Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

[2-(Hydroxyethoxy)ethyl]trimethylammonium iodide

Lingzhi Zhang, Galina A. Bikzhanova and Robert West*

Organosilicon Research Center, Department of Chemistry, University of Wisconsin-Madison, 1101 University Ave, Madison, WI 53706, USA

Correspondence e-mail: west@chem.wisc.edu

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.014
wR factor = 0.037
Data-to-parameter ratio = 16.3

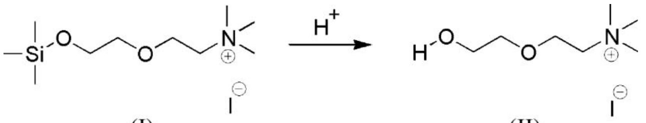
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 31 January 2007
Accepted 25 March 2007

In the crystal structure of the title compound, $C_7H_{18}NO_2^+\cdot I^-$, cations and anions are linked into ion pairs by means of a long O—H···I hydrogen-bonding interaction [O···I = 3.5299 (11) Å and O—H···I = 169.8 (19)°].

Comment

The synthesis of the title salt, (II), by the reaction of 2-[2-(dimethylamino)ethoxy]ethanol with methyl iodide was described earlier (De Amici *et al.*, 1987), but the crystal structure has not been reported. In our work, the trimethylsilyl derivative, (I), of the title compound was synthesized by the reaction of 2-[2-(dimethylamino)ethoxy]ethanol with trimethylchlorosilane, followed by methylation with methyl iodide.



(I) (II)

It is well known that the silylalkoxy compounds can be easily hydrolysed. The solution of (I) in CH_2Cl_2 was slowly hydrolysed by the trace amount of moisture present in the

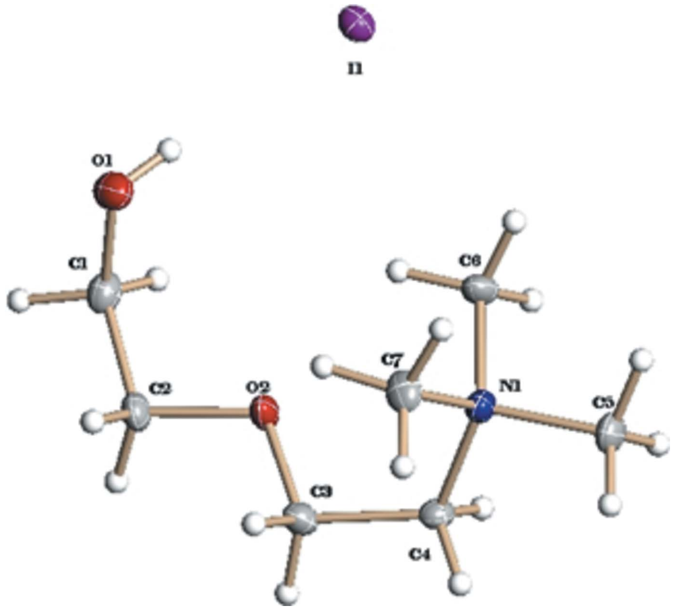


Figure 1
The asymmetric unit of (II); displacement ellipsoids are drawn at the 50% probability level.

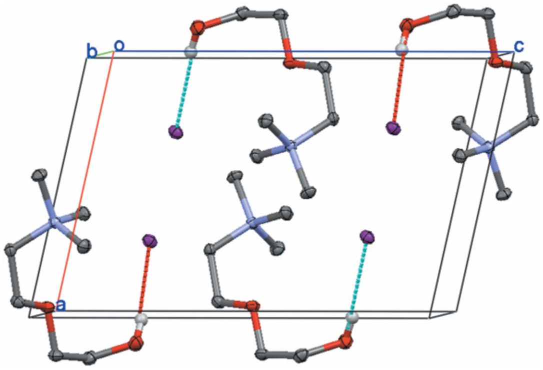


Figure 2
A packing diagram of (II), viewed approximately along the *b* axis, showing the O—H···I hydrogen bonds as dashed lines. Only H atoms involved in hydrogen bonds are shown. Displacement ellipsoids are drawn at the 50% probability level.

solution, producing the title compound (II). High-quality colorless crystals were obtained and the structure was determined (Fig. 1).

The conformation of the hydroxyethoxyethyl fragment is different from the planar zigzag chain typical for linear alkanes. The stereochemical arrangements for N1—C4—C3—O2, C4—C3—O2—C2, C3—O2—C2—C1 and O2—C2—C1—O1 are +*sc*, *ap*, *ap*, and −*sc*; the corresponding torsion angles are 60.99 (13), −179.84 (10), 176.43 (10) and −69.99 (13)°, respectively.

The cations and anions in the crystal structure are linked into ion pairs by means of a hydrogen bond between the hydroxyl group of the cation and the iodide anion (Fig. 2 and Table 2). The O1—H1···I1 hydrogen-bonding interaction is in excellent agreement with the average values for 184 similar interactions [O···I separation of 3.54 (9) Å and O—H···I angle of 166 (7)°] in 108 organic compounds found in the Cambridge Structural Database (Version 5.28, January 2007 release; Allen, 2002).

Experimental

Reactions and manipulations were carried out under an atmosphere of dry nitrogen using standard Schlenk techniques. Solvents were freshly distilled under nitrogen from sodium/benzophenone (THF) or calcium hydride (CH_2Cl_2). Trimethylchlorosilane (18 g, 0.15 mol) was added slowly to a mixture of 2-[2-(dimethylamino)ethoxy]ethanol (20 g, 0.15 mol) and triethylamine (17 g, 0.17 mol) in 200 ml of THF at 273 K. After the reaction was complete, the product was separated by filtration, and purified by fractional distillation. Reaction with methyl iodide (1.1 equivalents) yielded the trimethylsilyl derivative, (I), as a yellow solid. Compound (I) (400 mg) was dissolved in 15 ml of dry CH_2Cl_2 under nitrogen. The tube was sealed and left at 296 K for two weeks, resulting in the formation of colorless crystals of (II).

Crystal data

$C_7H_{18}NO_2^+\cdot I^-$
$M_r = 275.12$
Monoclinic, $P2_1/c$
$a = 7.5815$ (5) Å
$b = 12.6485$ (9) Å
$c = 11.4120$ (8) Å
$\beta = 102.537$ (1)°
$V = 1068.26$ (13) Å^3
$Z = 4$
Mo- $K\alpha$ radiation
$\mu = 2.96$ mm^{-1}
$T = 100$ (2) K
0.37 × 0.34 × 0.33 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{min} = 0.407$, $T_{max} = 0.442$ (expected range = 0.347–0.377)
14768 measured reflections
2819 independent reflections
2738 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.014$
$wR(F^2) = 0.037$
$S = 1.13$
2819 reflections
173 parameters
All H-atom parameters refined
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}

Table 1
Selected torsion angles (°).

C3—O2—C2—C1	176.43 (10)	C2—O2—C3—C4	−179.84 (10)
O1—C1—C2—O2	−69.99 (13)	O2—C3—C4—N1	60.99 (13)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···I1	0.79 (2)	2.75 (2)	3.5299 (11)	169.8 (19)

All H atoms were found in a difference map and refined isotropically [C—H = 0.94 (2)–1.02 (2) Å and O1—H1 = 0.79 (2) Å].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *publCIF* (Westrip, 2007) and *modiCIFer* (Guzei, 2007).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2003). *SADABS* (Version 2.05), *SAINT* (Version 6.22), *SHELXTL* (Version 6.10) and *SMART* (Version 5.622). Bruker AXS Inc., Madison, Wisconsin, USA.
De Amici, M., De Micheli, C., Pratesi, P., Toma, L., Grana, E. & Santagostino-Barbone, M. G. (1987). *Il Farmaco*, **42**, 921–930.
Guzei, I. A. (2007). *modiCIFer*. University of Wisconsin-Madison, USA.
Westrip, S. P. (2007). *publCIF*. In preparation.

Acta Cryst. (2007). E**63**, o2284–o2285 Zhang *et al.* • $C_7H_{18}NO_2^+\cdot I^-$ **o2285**