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N-(Methylacryloyl)glycine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.170
Data-to-parameter ratio = 15.9

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

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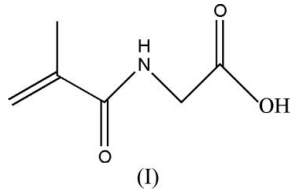
The title compound, $C_6H_9NO_3$, was prepared by the nucleophilic substitution reaction of methylacryloyl chloride with glycine. Intermolecular N—H···O and O—H···O hydrogen bonds link the molecules into a three-dimensional network, which may be effective in stabilizing the crystal structure.

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 the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C1/C3/C4/O3 and C3/O3/C4/C5/N1 units are nearly planar with r.m.s. deviations of 0.0337 and 0.0098 Å, respectively; the dihedral angle between them is 5.3 (3)°. 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, which may be effective in stabilizing 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 (I), methylacryloyl chloride (2.7 ml, 0.028 mol) containing diphenylpicrylhydrazyl polymerization inhibitor (0.01%) was added dropwise over a 30 min period to a well stirred aqueous solution of glycine (1.88 g, 0.025 mol in 40 ml water) and sodium hydroxide (2.4 g, 0.058 mol in 20 ml water) while maintaining the temperature at 273 K or lower. After the addition was complete, the reaction mixture was stirred in an ice bath for 2 h, and then acidified to about pH 2 with 6 *N* HCl. The *N*-methylacryloylglycine was extracted from the reaction mixture using ethyl acetate and subsequently crystallized from the same solvent (yield 1.8 g, 52%; m.p. 378 K).

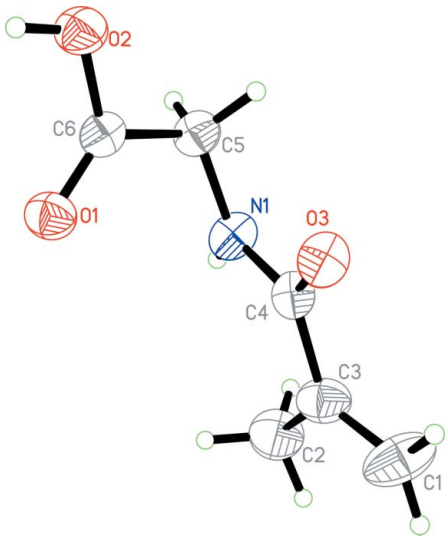


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

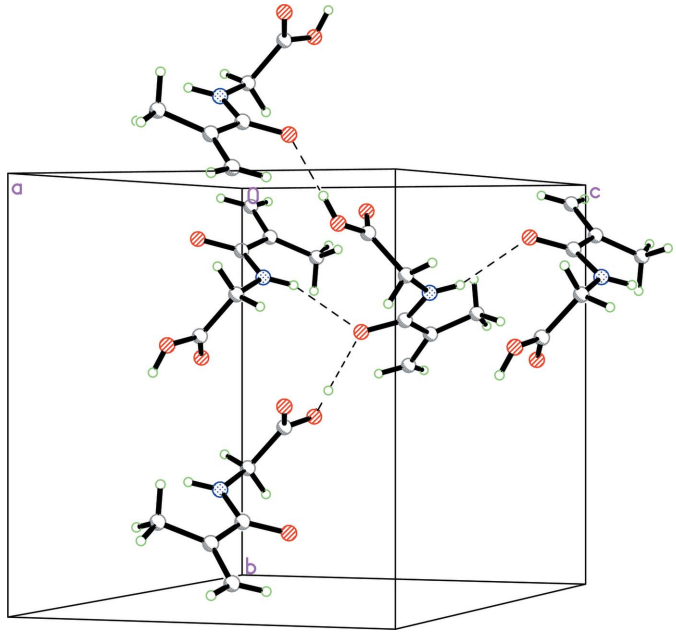


Figure 2
A packing diagram of (I). Intermolecular hydrogen bonds are shown as dashed lines.

Crystal data

$C_6H_9NO_3$
M_r = 143.14
Monoclinic, $P2_1/c$
a = 8.6340 (17) Å
b = 10.343 (2) Å
c = 9.1600 (18) Å
β = 115.04 (3)°
V = 741.1 (3) Å^3
Z = 4
D_x = 1.283 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.961, T_{max} = 0.988
1451 measured reflections
1448 independent reflections
1027 reflections with $I > 2\sigma(I)$
R_{int} = 0.008
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.170
S = 0.88
1451 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.103P)^2 + 0.3157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3^{i}	0.82	1.84	2.656 (3)	178
N1—H1···O3^{ii}	0.86	2.26	3.055 (3)	154

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

All H atoms were positioned geometrically, with O—H = 0.82 Å, N—H = 0.86 Å and C—H = 0.93 (sp^2) and 0.97 Å (sp^3), and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C,O).

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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