

The 7-azanorbornane nucleus of epibatidine: 7-azabicyclo[2.2.1]heptan-7-ium chloride

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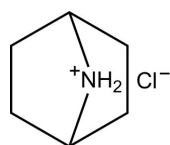
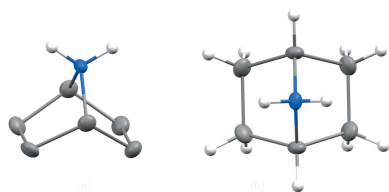
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7-Azabicyclo[2.2.1]heptane (7-azanorbornane) is a bridged heterocyclic nucleus found in epibatidine, the alkaloid isolated from the skin of the tropical poison frog *Epipedobates tricolor*. Since epibatidine is known as one of the most potent acetylcholine nicotinic receptor agonists, a plethora of literature has been devoted to this alkaloid. However, there are no structural data on the unsubstituted 7-azanorbornane, the parent bicyclic ring of epibatidine and its derivatives. We herein present the structural characterization of the 7-azabicyclo[2.2.1]heptane parent ring as its hydrochloride salt, namely 7-azabicyclo[2.2.1]heptan-7-ium chloride, $C_6H_{12}N^+ \cdot Cl^-$. The cation is generated by a crystallographic mirror plane with the N atom lying on the mirror, as does the chloride anion. In the crystal, the cations are linked to the anions by $N-H \cdots Cl$ hydrogen bonds, which generate [001] chains.

1. Chemical context

Since the discovery of the quinuclidine and tropane nuclei (Hamama *et al.*, 2006; Pollini *et al.*, 2006), elegant frameworks of bridged aza-heterocycles have been the focus of chemists exploring biologically active substances. One famous example in this series is epibatidine, (–)-2-(6-chloropyridin-3-yl)-7-azabicyclo[2.2.1]heptane, an active component of the skin poison extracted from the small tropical frog *Epipedobates tricolor* (Spande *et al.*, 1992; Gerzanich *et al.*, 1995; Sullivan & Bannon, 1996; Dukat & Glennon, 2003). Epibatidine comprises the first natural example of a compound incorporating an 7-azabicyclo[2.2.1]heptane (7-azanorbornane) ring system (Fletcher *et al.*, 1994). Due to the extreme binding affinity of the *exo* isomer of epibatidine towards nicotinic acetylcholine receptors, thousands of articles have been devoted to different aspects of its chemistry and biochemistry (see Carroll, 2004; Daly *et al.*, 2005; Yogeewari *et al.*, 2006; Garraffo *et al.*, 2009). We are not aware, however, that an X-ray structure determination of the alkaloid itself has ever been reported, in spite of numerous publications related to its



synthesis. Moreover, the molecular structure of 7-azanorbornane, the functional core of epibatidine, has also not been explored, in spite of the fact that 7-azanorbornane has been known since 1930 (Braun & Schwarz, 1930; Fraser & Swingle, 1970). In continuation of our studies related to bridged aza-heterocyclic systems (Britvin *et al.*, 2015, 2016,

Table 1
Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------|----------|-------------|-------------|---------------|
| $N7-H7B\cdots Cl1^i$ | 0.88 (3) | 2.25 (3) | 3.127 (2) | 175 (2) |
| $N7-H7A\cdots Cl1$ | 0.87 (4) | 2.25 (4) | 3.122 (2) | 178 (3) |

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

2017), we herein report on the structure of the unsubstituted 7-azabicyclo[2.2.1]heptane parent ring as its hydrochloride salt, namely 7-azabicyclo[2.2.1]heptan-7-ium chloride, **1**.

2. Structural commentary

The parent ring of 7-azabicyclo[2.2.1]heptane in **1** adopts a boat conformation (Fig. 1) resembling the molecular geometry of its nearest carbocyclic counterpart, bicyclo[2.2.1]heptane (norbornane), **2** (Fitch & Jobic, 1993). In order to achieve consistency of atomic labelling between the bicyclic cages of **1** and **2**, we herein apply the numbering scheme according to IUPAC nomenclature (Fig. 1) (Doms *et al.*, 1985). There are three unique C atoms (C1, C2 and C6) in the cation of **1**, with their clones $C1^i$ [= C4 by IUPAC; symmetry code: (i) $1 - x, y, z$], $C2^i$ (= C3 by IUPAC) and $C6^i$ (= C5 by IUPAC) generated by the mirror at $x = \frac{1}{2}$. Interatomic distances between the respective framework sites of **1** are shorter compared with the corresponding values of **2**. The distances (Å) in **1** and **2** are: C1–C2 = 1.528 (2) and 1.551 (3), C1–C6 = 1.523 (3) and 1.578 (1), and C1–N7(C7) = 1.508 (2) and 1.551 (3). The $C2^i-C2-C1-C6$ torsion angle determining the boat-like conformation is 109.4 (1)° in **1** and 108.7 (2)° in **2**. The s.u. values for **2** were generated using PLATON (Spek, 2009). Further details of the interatomic distances and angles of **1** can be found in the supporting information.

3. Supramolecular features

The structural integrity of **1** is maintained *via* intermolecular hydrogen bonding between the protonated secondary site N7 and the chloride counter-ion Cl1 (Table 1). Each chloride ion is linked to the two adjacent amine centres *via* N–H \cdots Cl hydrogen bonds so that the 7-azanorbornane cages are arranged into zigzag chains flattened on (010) and propagating along the *c*-axis direction (Fig. 2). That type of interleaved zigzag packing is known among chloride salts of secondary amines, both for alkyl- and arylamines (Adams *et al.*, 1997; Nancy *et al.*, 2003; Muller *et al.*, 2007) and heterocyclic systems (Gribkov *et al.*, 2006; Wang *et al.*, 2011; Fun *et al.*, 2011).

4. Database survey

Of more than 120 structures containing the 7-azanorbornane ring system in the Cambridge Structural Database (CSD, Version 5.38, latest update May 2017; Groom *et al.*, 2016), 17 entries represent the 7-azabicyclo[2.2.1]heptane parent ring unsubstituted at the carbon sites. All these compounds belong to *N*-substituted derivatives of 7-azanorbornane (Ohwada *et*

Table 2
Experimental details.

| | |
|----------------------------------------------------------------------------|------------------------------------------------------------------------|
| Crystal data | |
| Chemical formula | $C_6H_{12}N^+ \cdot Cl^-$ |
| M_r | 133.62 |
| Crystal system, space group | Orthorhombic, $Cmc2_1$ |
| Temperature (K) | 100 |
| a, b, c (Å) | 9.1532 (6), 8.7029 (8), 8.7336 (5) |
| V (Å ³) | 695.71 (9) |
| Z | 4 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 0.45 |
| Crystal size (mm) | 0.08 × 0.06 × 0.04 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (SADABS; Sheldrick, 2015) |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 3239, 777, 769 |
| R_{int} | 0.017 |
| $(\sin \theta/\lambda)_{max}$ (Å ⁻¹) | 0.638 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.017, 0.048, 1.15 |
| No. of reflections | 777 |
| No. of parameters | 47 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³) | 0.21, -0.12 |
| Absolute structure | Refined as an inversion twin |
| Absolute structure parameter | 0.19 (9) |

Computer programs: APEX2 (Bruker, 2015), SAINT (Bruker, 2015), SHELXT (Sheldrick, 2015a), OLEX2 (Dolomanov *et al.*, 2009), SHELXL2014 (Sheldrick, 2015b), Mercury (Macrae *et al.*, 2008) and publCIF (Westrip, 2010).

al. 1998; Cheng *et al.* 2002; Otani *et al.* 2003; Hori *et al.* 2008; Longobardi *et al.* 2015).

5. Synthesis and crystallization

7-Azabicyclo[2.2.1]heptane hydrochloride, **1**, was obtained from Sigma Aldrich. The purity of the substance has been proven by elemental analysis (analysis calculated for

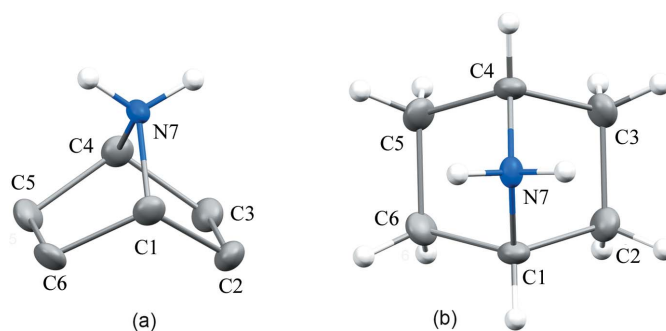
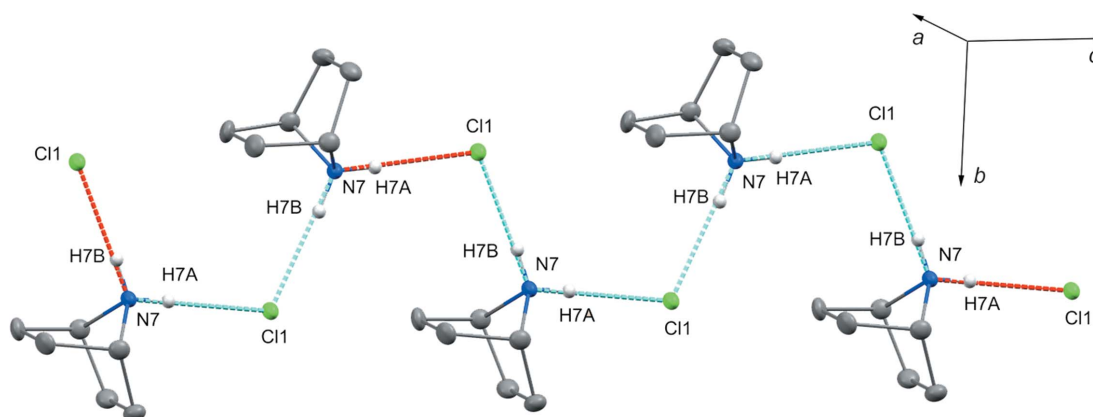


Figure 1
The molecular structure and systematic atomic numbering scheme of the 7-azabicyclo[2.2.1]heptane (7-azanorbornane) parent ring in **1**. Displacement ellipsoids are drawn at the 50% probability level. H atoms on C atoms in view (a) and the chloride counter-ion have been omitted for clarity. The labelling in the Figures corresponds to IUPAC notation (see text). Atoms C4, C3 and C5 are generated from C1, C2 and C6, respectively, by the symmetry operation $(1 - x, y, z)$.


Figure 2

Hydrogen bonding in the crystal structure of **1**. Protonated molecules of 7-azanorbornane are linked via N—H···Cl hydrogen bonds to form infinite zigzag chains propagated along the *c* axis. Displacement ellipsoids are drawn at the 50% probability level. H atoms not involved in hydrogen bonding have been omitted for clarity.

C₆H₁₂CIN: C 53.93, H 9.05, N 10.48%; found: C 53.89, H 9.08, N 10.44%). ¹H NMR (400 MHz) spectrum (Bruker Avance 400, SiMe₄ external standard, D₂O solution): δ 4.21–4.19 (*m*, 2H, 2 × CH at C1 and C4); 1.92–1.84 (*m*, 4H, 4 × *endo*-HCH at C2, C3, C5, C6), 1.78–1.71 (*m*, 4H, 4 × *exo*-HCH at C2, C3, C5, C6). ¹³C{¹H} NMR (101 MHz): δ 58.9 (*s*, C1 and C4), 26.7 (*s*, C2, C3, C5, C6). Crystals of **1** suitable for structural studies were obtained by slow evaporation of its aqueous solution.

6. Refinement

H atoms at the protonated N7 atom were refined freely, whereas H atoms on C atoms were refined based on a riding model. Crystal data, data collection and structure refinement details are summarized in Table 2.

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The 7-azanorbornane nucleus of epibatidine: 7-azabicyclo[2.2.1]heptan-7-ium chloride

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Computing details

Data collection: *APEX2* (Bruker, 2015); cell refinement: *SAINTE* (Bruker, 2015); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a) and *OLEX2* (Dolomanov *et al.*, 2009); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

7-Azabicyclo[2.2.1]heptan-7-ium chloride

Crystal data

$C_6H_{12}N^+ \cdot Cl^-$

$M_r = 133.62$

Orthorhombic, $Cmc2_1$

$a = 9.1532$ (6) Å

$b = 8.7029$ (8) Å

$c = 8.7336$ (5) Å

$V = 695.71$ (9) Å³

$Z = 4$

$F(000) = 288$

$D_x = 1.276$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2988 reflections

$\theta = 3.2\text{--}30.7^\circ$

$\mu = 0.45$ mm⁻¹

$T = 100$ K

Block, colourless

$0.08 \times 0.06 \times 0.04$ mm

Data collection

Bruker APEX-II CCD
diffractometer

Radiation source: fine focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2015)

3239 measured reflections

777 independent reflections

769 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 3.2^\circ$

$h = -11 \rightarrow 11$

$k = -4 \rightarrow 11$

$l = -11 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.017$

$wR(F^2) = 0.048$

$S = 1.15$

777 reflections

47 parameters

1 restraint

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 0.1322P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.21$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.12$ e Å⁻³

Absolute structure: Refined as an inversion twin

Absolute structure parameter: 0.19 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal data collection was performed using a Bruker Kappa APEX II DUO diffractometer equipped with microfocus optics. Refinement of lattice parameters and subsequent data reduction was carried out with the Bruker *S SAINT* software. The crystal structure of **1** was solved and refined using *SHELXT* and *SHELXL-2014* (Sheldrick, 2015) via the *OLEX2* v.1.2 graphical user interface (Dolomanov *et al.*, 2009).

Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| C1 | 0.62232 (18) | 0.2599 (3) | 0.5813 (2) | 0.0174 (4) |
| H1 | 0.7205 | 0.2960 | 0.5547 | 0.021* |
| C2 | 0.5850 (2) | 0.2715 (3) | 0.75142 (19) | 0.0202 (4) |
| H2B | 0.6233 | 0.3655 | 0.7956 | 0.024* |
| H2A | 0.6233 | 0.1843 | 0.8078 | 0.024* |
| C6 | 0.5848 (2) | 0.10083 (19) | 0.5202 (2) | 0.0209 (4) |
| H6A | 0.6231 | 0.0210 | 0.5864 | 0.025* |
| H6B | 0.6231 | 0.0863 | 0.4176 | 0.025* |
| N7 | 0.5000 | 0.3539 (2) | 0.5134 (2) | 0.0139 (4) |
| H7B | 0.5000 | 0.449 (4) | 0.548 (3) | 0.014 (7)* |
| H7A | 0.5000 | 0.347 (4) | 0.414 (5) | 0.030 (9)* |
| Cl1 | 0.5000 | 0.31735 (5) | 0.15788 (7) | 0.01568 (15) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|------------|------------|-------------|-------------|
| C1 | 0.0107 (7) | 0.0188 (10) | 0.0226 (9) | 0.0012 (7) | −0.0009 (6) | 0.0003 (7) |
| C2 | 0.0227 (10) | 0.0240 (10) | 0.0140 (8) | 0.0018 (8) | −0.0063 (7) | 0.0029 (7) |
| C6 | 0.0239 (9) | 0.0157 (9) | 0.0232 (9) | 0.0046 (6) | −0.0001 (7) | −0.0022 (8) |
| N7 | 0.0199 (10) | 0.0119 (9) | 0.0100 (9) | 0.000 | 0.000 | 0.0007 (8) |
| Cl1 | 0.0213 (2) | 0.0142 (2) | 0.0116 (2) | 0.000 | 0.000 | 0.0005 (2) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------------------|-------------|-----------------------|------------|
| C1—H1 | 0.9800 | C6—C6 ⁱ | 1.553 (4) |
| C1—C2 | 1.528 (2) | C6—H6A | 0.9700 |
| C1—C6 | 1.523 (3) | C6—H6B | 0.9700 |
| C1—N7 | 1.508 (2) | N7—C1 ⁱ | 1.508 (2) |
| C2—C2 ⁱ | 1.556 (4) | N7—H7B | 0.88 (3) |
| C2—H2B | 0.9700 | N7—H7A | 0.87 (4) |
| C2—H2A | 0.9700 | | |
| C2—C1—H1 | 114.5 | C1—C6—C6 ⁱ | 103.03 (9) |
| C6—C1—H1 | 114.5 | C1—C6—H6A | 111.2 |
| C6—C1—C2 | 110.50 (19) | C1—C6—H6B | 111.2 |

| | | | |
|--------------------------|-------------|--------------------------|-------------|
| N7—C1—H1 | 114.5 | C6 ⁱ —C6—H6A | 111.2 |
| N7—C1—C2 | 100.39 (16) | C6 ⁱ —C6—H6B | 111.2 |
| N7—C1—C6 | 100.82 (15) | H6A—C6—H6B | 109.1 |
| C1—C2—C2 ⁱ | 102.93 (9) | C1—N7—C1 ⁱ | 95.91 (18) |
| C1—C2—H2B | 111.2 | C1—N7—H7B | 111.8 (11) |
| C1—C2—H2A | 111.2 | C1 ⁱ —N7—H7B | 111.8 (11) |
| C2 ⁱ —C2—H2B | 111.2 | C1—N7—H7A | 110.6 (14) |
| C2 ⁱ —C2—H2A | 111.2 | C1 ⁱ —N7—H7A | 110.6 (14) |
| H2B—C2—H2A | 109.1 | H7B—N7—H7A | 115 (3) |
| C2—C1—C6—C6 ⁱ | 70.63 (12) | C6—C1—N7—C1 ⁱ | 56.31 (19) |
| C2—C1—N7—C1 ⁱ | -57.1 (2) | N7—C1—C2—C2 ⁱ | 35.24 (15) |
| C6—C1—C2—C2 ⁱ | -70.56 (14) | N7—C1—C6—C6 ⁱ | -34.89 (12) |

Symmetry code: (i) $-x+1, y, z$.

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N7—H7B \cdots C11 ⁱⁱ | 0.88 (3) | 2.25 (3) | 3.127 (2) | 175 (2) |
| N7—H7A \cdots C11 | 0.87 (4) | 2.25 (4) | 3.122 (2) | 178 (3) |

Symmetry code: (ii) $-x+1, -y+1, z+1/2$.