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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.052
wR factor = 0.135
Data-to-parameter ratio = 16.1

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

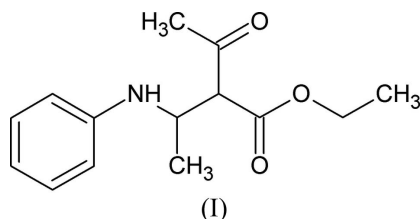
Ethyl 2-acetyl-3-anilinobutanoate

The title compound, $\text{C}_{14}\text{H}_{19}\text{NO}_3$, adopts an extended conformation and forms hydrogen-bonded dimers through intermolecular $\text{N}-\text{H}\cdots\text{O}$ interactions.

Received 20 September 2006
Accepted 25 October 2006

Comment

The structure of ethyl 2-acetyl-3-anilinobutanoate, (I), is reported here and the molecular structure is depicted in Fig. 1. There are three planar subunits in (I), *viz.* the aniline (atoms C1–C6/N7), acetyl (C10/C11/C13/O12) and ethyl acetate (C10/C14/O15/O16/C17/C18) groups. The aniline ring is inclined at angles of 79.9 (1) and 9.3 (1)° to the acetyl and ethyl acetate groups, respectively, with the acetyl group at an angle of 71.2 (1)° to the ethyl acetate group; torsion angles are reported in Table 1. Molecules of (I) adopt an extended conformation, with all of the main chain torsion angles associated with the ester and aniline groups, *i.e.* from C18–C17–O16–C14 to C10–C8–N7–C1, *trans*.



In the crystal structure, molecules of (I) associate into dimers through intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2), and stack along the *a* axis. The hydrogen-bonded centrosymmetric dimers are characterized by an $R_2^2(12)$ ring pattern (Bernstein *et al.*, 1995). There are no significant overlaps of the aromatic rings (Fig. 2).

Experimental

A mixture of acetaldehyde, ethyl acetoacetate and aniline, in the molar ratio 2:1:1, was stirred for 5 h. A paste-like solid was formed, which was repeatedly washed with diethyl ether. The resulting compound was recrystallized from diethyl ether (yield 90%; m.p. 367 K).

Crystal data

$\text{C}_{14}\text{H}_{19}\text{NO}_3$
 $M_r = 249.30$
Triclinic, $P\bar{1}$
 $a = 8.045$ (2) Å
 $b = 9.390$ (2) Å
 $c = 10.419$ (3) Å
 $\alpha = 72.77$ (1)°
 $\beta = 77.68$ (1)°
 $\gamma = 69.49$ (1)°

$V = 698.8$ (3) Å^3
 $Z = 2$
 $D_x = 1.185$ Mg m^{-3}
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm^{-1}
 $T = 295$ (2) K
Block, colourless
 $0.23 \times 0.14 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.931$, $T_{\max} = 0.998$

7266 measured reflections
 2734 independent reflections
 1672 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.135$
 $S = 1.01$
 2734 reflections
 170 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.1336P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{\AA}^{-3}$

Table 1

Selected torsion angles ($^\circ$).

C2—C1—N7—C8	24.3 (3)	C8—C10—C11—C13	51.4 (2)
C1—N7—C8—C9	79.4 (3)	C8—C10—C14—O16	139.35 (18)
C1—N7—C8—C10	-157.36 (18)	C10—C14—O16—C17	177.13 (18)
N7—C8—C10—C14	173.25 (17)	C14—O16—C17—C18	-177.5 (2)
N7—C8—C10—C11	51.7 (2)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N7-H7\cdots O12^i$	0.86 (2)	2.24 (2)	3.099 (3)	169 (2)

Symmetry code: (i) $-x, -y + 1, -z$.

C-bound H atoms were treated as riding atoms with fixed geometry (aryl C—H = 0.93 \AA , methyl C—H = 0.96 \AA , methylene C—H = 0.97 \AA and methine C—H = 0.98 \AA) riding on their carrier atoms, with U_{iso} values = $1.2U_{\text{eq}}$ ($1.5U_{\text{eq}}$ for methyl) of the parent atom. The amino H atom was located in a difference electron-density map and was refined isotropically, with N—H = 0.86 (2) \AA .

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PLATON.

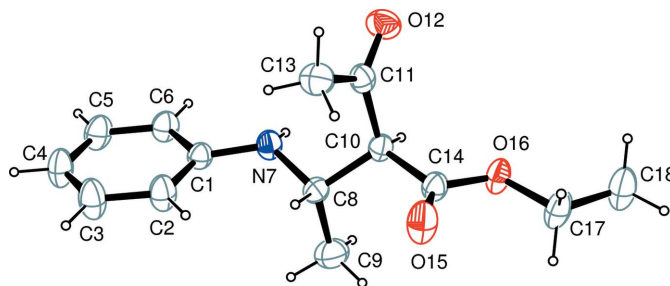


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

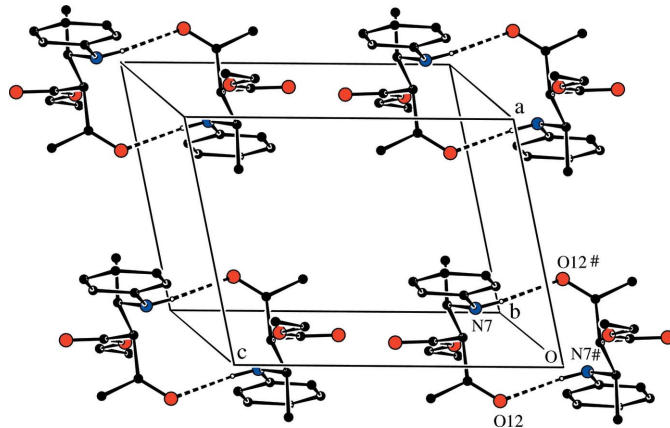


Figure 2

The packing in (I), showing the hydrogen-bonded (dashed lines) dimer. For clarity, of the H atoms, only amino atom H7 is shown. Symmetry code: (#) $-x, 1 - y, -z$. Colour key: C black, H white, N blue and O red.

The authors acknowledge the use of the CCD facility at the Indian Institute of Science, Bangalore, set up under the IRHPA–DST programme.

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