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Key indicators

Single-crystal X-ray study
 $T = 293$ K
 Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.025
 wR factor = 0.067
 Data-to-parameter ratio = 5.1

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

L-Histidinium tetrafluoroborate

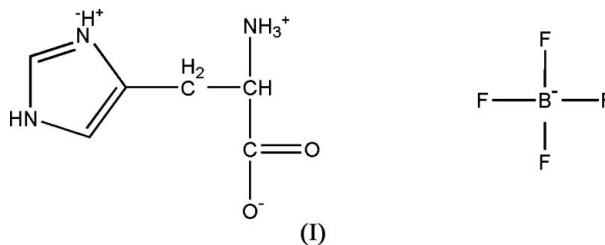
The title compound, $C_6H_{10}N_3O_2^+ \cdot BF_4^-$, crystallizes with one histidinium cation and one tetrafluoroborate anion in the asymmetric unit. The protonated cation and the deprotonated anion are linked through a number of intermolecular N—H...O and N—H...F hydrogen bonds, forming a three-dimensional network.

Received 30 January 2006

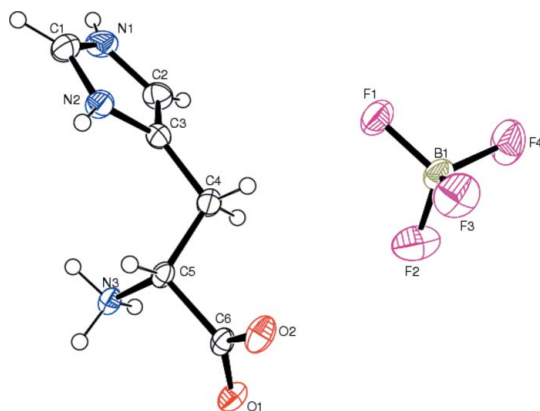
Accepted 20 February 2006

Comment

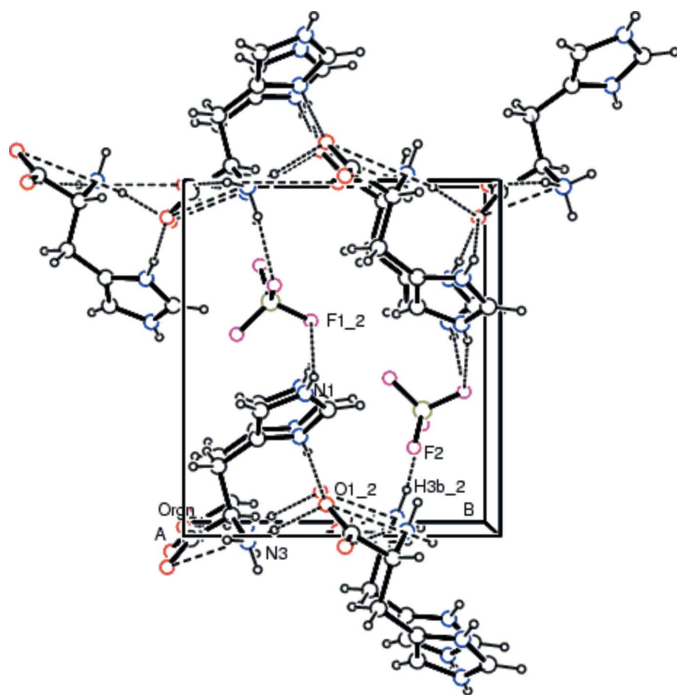
In our earlier studies, we have reported the crystal structure of L-histidinium trifluoroacetate (Gokul Raj *et al.*, 2006). The present work reports the crystal structure of L-histidinium tetrafluoroborate, (I). Other L-histidine complexes, such as L-histidine hydrochloride monohydrate (Fuess *et al.*, 1977), L-histidine sulfate (Kumar *et al.*, 2005), L-histidine dinitrate (Asath Bahadur *et al.*, 1992), L-histidine L-tartarate (Marchewka *et al.*, 2003), L-histidine dihydrogen arsenate orthoarsenic acid (Ratajczak *et al.*, 2000) and L-histidine tetrafluorosuccinate (Akkurt *et al.*, 2004), have been reported previously.



The asymmetric unit contains an L-histidine molecule protonated at a ring N atom and a tetrafluoroborate anion. The conformation of the histidine side chain can be described by two torsion angles, χ^1 [$C_3-C_4-C_5-N_3$] and χ^{21} [$N_2-C_3-C_4-C_5$] or χ^{22} [$C_2-C_3-C_4-C_5$] [IUPAC-IUB Commission on Biochemical Nomenclature, 1970]. The sum of χ^{22} and χ^{21} is 180° . χ^1 , which gives the orientation of the side chain with respect to main chain, can take values of -60° , 60° or 180° , corresponding to *gauche* I, *gauche* II and open conformations. The title compound has $\psi^1 = 61.3(3)^\circ$ and hence it is in the *gauche* II form, which gives a closed conformation (Pratap *et al.*, 2000). The torsion angles χ^{21} and χ^{22} are $-130.8(3)^\circ$ and $49.9(3)^\circ$, respectively. This deviation from the preferred value of 90° is due to interactions of the imidazole ring and is also observed in other compounds, for example, L-histidine tetrafluorosuccinate [$-102.7(2)^\circ$ and $79.2(3)^\circ$], L-histidinium trifluoroacetate [$-54.1(5)^\circ$ and $126.2(4)^\circ$] and L-histidine sulfate [$156.3(6)^\circ$ and $-28.0(12)^\circ$]. The imidazole group of L-histidine is in a *trans* conformation [$C3-C4-C5-C6$,

**Figure 1**

The cation and anion of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

**Figure 2**

The packing of the title compound, viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

$-175.68(19)^\circ$] with respect to the carboxylate group and in a *gauche* II conformation with respect to the amino N atom [$61.3(3)^\circ$]. The tetrafluoroborate anions play a vital role in hydrogen bonding with the histidinium cation *via* atoms N1 and N3 of the imidazole and amino groups through N—H...F bonds. Atoms N2 of the imidazole ring and N3 of the amino group form N—H...O bonds and link adjacent cations along the crystallographic *b* axis. The compound is stabilized by a network of both N—H...O and N—H...F bonds. An ORTEP representation of the pair of ions is given in Fig. 1 and the packing is shown in Fig. 2. Selected bond distances and angles are given in Table 1. Possible hydrogen bonds are summarized in Table 2.

Experimental

Crystals of the title compound were grown from a mixture of L-histidine and tetrafluoroboric acid in the molar ratio of 1:1 by slow evaporation of an aqueous solution at room temperature.

Crystal data

$C_6H_{10}N_3O_2^+ \cdot BF_4^-$
 $M_r = 242.98$
 Monoclinic, $P2_1$
 $a = 5.0259(8) \text{ \AA}$
 $b = 9.089(2) \text{ \AA}$
 $c = 10.218(2) \text{ \AA}$
 $\beta = 93.482(15)^\circ$
 $V = 465.91(17) \text{ \AA}^3$
 $Z = 2$

$D_x = 1.732 \text{ Mg m}^{-3}$
 Cu $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 20\text{--}30^\circ$
 $\mu = 1.59 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Prism, colourless
 $0.3 \times 0.2 \times 0.2 \text{ mm}$

Data collection

Enraf-Nonius CAD-4 diffractometer
 ω - 2θ scans
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.661$, $T_{\max} = 0.727$
 1008 measured reflections
 903 independent reflections
 902 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$
 $\theta_{\max} = 67.9^\circ$
 $h = 0 \rightarrow 6$
 $k = 0 \rightarrow 10$
 $l = -12 \rightarrow 12$
 2 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.067$
 $S = 1.09$
 903 reflections
 178 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.1648P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.088 (4)

Table 1

Selected geometric parameters (\AA , $^\circ$).

| | | | |
|-------------|-------------|-------------|---------------|
| C1—N1 | 1.311 (4) | C3—C4 | 1.489 (3) |
| C1—N2 | 1.322 (4) | C5—N3 | 1.485 (3) |
| C3—N2 | 1.378 (3) | C5—C6 | 1.531 (3) |
| N1—C1—N2 | 108.5 (3) | C2—C3—N2 | 106.2 (2) |
| C3—C2—N1 | 106.9 (3) | | |
| N1—C2—C3—C4 | 179.4 (2) | C3—C4—C5—N3 | 61.3 (3) |
| C2—C3—C4—C5 | $-130.8(3)$ | C3—C4—C5—C6 | $-175.68(19)$ |
| N2—C3—C4—C5 | 49.9 (3) | | |

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

| <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> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| N3—H3C...O1 ⁱ | 0.90 (4) | 2.14 (4) | 3.010 (3) | 161 (3) |
| N3—H3A...O2 ⁱⁱ | 0.90 (4) | 1.82 (4) | 2.722 (3) | 174 (3) |
| N2—H2'...O1 ⁱⁱⁱ | 0.91 (3) | 2.04 (3) | 2.953 (3) | 174 (3) |
| N3—H3B...F3 ⁱⁱⁱ | 0.93 (4) | 2.05 (4) | 2.945 (3) | 161 (3) |
| N1—H1'...F1 ^{iv} | 0.79 (4) | 2.09 (4) | 2.856 (3) | 161 (4) |

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

H atoms attached to C4 were refined using a riding model, with C–H distances constrained to 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. All other H atoms were located in a Fourier difference map and refined with isotropic displacement parameters. Refined C–H distances are in the range 0.83 (4)–0.95 (5) Å; N–H distances are given in Table 2. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1988); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* in *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SIR92* in *WinGX*; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-32* in *WinGX*; software used to prepare material for publication: *SHELXL97*.

SGR and GRK thank Professor A. K. Misra and Dr Babu Varghese of the Sophisticated Analytical Instrumentation Facility (SAIF), Indian Institute of Technology, Chennai 25, for providing the single-crystal X-ray diffraction facilities.

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