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Dipotassium hydrogencarbonate fluoride monohydrate

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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{O}-\text{C}) = 0.004$ Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 10.6.

Single crystals of the title compound, $\text{K}_2(\text{HCO}_3)\text{F}\cdot\text{H}_2\text{O}$, were obtained as a secondary product after performing flux synthesis experiments aimed at the preparation of potassium rare earth silicates. The basic building unit of the structure is an $[(\text{HCO}_3)(\text{H}_2\text{O})\text{F}]^{2-}$ zigzag chain running parallel to $[001]$. Both types of anions as well as the water molecules reside on mirror planes perpendicular to $[010]$ at $y = 0.25$ and $y = 0.75$, respectively. Linkage between the different constituents of the chains is provided by $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{F}$ hydrogen bonding. The K^+ cations are located between the chains and are coordinated by two F and five O atoms in form of a distorted monocapped trigonal prism.

Related literature

For phase equilibria in the system $(\text{Na},\text{K})-(\text{CO}_3,\text{HCO}_3,\text{F})-\text{H}_2\text{O}$, see: Soliev & Nizimov (2009, 2011, 2012). For structure determinations of phases in the system $\text{K}-(\text{CO}_3,\text{HCO}_3,\text{F})-\text{H}_2\text{O}$, see: Arlt & Jansen (1990); Beurskens & Jeffrey (1964); Broch *et al.* (1929); Cirpus & Adam (1995); Hill & Miller (1927); Preisinger *et al.* (1994); Skakle *et al.* (2001); Thomas *et al.* (1974). For phases related to the title compound, see: Dinnebier & Jansen (2008); Margraf *et al.* (2003); Pritchard & Islam (2003). For bond-valence parameters, see: Brown & Altermatt (1985). For details of the synthetic procedure, see: Vidican *et al.* (2003).

Experimental

Crystal data

 $\text{K}_2(\text{HCO}_3)\text{F}\cdot\text{H}_2\text{O}$ $M_r = 176.24$ Monoclinic, $P2_1/m$ $a = 5.4228$ (4) Å $b = 7.1572$ (6) Å $c = 7.4539$ (7) Å $\beta = 105.121$ (9)° $V = 279.28$ (4) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 1.64$ mm⁻¹ $T = 173$ K $0.18 \times 0.18 \times 0.06$ mm

Data collection

Agilent Xcalibur (Ruby, Gemini ultra) diffractometer

Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011) $T_{\min} = 0.946$, $T_{\max} = 1$

1008 measured reflections

551 independent reflections

475 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.027$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.075$ $S = 1.05$

551 reflections

52 parameters

4 restraints

All H-atom parameters refined

 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O4}-\text{H41}\cdots\text{O1}^{\text{i}}$	0.84 (2)	1.89 (2)	2.723 (3)	176 (3)
$\text{O4}-\text{H42}\cdots\text{F}^{\text{ii}}$	0.84 (2)	1.87 (2)	2.707 (3)	177 (3)
$\text{O3}-\text{H3}\cdots\text{F}^{\text{iii}}$	0.81 (2)	1.72 (2)	2.529 (3)	174 (4)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS for Windows* (Dowty, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010);.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2728).

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supporting information

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Dipotassium hydrogencarbonate fluoride monohydrate

Volker Kahlenberg and Timo Schwaier

S1. Comment

In the present paper we describe a previously unknown phase within the multinary system $\text{K}-(\text{CO}_3, \text{HCO}_3, \text{F})-\text{H}_2\text{O}$ which represents the first example of an alkali metal double salt containing hydrogencarbonate as well as fluoride anions.

Basic building units of the structure are $[(\text{HCO}_3)(\text{H}_2\text{O})\text{F}]^{2-}$ -zigzag-chains running along the [001]-direction. Within the unit cell the chains are located on mirror planes at $y = 0.25$ and $y = 0.75$, respectively. As can be seen from Fig. 1, a single water molecule in the chain provides two intermolecular hydrogen bonds with neighboring hydrogencarbonate and fluoride anions. Each fluorine atom in turn is the acceptor of two hydrogen bonds from adjacent H_2O and (HCO_3) -moieties (Table 1). The C—O bond lengths (1.250 (3)–1.350 (4) Å) and the O—C—O bond angles (114.7 (2)–127.6 (3) °) are in meaningful ranges. The distortions of the hydrogencarbonate group (point group symmetry m) follow the expected trends: the considerably longer C—O3 bond represents the linkage between the central carbon atom and the OH-group, which is also involved in hydrogen bonding. Consequently, the O1—C—O3 and O2—C—O3 angles are significantly smaller than 120°, whereas the O1—C—O2 angle is larger compared with the ideal undistorted case.

The potassium cations are coordinated by two fluorine and five oxygen atoms. The resulting coordination polyhedron can be described as a distorted monocapped trigonal prism (Fig. 2). Bond valence sum calculations were performed for the K^+ cations using the bond valence parameters for K—O and K—F of Brown & Altermatt (1985). The resulting value in valence units (v.u.) is 1.10 and thus is reasonably close to the expected value of 1.0 v.u..

A slightly different description of the structure results when anion-centred polyhedra are considered as well. Actually, each F^- anion is surrounded by two hydrogen atoms (belonging to a water molecule and a hydrogencarbonate group, respectively) and four additional equatorial potassium atoms in form of a distorted octahedron (Fig. 3). Edge-sharing between adjacent octahedra results in columns running along [010]. The linkage between the octahedral columns with the laterally attached H_2O and (HCO_3) -groups is realised by O4—H41... O1 hydrogen bonds (Fig. 4).

To our best knowledge, the present compound represents the first example of an alkali hydrogencarbonate halogenide hydrate. The structure of an alkaline earth hydrogencarbonate chloride hydrate with composition $\text{Mg}(\text{HCO}_3)_3\text{Cl}\cdot 6\text{H}_2\text{O}$ has been reported recently (Dinnebier & Jansen, 2008). However, there are no closer structural relationships between the two phases. On the other hand, anionic chains containing $(\text{CO}_3)/(\text{HCO}_3)$ -ions and water molecules have been observed in several other hydrous alkali/ammonium carbonates and hydrogencarbonates such as $\text{Na}_2\text{CO}_3\cdot\text{H}_2\text{O}$ (Pritchard & Islam, 2003), $\text{K}_2\text{CO}_3\cdot 1.5\text{H}_2\text{O}$ (Skakle *et al.*, 2001) and $\text{K}_4\text{H}_2(\text{CO}_3)_3\cdot 1.5\text{H}_2\text{O}$ (Cirpus & Adam, 1995). Concerning the general shape of the chains, the present compound and $(\text{NH}_4)_4[\text{H}_2(\text{CO}_3)_3]\cdot\text{H}_2\text{O}$ (Margraf *et al.*, 2003) are closely related (Fig. 5). As can be seen from Fig. 6, in both compounds the chains are located on mirror planes.

Only recently, the phase equilibria in the multinary system $(\text{Na}, \text{K})-(\text{CO}_3, \text{HCO}_3, \text{F})-\text{H}_2\text{O}$ have been studied at different temperatures in the range between 273 and 323 K (Soliev & Nizimov, 2009, 2011, 2012). The authors verified the existence of the following equilibrium solid phases containing potassium, for all of which detailed structural characterizations have been already performed in previous investigations: $\text{K}_2\text{CO}_3\cdot 1.5\text{H}_2\text{O}$ (Skakle *et al.*, 2001), KHCO_3

(Thomas *et al.*, 1974), $2\text{KHCO}_3 \cdot \text{K}_2\text{CO}_3 \cdot 1.5\text{H}_2\text{O}$ (or $\text{K}_4\text{H}_2(\text{CO}_3)_3 \cdot 1.5\text{H}_2\text{O}$) (Cirpus & Adam, 1995) and KF (Broch *et al.*, 1929). On the other hand, potassium carbonate hexahydrate ($\text{K}_2\text{CO}_3 \cdot 6\text{H}_2\text{O}$) has been identified as the stable hydrate below about 267 K (Hill & Miller, 1927). For potassium fluoride two hydrated forms have been described: $\text{KF} \cdot 2\text{H}_2\text{O}$ (Preisinger *et al.*, 1994) and $\text{KF} \cdot 4\text{H}_2\text{O}$ (Beurskens & Jeffrey, 1964). Furthermore, an anhydrous potassium fluoro-carbonate with composition $\text{K}_3\text{F}(\text{CO}_3)$ was reported (Arlt & Jansen, 1990).

S2. Experimental

Single crystals of $\text{K}_2(\text{HCO}_3)\text{F} \cdot \text{H}_2\text{O}$ were obtained by chance as a by-product during the preparation of K-*REE*-silicates (*REE* is an rare earth element) from a KF flux following the approach of Vidican *et al.* (2003). After the removal of the platinum crucible the solidified melt cake was immediately crashed in an agate mortar and transferred to a glass slide under a polarizing binocular. Due to the hygroscopic character of potassium fluoride under the given experimental conditions (temperature: 296 K, relative humidity: 43%) deliquescence of the halide became obvious after 30 min. After 2 h, 50 μm sized platy birefringent single crystals were observed in the solution droplets which continued to grow until the solution was completely evaporated. The sample was checked regularly over a period of two weeks. However, no indication for weathering or alteration could be detected. In order to study the compound in more detail a single-crystal of good optical quality showing sharp extinction when imaged between crossed polarizers was selected and mounted on the tip of a glass fibre using nail hardener as glue. A preliminary unit cell determination at ambient temperature using on Oxford Diffraction Gemini Ultra single-crystal diffractometer resulted in a set of lattice parameters that could not be found in the recent WEB-based version of the Inorganic Crystal Structure Database (ICSD). Therefore, we decided to perform a full data collection for structure solution. For the low temperature measurement the crystal was flash-cooled in a 173 (2) K dried air stream generated by an Oxford Cryosystems Desktop Cooler.

S3. Refinement

Difference Fourier calculations revealed the positions of all missing hydrogen atoms. For the subsequent refinement the positional parameters of the H atoms were optimized with restraints using *DFIX* 0.84 (2) commands for the O—H distances and *DFIX* 1.32 (2) commands for the H···H distances (giving H—O—H angles close to 105°).

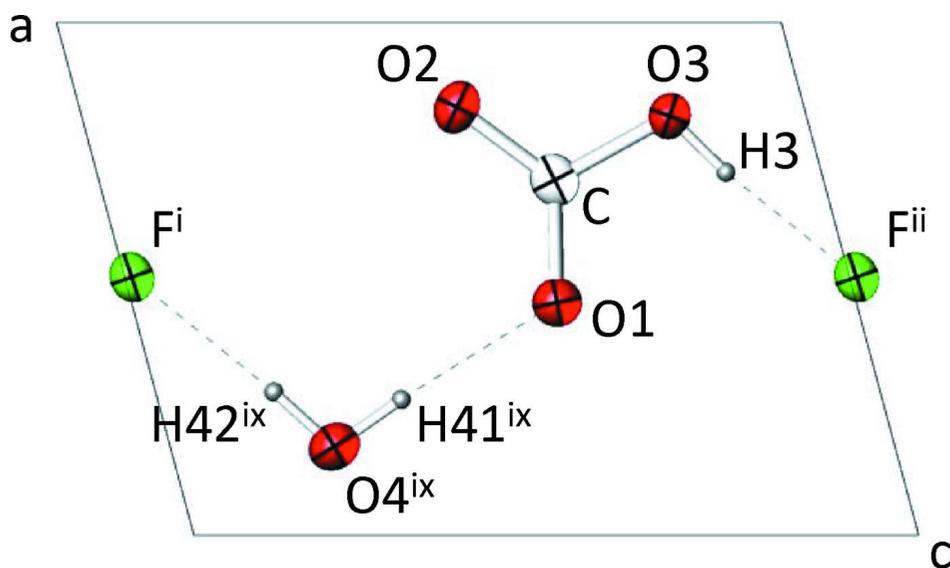


Figure 1

Projection of a single $[(\text{HCO}_3)(\text{H}_2\text{O})\text{F}]^{2-}$ chain in $y = 0.25$ parallel to $[010]$. C—O and O—H bonds are given as thick and thin open lines, respectively. Dashed lines correspond to $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{F}$ hydrogen bonds; thermal ellipsoids have been drawn on the 70% probability level. [Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x + 1, -y + 1, -z + 1$; (ix) $x - 1, y, z$].

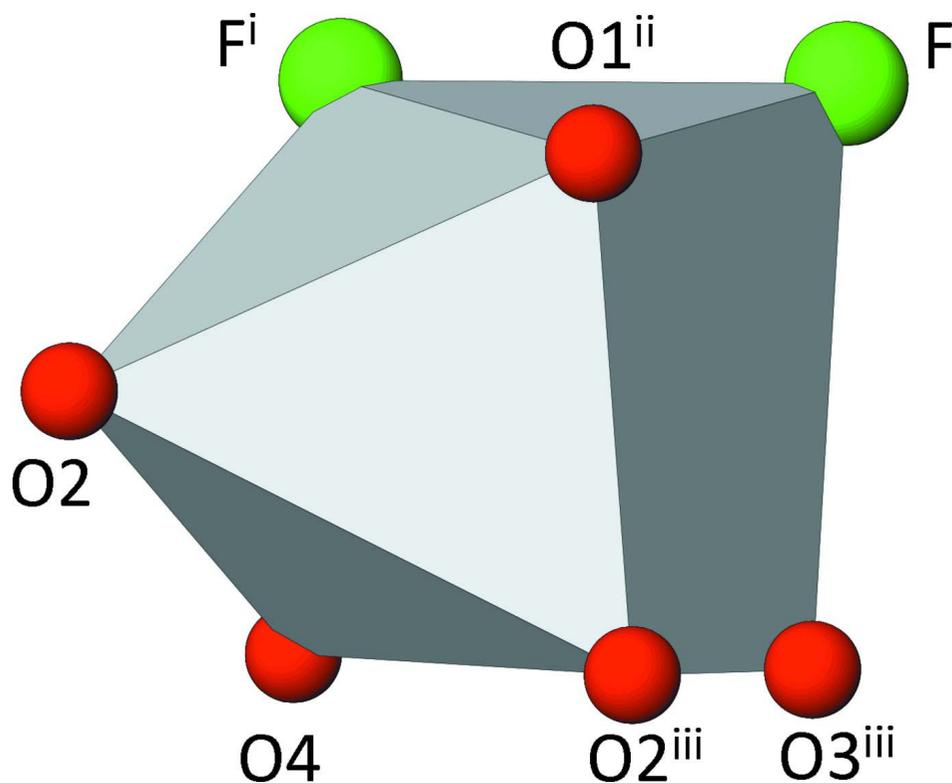


Figure 2

Side view of the coordination polyhedron around a single K^+ cation. [Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 2, -y + 1, -z + 1$].

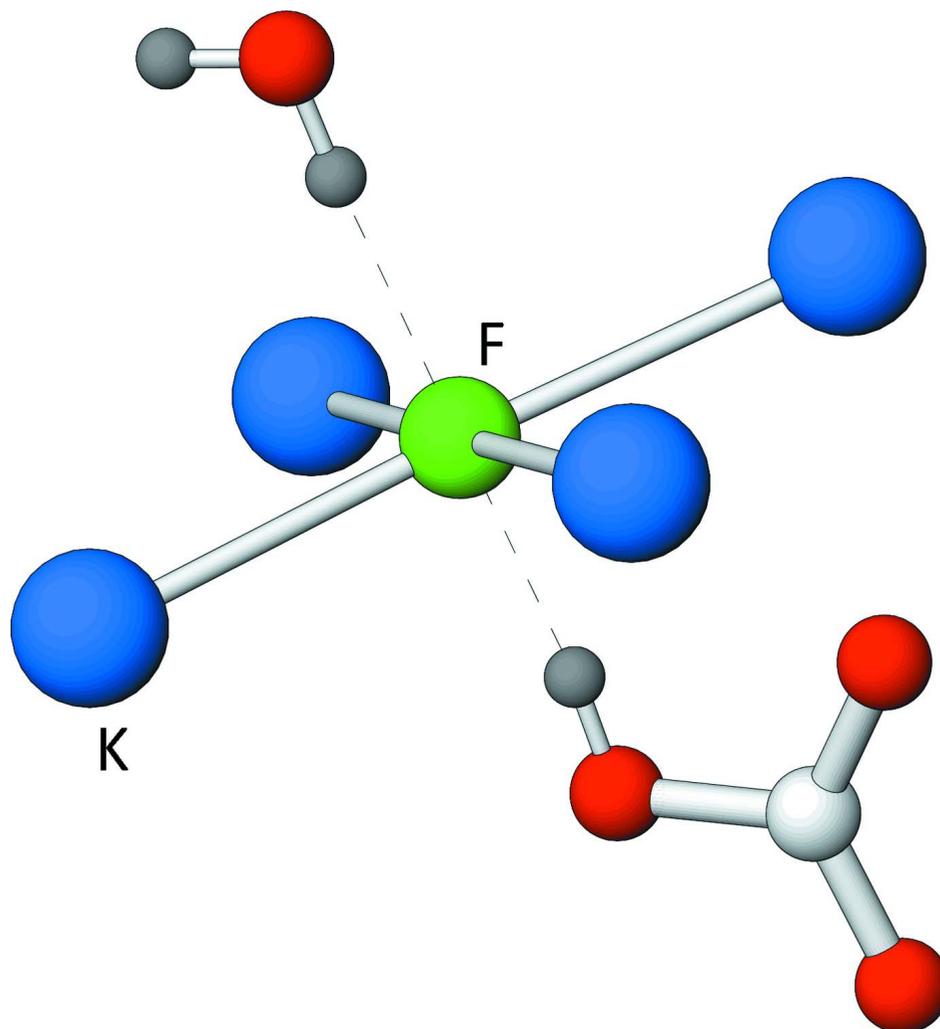
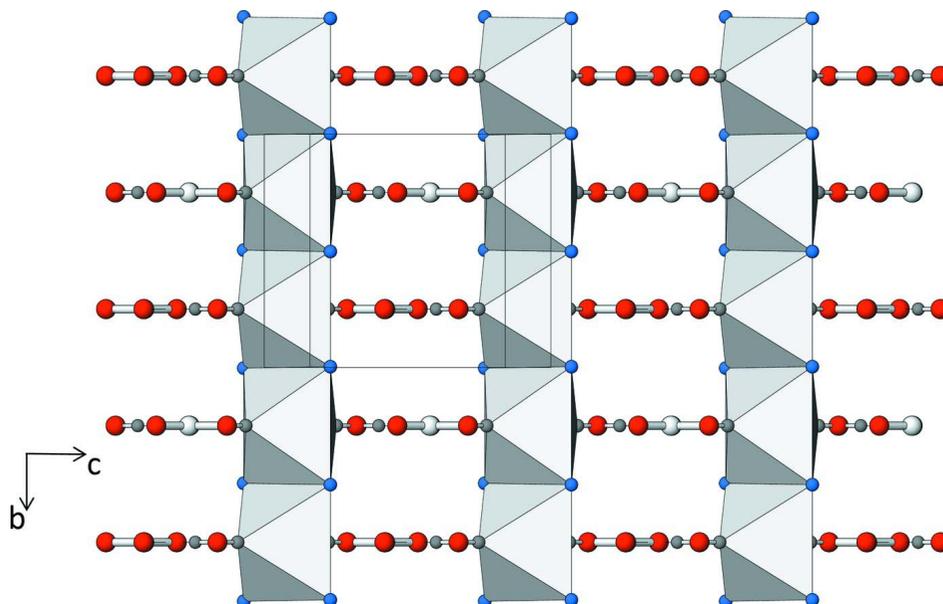
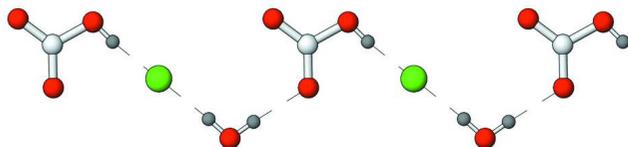


Figure 3
Coordination environment around a single F^- anion.

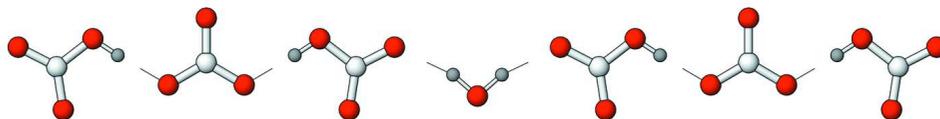
**Figure 4**

Projection of edge-sharing anion-centered chains (linked by H_2O and HCO_3^- moieties) perpendicular to (100). Small blue spheres correspond to the K^+ cations.

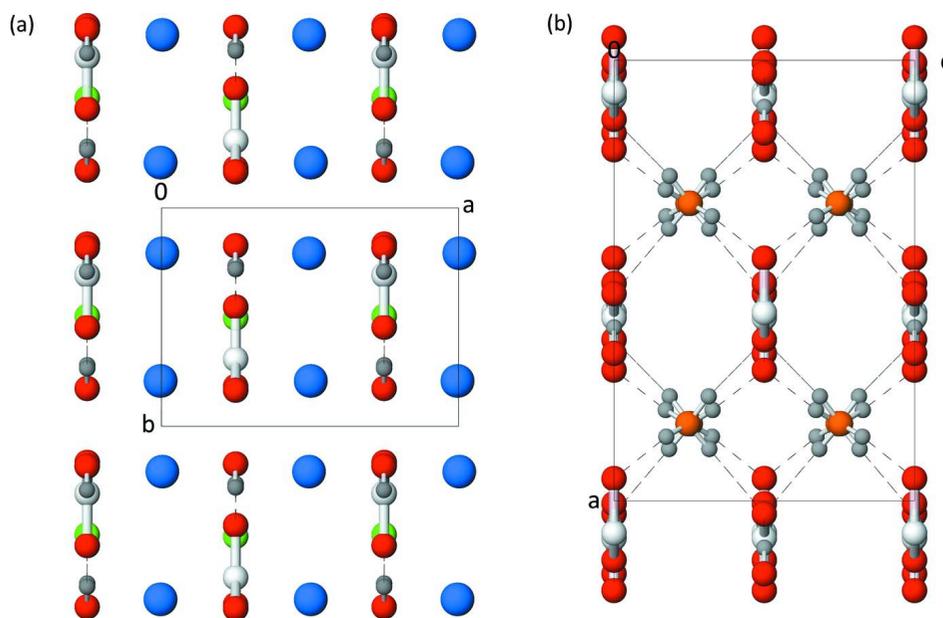
(a)



(b)

**Figure 5**

Chains containing carbonate/hydrogencarbonate and water moieties in (a) $\text{K}_2(\text{HCO}_3)\text{F}\cdot\text{H}_2\text{O}$ and (b) $(\text{NH}_4)_4[\text{H}_2(\text{CO}_3)_3]\cdot\text{H}_2\text{O}$.

**Figure 6**

Projections of the crystal structures of (a) $\text{K}_2(\text{HCO}_3)\text{F}\cdot\text{H}_2\text{O}$ and (b) $(\text{NH}_4)_4[\text{H}_2(\text{CO}_3)_3]\cdot\text{H}_2\text{O}$ parallel to the chain directions. Small blue spheres correspond to the K^+ cations.

Dipotassium hydrogen carbonate fluoride monohydrate

Crystal data

$\text{K}_2(\text{HCO}_3)\text{F}\cdot\text{H}_2\text{O}$

$M_r = 176.24$

Monoclinic, $P2_1/m$

Hall symbol: $-P\ 2_1y$

$a = 5.4228(4)\ \text{\AA}$

$b = 7.1572(6)\ \text{\AA}$

$c = 7.4539(7)\ \text{\AA}$

$\beta = 105.121(9)^\circ$

$V = 279.28(4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 176$

standard setting

$D_x = 2.096\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 538 reflections

$\theta = 2.8\text{--}28.5^\circ$

$\mu = 1.64\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Plate, colourless

$0.18 \times 0.18 \times 0.06\ \text{mm}$

Data collection

Agilent Xcalibur (Ruby, Gemini ultra)
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: $10.3575\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.946$, $T_{\max} = 1$

1008 measured reflections

551 independent reflections

475 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -5 \rightarrow 6$

$k = -8 \rightarrow 7$

$l = -8 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	All H-atom parameters refined
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
551 reflections	$(\Delta/\sigma)_{\max} < 0.001$
52 parameters	$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$
4 restraints	$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
K	0.79241 (9)	0.50302 (5)	0.23529 (7)	0.0170 (2)
F	0.4966 (3)	0.75	-0.0096 (2)	0.0164 (5)
O4	1.1731 (4)	0.25	0.2263 (3)	0.0231 (6)
H41	1.265 (6)	0.25	0.336 (2)	0.028*
H42	1.280 (5)	0.25	0.163 (4)	0.028*
O1	0.4539 (4)	0.25	0.5871 (3)	0.0212 (6)
O2	0.8344 (4)	0.25	0.5210 (3)	0.0186 (5)
O3	0.8172 (4)	0.25	0.8112 (3)	0.0182 (5)
H3	0.708 (5)	0.25	0.868 (4)	0.022*
C	0.6926 (6)	0.25	0.6289 (4)	0.0150 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K	0.0181 (3)	0.0121 (3)	0.0193 (4)	-0.00008 (16)	0.0021 (3)	-0.00045 (18)
F	0.0177 (10)	0.0170 (10)	0.0140 (10)	0	0.0034 (8)	0
O4	0.0165 (12)	0.0340 (14)	0.0198 (13)	0	0.0065 (9)	0
O1	0.0168 (12)	0.0290 (12)	0.0179 (12)	0	0.0046 (9)	0
O2	0.0198 (11)	0.0205 (11)	0.0171 (12)	0	0.0079 (9)	0
O3	0.0153 (11)	0.0262 (12)	0.0136 (12)	0	0.0049 (9)	0
C	0.0195 (17)	0.0082 (14)	0.0168 (17)	0	0.0037 (14)	0

Geometric parameters (Å, °)

K—F ⁱ	2.6816 (11)	O4—H42	0.838 (17)
K—F	2.7389 (11)	O1—C	1.250 (3)
K—O1 ⁱⁱ	2.7541 (17)	O1—K ^{vii}	2.7541 (17)
K—O2	2.7590 (17)	O1—K ⁱⁱ	2.7541 (17)
K—O4	2.7599 (17)	O2—C	1.250 (4)
K—O3 ⁱⁱⁱ	2.8477 (18)	O2—K ^{vi}	2.7590 (17)
K—O2 ⁱⁱⁱ	2.9330 (16)	O2—K ⁱⁱⁱ	2.9330 (16)
F—K ⁱ	2.6816 (11)	O2—K ^{viii}	2.9330 (16)
F—K ^{iv}	2.6816 (11)	O3—C	1.350 (4)
F—K ^v	2.7389 (11)	O3—K ⁱⁱⁱ	2.8477 (17)
O4—K ^{vi}	2.7599 (17)	O3—K ^{viii}	2.8477 (17)
O4—H41	0.838 (17)	O3—H3	0.814 (18)
F ⁱ —K—F	82.698 (16)	K ^{vi} —O4—H41	103.7 (16)
F ⁱ —K—O1 ⁱⁱ	117.24 (5)	K—O4—H41	103.7 (16)
F—K—O1 ⁱⁱ	68.47 (5)	K ^{vi} —O4—H42	130.3 (11)
F ⁱ —K—O2	87.60 (4)	K—O4—H42	130.3 (11)
F—K—O2	148.65 (6)	H41—O4—H42	103 (2)
O1 ⁱⁱ —K—O2	90.17 (5)	C—O1—K ^{vii}	118.72 (13)
F ⁱ —K—O4	81.96 (5)	C—O1—K ⁱⁱ	118.72 (13)
F—K—O4	135.97 (6)	K ^{vii} —O1—K ⁱⁱ	79.86 (6)
O1 ⁱⁱ —K—O4	153.18 (6)	C—O2—K ^{vi}	123.79 (11)
O2—K—O4	71.12 (6)	C—O2—K	123.79 (11)
F ⁱ —K—O3 ⁱⁱⁱ	132.40 (6)	K ^{vi} —O2—K	82.05 (6)
F—K—O3 ⁱⁱⁱ	80.97 (4)	C—O2—K ⁱⁱⁱ	92.42 (14)
O1 ⁱⁱ —K—O3 ⁱⁱⁱ	97.43 (4)	K ^{vi} —O2—K ⁱⁱⁱ	141.11 (8)
O2—K—O3 ⁱⁱⁱ	125.94 (6)	K—O2—K ⁱⁱⁱ	89.27 (3)
O4—K—O3 ⁱⁱⁱ	79.62 (5)	C—O2—K ^{viii}	92.42 (14)
F ⁱ —K—O2 ⁱⁱⁱ	172.55 (4)	K ^{vi} —O2—K ^{viii}	89.27 (3)
F—K—O2 ⁱⁱⁱ	102.32 (3)	K—O2—K ^{viii}	141.11 (8)
O1 ⁱⁱ —K—O2 ⁱⁱⁱ	70.01 (5)	K ⁱⁱⁱ —O2—K ^{viii}	74.13 (5)
O2—K—O2 ⁱⁱⁱ	90.73 (3)	C—O3—K ⁱⁱⁱ	94.04 (14)
O4—K—O2 ⁱⁱⁱ	90.63 (5)	C—O3—K ^{viii}	94.04 (14)
O3 ⁱⁱⁱ —K—O2 ⁱⁱⁱ	44.48 (6)	K ⁱⁱⁱ —O3—K ^{viii}	76.74 (6)
K ⁱ —F—K ^{iv}	84.96 (4)	C—O3—H3	106 (2)
K ⁱ —F—K ^v	177.20 (5)	K ⁱⁱⁱ —O3—H3	136.9 (10)
K ^{iv} —F—K ^v	97.302 (16)	K ^{viii} —O3—H3	136.9 (10)
K ⁱ —F—K	97.302 (16)	O1—C—O2	127.6 (3)
K ^{iv} —F—K	177.20 (5)	O1—C—O3	117.7 (3)
K ^v —F—K	80.39 (4)	O2—C—O3	114.7 (2)
K ^{vi} —O4—K	82.01 (6)		

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, y+1/2, -z$; (v) $x, -y+3/2, z$; (vi) $x, -y+1/2, z$; (vii) $-x+1, y-1/2, -z+1$; (viii) $-x+2, y-1/2, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O4—H41 \cdots O1 ^{ix}	0.84 (2)	1.89 (2)	2.723 (3)	176 (3)
O4—H42 \cdots F ^x	0.84 (2)	1.87 (2)	2.707 (3)	177 (3)
O3—H3 \cdots F ⁱⁱ	0.81 (2)	1.72 (2)	2.529 (3)	174 (4)

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (ix) $x+1, y, z$; (x) $-x+2, -y+1, -z$.