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Redetermination of racemic tartaric acid monohydrate

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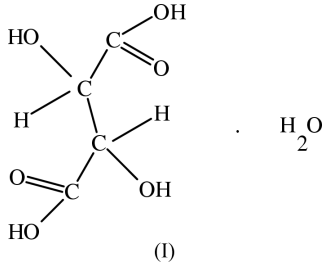
The structure of the title compound, 2,3-dihydroxysuccinic acid monohydrate, $C_4H_6O_6{\cdot}H_2O$, (I), was first determined (to $R = 0.22$) and reported by Parry [*Acta Cryst.* (1951), **4**, 131–138]. We present here a redetermination with significantly improved accuracy. In the centrosymmetric crystals (space group $P\overline{1}$, $Z = 2$), the enantiomeric molecules with both D- and L-configurations co-exist. An extensive intermolecular hydrogen-bond system involves hydrogen bonds formed by carboxyl and hydroxyl groups of the tartaric acid molecule, as well as the crystalline water molecule.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.114
Data-to-parameter ratio = 11.2

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



(I)

Experimental

Single crystals of racemic tartaric acid monohydrate (Parry, 1951) were obtained from an aqueous solution containing L-camphoramic acid and DL-tartaric acid in a 1:1 molar ratio when we tried to separate the racemic acid by L-camphoramic acid.

Crystal data

$C_4H_6O_6{\cdot}H_2O$
M_r = 168.10
Triclinic, $P\overline{1}$
a = 4.869 (5) Å
b = 8.052 (5) Å
c = 9.153 (5) Å
α = 109.260 (5)°
β = 99.862 (5)°
γ = 96.108 (5)°
V = 328.6 (4) Å^3
Z = 2
D_x = 1.699 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16 reflections
θ = 4.7–9.9°
μ = 0.17 mm^{-1}
T = 293 (2) K
Prism, colourless
0.70 × 0.60 × 0.40 mm

Data collection

Rigaku AFC-7*S* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.888, T_{max} = 0.934
1145 measured reflections
1145 independent reflections
1040 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
$h = -5 \rightarrow 5$
$k = 0 \rightarrow 9$
$l = -10 \rightarrow 9$
3 standard reflections
every 150 reflections
intensity decay: 1.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.114$
$S = 1.09$
1145 reflections
102 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o^2) + (0.0730P)^2 + 0.1479P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.64 (7)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.223 (2)	O5—C4	1.203 (2)
O2—C1	1.296 (2)	O6—C4	1.311 (2)
O3—C2	1.413 (2)	C1—C2	1.516 (2)
O4—C3	1.411 (2)	C2—C3	1.536 (3)
O1—C1—O2	124.9 (2)	O4—C3—C4	110.43 (14)
O3—C2—C1	108.47 (14)	O4—C3—C2	110.15 (14)
O3—C2—C3	111.51 (14)	C4—C3—C2	110.20 (15)
C1—C2—C3	110.67 (15)	O5—C4—O6	126.4 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.85	1.83	2.680 (2)	175
O3—H3···O4^{ii}	0.85	1.86	2.714 (3)	176
O6—H6···O*W*^{iii}	0.90	1.64	2.526 (2)	167
O*W*—H2*W*···O3	0.95	1.98	2.891 (2)	159
O*W*—H1*W*···O5^{iv}	0.96	1.90	2.824 (2)	159

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

H atoms were located from a difference Fourier map. They were included in the final cycles of least-squares refinement with fixed coordinates and U_{iso} (0.08 Å^2).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992*a*); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1992*b*); program(s) used to solve structure: *SHELXS*93 (Sheldrick, 1993); program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *XP* (Siemens, 1994).

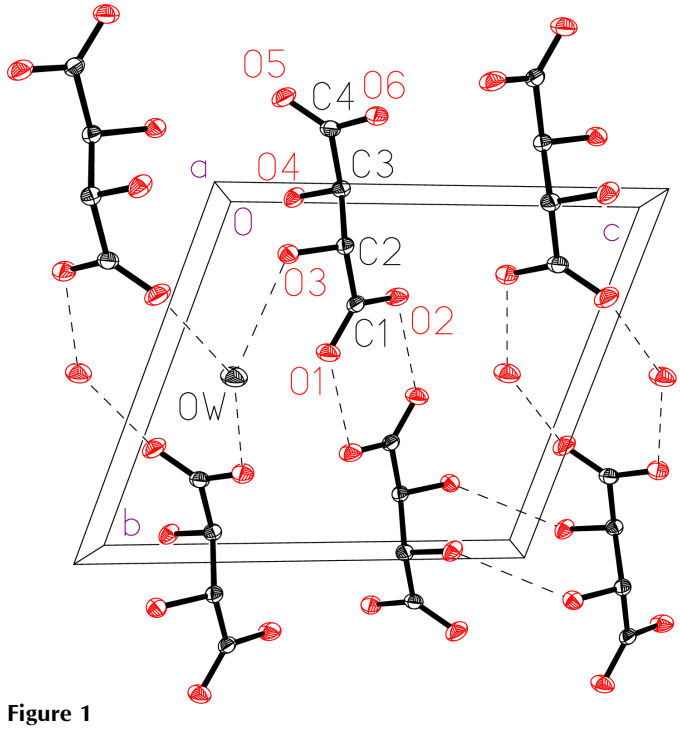


Figure 1
View of the crystal packing of the title compound with 50% probability displacement ellipsoids, with dashed lines showing the hydrogen-bond network. H atoms have been omitted for clarity.

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