

## Ethylammonium 2,4,5-tricarboxybenzoate

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## Key indicators

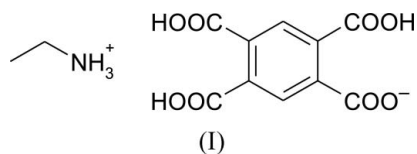
Single-crystal X-ray study  
 $T = 102$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.028  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 10.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_2\text{H}_8\text{N}^+\cdot\text{C}_{10}\text{H}_5\text{O}_8^-$ , contains discrete ethylammonium cations and singly deprotonated pyromellitate anions. The geometry of the ethylammonium cation is not significantly different from that in other structures containing this residue. The pyromellitate anion is non-planar. The network formed by these ions is based on strong  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

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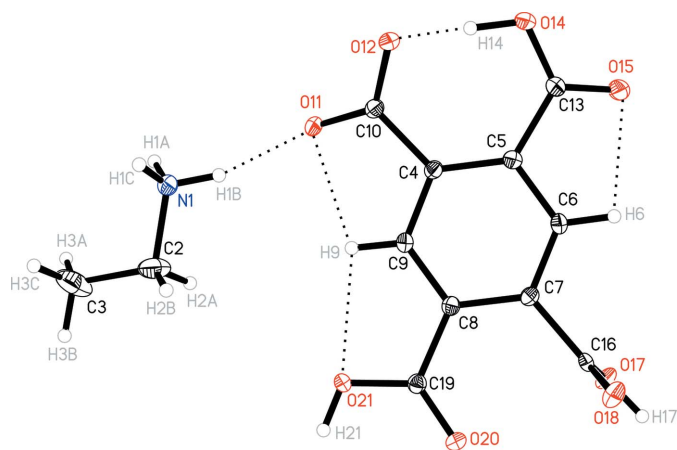
## Comment

Cocrystallization studies employing aromatic organic molecules containing carboxylate and/or carboxylic groups situated *ortho* to each other may potentially afford precursors for building hydrogen-bonded supramolecular networks in two or three directions. In the present work, pyromellitic acid (benzene-1,2,4,5-tetracarboxylic acid) was chosen as a building unit with various aza derivatives in crystal-engineering studies. This carboxylic acid and its deprotonated anions can form two and three-dimensional structures which differ in their stacking mode, *i.e.* channel structures, simple planar sheet structures and staircase structures (*e.g.* Arora & Pedireddi, 2003; Ruiz-Pérez *et al.*, 2004).



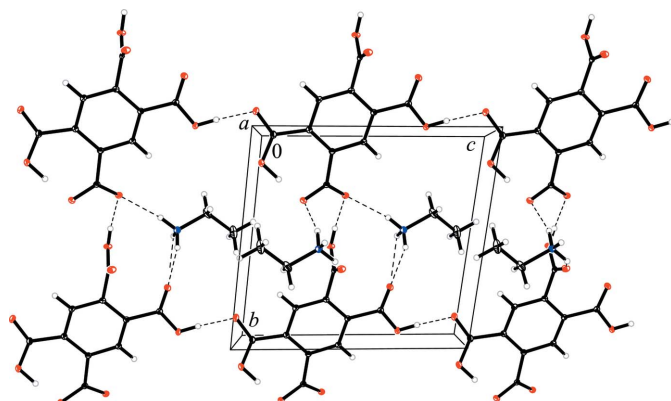
The asymmetric unit of the title compound, (I), consists of an ethylammonium cation and a singly deprotonated pyromellitate anion (Fig. 1 and Table 1). The structural parameters of the ethylammonium cation compare well with those found in other crystal structures which include this type of cation (Beach & Shea, 1994; Ishida & Kashino, 2000; Kalsbeek, 1991; Muthamizhchelvan *et al.*, 2005; Sada *et al.*, 1998).

Analysis of the structure of the pyromellitate anion reveals that there is one strong intramolecular  $\text{O}-\text{H}\cdots\text{O}$  and three relatively weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds (Fig. 1 and Table 2). The  $\text{O}14-\text{H}14\cdots\text{O}12$  hydrogen bond leads to the formation of a seven-membered ring. The three  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds result in the formation of three five-membered rings. Such a conformation decreases the repulsion between neighbouring groups. As a result, the pyromellitate monoanion is not planar. The  $\text{C}16/\text{O}17/\text{H}17/\text{O}18$  carboxyl group, for which O atoms do not participate in intramolecular hydrogen bonds, is most twisted with respect to the benzene ring [dihedral angle =  $85.1(4)^\circ$ ]. The neighbouring  $\text{C}19/\text{O}20/\text{O}21/\text{H}21$  carboxyl group is essentially coplanar with the



**Figure 1**

The asymmetric unit of (I), showing the hydrogen-bonding scheme (dotted lines). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**

The crystal packing of (I), viewed down the *a* axis. The O—H...O and N—H...O intermolecular hydrogen bonds are indicated by dashed lines. The intra-ion hydrogen bonds are not shown for clarity.

benzene ring [dihedral angle = 0.7 (4)°]. The analogous dihedral angles for the C10/O11/O12 carboxylate and C13/O14/H14/O15 carboxyl groups are 28.4 (1) and 20.6 (3)°, respectively. The other geometric parameters of the pyromellitate anion (Table 1) correlate well with corresponding values found in crystal structures containing these groups (*e.g.* Arora & Pedireddi, 2003; Dale *et al.*, 2004; Ruiz-Pérez *et al.*, 2004; Sun *et al.*, 2002; Zhu *et al.*, 2003).

In the crystal structure of (I), pyromellitate anions are connected by O—H...O hydrogen bonds, forming layers parallel to the *bc* plane (Fig. 2). These layers interact through an interanion contact [O11...O20<sup>i</sup> = 3.039 (2) Å; symmetry code: (i)  $-x, -y, 1 - z$ ]. The ethylammonium cations and pyromellitate anions are connected by N—H...O hydrogen bonds (Fig. 2 and Table 2).

## Experimental

Crystals of (I) were grown by slow evaporation of an aqueous solution containing ethylamine and benzene-1,2,4,5-tetracarboxylic acid in a 1:1 stoichiometric ratio at room temperature.

## Crystal data

$C_2H_8N^+ \cdot C_{10}H_5O_8^-$   
 $M_r = 299.23$   
 Triclinic,  $P\bar{1}$   
 $a = 7.4215$  (6) Å  
 $b = 9.5775$  (6) Å  
 $c = 9.7259$  (5) Å  
 $\alpha = 94.830$  (4)°  
 $\beta = 94.467$  (5)°  
 $\gamma = 110.874$  (6)°

$V = 639.31$  (8) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.554$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.13$  mm<sup>-1</sup>  
 $T = 102.0$  (1) K  
 Block, colourless  
 0.45 × 0.42 × 0.40 mm

## Data collection

Oxford Diffraction Xcalibur diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 4320 measured reflections

2466 independent reflections  
 2239 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.008$   
 $\theta_{max} = 26.0^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.085$   
 $S = 1.05$   
 2466 reflections  
 242 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.1846P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

C13—O15	1.226 (2)	C16—O17	1.319 (1)
C13—O14	1.296 (1)	C19—O20	1.216 (1)
C16—O18	1.2067 (15)	C19—O21	1.316 (1)
C9—C4—C10	114.56 (9)	O15—C13—C5	118.8 (1)
C5—C4—C10	126.83 (10)	O14—C13—C5	120.2 (1)
C6—C5—C13	113.77 (10)	O18—C16—O17	124.5 (1)
C4—C5—C13	127.57 (10)	O18—C16—C7	122.7 (1)
O11—C10—O12	123.2 (1)	O17—C16—C7	112.69 (9)
O11—C10—C4	117.47 (9)	O20—C19—O21	124.6 (1)
O12—C10—C4	119.33 (9)	O20—C19—C8	122.2 (1)
O15—C13—O14	121.0 (1)	O21—C19—C8	113.22 (9)
C9—C4—C10—O11	−27.0 (1)	C6—C7—C16—O18	92.5 (1)
C5—C4—C10—O11	155.3 (1)	C8—C7—C16—O18	−85.7 (1)
C9—C4—C10—O12	150.6 (1)	C6—C7—C16—O17	−83.7 (1)
C5—C4—C10—O12	−27.1 (2)	C8—C7—C16—O17	98.1 (1)
C6—C5—C13—O15	19.6 (2)	C9—C8—C19—O20	180.0 (1)
C4—C5—C13—O15	−158.7 (1)	C7—C8—C19—O20	−1.0 (2)
C6—C5—C13—O14	−159.1 (1)	C9—C8—C19—O21	−1.0 (1)
C4—C5—C13—O14	22.7 (2)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O14—H14...O12	1.00 (2)	1.44 (2)	2.426 (1)	171 (2)
C6—H6...O15	0.97 (2)	2.34 (2)	2.706 (1)	101 (1)
C9—H9...O11	0.96 (2)	2.37 (1)	2.735 (1)	102 (1)
C9—H9...O21	0.96 (2)	2.40 (1)	2.719 (1)	99.2 (9)
N1—H1B...O11	0.92 (2)	2.11 (2)	2.918 (1)	146 (1)
N1—H1A...O17 <sup>i</sup>	0.93 (2)	2.14 (2)	3.005 (1)	155 (2)
N1—H1A...O20 <sup>ii</sup>	0.93 (2)	2.29 (2)	2.815 (1)	115 (1)
N1—H1B...O18 <sup>iii</sup>	0.92 (3)	2.19 (2)	2.800 (1)	123 (1)
N1—H1C...O12 <sup>iv</sup>	0.90 (2)	2.06 (2)	2.924 (1)	161 (2)
O17—H17...O11 <sup>v</sup>	0.93 (2)	1.65 (2)	2.576 (1)	172 (2)
O21—H21...O15 <sup>vi</sup>	0.90 (2)	1.71 (2)	2.608 (1)	176 (2)

Symmetry codes: (i)  $-x, -y, -z + 1$ ; (ii)  $x, y + 1, z$ ; (iii)  $-x + 1, -y, -z + 1$ ; (iv)  $-x + 1, -y + 1, -z + 1$ ; (v)  $x, y - 1, z$ ; (vi)  $x, y, z + 1$ .

All H atoms were found in a difference map and refined freely.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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