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Redetermination of α-ammonio-α-methylpropionoate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.130
Data-to-parameter ratio = 15.3

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

The redetermined structure of the title compound, $C_4H_9NO_2$, comprises a simple amino acid derivative arranged in an extensive hydrogen-bonded network, with the three hydrogen-bond donor elements (N—H) associating with the two hydrogen-bond acceptor elements (carboxylate O atoms). The addition of one C—H···O close contact results in both carboxylate O atoms being involved in three-centre hydrogen-bonding associations.

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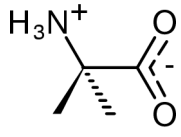
Comment

The redetermined structure of the title compound, (I), comprises a simple amino acid derivative arranged in an extensive hydrogen-bonded network, with the three hydrogen-bond donor elements (N—H) associating with the two hydrogen-bond acceptor elements (carboxylate O atoms). The addition of one C—H···O close contact results in both carboxylate O atoms being involved in three-centre hydrogen-bonding associations. The structure of (I) was initially determined in 1952 (Hirokawa *et al.*, 1952), using photographic techniques; the R value was 0.199. With such poor data it was impossible to confirm the zwiterionic nature of the compound, which is revealed in this current study. The title compound has been used as both a ligand and organic counter-ion in 19 other reported crystal structures.



(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_4H_9NO_2$
M_r = 103.12
Monoclinic, $C2/c$
a = 10.6273 (8) Å
b = 9.0102 (8) Å
c = 11.3370 (7) Å
β = 93.749 (6)°
V = 1083.2 (1) Å^3
Z = 8
D_x = 1.265 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2205 reflections
θ = 2.9–27.5°
μ = 0.10 mm^{-1}
T = 150 (2) K
Block, colourless
0.30 × 0.10 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.970, T_{max} = 0.992
3853 measured reflections
1208 independent reflections
755 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 27.4°
$h = -13 \rightarrow 11$
$k = -10 \rightarrow 11$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.00
1208 reflections
79 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.013 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	1.04 (2)	1.84 (2)	2.8645 (18)	167 (2)
N1—H2···O1^{ii}	0.96 (2)	1.88 (2)	2.828 (2)	170 (2)
N1—H3···O2^{iii}	0.97 (3)	1.90 (3)	2.841 (2)	163 (2)
C3—H31···O1^{i}	0.98	2.42	3.326 (2)	153

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

All methyl H atoms were included in the refinement, at calculated positions, as riding models with C—H distances set to 0.98 Å, whereas the ammonium H atoms were located in difference syntheses and both positional and displacement parameters were refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

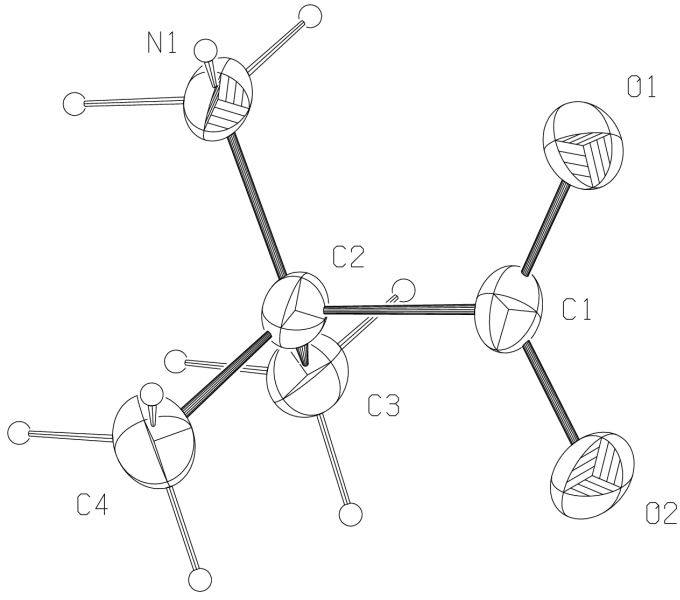


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 50% probability ellipsoids.

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