172 (3)	1.3127 (2)	0.0508 (7)
H9A	0.8392	−0.3465	1.3651	0.076*

H9B	1.0280	−0.3705	1.3114	0.076*
O10W	1.0768 (4)	−0.3539 (3)	1.1004 (2)	0.0399 (6)
H10A	1.0713	−0.3919	1.0576	0.060*
H10B	1.1789	−0.3893	1.1285	0.060*
O11W	1.0123 (5)	−0.1048 (3)	1.1442 (2)	0.0496 (8)
H11A	1.0628	−0.1281	1.1997	0.074*
H11B	0.9395	−0.0292	1.1392	0.074*
O12W	0.7652 (4)	−0.1549 (2)	1.01018 (18)	0.0327 (5)
H12A	0.7790	−0.2092	0.9766	0.049*
H12B	0.8172	−0.0931	0.9702	0.049*
O13W	−0.0153 (4)	0.4100 (2)	0.6226 (2)	0.0352 (6)
H13A	0.0081	0.4151	0.6794	0.053*
H13B	−0.0582	0.3411	0.6377	0.053*
O14W	1.5912 (6)	−0.1901 (3)	0.5556 (2)	0.0608 (9)
H14A	1.4965	−0.1913	0.6062	0.091*
H14B	1.5590	−0.1303	0.5022	0.091*
O15W	1.6115 (4)	0.0755 (2)	0.6342 (2)	0.0371 (6)
H15A	1.6390	0.1426	0.6361	0.056*
H15B	1.5541	0.0906	0.5830	0.056*
O16W	0.3399 (5)	−0.0597 (4)	1.0130 (3)	0.0642 (9)
H16A	0.3490	−0.1384	1.0455	0.096*
H16B	0.3618	−0.0500	0.9470	0.096*
O17W	0.9701 (5)	−0.3302 (3)	0.6995 (3)	0.0577 (8)
H17A	1.0121	−0.3888	0.7511	0.087*
H17B	1.0556	−0.3267	0.6449	0.087*
O18W	1.2910 (5)	−0.4540 (3)	1.2606 (3)	0.0584 (8)
H18A	1.3785	−0.4062	1.2377	0.088*
H18B	1.3035	−0.4956	1.3247	0.088*
O19W	0.7759 (4)	0.6085 (3)	0.9927 (2)	0.0436 (6)
H19A	0.6812	0.6080	0.9664	0.065*
H19B	0.8822	0.5733	0.9621	0.065*
C1	0.9180 (4)	0.2574 (3)	0.3402 (2)	0.0189 (6)
C2	0.9824 (4)	0.1244 (3)	0.3748 (2)	0.0223 (6)
H2	0.9591	0.0799	0.4454	0.027*
C3	1.0815 (5)	0.0614 (3)	0.3009 (2)	0.0213 (6)
C4	1.1186 (4)	0.1252 (3)	0.1949 (2)	0.0221 (6)
H4	1.1890	0.0809	0.1468	0.026*
C5	1.0486 (4)	0.2556 (3)	0.1624 (2)	0.0213 (6)
C6	0.9513 (5)	0.3224 (3)	0.2356 (2)	0.0232 (6)
H6	0.9090	0.4108	0.2136	0.028*
C7	0.8031 (4)	0.3279 (3)	0.4184 (2)	0.0201 (6)
C8	1.1374 (5)	−0.1446 (3)	0.4299 (2)	0.0280 (7)
H81	1.0049	−0.1570	0.4575	0.034*
H82	1.1717	−0.1008	0.4713	0.034*
C9	1.2758 (5)	−0.2724 (3)	0.4360 (3)	0.0287 (7)
C10	1.1395 (5)	0.2647 (3)	−0.0181 (2)	0.0228 (6)
H101	1.0651	0.2002	−0.0075	0.027*
H102	1.2750	0.2226	−0.0152	0.027*
C11	1.1210 (5)	0.3627 (3)	−0.1237 (2)	0.0255 (6)

C12	0.7946 (4)	0.1633 (3)	0.8330 (2)	0.0205 (6)
C13	0.6929 (4)	0.2321 (3)	0.9140 (2)	0.0192 (6)
C14	0.6166 (4)	0.3631 (3)	0.8811 (2)	0.0204 (6)
H14	0.6261	0.4068	0.8101	0.024*
C15	0.5266 (5)	0.4270 (3)	0.9558 (2)	0.0203 (6)
C16	0.5108 (5)	0.3619 (3)	1.0628 (2)	0.0216 (6)
H16	0.4486	0.4055	1.1124	0.026*
C17	0.5881 (4)	0.2331 (3)	1.0936 (2)	0.0215 (6)
C18	0.6809 (4)	0.1668 (3)	1.0196 (2)	0.0214 (6)
H18	0.7342	0.0797	1.0410	0.026*
C19	0.4421 (5)	0.6258 (3)	0.8262 (2)	0.0255 (6)
H191	0.3949	0.5789	0.7924	0.031*
H192	0.5716	0.6377	0.7898	0.031*
C20	0.3055 (5)	0.7552 (3)	0.8218 (3)	0.0257 (7)
C21	0.4896 (5)	0.2183 (3)	1.2755 (2)	0.0230 (6)
H211	0.3569	0.2610	1.2651	0.028*
H212	0.5591	0.2818	1.2740	0.028*
C22	0.4887 (5)	0.1164 (3)	1.3797 (2)	0.0262 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02845 (19)	0.02098 (16)	0.01952 (17)	0.00165 (13)	0.00168 (14)	−0.00723 (13)
Zn2	0.02831 (19)	0.02057 (16)	0.02017 (17)	0.00396 (13)	0.00093 (14)	−0.00687 (13)
Zn3	0.0371 (2)	0.02793 (17)	0.02684 (18)	−0.01000 (14)	0.00251 (14)	−0.00877 (13)
O1	0.0334 (13)	0.0195 (10)	0.0208 (11)	0.0062 (9)	−0.0004 (9)	−0.0062 (9)
O2	0.0397 (14)	0.0252 (11)	0.0163 (11)	0.0034 (9)	−0.0037 (10)	−0.0065 (9)
O3	0.0503 (15)	0.0132 (10)	0.0197 (11)	0.0030 (9)	−0.0022 (10)	−0.0047 (8)
O4	0.0476 (16)	0.0192 (11)	0.0351 (15)	0.0032 (10)	−0.0090 (12)	0.0045 (10)
O5	0.0424 (15)	0.0254 (12)	0.0460 (16)	0.0034 (11)	0.0103 (12)	−0.0114 (11)
O6	0.0452 (14)	0.0215 (10)	0.0134 (10)	0.0004 (9)	0.0024 (9)	−0.0036 (8)
O7	0.0444 (15)	0.0360 (13)	0.0164 (11)	−0.0086 (11)	−0.0006 (10)	−0.0066 (10)
O8	0.084 (2)	0.0280 (14)	0.0199 (13)	−0.0001 (13)	−0.0008 (13)	−0.0032 (10)
O9	0.0327 (12)	0.0171 (10)	0.0193 (11)	0.0057 (9)	0.0029 (9)	−0.0018 (8)
O10	0.0385 (14)	0.0295 (12)	0.0164 (11)	0.0041 (10)	−0.0020 (9)	−0.0077 (9)
O11	0.0410 (14)	0.0171 (10)	0.0186 (10)	0.0053 (9)	−0.0065 (9)	−0.0050 (8)
O12	0.0373 (14)	0.0198 (11)	0.0272 (13)	0.0067 (9)	−0.0037 (11)	−0.0023 (9)
O13	0.0489 (16)	0.0269 (12)	0.0340 (14)	0.0117 (11)	0.0027 (12)	−0.0086 (11)
O14	0.0470 (14)	0.0187 (9)	0.0111 (10)	0.0038 (9)	0.0006 (9)	−0.0017 (8)
O15	0.0392 (14)	0.0345 (12)	0.0169 (11)	−0.0066 (10)	0.0007 (9)	−0.0077 (9)
O16	0.093 (2)	0.0216 (12)	0.0236 (13)	−0.0081 (13)	−0.0045 (14)	0.0007 (10)
O1W	0.0258 (13)	0.0400 (14)	0.0219 (12)	0.0024 (10)	0.0001 (10)	0.0027 (10)
O2W	0.0360 (14)	0.0248 (12)	0.0333 (14)	−0.0025 (10)	−0.0044 (11)	−0.0074 (10)
O3W	0.0371 (15)	0.0339 (13)	0.0348 (14)	−0.0057 (10)	−0.0012 (11)	−0.0141 (11)
O4W	0.0324 (14)	0.0428 (15)	0.0239 (13)	0.0048 (11)	−0.0001 (10)	0.0074 (11)
O5W	0.0414 (17)	0.0362 (15)	0.060 (2)	−0.0015 (12)	−0.0167 (14)	−0.0154 (13)
O6W	0.0339 (14)	0.0367 (13)	0.0378 (14)	−0.0052 (10)	0.0033 (11)	−0.0196 (11)
O7W	0.0497 (17)	0.0349 (14)	0.0484 (17)	−0.0135 (12)	0.0128 (13)	−0.0196 (12)

O8W	0.0423 (14)	0.0256 (12)	0.0296 (13)	−0.0075 (10)	−0.0002 (11)	−0.0078 (10)
O9W	0.0516 (18)	0.0645 (19)	0.0272 (14)	−0.0151 (14)	0.0012 (12)	−0.0038 (13)
O10W	0.0406 (15)	0.0420 (15)	0.0324 (14)	−0.0018 (11)	−0.0030 (11)	−0.0117 (11)
O11W	0.063 (2)	0.0506 (17)	0.0454 (17)	−0.0336 (15)	0.0003 (14)	−0.0165 (14)
O12W	0.0400 (14)	0.0274 (11)	0.0269 (12)	−0.0050 (9)	0.0011 (10)	−0.0088 (9)
O13W	0.0367 (14)	0.0407 (14)	0.0301 (13)	−0.0129 (11)	−0.0093 (11)	−0.0060 (11)
O14W	0.101 (3)	0.0296 (14)	0.0300 (15)	0.0064 (15)	0.0015 (16)	−0.0034 (12)
O15W	0.0386 (15)	0.0384 (14)	0.0353 (14)	−0.0088 (11)	−0.0077 (11)	−0.0098 (11)
O16W	0.055 (2)	0.086 (2)	0.0464 (18)	−0.0137 (18)	−0.0028 (15)	−0.0156 (17)
O17W	0.082 (2)	0.0383 (16)	0.0396 (17)	0.0001 (15)	−0.0097 (16)	−0.0034 (13)
O18W	0.058 (2)	0.064 (2)	0.0541 (19)	−0.0144 (15)	−0.0220 (15)	−0.0067 (15)
O19W	0.0484 (16)	0.0448 (15)	0.0449 (16)	−0.0082 (12)	−0.0049 (12)	−0.0251 (12)
C1	0.0202 (15)	0.0184 (13)	0.0162 (13)	0.0018 (10)	−0.0030 (11)	−0.0068 (11)
C2	0.0277 (16)	0.0172 (13)	0.0181 (14)	0.0000 (11)	−0.0027 (12)	−0.0041 (11)
C3	0.0257 (16)	0.0150 (13)	0.0196 (14)	−0.0007 (11)	−0.0042 (12)	−0.0026 (11)
C4	0.0246 (16)	0.0215 (14)	0.0179 (14)	0.0005 (11)	−0.0008 (12)	−0.0086 (11)
C5	0.0248 (16)	0.0202 (13)	0.0156 (13)	−0.0018 (11)	−0.0046 (11)	−0.0021 (10)
C6	0.0313 (17)	0.0156 (12)	0.0196 (14)	−0.0010 (11)	−0.0039 (12)	−0.0039 (11)
C7	0.0235 (15)	0.0155 (12)	0.0166 (14)	0.0007 (11)	0.0017 (11)	−0.0058 (11)
C8	0.0371 (19)	0.0176 (14)	0.0206 (15)	0.0016 (12)	−0.0016 (13)	−0.0019 (12)
C9	0.0315 (18)	0.0187 (15)	0.0320 (19)	−0.0011 (12)	−0.0038 (15)	−0.0061 (13)
C10	0.0281 (16)	0.0219 (14)	0.0155 (14)	−0.0012 (11)	−0.0019 (11)	−0.0057 (11)
C11	0.0295 (17)	0.0266 (15)	0.0168 (14)	−0.0059 (12)	0.0011 (12)	−0.0046 (12)
C12	0.0221 (15)	0.0179 (13)	0.0166 (14)	−0.0035 (11)	0.0014 (11)	−0.0022 (11)
C13	0.0197 (15)	0.0183 (13)	0.0160 (13)	0.0000 (10)	−0.0013 (11)	−0.0045 (11)
C14	0.0242 (15)	0.0179 (13)	0.0142 (13)	−0.0010 (11)	−0.0033 (11)	−0.0009 (10)
C15	0.0249 (15)	0.0146 (13)	0.0198 (14)	−0.0003 (11)	−0.0043 (11)	−0.0052 (11)
C16	0.0279 (16)	0.0177 (13)	0.0176 (13)	−0.0003 (11)	−0.0027 (11)	−0.0071 (11)
C17	0.0235 (15)	0.0213 (14)	0.0166 (13)	−0.0021 (11)	−0.0024 (11)	−0.0036 (11)
C18	0.0221 (15)	0.0167 (13)	0.0192 (14)	0.0041 (11)	−0.0022 (11)	−0.0041 (11)
C19	0.0325 (18)	0.0150 (13)	0.0209 (15)	0.0051 (11)	−0.0050 (13)	−0.0019 (11)
C20	0.0322 (18)	0.0155 (13)	0.0264 (17)	−0.0011 (12)	−0.0060 (14)	−0.0042 (12)
C21	0.0272 (16)	0.0222 (14)	0.0171 (14)	−0.0011 (11)	−0.0001 (12)	−0.0079 (11)
C22	0.0289 (17)	0.0281 (16)	0.0182 (15)	−0.0058 (13)	−0.0031 (12)	−0.0025 (12)

Geometric parameters (Å, °)

Zn1—O1W	2.022 (2)	O9W—H9A	0.85
Zn1—O1	2.028 (2)	O9W—H9B	0.85
Zn1—O4^{i}	2.063 (3)	O10W—H10A	0.85
Zn1—O2W	2.099 (3)	O10W—H10B	0.85
Zn1—O3W	2.176 (3)	O11W—H11A	0.85
Zn2—O9	2.006 (2)	O11W—H11B	0.87
Zn2—O12^{ii}	2.030 (2)	O12W—H12A	0.85
Zn2—O4W	2.034 (2)	O12W—H12B	0.85
Zn2—O5W	2.075 (3)	O13W—H13A	0.86
Zn2—O6W	2.174 (3)	O13W—H13B	0.86
Zn3—O11W	2.042 (3)	O14W—H14A	0.85
Zn3—O7W	2.050 (3)	O14W—H14B	0.85

Zn3—O10W	2.110 (3)	O15W—H15A	0.84
Zn3—O9W	2.115 (3)	O15W—H15B	0.84
Zn3—O12W	2.116 (2)	O16W—H16A	0.85
Zn3—O8W	2.118 (2)	O16W—H16B	0.86
O1—C7	1.274 (4)	O17W—H17A	0.85
O2—C7	1.249 (4)	O17W—H17B	0.85
O3—C3	1.392 (3)	O18W—H18A	0.87
O3—C8	1.414 (4)	O18W—H18B	0.86
O4—C9	1.268 (4)	O19W—H19A	0.85
O4—Zn1^{ii}	2.063 (3)	O19W—H19B	0.85
O5—C9	1.218 (4)	C1—C6	1.375 (4)
O6—C5	1.361 (4)	C1—C2	1.401 (4)
O6—C10	1.418 (3)	C1—C7	1.503 (4)
O7—C11	1.283 (4)	C2—C3	1.380 (4)
O8—C11	1.225 (4)	C2—H2	0.9300
O9—C12	1.275 (4)	C3—C4	1.390 (4)
O10—C12	1.237 (4)	C4—C5	1.380 (4)
O11—C15	1.371 (3)	C4—H4	0.9300
O11—C19	1.429 (4)	C5—C6	1.396 (4)
O12—C20	1.274 (4)	C6—H6	0.9300
O12—Zn2^{i}	2.030 (2)	C8—C9	1.510 (4)
O13—C20	1.224 (4)	C8—H81	0.9700
O14—C17	1.365 (4)	C8—H82	0.9700
O14—C21	1.418 (3)	C10—C11	1.515 (4)
O15—C22	1.273 (4)	C10—H101	0.9700
O16—C22	1.226 (4)	C10—H102	0.9700
O1W—H1A	0.85	C12—C13	1.502 (4)
O1W—H1B	0.85	C13—C18	1.385 (4)
O2W—H2A	0.85	C13—C14	1.393 (4)
O2W—H2B	0.85	C14—C15	1.383 (4)
O3W—H3A	0.84	C14—H14	0.9300
O3W—H3B	0.84	C15—C16	1.400 (4)
O4W—H4A	0.85	C16—C17	1.372 (4)
O4W—H4B	0.85	C16—H16	0.9300
O5W—H5A	0.85	C17—C18	1.395 (4)
O5W—H5B	0.86	C18—H18	0.9300
O6W—H6A	0.84	C19—C20	1.521 (4)
O6W—H6B	0.84	C19—H191	0.9700
O7W—H7A	0.87	C19—H192	0.9700
O7W—H7B	0.85	C21—C22	1.512 (4)
O8W—H8A	0.86	C21—H211	0.9700
O8W—H8B	0.85	C21—H212	0.9700
O1W—Zn1—O1	122.32 (9)	H16A—O16W—H16B	109.5
O1W—Zn1—O4^{i}	95.06 (10)	H17A—O17W—H17B	110.7
O1—Zn1—O4^{i}	141.81 (10)	H18A—O18W—H18B	106.2
O1W—Zn1—O2W	93.32 (11)	H19A—O19W—H19B	110.3
O1—Zn1—O2W	90.19 (10)	C6—C1—C2	120.8 (3)
O4^{i}—Zn1—O2W	95.59 (10)	C6—C1—C7	120.1 (3)

O1W—Zn1—O3W	92.18 (11)	C2—C1—C7	119.1 (3)
O1—Zn1—O3W	83.45 (10)	C3—C2—C1	117.9 (3)
O4^{i}—Zn1—O3W	87.95 (11)	C3—C2—H2	121.0
O2W—Zn1—O3W	173.18 (10)	C1—C2—H2	121.0
O9—Zn2—O12^{ii}	143.70 (9)	C2—C3—C4	122.3 (3)
O9—Zn2—O4W	118.87 (10)	C2—C3—O3	124.1 (3)
O12^{ii}—Zn2—O4W	96.70 (10)	C4—C3—O3	113.6 (2)
O9—Zn2—O5W	90.34 (11)	C5—C4—C3	118.6 (3)
O12^{ii}—Zn2—O5W	93.23 (11)	C5—C4—H4	120.7
O4W—Zn2—O5W	95.78 (12)	C3—C4—H4	120.7
O9—Zn2—O6W	83.78 (9)	O6—C5—C4	124.6 (3)
O12^{ii}—Zn2—O6W	87.55 (10)	O6—C5—C6	115.0 (2)
O4W—Zn2—O6W	93.03 (12)	C4—C5—C6	120.3 (3)
O5W—Zn2—O6W	171.00 (12)	C1—C6—C5	120.0 (3)
O11W—Zn3—O7W	93.29 (12)	C1—C6—H6	120.0
O11W—Zn3—O10W	91.01 (12)	C5—C6—H6	120.0
O7W—Zn3—O10W	175.05 (13)	O2—C7—O1	122.6 (3)
O11W—Zn3—O9W	85.82 (13)	O2—C7—C1	119.6 (3)
O7W—Zn3—O9W	92.96 (13)	O1—C7—C1	117.8 (3)
O10W—Zn3—O9W	89.80 (11)	O3—C8—C9	108.5 (3)
O11W—Zn3—O12W	96.39 (11)	O3—C8—H81	110.0
O7W—Zn3—O12W	90.34 (11)	C9—C8—H81	110.0
O10W—Zn3—O12W	86.74 (10)	O3—C8—H82	110.0
O9W—Zn3—O12W	175.92 (12)	C9—C8—H82	110.0
O11W—Zn3—O8W	176.81 (13)	H81—C8—H82	108.4
O7W—Zn3—O8W	87.98 (10)	O5—C9—O4	121.4 (3)
O10W—Zn3—O8W	87.86 (10)	O5—C9—C8	122.0 (3)
O9W—Zn3—O8W	91.18 (11)	O4—C9—C8	116.6 (3)
O12W—Zn3—O8W	86.53 (10)	O6—C10—C11	108.4 (2)
C7—O1—Zn1	113.75 (19)	O6—C10—H101	110.0
C3—O3—C8	118.9 (2)	C11—C10—H101	110.0
C9—O4—Zn1^{ii}	102.3 (2)	O6—C10—H102	110.0
C5—O6—C10	117.7 (2)	C11—C10—H102	110.0
C12—O9—Zn2	116.53 (19)	H101—C10—H102	108.4
C15—O11—C19	117.6 (2)	O8—C11—O7	125.1 (3)
C20—O12—Zn2^{i}	102.0 (2)	O8—C11—C10	120.5 (3)
C17—O14—C21	118.0 (2)	O7—C11—C10	114.4 (3)
Zn1—O1W—H1A	122.6	O10—C12—O9	122.7 (3)
Zn1—O1W—H1B	125.9	O10—C12—C13	120.7 (3)
H1A—O1W—H1B	108.2	O9—C12—C13	116.5 (3)
Zn1—O2W—H2A	115.8	C18—C13—C14	120.8 (3)
Zn1—O2W—H2B	120.4	C18—C13—C12	120.3 (2)
H2A—O2W—H2B	109.8	C14—C13—C12	118.8 (3)
Zn1—O3W—H3A	104.6	C15—C14—C13	118.8 (3)
Zn1—O3W—H3B	123.5	C15—C14—H14	120.6
H3A—O3W—H3B	112.1	C13—C14—H14	120.6
Zn2—O4W—H4A	120.5	O11—C15—C14	124.3 (3)

Zn2—O4W—H4B	129.4	O11—C15—C16	114.6 (2)
H4A—O4W—H4B	110.1	C14—C15—C16	121.0 (3)
Zn2—O5W—H5A	113.7	C17—C16—C15	119.3 (3)
Zn2—O5W—H5B	118.3	C17—C16—H16	120.3
H5A—O5W—H5B	109.0	C15—C16—H16	120.3
Zn2—O6W—H6A	123.4	O14—C17—C16	125.0 (3)
Zn2—O6W—H6B	111.8	O14—C17—C18	114.3 (3)
H6A—O6W—H6B	111.5	C16—C17—C18	120.7 (3)
Zn3—O7W—H7A	113.4	C13—C18—C17	119.3 (3)
Zn3—O7W—H7B	116.6	C13—C18—H18	120.3
H7A—O7W—H7B	107.0	C17—C18—H18	120.3
Zn3—O8W—H8A	104.7	O11—C19—C20	108.5 (2)
Zn3—O8W—H8B	100.3	O11—C19—H191	110.0
H8A—O8W—H8B	104.5	C20—C19—H191	110.0
Zn3—O9W—H9A	121.0	O11—C19—H192	110.0
Zn3—O9W—H9B	112.6	C20—C19—H192	110.0
H9A—O9W—H9B	110.3	H191—C19—H192	108.4
Zn3—O10W—H10A	124.6	O13—C20—O12	123.3 (3)
Zn3—O10W—H10B	123.1	O13—C20—C19	122.1 (3)
H10A—O10W—H10B	109.9	O12—C20—C19	114.5 (3)
Zn3—O11W—H11A	107.3	O14—C21—C22	108.5 (2)
Zn3—O11W—H11B	108.5	O14—C21—H211	110.0
H11A—O11W—H11B	108.0	C22—C21—H211	110.0
Zn3—O12W—H12A	116.3	O14—C21—H212	110.0
Zn3—O12W—H12B	115.6	C22—C21—H212	110.0
H12A—O12W—H12B	108.5	H211—C21—H212	108.4
H13A—O13W—H13B	107.3	O16—C22—O15	125.6 (3)
H14A—O14W—H14B	109.8	O16—C22—C21	119.3 (3)
H15A—O15W—H15B	110.8	O15—C22—C21	115.2 (3)
O1W—Zn1—O1—C7	−6.0 (3)	O3—C8—C9—O4	−170.1 (3)
$O4^{i}$—Zn1—O1—C7	−172.6 (2)	C5—O6—C10—C11	172.2 (3)
O2W—Zn1—O1—C7	88.0 (2)	O6—C10—C11—O8	2.4 (4)
O3W—Zn1—O1—C7	−94.4 (2)	O6—C10—C11—O7	−177.9 (3)
$O12^{ii}$—Zn2—O9—C12	173.6 (2)	Zn2—O9—C12—O10	13.3 (4)
O4W—Zn2—O9—C12	6.3 (3)	Zn2—O9—C12—C13	−164.87 (19)
O5W—Zn2—O9—C12	−90.5 (2)	O10—C12—C13—C18	166.3 (3)
O6W—Zn2—O9—C12	96.3 (2)	O9—C12—C13—C18	−15.5 (4)
C6—C1—C2—C3	0.7 (5)	O10—C12—C13—C14	−15.7 (4)
C7—C1—C2—C3	177.7 (3)	O9—C12—C13—C14	162.5 (3)
C1—C2—C3—C4	0.0 (5)	C18—C13—C14—C15	−0.7 (5)
C1—C2—C3—O3	−178.9 (3)	C12—C13—C14—C15	−178.7 (3)
C8—O3—C3—C2	−6.6 (5)	C19—O11—C15—C14	7.4 (5)
C8—O3—C3—C4	174.4 (3)	C19—O11—C15—C16	−173.6 (3)
C2—C3—C4—C5	−1.9 (5)	C13—C14—C15—O11	178.7 (3)
O3—C3—C4—C5	177.1 (3)	C13—C14—C15—C16	−0.3 (5)
C10—O6—C5—C4	9.0 (5)	O11—C15—C16—C17	−178.3 (3)
C10—O6—C5—C6	−171.2 (3)	C14—C15—C16—C17	0.8 (5)
C3—C4—C5—O6	−177.1 (3)	C21—O14—C17—C16	0.4 (5)

C3—C4—C5—C6	3.1 (5)	C21—O14—C17—C18	−179.5 (3)
C2—C1—C6—C5	0.6 (5)	C15—C16—C17—O14	179.8 (3)
C7—C1—C6—C5	−176.4 (3)	C15—C16—C17—C18	−0.3 (5)
O6—C5—C6—C1	177.7 (3)	C14—C13—C18—C17	1.2 (5)
C4—C5—C6—C1	−2.5 (5)	C12—C13—C18—C17	179.1 (3)
Zn1—O1—C7—O2	−11.9 (4)	O14—C17—C18—C13	179.2 (3)
Zn1—O1—C7—C1	167.1 (2)	C16—C17—C18—C13	−0.7 (5)
C6—C1—C7—O2	−159.5 (3)	C15—O11—C19—C20	165.0 (3)
C2—C1—C7—O2	23.4 (4)	Zn2^{i}—O12—C20—O13	−5.1 (4)
C6—C1—C7—O1	21.5 (4)	Zn2^{i}—O12—C20—C19	172.5 (2)
C2—C1—C7—O1	−155.5 (3)	O11—C19—C20—O13	−15.8 (4)
C3—O3—C8—C9	−162.0 (3)	O11—C19—C20—O12	166.5 (3)
Zn1^{ii}—O4—C9—O5	5.4 (4)	C17—O14—C21—C22	175.8 (3)
Zn1^{ii}—O4—C9—C8	−171.9 (2)	O14—C21—C22—O16	−8.7 (4)
O3—C8—C9—O5	12.7 (5)	O14—C21—C22—O15	171.7 (3)

Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) *x*+1, *y*−1, *z*.

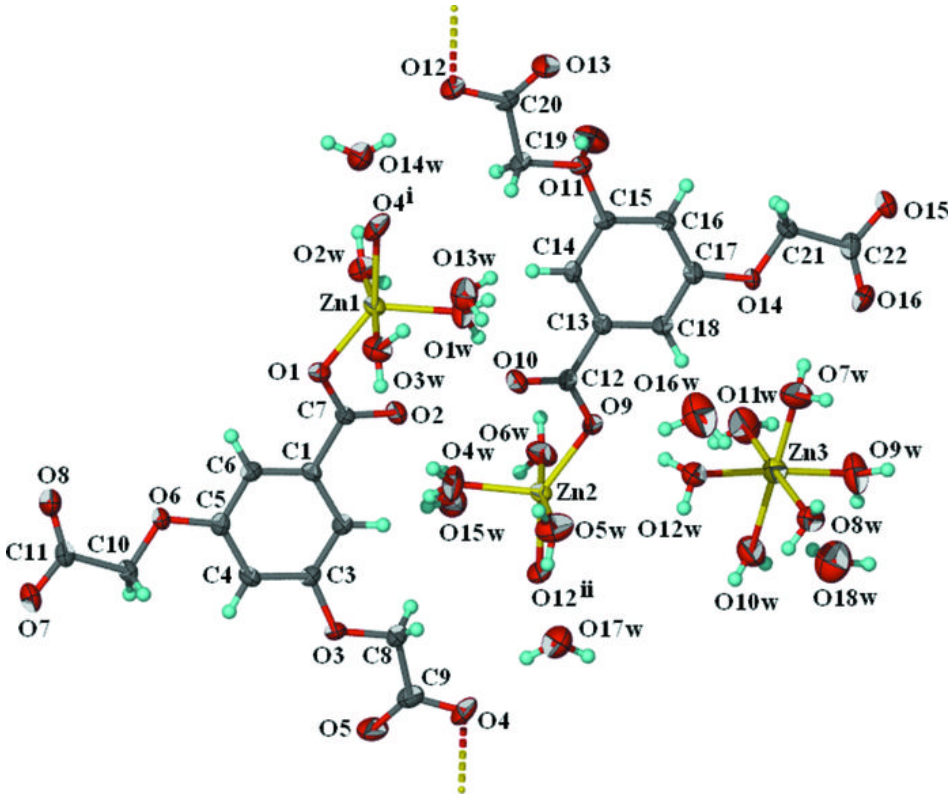
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O10	0.85	1.90	2.742 (3)	170
O1W—H1B···O7^{iii}	0.85	1.89	2.711 (3)	162
O2W—H2A···O13W^{iv}	0.85	1.94	2.769 (4)	165
O2W—H2B···O14W^{i}	0.85	1.74	2.591 (4)	173
O3W—H3A···O13W	0.84	1.91	2.747 (4)	176
O3W—H3B···O15^{v}	0.84	1.89	2.722 (3)	171
O4W—H4A···O15^{vi}	0.85	1.91	2.726 (3)	161
O4W—H4B···O2	0.85	1.95	2.765 (3)	163
O5W—H5A···O17W	0.85	1.84	2.651 (4)	159
O5W—H5B···O15W^{vii}	0.86	1.93	2.756 (4)	163
O6W—H6A···O7^{viii}	0.84	1.95	2.767 (4)	164
O6W—H6B···O15W	0.84	1.92	2.737 (4)	162
O7W—H7A···O5^{iii}	0.87	1.90	2.726 (4)	161
O7W—H7B···O16	0.85	2.12	2.868 (4)	147
O8W—H8A···O1^{ix}	0.86	2.06	2.893 (3)	163
O8W—H8B···O19W^{x}	0.85	1.93	2.694 (4)	151
O9W—H9A···O2W^{ix}	0.85	2.01	2.825 (4)	162
O9W—H9B···O18W	0.85	1.96	2.768 (5)	161
O10W—H10B···O18W	0.85	1.99	2.739 (4)	146
O11W—H11A···O3^{viii}	0.85	2.27	3.029 (4)	148
O11W—H11A···O3^{viii}	0.85	2.27	3.029 (4)	148
O12W—H12A···O19W^{x}	0.85	2.00	2.740 (3)	144
O12W—H12B···O9	0.85	1.95	2.788 (3)	171
O13W—H13A···O7^{iii}	0.86	2.09	2.814 (3)	142
O13W—H13B···O10^{vii}	0.86	2.07	2.849 (3)	150

O14W—H14A···O12^{ii}	0.85	1.96	2.782 (4)	164
O14W—H14B···O16^{vi}	0.85	1.84	2.678 (4)	168
O15W—H15A···O2^{iv}	0.84	2.30	2.914 (3)	131
O15W—H15B···O15^{vi}	0.84	1.93	2.759 (4)	169
O16W—H16B···O6W^{vii}	0.86	2.17	2.937 (5)	149
O17W—H17A···O8^{ix}	0.85	1.86	2.693 (4)	170
O17W—H17B···O4	0.85	2.01	2.845 (4)	168
O18W—H18A···O8W^{iv}	0.87	2.15	2.975 (4)	156
O18W—H18B···O3W^{xi}	0.86	1.91	2.769 (4)	173
O19W—H19A···O11	0.85	2.10	2.915 (4)	164
O19W—H19B···O8^{viii}	0.85	1.95	2.759 (4)	159

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

Fig. 1


O12
O13
C20
C19
O14w
O11
C15
C16
O15
O4i
O2w
O13w
C14
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C21
C22
Zn1
O14
O16
C13
C18
O1w
O1
O10
C12
O16w
O7w
O3w
C7
O2
O9
O11w
O6w
C6
C1
O4w
Zn3
O9w
O8
Zn2
O6
C5
O15w
O5w
O12w
O8w
C11
C10
C4
C3
O12ii
O10w
O18w
O7
O17w
O3
C8
C9
O5
O4