

Six molecules per unit cell is rather unusual for paraffin-chain salts, having been found previously only for the ζ phase of the sodium alkane sulfonates, although Buerger (1945) found 12 chains per unit cell in the triclinic β form of sodium acid stearate. By analogy with other paraffin-chain salts, it may be concluded that the molecules lie in sheets parallel to (001) with the chains tilted more or less from the normal to this plane. There are four possible arrangements which might be considered, having respectively 6, 3, 2 or 1 molecule in the a - b cross-section. The first and third of these seem very unlikely, since the ionic forces between the sulfonate groups and the sodium ions almost certainly lead to a 'head-to-head' arrangement, requiring an even number of molecules in the c direction, as is the case for all paraffin-chain salts which have been investigated. The second possibility, 3 molecules in the a - b cross-section and 2 molecules in the c direction, appears to be rather unlikely from a consideration of the dimensions of the unit cell. In the first place, this leads to an effective molecular length of 25.6 Å, which is considerably longer than the length observed for the alpha phase, 18.1 Å. It does not seem possible that this difference could be accounted for by poorer 'end-packing' and the increased hydration. In the second place, this arrangement leads to a cross-sectional area per molecule of 16.04 Å.² In a recent paper reviewing X-ray crystallographic data on a large number of paraffin-chain compounds, Kohlhaas (1949) has shown that, for most paraffin-chain compounds, the cross-sectional area is usually 18-19 Å.² He lists no case in which the cross-section is less than 17.8 Å.² Vand, Aitken & Campbell

(1949) have recently reported a cross-sectional area of 16.83 Å.² for silver hexanoate, but, since their results are based entirely on powder data, it is quite possible that they may be in error.

Thus it appears that, if the molecules in the η phase arrange themselves in sheets as is the case for other paraffin-chain compounds, there are 6 molecules in the c length and only one in the a - b cross-section. If we estimate the effective length of the sodium dodecane-sulfonate molecule to be 18.1 Å, as observed in the α phase, we can calculate the angle between the chain direction and the normal to the sheets to be about 61° ($\cos \tau = \frac{51.28}{6 \times 18.1}$), and the effective chain cross-section to be 22 Å.² Because of the fact that the chains are tilted slightly in the α phase and also since the η phase is more highly hydrated than the α phase, the actual tilt of the chains is probably greater than 61° and the cross-section less than 22 Å.²

References

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The monohydrate of ethylenediamine d -tartrate: optical properties and X-ray diffraction data. By E. G. STEWARD, *Research Laboratories, General Electric Company Limited, Wembley, England*

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Ethylenediamine d -tartrate monohydrate may be crystallized from an aqueous solution containing equimolecular proportions of ethylenediamine and d -tartaric acid. The hydrate is the stable form in contact with solution when the latter is saturated below approx. 41° C. The crystals belong to the orthorhombic sphenoidal class and exhibit the following forms: prisms {110}, domes {101}, {021} and sphenoids {111}.

The principal X-ray diffraction data and optical properties are given below and in Table 1.

$C_8H_{14}N_2O_6 \cdot H_2O$. Molecular weight = 228.20.

Specific gravity (18° C.) = 1.52₄.

Orthogonal structure cell dimensions (± 0.03 Å.):

$a = 11.56$, $b = 15.04$, $c = 5.80$ Å.

Molecules per unit cell = 4.

Probable space group $P2_12_12_1-V^4$.

Refractive indices (± 0.002), sodium light, 18° C.:

$\alpha = 1.542$ parallel to a ,

$\beta = 1.552$ parallel to c ,

$\gamma = 1.552$ parallel to b .

Birefringence negative, $\gamma - \alpha = 0.01$.

Optic axial angle ($2V$) approx. 26° at 18° C.

Table 1. Principal 'powder' lines

(Intensities visually estimated: d not corrected for absorption)

d (Å.)	intensity	d (Å.)	Intensity	d (Å.)	Intensity
9.23	0.5	3.78	2	2.58	2
7.51	0.5	3.63	10	2.46	8
6.31	3	3.46	1	2.44	3
5.80	2	3.24	4	2.36	1
5.44	1	3.17	5	2.31	3
5.22	4	3.04	1	2.25	3
4.91	0.5	2.93	4	2.15	3
4.55	10	2.87	5	2.12	3
4.31	4	2.78	4	2.06	3
4.13	3	2.72	5	1.99	3
3.99	9	2.59	1	—	—

With decrease in temperature, crossed-axial-plane dispersion was observed, crystals being in the uniaxial condition at $-34 \pm 5^\circ$ C. This is in contrast to the behaviour of the anhydrous tartrate (Steward, 1950), in which this effect occurred with increase in temperature. Both the anhydrous material and the hydrate are piezoelectric.

Reference

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