Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Triethylammonium hydrogen fumarate

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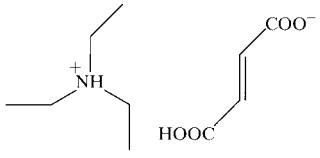
Received 17 February 2000
Accepted 1 March 2000

Data validation number: IUC0000053

In crystals of the title compound, the hydrogen fumarate anions form one-dimensional chains through an O—H···O hydrogen bonding along the *c* and (*a*+*b*)/2 directions. There are three sites of the hydrogen fumarate, two of which have an inversion centre.

Comment

The crystal structures of the ammonium and isopropylammonium salts of the fumaric acid dianion were reported by Hosomi *et al.* (1998). In the title crystals, (I), *trans–cis* photoisomerization was observed, but no photodimerization occurred. There is a strong O5—H5—O7 hydrogen bond; the O5—H5 and O7—H5 distances are 1.19 (3) and 1.26 (3) Å, respectively.



(I)

Experimental

The crystals of (I) were grown from a diethyl ether/2-propanol solution.

Crystal data

$C_6H_{16}N^+\cdot C_4H_3O_4^-$
M_r = 217.26
Triclinic, $P\overline{1}$
a = 13.409 (3) Å
b = 13.656 (3) Å
c = 7.432 (2) Å
α = 95.03 (3)°
β = 90.11 (2)°
γ = 113.99 (1)°
V = 1237.5 (5) Å^3
Z = 4
D_x = 1.166 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.4–15.0°
μ = 0.089 mm^{-1}
T = 295 (1) K
Prism, colourless
0.6 × 0.6 × 0.4 mm

Data collection

Rigaku AFC-5 diffractometer
θ–2θ scans
5071 measured reflections
4850 independent reflections
3040 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.0°
$h = 0 \rightarrow 17$
$k = -17 \rightarrow 17$
$l = -9 \rightarrow 9$
3 standard reflections
every 100 reflections
intensity decay: 4.4%

Refinement

Refinement on F^2
$R(F)$ = 0.045
$wR(F^2)$ = 0.117
S = 1.02
4850 reflections
424 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0510P)^2 + 0.1858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.026 (2)

Table 1
Selected geometric parameters (Å, °).

O1—C11	1.255 (2)	O5—C15	1.288 (2)
O2—C11	1.235 (2)	O6—C15	1.217 (2)
O3—C14	1.293 (2)	O7—C17	1.268 (3)
O4—C14	1.208 (2)	O8—C17	1.226 (3)
O1—C11—O2	126.1 (2)	O5—C15—O6	125.6 (1)
O3—C14—O4	124.3 (2)	O7—C17—O8	125.7 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	1.08 (3)	1.40 (3)	2.481 (2)	174 (3)
O5—H5···O7	1.19 (3)	1.26 (3)	2.445 (2)	175 (4)
N9—H9···O2^{ii}	0.90 (2)	1.81 (2)	2.708 (2)	170 (2)
N10—H10···O8	0.87 (2)	1.92 (2)	2.781 (2)	173 (2)

Symmetry codes: (i) $x, y, z-1$; (ii) $1-x, -y, 2-z$.

The C—H bond distances are in the range 0.89 (2)–1.05 (4) Å and the O—H distance not involving the H5 atom is 1.08 (3) Å.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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