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Poly[triaquabis(μ-benzene-1,2,4-tricarboxylato)zinc(II)dipotassium(I)]

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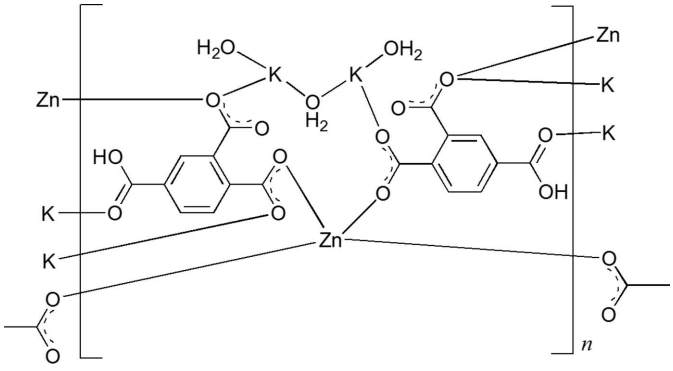
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.032; wR factor = 0.110; data-to-parameter ratio = 11.8.

In the crystal structure of the title metal–organic coordination polymer, $[K_2Zn(C_9H_4O_6)_2(H_2O)_3]_n$, the Zn^{II} ion exists in a tetrahedral coordination environment formed by four monodentate carboxylate O atoms. There are two crystallographically distinct K^I ions. Each is coordinated by one terminal water molecule and four carboxylate O atoms; in addition, these two K^I ions share one bridging water molecule. Thus, both K^I ions present a distorted octahedral coordination environment. Two crystallographically independent benzene-1,2,4-tricarboxylate dianions act as three-connected pillars to give a heterometallic three-dimensional layer-pillared network structure.

Related literature

A solely Zn^{II}-based layer-pillared coordination polymer, $[Zn_2(C_9H_4O_6)_2(H_2O)_3]_n$, was previously reported (Qin *et al.*, 2004).

For related literature, see: Rao *et al.* (2004); Yaghi *et al.* (2003).



Experimental

Crystal data

$[K_2Zn(C_9H_4O_6)_2(H_2O)_3]$
M_r = 613.86
Triclinic, $P\overline{1}$
a = 6.9626 (2) Å
b = 7.0317 (2) Å
c = 22.9019 (5) Å
α = 93.372 (1)°
β = 91.821 (1)°
γ = 102.932 (2)°
V = 1089.76 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 200 (2) K
0.24 × 0.16 × 0.14 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.697, T_{max} = 0.792
14633 measured reflections
3966 independent reflections
3510 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.110
S = 1.10
3966 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.0322 (19)	K1—O19	2.676 (2)
Zn1—O3^{i}	2.0343 (19)	K1—O29	2.874 (2)
Zn1—O7	2.0379 (19)	K2—O2^{iii}	2.833 (2)
Zn1—O10^{ii}	1.985 (2)	K2—O8A^{vi}	2.600 (19)
K1—O2	2.746 (2)	K2—O10	2.816 (2)
K1—O3^{iii}	2.807 (2)	K2—O11^{vii}	2.577 (2)
K1—O5^{iv}	2.696 (2)	K2—O19	2.827 (2)
K1—O9^{v}	2.655 (2)	K2—O39	2.883 (2)

Symmetry codes: (i) $x, y-1, z$; (ii) $x-1, y, z$; (iii) $x+1, y, z$; (iv) $-x+1, -y, -z$; (v) $x, y+1, z$; (vi) $x+1, y+1, z$; (vii) $-x+2, -y, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O29^{iv}	0.84	1.82	2.657 (3)	176
O12—H12A···O39^{viii}	0.84	1.83	2.668 (3)	176
O19—H19A···O7	0.83	2.02	2.805 (3)	159
O19—H19B···O1^{iii}	0.81	2.22	2.986 (3)	156
O29—H29A···O1^{vi}	0.84	2.10	2.903 (3)	159
O29—H29B···O4	0.85	1.96	2.790 (3)	165
O39—H39B···O7^{iii}	0.84	2.06	2.896 (3)	177

Symmetry codes: (iii) $x+1, y, z$; (iv) $-x+1, -y, -z$; (vi) $x+1, y+1, z$; (viii) $-x+3, -y, -z+1$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2244).

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supplementary materials

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Poly[triaquabis(μ-benzene-1,2,4-tricarboxylato)zinc(II)dipotassium(I)]

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Comment

Polycarboxylic acids such as 1,4-benzenedicarboxylic acid and 1,3,5-benzenetricarboxylic acid are recognized as efficient O donors exhibiting versatile coordination modes and hydrogen bonding interaction toward the assembly of metal-organic coordination polymers (Yaghi *et al.*, 2003; Rao *et al.*, 2004). Here we report the synthesis and structure of the title heterometallic coordination polymer, (I), on the basis of a unsymmetrical bridging ligand, benzene-1,2,4-tricarboxylic acid (H_3btc).

The asymmetric unit of (**I**) (Fig. 1) consists of two partially deprotonated $Hbtc^{2-}$ ligands, one Zn^{II} atom, two K^+ atoms, one bridging water molecule, and two coordinating water molecules with the formula of $[K_2Zn(Hbtc)_2(H_2O)_3]_n$. Program *PLATON*/*ADDSYM* (Spek, 2003) confirms that compound (I) is crystallized in a triclinic crystal system with space group of *P*-1. For (I), partially deprotonated $Hbtc^{2-}$ ligands are observed. There are two crystallographically distinct $Hbtc^{2-}$ ligands. The assignment of the carboxyl hydrogen atoms from the difference Fourier map, and asymmetrical carbon–oxygen bond lengths (C9—O5 and C9—O6; C18—O11 and C18—O12) of the carboxyl groups are revealed from crystallographic results. On the other hand, more symmetrical carbon–oxygen bond distances that range from 1.232 to 1.284 Å are observed for the rest of the carboxylate groups of the $Hbtc^{2-}$ ligands. The Zn^{II} exists in a tetrahedral coordination environment that is coordinated by four monodentate carboxylate oxygen atoms with Zn–O distances range from 1.985 to 2.038 Å. A close contacting distance of 2.482 (2) Å is observed between Zn1 and O4 carboxylate oxygen atom. There are two crystallographically distinct K atoms. Each K atom is coordinated by one coordinating water molecules, four carboxylate oxygen atoms, and these two K atoms share one bridging water molecule. Both of the K atoms present a distorted octahedral coordination environment. The ZnO_4 and KO_6 polyhedra are linked by carboxylate and carboxyl groups of $Hbtc^{2-}$ ligands as well as bridging water molecules to form a two dimensional layer network that lies parallel to the *ab* crystal plane (Fig. 2). The $Hbtc^{2-}$ ligands act as three-connected Pillars to give rise to a three-dimensional layer-pillared network structure (Fig. 3).

A solely Zn^{II} based layer-pillared coordination polymer, $[Zn_2(Hbtc)_2(H_2O)_3]_n$, which was crystallized in a monoclinic crystal system with higher space group symmetry of *C*2/*c* was previously reported (Qin *et al.*, 2004). The distinct coordination environment between main group K atoms and transition metal Zn atoms results in diverse solid state packing of the layer-pillared coordination networks.

Experimental

All reagents and solvents were used as obtained without further purification. $ZnCl_2$ (1.5 mmol), H_3btc (1.0 mmol) were dissolved in 10 ml of distilled water, and were added drop-wise of 4*M* KOH solution to the pH of 3.8. The mixture was sealed in a Teflon-lined stainless steel vessel and held at 383 K for 96 h. The vessel was gradually cooled to room temperature, and colorless crystals suitable for crystallographic analysis were obtained after 7 d.

Refinement

The C-bound H atoms were placed in calculated positions (C—H = 0.95 A) and refined in the riding-model approximation with U_{iso}(H) = 1.2 U_{eq}(C). The H atoms of the water molecules and carboxyl groups were located in a difference Fourier map, and refined as riding model with O—H distances range from 0.81 to 0.85 Å, and with U_{iso}(H) = 1.5 U_{eq}(O). The carboxylate oxygen atom O8 is disordered over two positions; the occupancies of O8A and O8B refined to 0.65 (14) and 0.35 (14), respectively.

Figures

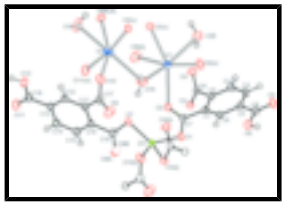

Fig. 1. The asymmetric unit, expanded to show the complete coordination of the Zn and K atoms, with displacement ellipsoids drawn at the 50% probability level. (Symmetry codes: (i) *x* − 1, *y*, *z*; (ii) *x*, *y* − 1, *z*; (iii) *x*, *y* + 1, *z*; (iv) −*x* + 1, −*y*, −*z*; (v) *x* + 1, *y*, *z*; (vi) −*x* + 2, −*y*, −*z* + 1; (vii) *x* + 1, *y* + 1, *z*)

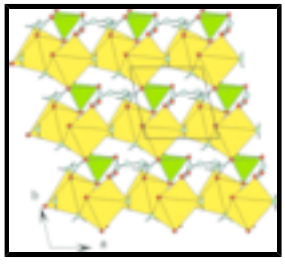

Fig. 2. A single polymeric two-dimensional layer within (I), which lies parallel to the *ab* crystal plane.

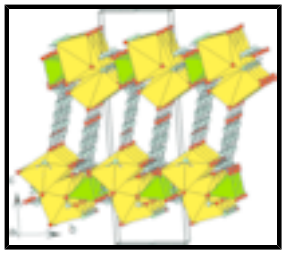

Fig. 3. Packing diagram illustrating the layer-pillared three-dimensional network of (I).

Poly[triaquabis(μ-benzene-1,2,4-tricarboxylato)zinc(II)dipotassium(I)]

Crystal data

$[K_2Zn(C_9H_4O_6)_2(H_2O)_3]$	$Z = 2$
$M_r = 613.86$	$F_{000} = 620$
Triclinic, $P\overline{1}$	$D_x = 1.871$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9626$ (2) Å	Cell parameters from 12853 reflections
$b = 7.0317$ (2) Å	$\theta = 2.0$–25.4°
$c = 22.9019$ (5) Å	$\mu = 1.59$ mm^{-1}
$\alpha = 93.372$ (1)°	$T = 200$ (2) K
$\beta = 91.821$ (1)°	Block, colorless

γ = 102.932 (2)º	0.24 × 0.16 × 0.14 mm
V = 1089.76 (5) Å^3	

Data collection

Nonius KappaCCD diffractometer	3966 independent reflections
Radiation source: fine-focus sealed tube	3510 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
T = 200(2) K	θ_{max} = 25.3º
CCD rotation images, thick slices scans	θ_{min} = 2.6º
Absorption correction: multi-scan (Blessing, 1995)	h = −8→8
T_{min} = 0.697, T_{max} = 0.792	k = −8→8
14633 measured reflections	l = −27→27

Refinement

Refinement on F^2	335 parameters
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.4828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.110	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.10	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
3966 reflections	$\Delta\rho_{min}$ = −0.82 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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.27940 (4)	−0.36692 (4)	0.253459 (12)	0.01718 (13)	
K1	0.77901 (9)	0.24823 (10)	0.19488 (3)	0.02317 (17)	
K2	1.16808 (11)	0.11542 (10)	0.31443 (3)	0.0338 (2)	
O1	0.1876 (3)	−0.2183 (3)	0.18857 (8)	0.0217 (4)	
O2	0.4098 (3)	0.0485 (3)	0.22169 (8)	0.0227 (4)	
O3	0.1914 (3)	0.3713 (3)	0.20653 (8)	0.0202 (4)	
O4	0.4817 (3)	0.5199 (3)	0.17720 (9)	0.0282 (5)	
O5	0.2264 (4)	−0.0941 (3)	−0.08408 (9)	0.0329 (5)	
O6	0.1906 (3)	−0.3381 (3)	−0.02374 (9)	0.0288 (5)	
H6A	0.1826	−0.4072	−0.0553	0.043*	
O7	0.5338 (3)	−0.2617 (3)	0.30286 (8)	0.0217 (4)	

O8A	0.376 (4)	−0.532 (4)	0.3400 (17)	0.028 (4)	0.65 (14)
O8B	0.418 (9)	−0.565 (7)	0.3281 (18)	0.028 (6)	0.35 (14)
O9	0.8514 (4)	−0.5486 (4)	0.29773 (10)	0.0434 (7)	
O10	1.1090 (3)	−0.2940 (3)	0.31484 (9)	0.0306 (5)	
O11	1.0028 (3)	−0.1760 (4)	0.59028 (9)	0.0373 (6)	
O12	1.2497 (3)	−0.2064 (3)	0.53400 (9)	0.0293 (5)	
H12A	1.3154	−0.1794	0.566	0.044*	
O19	0.8485 (3)	−0.0771 (3)	0.23775 (10)	0.0344 (5)	
H19A	0.746	−0.1471	0.2487	0.052*	
H19B	0.9172	−0.1474	0.2248	0.052*	
O29	0.8373 (3)	0.5706 (3)	0.12087 (9)	0.0328 (5)	
H29A	0.9323	0.6572	0.136	0.049*	
H29B	0.7313	0.5771	0.1377	0.049*	
O39	1.5575 (4)	0.1191 (4)	0.36191 (11)	0.0464 (7)	
H39A	1.596	0.2006	0.3385	0.07*	
H39B	1.5545	0.0113	0.3441	0.07*	
C1	0.2774 (4)	0.0367 (4)	0.12477 (11)	0.0170 (6)	
C2	0.3064 (4)	0.2379 (4)	0.11950 (11)	0.0170 (6)	
C3	0.3075 (4)	0.3100 (4)	0.06403 (12)	0.0225 (6)	
H3A	0.3281	0.4469	0.0604	0.027*	
C4	0.2788 (4)	0.1837 (4)	0.01401 (12)	0.0234 (6)	
H4A	0.2795	0.2339	−0.0236	0.028*	
C5	0.2490 (4)	−0.0174 (4)	0.01922 (11)	0.0196 (6)	
C6	0.2483 (4)	−0.0891 (4)	0.07450 (11)	0.0185 (6)	
H6B	0.2277	−0.226	0.078	0.022*	
C7	0.2941 (4)	−0.0466 (4)	0.18321 (11)	0.0171 (6)	
C8	0.3316 (4)	0.3842 (4)	0.17159 (11)	0.0182 (6)	
C9	0.2214 (4)	−0.1521 (5)	−0.03494 (12)	0.0226 (6)	
C10	0.6679 (4)	−0.3545 (4)	0.39147 (12)	0.0201 (6)	
C11	0.8697 (4)	−0.3471 (4)	0.38576 (11)	0.0180 (6)	
C12	0.9984 (4)	−0.2982 (4)	0.43456 (11)	0.0200 (6)	
H12B	1.1354	−0.2897	0.4306	0.024*	
C13	0.9280 (4)	−0.2618 (4)	0.48920 (12)	0.0198 (6)	
C14	0.7285 (4)	−0.2712 (5)	0.49488 (13)	0.0261 (7)	
H14A	0.6803	−0.2468	0.5323	0.031*	
C15	0.5998 (4)	−0.3157 (5)	0.44640 (12)	0.0258 (7)	
H15A	0.4636	−0.32	0.4505	0.031*	
C16	0.5225 (4)	−0.3940 (4)	0.33973 (12)	0.0230 (6)	
C17	0.9456 (4)	−0.4033 (5)	0.32786 (12)	0.0231 (6)	
C18	1.0629 (4)	−0.2102 (4)	0.54277 (12)	0.0223 (6)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0197 (2)	0.0186 (2)	0.01313 (19)	0.00488 (14)	−0.00094 (13)	−0.00035 (13)
K1	0.0247 (3)	0.0265 (4)	0.0166 (3)	0.0027 (3)	0.0002 (2)	−0.0008 (3)
K2	0.0454 (4)	0.0258 (4)	0.0249 (4)	−0.0029 (3)	0.0128 (3)	−0.0056 (3)
O1	0.0278 (11)	0.0211 (11)	0.0161 (9)	0.0049 (9)	0.0005 (8)	0.0037 (8)

O2	0.0265 (11)	0.0255 (11)	0.0151 (10)	0.0045 (9)	−0.0008 (8)	−0.0001 (8)
O3	0.0225 (10)	0.0214 (11)	0.0169 (9)	0.0055 (8)	0.0049 (8)	−0.0018 (8)
O4	0.0266 (11)	0.0280 (12)	0.0251 (11)	−0.0024 (10)	0.0027 (9)	−0.0062 (9)
O5	0.0528 (14)	0.0319 (13)	0.0132 (10)	0.0081 (11)	0.0021 (9)	0.0003 (9)
O6	0.0440 (13)	0.0226 (12)	0.0179 (10)	0.0049 (10)	0.0014 (9)	−0.0043 (8)
O7	0.0226 (10)	0.0261 (12)	0.0161 (10)	0.0043 (9)	−0.0007 (8)	0.0039 (8)
O8A	0.027 (5)	0.018 (4)	0.036 (7)	0.000 (3)	−0.009 (5)	0.001 (4)
O8B	0.033 (10)	0.022 (8)	0.028 (7)	0.002 (7)	−0.003 (7)	−0.002 (6)
O9	0.0389 (14)	0.0559 (17)	0.0301 (13)	0.0070 (12)	−0.0029 (10)	−0.0245 (12)
O10	0.0401 (13)	0.0324 (13)	0.0203 (11)	0.0089 (10)	0.0122 (9)	0.0018 (9)
O11	0.0357 (13)	0.0602 (17)	0.0169 (11)	0.0150 (12)	0.0005 (9)	−0.0061 (10)
O12	0.0244 (11)	0.0437 (14)	0.0194 (10)	0.0087 (10)	−0.0036 (8)	−0.0042 (9)
O19	0.0293 (12)	0.0308 (13)	0.0452 (14)	0.0084 (10)	0.0108 (10)	0.0099 (11)
O29	0.0361 (13)	0.0312 (13)	0.0266 (11)	0.0004 (10)	0.0056 (9)	−0.0089 (10)
O39	0.0659 (18)	0.0344 (14)	0.0400 (14)	0.0210 (13)	−0.0280 (13)	−0.0098 (11)
C1	0.0155 (13)	0.0198 (15)	0.0160 (13)	0.0043 (11)	0.0023 (10)	0.0011 (11)
C2	0.0148 (13)	0.0207 (15)	0.0156 (13)	0.0040 (11)	0.0023 (10)	0.0005 (11)
C3	0.0290 (16)	0.0197 (16)	0.0199 (14)	0.0073 (13)	0.0022 (12)	0.0031 (12)
C4	0.0298 (16)	0.0277 (17)	0.0142 (13)	0.0091 (13)	0.0011 (11)	0.0049 (12)
C5	0.0194 (14)	0.0229 (16)	0.0149 (13)	0.0024 (12)	0.0008 (11)	−0.0015 (11)
C6	0.0197 (14)	0.0185 (15)	0.0169 (13)	0.0031 (11)	0.0020 (11)	0.0014 (11)
C7	0.0195 (14)	0.0204 (15)	0.0137 (13)	0.0094 (12)	0.0045 (11)	−0.0011 (11)
C8	0.0216 (14)	0.0196 (15)	0.0143 (13)	0.0073 (12)	−0.0012 (11)	0.0006 (11)
C9	0.0224 (15)	0.0277 (17)	0.0172 (14)	0.0047 (13)	0.0017 (11)	−0.0001 (12)
C10	0.0236 (15)	0.0196 (15)	0.0167 (13)	0.0043 (12)	−0.0027 (11)	0.0030 (11)
C11	0.0225 (14)	0.0181 (15)	0.0133 (13)	0.0048 (12)	0.0004 (10)	0.0009 (10)
C12	0.0212 (14)	0.0246 (16)	0.0154 (13)	0.0075 (12)	0.0011 (11)	0.0017 (11)
C13	0.0223 (14)	0.0205 (15)	0.0162 (13)	0.0043 (12)	−0.0001 (11)	0.0008 (11)
C14	0.0258 (16)	0.0369 (19)	0.0163 (14)	0.0082 (14)	0.0057 (12)	−0.0001 (12)
C15	0.0179 (14)	0.0389 (19)	0.0211 (15)	0.0067 (13)	0.0021 (11)	0.0029 (13)
C16	0.0244 (15)	0.0224 (16)	0.0212 (15)	0.0037 (13)	−0.0032 (12)	0.0011 (12)
C17	0.0261 (16)	0.0297 (17)	0.0161 (14)	0.0129 (14)	−0.0016 (12)	−0.0015 (12)
C18	0.0281 (16)	0.0232 (16)	0.0168 (14)	0.0084 (13)	0.0012 (12)	−0.0002 (11)

Geometric parameters (Å, °)

Zn1—O1	2.0322 (19)	O12—H12A	0.8399
Zn1—O3^{i}	2.0343 (19)	O19—H19A	0.8262
Zn1—O4^{i}	2.482 (2)	O19—H19B	0.8125
Zn1—O7	2.0379 (19)	O29—H29A	0.8421
Zn1—O10^{ii}	1.985 (2)	O29—H29B	0.8527
K1—O2	2.746 (2)	O39—H39A	0.8147
K1—O3^{iii}	2.807 (2)	O39—H39B	0.835
K1—O5^{iv}	2.696 (2)	C1—C6	1.390 (4)
K1—O9^{v}	2.655 (2)	C1—C2	1.397 (4)
K1—O19	2.676 (2)	C1—C7	1.504 (4)
K1—O29	2.874 (2)	C2—C3	1.395 (4)
K2—O2^{iii}	2.833 (2)	C2—C8	1.508 (4)

K2—O8A^{vi}	2.600 (19)	C3—C4	1.388 (4)
K2—O8B^{vi}	2.51 (2)	C3—H3A	0.95
K2—O10	2.816 (2)	C4—C5	1.395 (4)
K2—O11^{vii}	2.577 (2)	C4—H4A	0.95
K2—O19	2.827 (2)	C5—C6	1.390 (4)
K2—O39	2.883 (2)	C5—C9	1.496 (4)
O1—C7	1.283 (3)	C6—H6B	0.95
O2—C7	1.232 (3)	C10—C15	1.392 (4)
O3—C8	1.272 (3)	C10—C11	1.405 (4)
O4—C8	1.245 (3)	C10—C16	1.505 (4)
O5—C9	1.218 (4)	C11—C12	1.387 (4)
O6—C9	1.319 (4)	C11—C17	1.507 (4)
O6—H6A	0.8401	C12—C13	1.389 (4)
O7—C16	1.284 (3)	C12—H12B	0.95
O8A—C16	1.239 (14)	C13—C14	1.386 (4)
O8B—C16	1.27 (3)	C13—C18	1.497 (4)
O9—C17	1.240 (4)	C14—C15	1.380 (4)
O10—C17	1.278 (4)	C14—H14A	0.95
O11—C18	1.208 (4)	C15—H15A	0.95
O12—C18	1.317 (4)		
O10^{ii}—Zn1—O1	97.31 (8)	C1—C2—C8	123.0 (2)
O10^{ii}—Zn1—O3^{i}	119.28 (9)	C4—C3—C2	120.7 (3)
O1—Zn1—O3^{i}	92.78 (8)	C4—C3—H3A	119.7
O10^{ii}—Zn1—O7	93.83 (9)	C2—C3—H3A	119.7
O1—Zn1—O7	122.86 (8)	C3—C4—C5	119.7 (3)
O3^{i}—Zn1—O7	128.48 (8)	C3—C4—H4A	120.1
O9^{v}—K1—O19	93.43 (8)	C5—C4—H4A	120.1
O9^{v}—K1—O5^{iv}	168.09 (8)	C6—C5—C4	119.6 (3)
O19—K1—O5^{iv}	91.36 (7)	C6—C5—C9	121.1 (3)
O9^{v}—K1—O2	94.31 (7)	C4—C5—C9	119.3 (2)
O19—K1—O2	77.08 (7)	C5—C6—C1	121.0 (3)
O5^{iv}—K1—O2	97.39 (7)	C5—C6—H6B	119.5
O9^{v}—K1—O3^{iii}	74.95 (7)	C1—C6—H6B	119.5
O19—K1—O3^{iii}	82.82 (6)	O2—C7—O1	124.4 (2)
O5^{iv}—K1—O3^{iii}	94.87 (7)	O2—C7—C1	119.4 (3)
O2—K1—O3^{iii}	156.63 (6)	O1—C7—C1	116.1 (2)
O9^{v}—K1—O29	98.37 (8)	O4—C8—O3	122.1 (3)
O19—K1—O29	156.20 (7)	O4—C8—C2	119.5 (2)
O5^{iv}—K1—O29	73.45 (6)	O3—C8—C2	118.3 (2)
O2—K1—O29	122.18 (6)	O5—C9—O6	124.1 (3)
O3^{iii}—K1—O29	80.42 (6)	O5—C9—C5	122.9 (3)
O11^{vii}—K2—O8A^{vi}	83.8 (11)	O6—C9—C5	113.0 (2)
O11^{vii}—K2—O10	98.29 (7)	C15—C10—C11	119.3 (3)
O8A^{vi}—K2—O10	152.0 (5)	C15—C10—C16	118.3 (3)

O11^{vii}—K2—O19	102.72 (7)	C11—C10—C16	122.4 (2)
O8A^{vi}—K2—O19	138.6 (3)	C12—C11—C10	119.7 (2)
O10—K2—O19	68.50 (7)	C12—C11—C17	119.7 (2)
O11^{vii}—K2—O2^{iii}	170.71 (7)	C10—C11—C17	120.5 (2)
O8A^{vi}—K2—O2^{iii}	92.8 (12)	C11—C12—C13	120.4 (3)
O10—K2—O2^{iii}	80.66 (6)	C11—C12—H12B	119.8
O19—K2—O2^{iii}	85.54 (6)	C13—C12—H12B	119.8
O11^{vii}—K2—O39	99.85 (7)	C14—C13—C12	119.9 (3)
O8A^{vi}—K2—O39	67.6 (6)	C14—C13—C18	118.5 (2)
O10—K2—O39	84.58 (7)	C12—C13—C18	121.6 (3)
O19—K2—O39	146.89 (7)	C15—C14—C13	120.2 (3)
O2^{iii}—K2—O39	70.88 (7)	C15—C14—H14A	119.9
C7—O1—Zn1	115.32 (17)	C13—C14—H14A	119.9
C8—O3—Zn1^{v}	99.94 (17)	C14—C15—C10	120.5 (3)
C8—O4—Zn1^{v}	80.11 (16)	C14—C15—H15A	119.7
C9—O6—H6A	109.5	C10—C15—H15A	119.7
C16—O7—Zn1	100.78 (17)	O8A—C16—O7	121.6 (6)
C17—O10—Zn1^{iii}	124.00 (19)	O8B—C16—O7	121.3 (10)
K1—O19—K2	95.75 (8)	O8A—C16—C10	119.0 (9)
H19A—O19—H19B	108.3	O8B—C16—C10	119.6 (14)
H29A—O29—H29B	110.1	O7—C16—C10	117.9 (3)
H39A—O39—H39B	105.4	O9—C17—O10	125.5 (3)
C6—C1—C2	119.4 (2)	O9—C17—C11	119.6 (3)
C6—C1—C7	118.8 (2)	O10—C17—C11	114.8 (3)
C2—C1—C7	121.6 (2)	O11—C18—O12	123.2 (3)
C3—C2—C1	119.7 (2)	O11—C18—C13	121.9 (3)
C3—C2—C8	117.4 (2)	O12—C18—C13	114.9 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O29^{iv}	0.84	1.82	2.657 (3)	176
O12—H12A···O39^{viii}	0.84	1.83	2.668 (3)	176
O19—H19A···O7	0.83	2.02	2.805 (3)	159
O19—H19B···O1^{iii}	0.81	2.22	2.986 (3)	156
O29—H29A···O1^{vi}	0.84	2.10	2.903 (3)	159
O29—H29B···O4	0.85	1.96	2.790 (3)	165
O39—H39B···O7^{iii}	0.84	2.06	2.896 (3)	177

Symmetry codes: (iv) −*x*+1, −*y*, −*z*; (viii) −*x*+3, −*y*, −*z*+1; (iii) *x*+1, *y*, *z*; (vi) *x*+1, *y*+1, *z*.

Fig. 1

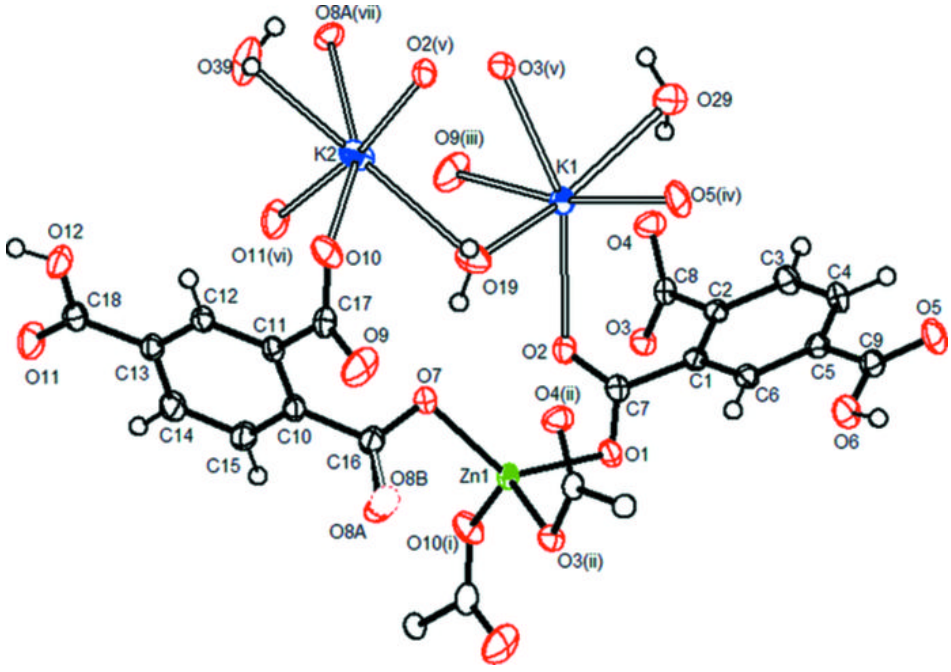
O8A(vii)
O2(v)
O39
O3(v)
O29
K2
O9(iii)
K1
O5(iv)
O12
O11(vi)
O10
O19
O4
C8
C3
C4
C18
C12
C17
C2
O5
O3
O9
O2
C9
O11
C13
C11
O7
C1
C5
C6
O4(ii)
C7
C14
C10
O1
O6
C15
C16
O8B
Zn1
O8A
O10(i)
O3(ii)

Fig. 2

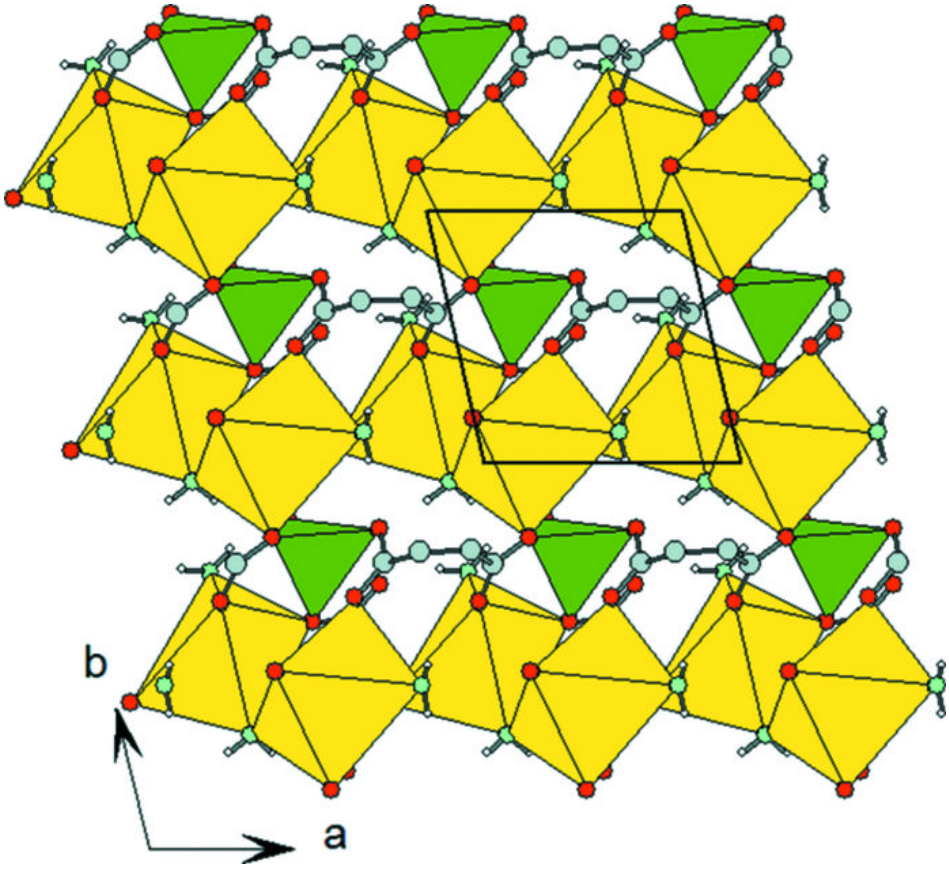

Fig. 3