DL-Piperidine-2-carboxylic acid

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Key indicators

Single-crystal X-ray study
$T = 173$ K
Mean $\sigma(C–C) = 0.002$ Å
R factor = 0.035
wR factor = 0.128
Data-to-parameter ratio = 18.2

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

A chair conformation is found for zwitterionic DL-piperidinium-2-carboxylate, $C_6H_{11}NO_2$. Hydrogen-bonding interactions involving the carboxylate groups and ammonium H atoms give rise to a two-dimensional structure comprised of interconnected 12-membered rings.

Comment

The title molecule, (I), exists as a zwitterion [C21—O21 = 1.2508 (15) Å and C21—O22 = 1.2468 (15) Å] and adopts a chair conformation with the carboxylate occupying an equatorial position. The molecular structure is consistent with that found for the tetrahydrate (Bhattacharjee & Chacko, 1979) but features a different packing arrangement.

(I)
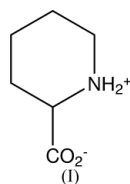
As shown in Fig. 1, two centrosymmetrically related carboxylate residues are linked by two ammonium cations, leading to the formation of 12-membered rings. As each molecule is involved in two donor and two acceptor hydrogen-bonding interactions that extend in the b and c directions, a two-dimensional network is formed. Layers stack along the a axis via hydrophobic interactions.

Experimental

Crystals were obtained by the vapour diffusion of diethyl ether into an ethanol/benzene (5:1 v/v) solution of commercial DL-piperidine-2-carboxylic acid (Sigma).

Crystal data

$C_6H_{11}NO_2$	$D_x = 1.304$ Mg m^{-3}
$M_r = 129.16$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 14
$a = 11.148$ (3) Å	reflections
$b = 5.822$ (2) Å	$\theta = 7.4–12.1°$
$c = 10.813$ (4) Å	$\mu = 0.10$ mm^{-1}
$\beta = 110.39$ (2)°	$T = 173$ (1) K
$V = 657.8$ (4) Å^3	Block, colourless
$Z = 4$	$0.3 \times 0.2 \times 0.1$ mm

Data collection

Rigaku AFC-7R diffractometer	$h = -14 \rightarrow 14$
$\omega–2\theta$ scans	$k = -7 \rightarrow 0$
3323 measured reflections	$l = -14 \rightarrow 13$
1513 independent reflections	3 standard reflections
1191 reflections with $I > 2\sigma(I)$	every 400 reflections
$R_{int} = 0.018$	intensity decay: 0.7%
$\theta_{max} = 27.5°$	
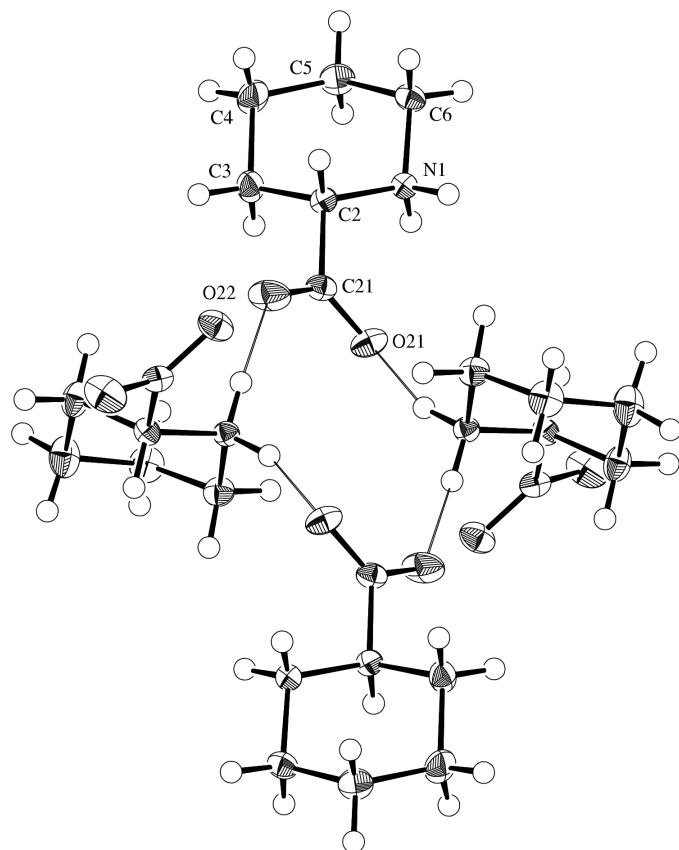
Figure 1
The molecular structure, crystallographic numbering scheme and hydrogen-bonding scheme for (I). Displacement ellipsoids are shown at the 50% probability level.

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F) = 0.035$	$w = 1/[\sigma^2(F_o{}^2) + (0.1P)^2]$
$wR(F^2) = 0.128$	where $P = (F_o{}^2 + 2F_c{}^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
1513 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
83 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1996); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

References

Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bhattacharjee, S. K. & Chacko, K. K. (1979). *Acta Cryst.* B**35**, 396–398.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Molecular Structure Corporation (1996). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1997). *TEXSAN for Windows*. Version 1.05. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.