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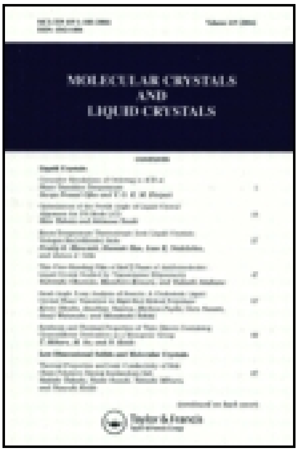

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X-Ray Crystal Structures and Directional Diamagnetic Susceptibility Calculations of Decyl and Dodecylammonium Chlorides

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X-Ray Crystal Structures and Directional Diamagnetic Susceptibility Calculations of Decyl and Dodecylammonium Chlorides

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The crystal and molecular structures of decylammonium chloride (DACl) and dodecylammonium chloride (DDACl) were determined. The crystal data for DACl is: $a = 5.700(3)$, $b = 7.173(1)$, $c = 15.507(2)$ Å, $\beta = 91.23(3)°$; monoclinic, space group $P2_1$ with two molecules in the unit cell and for DDACl is: $a = 5.676(3)$, $b = 7.186(2)$, $c = 17.770(4)$ Å, $\beta = 92.72(3)°$; monoclinic, space group $P2_1$ with two molecules in the unit cell. The structures were solved by direct methods and refined anisotropic (DACl) and isotropically (DDACl) to R-values of 0.083 and 0.091 for 975 and 337 observed reflections, respectively. Each NH_3^+ group in both structures is involved in hydrogen bonds and ionic bonds with three Cl^- ions, with mean distance of 3.144 Å.

The directional diamagnetic susceptibilities of the title compounds were calculated by the Flygare method using the structural data as determined. The values of $\bar{\chi}$ calculated by this method are shown to be in good agreement with those given by the Pascal method.

While it is not possible to make a direct comparison of the calculated directional susceptibility of the molecule and the measured directional susceptibility of the lyomesophase, it is possible to compare the calculated and the measured anisotropies. When reasonable assumptions are made as to the order and structure of the nematic mesophase, our calculated anisotropy for DACl is well within the range of the available experimental values.

Keywords: crystal structure, directional susceptibility, lyotropic systems, surfactants, diamagnetic anisotropy

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INTRODUCTION

Lyotropic liquid crystals are being studied by an ever increasing number of techniques. One possible path toward a better understanding of the lyotropic mesophases is to study the molecular properties of the surfactant that forms the mesophase. The determination of the crystal structures has proved helpful for the understanding of the anhydrous mesophases of the surfactants[1-7] and we believe can also be of value in understanding certain properties of the lyomesophases.

One of the most studied lyotropic systems is that which contains decylammonium chloride.[2,8-10] Some members of our group have recently completed a study of the anhydrous thermotropic liquid crystalline phases and a phase diagram study comparing the lyomesophases of octyl-, decyl-, and dodecylammonium chloride (OACl, DACl and DDACl).[2,10] As a complement to this work we decided to investigate crystal structures of these compounds. A further motive for determining these structures was our desire to apply the Flygare method for calculating the magnetic susceptibilities of the molecules used in the lyotropic nematic phase, and knowledge of the molecular structure is necessary for this calculation. Once the molecular susceptibilities are known one can hope to use this information to test models of the lyomesophases.

When a literature search was able to locate only a preliminary (projection) structure[11] determination of DDACl and nothing on the structure of OACl or DACl, the present study was undertaken. The structural study of OACl was abandoned due to the existence of a phase transition close to room temperature[2] which made the crystal structure unstable.

EXPERIMENTAL

The DACl and DDACl were produced by the addition of HCl to decylamine (or dodecylamine) and recrystallized as described in Reference 12. An Enraf-Nonius CAD-4 diffractometer was used to obtain the structural data. The crystal data and the data collection parameters for both DACl and DDACl are given in Table I. During data collection two standard reflections were monitored every 120 min. The LP correction was applied but the absorption was ignored. The systematic absences O k O, with k odd, indicated space group $P2_1$ for both compounds. The structures were solved by direct methods using MULTAN-80[13] and were refined using a full-matrix least-squares. For DACl the refinement was carried out using anisotropic thermal

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TABLE I

A. Crystal data for DACl and DDACl

Molecular formula	$C_{10}H_{24}N^+Cl^-$	$C_{12}H_{28}N^+Cl^-$
Molecular weight [g·mol^{-1}]	193.66	221.81
F(000)	216	248
Space group	$P2_1$	$P2_1$
a(Å)	5.700(3)	5.676(3)
b(Å)	7.173(1)	7.186(2)
c(Å)	15.507(2)	17.770(4)
β(°)	93.23(3)	92.72(3)
D_c(g·cm^{-3})	1.01	1.02
V(Å^3)	633.9(5)	723.9(8)

B. Data collection parameters and refinement results for DACl and DDACl

Crystal size (mm)	0.58 × 0.45 × 0.18	0.25 × 0.25 × 0.08
Radiation (graphite monochromatized)	MoKα (λ = 0.71073 Å)	
Range of measured hkl	−6/6, 0/8, 0/18	0/6, 0/7, −19/19
Scan widths and speeds (θ–2θ scan)	3-50°, 5-7°/min	3-46°, 5-7°/min
Absorption coefficient, μ(cm^{-1})	2.24	2.00
Number of measured reflection	1402	1100
Reflections with $I \geq 3\sigma(I)$	975	337
R	0.083	0.091
R_w	0.075	0.091
R_{all}	0.10	0.26
Parameters *k* and *g* in weighting scheme	1,000, 0.016724	5.0019, 0.000600
Maximum residuals on final difference-maps (e$^-$/Å^3)	0.62 and −0.49	0.26 and −0.21

factors, but the DDACl data would only allow the use of isotropic thermal factors. The reflection intensities for both compounds were quite weak, perhaps due to closeness of a phase transition (see Reference 2) which could provoke crystalline disorder. The position of the H atoms of the NH_3^+ group were located by difference Fourier, all other H atoms being included in their idealized positions (C—H = 1.0 Å) as fixed contributions. In their final cycle the shifts in all the parameters were less than their standard deviations. The calculations were carried out on a VAX computer with SHELX-76[14] and the scattering factors were taken from the International Tables of X-ray Crystallography.[15]

CRYSTAL STRUCTURE RESULTS AND DISCUSSION

The atomic coordinates and the equivalent isotropic temperature factors for the non-hydrogen atoms of both compounds are given in

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TABLE II

Final positional parameters and isotropic temperature factors for DACl and DDACl

Atom	x/a	y/b	z/c	B_{isoa}
Cl	0.2662(2)	0.0804[b]	0.0390(1)	4.68(4)
	0.743 (1)	0.1974[b]	0.0340(4)	4.6 (1)
N	0.7654(8)	0.020(1)	0.9565(3)	4.4 (2)
	0.233 (4)	0.262(3)	0.964 (1)	4.1 (6)
C(1)	0.785 (1)	0.090(2)	0.8670(3)	4.3 (2)
	0.194 (5)	0.203(9)	0.885 (1)	5.3 (6)
C(2)	0.578 (1)	0.030(1)	0.8119(4)	4.2 (2)
	0.393 (4)	0.251(5)	0.838 (1)	4.4 (8)
C(3)	0.601 (1)	0.101(2)	0.7182(4)	4.4 (2)
	0.359 (4)	0.178(7)	0.757 (1)	2.9 (6)
C(4)	0.395 (1)	0.033(1)	0.6611(4)	4.1 (2)
	0.548 (4)	0.246(5)	0.703 (1)	3.7 (7)
C(5)	0.4060(9)	0.101(2)	0.5674(3)	4.1 (2)
	0.512 (4)	0.176(7)	0.625 (1)	2.8 (6)
C(6)	0.201 (1)	0.034(1)	0.5114(4)	4.0 (2)
	0.708 (4)	0.241(5)	0.574 (1)	3.2 (7)
C(7)	0.2075(9)	0.101(2)	0.4193(4)	4.1 (2)
	0.677 (5)	0.183(8)	0.493 (1)	4.8 (7)
C(8)	0.004 (1)	0.033(1)	0.3628(4)	4.2 (2)
	0.872 (6)	0.250(6)	0.447 (2)	4.5 (7)
C(9)	0.005 (1)	0.109(2)	0.2709(4)	4.5 (2)
	0.862 (5)	0.172(9)	0.364 (1)	5.8 (9)
C(10)	−0.201 (1)	0.033(2)	0.2159(5)	6.7 (4)
	1.063 (6)	0.247(7)	0.321 (2)	7.0 (1)
C(11)	—	—	—	—
	1.048 (5)	0.171(7)	0.236 (1)	5.4 (8)
C(12)	—	—	—	—
	1.252 (5)	0.251(4)	0.191 (1)	4.4 (8)

[a] For DACl; $B_{iso} = \frac{4}{3} \Sigma_{ij} T_{ij} B_{ij}$ and $\sigma(B_{iso}) = T_{ij}\, \sigma(B_{ij})$.
[b] Not refined.

Table II. The bond distances and angles are given in Table III. Tables of the observed and calculated structure factors, the anisotropic thermal parameters (DACl only), the hydrogen atom coordinates and the hydrogen bonds are included in the Supplementary Material on file with the publisher. The stereoscopic projection of the molecular packing of DACl as calculated by the program ORTEP[16] is shown in Figure 1.

The average distance between alternate carbon atoms is 2.54 Å for both DACl and DDACl. This is about the same as observed in lauric acid,[17] but is less than that observed in strontium laurate (2.610 Å).[18]

The chain length, as measured from the nitrogen atom to the last carbon in the chain is 12.7 Å for DACl and 14.9 Å for DDACl. The angles between the chains and the normal to the planes containing

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TABLE III

Intramolecular bond distances (Å) and angles (°) for DACl and DDACl

N—C(1)	1.482(9) 1.48 (3)	N—C(1)—C(2)	111.1(6) 112(3)
C(1)—C(2)	1.506(8) 1.47(3)	C(1)—C(2)—C(3)	111.0(5) 112(3)
C(2)—C(3)	1.549(9) 1.55(3)	C(2)—C(3)—C(4)	111.1(6) 114(3)
C(3)—C(4)	1.530(9) 1.55(3)	C(3)—C(4)—C(5)	113.8(6) 114(3)
C(4)—C(5)	1.534(9) 1.49(3)	C(4)—C(5)—C(6)	113.3(6) 112(3)
C(5)—C(6)	1.520(9) 1.54(3)	C(5)—C(6)—C(7)	113.8(5) 115(3)
C(6)—C(7)	1.509(9) 1.50(3)	C(6)—C(7)—C(8)	114.1(6) 113(3)
C(7)—C(8)	1.519(9) 1.49(3)	C(7)—C(8)—C(9)	114.1(6) 114(3)
C(8)—C(9)	1.524(9) 1.57(4)	C(8)—C(9)—C(10)	112.1(7) 111(4)
C(9)—C(10)	—	C(9)—C(10)—C(11)	— 111(4)
C(10)—C(11)	— 1.60(4)	C(10)—C(11)—C(12)	— 111(3)
C(11)—C(12)	— 1.55(4)	—	—

the Cl is 30.0° for DACl and 29.5° for DDACl. Crystalline cohesion is attained via ionic bonds involving $—NH_3^+$ and Cl^- ions and van der Waals interactions between the carbon chains. The mean distance between the N and the Cl is 3.155(9) Å for DACl and 3.13(3) Å for DDACl. There is also hydrogen bonding in this ionic layer with the mean H . . . Cl distances for the two compounds being 2.099 Å and 2.12 Å. The angles between the H—N and H . . . Cl axis are 165.3° and 161°, respectively.

As would be expected, the structures of DACl and DDACl are

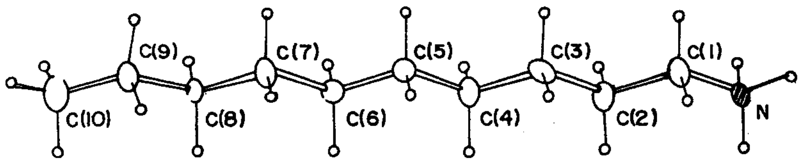

FIGURE 1 Perspective view of the molecule showing the atomic numbering.

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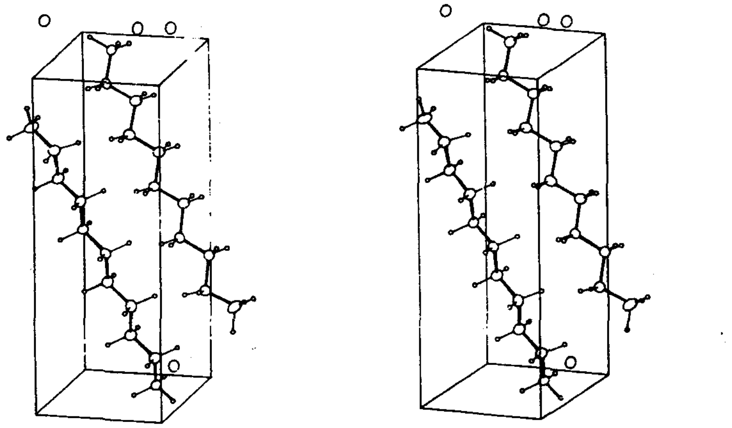

FIGURE 2 Stereoscopic view of the molecular packing. The ionic bonds are indicated. The z axis is vertical, the x axis horizontal, and the origin is in the lower, right hand bottom corner. Thermal ellipsoids are drawn at the 20% probability level while hydrogen atoms are represented by spheres of arbitrary radius.

very similar. Both consist of ionic layers alternating with layers of carbon–hydrogen chains, the chains making an angle of about 30° with the ionic layer. The chains are somewhat stressed resulting in a slight curvature. The *a* and *b* parameters of the unit cell for both compounds are practically equal. A previous temperature study[2] of these substances has shown that there are phase transitions at 32.5 C for DACl and 45 C for DDACl in which the structure almost doubles the distance between ionic layers, the interlayer spacing in the DACl going to 24 Å and the DDACl to 30 Å. As previously stated, the closeness of these transitions may well account for the low quality of the crystals we are able to grow (i.e., the low number of observed reflections). These phase transitions are probably driven by the necessity of the C—H chain to have more freedom (rotate).

We believe the structure of the ionic layer in which each Cl^- is surrounded by a network of three $—NH_3^+$ groups and each $—NH_3^+$ by three Cl^- ions to be of special interest in the formation of the higher temperature anhydrous mesophases studied in Reference 2 and probably also of help in understanding structures in the lyomesophases (for example see the work of Radley[19]).

After our experimental work was complete, we became aware of Reference 20 which also presents the crystal structure of DACl, in excellent agreement with our results.

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DIRECTIONAL DIAMAGNETIC SUSCEPTIBILITY CALCULATIONS

Flygare has developed a method which enables calculation of the molecular directional diamagnetic susceptibilities.[21-23] The most serious limitation of this method is the necessity of knowing the Directional Atomic Susceptibilities (DAS) as these have been determined for a limited number of atoms. However, for DACl and DDACl the DAS are known for all the atoms with the exception of that of Cl, and in the lyomesophases we can, to a first approximation, assume that the Cl will be separated from the $[DA]^+$ and $[DDA]^+$ radicals and therefore neglect its contribution (which should be in any case isotropic). What we calculate and what is of interest for the lyomesophases are the susceptibilities of the $[DA]^+$ and $[DDA]^+$ ions.

The Flygare method obtains the Directional Molecular Susceptibility (DMS) by projecting the Local Atom Susceptibilities (LAS) on the principal axes of inertia of the molecule (a, b, c) assuming that the principal axes of inertia of the molecule coincide with the principal axes of the diamagnetic susceptibility tensor. The values of the susceptibility are then given by the following equations:

$$\begin{aligned}
\chi_{aa} &= \sum_{i}^{n} [\chi_{xx_i}\,\theta^2_{ax_i} + \chi_{yy_i}\,\theta^2_{ay_i} + \chi_{zz_i}\,\theta^2_{az_i}] \\
\chi_{bb} &= \sum_{i}^{n} [\chi_{xx_i}\,\theta^2_{bx_i} + \chi_{yy_i}\,\theta^2_{by_i} + \chi_{zz_i}\,\theta^2_{bz_i}] \qquad (1) \\
\chi_{cc} &= \sum_{i}^{n} [\chi_{xx_i}\,\theta^2_{cx_i} + \chi_{yy_i}\,\theta^2_{cy_i} + \chi_{zz_i}\,\theta^2_{cz_i}]
\end{aligned}$$

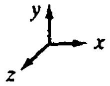
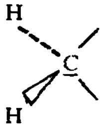
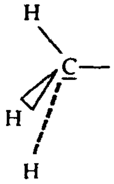
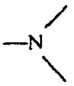
where χ_{xx} . . . are the LAS (values given in Table IV); θ_{ax} . . . are the cosines of the angles between the principal molecular axis of inertia, a . . . , and the atomic axis x . . . ; with the sums ranging over the atomic contributions of the n atoms of the molecule.

The inertial tersor components in the Center of Mass (CM) system are calculated using the equation:

$$I_{ij} = \sum_{\alpha}^{n} m_\alpha \left(\delta_{ij} \sum_{k} R^2_{\alpha k} - R_{\alpha i} R_{\alpha j}\right) \qquad (2)$$

TABLE IV

Local atom susceptibilities[a,b]

 (out of plane)	x	y	z
H	−2.0	−2.3	−2.3
	−6.5	−8.0	−7.1
	−9.5	−6.7	−6.7
	−11.3	−14.8	−2.5

[a] From Reference 22.
[b] Units are $\times 10^{-6}$ erg/(G^2·mol).

where the sum in α ranges over the n atoms of the molecule (except for the hydrogen), the subscript $i, j, k, = x, y, z$ and R is the projection of the interatomic distances on the axes of the CM system.

The inertial tensor matrix is then diagonalized to obtain the position of the principal axis of the inertial (a, b, c) system in relation to the CM system. The cosines of the angles between the atomic coordinate axes (x, y, z) of the LAS, and the principal inertial axes (a, b, c) as needed for equation 1, are given in Table V.

We will now make the following simplifications:

a) The hydrogen atoms will be ignored in the calculation of the moments of inertia of the molecule. This is justified by their low mass and symmetric distribution.

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TABLE V

Angles (°) between atomic axes systems and the inertial moments systems for $[DA]^+$ and $[DDA]^+$

	$\hat{\theta}$§	$\hat{\theta}$§§	$\hat{\theta}$§§§
ax	56.5	54.5	53.0
ay	33.5	90.0	37.0
az	90.0	35.5	90.0
bx	33.5	90.0	37.0
by	56.5	0.0	53.0
bz	90.0	90.0	90.0
cx	90.0	35.5	90.0
cy	90.0	90.0	90.0
cz	0.0	54.5	0.0

§ All C atoms and N atom.
§§ H atoms of all CH_2, NH_3 and CH_3 out of the XY plane.
§§§ H atoms of NH_3 and CH_3 in the XY plane.

b) As the molecule in the lyomesophase (micelle) is relatively free, we believe the best molecular structure to assume is an "idealized" one in which all the carbon–carbon and carbon–hydrogen distances and angles are those of the mean values of the crystal, and the carbon atoms are assumed to lie in a plane. Therefore interatomic distances and angles are all assumed to have their mean crystallographic values, i.e., $d_{cc} = d_{cN} = 1.53$ Å, $d_{cH} = d_{NH} = 1.08$ Å.

c) Both hydrogen atoms in the CH_2 groups and two each in the CH_3 and NH_3 groups are assumed to stay out of the plane through nitrogen and carbon atoms and for these the column labeled §§ in table V was used to calculate their angles. The remaining hydrogen atoms are assumed to stay in the N—C plane and for these the §§§ column of this table was used.

d) The axes of the CM and of the principal inertial systems are assumed to coincide. (Calculations show this error to be about 0.1%, which is less than the crystallographic standard deviations).

If this procedure is carried out for the uniaxial case, we find for the mean value of the susceptibility, χ, and its anisotropy $\Delta\chi$:

$$\begin{aligned} \bar{\chi} &= \frac{1}{3}(\chi_\parallel + 2\chi_\perp) \\ \Delta\chi &= \chi_\parallel - \chi_\perp \end{aligned} \tag{3}$$

where $\chi_\parallel$ and $\chi_\perp$ are the DMS that correspond to the orientation

TABLE VI

Calculated diamagnetic susceptibilities[a]

	χ_{aa}	χ_{bb}	χ_{cc}	$\bar{\chi}$	$\Delta\chi$
$[DA]^+$	−142	−138	−124	−135	−5
$[DDA]^+$	−166	−162	−146	−158	−6

[a] Units are $\times 10^{-6}$ erg/(G^2·mol).

which coincide with the long axis of the molecule, and the perpendicular to that axis, respectively. In other words,

$$\chi_{\parallel} = \chi_{bb}; \quad \chi_{\perp} = \frac{1}{2}(\chi_{aa} + \chi_{cc}) \tag{4}$$

Equations (1), (2) and (3) together with the values of the LAS taken from Table IV and the direction cosines taken from Table V can now be used to calculate the susceptibilities. The results for both DACl and DDACl are given in Table VI. From these we can now obtain the anisotropy of the mass diamagnetic susceptibilities and therefore both DACl and DDACl:

$$\Delta\chi_m = 3.1.10^{-8} \text{ cgs } [DA]^+$$

$$\Delta\chi_m = 3.2.10^{-8} \text{ cgs } [DDA]^+$$

DISCUSSION OF SUSCEPTIBILITY RESULTS

A literature search was unable to locate data on the directional susceptibilities, either experimental or theoretical, which would allow a direct check of our results. We can, however, calculate the expected value of the susceptibility of an isotropic liquid by Pascal's method, which is an empirical method that often gives good results for liquids.[24] The result obtained by this method is 135 × 10^{-6} erg/(G^2 · mol) for DACl and 159 × 10^{-6} for DDACl, in excellent agreement with our data in Table VI.

In order to further check the applicability to systems such as ours, we have the Flygare method to calculate the directional susceptibilities of the corresponding saturated hydrocarbons, decane and dodecane, the position of the hydrogen and carbon being the same we

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used in the DACl and DDACl calculations. When this is done and the results averaged over all orientations, the results for these substances is within 1% of their measured experimental values.[24] The same calculation was performed for decanol and dodecanol, using CRC handbook values for the positions of the atoms of the OH group and the error is also of the order of a percent.

Stefanov and Saupe[25] have measured the anisotropy in the diamagnetic susceptibility in the nematic phase of DACl obtaining a value $3 \times 10^{-9} < \Delta\chi < 6 \times 10^{-9}$ (in cgs units). In order to compare this to our calculated result of 3.1×10^{-8} cgs units, several factors must be taken into consideration, the most important of which is the order within the lyomesophase. The result of our calculation assumes that all the molecules are aligned and this is far from the case, even when the sample is optically aligned. If we consider the micelles to be as described by Charvolin[26] (a diameter of ~60 Å and a thickness of ~28 Å), then approximately 1/4 of the molecules within each micelle are aligned (those at the center of the disk), the average contribution to the anisotropy of those on the micelle edge being zero. The order between micelles is also not perfect, and is usually described by the order parameter S. In order for our results to agree with those measured by Stefanov and Saupe we only need a factor that ranges from .38 to .78, not at all incompatible with order parameters for a nematic phase. Another factor which would tend to lower the number we calculated is the disorder within a single chain (as in our calculation the C—H chain is assumed to be extended and in the same configuration as in the crystal). This assumption is supported by the NMR measurements made by Fujiwara and Reeves[27] which have shown that, in the nematic phase, the chains are extended with little disorder until the terminal methyl group is reached; and thus this type of disorder should have a small effect on the anisotropy of the susceptibility.

CONCLUSIONS

We have determined the crystalline structure of DACl and DDACl. The atomic configuration in these structures was used to calculate the directional diamagnetic susceptibilities. When reasonable assumptions are made, our calculated anisotropy is in agreement with that measured by Stefanov and Saupe.[25] We believe that we have shown that the crystalline structure of surfactants can be helpful in the understanding of their thermotropic and lyotropic mesophases.

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