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Poly[propane-1,2-diammonium [(μ_4-benzene-1,2,4,5-tetracarboxylato-$\kappa^4O:O':O'':O'''$)zinc(II)] tetrahydrate]

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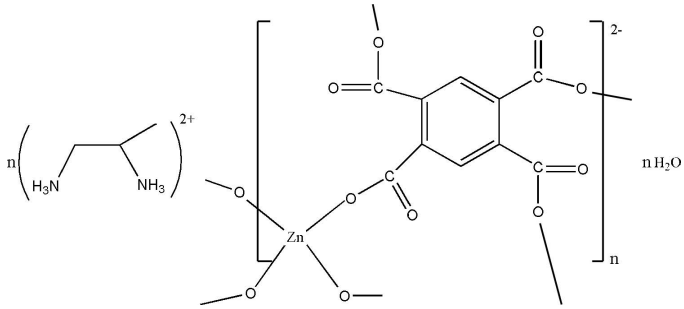
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.038; wR factor = 0.111; data-to-parameter ratio = 17.0.

In the title compound, $\{[Zn(C_{10}H_2O_8)(C_3H_{12}N_2)]\cdot 4H_2O\}_n$, the Zn^{2+} ions are in a distorted tetrahedral environment made up of four O atoms from four benzene-1,2,4,5-tetracarboxylate anions, which leads to the formation of a polymeric three-dimensional network. The disordered (3:1) propane-1,2-diammonium counter-cations and the water molecules are located in the voids of the network. Intermolecular N—H···O and O—H···O hydrogen bonds help to consolidate the crystal packing.

Related literature

Transition metal complexes with benzene-1,2,4,5-tetracarboxylate (btec) ligands include those with Mn (Rochon & Massarweh, 2000; Hu *et al.*, 2001), Fe (Chu *et al.*, 2001), Co (Murugavel *et al.*, 2002; Kumagai *et al.*, 2002; Poleti & Karanović, 1989; Cheng *et al.*, 2002), Ni (Murugavel *et al.*, 2002; Rochon & Massarweh, 2000; Poleti *et al.*, 1988), Cu (Zou *et al.*, 1998; Cheng *et al.*, 2001; Cao, Shi *et al.*, 2002), Ag (Jaber *et al.*, 1997) and Zn (Murugavel *et al.*, 2002; Yang *et al.*, 2004). Main group and metal complexes with the same ligand include those with Ca (Robl, 1988) and Tl (Day & Luehrs, 1988); for rare earth metal complexes, see Cao, Sun *et al.* (2002) and Daiguebonne *et al.* (2003). The Zn—O bond lengths and angles are comparable to those in similar structures (Murugavel *et al.*, 2002; Yang *et al.*, 2004).



Experimental

Crystal data

$[Zn(C_{10}H_2O_8)(C_3H_{12}N_2)]\cdot 4H_2O$
M_r = 463.70
Monoclinic, $P2_1/c$
a = 9.4116 (5) Å
b = 13.2967 (7) Å
c = 14.9365 (7) Å
β = 98.019 (1)°
V = 1850.92 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.39 mm^{-1}
T = 100 (2) K
0.21 × 0.18 × 0.17 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.758, T_{max} = 0.797
20525 measured reflections
4454 independent reflections
4001 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.08
4454 reflections
262 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3	1.9519 (16)	Zn1—O7^{i}	1.9705 (16)
Zn1—O6	1.9526 (16)	Zn1—O1^{ii}	2.0047 (17)
O3—Zn1—O6	118.41 (7)	O3—Zn1—O1^{ii}	98.78 (7)
O3—Zn1—O7^{i}	112.19 (7)	O6—Zn1—O1^{ii}	101.10 (7)
O6—Zn1—O7^{i}	104.51 (7)	O7^{i}—Zn1—O1^{ii}	122.33 (7)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1NA···O8^{i}	0.87	2.05	2.901 (4)	165
N1—H1NB···O2W^{iii}	0.87	1.92	2.771 (4)	164
N1—H1NC···O2^{iv}	0.87	2.11	2.964 (4)	165
N2—H2NA···O4^{ii}	0.90	1.94	2.788 (3)	156
N2—H2NB···O8^{i}	0.89	1.87	2.755 (3)	173
N2—H2NC···O1	0.97	2.16	2.968 (3)	139
N2—H2NC···O3	0.97	2.37	2.992 (3)	121
O1W—H1WA···O3W^{v}	0.82	2.02	2.838 (4)	173
O1W—H1WB···O4W	0.82	2.02	2.792 (3)	157
O2W—H2WA···O5	0.82	2.14	2.962 (3)	177
O2W—H2WB···O1W	0.82	2.00	2.819 (4)	179
O3W—H3WA···O5^{vi}	0.82	2.11	2.911 (3)	165

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D—H···A	D—H	H···A	D···A	D—H···A
O3W—H3WB···O2	0.82	2.02	2.817 (3)	164
O4W—H4WA···O5^{vi}	0.82	2.06	2.859 (3)	166
O4W—H4WB···O4	0.82	2.12	2.911 (3)	163

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, -y+2, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, -y+\frac{5}{2}, z+\frac{1}{2}$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (vi) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); 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: WM2117).

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supplementary materials

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Poly[propane-1,2-diammonium [(μ_4-benzene-1,2,4,5-tetracarboxylato-$\kappa^4O:O':O'':O'''$)zinc(II)] tetrahydrate]

M. Rafizadeh, V. Amani and S. Zahiri

Comment

In the past, considerable attention has been paid to the exploration of the structures and properties of metal complexes or salts containing benzenepolycarboxylate ligands. In the case of benzene-1,2,4,5-tetracarboxylate (btec) ligands, the coordination chemistry is well represented, although there are not as many structures as reported for benzene-1,3,5-tricarboxylate (btc). Among the many known compounds containing btec ligands, most are transition metal complexes, including Mn (Rochon & Massarweh, 2000; Hu *et al.*, 2001), Fe (Chu *et al.*, 2001), Co (Murugavel *et al.*, 2002; Kumagai *et al.*, 2002; Poleti & Karanović, 1989; Cheng *et al.*, 2002), Ni (Murugavel *et al.*, 2002; Rochon & Massarweh, 2000; Poleti *et al.*, 1988), Cu (Zou *et al.*, 1998; Cheng *et al.*, 2001; Cao, Shi *et al.*, 2002), Ag (Jaber *et al.*, 1997) and Zn (Murugavel *et al.*, 2002; Yang *et al.*, 2004). Examples of compounds with main group metals such as Ca (Robl, 1988) and Tl (Day & Luehrs, 1988) also exist. Recently, compounds of the rare earth elements were also reported (Cao, Sun *et al.*, 2002; Daiguebonne *et al.*, 2003). However, compounds with btec ligands and organic ammonium counter cations are rare and may have an interesting polymeric structure.

Indeed, the title compound, (I), forms a polymeric three-dimensional structure. The Zn atom is in the center of a distorted tetrahedron made up of four O atoms from four benzene-1,2,4,5-tetracarboxylate anions. The Zn—O bond lengths and bond angles in (I) (Table 1) are within the normal range (Murugavel *et al.*, 2002; Yang *et al.*, 2004). The propane-1,2-diammonium counter cations and the water molecules are located in the voids of the polymeric anionic moieties (Fig. 1). Intermolecular hydrogen bonds of the type N—H···O and O—H···O (Table 2) stabilize the crystal packing (Fig. 2).

Experimental

At room temperature propane-1,2-diamine (0.87 g (1.0 ml), 11.6 mmol) was added to a solution of benzene-1,2,4,5-tetracarboxylic acid (1.52 g, 5.81 mmol) in ethanol (20 ml), resulting in a milky suspension which subsequently was added to a solution of $ZnCl_2$ (0.41 g, 2.93 mmol) in water (30 ml). The resulting colorless solution was stirred for 5 min and was left to evaporate slowly at room temperature. After three days, colorless prismatic crystals of (I) were isolated (yield 1.15 g, 84.1%).

Refinement

The H atoms bonded to C atoms were placed in calculated positions. The H atoms of the NH_3^+ groups and of the water molecules were found in difference Fourier maps. All H atoms were refined in the riding model approximation with the U_{iso}(H) parameters equal to 1.2U_{eq}(X) (X = C, N and O). The propane-1,2-diammonium cation is disordered. One NH_3^+, the CH_3 and the CH groups are split in two positions. They were refined with fixed occupancies of 0.75 and 0.25. Four restrains were used to fix distances d(C11—C12), d(C11—C12'), d(C12—C13) and d(C12'-C13) for the disordered cation. The highest peak and the deepest hole in the final Fourier map are located 1.02 and 0.48 Å from atom OW2.

Figures

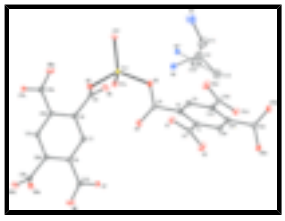

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 40% probability level. The disorder of the propane-1,2-diammonium cation is indicated with dotted lines.

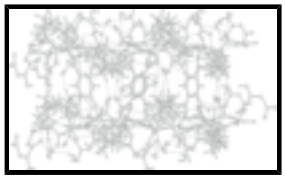

Fig. 2. Unit-cell packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Poly[propane-1,2-diammonium [(μ_4-benzene-1,2,4,5-tetracarboxylato-$\kappa^4O:O':O'':O'''$)zinc(II)] tetrahydrate]

Crystal data

$[Zn(C_{10}H_2O_8)(C_3H_{12}N_2)]\cdot 4H_2O$	$F_{000} = 960$
$M_r = 463.70$	$D_x = 1.664$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 8669 reflections
$a = 9.4116$ (5) Å	$\theta = 2.8$–$33.7°$
$b = 13.2967$ (7) Å	$\mu = 1.39$ mm^{-1}
$c = 14.9365$ (7) Å	$T = 100$ (2) K
$\beta = 98.019$ (1)°	Prism, colourless
$V = 1850.92$ (16) Å^3	0.21 × 0.18 × 0.17 mm
$Z = 4$	

Data collection

Bruker APEX II CCD area-detector diffractometer	4454 independent reflections
Radiation source: fine-focus sealed tube	4001 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 100(2)$ K	$\theta_{max} = 28.0°$
ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -12 \rightarrow 12$
$T_{min} = 0.758$, $T_{max} = 0.797$	$k = -17 \rightarrow 17$
20525 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.111$

$S = 1.08$

4454 reflections

262 parameters

4 restraints

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 2.3619P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.62$ e Å^{-3}

$\Delta\rho_{min} = -0.94$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.03224 (3)	0.868391 (18)	0.655799 (16)	0.00834 (10)	
O1	0.12169 (17)	1.06008 (13)	0.42654 (12)	0.0154 (3)	
O2	0.2471 (2)	1.11654 (15)	0.32229 (13)	0.0230 (4)	
O3	0.19966 (17)	0.92584 (13)	0.61094 (11)	0.0146 (3)	
O4	0.17684 (18)	0.83944 (13)	0.48050 (12)	0.0161 (3)	
C1	0.3718 (2)	1.02922 (17)	0.44759 (15)	0.0123 (4)	
C2	0.3698 (2)	0.95572 (17)	0.51446 (15)	0.0117 (4)	
C3	0.4976 (2)	0.92813 (17)	0.56651 (15)	0.0126 (4)	
H3A	0.4963	0.8792	0.6127	0.015*	
C4	0.2385 (2)	1.07046 (17)	0.39364 (15)	0.0130 (4)	
C5	0.2357 (2)	0.90262 (17)	0.53424 (15)	0.0117 (4)	
O5	0.20752 (18)	0.67090 (13)	0.66424 (12)	0.0177 (3)	
O6	−0.01647 (18)	0.72814 (12)	0.62750 (12)	0.0154 (3)	
O7	0.04691 (18)	0.62364 (12)	0.28851 (11)	0.0135 (3)	
O8	0.0393 (2)	0.45944 (14)	0.26156 (12)	0.0253 (4)	
C6	0.0402 (2)	0.57553 (16)	0.56367 (15)	0.0110 (4)	
C7	0.0576 (2)	0.58931 (16)	0.47342 (15)	0.0117 (4)	
H7A	0.0973	0.6504	0.4552	0.014*	
C8	0.0176 (2)	0.51486 (16)	0.40971 (15)	0.0116 (4)	
C9	0.0823 (2)	0.66294 (17)	0.62596 (15)	0.0121 (4)	
C10	0.0358 (2)	0.53321 (17)	0.31313 (15)	0.0123 (4)	
N1	0.2934 (3)	1.1642 (3)	0.8054 (2)	0.0430 (7)	
H1NA	0.2231	1.1212	0.8016	0.052*	

H1NB	0.3625	1.1541	0.8497	0.052*	
H1NC	0.2726	1.2256	0.8189	0.052*	
C11	0.3328 (3)	1.1789 (3)	0.7146 (2)	0.0347 (7)	
H11A	0.4383	1.2117	0.7123	0.042*	
H11B	0.3743	1.1080	0.6924	0.042*	
C13	0.2738 (3)	1.2619 (2)	0.56495 (19)	0.0297 (6)	
H13A	0.1951	1.2867	0.5206	0.045*	0.75
H13B	0.3275	1.2103	0.5370	0.045*	0.75
H13C	0.3380	1.3178	0.5857	0.045*	0.75
H13D	0.3753	1.2534	0.5585	0.045*	0.25
H13E	0.2591	1.3288	0.5896	0.045*	0.25
H13F	0.2152	1.2551	0.5057	0.045*	0.25
N2	0.1015 (3)	1.1399 (2)	0.6099 (2)	0.0171 (5)	0.75
H2NA	0.0212	1.1639	0.5766	0.021*	0.75
H2NB	0.0766	1.1045	0.6556	0.021*	0.75
H2NC	0.1427	1.0946	0.5692	0.021*	0.75
C12	0.2138 (3)	1.2175 (4)	0.6440 (2)	0.0248 (8)	0.75
H12A	0.1646	1.2717	0.6718	0.030*	0.75
N2'	0.0784 (8)	1.1905 (6)	0.6487 (5)	0.0112 (14)*	0.25
H2'A	0.0674	1.1496	0.6961	0.017*	0.25
H2'B	0.0166	1.1713	0.5994	0.017*	0.25
H2'C	0.0596	1.2551	0.6632	0.017*	0.25
C12'	0.2306 (12)	1.1829 (10)	0.6281 (6)	0.038 (4)*	0.25
H12B	0.2389	1.1173	0.5993	0.045*	0.25
O1W	0.3900 (3)	0.5682 (2)	0.3988 (2)	0.0468 (6)	
H1WA	0.4572	0.5478	0.3743	0.056*	
H1WB	0.3578	0.6178	0.3702	0.056*	
O2W	0.4618 (3)	0.6631 (2)	0.56783 (19)	0.0480 (6)	
H2WA	0.3901	0.6640	0.5933	0.058*	
H2WB	0.4418	0.6355	0.5186	0.058*	
O3W	0.3873 (3)	1.0068 (2)	0.1991 (2)	0.0512 (7)	
H3WA	0.3241	0.9640	0.1902	0.061*	
H3WB	0.3608	1.0369	0.2417	0.061*	
O4W	0.3356 (2)	0.76559 (16)	0.33999 (13)	0.0266 (4)	
H4WA	0.2875	0.7767	0.2909	0.032*	
H4WB	0.3032	0.7964	0.3802	0.032*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01004 (14)	0.00727 (14)	0.00786 (14)	0.00064 (8)	0.00181 (9)	−0.00028 (8)
O1	0.0107 (7)	0.0166 (8)	0.0189 (8)	0.0027 (6)	0.0019 (6)	0.0031 (6)
O2	0.0160 (8)	0.0314 (10)	0.0213 (9)	0.0027 (7)	0.0014 (7)	0.0113 (8)
O3	0.0124 (7)	0.0148 (8)	0.0177 (8)	−0.0012 (6)	0.0062 (6)	−0.0010 (6)
O4	0.0159 (8)	0.0142 (8)	0.0184 (8)	−0.0028 (6)	0.0031 (6)	−0.0011 (6)
C1	0.0097 (10)	0.0137 (10)	0.0137 (10)	0.0014 (8)	0.0027 (8)	0.0000 (8)
C2	0.0108 (10)	0.0111 (10)	0.0136 (10)	0.0000 (8)	0.0038 (8)	−0.0013 (8)
C3	0.0119 (10)	0.0120 (10)	0.0143 (10)	0.0016 (8)	0.0034 (8)	0.0013 (8)

C4	0.0117 (10)	0.0117 (10)	0.0152 (10)	0.0014 (8)	0.0001 (8)	−0.0001 (8)
C5	0.0081 (9)	0.0120 (10)	0.0149 (10)	0.0022 (8)	0.0011 (8)	0.0031 (8)
O5	0.0163 (8)	0.0196 (9)	0.0165 (8)	0.0016 (7)	0.0002 (6)	−0.0043 (7)
O6	0.0158 (8)	0.0096 (7)	0.0209 (8)	0.0010 (6)	0.0025 (6)	−0.0052 (6)
O7	0.0169 (8)	0.0143 (8)	0.0092 (7)	−0.0024 (6)	0.0016 (6)	0.0022 (6)
O8	0.0473 (12)	0.0180 (9)	0.0129 (8)	−0.0027 (8)	0.0120 (8)	−0.0032 (7)
C6	0.0143 (10)	0.0087 (9)	0.0099 (9)	0.0018 (8)	0.0017 (8)	−0.0002 (8)
C7	0.0163 (10)	0.0079 (9)	0.0116 (10)	0.0005 (8)	0.0038 (8)	0.0013 (8)
C8	0.0159 (10)	0.0098 (10)	0.0098 (10)	0.0011 (8)	0.0048 (8)	0.0007 (8)
C9	0.0180 (11)	0.0100 (9)	0.0089 (9)	−0.0008 (8)	0.0041 (8)	0.0000 (8)
C10	0.0144 (10)	0.0135 (10)	0.0094 (9)	0.0000 (8)	0.0029 (8)	0.0017 (8)
N1	0.0316 (14)	0.064 (2)	0.0327 (15)	−0.0096 (14)	0.0020 (12)	−0.0115 (14)
C11	0.0187 (13)	0.0481 (19)	0.0379 (17)	0.0005 (13)	0.0059 (12)	0.0085 (14)
C13	0.0271 (14)	0.0341 (15)	0.0283 (14)	−0.0050 (12)	0.0046 (11)	−0.0003 (12)
N2	0.0198 (14)	0.0159 (13)	0.0162 (13)	−0.0009 (10)	0.0045 (11)	0.0007 (10)
C12	0.0245 (19)	0.029 (2)	0.0220 (18)	−0.0111 (15)	0.0080 (14)	−0.0077 (16)
O1W	0.0398 (14)	0.0443 (14)	0.0599 (17)	0.0103 (11)	0.0192 (12)	0.0098 (12)
O2W	0.0338 (13)	0.0690 (18)	0.0413 (14)	−0.0020 (13)	0.0063 (11)	−0.0043 (13)
O3W	0.0552 (16)	0.0491 (16)	0.0555 (16)	−0.0195 (13)	0.0292 (13)	−0.0152 (13)
O4W	0.0228 (9)	0.0342 (11)	0.0221 (9)	0.0038 (8)	0.0010 (7)	−0.0006 (8)

Geometric parameters (Å, °)

Zn1—O3	1.9519 (16)	C11—C12'	1.501 (3)
Zn1—O6	1.9526 (16)	C11—C12	1.517 (3)
Zn1—O7^{i}	1.9705 (16)	C11—H11A	1.0900
Zn1—O1^{ii}	2.0047 (17)	C11—H11B	1.0900
O1—C4	1.273 (3)	C13—C12	1.500 (3)
O1—Zn1^{ii}	2.0047 (16)	C13—C12'	1.505 (3)
O2—C4	1.242 (3)	C13—H13A	0.9800
O3—C5	1.277 (3)	C13—H13B	0.9800
O4—C5	1.238 (3)	C13—H13C	0.9800
C1—C3^{iii}	1.396 (3)	C13—H13D	0.9800
C1—C2	1.399 (3)	C13—H13E	0.9800
C1—C4	1.497 (3)	C13—H13F	0.9799
C2—C3	1.388 (3)	N2—C12	1.513 (5)
C2—C5	1.511 (3)	N2—H2NA	0.9031
C3—C1^{iii}	1.396 (3)	N2—H2NB	0.8871
C3—H3A	0.9500	N2—H2NC	0.9737
O5—C9	1.240 (3)	C12—H12A	0.9801
O6—C9	1.274 (3)	N2'—C12'	1.510 (17)
O7—C10	1.266 (3)	N2'—H2NA	1.1886
O7—Zn1^{iv}	1.9705 (16)	N2'—H2NB	1.1475
O8—C10	1.250 (3)	N2'—H2'A	0.9100
C6—C7	1.392 (3)	N2'—H2'B	0.9100
C6—C8^{v}	1.400 (3)	N2'—H2'C	0.9100
C6—C9	1.507 (3)	C12'—H12B	0.9799
C7—C8	1.388 (3)	O1W—H1WA	0.8200

C7—H7A	0.9500	O1W—H1WB	0.8204
C8—C6^{v}	1.400 (3)	O2W—H2WA	0.8199
C8—C10	1.496 (3)	O2W—H2WB	0.8201
N1—C11	1.468 (4)	O3W—H3WA	0.8202
N1—H1NA	0.8701	O3W—H3WB	0.8198
N1—H1NB	0.8699	O4W—H4WA	0.8200
N1—H1NC	0.8701	O4W—H4WB	0.8204
O3—Zn1—O6	118.41 (7)	C12—C13—H13D	120.8
O3—Zn1—O7^{i}	112.19 (7)	C12'—C13—H13D	109.5
O6—Zn1—O7^{i}	104.51 (7)	H13A—C13—H13D	128.8
O3—Zn1—O1^{ii}	98.78 (7)	H13B—C13—H13D	46.3
O6—Zn1—O1^{ii}	101.10 (7)	H13C—C13—H13D	63.4
O7^{i}—Zn1—O1^{ii}	122.33 (7)	C12—C13—H13E	88.4
C4—O1—Zn1^{ii}	107.52 (14)	C12'—C13—H13E	109.5
C5—O3—Zn1	122.78 (15)	H13A—C13—H13E	79.4
C3^{iii}—C1—C2	119.4 (2)	H13B—C13—H13E	154.7
C3^{iii}—C1—C4	117.3 (2)	H13C—C13—H13E	46.1
C2—C1—C4	123.1 (2)	H13D—C13—H13E	109.5
C3—C2—C1	119.2 (2)	C12—C13—H13F	116.6
C3—C2—C5	116.7 (2)	C12'—C13—H13F	109.5
C1—C2—C5	124.1 (2)	H13B—C13—H13F	79.0
C2—C3—C1^{iii}	121.4 (2)	H13C—C13—H13F	126.9
C2—C3—H3A	119.3	H13D—C13—H13F	109.5
C1^{iii}—C3—H3A	119.3	H13E—C13—H13F	109.5
O2—C4—O1	123.2 (2)	C12—N2—H2NA	115.8
O2—C4—C1	119.5 (2)	C12—N2—H2NB	110.4
O1—C4—C1	117.2 (2)	H2NA—N2—H2NB	108.7
O4—C5—O3	126.5 (2)	C12—N2—H2NC	108.2
O4—C5—C2	120.0 (2)	H2NA—N2—H2NC	104.5
O3—C5—C2	113.33 (19)	H2NB—N2—H2NC	108.9
C9—O6—Zn1	120.26 (15)	C12—N2—H12B	63.8
C10—O7—Zn1^{iv}	110.26 (14)	H2NA—N2—H12B	138.7
C7—C6—C8^{v}	119.4 (2)	H2NB—N2—H12B	109.3
C7—C6—C9	116.09 (19)	H2NC—N2—H12B	47.3
C8^{v}—C6—C9	124.5 (2)	C13—C12—N2	109.0 (3)
C8—C7—C6	120.8 (2)	C13—C12—C11	111.0 (3)
C8—C7—H7A	119.6	N2—C12—C11	114.6 (3)
C6—C7—H7A	119.6	C13—C12—H12A	107.2
C7—C8—C6^{v}	119.8 (2)	N2—C12—H12A	107.1
C7—C8—C10	119.2 (2)	C11—C12—H12A	107.5
C6^{v}—C8—C10	121.0 (2)	C13—C12—H12B	84.3
O5—C9—O6	125.6 (2)	N2—C12—H12B	53.1
O5—C9—C6	120.1 (2)	C11—C12—H12B	82.2
O6—C9—C6	114.0 (2)	H12A—C12—H12B	160.1
O8—C10—O7	123.8 (2)	C12'—N2'—H2NA	96.7

O8—C10—C8	118.8 (2)	C12'—N2'—H2NB	88.7
O7—C10—C8	117.4 (2)	H2NA—N2'—H2NB	77.0
C11—N1—H1NA	108.3	C12'—N2'—H12A	63.8
C11—N1—H1NB	117.7	H2NA—N2'—H12A	129.9
H1NA—N1—H1NB	115.4	H2NB—N2'—H12A	141.3
C11—N1—H1NC	100.6	C12'—N2'—H2'A	109.5
H1NA—N1—H1NC	116.0	C12'—N2'—H2'B	109.5
H1NB—N1—H1NC	97.9	H2'A—N2'—H2'B	109.5
N1—C11—C12'	125.9 (5)	C12'—N2'—H2'C	109.5
N1—C11—C12	115.5 (3)	H2'A—N2'—H2'C	109.5
N1—C11—H11A	115.6	H2'B—N2'—H2'C	109.5
C12'—C11—H11A	115.8	C11—C12'—C13	111.6 (3)
C12—C11—H11A	115.5	C11—C12'—N2'	109.8 (8)
N1—C11—H11B	108.3	C13—C12'—N2'	115.4 (9)
C12'—C11—H11B	89.0	C11—C12'—H12A	84.7
C12—C11—H11B	110.0	C13—C12'—H12A	83.7
H11A—C11—H11B	88.2	N2'—C12'—H12A	53.5
C12—C13—H13A	109.5	C11—C12'—H12B	105.4
C12'—C13—H13A	114.4	C13—C12'—H12B	107.6
C12—C13—H13B	109.5	N2'—C12'—H12B	106.6
C12'—C13—H13B	88.8	H12A—C12'—H12B	160.0
H13A—C13—H13B	109.5	H1WA—O1W—H1WB	106.5
C12—C13—H13C	109.5	H2WA—O2W—H2WB	108.7
C12'—C13—H13C	122.7	H3WA—O3W—H3WB	99.9
H13A—C13—H13C	109.5	H4WA—O4W—H4WB	110.6
H13B—C13—H13C	109.5		
O6—Zn1—O3—C5	35.90 (19)	$C8^{v}$—C6—C7—C8	0.3 (4)
$O7^{i}$—Zn1—O3—C5	157.79 (16)	C9—C6—C7—C8	−177.8 (2)
$O1^{ii}$—Zn1—O3—C5	−71.86 (18)	C6—C7—C8—$C6^{v}$	−0.3 (4)
$C3^{iii}$—C1—C2—C3	1.2 (4)	C6—C7—C8—C10	179.0 (2)
C4—C1—C2—C3	−174.5 (2)	Zn1—O6—C9—O5	21.3 (3)
$C3^{iii}$—C1—C2—C5	−178.5 (2)	Zn1—O6—C9—C6	−152.37 (15)
C4—C1—C2—C5	5.9 (3)	C7—C6—C9—O5	−88.7 (3)
C1—C2—C3—$C1^{iii}$	−1.2 (4)	$C8^{v}$—C6—C9—O5	93.2 (3)
C5—C2—C3—$C1^{iii}$	178.5 (2)	C7—C6—C9—O6	85.4 (3)
$Zn1^{ii}$—O1—C4—O2	−0.9 (3)	$C8^{v}$—C6—C9—O6	−92.7 (3)
$Zn1^{ii}$—O1—C4—C1	175.71 (16)	$Zn1^{iv}$—O7—C10—O8	10.9 (3)
$C3^{iii}$—C1—C4—O2	21.3 (3)	$Zn1^{iv}$—O7—C10—C8	−169.08 (15)
C2—C1—C4—O2	−163.0 (2)	C7—C8—C10—O8	160.0 (2)
$C3^{iii}$—C1—C4—O1	−155.4 (2)	$C6^{v}$—C8—C10—O8	−20.6 (3)
C2—C1—C4—O1	20.3 (3)	C7—C8—C10—O7	−20.0 (3)
Zn1—O3—C5—O4	−3.5 (3)	$C6^{v}$—C8—C10—O7	159.4 (2)
Zn1—O3—C5—C2	−179.39 (14)	C12'—C13—C12—N2	−54.4 (9)
C3—C2—C5—O4	−107.6 (3)	C12'—C13—C12—C11	72.8 (6)
C1—C2—C5—O4	72.1 (3)	N1—C11—C12—C13	161.0 (3)
C3—C2—C5—O3	68.6 (3)	N1—C11—C12—N2	−74.9 (4)

C1—C2—C5—O3	−111.7 (2)	N1—C11—C12'—C13	140.5 (7)
O3—Zn1—O6—C9	37.10 (19)	C12—C11—C12'—C13	74.2 (7)
O7^{i}—Zn1—O6—C9	−88.60 (17)	N1—C11—C12'—N2'	11.3 (12)
O1^{ii}—Zn1—O6—C9	143.54 (17)	C12—C11—C12'—N2'	−55.0 (13)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1NA···O8^{i}	0.87	2.05	2.901 (4)	165
N1—H1NB···O2W^{vi}	0.87	1.92	2.771 (4)	164
N1—H1NC···O2^{vii}	0.87	2.11	2.964 (4)	165
N2—H2NA···O4^{ii}	0.90	1.94	2.788 (3)	156
N2—H2NB···O8^{i}	0.89	1.87	2.755 (3)	173
N2—H2NC···O1	0.97	2.16	2.968 (3)	139
N2—H2NC···O3	0.97	2.37	2.992 (3)	121
O1W—H1WA···O3W^{viii}	0.82	2.02	2.838 (4)	173
O1W—H1WB···O4W	0.82	2.02	2.792 (3)	157
O2W—H2WA···O5	0.82	2.14	2.962 (3)	177
O2W—H2WB···O1W	0.82	2.00	2.819 (4)	179
O3W—H3WA···O5^{iv}	0.82	2.11	2.911 (3)	165
O3W—H3WB···O2	0.82	2.02	2.817 (3)	164
O4W—H4WA···O5^{iv}	0.82	2.06	2.859 (3)	166
O4W—H4WB···O4	0.82	2.12	2.911 (3)	163

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (vi) −*x*+1, *y*+1/2, −*z*+3/2; (vii) *x*, −*y*+5/2, *z*+1/2; (ii) −*x*, −*y*+2, −*z*+1; (viii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*, −*y*+3/2, *z*−1/2.

Fig. 1

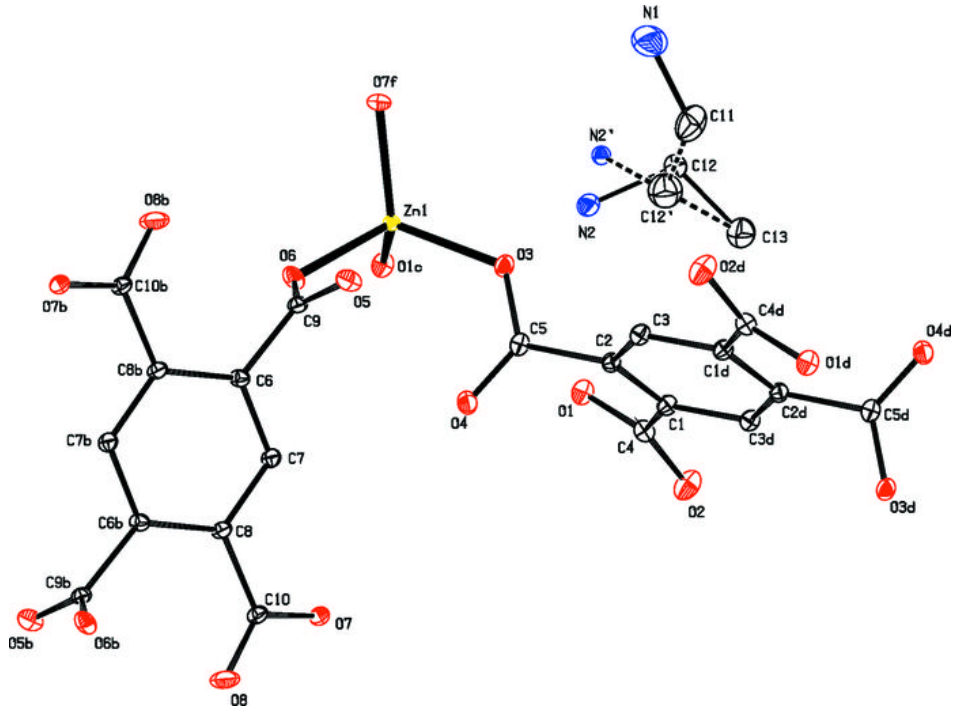
N1
C11
N2'
C12
C12'
N2
C13
O7f
Zn1
O8b
O6
O1o
O3
O2d
C10b
O7b
O5
C9
C5
C3
C4d
C2
O1d
O4d
C8b
C6
C1d
O4
O1
C1
C2d
C5d
C7b
C7
C4
C3d
O2
O3d
C6b
C8
C9b
C10
O7
O5b
O6b
O8

Fig. 2