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1,10-Phenanthroline (2*R*,3*R*)-tartaric acid trihydrate

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In the title compound, $C_{12}H_8N_2 \cdot C_4H_6O_6 \cdot 3H_2O$, the molecules are linked by strong O—H⋯O hydrogen bonds and π–π interactions, generating an infinite three-dimensional framework.

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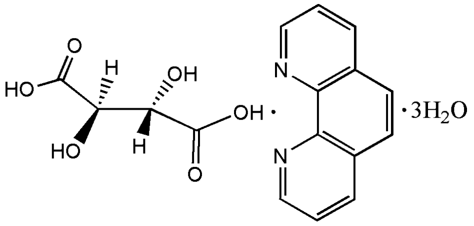
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.053
wR factor = 0.140
Data-to-parameter ratio = 7.3

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

Comment

Our research groups are currently investigating supramolecular structures of cocrystals containing tartaric acid and various organic bases (Wang *et al.*, 2006). We are attempting to understand the relationships between the stabilized crystal structures and the organic base and solvents used in the synthesis, reaction temperature, reaction times and so on. Here, we report a 1:1 co-crystal, (I), of 1,10-phenanthroline and (L)-(+)-tartaric acid as a trihydrate.



(I)

The asymmetric unit of the title complex consists of one (L)-(+)-tartaric acid molecule, one 1,10-phenanthroline molecule and three water molecules, all in general positions (Fig. 1). An infinite three-dimensional supramolecular framework is built

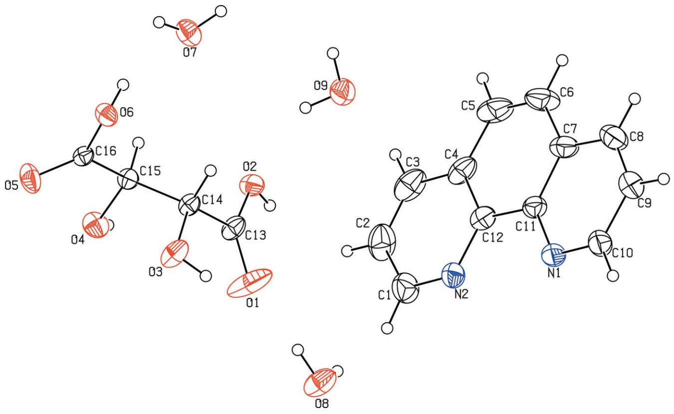


Figure 1
The asymmetric unit of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level. The following symmetry operations have been applied: (x, y, z) for 1,10-phenanthroline and O8, ($\frac{1}{2} + x$, $\frac{3}{2} - y$, $1 - z$) for tartaric acid, and ($\frac{3}{2} - x$, $1 - y$, $\frac{1}{2} + z$) for O7 and O9.

up through strong O—H···O hydrogen bonds (Table 1 and Fig. 2). Additionally, π–π interactions are observed between the N1/C7–C11 ring at (x, y, z) and symmetry-related N2/C1–C4/C12 rings at ($\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$) and ($-\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$) [centroid–centroid separations are 3.842 (3) and 3.700 (3) Å, respectively]. Likewise, the N2/C1–C4/C12 ring makes contacts with rings C4–C7/C11/C12, at positions ($\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$) and ($-\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$), with centroid–centroid separations of 3.773 (3) and 3.797 (3) Å, respectively.

Experimental

All reagents are commercially available and of analytical grade. (L)-(+)-Tartaric acid (2 mmol, 0.30 g) and 1,10-phenanthroline (0.33 mmol, 0.06 g) were dissolved in a beaker filled with 25 ml distilled water. The resulting solution was stirred for about 20 min at 353 K. Colourless crystals of (I) were obtained from the filtrate after 3 d.

Crystal data

$C_{12}H_8N_2 \cdot C_4H_6O_6 \cdot 3H_2O$
$M_r = 384.34$
Orthorhombic, $P2_12_12_1$
$a = 7.1625$ (11) Å
$b = 12.680$ (2) Å
$c = 19.573$ (5) Å
$V = 1777.6$ (6) Å^3
$Z = 4$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.965$, $T_{\max} = 0.977$
7952 measured reflections
2011 independent reflections
1607 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.140$
$S = 1.06$
2011 reflections
274 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 0.2889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O9	0.84 (3)	1.91 (3)	2.740 (4)	173 (5)
O8—H82···O1	0.87 (4)	1.80 (4)	2.663 (5)	178 (6)
O2—H2···O6$^{\rm i}$	0.82 (2)	1.70 (2)	2.479 (3)	161 (4)
O3—H3···O8$^{\rm ii}$	0.82 (4)	1.91 (4)	2.699 (4)	163 (5)
O6—H6···O7$^{\rm iii}$	0.80 (3)	2.04 (4)	2.808 (4)	159 (4)
O7—H72···O5$^{\rm i}$	0.86 (2)	1.91 (3)	2.747 (4)	163 (6)
O7—H71···O6$^{\rm iv}$	0.84 (2)	2.41 (4)	2.808 (4)	110 (3)
O8—H81···O3$^{\rm i}$	0.83 (4)	1.95 (4)	2.765 (4)	167 (4)
O9—H91···O2$^{\rm iv}$	0.86 (3)	2.29 (3)	3.016 (5)	142 (4)
O9—H92···O5$^{\rm i}$	0.88 (4)	1.94 (4)	2.772 (4)	159 (4)

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

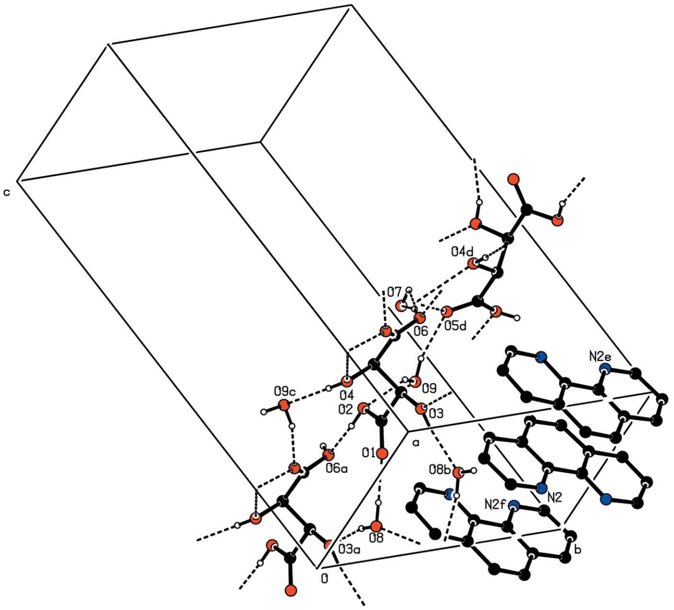


Figure 2
Part of the crystal structure of (I). H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity. [Symmetry codes: (a) $-1 + x, y, z$; (b) $\frac{1}{2} + x, \frac{1}{2} - y, -z$; ($c$) $1\ x, -\frac{1}{2} + y, \frac{1}{2} - z$; ($d$) $2 - x, \frac{1}{2} + y, \frac{1}{2} - z$; ($e$) $-\frac{1}{2} + x, \frac{3}{2} - y, -z$; ($f$) $\frac{1}{2} + x, \frac{3}{2} - y, -z$.]

All C-bound H atoms were placed in calculated positions and refined using a riding approximation, with C—H bond lengths constrained to 0.93 (aromatic CH) or 0.98 Å (methine CH), and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). H atoms bonded to O atoms were located in a difference map. For water molecules, O—H and H···H distances were restrained to 0.85 (1) and 1.34 (1) Å. For tartaric acid, O—H bond lengths of carboxylic groups were restrained to 0.82 (1) Å. 735 Friedel pairs were merged, and the absolute configuration for the chiral centres was assigned assuming the configuration of the (L)-(+)-tartaric acid used in the synthesis.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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