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Monoclinic form of ethyl 4-aminobenzoate (benzocaine)

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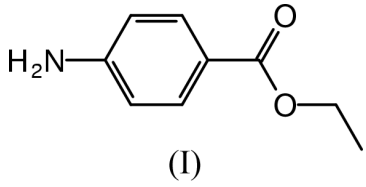
The structure of the title compound, $C_9H_{11}NO_2$, (I), comprises a flat molecule arranged, head-to-tail, in linear ribbon arrays *via* a N—H···O=C association. These ribbons end-on form a herring-bone structure interconnected *via* N—H···N association. The structure was first determined in 1987 [Sinha & Pattabhi (1987). *Proc. Indian Acad. Sci. Chem. Sci.* **98**, 229–234] in the orthorhombic space group $P2_12_12_1$, with $R = 0.120$, whereas similar cell dimensions and an increased β angle in the present study resulted in monoclinic space group $P2_1/c$, with $R = 0.065$.

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.065
wR factor = 0.181
Data-to-parameter ratio = 12.3

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



(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_9H_{11}NO_2$
M_r = 165.19
Monoclinic, $P2_1/c$
a = 8.198 (2) Å
b = 5.430 (1) Å
c = 19.592 (5) Å
β = 91.350 (6)°
V = 871.8 (4) Å^3
Z = 4
D_x = 1.259 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3445 reflections
θ = 1.0–27.5°
μ = 0.09 mm^{-1}
T = 120 (2) K
Block, colourless
0.10 × 0.08 × 0.03 mm

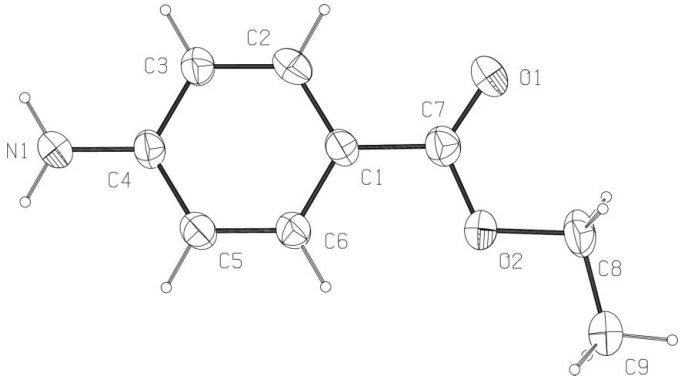


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 50% probability ellipsoids.

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	1352 independent reflections
φ and ω scans	686 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$R_{int} = 0.097$
$T_{min} = 0.991$, $T_{max} = 0.997$	$\theta_{max} = 25.0^\circ$
3445 measured reflections	$h = -9 \rightarrow 9$
	$k = -6 \rightarrow 5$
	$l = -21 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.181$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
1352 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
110 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O1^{i}	0.88	2.10	2.934 (4)	158
N1—H12···N1^{ii}	0.88	2.38	3.252 (3)	174

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

An R_{int} value of 0.097 was the result of weak high-angle data. All H atoms were included in the refinement, at calculated positions, as riding models, with C—H distances set to 0.95 (Ar–H), 0.99 (CH_2) and 0.98 Å (CH_3), and N—H distances set to 0.88 Å.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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