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N-Acryloyl-L-alanine

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.082
Data-to-parameter ratio = 9.7

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

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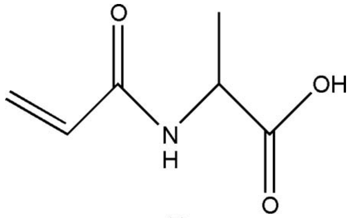
The title compound, $C_6H_9NO_3$, was prepared by a nucleophilic substitution reaction of acryloyl chloride with L-alanine. In the crystal structure, intermolecular N—H···O and O—H···O hydrogen bonds link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the crystal structure.

Comment

The title compound, (I), is an important intermediate and also a free radical addition monomer for the syntheses of radiation-sensitive (Heilmann & Palensky, 1981), hydropholic (Heilmann & Rasmussen, 1984) and pressure-sensitive (Heilmann, 1979) polymers. The crystal structure determination of (I) has been carried out in order to elucidate the molecular conformation. We report here the synthesis and the crystal structure of (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Atoms C2, C3, O2, N1 and C4 are nearly coplanar, with a dihedral angle of 1.2 (3)° between the C2/C3/O2 and C3/N1/C4 planes.

As can be seen from the packing diagram (Fig. 2), intermolecular N—H···O and O—H···O hydrogen bonds (Table 1) link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

For the preparation of the title compound, acryloyl chloride (7.5 ml, 0.11 mol) containing diphenylpicrylhydrazyl polymerization inhibitor (0.01%) and sodium hydroxide solution (0.1 mol in 40 ml of water) were simultaneously added dropwise over a 30 min period to give a well stirred solution containing L-alanine (0.1 mol in 100 ml of water) and sodium hydroxide (0.1 mol). The solution was stirred for a further 1 h at 273 K in an ice–water bath, and the pH of the reaction mixture was maintained at 2 by the addition of HCl (6 *M*). The resulting solid was filtered off and crystallized from ethyl acetate (yield 6.4 g, 45%; m.p. 402.5 K).

Crystal data

$C_6H_9NO_3$
$M_r = 143.14$
Orthorhombic, $P2_12_12_1$
$a = 8.3670$ (17) Å
$b = 8.7730$ (18) Å
$c = 10.350$ (2) Å
$V = 759.7$ (3) Å^3
$Z = 4$
$D_x = 1.251$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Block, colorless
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.962$, $T_{\max} = 0.972$
1686 measured reflections
888 independent reflections
805 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 26.0°$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.082$
$S = 1.08$
888 reflections
92 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.05P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.317 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1$^{\rm i}$	0.86	2.01	2.861 (2)	171
O3—H3···O2$^{\rm ii}$	0.82	1.80	2.616 (2)	175

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (ii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically, with O—H = 0.82 Å, N—H = 0.86 Å and C—H = 0.93, 0.98, 0.93 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = xU_{\rm eq}({\rm C,N,O})$, where $x = 1.5$ for OH and methyl H, and $x = 1.2$ for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration is known from the synthesis.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; 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: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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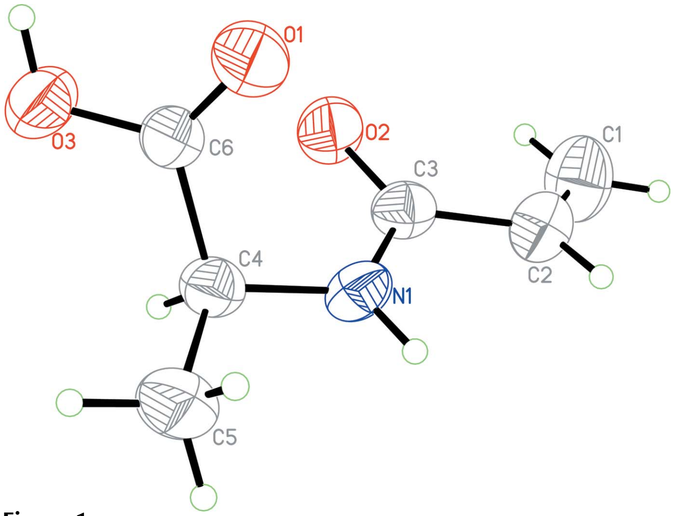

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

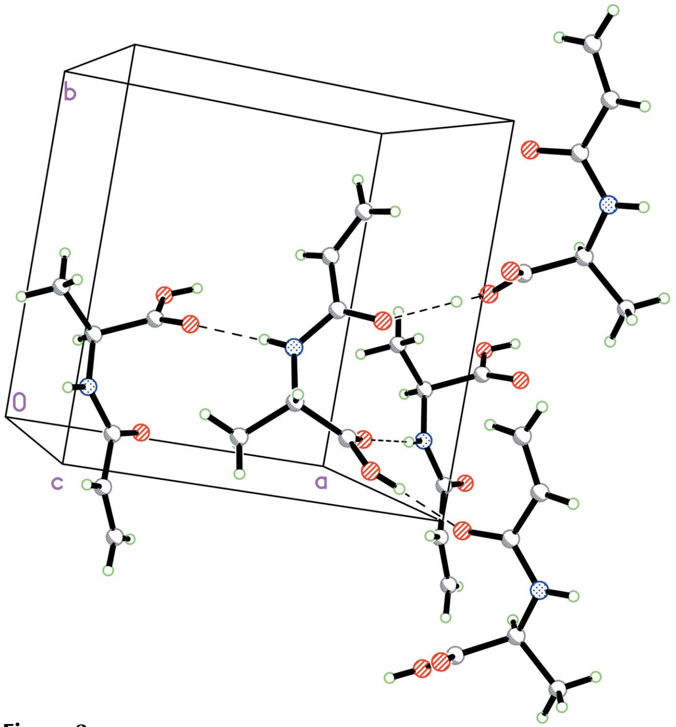

Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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