Elastic and flexoelectric properties of liquid crystal dimers: dramatic effects of a bent-shape

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We have calculated the elastic constants (K_{11}, K_{22}, K_{33}) and the flexoelectric coefficients (e_1, e_3) for the nematic phase formed by liquid crystal dimers, made of biphenyl units linked by a flexible spacer. To do this we have used a recently developed methodology,[1,2] which combines a molecular field theory with atomistic modelling. The orienting molecular field in the presence of director distortions is parameterized according to the anisometry of the molecular shape. The main results can be summarized as follows.

-Good agreement with the available experimental data (splay elastic constants and flexoelastic ratios) [3-6] is found. Thus, a shape model seems able to account for the elasticity of nematics, provided that the conformational distribution of the molecules is properly considered. The flexoelectric behaviour cannot be described in terms of molecular dipoles, but a more detailed representation, e.g. by atomic charges, is needed. The odd-even effects observed for K_{11}, K_{22} and e_1 simply reflect the alternating degree of orientational order in the nematic phase of odd and even dimers.[5]

-Peculiar behaviour is found for the bend elastic constants, with exceptionally low values for odd dimers, in keeping with their bent shape. The effect is much stronger than previously predicted.[7] In our communication this result will be discussed, in relation to a number of different and unexplained observations[8-10] and theoretical results[11] for the nematics formed from bent-core mesogens, which might have a common origin in the unusual propensity of these systems for bend deformations of the director.

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