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n-Decyltrimethylammonium bromide

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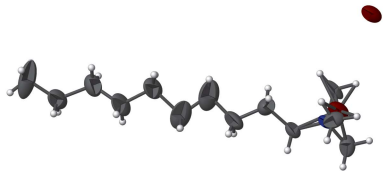
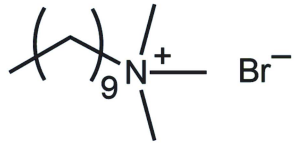
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{13}H_{30}N^{+}\cdot Br^{-}$ (systematic name: *N*,*N*,*N*-trimethyl-1-decanaminium bromide), forms crystals having a bilayer structure, comprised of layers of trimethylammonium cations and bromide anions separated by the inter-digitated *n*-decyl groups of the cation; close ammonium-methyl-C—H···Br contacts connect the ions. The *n*-decyl chain adopts a slightly distorted all-*trans* conformation. The *n*-decyl chain exhibits positional disorder with all atoms at half occupancy. The sample was a racemic twin.

3D view



Chemical scheme



Structure description

One component of the statistically disordered *n*-decyl chain in the cation along with the bromide counter-ion are shown in Fig. 1. The cation comprises an *n*-decyl chain bound to a trimethyl ammonium group at one end (cation). The bromide counter-ion is in close proximity to the cation. The ionic aggregate spans much of the *c* axis of the unit cell. In the crystal, Fig. 2, a bilayer structure comprised of layers of trimethylamino groups packed closely with bromide anions separated by the interdigitated 'all-*trans*' *n*-decyl chains of the cations; the maximum deviation from the ideal 180° torsion angle is −162 (2)° for C7—C8—C9—C10. Close ammonium-methyl-C—H···Br links connect the ions, Table 1. The packing motif is similar to those of longer *n*-alkyltetramethyl-ammonium bromides summarized in Alonso *et al.* (2009).

Synthesis and crystallization

The sample (>99% purity) was obtained from TCI, and needle-shaped colourless crystals were grown by slow evaporation of its ethyl acetate solution.

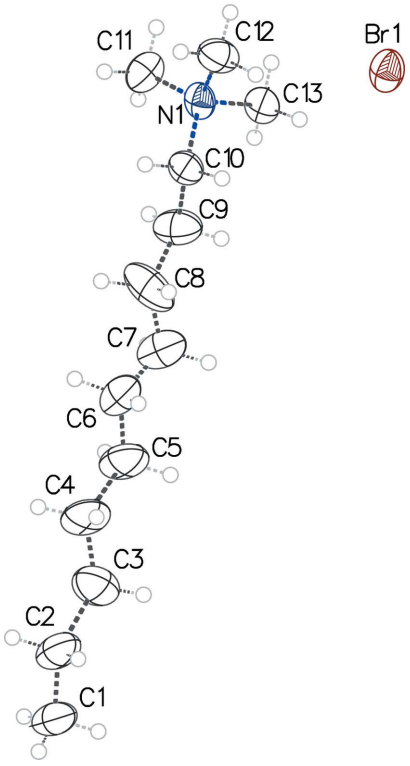


Figure 1
The asymmetric unit of the title salt, $[C_{13}H_{30}N]Br$, showing one conformation of the statistically disordered *n*-decyl chain. The displacement ellipsoids are drawn at the 50% probability level.

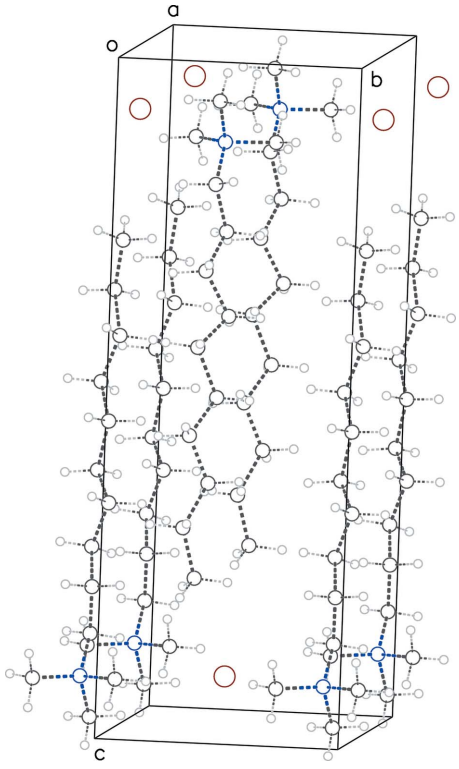


Figure 2
Schematic packing diagram showing one orientation of the statistically disordered *n*-decyl chains only. The alternating hydrophobic and hydrophilic regions of the structure are clearly evident.

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···Br1^{i}	0.96	2.89	3.82 (2)	162

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{30}N^{+}\cdot Br^{-}$
M_r	280.28
Crystal system, space group	Monoclinic, *C*2
Temperature (K)	298
a, *b*, *c* (Å)	5.6390 (9), 7.2545 (12), 19.586 (3)
β (°)	98.186 (3)
V (Å^3)	793.1 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.57
Crystal size (mm)	0.28 × 0.08 × 0.01
Data collection	
Diffractometer	Bruker *SMART* CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.097, 0.9
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3515, 1803, 1477
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.143, 1.07
No. of reflections	1803
No. of parameters	139
No. of restraints	118
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.36
Absolute structure	Flack (1983)
Absolute structure parameter	0.0 (3)

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Positional disorder in the *n*-decyl chain was resolved over two positions of equal occupancy. Further, an inversion matrix was used to address racemic twinning; the major fraction = 0.57 (4).

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190933 [https://doi.org/10.1107/S2414314619009337]

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N,*N*,*N*-Trimethyl-1-decanaminium

Crystal data

$C_{13}H_{30}N^+\cdot Br^-$
M_r = 280.28
Monoclinic, *C*2
a = 5.6390 (9) Å
b = 7.2545 (12) Å
c = 19.586 (3) Å
β = 98.186 (3)°
V = 793.1 (2) Å^3
Z = 2
F(000) = 300
D_x = 1.174 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1233 reflections
θ = 2.8–27.3°
μ = 2.57 mm^{-1}
T = 298 K
Needle, colorless
0.28 × 0.08 × 0.01 mm

Data collection

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.34 pixels mm^{-1}
phi and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.097, T_{max} = 0.9
3515 measured reflections
1803 independent reflections
1477 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −7→6
k = −9→9
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.143
S = 1.07
1803 reflections
139 parameters
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2 + 0.1533P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (4)
Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Absolute structure parameter: 0.0 (3)

Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 4 sets of ω scans each set at different φ and/or 2θ angles and each scan (30 s exposure) covering -0.300° degrees in ω. The crystal to detector distance was 5.82 cm.

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.
The H atoms were placed geometrically and allowed to ride on their parent C atoms during refinement, with C—H distances of 0.97 Å (methylene) and 0.96 Å (methyl), and with $U_{iso}(H) = 1.2U_{eq}$(methylene-C) or $1.5U_{eq}$(methyl-C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	1.41220 (13)	1.006 (3)	0.09518 (3)	0.0629 (3)	0.50
N1	0.7948 (10)	0.495 (4)	0.1062 (2)	0.0455 (13)	0.50
C1	0.387 (4)	0.520 (5)	0.7267 (6)	0.143 (8)	0.50
H1A	0.4299	0.6480	0.7331	0.215*	0.50
H1B	0.5192	0.4448	0.7462	0.215*	0.50
H1C	0.2504	0.4944	0.7492	0.215*	0.50
C2	0.327 (3)	0.480 (5)	0.6504 (10)	0.080 (6)	0.50
H2A	0.1676	0.5291	0.6365	0.096*	0.50
H2B	0.3123	0.3468	0.6467	0.096*	0.50
C3	0.483 (3)	0.542 (5)	0.5916 (7)	0.086 (5)	0.50
H3A	0.4618	0.6743	0.5864	0.103*	0.50
H3B	0.6497	0.5228	0.6107	0.103*	0.50
C4	0.454 (3)	0.465 (4)	0.5214 (9)	0.085 (5)	0.50
H4A	0.2888	0.4852	0.5008	0.102*	0.50
H4B	0.4775	0.3329	0.5253	0.102*	0.50
C5	0.613 (3)	0.537 (4)	0.4721 (8)	0.084 (6)	0.50
H5A	0.7733	0.4887	0.4844	0.100*	0.50
H5B	0.6204	0.6704	0.4749	0.100*	0.50
C6	0.508 (5)	0.475 (4)	0.3944 (9)	0.106 (6)	0.50
H6A	0.5093	0.3421	0.3893	0.127*	0.50
H6B	0.3456	0.5201	0.3810	0.127*	0.50
C7	0.672 (5)	0.562 (5)	0.3553 (12)	0.121 (7)	0.50
H7A	0.8368	0.5285	0.3720	0.145*	0.50
H7B	0.6559	0.6949	0.3551	0.145*	0.50
C8	0.5880	0.4800	0.2860	0.092 (6)	0.50
H8A	0.5758	0.3473	0.2905	0.110*	0.50
H8B	0.4296	0.5271	0.2691	0.110*	0.50
C9	0.7516 (13)	0.523 (5)	0.2354 (3)	0.074 (4)	0.50
H9A	0.8917	0.4443	0.2445	0.089*	0.50
H9B	0.8049	0.6497	0.2419	0.089*	0.50
C10	0.6380 (8)	0.497 (5)	0.1611 (3)	0.0502 (13)	0.50

H10A	0.5508	0.3813	0.1583	0.060*	0.50
H10B	0.5208	0.5942	0.1501	0.060*	0.50
C11	0.9609 (19)	0.338 (4)	0.1088 (6)	0.058 (3)	0.50
H11A	1.0753	0.3453	0.1500	0.087*	0.50
H11B	1.0434	0.3412	0.0691	0.087*	0.50
H11C	0.8723	0.2250	0.1088	0.087*	0.50
C12	0.6316 (10)	0.504 (5)	0.0383 (2)	0.0638 (14)	0.50
H12A	0.5330	0.3956	0.0330	0.096*	0.50
H12B	0.7261	0.5106	0.0013	0.096*	0.50
H12C	0.5316	0.6114	0.0374	0.096*	0.50
C13	0.941 (2)	0.672 (4)	0.1112 (8)	0.061 (3)	0.50
H13A	0.8347	0.7760	0.1044	0.091*	0.50
H13B	1.0444	0.6718	0.0763	0.091*	0.50
H13C	1.0352	0.6797	0.1559	0.091*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0516 (4)	0.0489 (4)	0.0914 (5)	−0.0035 (9)	0.0210 (3)	0.0014 (10)
N1	0.0364 (18)	0.041 (3)	0.060 (2)	−0.011 (5)	0.0113 (17)	0.003 (5)
C1	0.29 (2)	0.089 (12)	0.065 (4)	0.070 (18)	0.062 (8)	0.000 (9)
C2	0.083 (6)	0.072 (15)	0.096 (8)	−0.014 (8)	0.048 (6)	−0.029 (8)
C3	0.087 (6)	0.099 (14)	0.079 (6)	−0.007 (7)	0.036 (6)	0.004 (7)
C4	0.070 (8)	0.095 (12)	0.104 (6)	0.004 (6)	0.057 (5)	−0.018 (6)
C5	0.075 (8)	0.094 (17)	0.093 (5)	−0.007 (7)	0.048 (5)	−0.025 (7)
C6	0.181 (13)	0.061 (15)	0.080 (6)	0.016 (9)	0.029 (7)	−0.015 (7)
C7	0.193 (19)	0.092 (12)	0.086 (7)	0.027 (10)	0.048 (10)	−0.018 (8)
C8	0.070 (4)	0.127 (15)	0.079 (6)	−0.042 (9)	0.014 (4)	0.031 (8)
C9	0.070 (3)	0.097 (10)	0.056 (3)	−0.017 (7)	0.012 (3)	−0.018 (7)
C10	0.044 (2)	0.053 (3)	0.057 (2)	−0.007 (6)	0.0199 (17)	0.003 (6)
C11	0.048 (5)	0.056 (5)	0.065 (5)	0.011 (4)	−0.009 (4)	−0.009 (4)
C12	0.061 (3)	0.081 (4)	0.052 (2)	0.024 (6)	0.015 (2)	0.011 (7)
C13	0.049 (5)	0.052 (4)	0.093 (7)	−0.007 (4)	0.048 (4)	0.003 (5)

Geometric parameters (Å, º)

N1—C10	1.485 (8)	C6—C7	1.43 (3)
N1—C11	1.473 (18)	C7—H7A	0.9700
N1—C12	1.507 (7)	C7—H7B	0.9700
N1—C13	1.518 (18)	C7—C8	1.50 (2)
C1—H1A	0.9600	C8—H8A	0.9700
C1—H1B	0.9600	C8—H8B	0.9700
C1—H1C	0.9600	C8—C9	1.479 (10)
C1—C2	1.51 (2)	C9—H9A	0.9700
C2—H2A	0.9700	C9—H9B	0.9700
C2—H2B	0.9700	C9—C10	1.518 (9)
C2—C3	1.61 (2)	C10—H10A	0.9700
C3—H3A	0.9700	C10—H10B	0.9700

C3—H3B	0.9700	C11—H11A	0.9600
C3—C4	1.47 (2)	C11—H11B	0.9600
C4—H4A	0.9700	C11—H11C	0.9600
C4—H4B	0.9700	C12—H12A	0.9600
C4—C5	1.500 (14)	C12—H12B	0.9600
C5—H5A	0.9700	C12—H12C	0.9600
C5—H5B	0.9700	C13—H13A	0.9600
C5—C6	1.62 (2)	C13—H13B	0.9600
C6—H6A	0.9700	C13—H13C	0.9600
C6—H6B	0.9700		

C10—N1—C12	106.6 (4)	C5—C6—H6A	111.4
C10—N1—C13	108.7 (12)	C5—C6—H6B	111.4
C11—N1—C10	115.0 (13)	H6A—C6—H6B	109.3
C11—N1—C12	111.5 (11)	C7—C6—C5	101.7 (19)
C11—N1—C13	108.4 (5)	C7—C6—H6A	111.4
C12—N1—C13	106.2 (12)	C7—C6—H6B	111.4
C1—C2—H2A	105.9	C6—C7—H7A	111.9
C1—C2—H2B	105.9	C6—C7—H7B	111.9
C1—C2—C3	125.7 (17)	C6—C7—C8	99.5 (18)
H2A—C2—H2B	106.2	H7A—C7—H7B	109.6
C3—C2—H2A	105.9	C8—C7—H7A	111.9
C3—C2—H2B	105.9	C8—C7—H7B	111.9
C2—C3—H3A	106.3	C7—C8—H8A	109.2
C2—C3—H3B	106.3	C7—C8—H8B	109.2
H3A—C3—H3B	106.4	H8A—C8—H8B	107.9
C4—C3—C2	124.1 (16)	C9—C8—C7	112.1 (14)
C4—C3—H3A	106.3	C9—C8—H8A	109.2
C4—C3—H3B	106.3	C9—C8—H8B	109.2
C3—C4—H4A	107.8	C8—C9—H9A	108.9
C3—C4—H4B	107.8	C8—C9—H9B	108.9
C3—C4—C5	118.1 (13)	C8—C9—C10	113.5 (7)
H4A—C4—H4B	107.1	H9A—C9—H9B	107.7
C5—C4—H4A	107.8	C10—C9—H9A	108.9
C5—C4—H4B	107.8	C10—C9—H9B	108.9
C4—C5—H5A	109.7	N1—C10—C9	118.8 (5)
C4—C5—H5B	109.7	N1—C10—H10A	107.6
C4—C5—C6	109.7 (12)	N1—C10—H10B	107.6
H5A—C5—H5B	108.2	C9—C10—H10A	107.6
C6—C5—H5A	109.7	C9—C10—H10B	107.6
C6—C5—H5B	109.7	H10A—C10—H10B	107.0

C1—C2—C3—C4	165 (2)	C7—C8—C9—C10	−162 (2)
C2—C3—C4—C5	−180.0 (19)	C8—C9—C10—N1	−167 (2)
C3—C4—C5—C6	−166 (2)	C11—N1—C10—C9	66 (2)
C4—C5—C6—C7	177.3 (18)	C12—N1—C10—C9	−169.5 (18)
C5—C6—C7—C8	172.7 (15)	C13—N1—C10—C9	−55 (2)
C6—C7—C8—C9	−171 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···Br1^{i}	0.96	2.89	3.82 (2)	162

Symmetry code: (i) *x*−1, *y*, *z*.