C(10) and the alkyl chain at C(8) are equatorial in ring *B* while the chain at C(9) is axial. Presumably, such a conformation avoids strong 1,3-diaxial interactions between the methoxycarbonyl group and the C(8)—C(9) region of ring *B*. This conformation corresponds to one epimer in the (1:1) mixture after equilibration and this molecular structure was used to determine the second epimeric structure. Total conformational energies of possible structures for C(8) epimers have been calculated using the *MAXIMIN* program of the *SYBYL* molecular modeling system (Tripos Associates, 1988). The structure CCC-8*R** observed for the crystal structure corresponds to the global minimum for this structure ($-26{\cdot}4$ kJ mol^{-1}). Another possible isomer was CBC-8*S* obtained by modification of the conformation of ring *B* (chair→boat) and inversion of carbon C(8). The corresponding energy was much higher ($-2{\cdot}9$ kJ mol^{-1}) due to torsional contributions at the C(10)—C(9) bond. The CCC-8*S* epimer (2) structure was obtained by inversion of the C(8) center, reorganization of the rings and energy minimization. The inversion at C(8) induces extensive reorganization involving rings *A* and *B* in order to reach an all-chair conformation with conformational energy of $-23{\cdot}9$ kJ mol^{-1}. Similar values of conformational energies obtained for the crystalline structure of (1) (Fig. 2) and the computer-generated structure of (2) (Fig.3) account for the 1:1 equilibration.

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* CCC-8*R* is the abbreviation of chair (ring *A*), chair (ring *B*), chair (ring *C*) with the C(8) in the *R* configuration. The meaning of further similar abbreviations can be easily deduced.

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Structure of Butyldodecyldimethylammonium Bromide Monohydrate

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Abstract. $C_{18}H_{40}N^+.Br^-.H_2O$, $M_r = 368{\cdot}4$, triclinic, $P\bar{1}$, $a = 8{\cdot}164\,(1)$, $b = 8{\cdot}486\,(2)$, $c = 17{\cdot}531\,(1)$ Å, $\alpha = 74{\cdot}72\,(1)$, $\beta = 86{\cdot}28\,(1)$, $\gamma = 71{\cdot}57\,(1)°$, $V = 1111{\cdot}3\,(1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}10$ Mg m^{-3}, λ(Cu $K\alpha$) $= 1{\cdot}54178$ Å, $\mu = 2{\cdot}5$ mm^{-1}, $F(000) = 400$, $T = 295$ K, $R = 0{\cdot}061$ for 2695 reflections. The molecules are packed in bilayers parallel to the (001) plane. The Br ions and water molecules form an anionic group. The Br···O hydrogen-bond distances are 3·410 (1) and 3·414 (1) Å.

Introduction. The structure of the title crystal was determined as part of our continuing studies on the crystal properties and molecular packing of alkylammonium halides with various alkyl chain lengths. The molecule has a butyl group as the secondary long hydrocarbon chain which is different from that of the dodecyldimethylpropylammonium bromides studied so far (Taga, Machida, Kimura, Hayashi, Umemura & Takenaka, 1986, 1987). Thus the crystal structure allows a comparison of the effects of the different chain lengths on the molecular packing in these crystal structures.

Experimental. Crystals grown from ethyl acetate solution; colorless prism; 0·2 × 0·2 × 0·15 mm; Rigaku AFC-5RU diffractometer with graphite-monochromated Cu $K\alpha$ radiation; lattice parameters from 22 reflections with $18{\cdot}8 < \theta < 27{\cdot}2°$; 3677 reflections measured within $2\theta < 120°$; $-9 \le h \le 0$,

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Table 1. *Atomic parameters and equivalent isotropic thermal parameters for non*-H *atoms in butyldodecyldimethylammonium bromide monohydrate*

$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
Br(1)	0·6853 (1)	0·2951 (1)	0·3985 (1)	7·64 (3)
C(1)	0·1783 (7)	0·2238 (6)	0·3016 (3)	6·2 (4)
C(2)	0·2596 (7)	0·3656 (6)	0·2909 (3)	6·4 (4)
C(3)	0·2152 (7)	0·4897 (6)	0·2104 (3)	6·4 (4)
C(4)	0·2736 (8)	0·6460 (7)	0·2015 (3)	7·0 (4)
C(5)	0·2275 (8)	0·7770 (7)	0·1212 (3)	7·5 (4)
C(6)	0·2761 (8)	0·9370 (8)	0·1125 (3)	7·5 (5)
C(7)	0·2262 (9)	1·0676 (8)	0·0335 (3)	7·8 (5)
C(8)	0·2709 (9)	1·2297 (8)	0·0231 (3)	7·7 (5)
C(9)	0·2227 (9)	1·3568 (8)	−0·0549 (3)	7·7 (5)
C(10)	0·2671 (8)	1·5204 (8)	−0·0676 (4)	7·9 (5)
C(11)	0·2109 (10)	1·6461 (9)	−0·1461 (4)	9·2 (6)
C(12)	0·2584 (13)	1·8054 (10)	−0·1606 (5)	11·3 (8)
C(13)	0·4161 (7)	−0·0092 (6)	0·3899 (3)	5·9 (4)
C(14)	0·5021 (8)	−0·0967 (7)	0·3270 (3)	7·1 (4)
C(15)	0·6911 (9)	−0·1819 (8)	0·3449 (4)	8·7 (5)
C(16)	0·7873 (11)	−0·2722 (9)	0·2849 (5)	10·7 (7)
C(17)	0·1273 (8)	−0·0381 (8)	0·3801 (4)	7·4 (5)
C(18)	0·1695 (8)	0·1623 (8)	0·4473 (3)	7·2 (5)
N(1)	0·2257 (5)	0·0860 (5)	0·3780 (2)	5·9 (3)
O(1)	0·2910 (9)	0·5260 (8)	0·4511 (4)	14·1 (7)

Table 2. *Bond lengths* (Å) *and valence angles* (°) *in butyldodecyldimethylammonium bromide monohydrate*

C(1)—C(2)	1·514 (9)	C(1)—N(1)	1·506 (5)
C(2)—C(3)	1·508 (6)	C(3)—C(4)	1·514 (9)
C(4)—C(5)	1·529 (7)	C(5)—C(6)	1·499 (10)
C(6)—C(7)	1·514 (7)	C(7)—C(8)	1·495 (11)
C(8)—C(9)	1·487 (7)	C(9)—C(10)	1·501 (11)
C(10)—C(11)	1·497 (8)	C(11)—C(12)	1·476 (13)
C(13)—C(14)	1·504 (8)	C(13)—N(1)	1·507 (6)
C(14)—C(15)	1·497 (9)	C(15)—C(16)	1·499 (11)
C(17)—N(1)	1·505 (9)	C(18)—N(1)	1·503 (7)
C(2)—C(1)—N(1)	115·0 (5)	C(1)—C(2)—C(3)	111·0 (5)
C(2)—C(3)—C(4)	112·5 (5)	C(3)—C(4)—C(5)	114·1 (5)
C(4)—C(5)—C(6)	115·1 (5)	C(5)—C(6)—C(7)	114·7 (6)
C(6)—C(7)—C(8)	116·1 (6)	C(7)—C(8)—C(9)	115·8 (6)
C(8)—C(9)—C(10)	117·2 (6)	C(9)—C(10)—C(11)	115·0 (7)
C(10)—C(11)—C(12)	115·7 (7)	C(14)—C(13)—N(1)	116·4 (5)
C(13)—C(14)—C(15)	110·9 (5)	C(14)—C(15)—C(16)	114·5 (6)
C(1)—N(1)—C(13)	114·6 (4)	C(1)—N(1)—C(17)	107·6 (4)
C(1)—N(1)—C(18)	110·3 (4)	C(13)—N(1)—C(17)	110·0 (4)
C(13)—N(1)—C(18)	106·8 (4)	C(17)—N(1)—C(18)	107·4 (5)

$-9 \leq k \leq 9$, $-18 \leq l \leq 18$; no significant change in intensity for three standard reflections measured every 56 reflections; no absorption correction; 2695 unique reflections with $F_o > 3\sigma(F_o)$ used; structure solved by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); refined by full-matrix least squares; $\sum w(|F_o| - |F_c|)^2$ minimized; $w = [\sigma(F) + (0{\cdot}023F)^2]^{-1}$; non-H atoms anisotropic; H atoms from difference map, isotropic; $R = 0{\cdot}061$, $wR = 0{\cdot}083$, $S = 2{\cdot}11$; $(\Delta/\sigma)_{\max} = 0{\cdot}25$, $\Delta\rho_{\max} = 0{\cdot}52$ e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); all computations performed on a FACOM M382 in the Data Processing Center of Kyoto University using *KPPXRAY* programs (Taga, Higashi & Iizuka, 1985).

Discussion. The final atomic parameters are listed in Table 1.* A perspective view of the molecule with atomic numbering is illustrated in Fig. 1. Bond distances and angles are listed in Table 2. The average C—C and C—N distances are 1·501 and 1·504 Å, respectively, and the average C—C—C bond angle is 114·8°. The dodecyl and butyl chains have an extended *trans*-zigzag form. The torsion angle of 172·4 (4)° for C(1)—C(2)—C(3)—C(4) is the largest deviation from the ideal value.

The crystal structure veiwed along the *a* axis is illustrated in Fig. 2. The molecules are packed in bilayers parallel to the (001) crystal plane. The molecular packing resembles that of dodecyldimethylpropylammonium bromide monohydrate (Taga, Machida, Kimura, Hayashi, Umemura & Takenaka, 1986). Comparable unit-cell dimensions

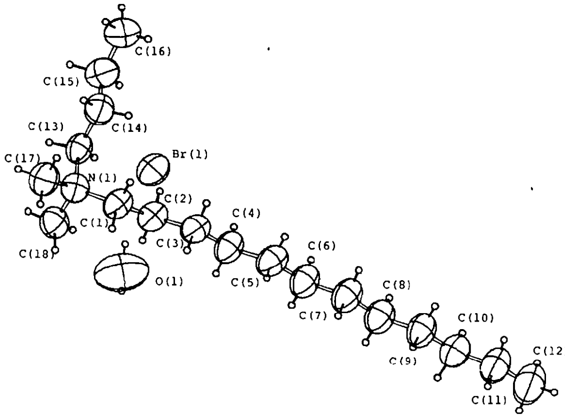

Fig. 1. Perspective drawing of the molecule.

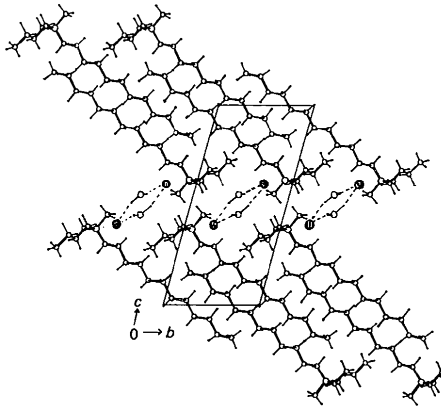

Fig. 2. Packing diagram projected along the *a* axis.

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* Lists of atomic parameters for H atoms, anisotropic thermal parameters for non-H atoms and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52270 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

of the propyl derivative are $a' = 8\cdot502$, $b' = 8\cdot234$, $c' = 17\cdot494$ Å, $\alpha' = 78\cdot41$, $\beta' = 84\cdot96$ and $\gamma' = 61\cdot24°$, which were obtained by exchanging the axes $a \rightarrow -b'$, $b \rightarrow -a'$, $c \rightarrow -c'$. The $a \times b$ dimension for the butyl derivative (65·7 Å^2) is larger than the 61·4 Å^2 found for the propyl derivative, while the (001) interplanar distance (16·9 Å) is slightly smaller than the 17·1 Å found for the propyl derivative. Thus, exchange of the propyl group by the butyl group causes the tilt of the dodecyl chain from the (001) plane to change from 52 to 53°. This small change reflects a similar packing form of dodecyl chains; a triclinic subcell assuming the a_s axis parallel to the long-chain axis has similar dimensions $a_s = 2\cdot54\,(1)$, $b_s = 4\cdot35\,(4)$, $c_s = 4\cdot90\,(4)$ Å, $\alpha_s = 66\cdot5\,(6)$, $\beta_s = 88\cdot2\,(4)$ and $\gamma_s = 77\cdot4\,(4)°$. The short intermolecular C···C contacts are 3·888 (1) Å for C(17)···C(18) and 3·899 (1) Å for C(12)···C(16).

The Br ions and water molecules form an isolated anionic group in a square shape. The Br···O hydrogen-bond distances are 3·410 (1) and 3·414 (1) Å, and the Br···O···Br and O···Br···O angles are 112·9 (3) and 67·1 (2)°. In comparison with the propyl derivative, the Br···O distances are long and the Br···O···Br angle is open. The anionic group is surrounded by cationic ammonium groups with shortest O···N distance 4·443 (1) Å and Br···N distances 4·233 (1) Å.

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Structure of 1,4-Cubanediyldiammonium Bis(trinitromethanide)*

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Abstract. $C_8H_{12}N_2^+.2CN_3O_6^-$, $M_r = 436\cdot27$, monoclinic, $C2/m$, $a = 14\cdot298\,(2)$, $b = 8\cdot408\,(1)$, $c = 7\cdot354\,(2)$ Å, $\beta = 103\cdot42\,(2)°$, $V = 859\cdot9\,(5)$ Å^3, $Z = 2$, $D_x = 1\cdot68$ g cm^{-3}, $\lambda(\mathrm{Mo}\,K\alpha) = 0\cdot71069$ Å (graphite monochromator), $\mu = 1\cdot66$ cm^{-1}, $F(000) = 448$, $T = 293$ K, final $R = 0\cdot039$ for 672 reflections with $I \geq 3\sigma(I)$. The cubanediyldiammonium cation and trinitromethanide anion have $2/m$ and m crystallographic symmetries, respectively. The cation is linked to six trinitromethanide anions, three at each end, by a total of 12 N—H···O hydrogen bonds through the six cation H atoms. The cubane cage has a local threefold axis of symmetry along the long axis (N1···N1) of the cation and undergoes a large librational motion, 17° r.m.s. amplitude, about this axis.

Introduction. There is a continued interest in the synthesis and chemistry of cubane derivatives because of the potential of cubane as a molecular template for the formation of high-density energetic materials (Alster & Iyer, 1983–1988). In the case of octanitrocubane, various estimates of the crystal density have been in the 1·99–2·10 g cm^{-3} range. The crystal structures of several nitrocubanes are known at this time; only that of 1,4-dinitrocubane has been published (Eaton, Ravi Shanka, Price, Pluth, Gilbert, Alster & Sandus, 1984; Umrigar, Vaz, Kirschenheuter, Griffin, Majeste, Klein, Stevens, Gilbert, Alster, Sandus & Legendre, 1988). The

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* Cubane is pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane.

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