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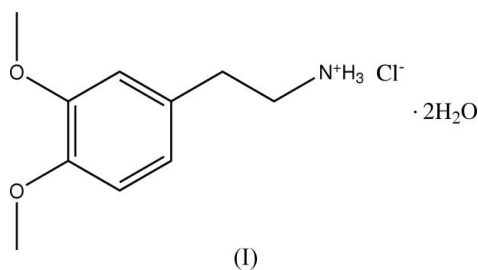
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(C-C) = 0.003$  Å  
 $R$  factor = 0.055  
 $wR$  factor = 0.161  
Data-to-parameter ratio = 17.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Redetermination of 3,4-dimethoxyphenylethyl-  
ammonium chloride dihydrateThe structure of the title compound,  $C_{10}H_{16}NO_2^+ \cdot Cl^- \cdot 2H_2O$ , has been redetermined. It is stabilized by  $O-H \cdots Cl$ ,  $O-H \cdots O$ ,  $N-H \cdots O$  and  $N-H \cdots Cl$  hydrogen-bonding interactions, which build up an intricate three-dimensional network.

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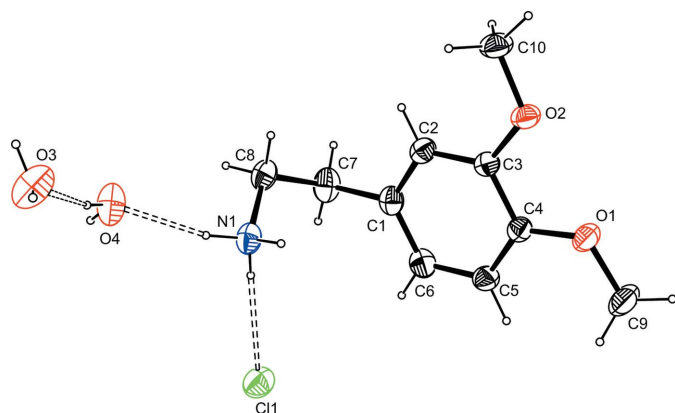
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## Comment

This work is a redetermination of the structure of 3,4-dimethoxyphenylethylamine hydrochloride dihydrate, (I), previously reported by Pattanayek *et al.* (1984), leading to an improved refinement; the  $R$  factor reduced from 0.1150 to 0.055.The asymmetric unit of (I) consists of a 3,4-dimethoxyphenylethylammonium cation, a  $Cl^-$  anion and two water molecules (Fig. 1). The benzene ring, methylene atom C7 and the two methoxy groups are roughly coplanar, with the largest deviation from the mean plane being 0.109 (2) Å for C9. Atoms C8 and N1 are displaced from this plane by 1.140 (3) and 2.368 (3) Å, respectively.The cations adopt a dimer structure, through a head-to-tail hydrogen bond between the dimethoxy and ammonium groups (Table 1, Fig. 2), as already observed in 2-(3,4-dimethoxyphenyl)ethylammonium 3,5-dinitrobenzoate (Ohba & Ito, 2002). These dimers are further connected to each other through  $N-H \cdots O$ ,  $O-H \cdots O$  and  $O-H \cdots Cl$  hydrogen bonds involving the water molecules and the  $Cl^-$  anions (Table 1, Fig. 2), thus forming an intricate three-dimensional network.

## Experimental

To a solution of 3,4-dimethoxyphenylethylamine (1.0 g, 5.52 mmol) in MeOH (20 ml), concentrated hydrochloric acid (0.8 ml) was added at room temperature. The solution was then evaporated *in vacuo* and the title compound was obtained as a white powder. Colourless crystals of (I) suitable for X-ray structure analysis were grown by slow evaporation of a solution in methanol at room temperature.


**Figure 1**

The asymmetric unit of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii. Hydrogen bonds are indicated as dashed lines.

#### Crystal data

$C_{10}H_{16}NO_2^+ \cdot Cl^- \cdot 2H_2O$   
 $M_r = 253.72$   
 Monoclinic,  $P2_1/c$   
 $a = 11.565$  (2) Å  
 $b = 13.760$  (3) Å  
 $c = 8.3165$  (16) Å  
 $\beta = 94.955$  (4)°  
 $V = 1318.5$  (4) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.278$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.29$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, colourless  
 $0.50 \times 0.50 \times 0.15$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{min} = 0.858$ ,  $T_{max} = 0.923$

7595 measured reflections  
 2861 independent reflections  
 2161 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.099$   
 $\theta_{max} = 27.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.055$   
 $wR(F^2) = 0.161$   
 $S = 1.00$   
 2861 reflections  
 160 parameters

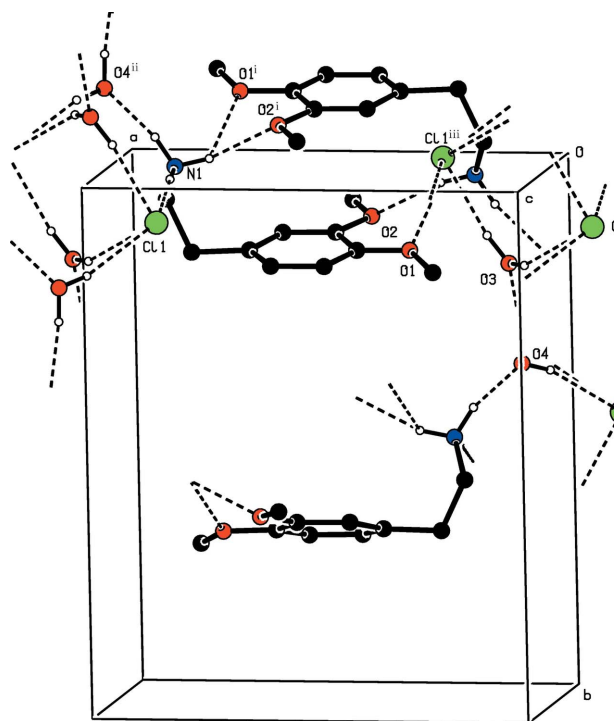
H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0915P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.33$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1C \cdots O2^i$	0.89	2.10	2.952 (2)	161
$N1-H1C \cdots O1^i$	0.89	2.41	2.962 (2)	120
$O3-H3A \cdots Cl1^{ii}$	0.83 (3)	2.39 (3)	3.211 (2)	172 (4)
$O3-H3B \cdots Cl1^{iii}$	0.82 (3)	2.55 (3)	3.229 (2)	141 (4)
$O4-H4A \cdots Cl1^{iv}$	0.83 (3)	2.42 (3)	3.233 (2)	169 (3)
$N1-H1B \cdots O4$	0.89	1.90	2.768 (2)	164
$N1-H1A \cdots Cl1$	0.89	2.40	3.2833 (19)	170

Symmetry codes: (i)  $-x + 1, -y + 1, -z + 2$ ; (ii)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (iii)  $-x, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iv)  $-x, -y + 1, -z + 1$ .


**Figure 2**

A partial view of the packing, showing the formation of dimers and the different hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i)  $1-x, 1-y, 2-z$ ; (ii)  $x, -\frac{1}{2}-y, \frac{1}{2}+z$ ; (iii)  $-x, y-\frac{1}{2}, \frac{3}{2}-z$ ; (iv)  $-x, 1-y, 1-z$ .]

H atoms attached to C and N atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.96 (CH<sub>3</sub>), 0.97 (CH<sub>2</sub>) or 0.93 Å (CH) and N—H = 0.89 Å, and with  $U_{iso}(H) = 1.5U_{eq}(CH_3, NH_3)$  or  $1.2U_{eq}(CH_2, CH)$ . The H atoms of the water molecules were positioned from a difference map and allowed to refine with restrained O—H [90 (2) Å] distances and with  $U_{iso}(H) = 1.5U_{eq}(O)$ .

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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