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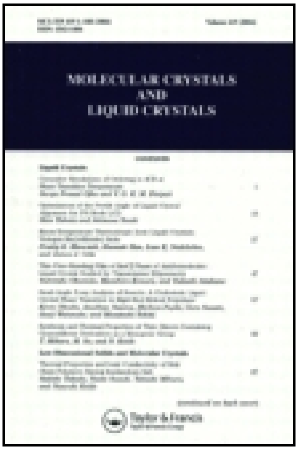

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Mesomorphism in the System Disodium Chromoglycate (DSCG)-Water

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MESOMORPHISM IN THE SYSTEM DISODIUM CHROMOGLYCATE (DSCG)-WATER

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(Submitted for publication 14th November, 1980)

A recent letter to this journal by Dr John E Lydon[1] criticises the conclusions drawn by us in some earlier work on this subject[2] and proposes new structures for the mesophases. In particular, he suggests that the rods in the "middle"-type M phase are square-sectioned boxes *containing water* as well as being arrayed hexagonally in a water continuum, instead of the cylindrical rods pictured by us. He quotes our figure of 16 Å for the diameter of the rods, which we obtained in an early calculation, but he omits to state that this was based on a hypothetical structure in which there was complete separation between the water and the DSCG, ie, a structure in which there was no water in the rods. (Actually, we mainly referred to this calculation because we thought it afforded some evidence that the structure was not of the inverse type, ie, one in which the rods are in a lipophilic continuum.)

In view of the strong affinity of DSCG for water, and the fact that the crystalline phase acquires *ca*. 10% of interstitial water before it collapses to the M mesophase, we always considered it most unlikely that the M rods contained no water. Our paper discussed this at some length and reported some values of the rod diameter calculated for a plausible range of water percentages. Dr Lydon's letter makes no mention of this discussion.

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The Lydon M rods are based on the molecular structure of DSCG obtained from an X-ray study of the crystalline phase by Hamodrakas, Geddes, and Sheldrick.[3] The molecules in the rods are arranged transversely with their long axes forming the sides of the square boxes and with the bridge -OH groups pointing outwards. Such a general arrangement of the molecules with respect to the rod axes is consistent with the fact that there are centres of potential hydrophilic interactions (the negative oxygen atoms) along both sides of the extended molecules, but that with the exception of the bridge -OH group these occur in oppositely directed pairs (eg, the two carbonyl groups) the members of which will roughly balance each others' effects. The lone bridge -OH will increase the total hydrophilic interaction on that side, and by an extension of Winsor's "R" theory,[4] this could result in the molecules arranging themselves in rings with the bridge -OH groups on the outer (convex) sides, in fact as in Dr Lydon's cross-sectional pattern for the rods, but without any necessary restrictions as to shape, square or otherwise. With this qualification we are prepared to support his ideas, and to admit that in the past we have tended to think of the rods with the molecules oriented so that only the carboxylic groups were in association with the water continuum, by analogy with the soaps.

As regards Dr Lydon's views on the N phase, we have open minds. Possibly the answer lies in the reason for the diffuse X-ray reflection corresponding to a spacing of 3.4 - 3.8 Å, shown by both the M and the N phases, and as yet unexplained so far as we are aware.

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