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Potassium 2-benzoylbenzoate 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

Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.005 Å
R factor = 0.105
wR factor = 0.243
Data-to-parameter ratio = 20.7

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

The title compound, $K^+\cdot C_{14}H_9O_3^-\cdot 2H_2O$, was prepared by slow evaporation of an aqueous solution of potassium 2-benzoylbenzoate. Potassium cations are coordinated by six O atoms of two 2-benzoylbenzoate anions and three water molecules in a polymeric structure with bridging ligands. There are intermolecular O—H···O hydrogen bonds in the crystal structure.

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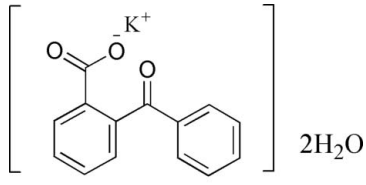
Comment

2,5-Dibenzoylterephthalic acid and 2-benzoylbenzoic acid are significant materials in the synthesis of supramolecular coordination compounds (Jullian *et al.*, 2003; Nakamura & Ukita, 2002). They are also important compounds in the preparation of electron-transport materials (Pika *et al.*, 2003). The synthesis and crystal structures of 2,5-dibenzoylterephthalic acid and $[Na_2(H_2O)_6(2,5\text{-dibenzoylterephthalate})]\cdot 4H_2O$ have been reported (Zhu *et al.*, 2005; Wang *et al.*, 2005), as well as 2-benzoylbenzoic acid (Lalancette *et al.*, 1990). This paper presents the results of a single-crystal X-ray diffraction analysis of K(2-benzoylbenzoate)$(H_2O)_2$.



(I)

The structure of (I) is shown in Fig.1, and selected bond lengths and angles are given in Table 1. The coordination around K^+ is defined by six O atoms of two 2-benzoylbenzoate anions and three water molecules, giving a polymeric structure with bridging ligands.

In the crystal structure, water molecules and carboxylate O atoms are also linked by O—H···O intermolecular hydrogen bonds, forming a two-dimensional layer structure (Fig. 2 and Table 2).

Experimental

2-Benzoylbenzoic acid was prepared by reaction of phthalic anhydride (9.0 g, 60 mmol) and powdered $AlCl_3$ (15 g, 120 mmol) in benzene (150 ml) with stirring at 338–343 K for three h. Crystals of (I) suitable for diffraction measurements were obtained by slow evaporation of an aqueous solution (10 ml) containing potassium hydroxide (0.2 g, 3 mmol) and 2-benzoylbenzoic acid (0.6 g, 3 mmol) at room temperature. Analysis calculated (%) for compound: C 55.99, H 4.36; found (%): C 55.92, H 4.44.

Crystal data

$K^+ \cdot C_{14}H_9O_3^- \cdot 2H_2O$
$M_r = 300.34$
Orthorhombic, *Pbca*
$a = 10.391\ (4)$ Å
$b = 7.771\ (3)$ Å
$c = 33.314\ (13)$ Å
$V = 2690.1\ (18)$ Å^3
$Z = 8$
$D_x = 1.483$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4649 reflections
$\theta = 1.2$–31.3°
$\mu = 0.41$ mm^{-1}
$T = 180\ (2)$ K
Block, colourless
$0.24 \times 0.18 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.908$, $T_{max} = 0.965$
24641 measured reflections
4104 independent reflections
3667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 31.3^\circ$
$h = -14 \rightarrow 12$
$k = -11 \rightarrow 10$
$l = -46 \rightarrow 47$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.105$
$wR(F^2) = 0.243$
$S = 1.37$
4104 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0749P)^2 + 2.9686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

K1—O3^{i}	2.746 (3)	K1—O5	2.835 (3)
K1—O4	2.776 (3)	K1—O1	2.959 (3)
K1—O4^{i}	2.800 (3)	K1—O3	3.146 (3)
O3^{i}—K1—O4	146.49 (9)	O4^{i}—K1—O1	119.42 (9)
O3^{i}—K1—O4^{i}	75.09 (9)	O5—K1—O1	155.42 (8)
O4—K1—O4^{i}	90.31 (9)	O3^{i}—K1—O3	140.70 (9)
O3^{i}—K1—O5	70.92 (8)	O4—K1—O3	69.29 (8)
O4—K1—O5	76.14 (9)	O4^{i}—K1—O3	95.08 (9)
O4^{i}—K1—O5	74.01 (9)	O5—K1—O3	143.71 (8)
O3^{i}—K1—O1	91.86 (8)	O1—K1—O3	59.52 (7)
O4—K1—O1	121.37 (9)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*B*2···O2^{i}	0.83 (5)	1.93 (5)	2.760 (4)	175 (5)
O5—H5*B*1···O2^{ii}	1.04 (7)	1.81 (6)	2.839 (4)	169 (5)
O4—H4*B*2···O5^{iii}	0.87 (6)	1.91 (6)	2.757 (4)	167 (5)
O4—H4*B*1···O2^{iv}	0.84 (6)	2.14 (6)	2.972 (4)	170 (6)

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

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

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*.

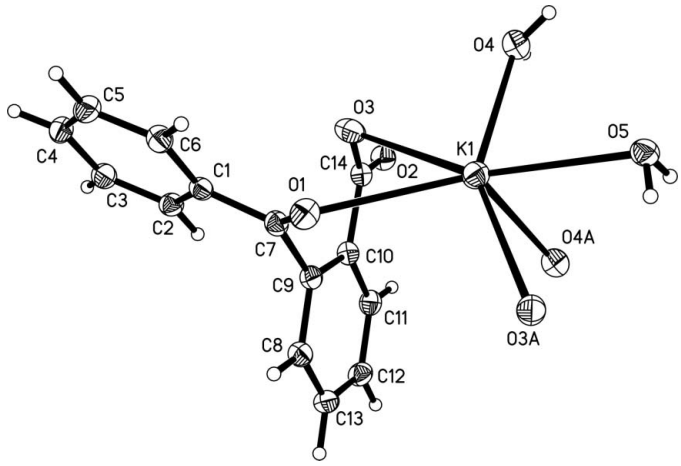


Figure 1
The structure of the asymmetric unit of (I), together with additional O atoms to complete the K^+ coordination. Displacement ellipsoids are drawn at the 30% probability level. The suffix A corresponds to symmetry code (i) in Table 1.

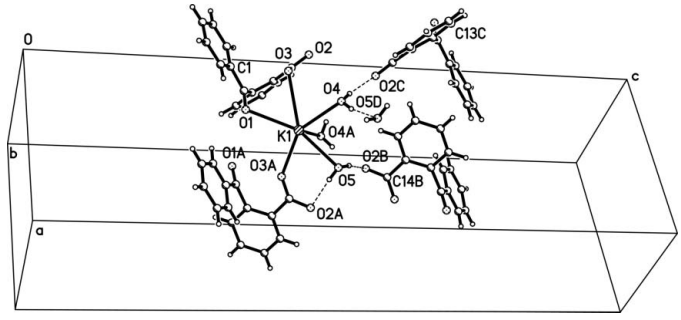


Figure 2
Intermolecular O—H···O hydrogen bonds (dashed lines) in (I). The suffixes A–D correspond to symmetry codes (i), (ii), (iv) and (iii), respectively, in Table 2.

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