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DL-Alanine

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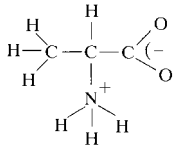
A determination of the structure of the title compound, $C_3H_7NO_2$, leads to an accurate description of its molecular dimensions and crystal packing. As in the structure of the L-isomer, the molecules aggregate into alternating layers, each consisting of only one type of isomer. The molecules in each layer are interconnected through head-to-tail sequences generated by a cell translation and a 2_1 screw axis. Adjacent layers are interconnected by head-to-tail sequences generated by a glide plane.

Comment

DL-Alanine, (I), is one of the few amino acids for which an accurate X-ray crystal structure is not known. Previous work on this amino acid reports the cell dimensions (Bernal, 1931) and X-ray crystal structures derived from two-dimensional intensity data (Levy & Corey, 1941; Donohue, 1950). We report here an accurate determination of the crystal structure of DL-alanine at room temperature. This structure represents a rare case of an amino acid racemate crystallizing in a non-centrosymmetric space group. Another such structure is DL-tyrosine (Mostad & Romming, 1973).



(I)

The DL-alanine molecule (Fig. 1) exists as a zwitterion. The C—O distances in the carboxylate group are unequal, presumably due to the participation of one atom (O1) in one hydrogen bond and the second (O2) in two other hydrogen bonds. The C—N distance, formerly thought to be unusually short by Levy & Corey (1941) with a value of 1.427 Å, is found to be 1.483 (3) Å in the present work. This is slightly less than the value of 1.496 Å quoted by Donohue (1950). The N atom deviates by 0.392 (5) Å from the carboxylate plane and the methyl carbon deviates by 1.356 (4) Å in the opposite direction.

The crystal structure is stabilized by a network of characteristic head-to-tail hydrogen-bond sequences (Fig. 2). The structure contains three types of such sequences, *viz*. S2 (straight sequence along the *c* axis with O2 of the carboxylate group as acceptor), Z1 (zigzag sequence along the 2_1 screw axis with O1 of the carboxylate group as acceptor) and DL2 (zigzag-DL sequence among the glide-related molecules with O2 of the carboxylate group as acceptor) (Suresh & Vijayan, 1983). While the sequences S2 and Z1 connect molecules in each layer, the zigzag-DL sequence connects alternating layers, each containing one isomer. The direction of the DL2 sequence is parallel to the plane of the amino acid layers. There is a striking similarity between this structure and that of its L-isomer (Simpson & Marsh, 1966; Destro *et al.*, 1988) which is not uncommon in most other hydrophobic amino acids (Soman & Vijayan, 1989). The cell dimensions of the L- and DL- isomers are nearly identical. Both structures belong to the orthorhombic system, but the space group is $P2_12_12_1$ for the

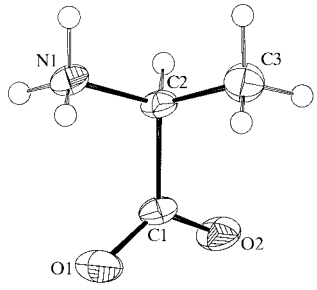


Figure 1
The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

L-isomer and $Pna2_1$ for the racemate. Furthermore, the arrangements of molecules within layers in the crystal structures of both L- and DL-alanine are identical. However, the DL2 sequence observed in the racemate is replaced by a Z2 sequence in its L-isomer. In addition, a weak C—H···O hydrogen bond, with the carboxylate O1 atom as acceptor, is observed among the glide-related molecules, interconnecting alternate layers, each containing one isomer.

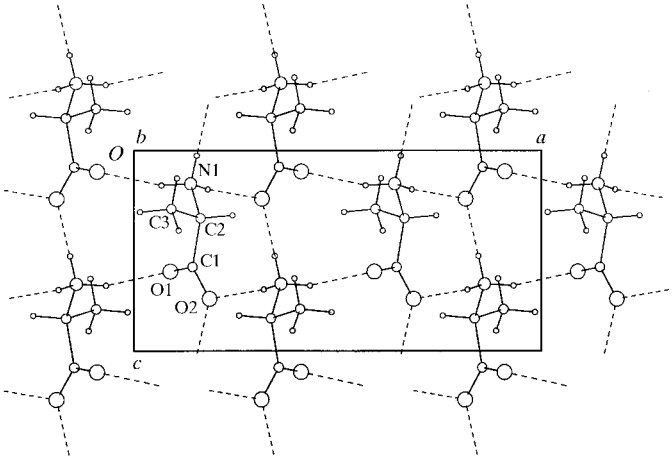


Figure 2
Packing diagram of the title molecule viewed down the *b* axis.

Experimental

Colourless single crystals of the title amino acid were grown as fine transparent needles from a saturated aqueous solution.

Crystal data

$C_3H_7NO_2$
M_r = 89.10
Orthorhombic, $Pna2_1$
a = 12.0263 (17) Å
b = 6.0321 (9) Å
c = 5.829 (2) Å
V = 422.88 (19) Å^3
Z = 4
D_x = 1.399 Mg m^{-3}
D_m = 1.39 Mg m^{-3}
D_m measured by flotation in carbon tetrachloride and xylene
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 15–27°
μ = 0.998 mm^{-1}
T = 293 (2) K
Fine needle, colourless
0.42 × 0.24 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.97, T_{max} = 0.99
422 measured reflections
422 independent reflections
417 reflections with $I > 2\sigma(I)$
θ_{max} = 67.58°
$h = -14 \rightarrow 0$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 7$
2 standard reflections
frequency: 60 min
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.072
S = 1.089
422 reflections
56 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.0571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.012 (3)

All the H atoms were generated geometrically and treated as riding with U_{iso} fixed at 1.2U_{eq} of the bonded atoms or 1.5U_{eq} for amino and methyl groups.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: C*AD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.89	1.96	2.817 (2)	160
N1—H1B···O1^{ii}	0.89	2.00	2.865 (2)	165
N1—H1C···O2^{iii}	0.89	1.92	2.804 (3)	173
C2—H2···O1^{iv}	0.98	2.67	3.566 (3)	153

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1132). Services for accessing these data are described at the back of the journal.

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