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(2*S*,3*S*)-2,3-Dihydroxysuccinic acid monohydrate

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The crystal structure of the title compound, $C_4H_6O_6\cdot H_2O$, displays a two-dimensional network formed by O—H···O hydrogen bonds.

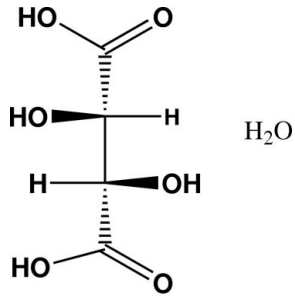
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.126
Data-to-parameter ratio = 6.6

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

Comment

D-Tartaric acid is an important material in biochemistry and racemic resolution. The structure of racemic tartaric acid monohydrate was first determined and reported by Stern & Beevers (1950) and Parry (1951), and redetermined by Nie *et al.* (2001). The structure of D-tartaric acid tetrahydrate was determined by Okaya *et al.* (1966). However, D-tartaric acid monohydrate, (I), has not been reported until now.



(I)

In the crystal structure of (I), the molecules are linked by O—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

D-Tartaric acid (15.0 g, 0.10 mol) in water (9.0 ml) was heated to 343 K until the acid dissolved; the solution was then cooled to room temperature to give colourless prismatic crystals of (I) (5.5 g) after 5 d.

Crystal data

$C_4H_6O_6\cdot H_2O$
M_r = 168.10
Orthorhombic, $P2_12_12_1$
a = 7.6377 (7) Å
b = 7.8268 (7) Å
c = 11.0427 (10) Å
V = 660.12 (10) Å^3
Z = 4
D_x = 1.691 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 293 (2) K
Prism, colourless
0.51 × 0.44 × 0.43 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.779, T_{max} = 1.000
(expected range = 0.724–0.930)
3853 measured reflections
852 independent reflections
818 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 27.0°

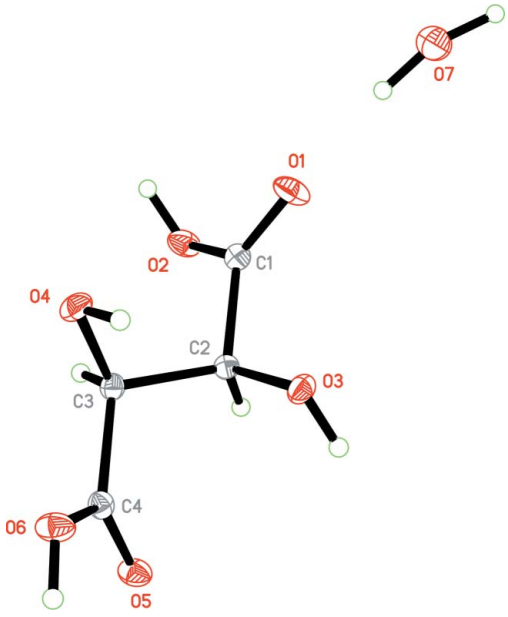


Figure 1
The asymmetric unit of the title compound, showing 40% probability displacement ellipsoids and the atom-numbering scheme.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.2665P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.047$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.126$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.32$ e Å^{-3}
852 reflections	Extinction correction: *SHELXL97*
129 parameters	Extinction coefficient: 1.13 (8)
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7*B*···O1	0.92 (2)	2.04 (3)	2.882 (3)	151 (5)
O7—H7*A*···O2^{i}	0.93 (2)	2.43 (4)	3.120 (4)	131 (4)
O7—H7*A*···O1^{ii}	0.93 (2)	2.13 (4)	2.848 (3)	133 (4)
O3—H5···O6^{iii}	0.90 (2)	1.88 (2)	2.737 (3)	158 (4)
O4—H4···O5^{iv}	0.89 (2)	1.97 (2)	2.808 (3)	156 (4)
O2—H1···O6^{v}	0.90 (2)	1.98 (7)	2.549 (3)	120 (6)
O6—H6···O2^{vi}	0.82	1.74	2.549 (3)	169

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

Atom H6 was placed in a calculated position and allowed to ride on its parent atom at an O—H distance of 0.82 Å. Other H atoms were refined freely [O—H = 0.89 (2)–0.93 (2) Å and C—H = 0.88 (4)–0.99 (4) Å].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT*; data reduction: *SAINT* (Bruker, 2000) and *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

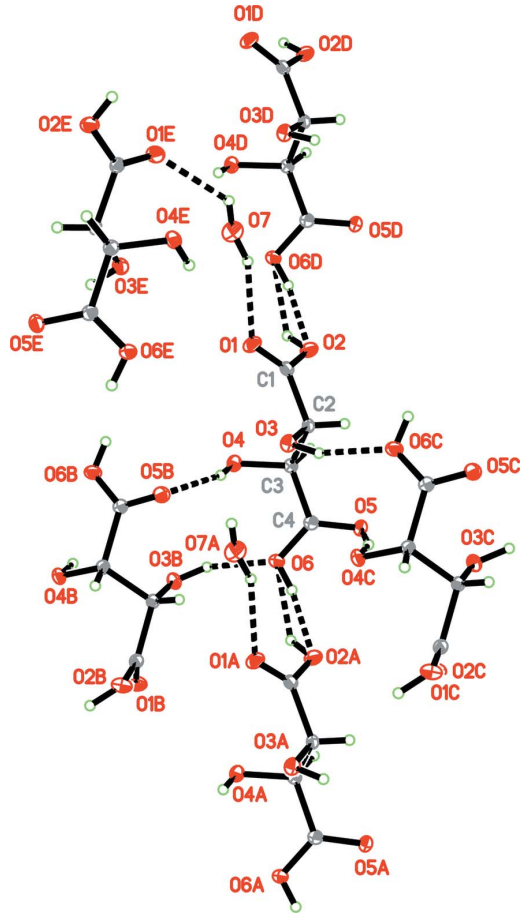


Figure 2
The O—H···O hydrogen bonds (dashed lines) in (I).

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