Ethylammonium hydrogen oxalate hemihydrate

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The structure of the title compound, $C_2H_8N^+ \cdot C_2HO_4^- \cdot 0.5$ H_2O, contains discrete ethylammonium cations, hydrogen oxalate anions and water molecules. The cations and anions occupy general positions, whereas the water molecules are located on twofold axes. The cations and anions are connected to each other and to water molecules by N—H···O and O—H···O hydrogen bonds.

Comment

Oxalic acid, together with its anions, is one of the best building blocks for the construction of supramolecular structures based on hydrogen bonds. There are four O atoms, which can be acceptors and/or donors in hydrogen bonding. Oxalates of organic amines (alkylammonium, guanidine, 1,4-diazabicyclo[2.2.2]octane, *etc.*) have been examined by single-crystal X-ray diffraction and other techniques (MacDonald *et al.*, 2001; Vaidhyanathan *et al.*, 2001, 2002).

(I)
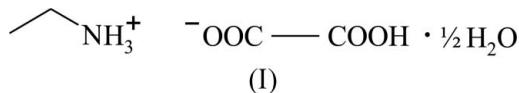
The crystal structure of the title salt, (I), consists of ethylammonium cations, oxalate monoanions and water molecules (Fig. 1). The geometric parameters of the ethylammonium cation are not significantly different from those observed in other structures including this cation (Beach & Shea, 1994; Ishida & Kashino, 2000; Kalsbeek, 1991; Muthamizhchelvan *et al.*, 2005; Sada *et al.*, 1998). The oxalate monoanions are nearly planar and are connected to each other by strong O—H···O hydrogen bonds along the *b* axis. The ethylammonium cations form N—H···O hydrogens bonds to the anions and water molecules (Fig. 2 and Table 2).

Experimental

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

Crystal data

$C_2H_8N^+ \cdot C_2HO_4^- \cdot 0.5H_2O$
$M_r = 144.13$
Monoclinic, $C2/c$
$a = 18.1163$ (15) Å
$b = 5.6775$ (5) Å
$c = 14.1207$ (7) Å
$\beta = 102.064$ (5)°
$V = 1420.31$ (19) Å^3

$Z = 8$
$D_x = 1.348$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 86$ (1) K
Block, colourless
$0.48 \times 0.46 \times 0.42$ mm

organic papers

Data collection

Oxford Diffraction Xcalibur diffractometer	1705 independent reflections
	1439 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.026$
Absorption correction: none	$\theta_{max} = 28.0°$
10130 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.9997P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.097$	
$S = 1.14$	$(\Delta/\sigma)_{max} < 0.001$
1705 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
127 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

C4—O9	1.2089 (14)	C5—O7	1.2454 (14)
C4—O6	1.3166 (14)	C5—O8	1.2569 (14)
C4—C5	1.5499 (16)		
O9—C4—O6	125.90 (11)	O7—C5—C4	118.54 (10)
O9—C4—C5	121.58 (10)	O8—C5—C4	115.22 (9)
O6—C4—C5	112.52 (9)	C4—O6—H6	110.2 (12)
O7—C5—O8	126.24 (11)		
O9—C4—C5—O7	−171.59 (12)	O9—C4—C5—O8	8.22 (17)
O6—C4—C5—O7	8.29 (15)	O6—C4—C5—O8	−171.90 (10)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$B\cdots$O7	0.917 (18)	1.921 (18)	2.8274 (14)	169.6 (15)
N1—H1$A\cdots$O10	0.906 (18)	1.911 (17)	2.7816 (15)	160.5 (14)
N1—H1$C\cdots$O8^i	0.878 (19)	1.999 (19)	2.8104 (15)	153.1 (17)
O6—H6$\cdots$O8^{ii}	0.90 (2)	1.69 (2)	2.5885 (12)	176.6 (18)
O10—H10$\cdots$O7^{ii}	0.852 (19)	1.89 (2)	2.7368 (13)	171.9 (19)

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

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); 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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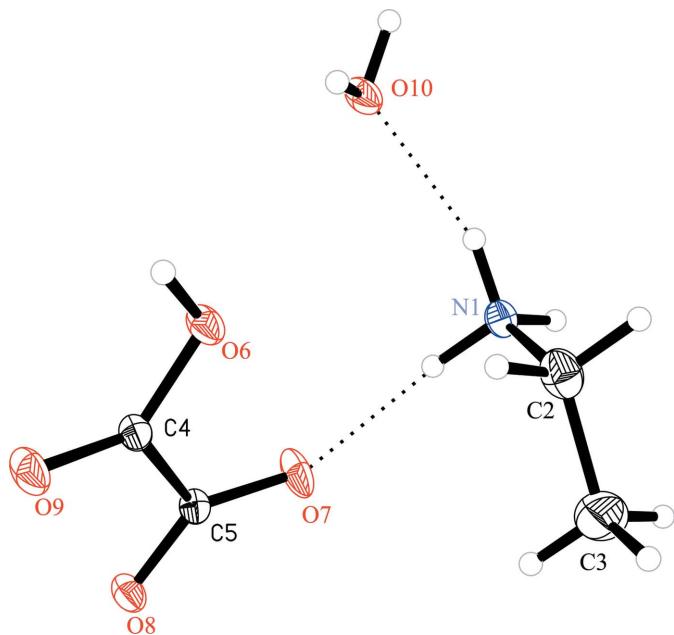
Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Hydrogen bonds are shown as dotted lines.
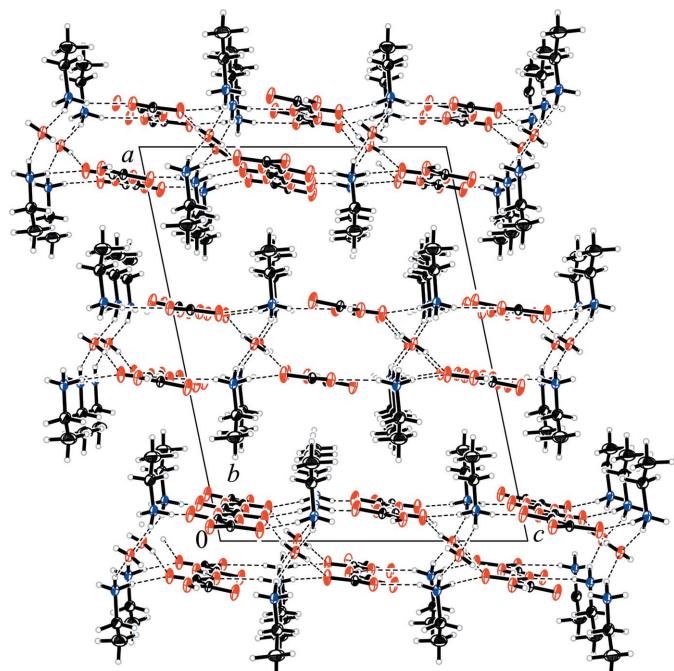

Figure 2
Packing diagram of (I), viewed along the *b* axis, showing the intermolecular hydrogen-bonding scheme (dashed lines).

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