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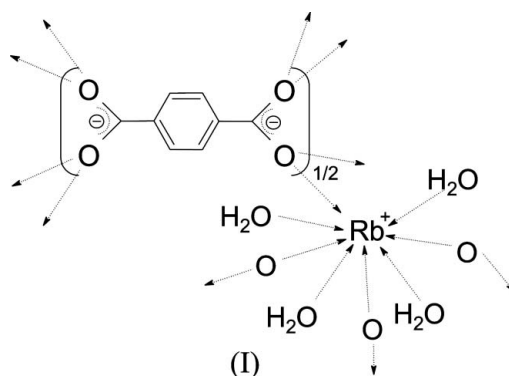
Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.007$ Å
 R factor = 0.042
 wR factor = 0.103
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[di- μ_3 -aqua- μ_4 -terephthalato-dirubidium]

Colourless platelets of dirubidium terephthalate dihydrate, $[\text{Rb}_2(\text{C}_8\text{O}_4\text{H}_4)(\text{H}_2\text{O})_2]_n$, were obtained by hydrothermal reaction of Rb_2CO_3 and terephthalic acid in demineralized water followed by slow evaporation of the solvent at room temperature. Rubidium is coordinated by four O atoms from four water molecules and four O atoms from four different centrosymmetric terephthalates. The metal centers are connected by the water molecules, forming a double layer perpendicular to $[100]$. These double layers are linked by the terephthalate dianions, forming a three-dimensional framework structure.

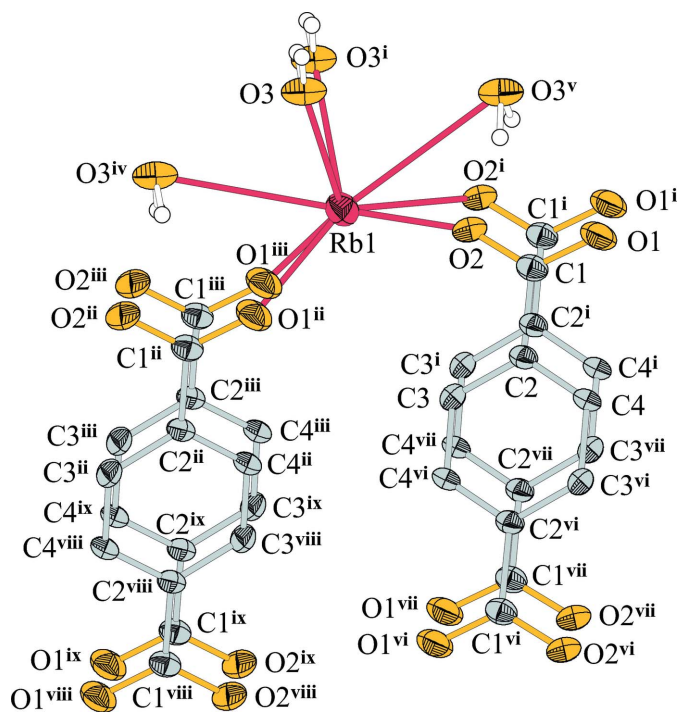
Comment

The dianion of terephthalic acid (benzene-1,4-dicarboxylic acid) is a versatile and well established ligand for the construction of coordination polymers. Surprisingly, only little is known about the structural chemistry of simple terephthalate salts of monovalent cations. Only in 2000, Kaduk investigated the crystal structures of dilithium, disodium and dipotassium terephthalate, which crystallized as anhydrous salts (Kaduk, 2000). This mainly confirmed former work by Ebara and Furuyama (Furuyama & Ebara, 1967; Ebara & Furuyama 1973), who also investigated the crystal structure of anhydrous dirubidium terephthalate (Furuyama & Ebara, 1967).

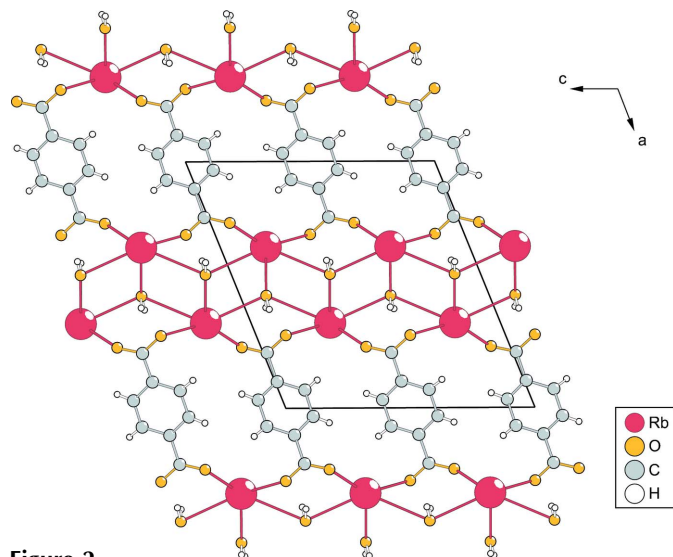


By hydrothermal reaction of Rb_2CO_3 and terephthalic acid followed by a slow evaporation of the solvent, we were able to obtain single crystals of the first hydrate of a di(alkali metal) terephthalate, $[\text{Rb}_2(\text{C}_8\text{O}_4\text{H}_4)(\text{H}_2\text{O})_2]_n$, (I). The crystal structure contains distorted RbO_8 square antiprisms (Fig. 1). Four of the eight O atoms are from four different but symmetry-equivalent centrosymmetric terephthalate anions [$\text{Rb}-\text{O} = 2.847(4)-3.005(4)$ Å]. The coordination is completed by four water molecules [$\text{Rb}-\text{O} = 2.980(4)-3.327(4)$ Å]. Each terephthalate anion connects eight rubidium ions and each

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Figure 1

Part of the polymeric structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, 1 + y, z$; (ii) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (iii) $x, \frac{3}{2} - y, z - \frac{1}{2}$; (iv) $1 - x, 1 - y, -z$; (v) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (vi) $2 - x, -y, 1 - z$; (vii) $2 - x, 1 - y, 1 - z$; (viii) $2 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ix) $2 - x, \frac{3}{2} + y, \frac{1}{2} - z$.]


Figure 2

View of the crystal structure of (I) in a projection along [010].

water molecule four rubidium ions so that the rubidium ions and water molecules form a double layer perpendicular to [100]. The shortest Rb...Rb distance within the double layers is 3.9531 (5) Å. These layers are linked by the terephthalate anions along [100], forming a three-dimensional framework structure (Fig. 2).

In a similar reaction we obtained $[\text{Cs}_2(\text{C}_8\text{O}_4\text{H}_4)(\text{H}_2\text{O})_2]$, which is isotopic with (I). The crystal structure of the caesium compound will be reported in the near future.

Experimental

Terephthalic acid (0.06 g, 0.36 mmol) and rubidium carbonate (0.28 g, 1.2 mmol) were suspended in 6 ml of demineralized water and poured into a Teflon-coated beaker, which was inserted into a steel autoclave. The reaction was carried out at 423 K for 100 h. After cooling to room temperature, the solvent was allowed to evaporate in a beaker sealed with a perforated foil. After a few days, colorless platelets of (I) were obtained. X-ray powder patterns revealed that the sample is not a single phase; accordingly, no yield was determined.

Crystal data

$[\text{Rb}_2(\text{C}_8\text{H}_4\text{O}_4)(\text{H}_2\text{O})_2]$
 $M_r = 371.08$
 Monoclinic, $P2_1/c$
 $a = 12.663$ (3) Å
 $b = 3.9531$ (5) Å
 $c = 11.873$ (3) Å
 $\beta = 111.87$ (3)°
 $V = 551.6$ (2) Å³

$Z = 2$
 $D_x = 2.234$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 8.88$ mm⁻¹
 $T = 295$ (2) K
 Plate, colorless
 $0.4 \times 0.3 \times 0.07$ mm

Data collection

Stoe IPDS IP diffractometer
 φ scans
 Absorption correction: numerical
 [X-RED32 (Stoe & Cie, 2001);
 crystal shape optimized by
 X-SHAPE (Stoe & Cie, 1999)]
 $T_{\min} = 0.248, T_{\max} = 0.333$

5609 measured reflections
 1243 independent reflections
 874 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.091$
 $\theta_{\max} = 28.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.103$
 $S = 0.96$
 1243 reflections
 84 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.87$ e Å⁻³
 $\Delta\rho_{\min} = -1.48$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.015 (3)

Table 1

Selected bond lengths (Å).

Rb1—O1 ⁱ	2.847 (4)	Rb1—O3 ^v	3.327 (4)
Rb1—O1 ⁱⁱ	2.859 (4)	O2—C1	1.265 (6)
Rb1—O2	2.927 (4)	O1—C1	1.240 (5)
Rb1—O3 ⁱⁱⁱ	2.980 (4)	C1—C2	1.511 (6)
Rb1—O2 ⁱⁱⁱ	3.005 (4)	C2—C3	1.395 (6)
Rb1—O3	3.136 (4)	C2—C4	1.396 (7)
Rb1—O3 ^{iv}	3.172 (4)	C3—C4 ^{vi}	1.389 (6)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H1...O2 ^{vii}	0.94 (2)	1.86 (3)	2.775 (5)	164 (5)
O3—H2...O2 ^v	0.94 (2)	2.15 (4)	3.018 (6)	153 (6)
O3—H2...O1 ^v	0.94 (2)	2.42 (5)	3.215 (6)	141 (6)

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

H3 and H4 of the terephthalate anion were placed at calculated positions and refined as riding, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) =$

1.2 $U_{eq}(C)$. The H atoms of the water molecule were located in difference Fourier maps and refined isotropically with a restrained O—H distance of 0.94 (2) Å. The deepest hole in the final difference Fourier map was 0.88 Å from the Rb atom.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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