4-Aminobenzoic acid–nicotinic acid (2/1)

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Key indicators

Single-crystal X-ray study
$T = 303$ K
Mean σ(C–C) = 0.011 Å
R factor = 0.075
wR factor = 0.234
Data-to-parameter ratio = 6.2

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

In the title compound, $2C_7H_7NO_2 \cdot C_6H_5NO_2$, the 4-aminobenzoic acid and the nicotinic acid molecules are approximately planar. The crystal structure is stabilized by an extensive network of N—H···O, O—H···O and O—H···N hydrogen bonds.

Comment

4-Aminobenzoic acid is involved in the biosynthesis of folic acid, which is a constituent of the vitamin B complex and is found in animal and plant tissues (Zoroddu *et al.*, 1996). Nicotinic acid (vitamin B3), known as niacin, is a lipid-lowering agent widely used to treat hypertriglyceridemia by the inhibition of lipolysis in adipose tissue (Athimoolam & Rajaram, 2005). The nicotinic acid complex 5-methylpyrazine-2-carboxylic acid 4-oxide is a commonly used drug for the treatment of hypercholesterolemia (Lorenzen *et al.*, 2001). Coordination complexes of nicotinic acid with metals such as Sn possess antitumour activity greater than that of the well known *cis*-platin or doxorubicin (Gielen *et al.*, 1992). The enzyme nicotinic acid mononucleotide adenyltransferase is essential for the synthesis of nicotinamide adenine dinucleotide in all living cells and is a potential target for antibiotics (Kim *et al.*, 2004). As a part of our investigation of interactions between acids, we report here the crystal structure of 4-aminobenzoic acid–nicotinic acid (2/1), (I).
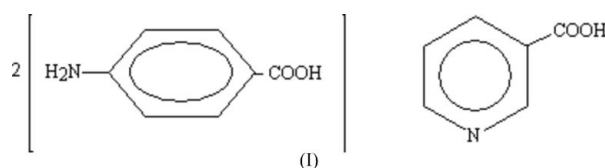
The asymmetric unit of (I) contains two independent aminobenzoic acid molecules and a nicotinic acid molecule. The bond lengths and angles of the nicotinic acid are normal (Kutoglu & Scheringer, 1983). The nicotinic acid molecule is
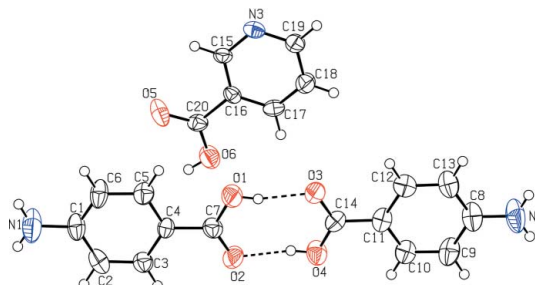

Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.
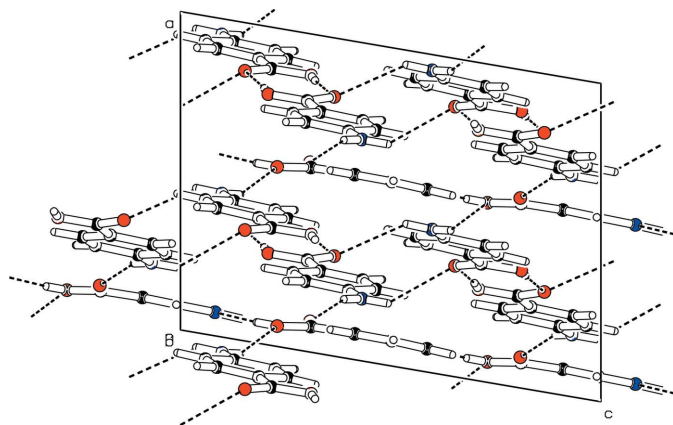
Figure 2
A packing diagram for (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

approximately planar, with a maximum deviation from the mean plane of 0.138 (4) Å for atom O6. Each of the 4-aminobenzoic acid molecules is almost planar, the maximum deviation from the mean planes being 0.077 (5) Å for atom O2 and 0.077 (5) Å for atom O3. The bond lengths and angles of *p*-aminobenzoic acid in (I) are similar to those reported for 4-aminobenzoic acid (Gracin & Fischer, 2005).

The crystal structure is stabilized by N—H···O, O—H···O and O—H···N hydrogen bonds.

Experimental

Solutions of 4-aminobenzoic acid and nicotinic acid were mixed in 2:1 molar ratio in ethanol and warmed in a water bath for 2 h. Yellow crystals were obtained after two weeks *via* slow evaporation.

Crystal data

$2C_7H_7NO_2 \cdot C_6H_5NO_2$	$Z = 4$
$M_r = 397.38$	$D_x = 1.395$ Mg m^{-3}
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 10.1803$ (4) Å	$\mu = 0.11$ mm^{-1}
$b = 13.8050$ (7) Å	$T = 303$ (2) K
$c = 13.6530$ (8) Å	Block, yellow
$\beta = 99.680$ (4)°	$0.4 \times 0.25 \times 0.2$ mm
$V = 1891.46$ (16) Å^3	

Data collection

Nonius MACH3 diffractometer	1281 reflections with $I > 2\sigma(I)$
ω–2θ scans	$R_{int} = 0.043$
Absorption correction: ψ scan	$\theta_{max} = 25.0°$
(North *et al.*, 1968)	3 standard reflections
$T_{min} = 0.969$, $T_{max} = 0.979$	frequency: 60 min
3471 measured reflections	intensity decay: none
1614 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$
$wR(F^2) = 0.234$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.006$
1614 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···N3^i	0.82	1.73	2.549 (7)	177
N2—H2A···O2^{ii}	0.86	2.56	3.278 (10)	141
N2—H2B···O5^{iii}	0.86	2.11	2.930 (11)	160
N1—H1A···O6^{iv}	0.86	2.32	3.113 (10)	154
N1—H1B···O3^i	0.86	2.57	3.303 (11)	144
O4—H4···O2	0.82	1.81	2.620 (8)	168
O1—H1···O3	0.82	1.79	2.596 (8)	167

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

After checking their presence in a difference map, H atoms were placed in calculated positions, with C—H = 0.93 Å, O—H = 0.82 Å and N—H = 0.82 Å, and refined using a riding model, with U_{iso}(H) = $1.2U_{eq}$(C,N) and $1.5U_{eq}$(O). In the absence of significant anomalous scattering effects, 158 Friedel pairs were averaged.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *SHELXL97*.

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