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5-Methyl L-glutamate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.160
Data-to-parameter ratio = 9.3

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

In the title compound, $C_6H_{11}NO_4$, the ψ^1 and ψ^2 torsion angles are −34.1 (3) and 149.1 (4)°, respectively. Atom C^{γ} is *gauche* to N and atom C^{δ} is *trans* to C^{α}. Translationally and screw-related molecules are connected by N—H···O hydrogen bonds to form layers parallel to the *ab* plane.

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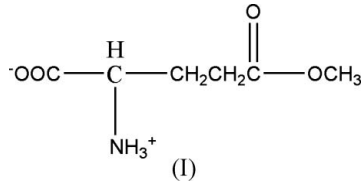
Comment

It is well known that many esters of amino acids display a broad range of biological activities, as antioxidants, bactericides, food additives, cosmetics and so on (Wang & Li, 1995). Furthermore, these esters can also be used as ligands. As part of our work to find new methods to synthesize these compounds and study their structures and activities, we report here the crystal stucture of one such ester of L-glutamic acid, namely 5-methyl L-glutamate, (I).



(I)

Compound (I) exists as a zwitterion in the crystal structure (Fig. 1). The N1—C2—C1—O1 (ψ^1) and N1—C2—C1—O2 (ψ^2) torsion angles are −34.1 (3) and 149.1 (4)°, respectively. Atom C^{γ} is *gauche* to N [N1—C2—C3—C4 (χ^1) = −56.2 (4)°] and atom C^{δ} is *trans* to C^{α} [C2—C3—C5—C5 (χ^2) = 173.5 (3)°]. The C—O lengths of the ionized carboxylate group are almost equal (Table 1).

In the crystal structure, translationally and screw-related molecules are connected by N—H···O hydrogen bonds to form a layer structure parallel to the *ab* plane (Table 2). Each molecule forms eight N—H···O or O···H—N hydrogen bonds with six adjacent molecules (Fig. 2).

Experimental

Compound (I) was synthesized according to the literature procedure of Li & Wang (1999). Colourless plate-like crystals were grown from an aquous solution, by slow evaporation at room temperature.

Crystal data

$C_6H_{11}NO_4$
M_r = 161.16
Monoclinic, $C2$
a = 10.286 (3) Å
b = 4.6163 (11) Å
c = 17.111 (4) Å
β = 104.995 (4)°
V = 784.9 (3) Å^3
Z = 4
D_x = 1.364 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1287 reflections
θ = 2.5–28.2°
μ = 0.12 mm^{-1}
T = 292 (2) K
Plate, colourless
0.30 × 0.30 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.993
953 measured reflections
953 independent reflections
903 reflections with $I > 2\sigma(I)$
θ_{max} = 27.0°
$h = -12 \rightarrow 12$
$k = 0 \rightarrow 5$
$l = 0 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.160
S = 1.15
953 reflections
103 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1191P)^2 + 0.0947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.252 (6)	C3—C4	1.523 (4)
C1—O2	1.253 (4)	C4—C5	1.494 (5)
C1—C2	1.529 (3)	C5—O3	1.179 (7)
C2—N1	1.486 (3)	C5—O4	1.309 (5)
C2—C3	1.530 (4)	C6—O4	1.442 (6)
O1—C1—O2	125.9 (3)	N1—C2—C3	110.0 (2)
O1—C1—C2	116.5 (2)	O3—C5—C4	126.4 (3)
N1—C2—C1	108.7 (2)	O4—C5—C4	110.7 (4)
O1—C1—C2—C3	86.4 (3)	C3—C4—C5—O3	16.6 (8)
O2—C1—C2—C3	−90.4 (3)	C3—C4—C5—O4	−161.9 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1^{i}	0.89	1.90	2.769 (3)	166
N1—H1A···O2^{ii}	0.89	2.12	2.994 (4)	167
N1—H1C···O2^{iii}	0.89	1.91	2.797 (4)	171
N1—H1C···O1^{iii}	0.89	2.49	3.124 (3)	129

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

All H atoms were placed in calculated positions, with N—H distances of 0.89 Å and C—H distances of 0.96 (CH_3), 0.97 (CH_2) and 0.98 Å (CH). They were included in the refinement in the riding-model approximation, with U_{iso}(H) set to 1.2U_{eq} of the carrier atom (1.5U_{eq} for CH_3 and NH_3 H atoms). A rotating-group model was used for the –CH_3 and –NH_3 groups. In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement; the absolute configuration is known from the synthesis.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

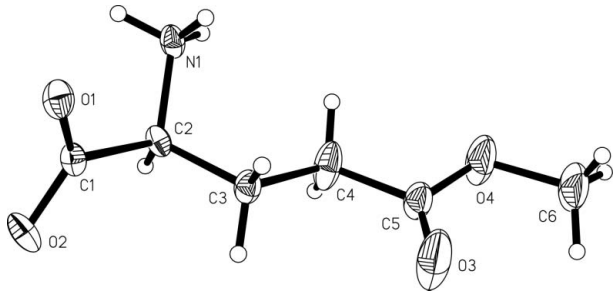


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

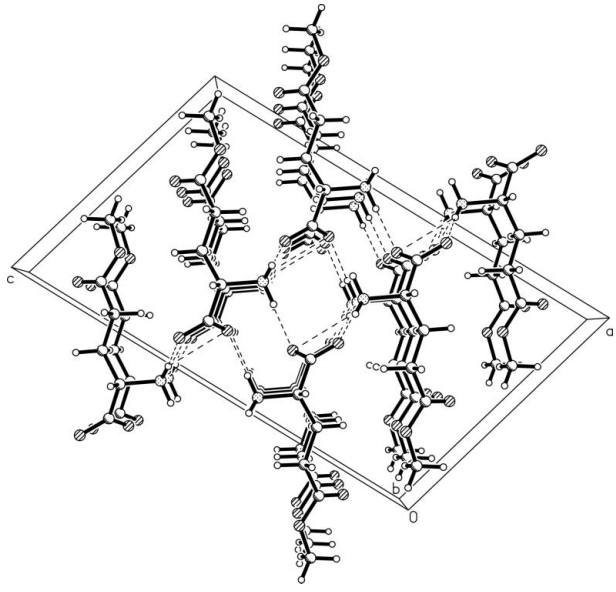


Figure 2
A packing diagram for (I). N—H···O hydrogen bonds are shown as dashed lines.

References

Bruker (2001). *SMART* (Version 5.628), *SAINT-Plus* (Version 6.45) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, W.-M. & Wang, X.-M. (1999). *Adv. Sci. Technol.* **9**, 16–19.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, B.-Q. & Li, Z.-C. (1995). *Amino Acids Biotic Resources*, **17**, 40–45.