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(3-Methylbut-2-enyl)ammonium chloride

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.139
Data-to-parameter ratio = 18.8

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

All interatomic distances of the title compound, $C_5H_{12}N^+\cdot Cl^-$, are normal. All C atoms lie in a common plane. Molecules of the title compound are assembled by intermolecular weak N—H···Cl hydrogen bonds into an infinite zigzag ribbon structure along the y axis. The ribbon is bent repeatedly with angles of 34.15 (6)°.

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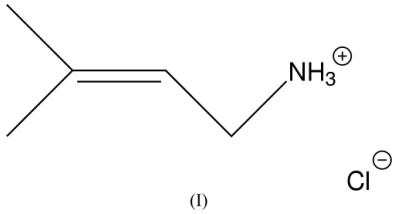
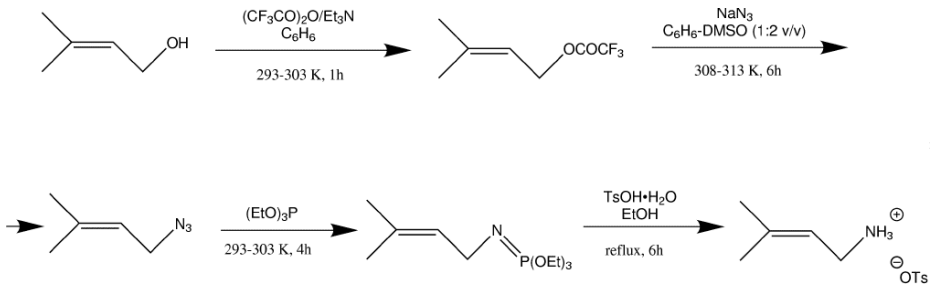
Comment

A perspective view of the title structure, (I), together with the atom-numbering scheme is shown in Fig. 1. All interatomic distances are normal. The part of the molecule consisting of C atoms is only insignificantly distorted from planarity (see Table 1); the maximum deviation of −0.012 (3) Å occurs for the C3 atom. The N1 atom deviates by 1.241 (4) Å from the above plane.



(I)

Molecules of (I) are assembled by intermolecular weak N—H···Cl hydrogen bonds into an infinite zigzag ribbon structure along the y axis (Fig. 2 and Table 2). The least-squares plane calculated through N1/Cl1/N1^{i}/Cl1^{i}/N1^{ii}/Cl1^{ii} [ribbon plane equation 9.315 (6)x + 6.184 (4)z = 4.777 (3); symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$], with a maximum deviation of −0.672 (2) Å for the N1 atom, makes an angle of 29.29 (13)° with the least-squares plane calculated through all C atoms and an angle of 17.55 (7)° with the N1/Cl1/N1^{i}/Cl1^{i} plane. The ribbon is bent repeatedly at angles of 34.15 (6)° [angle between planes indicated by N1/Cl1/N1^{i}/Cl1^{i} and N1/Cl1/N1^{ii}/Cl1^{ii} atoms].



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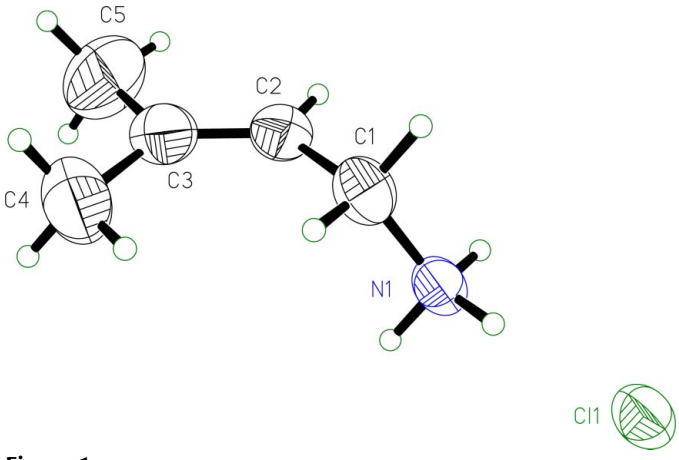

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The 3-methylbut-2-enyloammonium tosylate was synthesized in a single-point reaction (see reaction scheme above) (47.2% theoretical yield), based on the method of Tomassy & Zwierzak (1998). ^{1}H NMR (in $CDCl_3$/TMS, chemical shifts in p.p.m.): δ(Ts, *AA′XX′* system) 7.17–7.77 (4H, aromatic); $\delta(NH_3^+)$ 7.65 (*bs*); $\delta[(CH_3)_2CCHCH_2]$ 5.09–5.15 (*m*, 1H), 3.34–3.39 (*m*, 2H), 1.60 (*s*, 3H), 1.51 (*s*, 3H); δ(Ts, CH_3) 2.36 (*s*, 3H). The 3-methylbut-2-enyloammonium tosylate was dissolved in a 30% aqueous solution of NaOH containing a few drops of 95% EtOH. The solution was extracted three times with ethyl ether. The extract was dried over anhydrous $CaCl_2$ and then had gaseous HCl bubbled into it. After 30 min, a fine white crystalline product was obtained (total yield 20.1%). This was filtered off and dissolved in a small amount of fresh distilled EtOH. The solution was kept at 277 K in a sealed vessel. After one month, EtOH almost completely evaporated leaving plate-shaped colourless crystals. ^{1}H NMR (in $CDCl_3$/TMS, chemical shifts in p.p.m.): $\delta(NH_3^+)$ 8.03–8.35 (*bs*); $\delta[(CH_3)_2CCHCH_2]$ 5.38 (*bs*, 1H), 3.60 (*bs*, 2H), 1.79 (*s*, 3H), 1.75 (*s*, 3H).

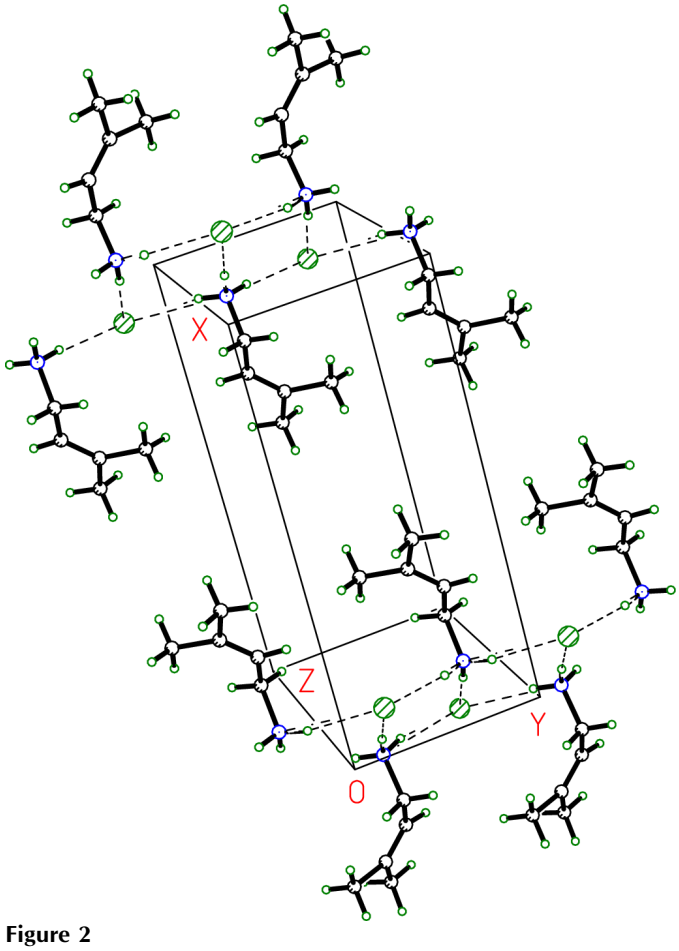

Figure 2
Part of the molecular packing of the title compound showing intermolecular hydrogen bonds creating a ribbon structure along the *y* axis. Hydrogen bonds are indicated by dashed lines.

Crystal data

$C_5H_{12}N^+\cdot Cl^-$	D_x = 1.102 Mg m^{-3}
M_r = 121.61	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2025 reflections
a = 14.1286 (12) Å	θ = 5–22°
b = 5.8874 (7) Å	μ = 0.42 mm^{-1}
c = 8.8335 (9) Å	T = 291 (2) K
β = 94.321 (8)°	Plate, colourless
V = 732.69 (13) Å^3	0.44 × 0.25 × 0.04 mm
Z = 4	

Data collection

Kuma KM-4–CCD diffractometer	R_{int} = 0.050
ω scans	θ_{max} = 25.1°
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1999)	$h = -16 \rightarrow 16$
T_{min} = 0.837, T_{max} = 0.983	$k = -7 \rightarrow 5$
7034 measured reflections	$l = -10 \rightarrow 10$
1241 independent reflections	2 standard reflections every 50 reflections
1223 reflections with $I > 2\sigma(I)$	intensity decay: 0.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.2647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.139	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
S = 1.18	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
1241 reflections	
66 parameters	
H-atom parameters constrained	

Table 1
Selected torsion angles (°).

N1—C1—C2—C3	117.1 (3)	C1—C2—C3—C5	−179.7 (3)
C1—C2—C3—C4	−2.2 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1	0.89	2.32	3.201 (2)	173
N1—H1B···Cl1^{i}	0.89	2.36	3.2178 (16)	163
N1—H1C···Cl1^{ii}	0.89	2.35	3.2173 (16)	165

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

Data collection: *CrysAlis CCD* (UNIL IC & Kuma, 2000); cell refinement: *CrysAlis RED* (UNIL IC & Kuma, 2000); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1990*b*) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1990*a*). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1990*b*). *SHELXTL/PC.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Stoe & Cie (1999). *X-RED.* Version 1.18. Stoe & Cie GmbH, Darmstadt, Germany.
Tomassy, B. & Zwierzak, A. (1998). *Synth. Commun.* **28**, 1201–1214.
UNIL IC & Kuma (2000). *CrysAlis CCD* (Version 1.163) and *CrysAlis RED* (Version 1.163). Kuma Diffraction Instruments GmbH, Wrocław, Poland.