The Crystal Structure of Sodium Dodecylsulfate

STAFFAN SUNDELL

Dept. of Structural Chemistry, Institute of Medical Biochemistry, University of Göteborg, P.O.B., S-400 33 Göteborg, Sweden

Sodium dodecylsulfate $(CH_3(CH_2)_{11}OSO_3^-Na^+)$ which has been studied as a model sulfolipid is monoclinic $(C2/c)$ with $a = 78.69$, $b = 10.22$, $c = 16.41$ Å, $\beta = 98.28°$. The unit cell contains 32 molecules and in addition 4 molecules of water. The lipid molecules are arranged tail to tail in double layers. Favourable electrostatic interactions within the polar region are achieved by an alternating 2 Å displacement of adjacent molecules perpendicular to the layer plane. This arrangement of the polar head groups determines the lateral packing of the molecules and leaves the hydrocarbon chains with about 10 % larger cross section area than usual in solid state chain packing arrangements. Still the hydrocarbon chains are fully extended and only slightly tilted (79°) to the layer plane. The chain packing, however, is irregular and can be described as an intermediate between the orthorhombic $O\perp$ and the hexagonal chain packing mode.

A variety of complex sulfolipids have been isolated from different organisms.[1] For sulfatide (cerebroside sulfate), the dominating sulfolipid in vertebrates, an interesting correlation with $Na^+ - K^+$ ATPase has been shown.[2] Other sulfolipids like lactosylceramide sulfate of kidney,[3] the sulfate ester of 2,3-di-O-phytanyl-1-O-triglycosyl-L-glycerol of halophilic bacteria,[4] the plant sulfonolipid 6-sulfo-quinovosyl-diglycerid [5] have similar structures in their polar parts and may have the same biological function as sulfatide. In the sea star *Asterias rubens* large amounts of cholesteryl sulfate were detected while other types of common sulfolipids were missing.[6] This finding suggests that also cholesteryl sulfate may participate in ion transport phenomena. In our structural studies of membrane lipids we have started X-ray work on sulfatides and cholesteryl sulfate. Sodium dodecylsulfate (SDS) has been included in this

study as it represents a simple alkyl sulfate. Alkyl sulfates and chloroalkyl sulfates have been found in nature in phytoflagellates.[7] The molecular arrangement and phase behaviour of SDS is also of interest with regard to its role as an important detergent.

EXPERIMENTAL

The synthetic sodium dodecylsulfate used in this study was shown by gas chromatographic analysis to contain dodecanol with a purity of better than 99 %. Single crystals were obtained as thin plates from a chloroform-methanol (9:1, v:v) solution on slow evaporation.

The intensity data were collected on a Picker FACS I automatic diffractometer [8] using graphite monochromated $CuK\alpha$ radiation. The crystal used had the dimensions 0.36 × 0.32 × 0.03 mm. The $\theta - 2\theta$ scanning mode was used with a scan speed of 1 degree/min and a scan width of 2.5° plus a dispersion term. On each side of the reflexion the background level was determined from 10 s counts. After every 50th reflexion, three standards were measured in order to make a correction for the decaying scattering power of the crystal. It was found at the end of the measurement that the standard reflexions had decreased in intensity to about 70 % of the original values. 5841 independent reflexions were measured. 3666 of these were considered observed $[I > 4\sigma(I)]$ and used in the analysis. The intensities were corrected for Lorentz, polarization and absorption effects. No extinction correction was made.

CRYSTAL DATA

Molecular formula: $CH_3(CH_2)_{11}OSO_3^-Na^+.1/8H_2O$. Crystal system: monoclinic. Space group: $C2/c$. Unit cell: $a = 78.69(26)$, $b = 10.220(22)$, $c = 16.410(45)$Å, $\beta = 98.28(8)°$, $V = 13060$ Å^3, $M = 289.73$, $Z = 32$, $D_c = 1.19$ g

cm^{-3}, $D_m = 1.18$ g cm^{-3}, $\lambda = 1.54051$ Å (CuKα_1 radiation), $\mu = 20.1$ cm^{-1}.

Systematic absences: hkl: $h + k = 2n + 1$
                        $h0l$: $l = 2n + 1$.

STRUCTURE DETERMINATION AND REFINEMENT

As there are four heavy atoms in the asymmetric unit the solution of the Patterson series was not straight-forward. However, a vector set was selected which appeared to define the positions of three sulfur atoms. The phases of one of these atoms were used for a Fourier synthesis, which showed that the two other sulfur positions had been correctly determined from the Patterson function. The following two Fourier syntheses — the first based on the phases of the three sulfur atoms — revealed the structure of the whole polar region including a peak that could only represent a crystal water oxygen. At this stage the R-value was 0.32. After three cycles of block diagonal refinement using anisotropic temperature factors for the sulfur, sodium and oxygen atoms the R-value had dropped to 0.25. An electron density and a difference synthesis were then calculated. In both cases the carbon atoms of the chains were poorly resolved. The resolution was nevertheless sufficient near the polar regions to determine the direction of the chains and the tilt of the zigzag planes to the ac-plane. One chain (2) (Fig. 2) was better defined than the others. About a quarter of the carbon atoms were incorporated in the next structure factor calculation. In the following three Fourier syntheses the remaining carbons were successively included to give the best fit to the electron density. Anisotropic temperature factors were assigned to the carbon atoms but after a few cycles of refinement many of the U_{ij} values of atoms belonging to chain (1), (3) and (4) had become unrealistically high. The refinement was then restarted with isotropic temperature factors for the carbons in chains (1), (3) and (4), while anisotropic ones were still used in chain (2). The structure was refined by six cycles of full matrix refinement to $R = 0.103$ and $R_w = 0.118$. The temperature factors for the carbons of chains (1), (2) and (3) became very large (on the average 26 Å^2). The poor resolution of these atoms was also clear from the electron density map (Fig. 1). Finally a check of the space group choice was made.
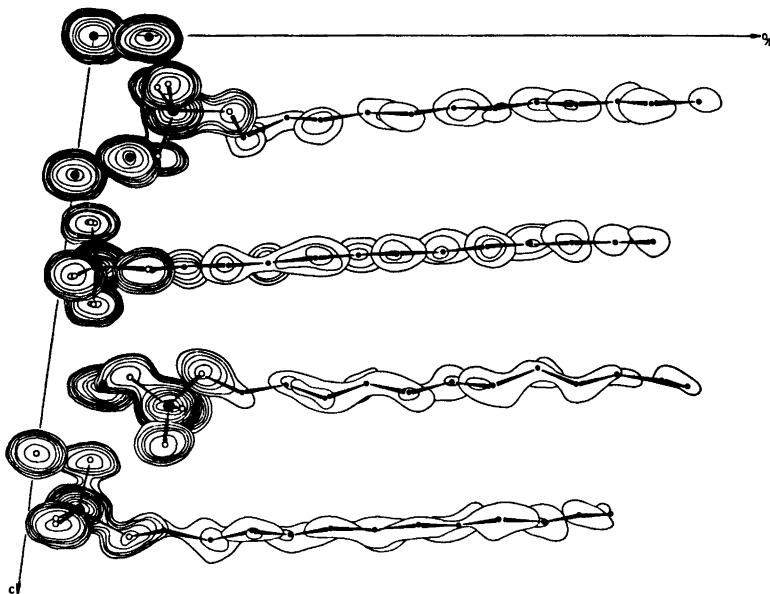

Fig. 1. Composite electron map of one asymmetric unit (0,0,0), (1/4,1/2,1). Contours are drawn at intervals of 1.5, 2.0, 2.5, 3.0, 4.0, 6.0, 8.0, 10.0, 12.0, 14.0, 16.0 and 18.0 e/Å^3.

The structure was solved as before starting with the phases of one sulfur atom but this time in Cc. The resulting atom positions, however, did not differ significantly from the centrosymmetrically related positions in $C2/c$. The form factors used were those given in *International Tables for X-Ray Crystallography*.[9] All calculations were performed on a DEC 10 computer using the X-RAY 72 program system.[10] The weight assigned to each observation[11] in the least-squares refinement was:

$$w = 1/[1 + (|F_o| - 5.6F_{min})^2/(11.1F_{min})^2]$$

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

Lists of observed and calculated structure factors can be obtained from this Department.

Table 1. Fractional coordinates and thermal parameters ($\times 10^3$) with estimated standard deviations in parentheses. The isotropic and anisotropic thermal parameters are in the form exp $-8\pi U(\sin^2\theta/\lambda^2)$ and exp $-2\pi^2(h^2a^{*2}U_{11} + \cdots + 2kl2b^*c^*U_{23})$, respectively.

Atom	x	y	z	U or U11	U22	U33	U12	U13	U23
Na(11)	0.0000(-)	0.0000(-)	0.0000(-)	95(7)	22(3)	23(3)	3(4)	11(3)	3(2)
Na(12)	0.0000(-)	0.0590(6)	0.2500(-)	93(7)	31(3)	21(3)	0(-)	7(3)	0(-)
Na(2)	0.0208(1)	0.4134(4)	0.0019(2)	96(5)	26(2)	23(2)	-2(3)	7(2)	0(2)
Na(3)	0.0200(1)	0.3628(4)	0.2197(3)	102(5)	37(3)	45(3)	-2(3)	22(3)	-6(2)
Na(4)	0.0216(1)	0.2111(4)	0.6279(2)	91(5)	37(3)	23(2)	-6(3)	10(2)	0(2)
O(5)	0.0000(-)	0.4832(9)	0.7500(-)	98(12)	24(6)	21(5)	0(-)	9(6)	0(-)
S(1)	0.0338(1)	0.1239(3)	0.1348(2)	66(3)	23(2)	25(1)	5(2)	6(2)	-1(1)
O(11)	0.0302(1)	0.2400(8)	0.0878(5)	98(9)	39(5)	56(5)	6(5)	12(5)	10(4)
O(12)	0.0261(1)	0.0117(7)	0.0954(5)	130(10)	23(4)	53(5)	-11(5)	1(5)	-6(4)
O(13)	0.0301(1)	0.1383(9)	0.2170(4)	121(10)	63(6)	34(5)	27(6)	9(5)	-6(4)
O(14)	0.0531(1)	0.1104(9)	0.1383(6)	96(10)	54(6)	88(7)	0(6)	8(6)	7(5)
C(11)	0.0617(3)	0.0089(24)	0.1837(14)	155(9)					
C(12)	0.0776(5)	-0.0420(35)	0.1571(20)	239(15)					
C(13)	0.0923(4)	0.0315(29)	0.1547(17)	191(11)					
C(14)	0.1089(4)	-0.0469(31)	0.1478(18)	220(13)					
C(15)	0.1234(4)	0.0265(34)	0.1435(19)	224(13)					
C(16)	0.1387(5)	-0.0416(33)	0.1310(19)	211(13)					
C(17)	0.1532(4)	0.0397(34)	0.1321(19)	226(14)					
C(18)	0.1700(5)	-0.0422(34)	0.1273(19)	224(14)					
C(19)	0.1856(6)	0.0376(42)	0.1311(23)	270(18)					
C(110)	0.2014(7)	-0.0414(47)	0.1201(27)	293(21)					
C(111)	0.2158(9)	0.0359(59)	0.1273(34)	393(29)					
C(112)	0.2309(7)	-0.0271(54)	0.1173(29)	350(26)					
S(2)	0.0135(1)	0.2945(3)	0.4187(1)	57(3)	23(1)	14(1)	-4(2)	7(1)	-1(1)
O(21)	0.0081(1)	0.2428(7)	0.3369(4)	117(9)	28(4)	15(4)	5(5)	9(4)	-3(3)
O(22)	0.0047(1)	0.4124(7)	0.4334(4)	94(8)	25(4)	27(4)	-14(5)	14(4)	-1(3)
O(23)	0.0136(1)	0.1993(7)	0.4826(4)	98(8)	32(4)	20(4)	-7(5)	5(4)	5(3)
O(24)	0.0319(1)	0.3404(8)	0.4203(4)	44(7)	59(5)	44(4)	12(5)	11(4)	5(4)
C(21)	0.0462(2)	0.2532(17)	0.4202(8)	44(14)	120(14)	61(9)	35(11)	0(8)	8(9)
C(22)	0.0631(3)	0.3205(21)	0.4160(10)	94(18)	147(19)	87(12)	-15(15)	5(11)	4(12)
C(23)	0.0772(3)	0.2286(18)	0.4106(10)	111(20)	105(14)	100(13)	-3(14)	32(13)	-1(11)
C(24)	0.0937(3)	0.3024(20)	0.4036(11)	104(20)	125(16)	118(15)	-3(15)	28(13)	3(13)
C(25)	0.1086(3)	0.2210(24)	0.3986(13)	55(20)	171(21)	150(18)	-3(17)	1(14)	-3(16)
C(26)	0.1259(4)	0.2896(28)	0.3947(14)	75(27)	187(26)	161(21)	25(21)	17(17)	4(18)
C(27)	0.1413(4)	0.2144(26)	0.3874(15)	90(26)	170(23)	181(23)	0(19)	34(18)	-12(18)
C(28)	0.1581(4)	0.2821(31)	0.3881(16)	144(28)	220(31)	183(24)	-31(24)	72(20)	-2(22)
C(29)	0.1731(4)	0.2108(31)	0.3754(18)	139(28)	207(30)	235(29)	-21(23)	60(22)	-17(24)
C(210)	0.1888(4)	0.2829(37)	0.3769(19)	58(31)	300(41)	263(33)	15(27)	49(24)	1(29)
C(211)	0.2039(5)	0.2116(46)	0.3716(23)	59(41)	334(52)	351(45)	3(33)	77(32)	0(36)
C(212)	0.2196(5)	0.2773(47)	0.3684(24)	106(37)	390(57)	357(49)	19(36)	100(32)	34(41)

Table 1. Continued.

Atom	x	y	z	U or U11	U22	U33	U12	U13	U23
S(3)	0.0469(1)	0.4389(3)	0.6647(2)	94(4)	35(2)	39(2)	-5(2)	4(2)	0(1)
O(31)	0.0306(2)	0.4471(9)	0.6135(6)	145(12)	63(6)	69(7)	5(7)	3(7)	1(5)
O(32)	0.0468(2)	0.5130(9)	0.7373(5)	139(11)	69(7)	56(6)	-7(7)	11(6)	-20(5)
O(33)	0.0517(2)	0.3057(9)	0.6758(6)	132(11)	54(6)	90(7)	24(7)	23(7)	17(6)
O(34)	0.0583(2)	˙0.5087(13)	0.6103(8)	222(17)	122(11)	141(11)	-64(12)	98(11)	-51(9)
C(31)	0.0735(3)	0.5769(27)	0.6488(15)	181(11)					
C(32)	0.0876(4)	0.4967(30)	0.6299(17)	203(11)					
C(33)	0.1042(4)	0.5526(29)	0.6547(17)	189(11)					
C(34)	0.1198(5)	0.4854(35)	0.6327(20)	242(14)					
C(35)	0.1360(4)	0.5508(28)	0.6477(16)	194(11)					
C(36)	0.1519(5)	0.4759(36)	0.6270(20)	239(15)					
C(37)	0.1678(6)	0.5423(41)	0.6418(23)	268(18)					
C(38)	0.1828(6)	0.4695(41)	0.6168(23)	268(17)					
C(39)	0.1993(7)	0.5398(47)	0.6350(26)	299(21)					
C(310)	0.2138(7)	0.4659(49)	0.6099(27)	317(22)					
C(311)	0.2303(9)	0.5484(66)	0.6244(38)	436(34)					
C(312)	0.2421(9)	0.4419(73)	0.6239(40)	449(41)					
S(4)	0.0186(1)	0.1847(3)	0.8508(2)	73(3)	27(2)	17(1)	-4(2)	5(2)	-3(1)
O(41)	0.0204(1)	0.1838(8)	0.7649(4)	117(8)	71(6)	17(4)	-3(6)	22(5)	0(4)
O(42)	0.0100(1)	0.0738(8)	0.8748(4)	147(11)	34(5)	35(5)	-17(6)	17(5)	3(4)
O(43)	0.0116(1)	0.3007(8)	0.8766(5)	164(11)	33(5)	33(5)	4(6)	18(5)	5(4)
O(44)	0.0376(2)	0.1678(15)	0.9010(6)	126(12)	236(15)	43(6)	-50(11)	14(7)	6(8)
C(41)	0.0528(4)	0.2436(27)	0.8968(15)	172(10)					
C(42)	0.0683(4)	0.1776(29)	0.9080(16)	191(11)					
C(43)	0.0821(4)	0.2675(31)	0.8961(18)	216(12)					
C(44)	0.0991(3)	0.2105(27)	0.9010(16)	186(11)					
C(45)	0.1145(4)	0.2813(32)	0.8885(19)	230(13)					
C(46)	0.1302(4)	0.2127(32)	0.8975(19)	229(14)					
C(47)	0.1462(4)	0.2817(35)	0.8817(21)	255(15)					
C(48)	0.1614(4)	0.2107(33)	0.8918(19)	235(14)					
C(49)	0.1759(5)	0.2832(38)	0.8713(22)	264(17)					
C(410)	0.1924(6)	0.2269(42)	0.8840(24)	286(19)					
C(411)	0.2072(6)	0.2874(48)	0.8604(27)	336(23)					
C(412)	0.2234(7)	0.2272(49)	0.8668(28)	342(24)					

Table 2. Average interatomic distances and angles with standard deviations in parentheses.

| Distance	Å	Angle	Degrees
S − O(1)	1.44(1)	O(1) − S − O(2)	112.2(0.5)
S − O(2)	1.42(1)	O(1) − S − O(3)	112.2(0.5)
S − O(3)	1.42(1)	O(1) − S − O(4)	104.8(0.6)
S − O(4)	1.55(1)	O(2) − S − O(3)	113.6(0.6)
O(4) − C(1)	1.43(2)	O(2) − S − O(4)	105.4(0.6)
C(1) − C(2)	1.43(4)	O(3) − S − O(4)	108.6(0.6)
C(2) − C(3)	1.44(4)	O(4) − C(1) − C(2)	113.4(2.0)
C(3) − C(4)	1.51(4)	C(1) − C(2) − C(3)	115.3(2.4)
C(4) − C(5)	1.43(4)	C(2) − C(3) − C(4)	115.5(2.4)
C(5) − C(6)	1.48(4)	C(3) − C(4) − C(5)	118.8(2.5)
C(6) − C(7)	1.44(5)	C(4) − C(5) − C(6)	117.8(2.7)
C(7) − C(8)	1.49(5)	C(5) − C(6) − C(7)	117.8(2.8)
C(8) − C(9)	1.46(5)	C(6) − C(7) − C(8)	116.2(3.0)
C(9) − C(10)	1.46(6)	C(7) − C(8) − C(9)	115.6(3.1)
C(10) − C(11)	1.44(7)	C(8) − C(9) − C(10)	115.9(3.5)
C(11) − C(12)	1.41(8)	C(9) − C(10) − C(11)	115.8(4.0)
		C(10) − C(11) − C(12)	114.2(4.8)
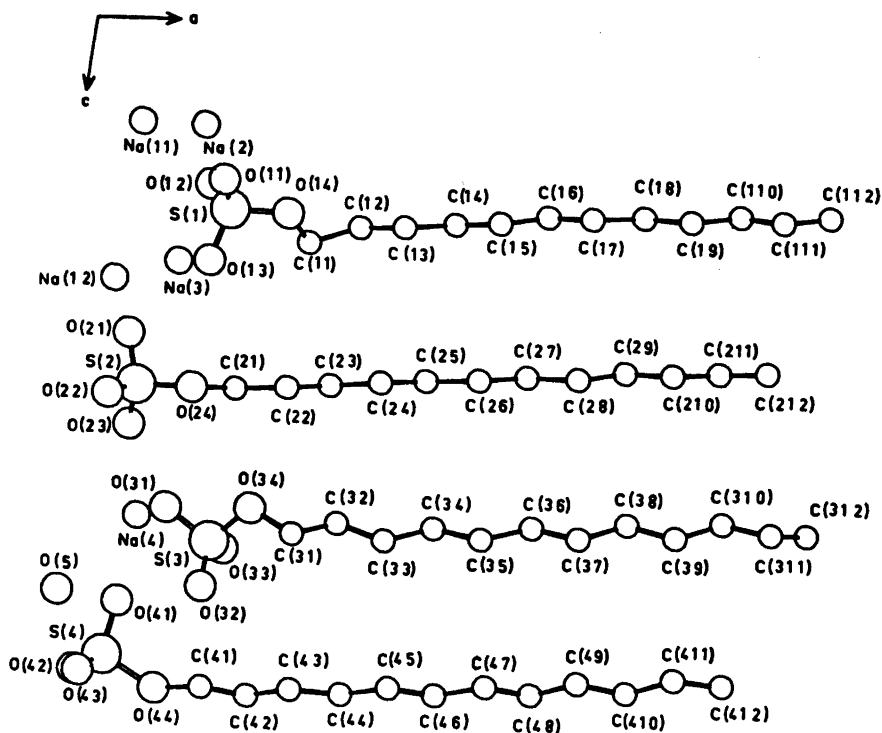
Fig. 2. The numbering of atoms. The first figure of the atom index gives the number of the molecule.
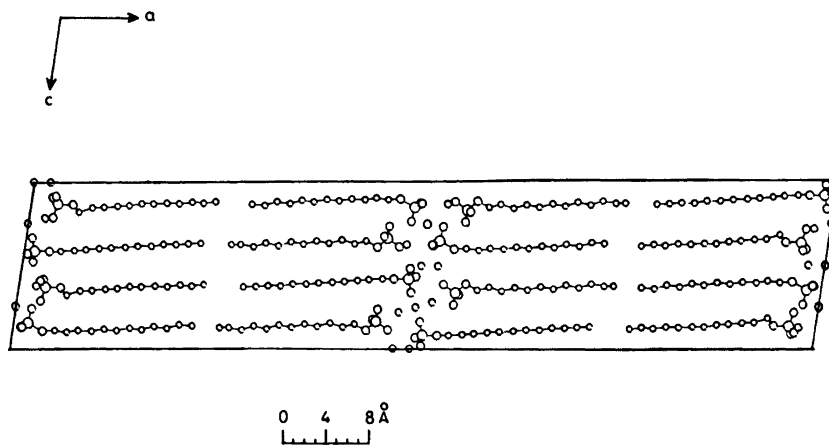

0   4   8 Å

Fig. 3. The molecular arrangement of SDS viewed along the b-axis.

The final atomic parameters are listed in Table 1 and average interatomic parameters are listed in Table 2. The numbering of the atoms is shown in Fig. 2. The structure is built up of double layers of molecules in a tail

to tail arrangement (Fig. 3). The carbon chain axes are tilted 79° to the layer plane.

The polar part. The sulfate head groups of adjacent molecules are alternatingly displaced by about 2 Å in direction of the a-axis. The
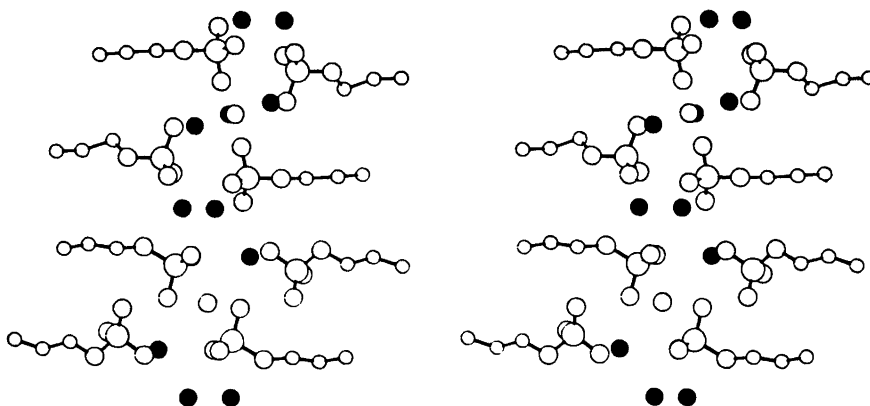
Fig. 4. Stereogram of the polar region.

rippled structure thereby produced allows favourable electrostatic interaction within the polar region as sodium ions become distributed between sulfate groups both within each layer and between opposite layers. A stereo drawing of the polar region is shown in Fig. 4. The average S−O distance and O−S−O angle excluding those containing the ester oxygen are 1.43 Å and 112.7°. The corresponding values for the ester oxygen are 1.54 Å and 106.0°. The sodium ions Na(11) and Na(12) situated in special positions are coordinated by six oxygens each, forming a distorted octahedron (Fig. 5). The Na−O distance intervals are 2.34−2.42 and 2.39−2.63 Å, respectively.

Na(2) is surrounded by five oxygens at a distance between 2.32 and 2.40 Å where the O−Na−O angles deviate less than 16° from
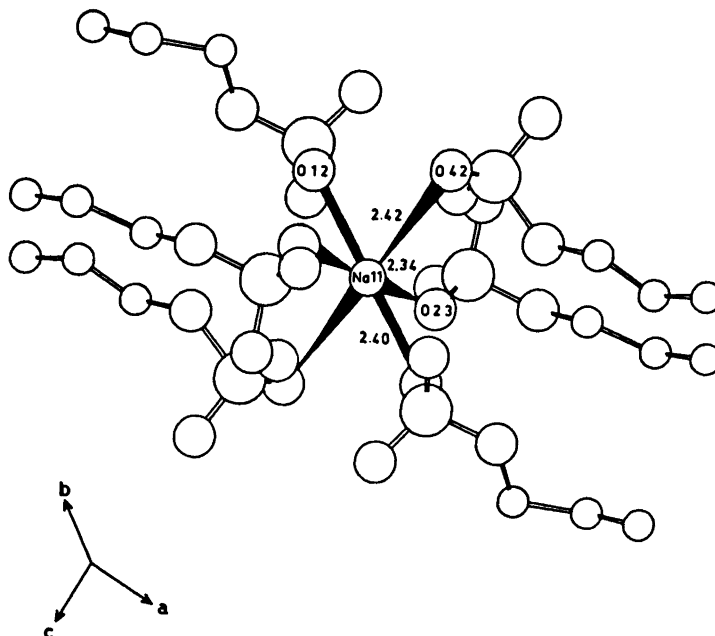
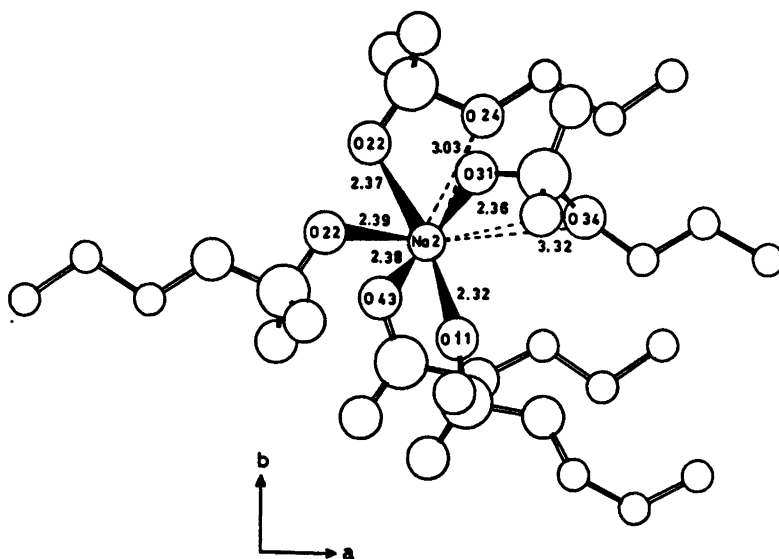

Fig. 5. The environment of Na(11).

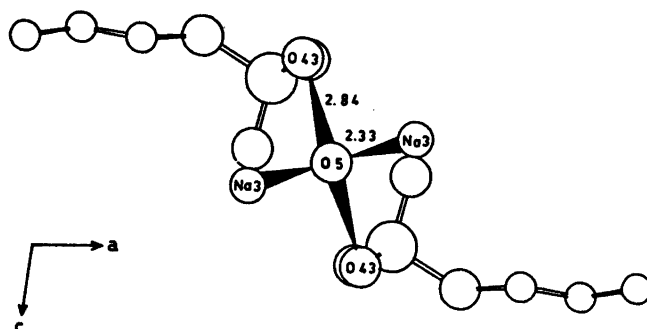*Fig. 6.* The environment of Na(2) viewed along the *c*-axis.

Fig. 7. The environment of the crystal water oxygen O(5) viewed along the *b*-axis.

those of a regular octahedron. In the vicinity of the sixth corner of the octahedron there are two oxygens at 3.03 and 3.32 Å from the sodium ion (Fig. 6). A similar oxygen arrangement is also found around Na(3) and Na(4). The Na — O distance intervals for the five closest oxygens are in the latter cases 2.30 − 2.57 and 2.28 − 2.57 Å respectively. For Na(3) the distances to the two more remote oxygens are 2.72 and 2.82 Å while for Na(4) the distances are 2.76 and 2.85 Å.

The crystal water oxygen O(5) placed on a twofold axis is hydrogen bonded to O(43) and its symmetry equivalent generated by the

twofold axis (Fig. 7). The O---O distance is 2.84 Å and the O − O − O angle 98.0°. The lone pair valence orbitals point towards Na(3) and its symmetry equivalent, the Na − O distance being 2.33 Å and Na − O − Na angle 95.0°. A list of sodium-oxygen distances is given in Table 3.

The non-polar part. The strong ionic forces and the hydrogen bond system in the polar region dominate the molecular structure to the extent that the hydrocarbon chains cannot adopt any of the common side packing arrangements with optimum van der Waals interactions.[12,13] Despite the alternating dis-

Table 3. Sodium-oxygen distances (Å) less than 3.5 Å and their estimated standard deviations.

Na(11)	O(12)	(0,0,0)1 [a]	2.40(1)
Na(11)	O(12)	(0,0,0)2	2.40(1)
Na(11)	O(23)	(0,0,0)3	2.34(1)
Na(11)	O(23)	(0,0,−1)4	2.34(1)
Na(11)	O(42)	(0,0,−1)1	2.42(1)
Na(11)	O(42)	(0,0,1)2	2.42(1)
Na(12)	O(13)	(0,0,0)1	2.63(1)
Na(12)	O(13)	(0,0,0)3	2.63(1)
Na(12)	O(21)	(0,0,0)1	2.39(1)
Na(12)	O(21)	(0,0,0)3	2.39(1)
Na(12)	O(41)	(0,0,1)2	2.95(1)
Na(12)	O(41)	(0,0,−1)4	2.95(1)
Na(12)	O(42)	(0,0,1)2	2.49(1)
Na(12)	O(42)	(0,0,−1)4	2.49(1)
Na(2)	O(11)	(0,0,0)1	2.32(1)
Na(2)	O(22)	(0,0,0)3	2.40(1)
Na(2)	O(22)	(0,1,−1)4	2.37(1)
Na(2)	O(24)	(0,1,−1)4	3.03(1)
Na(2)	O(31)	(0,1,−1)4	2.36(1)
Na(2)	O(34)	(0,1,−1)4	3.31(2)
Na(2)	O(43)	(0,0,−1)1	2.38(1)
Na(2)	O(44)	(0,0,−1)1	3.38(2)
Na(3)	O(11)	(0,0,0)1	2.72(1)
Na(3)	O(13)	(0,0,0)1	2.43(1)
Na(3)	O(21)	(0,0,0)1	2.57(1)
Na(3)	O(21)	(0,0,0)3	2.58(1)
Na(3)	O(22)	(0,0,0)3	2.99(1)
Na(3)	O(24)	(0,0,0)1	3.30(1)
Na(3)	O(31)	(0,1,−1)4	2.82(1)
Na(3)	O(32)	(0,1,−1)4	2.44(1)
Na(3)	O(5)	(0,0,1)2	2.33(1)
Na(4)	O(12)	(0,0,0)4	2.38(1)
Na(4)	O(23)	(0,0,0)1	2.38(1)
Na(4)	O(31)	(0,0,0)1	2.53(1)
Na(4)	O(33)	(0,0,0)1	2.57(1)
Na(4)	O(41)	(0,0,0)1	2.28(1)
Na(4)	O(42)	(0,0,1)3	2.85(1)
Na(4)	O(43)	(0,0,1)3	2.76(1)

[a] The figures within parentheses indicate translations in the directions a, b and c of the second atom and the last figure to the equivalent position. 1: x, y, z; 2: $\bar{x}, \bar{y}, \bar{z}$; 3: $\bar{x}, y, 1/2−z$; 4: $x, \bar{y}, 1/2+z$.

placement of adjacent molecules the area occupied per sulfate group is larger than the cross section area normally required by a hydrocarbon chain in the solid state. The chains are only slightly tilted and the average area per chain is 20.9 Å² compared with a value of about 19 Å² for the common orthorhombic chain packing O⊥. Only in the hexagonal chain arrangement which is often adopted near the melting point chains pack as cylindrical rods with a cross section of 21.1 Å. The chains in SDS must, however, be considered to

be in an intermediate state between O⊥ and the hexagonal packing (Fig. 8) as the symmetry along the chain axis is still clearly twofold.

The chains in SDS are too irregular to allow any formal subcell description of the arrangement. On the other hand, all attempts to use an idealized model for the chains have resulted in a higher R-value and/or too close contacts between hydrogen atoms when included at their expected positions. This indicates that the chain structure reported here — though very unusual — must be essentially correct.

As the space available for each chain is large, high thermal vibrations and disorder is expected. This is also indicated by the short average C − C distance of 1.45 Å and the large carbon valence angles of 116° with estimated standard deviations $(s = [(\sum_N(\overline{X}_N − X^2/N − 1)]^{1/2})$ 0.05 Å and 5.2°, respectively. The normal values for long chains are around 1.51 Å and 114°, respectively. The molecular arrangement of SDS is interesting in connection with biological lipid systems such as the cell membranes. In these it is generally concluded that the polar regions of lipid bilayers can have a fairly ordered arrangement whereas the carbon chains are in a more fluid state. The present analysis shows that the rigid arrangement of the polar head groups leaves the hydrocarbon chains with 10 % more space than normally required in the solid state, thereby allowing disorder and high thermal motion in the hydrocarbon matrix. On heating SDS undergoes a phase transition at 85 °C which is accompanied by a layer thickness decrease of 5 Å and a change to hexagonal chain packing as indicated in the powder diagram by a single short-spacing line at 4.28 Å.

The decrease in lamellar thickness can be explained by a change in tilt of the hydrocarbon chains from 79° to about 60°. However, this tilt and the hexagonal chain packing require an increase of the molecular area in the *ac*-plane from 20.9 to approximately 24.5 Å. This suggests that the transition to the high temperature phase involves a change of the sulfate groups from a rippled to a planar arrangement.

	orthorhombic	SDS	hexagonal	
a	5.0	5.1	4.9	Å
b	7.4 – 7.8	8.2	8.6	
cross section area per chain	18.5 – 19.5	20.9	21.1	Å²
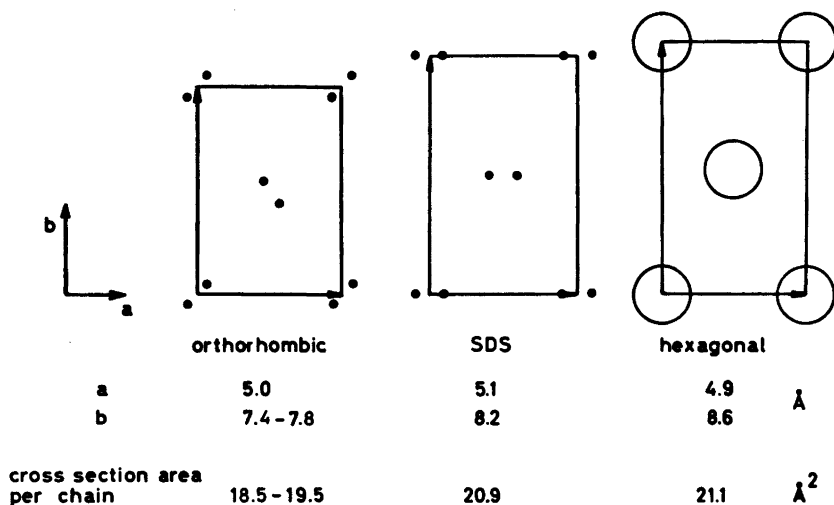
Fig. 8. The idealized subcell of SDS compared with an orthorhombic and a hexagonal subcell.

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