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Triethanolammonium 2-formylbenzoate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.066
wR factor = 0.221
Data-to-parameter ratio = 14.5

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

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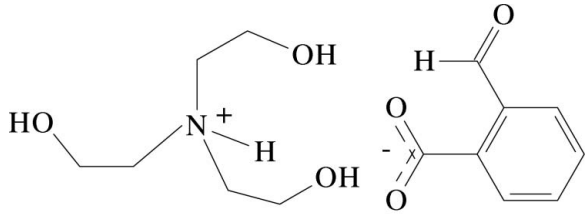
The title compound, $C_6H_{16}NO_3^+\cdot C_8H_5O_3^-$, contains edge-fused $R_2^2(12)R_2^2(10)R_2^2(12)$ motifs involving triethanolammonium and 2-carbonylbenzoate ions. These motifs are connected by $C(9)$ chains with $R_2^2(12)$ rings.

Comment

The title compound, (I), was obtained by the reaction of triethanolamine and 2-formylbenzoic acid. We have been interested in supramolecularly hydrogen-bonded systems formed by organic amines and carboxylic acids (Odabaşoğlu, Büyükgüngör & Lönnecke, 2003; Odabaşoğlu, Büyükgüngör *et al.*, 2003; Büyükgüngör *et al.*, 2004; Büyükgüngör & Odabaşoğlu, 2002, 2003, 2006; Odabaşoğlu & Büyükgüngör, 2006*a*,*b*). The present work is part of a structural study of compounds of organic ammonium systems with hydrogen-bond donors and we report here the structure of triethanolammonium 2-formylbenzoate, (I) (Fig. 1).



(I)

In compound (I), the triethanolammonium ions are linked to the 2-formylbenzoate ions through N—H···O and O—H···O hydrogen bonds (Table 1) and generate centrosymmetric edge-fused $[R_2^2(12)R_2^2(10)R_2^2(12)]$ motifs (Fig. 2) (Etter,

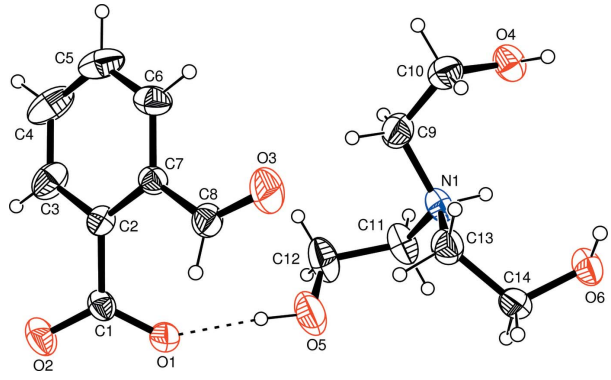


Figure 1
The molecular structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates a hydrogen bond.

1990). These motifs are connected by $C(9)$ chains with $R_2^2(12)$ rings (Fig. 3). Bond lengths and angles for the 2-formylbenzoate ion are similar to those reported in our previous work (Büyükgüngör & Odabaşoğlu, 2006).

Experimental

The title compound was prepared by mixing triethanolamine (1.49 g, 0.01 mol) and 2-formylbenzoic acid (1.50 g, 0.01 mol) in water (50 ml) at room temperature. Crystals of (I) were obtained by slow evaporation of the solvent (m.p. 354–357 K).

Crystal data

$C_6H_{16}NO_3^+\cdot C_8H_5O_3^-$
M_r = 299.32
Monoclinic, $P2_1/c$
a = 11.5316 (8) Å
b = 7.5990 (4) Å
c = 19.2535 (14) Å
β = 117.470 (5)°
V = 1496.93 (17) Å^3
Z = 4
D_x = 1.328 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
Prism, colourless
0.76 × 0.61 × 0.38 mm

Data collection

Stoe IPDS II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.752, T_{max} = 0.949
13959 measured reflections
2947 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.221
S = 1.10
2947 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.128P)^2 + 0.5183P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.008 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O6^{i}	0.88 (4)	2.06 (3)	2.867 (3)	153 (3)
O4—H4A···O1^{ii}	0.82 (4)	1.88 (4)	2.706 (3)	178 (3)
O5—H5A···O1	0.92 (5)	1.79 (5)	2.709 (3)	175 (5)
O6—H6A···O2^{ii}	0.84 (5)	1.82 (5)	2.645 (3)	168 (5)

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

All C-bound H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic and aldehydic H, and C—H = 0.97 Å for methylene C—H [U_{iso}(H) = 1.2U_{eq}(parent atom)]. The amino and hydroxy H atoms were located in a difference Fourier map and refined freely with an isotropic displacement parameter.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

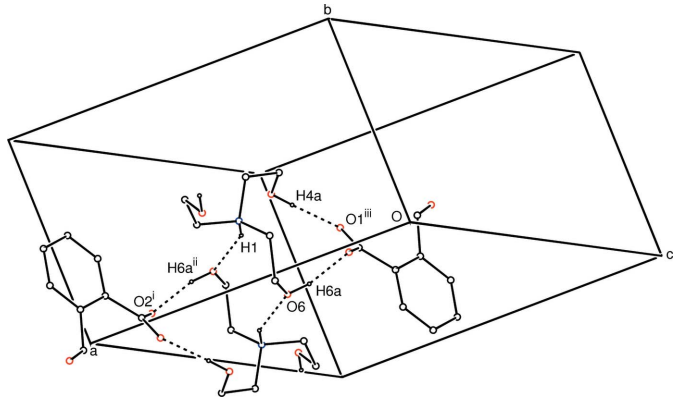


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded $[R_2^2(12)R_2^2(10)R_2^2(12)]$ motif. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $1-x, y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $1-x, -y, -z$; (iii) $x-\frac{1}{2}, -y, z-\frac{1}{2}$].

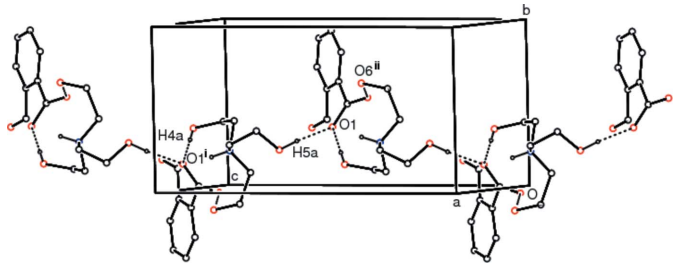


Figure 3
Part of the crystal structure of (I), showing the formation of a $C(9)$ chain with $R_2^2(12)$ ring. The N—H···O and C—H···O interactions are represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.]

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References

Büyükgüngör, O. & Odabaşoğlu, M. (2002). *Acta Cryst.* C**58**, o691–o692.
Büyükgüngör, O. & Odabaşoğlu, M. (2003). *Acta Cryst.* C**59**, o105–o106.
Büyükgüngör, O. & Odabaşoğlu, M. (2006). *Acta Cryst.* E**62**, o2749–o2750.
Büyükgüngör, O., Odabaşoğlu, M., Albayrak, Ç. & Lönnecke, P. (2004). *Acta Cryst.* C**60**, o470–o472.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Odabaşoğlu, M. & Büyükgüngör, O. (2006*a*). *Acta Cryst.* E**62**, o739–o741.
Odabaşoğlu, M. & Büyükgüngör, O. (2006*b*). *Acta Cryst.* E**62**, o1524–o1525.
Odabaşoğlu, M., Büyükgüngör, O. & Lönnecke, P. (2003). *Acta Cryst.* C**59**, o51–o52.
Odabaşoğlu, M., Büyükgüngör, O., Turgut, G., Karadağ, A., Bulak, E. & Lönnecke, P. (2003). *J. Mol. Struct.* **648**, 133–138.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.