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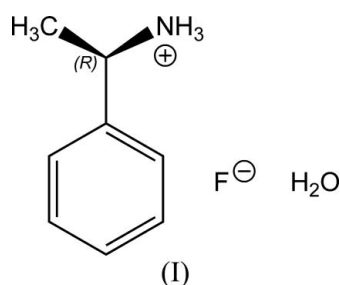
Key indicators

Single-crystal X-ray study
 $T = 299$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.045
 wR factor = 0.113
Data-to-parameter ratio = 10.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(*R*)-Phenylethanaminium fluoride monohydrate**The title compound, $C_8H_{12}FN \cdot H_2O$, was crystallized from an aqueous solution. The crystal structure features $N-H \cdots F$, $N-H \cdots O$ and $O-H \cdots F$ hydrogen bonding.

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Comment

Recently, the crystal structure of (*R*)-phenylethanaminium bromide was reported (Fischer, 2006), which is, to the author's knowledge, the first crystal structure of an (*R*)-phenylethanaminium halide. In order to study the nature of the influence of the type of halogen atom on hydrogen bonding, we decided to determine the crystal structures of other halide salts. Attempts to crystallize the fluoride salt from an aqueous solution of the amine and HF yielded (*R*)-phenylethanaminium fluoride monohydrate, (I).The asymmetric unit of (I) is shown in Fig. 1. The geometry is unexceptional. All N-bonded H atoms are involved in hydrogen bonds, giving two $N-H \cdots F$ bonds and one $N-H \cdots O$ bond. Both O-bonded H atoms form $O-H \cdots F$ bonds; details of hydrogen-bond geometries can be found in Table 1 and Fig. 2 displays the hydrogen-bonding pattern.

Experimental

(R)-Phenylethanamine (1.5 ml; Fluka, purum) and hydrofluoric acid (0.5 ml; Mallinckrodt, 48.75–49.25%) were dissolved in demineralized water (1 ml). The enantiomeric purity of the amine was confirmed prior to synthesis by measuring the optical rotation. The solution was allowed to stand at room temperature for evaporation. Withing a couple of days, single crystals of the title compound were obtained.

Crystal data

 $C_8H_{12}N^+ \cdot F^- \cdot H_2O$
 $M_r = 159.20$
Orthorhombic, $P2_12_12_1$
 $a = 6.1754$ (2) Å
 $b = 6.6276$ (5) Å
 $c = 22.772$ (2) Å
 $V = 932.01$ (11) Å³ $Z = 4$
 $D_x = 1.135$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 299$ K
Fragment, colourless
 $0.60 \times 0.23 \times 0.15$ mm

Data collection

Bruker–Nonius KappaCCD
diffractometer
 φ and ω scans
Absorption correction: none
5560 measured reflections

1085 independent reflections
866 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.081$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.113$
 $S = 1.13$
1085 reflections
100 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.166P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.18 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{Å}^{-3}$

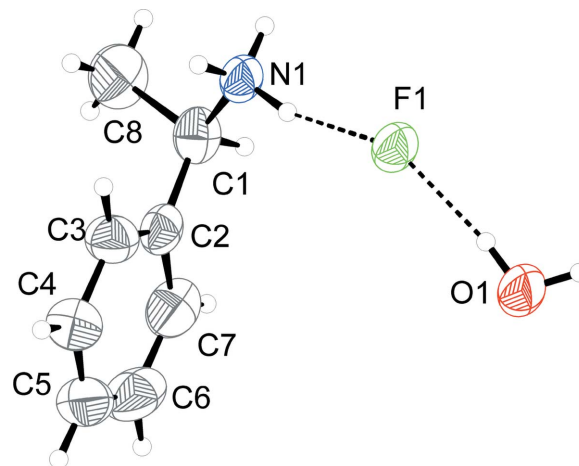


Figure 1

The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and hydrogen bonds are indicated by dashed lines.

Table 1

Hydrogen-bond geometry ($\text{Å}, ^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------|-------|-------------|-------------|---------------|
| $N1-H1A\cdots F1$ | 0.89 | 1.83 | 2.699 (2) | 164 |
| $N1-H1B\cdots F1^i$ | 0.89 | 1.80 | 2.673 (3) | 166 |
| $N1-H1C\cdots O1^{ii}$ | 0.89 | 1.84 | 2.722 (3) | 169 |
| $O1-H1O\cdots F1$ | 0.86 | 1.87 | 2.732 (3) | 172 |
| $O1-H2O\cdots F1^{iii}$ | 0.86 | 1.82 | 2.663 (2) | 165 |

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

Due to the absence of significant anomalous dispersion, Friedel pairs were merged prior to refinement. The absolute configuration was assigned with reference to the enantiomerically pure amine. H atoms were placed at calculated positions ($C-H = 0.93 \text{ Å}$ for aromatic H atoms, $C-H = 0.96 \text{ Å}$ for methyl H atoms and $C-H = 0.98 \text{ Å}$ for C1). Local maxima could be found in the difference Fourier map in the proximity of the O atom. The corresponding O—H H atoms were refined using an idealized model ($O-H = 0.86 \text{ Å}$). All H atoms were refined riding on their carrier atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}, \text{O})$ or $1.2U_{\text{eq}}(\text{C}1)$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MAXUS* (Mackay *et al.*, 1999).

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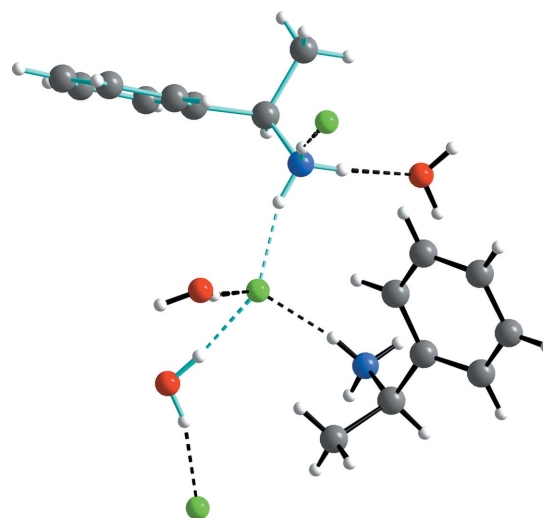


Figure 2

The hydrogen bonding pattern in (I). Components of the asymmetric unit are indicated by blue bonds. Hydrogen bonds are indicated by dashed lines.

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