Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[tetra-μ_2-aqua-diaqua-μ_2-2,5-dibenzoylterephthalatodipotassium(I)] dihydrate]

Dan-Dan Wang,[a] Hong-Jun Zhu,[a]* Ning Shan,[b] Guang-Liang Song[a] and Jin-Tang Wang[a]

[a]Department of Applied Chemistry, College of Science, Nanjing University of Technology, Nanjing 210009, People's Republic of China, and [b]Institute of Chemical and Engineering Sciences, The Singapore Government Agency for Science,Technology and Research, 627833, Singapore

Correspondence e-mail: zhuhj@njut.edu.cn

Received 16 December 2005
Accepted 22 December 2005
Online 7 January 2006

The title compound, $\{[K_2(C_{22}H_{12}O_6)(H_2O)_6]\cdot 2H_2O\}_n$, was prepared by slow evaporation of an aqueous solution of potassium dibenzoylterephthalate. The molecular complex contains two potassium cations, one 2,5-dibenzoylterephthalate anion, six coordinated water molecules and two uncoordinated water molecules. The 2,5-dibenzoylterephthalate anion lies on a center of symmetry. Each potassium cation is coordinated by seven O atoms, two from 2,5-dibenzoylterephthalate anions and the remainder from four bridging and one terminal water molecules. The uncoordinated water molecules are linked to the carboxylate O atoms and the coordinated water molecules by a network of intermolecular O—H···O hydrogen bonds, forming a layer structure.

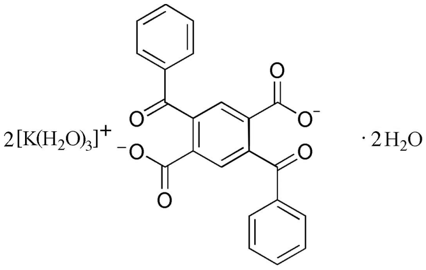
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
Some non-H atoms missing
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

2,5-Dibenzoylterephthalic acid with its centrosymmetric unit is a significant material in the synthesis of supramolecular coordination compounds. The synthesis of 2,5-dibenzoylterephthalic acid has been reported (Imai *et al.*, 1975), as have the structures of 2,5-dibenzoylterephthalic acid and $Na_2(6H_2O)$(2,5-dibenzoylterephthalate)$\cdot 4H_2O$ (Zhu *et al.*, 2005; Wang *et al.*, 2005). This paper reports the structure of K_2(2,5-dibenzoylterephthalate)$(6H_2O)\cdot 2H_2O$, (I) (Fig. 1 and Table 1).



(I)

The asymmetric unit consists of one-half of the formula unit, as the 2,5-dibenzoylterephthalate anion lies on a center of symmetry, at the centroid of the (C2/C3/C4/C2A/C3A/C4A) terephthalate ring. The coordination of each K^+ cation is defined by seven coordinated O atoms, two from 2,5-dibenzoylterephthalate anions and the remainder from four bridging and one terminal water molecules (Fig. 2). In the crystal structure, the uncoordinated water molecules are linked to the carboxylate O atoms and the coordinated water molecules by a network of intermolecular O—H···O hydrogen bonds (Fig. 3), forming a two-dimensional layer structure.

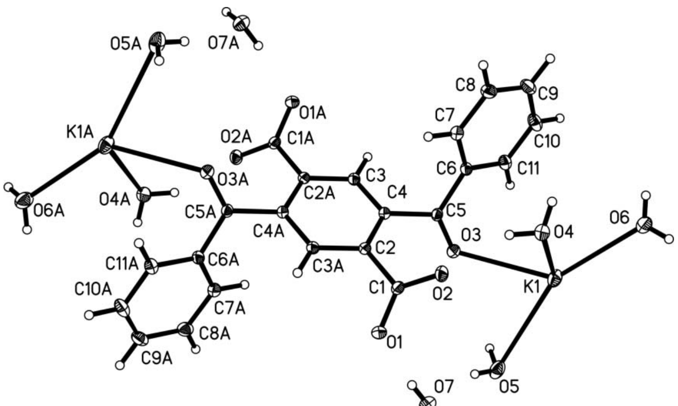


Figure 1
A segment of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $-x + 1, -y, -z - 1$.]

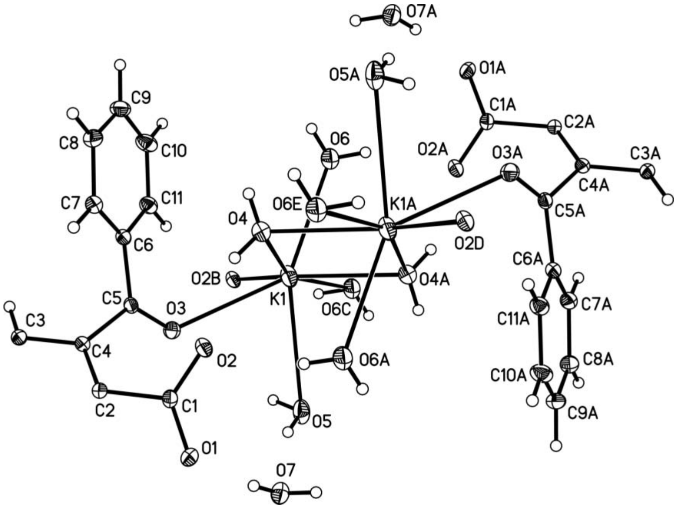


Figure 2
The coordination environment of the K$^+$ ions in (I). The symmetry operations for the atoms labelled with suffixes A–E are as follows: (A) $-x, -y - 1, -z$; (B) $x - 1, y, z$; (C) $-x - 1, -y, -z$; (D) $1 - x, -1 - y, -z$; (E) $x + 1, y, z$.

Experimental

2,5-Dibenzoylterephthalic acid was prepared by the method of Imai *et al.* (1975). Crystals of (I) suitable for diffraction measurements were obtained by slow evaporation of an aqueous solution (15 ml) containing potassium hydroxide (0.4 g, 6 mmol) and 2,5-dibenzoylterephthalic acid (1.1 g, 3 mmol) at room temperature. Analysis calculated for $C_{11}H_{14}O_7K$: C 44.59, H 4.77%; found: C 44.65, H 4.82%. IR (KBr, cm^{-1}): 3386, 3255, 2912, 2835, 1671, 1584, 1453, 1405, 1338, 1291, 1259, 1144.

Crystal data

$[K_2(C_{22}H_{12}O_6)(H_2O)_6]\cdot 2H_2O$
$M_r = 594.64$
Triclinic, $P\overline{1}$
$a = 6.153$ (2) Å
$b = 8.455$ (3) Å
$c = 13.769$ (4) Å
$\alpha = 69.441$ (11)°
$\beta = 79.673$ (13)°
$\gamma = 87.265$ (14)°
$V = 659.7$ (4) Å^3
$Z = 1$
$D_x = 1.492$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3510 reflections
$\theta = 2.5$–28.1°
$\mu = 0.43$ mm^{-1}
$T = 180$ (2) K
Plate, colorless
0.46 × 0.40 × 0.18 mm

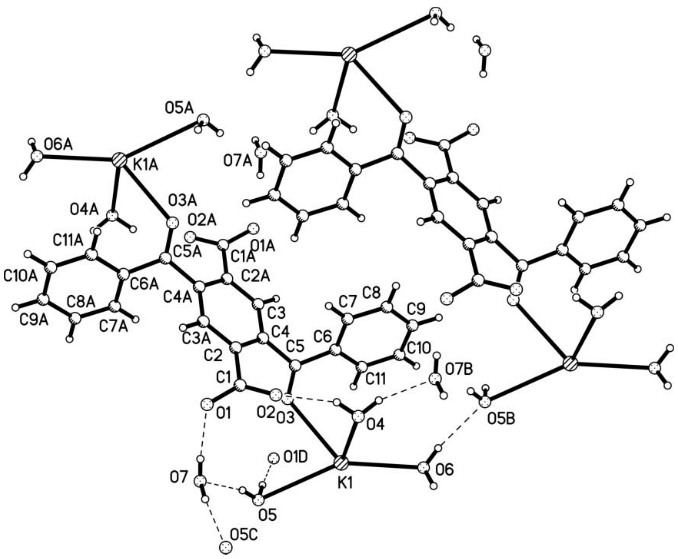


Figure 3
Intermolecular O—H···O hydrogen bonds (dashed lines) in (I). The symmetry operations for the atoms labelled with suffixes A–D are as follows: (A) $-x + 1, -y, -z - 1$; (B) $x, y - 1, z$; (C) $-x, -y, -z$; (D) $x - 1, y, z$.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min} = 0.827$, $T_{\max} = 0.927$
9790 measured reflections
3699 independent reflections
3553 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 31.1°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.119$
$S = 1.02$
3699 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.4465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

K1—O4	2.7263 (16)	K1—O2^{ii}	2.8918 (14)
K1—O4^{i}	2.7375 (15)	K1—O6^{iii}	2.9244 (19)
K1—O6	2.8042 (18)	K1—O5	3.143 (2)
K1—O3	2.8803 (14)		
O4—K1—O4^{i}	84.62 (4)	O4^{i}—K1—O6^{iii}	77.76 (5)
O4—K1—O6	77.62 (5)	O6—K1—O6^{iii}	83.57 (5)
O4^{i}—K1—O6	71.86 (4)	O3—K1—O6^{iii}	124.09 (4)
O4—K1—O3	78.31 (4)	O2^{ii}—K1—O6^{iii}	58.36 (4)
O4^{i}—K1—O3	143.29 (4)	O4—K1—O5	121.85 (4)
O6—K1—O3	133.66 (4)	O4^{i}—K1—O5	89.35 (4)
O4—K1—O2^{ii}	136.24 (4)	O6—K1—O5	152.23 (4)
O4^{i}—K1—O2^{ii}	135.96 (4)	O3—K1—O5	73.10 (4)
O6—K1—O2^{ii}	97.85 (5)	O2^{ii}—K1—O5	81.34 (4)
O3—K1—O2^{ii}	74.11 (4)	O6^{iii}—K1—O5	72.33 (4)
O4—K1—O6^{iii}	157.46 (4)		

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

m202 Wang *et al.* • $[K_2(C_{22}H_{12}O_6)(H_2O)_6]\cdot 2H_2O$ *Acta Cryst.* (2006). E**62**, m201–m203

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*B*1···O5$^{\mathrm{iv}}$	0.86 (4)	1.93 (4)	2.772 (2)	166 (3)
O4—H4*B*2···O7$^{\mathrm{v}}$	0.86 (3)	1.98 (4)	2.815 (2)	163 (2)
O4—H4*B*1···O2	0.86 (3)	2.02 (3)	2.810 (2)	154 (2)
O5—H5*B*2···O1$^{\mathrm{ii}}$	0.88 (4)	1.89 (4)	2.764 (2)	174 (4)
O5—H5*B*1···O7	0.77 (3)	2.06 (3)	2.800 (2)	162 (3)
O7—H7*B*2···O1	0.80 (3)	1.98 (3)	2.778 (2)	174 (3)
O6—H6*B*2···O5$^{\mathrm{v}}$	0.84 (4)	2.23 (4)	3.067 (3)	170 (4)

Symmetry codes: (ii) $x-1, y, z$; (iv) $-x, -y, -z$; (v) $x, y-1, z$.

H atoms attached to O were located in a difference Fourier map and refined freely. The H atoms bound to C were placed in calculated positions (C—H = 0.95 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center of Test and Analysis of the Singapore Government Agency for Science, Technology and Research for support.

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Imai,Y., Johnson, E. F., Katto, T., Kurihara, M. & Stille, J. K. (1975). *J. Polymer Sci.* **13**, 2233–2249.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (2001). *SHELXTL*. Version 5. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2002). *SADABS*. University of Göttingen, Germany.

Wang, D. D., Zhu, H. J. & Song, G. L. (2005). *Acta Cryst.* E**61**, m2610–m2612.

Zhu, H. J., Wang, D. D. & Song, G. L. (2005). *Acta Cryst.* E**61**, o2237–o2238.

Acta Cryst. (2006). E**62**, m201–m203 Wang *et al.* • $[{\rm K_2(C_{22}H_{12}O_6)(H_2O)_6}]\cdot 2{\rm H_2O}$ **m203**