*Xtal*2.6 *DIFDAT* (Hall & Stewart, 1989). Structure solution: *SHELXS*86 (Sheldrick, 1985). Structure refinement: *Xtal*2.6 *CRYLSQ*. Molecular graphics: *Xtal*2.6. Preparation of material for publication: *Xtal*2.6 *BONDLA*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the IUCr (Reference: BK1104). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.

Hall, S. R. & Stewart, J. M. (1989). Editors. *Xtal*2.6 *Users Manual*. Univs. of Western Australia, Australia, and Maryland, USA.

Le Page, Y. (1982). *J. Appl. Cryst.* **15**, 255–259.

Le Page, Y. (1987). *J. Appl. Cryst.* **20**, 264–269.

Matkovics, B., Tarodi, B. & Belaspira, L. (1974). *Acta Chim. (Budapest)*, **80**, 79–87.

Sheldrick, G. M. (1985). *SHELX*86. *Program for the Solution of Crystal Structures*. Univ. of Göttingen, Germany.

Acta Cryst. (1995). **C51**, 1940–1941

1-Dodecylpyridinium Chloride Monohydrate

KULTHIDA VONGBUPNIMIT, KEIICHI NOGUCHI AND KENJI OKUYAMA

Faculty of Technology, Tokyo University of Agriculture and Technology, 2-24-16 Naka-cho, Koganei-shi, Tokyo 184, Japan

(*Received* 2 *February* 1995; *accepted* 29 *March* 1995)

Abstract

The molecular and crystal structure of 1-dodecylpyridinium chloride monohydrate, $C_{17}H_{30}N^+.Cl^-.H_2O$, has been determined. It was found that the hydrocarbon chains are arranged in a parallel fashion and that they interlink in a bimolecular layer. The conformation of the hydrocarbon chain is almost completely *trans*-planar with a mean deviation from the plane of 0.005 Å. The pyridine ring also has a mean deviation of 0.005 Å. The angle between the planes of the hydrocarbon chain and the pyridine ring is 79.16°.

Comment

Structural knowledge of molecular aggregation is important for the understanding of chemical and physical properties, as well as other related phenomena. 1-Dodecylpyridinium chloride, (I), is a cationic amphiphilic molecule which possesses a non-polar hydrocarbon chain ending with a methyl group, nitrogen as the element capable of forming an 'onium' structure, and chloride as the counterion. It has a critical micelle concentration (CMC) of 1.5×10^{-2} mol dm^{-3} at 298 K. Furthermore, it can form thin films by solvent evaporation. The present work was aimed at elucidating the molecular aggregation of this compound in the crystalline phase.

(I)

The observed density suggested the presence of one water molecule for each 1-dodecylpyridinium chloride molecule. The molecular structure exhibits normal geometry. The average C—C bond length found in the hydrocarbon chain is 1.529 (7) Å and the average C—C—C bond angle is 111.9 (12)°. These values are close to those found in other long-chain structures, *e.g.* 1.523 (6) Å and 113.8 (3)° for *n*-dodecylammonium bromide (Lundén, 1974), and 1.523 (8) Å and 113.2 (5)° for hexadecyltrimethylammonium bromide (Campanelli & Scaramuzza, 1986).

The torsion angles in the hydrocarbon chain show that the largest deviation from the *trans*-conformation is 179.0 (4)° for N—C6—C7—C8. The molecular packing is governed by coulombic and van der Waals inter-

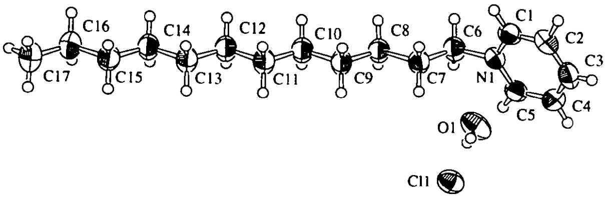

Fig. 1. The molecular structure of 1-dodecylpyridinium chloride monohydrate with the atomic numbering scheme and non-H atoms represented by 50% probability ellipsoids.

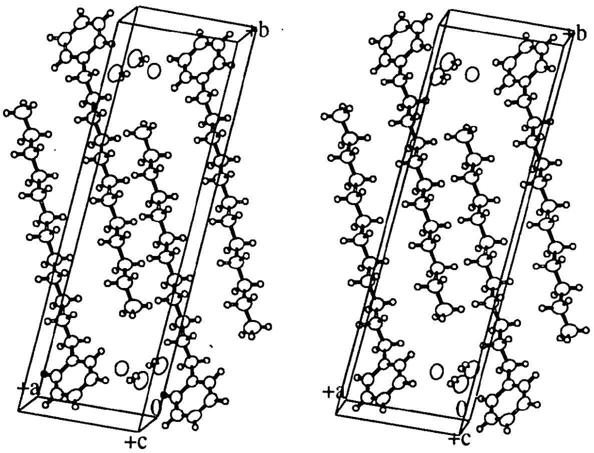

Fig. 2. Stereoview of the crystal structure of the title compound.

Acta Crystallographica Section C
ISSN 0108-2701 ©1995

actions, which cause the formation of bilayers. Hydrocarbon chains are arranged in a parallel fashion and interlink within the bimolecular layer.

Experimental

The title compound was obtained from Tokyo Kasei Organic Chemicals (D-0995) and recrystallized as colorless platelets by slow evaporation from an ethyl acetate/acetone solution. The density D_m was measured by flotation in a toluene–carbon tetrachloride mixture.

Crystal data

$C_{17}H_{30}N^+.Cl^-.H_2O$
$M_r = 301.90$
Triclinic
$P\bar{1}$
$a = 7.6582\ (5)$ Å
$b = 23.765\ (3)$ Å
$c = 5.2255\ (3)$ Å
$\alpha = 95.680\ (7)^\circ$
$\beta = 99.073\ (5)^\circ$
$\gamma = 96.759\ (7)^\circ$
$V = 925.9\ (1)$ Å^3
$Z = 2$
$D_x = 1.083$ Mg m^{-3}
$D_m = 1.08$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 17 reflections
$\theta = 38.9–40.0^\circ$
$\mu = 1.786$ mm^{-1}
$T = 23.0$ K
Platelet
0.70 × 0.50 × 0.10 mm
Colorless

Data collection

Rigaku AFC-5*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.519$, $T_{\max} = 1.000$
2987 measured reflections
2750 independent reflections

2501 observed reflections $[F_o > 3\sigma(F_o)]$
$R_{\rm int} = 0.024$
$\theta_{\max} = 60.05^\circ$
$h = 0 \rightarrow 8$
$k = -26 \rightarrow 26$
$l = -5 \rightarrow 5$
3 standard reflections monitored every 100 reflections intensity decay: 0.46%

Refinement

Refinement on *F*
$R = 0.063$
$wR = 0.073$
$S = 9.330$
2501 reflections
309 parameters
H atoms were refined isotropically

$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{\max} = 0.350$
$\Delta\rho_{\max} = 0.278$ e Å^{-3}
$\Delta\rho_{\min} = -0.377$ e Å^{-3}
Atomic scattering factors from Cromer & Waber (1974)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Cl1	0.3313 (1)	0.12522 (5)	0.4455 (2)	0.0685 (4)
O1	0.0960 (4)	0.1230 (2)	−0.1118 (8)	0.0825 (13)
N1	−0.2365 (4)	0.1147 (1)	0.2538 (6)	0.0510 (9)
C1	−0.3488 (5)	0.1084 (2)	0.0232 (8)	0.0584 (13)
C2	−0.3728 (5)	0.0592 (2)	−0.1424 (9)	0.0640 (13)
C3	−0.2827 (6)	0.0150 (2)	−0.0674 (10)	0.0675 (13)
C4	−0.1704 (6)	0.0214 (2)	0.1648 (10)	0.0667 (13)
C5	−0.1465 (5)	0.0721 (2)	0.3254 (9)	0.0593 (13)
C6	−0.2107 (6)	0.1694 (2)	0.4300 (9)	0.0609 (13)
C7	−0.0869 (6)	0.2150 (2)	0.3415 (9)	0.0596 (13)
C8	−0.0698 (6)	0.2700 (2)	0.5288 (9)	0.0623 (13)
C9	0.0525 (6)	0.3191 (2)	0.4577 (9)	0.0654 (13)
C10	0.0642 (6)	0.3734 (2)	0.6487 (10)	0.0666 (13)
C11	0.1863 (6)	0.4238 (2)	0.5840 (9)	0.0672 (13)
C12	0.1944 (6)	0.4773 (2)	0.7784 (9)	0.0675 (13)
C13	0.3161 (6)	0.5280 (2)	0.7164 (9)	0.0670 (13)
C14	0.3238 (6)	0.5814 (2)	0.9124 (10)	0.0684 (13)
C15	0.4454 (6)	0.6324 (2)	0.8536 (10)	0.0676 (13)
C16	0.4532 (7)	0.6855 (2)	1.049 (1)	0.0787 (13)
C17	0.5770 (9)	0.7365 (2)	0.992 (2)	0.097 (3)

Table 2. *Selected geometric parameters* (Å, °)

N1—C1	1.349 (5)	C8—C9	1.522 (6)
N1—C5	1.342 (5)	C9—C10	1.535 (6)
N1—C6	1.491 (5)	C10—C11	1.530 (6)
C1—C2	1.359 (6)	C11—C12	1.536 (6)
C2—C3	1.380 (6)	C12—C13	1.528 (6)
C3—C4	1.356 (6)	C13—C14	1.539 (6)
C4—C5	1.373 (6)	C14—C15	1.525 (6)
C6—C7	1.512 (5)	C15—C16	1.533 (6)
C7—C8	1.532 (5)	C16—C17	1.533 (7)
C1—N1—C5	120.4 (4)	C7—C8—C9	113.2 (3)
C1—N1—C6	120.1 (4)	C8—C9—C10	111.4 (4)
C5—N1—C6	119.5 (3)	C9—C10—C11	113.0 (4)
N1—C1—C2	121.2 (4)	C10—C11—C12	111.6 (4)
C1—C2—C3	118.5 (4)	C11—C12—C13	112.2 (4)
C2—C3—C4	120.0 (5)	C12—C13—C14	111.9 (4)
C3—C4—C5	120.0 (4)	C13—C14—C15	112.5 (4)
N1—C5—C4	119.8 (4)	C14—C15—C16	112.4 (4)
N1—C6—C7	111.8 (3)	C15—C16—C17	112.4 (5)
C6—C7—C8	108.7 (3)		

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Data reduction: *TEXSAN* (Molecular Structure Corporation, 1993). The structure was solved by direct methods using the *SIR*88 program (Burla *et al.*, 1989). Refinement was by full-matrix least squares using *ORFLS* (Busing, Martin & Levy, 1962). The figures were drawn with *ORTEP*II (Johnson, 1976). All calculations were performed using *TEXSAN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: AS1176). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Polidori, G., Spagna, R. & Viterbo, D. (1989). *J. Appl. Cryst.* **22**, 389–393.

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *ORFLS. Fortran Crystallographic Function and Error Program.* Report ORNL-TM-305. Oak Ridge National Laboratory, Tennessee, USA.

Campanelli, A. R. & Scaramuzza, L. (1986). *Acta Cryst.* C**42**, 1380–1383.

Cromer, D. T. & Waber, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Tables 2.2A, 2.3.1. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Lundén, B.-M. (1974). *Acta Cryst.* B**30**, 1756–1760.

Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Molecular Structure Corporation (1993). *TEXSAN. Single Crystal Structure Analysis Software.* Version 1.6. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.