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n-Dodecylammonium bromide monohydrate

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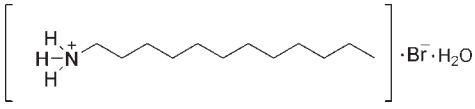
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.081; data-to-parameter ratio = 18.2.

In the title compound, $C_{12}H_{28}N^{+}\cdot Br^{-}\cdot H_2O$, the ionic pairs formed by *n*-dodecylammonium cations and bromide anions are arranged into thick layers; these layers are linked in a nearly perpendicular fashion [the angle between the layers is 85.84 (5)°] by hydrogen-bonding interactions involving the water molecules. The methylene part of the alkyl chain in the cation adopts an all-*trans* conformation. In the crystal structure, molecules are linked by intermolecular N—H···Br, O—H···Br and N—H···O hydrogen bonds.

Related literature

Long-chain *n*-alkylammonium halides are widely used as surfactants (Aratono *et al.*, 1998; Tornblom *et al.*, 2000) and as models for biological membranes (Ringsdorf *et al.*, 1988). They exhibit polymorphism at room temperature: for solid-solid phase transitions in *n*–alkylammonium chlorides, see: Terreros *et al.* (2000). For a related structure, see: Lundén (1974).



Experimental

Crystal data

$C_{12}H_{28}N^{+}\cdot Br^{-}\cdot H_2O$
M_r = 284.28
Monoclinic, *Cc*
a = 4.7921 (5) Å
b = 42.810 (4) Å
c = 7.8573 (8) Å
β = 105.798 (2)°
V = 1551.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.63 mm^{-1}
T = 293 K
0.42 × 0.14 × 0.06 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.404, T_{max} = 0.858
4760 measured reflections
2644 independent reflections
1665 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.081
S = 0.92
2644 reflections
145 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 945 Friedel pairs
Flack parameter: 0.048 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1^{i}	0.89	2.53	3.380 (4)	159
N1—H1B···Br1	0.89	2.47	3.340 (4)	166
N1—H1C···O1	0.89	1.97	2.834 (7)	165
O1—H1···Br1^{ii}	0.83 (4)	2.76 (6)	3.329 (5)	128 (6)
O1—H2···Br1^{iii}	0.97 (4)	2.49 (5)	3.361 (5)	149 (5)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2141).

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supporting information

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S1. Comment

Long-chain *n*-alkylammonium halides are widely used as surfactants (Aratono *et al.*, 1998; Tornblom *et al.*, 2000) and as models for biological membranes (Ringsdorf *et al.*, 1988). They exhibit polymorphism at room temperature; solid-solid phase transitions occurred in *n*-alkylammonium chlorides (Terreros *et al.*, 2000). As a part of the studies on novel potential phase transfer materials with the thermochemical properties such as *n*-alkylammonium chlorides, we report the crystal structure of the title compound (Fig. 1).

Atoms C3–C12 are coplanar in the title compound; however, atoms C2–C12 are coplanar in *n*–dodecylammonium bromide (Ludén, 1974). Although the methylene chain had the extended all–*trans* conformation, it is slightly curved in the vicinity of the ammonium group, to accommodate the hydrogen–bonding interactions. The hydrogen bonds of *n*–dodecylammonium bromide monohydrate are more stronger than that of *n*–dodecylammonium bromide because of N—H···O and O—H···Br hydrogen bonds. Only torsion angle C1–C2–C3–C4 deviates significantly from 180 °, with a value of 170.6 (5)°. The crystal packing (Fig. 2) is stabilized by intermolecular N—H···Br, N—H···O and O—H···Br hydrogen bonds (Table 1).

S2. Experimental

n–Dodecylammonium bromide monohydrate was prepared by the addition of hydrobromic acid to an ethanol solution of *n*–dodecylamine. The resulting precipitate was filtered off and recrystallized several times from chloroform. Single crystals suitable for X–ray diffraction were prepared by evaporation of a solution of the title compound in chloroform at room temperature. Analysis, calculated for $C_{12}H_{30}BrNO$ (Mr = 284.28): C 50.69, H 10.64, N 4.93, O 5.63, Br 28.11%; found: C 50.67, H 10.65, N 4.91, O 5.64, Br 28.13%.

S3. Refinement

The reported Flack parameter was obtained by TWIN/BASF procedure in SHELXL (Sheldrick, 2008). Water molecule bound H atoms were located in difference Fourier maps and their positional parameters refined with a distance restraint [O1—H1 = 0.85 (5) & O1—H2 = 0.80 (5) Å] and a angle restraint. The H atoms of C and N atoms were positioned geometrically, with methylene C—H distances of 0.97 Å, methyl C—H distances of 0.96 Å, N—H 0.89 Å and refined as riding on their parent atoms. TheU_{iso}(H) values were set at $1.2U_{eq}$ for the methylene H atoms and at $1.5U_{eq}$ for other H atoms.

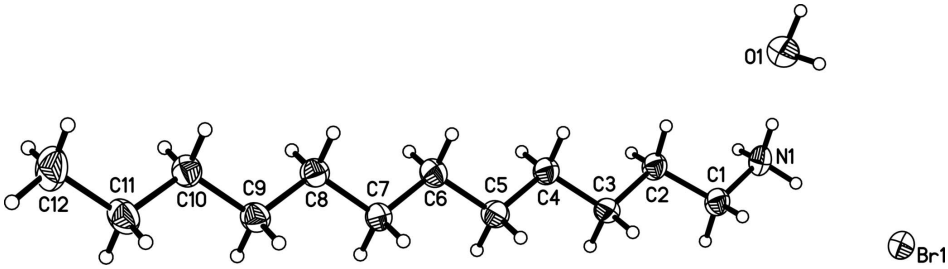

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

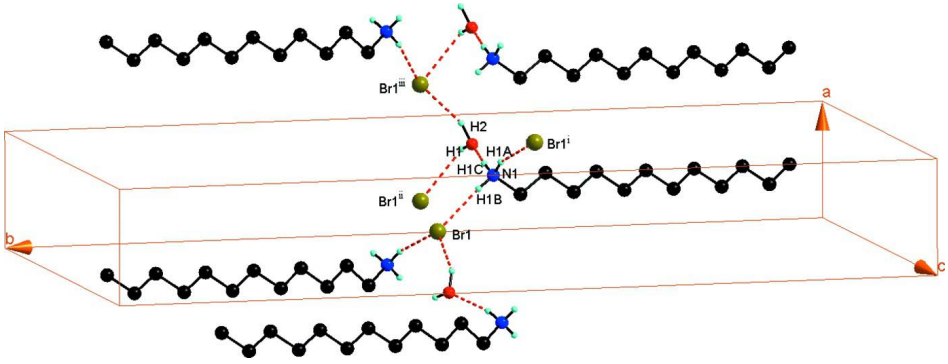

Figure 2

N—H···Br, N—H···O and O—H···Br interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $x + 1, - y + 1, z + 1/2$; (ii) $x, - y +1 , z - 1/2$; (iii) $x + 1, - y + 1, z - 1/2$]

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$b = 42.810$ (4) Å
$c = 7.8573$ (8) Å
$\beta = 105.798$ (2)°
$V = 1551.0$ (3) Å^3
$Z = 4$

$F(000) = 608$
$D_x = 1.217$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1266 reflections
$\theta = 2.9$–$25.0°$
$\mu = 2.63$ mm^{-1}
$T = 293$ K
Acicular, colourless
0.42 × 0.14 × 0.06 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.404$, $T_{max} = 0.858$

4760 measured reflections
2644 independent reflections
1665 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.9°$
$h = -6 \rightarrow 5$
$k = -54 \rightarrow 50$
$l = -6 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.081$
$S = 0.92$
2644 reflections
145 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983), 945 Friedel pairs
Absolute structure parameter: 0.048 (19)

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.2086 (2)	0.524590 (10)	0.38293 (16)	0.05643 (18)
O1	0.8268 (12)	0.45062 (13)	0.1580 (6)	0.0760 (15)
H1	0.734 (13)	0.4485 (18)	0.053 (6)	0.114*
H2	0.993 (11)	0.4589 (15)	0.124 (9)	0.114*
N1	0.7249 (9)	0.46990 (8)	0.4809 (6)	0.0502 (12)
H1A	0.8831	0.4731	0.5697	0.075*
H1B	0.6083	0.4864	0.4696	0.075*
H1C	0.7755	0.4671	0.3810	0.075*
C1	0.5729 (12)	0.44200 (13)	0.5176 (8)	0.0496 (17)
H1D	0.3952	0.4392	0.4238	0.059*
H1E	0.5212	0.4449	0.6276	0.059*
C2	0.7567 (11)	0.41323 (10)	0.5313 (7)	0.0480 (14)
H2A	0.9345	0.4161	0.6249	0.058*
H2B	0.8084	0.4104	0.4213	0.058*
C3	0.6028 (11)	0.38403 (11)	0.5696 (7)	0.0496 (14)
H3A	0.5795	0.3855	0.6881	0.059*
H3B	0.4108	0.3831	0.4875	0.059*
C4	0.7635 (11)	0.35416 (10)	0.5545 (7)	0.0466 (14)
H4A	0.7908	0.3531	0.4367	0.056*
H4B	0.9540	0.3550	0.6382	0.056*
C5	0.6137 (11)	0.32477 (11)	0.5877 (7)	0.0484 (14)
H5A	0.5955	0.3254	0.7076	0.058*
H5B	0.4194	0.3245	0.5082	0.058*

C6	0.7625 (11)	0.29500 (11)	0.5641 (7)	0.0488 (14)
H6A	0.9550	0.2951	0.6458	0.059*
H6B	0.7859	0.2947	0.4453	0.059*
C7	0.6105 (11)	0.26515 (11)	0.5920 (7)	0.0454 (13)
H7A	0.5909	0.2651	0.7117	0.055*
H7B	0.4168	0.2651	0.5117	0.055*
C8	0.7621 (11)	0.23602 (11)	0.5640 (7)	0.0484 (14)
H8A	0.9555	0.2361	0.6447	0.058*
H8B	0.7827	0.2362	0.4446	0.058*
C9	0.6128 (11)	0.20610 (11)	0.5905 (7)	0.0495 (14)
H9A	0.4180	0.2062	0.5116	0.059*
H9B	0.5957	0.2058	0.7107	0.059*
C10	0.7642 (12)	0.17604 (11)	0.5585 (7)	0.0508 (14)
H10A	0.7842	0.1766	0.4389	0.061*
H10B	0.9579	0.1757	0.6387	0.061*
C11	0.6143 (13)	0.14651 (12)	0.5818 (8)	0.0592 (16)
H11A	0.5946	0.1459	0.7014	0.071*
H11B	0.4205	0.1468	0.5016	0.071*
C12	0.7623 (15)	0.11758 (13)	0.5502 (9)	0.080 (2)
H12A	0.7850	0.1179	0.4325	0.121*
H12B	0.6483	0.0998	0.5634	0.121*
H12C	0.9496	0.1163	0.6342	0.121*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0519 (3)	0.0577 (3)	0.0587 (3)	0.0057 (6)	0.0134 (2)	0.0063 (5)
O1	0.078 (3)	0.085 (4)	0.069 (3)	0.006 (3)	0.025 (3)	0.006 (3)
N1	0.051 (3)	0.038 (3)	0.056 (3)	0.006 (2)	0.005 (2)	0.0026 (19)
C1	0.050 (4)	0.032 (3)	0.067 (5)	0.001 (3)	0.017 (3)	0.004 (3)
C2	0.052 (3)	0.036 (3)	0.057 (4)	−0.001 (3)	0.016 (3)	0.000 (2)
C3	0.053 (4)	0.043 (3)	0.059 (4)	0.001 (3)	0.027 (3)	0.007 (3)
C4	0.047 (3)	0.039 (3)	0.056 (4)	0.000 (3)	0.017 (3)	0.001 (3)
C5	0.057 (4)	0.041 (3)	0.052 (3)	0.001 (3)	0.024 (3)	−0.005 (3)
C6	0.053 (3)	0.044 (3)	0.049 (3)	−0.003 (3)	0.013 (3)	0.000 (3)
C7	0.048 (3)	0.036 (3)	0.056 (3)	−0.001 (3)	0.020 (3)	0.001 (3)
C8	0.050 (3)	0.042 (3)	0.055 (3)	−0.003 (3)	0.017 (3)	−0.001 (3)
C9	0.051 (4)	0.046 (3)	0.056 (4)	−0.007 (3)	0.021 (3)	−0.001 (3)
C10	0.058 (4)	0.048 (3)	0.047 (3)	0.000 (3)	0.015 (3)	0.001 (3)
C11	0.073 (4)	0.041 (3)	0.067 (4)	−0.011 (3)	0.026 (3)	−0.001 (3)
C12	0.104 (5)	0.041 (4)	0.097 (5)	0.003 (4)	0.028 (4)	−0.007 (3)

Geometric parameters (Å, º)

O1—H1	0.83 (4)	C6—C7	1.516 (6)
O1—H2	0.97 (4)	C6—H6A	0.9700
N1—C1	1.468 (7)	C6—H6B	0.9700
N1—H1A	0.8900	C7—C8	1.490 (6)

N1—H1B	0.8900	C7—H7A	0.9700
N1—H1C	0.8900	C7—H7B	0.9700
C1—C2	1.501 (7)	C8—C9	1.509 (7)
C1—H1D	0.9700	C8—H8A	0.9700
C1—H1E	0.9700	C8—H8B	0.9700
C2—C3	1.522 (6)	C9—C10	1.532 (7)
C2—H2A	0.9700	C9—H9A	0.9700
C2—H2B	0.9700	C9—H9B	0.9700
C3—C4	1.514 (7)	C10—C11	1.490 (7)
C3—H3A	0.9700	C10—H10A	0.9700
C3—H3B	0.9700	C10—H10B	0.9700
C4—C5	1.506 (6)	C11—C12	1.481 (8)
C4—H4A	0.9700	C11—H11A	0.9700
C4—H4B	0.9700	C11—H11B	0.9700
C5—C6	1.496 (6)	C12—H12A	0.9600
C5—H5A	0.9700	C12—H12B	0.9600
C5—H5B	0.9700	C12—H12C	0.9600

H1—O1—H2	91 (5)	C5—C6—H6B	108.3
C1—N1—H1A	109.5	C7—C6—H6B	108.3
C1—N1—H1B	109.5	H6A—C6—H6B	107.4
H1A—N1—H1B	109.5	C8—C7—C6	114.3 (4)
C1—N1—H1C	109.5	C8—C7—H7A	108.7
H1A—N1—H1C	109.5	C6—C7—H7A	108.7
H1B—N1—H1C	109.5	C8—C7—H7B	108.7
N1—C1—C2	111.6 (5)	C6—C7—H7B	108.7
N1—C1—H1D	109.3	H7A—C7—H7B	107.6
C2—C1—H1D	109.3	C7—C8—C9	114.9 (4)
N1—C1—H1E	109.3	C7—C8—H8A	108.5
C2—C1—H1E	109.3	C9—C8—H8A	108.5
H1D—C1—H1E	108.0	C7—C8—H8B	108.5
C1—C2—C3	112.4 (4)	C9—C8—H8B	108.5
C1—C2—H2A	109.1	H8A—C8—H8B	107.5
C3—C2—H2A	109.1	C8—C9—C10	115.3 (4)
C1—C2—H2B	109.1	C8—C9—H9A	108.5
C3—C2—H2B	109.1	C10—C9—H9A	108.5
H2A—C2—H2B	107.9	C8—C9—H9B	108.5
C4—C3—C2	113.2 (4)	C10—C9—H9B	108.5
C4—C3—H3A	108.9	H9A—C9—H9B	107.5
C2—C3—H3A	108.9	C11—C10—C9	115.3 (4)
C4—C3—H3B	108.9	C11—C10—H10A	108.5
C2—C3—H3B	108.9	C9—C10—H10A	108.5
H3A—C3—H3B	107.8	C11—C10—H10B	108.5
C5—C4—C3	114.6 (4)	C9—C10—H10B	108.5
C5—C4—H4A	108.6	H10A—C10—H10B	107.5
C3—C4—H4A	108.6	C12—C11—C10	114.8 (5)
C5—C4—H4B	108.6	C12—C11—H11A	108.6
C3—C4—H4B	108.6	C10—C11—H11A	108.6

H4A—C4—H4B	107.6	C12—C11—H11B	108.6
C6—C5—C4	115.1 (4)	C10—C11—H11B	108.6
C6—C5—H5A	108.5	H11A—C11—H11B	107.5
C4—C5—H5A	108.5	C11—C12—H12A	109.5
C6—C5—H5B	108.5	C11—C12—H12B	109.5
C4—C5—H5B	108.5	H12A—C12—H12B	109.5
H5A—C5—H5B	107.5	C11—C12—H12C	109.5
C5—C6—C7	115.9 (4)	H12A—C12—H12C	109.5
C5—C6—H6A	108.3	H12B—C12—H12C	109.5
C7—C6—H6A	108.3		

N1—C1—C2—C3	179.9 (4)	C5—C6—C7—C8	178.9 (4)
C1—C2—C3—C4	170.6 (5)	C6—C7—C8—C9	−179.7 (5)
C2—C3—C4—C5	−178.7 (4)	C7—C8—C9—C10	178.9 (4)
C3—C4—C5—C6	177.0 (5)	C8—C9—C10—C11	−179.1 (5)
C4—C5—C6—C7	−178.4 (4)	C9—C10—C11—C12	179.9 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br1^{i}	0.89	2.53	3.380 (4)	159
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O1—H1···Br1^{ii}	0.83 (4)	2.76 (6)	3.329 (5)	128 (6)
O1—H2···Br1^{iii}	0.97 (4)	2.49 (5)	3.361 (5)	149 (5)

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