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(*S*)-Phenylsuccinic acid

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.074
Data-to-parameter ratio = 8.5

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

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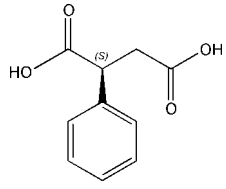
(*S*)-Phenylsuccinic acid, $C_{10}H_{10}O_4$, crystallizes from water with two molecules per asymmetric unit. In the crystal structure, the carboxyl groups of each acid molecule are connected to those of adjacent molecules *via* hydrogen bonds; each molecule is connected to three other molecules, forming infinite chains.

Comment

Phenylsuccinic acid (PSA) is an aromatic dicarboxylic acid used as a classical resolving agent for pharmaceuticals (Bayley & Vaidya, 1992; Kozma, 2002). To be able to study and understand the solid-state properties of PSA and its interactions with solvents or with other common reagents, it is essential to know the crystal structures of both the pure enantiomer and the racemate. Since the structures of neither (*S*)- nor (*RS*)-PSA were known, we grew crystals of both compounds in order to determine how the acid molecules are assembled in each structure. The structure of (*S*)-PSA is presented here.



PSA

In (*S*)-PSA, two molecules are present in the asymmetric unit (see Fig. 1) and the geometry of these is unexceptional.

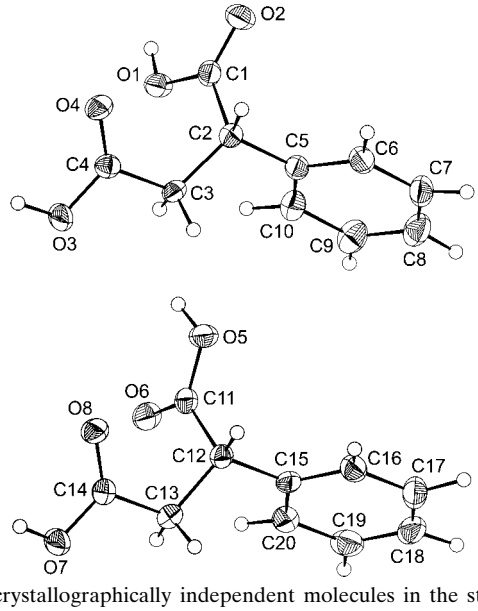


Figure 1
The two crystallographically independent molecules in the structure of (*S*)-PSA. Displacement ellipsoids are drawn at the 70% probability level.

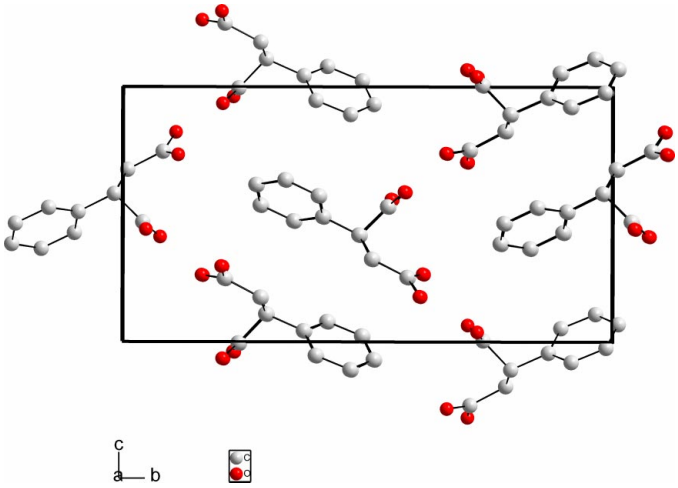


Figure 2
The unit cell contents of (*S*)-PSA, viewed along *a*. H atoms have been omitted.

Fig. 2 displays the packing in the unit cell. The acid molecules are connected *via* hydrogen bonds (Table 1), each molecule binding to one adjacent molecule *via* both O atoms of one carboxyl group. The other carboxyl group binds to two different molecules *via* two H bonds. Fig. 3 shows the network which is formed. Molecule 1 of the asymmetric unit is connected to three molecules of the second and *vice versa*. The screw axis then generates a second network which is crystallographically equivalent, but not connected to the first.

Experimental

Crystals were grown from aqueous solutions by dissolving the purchased material (Fluka, >99%) in pure, distilled and deionized water at room temperature. The clear solutions were evaporated to dryness under low-pressure conditions at room temperature, yielding single crystals of (*S*)-PSA.

Crystal data

$C_{10}H_{10}O_4$
M_r = 194.19
Monoclinic, $P2_1$
a = 5.4193 (2) Å
b = 18.0847 (5) Å
c = 9.4713 (3) Å
β = 95.7044 (11)°
V = 923.65 (5) Å^3
Z = 4
D_x = 1.396 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4591 reflections
θ = 4.1–27.5°
μ = 0.11 mm^{-1}
T = 100 K
Irregular, colourless
0.35 × 0.15 × 0.07 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
7099 measured reflections
2162 independent reflections
2009 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.4°
$h = -7 \rightarrow 6$
$k = -22 \rightarrow 23$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.074
S = 1.03
2162 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.1504P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

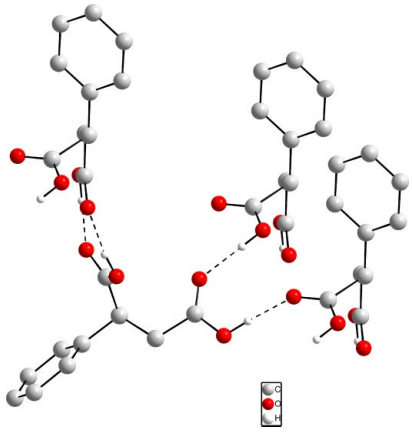


Figure 3
The chains formed by the molecules of (*S*)-PSA. Only the carboxy H atoms are shown. Hydrogen bonds are indicated by dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O8^{i}	0.92	1.75	2.659 (2)	170
O3—H3O···O6^{ii}	0.92	1.71	2.627 (2)	177
O5—H5O···O4^{iii}	0.89	1.82	2.714 (2)	178
O7—H7O···O2^{iv}	0.92	1.70	2.615 (2)	178

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

The *S* configuration is known from a commercial sample. A whole sphere of data was collected and Friedel pairs were merged. All H atoms were located in a difference Fourier map and were refined using a riding model, with U_{iso} set equal to 1.2U_{eq} of the parent atoms.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *maXus* (Mackay *et al.*, 1998).

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