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N-Acetyl-L-phenylalanine

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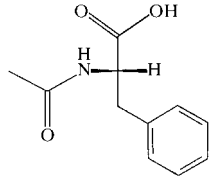
The structure of the title compound, $C_{11}H_{13}NO_3$, is characterized by a two-dimensional infinite network of intermolecular N—H···O and O—H···O hydrogen bonds.

Comment

It is important to determine the crystal structures of amino acids and their derivatives because of their importance in defining the preferred conformations of large peptides and proteins. We have determined the structure of the title compound, (I), for a solid-state NMR tensor study. Few N^{15}



(I)

chemical-shielding tensors have been determined (Harbison *et al.*, 1984) and chemical-shielding tensors are important for accurate solution and solid-state NMR experiments (Oas *et al.*, 1987; Hartzell *et al.*, 1987; Lee & Ramamoorthy, 1998; Lee *et al.*, 1998).

Experimental

(I) was obtained from Sigma Chemical Corporation (St Louis, Missouri). Crystals were grown from water and analyzed.

Crystal data

$C_{11}H_{13}NO_3$, M_r = 207.22
Orthorhombic, $P2_12_12_1$
a = 5.6528 (1) Å
b = 11.1532 (2) Å
c = 16.9897 (1) Å
V = 1071.15 (3) Å^3
Z = 4
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6900 reflections
θ = 2.40–30.49°
μ = 0.094 mm^{-1}
T = 158 (2) K
Needle, colourless
0.54 × 0.14 × 0.12 mm

Data collection

CCD area-detector diffractometer
ω scans
15 627 measured reflections
1866 independent reflections
1778 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 30.49°
$h = -8 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.077
S = 1.077
1866 reflections
190 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.010 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.86 (2)	2.14 (2)	2.9835 (11)	171.3 (14)
O2—H2···O1^{ii}	0.87 (2)	1.74 (2)	2.5502 (10)	158.4 (18)

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

H atoms were allowed to refine isotropically. The range of C—H distances is 0.92 (2)-1.01 (2) Å; N—H = 0.86 (2) Å; O—H = 0.87 (2) Å.

Data collection and cell refinement: *SMART* (Bruker, 1997); data reduction, program used to solve and refine structure, software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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