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N-Acetyl-L-alanine

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Key indicators

Single-crystal X-ray study
T = 105 K
Mean σ(C–C) = 0.001 Å
R factor = 0.037
wR factor = 0.100
Data-to-parameter ratio = 28.6

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

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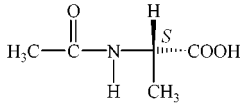
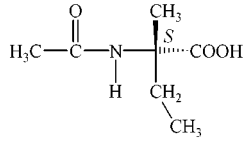
The crystal structure of the title compound, $C_5H_9NO_3$, has been investigated as part of a search for suitable materials for electron paramagnetic resonance (EPR) radiation dosimetry.

Comment

The simple amino acid alanine has, during the last 15 years, been developed to be the standard material for radiation dosimetry using electron paramagnetic resonance (EPR) spectrometry as the readout technique (Regulla & Deffner, 1982). EPR/alanine dosimetry is simple, versatile, reproducible and non-destructible upon dose readout. The disadvantage is the sensitivity; alanine is, for all practical purposes, usable only for doses above 1 Gy and is thus not well suited for clinical work. A search for more suitable materials for EPR dosimetry has been pursued in several laboratories over recent years (Vestad *et al.*, 2003; Lund *et al.*, 2004). *N*-Acetyl-L-alanine, (I), is one such possible material. However, to learn the dosimetric properties of this compound and to understand the prospects of enhancing the sensitivity, there is a need to characterize the physical properties of radiation-induced radicals in crystalline (I) using EPR spectroscopy. Accordingly, knowledge of the crystal structure of (I) is necessary.



(I)



(II)

The molecular structure of (I) is illustrated in Fig. 1. Bond lengths and angles are normal. Crystal structures are available (Cambridge Structural Database, Version 5.25 of November 2003; Allen, 2002) for seven other *N*-acetyl derivatives of the 20 common L-amino acids: *N*-acetylglycine (Mackay, 1975), *N*-acetyl-L-phenylalanine (Stout *et al.*, 2000), *N*-acetyl-L-cysteine (Takusagawa *et al.*, 1981), *N*-acetyl-L-glutamine (Narasimhamurthy *et al.*, 1976), *N*-acetyl-L-tyrosine (Koszelak & van der Helm, 1981), *N*-acetyl-L-tryptophan (Yamane *et al.*, 1977) and *N*-acetyl-L-glutamic acid (Dobson & Gerkin, 1997). The structures of *N*-acetyl-L-norvaline (Lovas *et al.*, 1974) and the racemates *N*-acetyl-DL-methionine (Ponnuswamy & Trotter, 1985) and *N*-acetyl-DL-valine (Carroll *et al.*, 1990) are relevant additions to this group. A typical feature for these compounds (and indeed for *N*-acyl amino acids in general; Chen & Parthasarathy, 1977) is the presence of —COOH···O═C(amide) and >N—H···O═C(carboxyl) hydrogen bonds. The former is missing only for *N*-acetyl-DL-valine, the

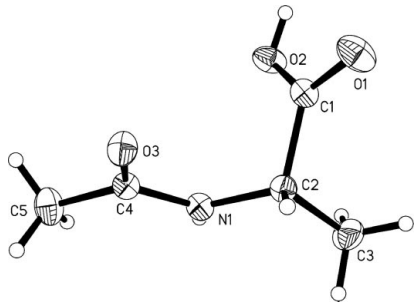


Figure 1
The molecular structure of *N*-acetyl-L-alanine. Displacement ellipsoids are shown at the 50% probability level and H atoms are shown as spheres of arbitrary size.

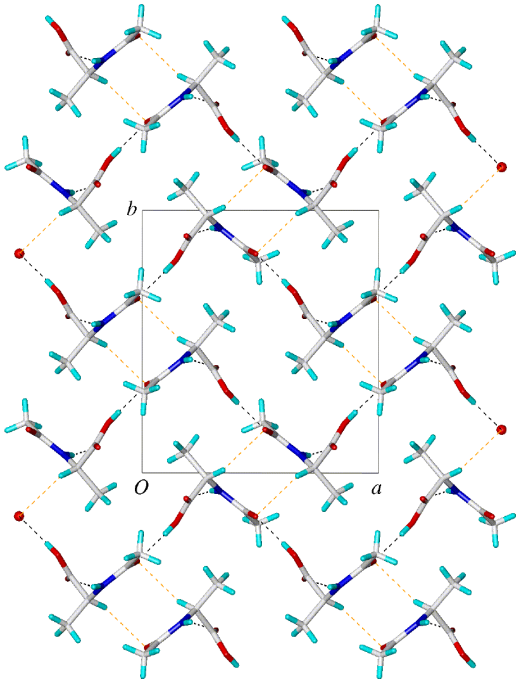


Figure 2
The molecular packing and unit cell viewed along the *c* axis. Spheres show the positions of O3 atoms in neighbouring molecules, included here to illustrate the hydrogen-bond network. Hydrogen bonds with N—H and O—H donors are shown as dashed black lines and the C2—H21···O3 hydrogen bonds are shown as dashed orange lines (the C5—H53···O3 interaction runs parallel to the viewing direction and is not visible).

latter only for *N*-acetyl-L-cysteine. Compound (I) thus shares its two most important intermolecular interactions (Table 2) with almost all other *N*-acetyl amino acids, and even has essentially the same folded molecular conformation [C1—C2—N1—C4 = −70.77 (7)°; Table 1] as *N*-acetyl-L-phenylalanine, *N*-acetyl-L-tyrosine, *N*-acetyl-L-norvaline and the L-enantiomer in *N*-acetyl-DL-methionine. Nevertheless, the specific hydrogen-bond pattern of (I) is not found for any of the compounds listed above. A very similar structure with the same overall crystal packing pattern has, however, been observed for *N*-acetyl-(*S*)-isovaline, (II) (Crisma *et al.*, 1998). The only difference between the two pertains to the weak C2—H21···O3 hydrogen bonds of (I) (Table 2), which are broken in (II) as the separation of hydrogen-bonded zigzag layers of peptide molecules is increased to make room for the two extra methyl groups (Fig. 2). In the process, the length of the longest axis is increased from 11.5449 (3) Å for (I) to 14.577 (2) Å for (II).

Experimental

N-Acetyl-L-alanine was obtained from Sigma–Aldrich. Crystals were prepared by recrystallization from a methanol solution at room temperature.

Crystal data

$C_5H_9NO_3$
M_r = 131.13
Orthorhombic, $P2_12_12$
a = 10.3879 (2) Å
b = 11.5449 (3) Å
c = 5.74260 (10) Å
V = 688.69 (3) Å^3
Z = 4
D_x = 1.265 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 042 reflections
θ = 2.6–44.8°
μ = 0.11 mm^{-1}
T = 105 (2) K
Plate, colourless
1.15 × 1.00 × 0.03 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.688, T_{max} = 0.997
14 223 measured reflections
3149 independent reflections
2839 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 44.8°
$h = -19 \rightarrow 20$
$k = -22 \rightarrow 22$
$l = -11 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.12
3149 reflections
110 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.0041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected torsion angles (°).

O1—C1—C2—N1	149.71 (7)	C2—N1—C4—O3	−1.92 (9)
C1—C2—N1—C4	−70.77 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.783 (15)	2.190 (15)	2.9586 (8)	167.0 (12)
O2—H2···O3^{ii}	0.83 (2)	1.793 (19)	2.5831 (7)	158 (2)
C2—H21···O3^{iii}	0.995 (14)	2.624 (13)	3.3211 (8)	127.1 (11)
C5—H53···O3^{i}	0.903 (18)	2.65 (2)	3.3641 (9)	136.8 (13)

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

Positional parameters were refined for all H atoms. U_{iso} values were $1.2U_{eq}$ (methylene and amide) or $1.5U_{eq}$ (carboxylate and methyl) of the carrier atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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