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Potassium sodium (2*R*,3*R*)-tartrate tetrahydrate: the paraelectric phase of Rochelle salt at 105 K

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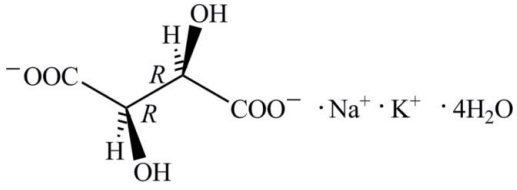
Key indicators: single-crystal X-ray study; T = 105 K; mean σ(C–C) = 0.001 Å; R factor = 0.030; wR factor = 0.069; data-to-parameter ratio = 51.5.

Rochelle salt, $K^+ \cdot Na^+ \cdot C_4H_4O_6^{2-} \cdot 4H_2O$, is known for its remarkable ferroelectric state between 255 and 297 K. The current investigation, based on data collected at 105 K, provides very accurate structural information for the low-temperature paraelectric form. Unlike the ferroelectric form, there is only one tartrate molecule in the asymmetric unit, and the structure displays no disorder to large anisotropic atomic displacements.

Related literature

For previous and related structures, see: Beevers & Hughes (1941); Iwata *et al.* (1989); Solans *et al.* (1997); Ottenz *et al.* (1998); Hinazumi & Mitsui (1972); Kay (1978); Kuroda & Mason (1981); Brożek & Stadnicka (1994); Suzuki *et al.* (1996*a*,*b*); Ambady & Kartha (1968); Boese *et al.* (1995). For irradiation studies, see: Suzuki (1974); Treeck, van & Windsch (1977). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$K^+ \cdot Na^+ \cdot C_4H_4O_6^{2-} \cdot 4H_2O$
M_r = 282.23
Orthorhombic, $P2_12_12$
a = 11.7859 (6) Å
b = 14.1972 (7) Å
c = 6.1875 (3) Å
V = 1035.33 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 105 (2) K
0.5 mm (radius)

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.398, T_{max} = 0.551
(expected range = 0.722–1.000)
33523 measured reflections
10040 independent reflections
8947 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.06
10040 reflections
195 parameters
12 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Absolute structure: Flack, 1983, 4266 Friedel pairs
Flack parameter: 0.044 (14)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O2	0.789 (17)	2.031 (16)	2.5946 (6)	128.2 (14)
O6—H6···O4W^{i}	0.861 (16)	1.968 (16)	2.8119 (7)	166.5 (16)
O1W—H11W···O6	0.824 (8)	1.960 (8)	2.7832 (6)	176.8 (15)
O1W—H12W···O4^{ii}	0.843 (9)	2.010 (9)	2.8500 (7)	174.8 (18)
O2W—H21W···O3^{iii}	0.868 (9)	1.830 (9)	2.6941 (7)	173.4 (19)
O2W—H22W···O2^{iv}	0.862 (9)	1.890 (9)	2.7505 (7)	175.5 (19)
O3W—H31W···O6^{v}	0.843 (9)	2.391 (15)	3.1029 (7)	142.5 (19)
O3W—H31W···O2^{vi}	0.843 (9)	2.499 (17)	3.1181 (7)	131.0 (17)
O3W—H31W···O3^{v}	0.843 (9)	2.584 (14)	3.1569 (8)	126.2 (15)
O3W—H32W···O4^{vii}	0.862 (8)	1.926 (8)	2.7842 (8)	173.8 (16)
O4W—H41W···O1^{viii}	0.858 (9)	1.888 (10)	2.7124 (6)	160.4 (19)
O4W—H42W···O3W^{iv}	0.836 (8)	1.939 (9)	2.7532 (8)	164.4 (16)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2163).

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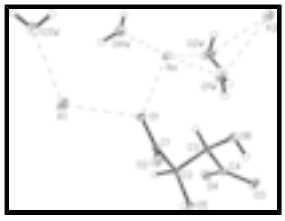

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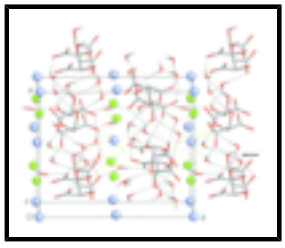

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