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A 1:1 cocrystal of pyridine and 4-hydroxybenzoic acid

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.167
Data-to-parameter ratio = 13.8

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

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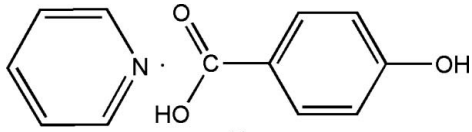
The title cocrystal, $C_5H_5N{\cdot}C_7H_6O_3$, consists of pyridine and 4-hydroxybenzoic acid molecules which are linked by O—H···N and O—H···O hydrogen bonds, leading to zigzag chains along the b axis.

Comment

In recent years, hydrogen bonds have attracted the interest of chemists and have been widely used to design and synthesize one-, two- and three-dimensional supramolecular compounds (Aakeröy *et al.*, 2002). 4-Hydroxybenzoic acid is a good hydrogen-bond donor and can form cocrystals with other organic molecules (Vishweshwar *et al.*, 2003). Here we report the crystal structure of the title cocrystal, (I).



(I)

Compound (I) consists of pyridine and 4-hydroxybenzoic acid neutral molecules (Fig. 1 and Table 1). 4-Hydroxybenzoic acid forms O—H···N hydrogen bonds with pyridine and O—H···O hydrogen bonds with two neighboring 4-hydroxybenzoic acid molecules, forming zigzag chains along the b axis (Fig. 2).

Experimental

All reagents were commercially available and of analytical grade. 4-Hydroxybenzoic acid (2.0 mmol, 0.28 g) was dissolved in pyridine (12 ml). The mixture was stirred for 30 min at room temperature and was then filtered. Colorless crystals were obtained after 8 d by slow evaporation of the filtrate.

Crystal data

$C_5H_5N{\cdot}C_7H_6O_3$
M_r = 217.22
Monoclinic, $P2_1/c$
a = 12.163 (5) Å
b = 9.002 (4) Å
c = 11.171 (5) Å
β = 117.34 (1)°
V = 1086.6 (8) Å^3
Z = 4
D_x = 1.328 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: none
6841 measured reflections
2118 independent reflections
1602 reflections with $I > 2\sigma(I)$
R_{int} = 0.174
θ_{max} = 26.0°

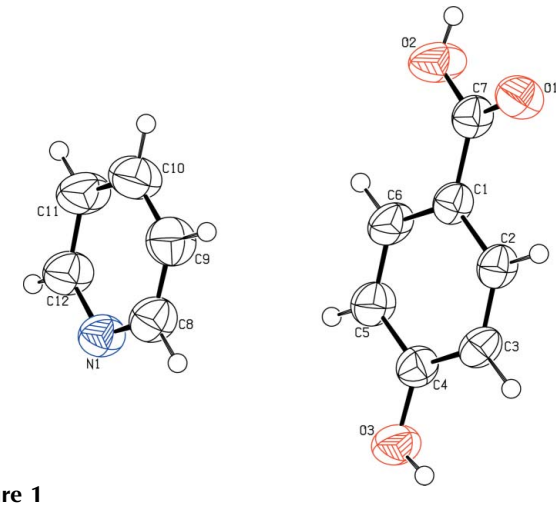


Figure 1
The asymmetric unit of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

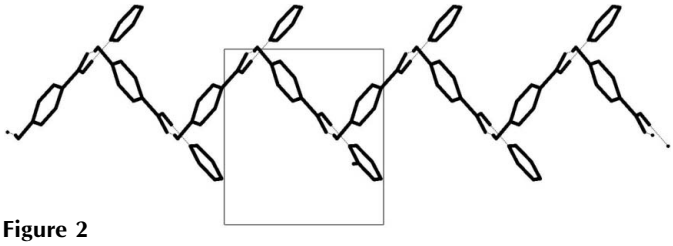


Figure 2
The crystal structure of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.167$
$S = 1.00$
2118 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C7—O1	1.228 (2)	C7—O2	1.297 (2)
O1—C7—C1	122.53 (15)	O2—C7—C1	115.63 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H*O2*···N1^{i}	0.843 (10)	1.753 (11)	2.592 (2)	173 (3)
O3—H*O3*···O1^{ii}	0.825 (10)	1.868 (11)	2.686 (2)	171 (2)

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

The value of R_{int} is very large because the crystal is not stable at room temperature and effloresces easily. Therefore, there were some difficulties in collecting the data. H atoms of the hydroxy and carboxyl groups were located in difference maps, and O—H lengths were restrained to 0.82 (1) Å. Other H atoms were positioned geometrically, with C—H = 0.93 Å, and were refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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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