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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.046  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 17.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## A 1:1 cocrystal of sebacic acid and 4,4'-bipyridine

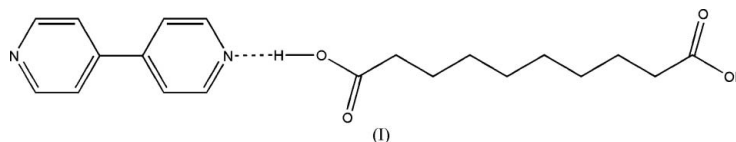
The crystal structure of the title compound,  $\text{C}_{10}\text{H}_{18}\text{N}_2 \cdot \text{C}_{10}\text{H}_{18}\text{O}_4$ , consists of sebacic acid and 4,4'-bipyridine molecules. The sebacic acid molecule displays an extended planar structure, but the pyridine rings of the 4,4'-bipyridine molecule are twisted relative to each other, with a dihedral angle of  $15.78(7)^\circ$ . The centroid-to-centroid separation of  $3.6366(11)$  Å indicates  $\pi$ - $\pi$  stacking between parallel pyridine rings.

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## Comment

As part of our ongoing investigation of non-covalent interactions, we report here the crystal structure of the title compound, (I).



The crystal structure of (I) consists of sebacic acid molecules and 4,4'-bipyridine molecules (Fig. 1). The two pyridine rings of the 4,4'-bipyridine molecule are twisted relative to each other, with a dihedral angle of  $15.78(7)^\circ$ . The torsion angles (Table 1) indicate the extended planar conformation of the skeleton of sebacic acid.

Classical  $\text{O}-\text{H} \cdots \text{N}$  and weak  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds occur (Table 2), which help to stabilize the crystal structure of (I). The centroid-to-centroid separation of  $3.6366(11)$  Å indicates the existence of  $\pi$ - $\pi$  stacking between parallel  $\text{N}2$ -pyridine and  $\text{N}2^v$ -pyridine rings [symmetry code: (v)  $1 - x, 2 - y, 1 - z$ ].

## Experimental

An aqueous solution (15 ml) of sebacic acid (0.101 g, 1 mmol) and 4,4'-bipyridine (0.096 g, 1 mmol) was sealed in a Parr Teflon-lined stainless steel vessel (25 ml) and heated at 453 K for 72 h. After

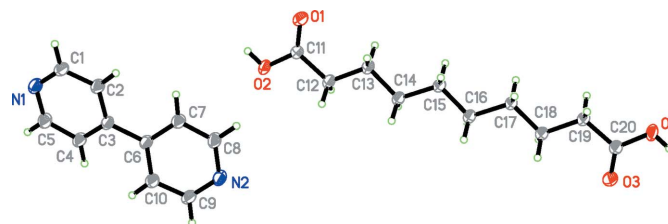


Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

cooling the mixture to room temperature, single crystals of (I) were obtained.

Crystal data

$C_{10}H_{18}O_4 \cdot C_{10}H_8N_2$	$V = 912.8 (4) \text{ \AA}^3$
$M_r = 358.43$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.304 \text{ Mg m}^{-3}$
$a = 8.9652 (18) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.5699 (19) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 11.700 (2) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\alpha = 90.67 (3)^\circ$	Lath, colourless
$\beta = 95.82 (3)^\circ$	$0.45 \times 0.17 \times 0.09 \text{ mm}$
$\gamma = 113.71 (3)^\circ$	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	4146 independent reflections
$\omega$ scans	2837 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.040$
9086 measured reflections	$\theta_{max} = 27.5^\circ$

Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2]$
$wR(F^2) = 0.132$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.002$
4146 reflections	$\Delta\rho_{max} = 0.27 \text{ e \AA}^{-3}$
235 parameters	$\Delta\rho_{min} = -0.25 \text{ e \AA}^{-3}$

Table 1

Selected torsion angles ( $^\circ$ ).

O1—C11—C12—C13	2.8 (2)	C15—C16—C17—C18	-178.14 (12)
O2—C11—C12—C13	-178.02 (12)	C16—C17—C18—C19	-179.48 (12)
C11—C12—C13—C14	-179.91 (12)	C17—C18—C19—C20	178.61 (12)
C12—C13—C14—C15	179.23 (12)	C18—C19—C20—O3	1.8 (2)
C13—C14—C15—C16	-178.32 (12)	C18—C19—C20—O4	-178.02 (12)
C14—C15—C16—C17	179.65 (12)		

Table 2

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H2A $\cdots$ N1 <sup>i</sup>	0.82	1.84	2.6418 (15)	165
O4—H4B $\cdots$ N2 <sup>ii</sup>	0.82	1.84	2.6436 (15)	167
C2—H2B $\cdots$ O1 <sup>iii</sup>	0.93	2.56	3.486 (2)	174
C4—H4A $\cdots$ O3 <sup>iv</sup>	0.93	2.59	3.511 (2)	173

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

Carboxyl H atoms were located in a difference Fourier map and refined as riding with  $O-H = 0.82 \text{ \AA}$  and  $U_{iso}(H) = 1.5U_{eq}(O)$ . Other H atoms were placed in calculated positions, with  $C-H = 0.93$  (aromatic) or  $0.97 \text{ \AA}$  (methylene), and refined in riding mode, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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