Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Hydroxyethylammonium iodide

Christina Kohrt, Anke Spannenberg and Thomas Werner*

Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany
Correspondence e-mail: thomas.werner@catalysis.de

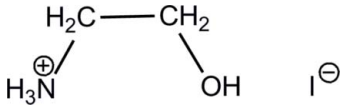
Received 17 April 2014; accepted 28 April 2014

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.014; wR factor = 0.032; data-to-parameter ratio = 27.5.

In the crystal structure of the title salt, $C_2H_8NO^+\cdot I^-$, N—H···O, N—H···I and O—H···I hydrogen bonds lead to the formation of layers staggered along the c axis.

Related literature

A variety of compounds are known in the literature involving the cation $[NH_3CH_2CH_2OH]^+$. A WebCSD search (Release April 2014) yielded 85 examples (Thomas *et al.*, 2010), see for example: Koo *et al.* (1974) for 2-hydroxyethylammonium bromide, or Koo *et al.* (1972) for 2-hydroxyethylammonium chloride.



Experimental

Crystal data

$C_2H_8NO^+\cdot I^-$
M_r = 188.99
Triclinic, $P\overline{1}$
a = 4.6557 (4) Å
b = 7.5432 (6) Å
c = 8.1787 (7) Å
α = 85.235 (2)°
β = 78.091 (2)°
γ = 77.544 (2)°
V = 274.21 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.70 mm^{-1}
T = 150 K
0.34 × 0.12 × 0.03 mm

Data collection

Bruker Kappa APEXII DUO diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.672, T_{max} = 0.843
4884 measured reflections
1319 independent reflections
1254 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.032
S = 1.08
1319 reflections
48 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.91	1.93	2.800 (2)	158
N1—H1B···I1^{ii}	0.91	2.75	3.5825 (18)	152
N1—H1C···I1^{iii}	0.91	2.78	3.6322 (18)	155
O1—H1D···I1	0.84	2.72	3.5100 (15)	157

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We wish to thank the Federal Ministry of Research and Education (BMBF) for financial support (Chemische Prozesse und stoffliche Nutzung von CO_2: Technologien für Nachhaltigkeit und Klimaschutz, grant 01 RC 1004A).

Supporting information for this paper is available from the IUCr electronic archives (Reference: ZL2586).

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supporting information

Acta Cryst. (2014). E**70**, o628 [doi:10.1107/S1600536814009581]

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S1. Comment

Recently we were interested in the synthesis of perfluorinated organocatalysts. In this context we tried to alkylate 2-aminoethanol with 1*H*,1*H*,2*H*,2*H*-perfluorooctyliodide. Unfortunately we did not obtain the desired product under the chosen reaction conditions. However, instead we were able to isolate the title compound in excellent yield. The molecular structure of the ammonium iodide shows a nitrogen atom carrying three protons and one 2-hydroxyethyl-group and the iodide as anion (Fig. 1). The cations are aggregated through N—H···O hydrogen bonds in a linear arrangement parallel to the *a* axis. These chains are extended by N—H···I and O—H···I hydrogen bonds into layers staggered along the *c* axis (Fig. 2).

A variety of compounds involving the same cation had been reported in the literature. A WebCSD search (Release April 2014, Thomas *et al.* (2010)) yielded 85 examples of hydroxyethylammonium salts; for the bromide and chloride salts most closely related to the iodide title compound, please see Koo *et al.* (1974) and Koo *et al.* (1972), respectively.

S2. Experimental

2-Aminoethanol (4.09 mmol, 250 mg, 1 eq) was added to 1*H*,1*H*,2*H*,2*H*-perfluorooctyliodide (12.3 mmol, 5.80 g, 3 eq) in a pressure pipe under argon. The solution was stirred at 80°C for 24 h. Afterwards the resulting yellow solution was layered with 2,2,2-trifluoroethanol and crystals precipitated directly from the mixture. 84% (3.43 mmol, 649 mg) of the title compound were obtained as colorless crystals. ^{1}H NMR (CF_3—CD_2—OD): δ 3.59–3.48 (br m, 2H); 2.78–2.67 (br m, 2H) ppm. ^{13}C NMR (CF_3—CD_2—OD): δ 62.47 (s, CH_2); 44.03 (s, CH_2) ppm. Elemental analysis calculated (%) for C_2H_8INO: C 12.71, H 4.27, N 7.41; found: C 12.97, H 4.10, N 7.48.

S3. Refinement

H1A - H1D were clearly identified in difference Fourier maps. All H atoms were placed in idealized positions with d(O—H) = 0.84, d(N—H) = 0.91, d(C—H) = 0.99 Å and refined using a riding model with U_{iso}(H) fixed at 1.2 U_{eq}(C) and 1.5 U_{eq}(N, O)

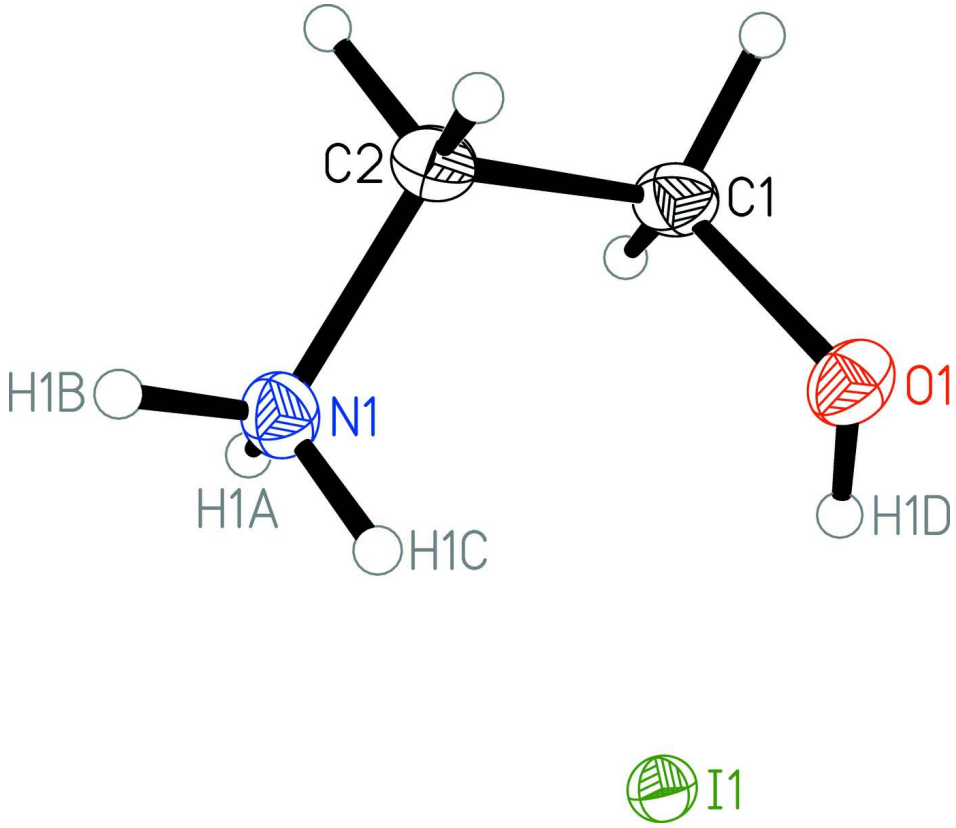

Figure 1

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

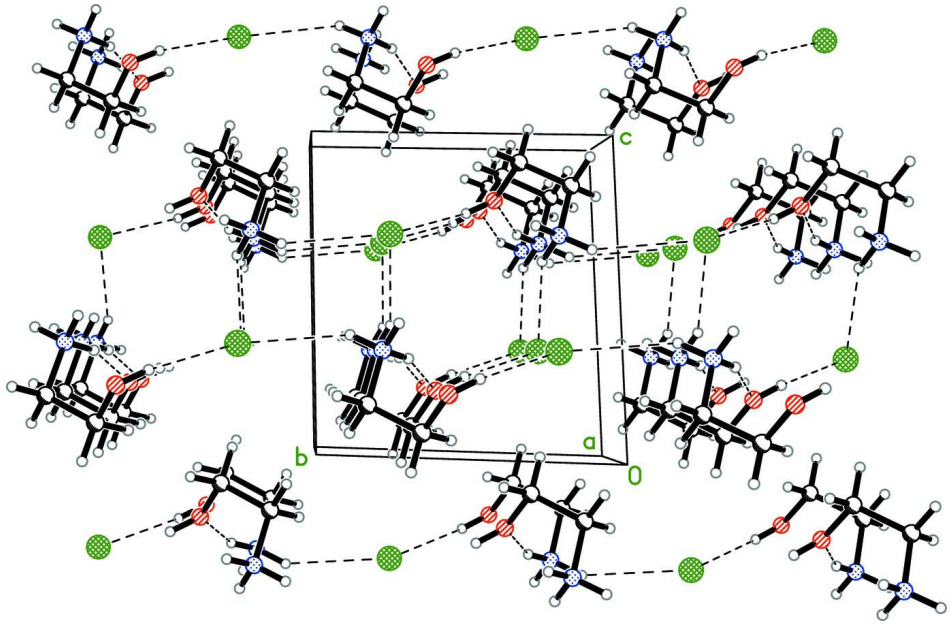

Figure 2

Packing plot; hydrogen bonds are shown as dashed lines.

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Crystal data

$C_2H_8NO^+·I^-$
M_r = 188.99
Triclinic, $P\overline{1}$
a = 4.6557 (4) Å
b = 7.5432 (6) Å
c = 8.1787 (7) Å
α = 85.235 (2)°
β = 78.091 (2)°
γ = 77.544 (2)°
V = 274.21 (4) Å^3
Z = 2
$F(000)$ = 176
D_x = 2.289 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3767 reflections
θ = 2.8–29.0°
μ = 5.70 mm^{-1}
T = 150 K
Plate, colorless
0.34 × 0.12 × 0.03 mm

Data collection

Bruker Kappa APEXII DUO diffractometer
Radiation source: fine-focus sealed tube
Curved graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.672, T_{max} = 0.843
4884 measured reflections
1319 independent reflections
1254 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 28.0°, θ_{min} = 2.6°
h = −6→6
k = −9→9
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.032
S = 1.08
1319 reflections
48 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 0.0136P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.63581 (3)	0.752733 (16)	0.669449 (16)	0.01732 (5)

O1	1.1624 (3)	0.3874 (2)	0.79532 (19)	0.0204 (3)
H1D	1.0844	0.4856	0.7510	0.031*
N1	0.7519 (4)	0.2059 (2)	0.6780 (2)	0.0182 (4)
H1A	0.5779	0.2898	0.7009	0.027*
H1B	0.7164	0.1061	0.6366	0.027*
H1C	0.8882	0.2542	0.6011	0.027*
C1	0.9351 (5)	0.3140 (3)	0.9069 (3)	0.0189 (4)
H1E	0.7493	0.4085	0.9290	0.023*
H1F	1.0004	0.2765	1.0146	0.023*
C2	0.8719 (5)	0.1527 (3)	0.8344 (3)	0.0182 (4)
H2A	1.0590	0.0596	0.8098	0.022*
H2B	0.7245	0.0988	0.9174	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01634 (8)	0.01767 (8)	0.01768 (8)	−0.00360 (5)	−0.00336 (5)	0.00129 (5)
O1	0.0182 (7)	0.0167 (7)	0.0249 (8)	−0.0035 (6)	−0.0021 (6)	0.0012 (6)
N1	0.0164 (9)	0.0213 (9)	0.0175 (9)	−0.0048 (7)	−0.0027 (7)	−0.0022 (7)
C1	0.0218 (11)	0.0203 (11)	0.0139 (10)	−0.0046 (8)	−0.0020 (8)	0.0000 (8)
C2	0.0188 (10)	0.0176 (11)	0.0182 (10)	−0.0023 (8)	−0.0058 (8)	0.0018 (8)

Geometric parameters (Å, º)

O1—C1	1.425 (3)	C1—C2	1.505 (3)
O1—H1D	0.8400	C1—H1E	0.9900
N1—C2	1.490 (3)	C1—H1F	0.9900
N1—H1A	0.9100	C2—H2A	0.9900
N1—H1B	0.9100	C2—H2B	0.9900
N1—H1C	0.9100		
C1—O1—H1D	109.5	O1—C1—H1F	109.5
C2—N1—H1A	109.5	C2—C1—H1F	109.5
C2—N1—H1B	109.5	H1E—C1—H1F	108.0
H1A—N1—H1B	109.5	N1—C2—C1	111.23 (16)
C2—N1—H1C	109.5	N1—C2—H2A	109.4
H1A—N1—H1C	109.5	C1—C2—H2A	109.4
H1B—N1—H1C	109.5	N1—C2—H2B	109.4
O1—C1—C2	110.92 (17)	C1—C2—H2B	109.4
O1—C1—H1E	109.5	H2A—C2—H2B	108.0
C2—C1—H1E	109.5		
O1—C1—C2—N1	−63.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.91	1.93	2.800 (2)	158

N1—H1*B*···I1^{ii}	0.91	2.75	3.5825 (18)	152
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