Spontaneous Enantiomer Separation in Liquid Crystals Composed of Achiral Rod-Shaped Esters

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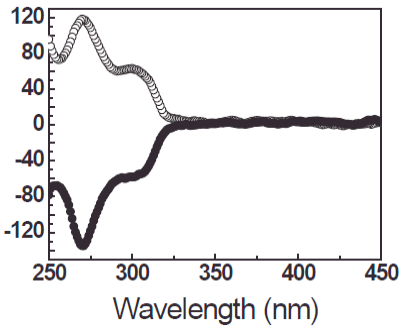
The discovery of spontaneously induced chirality and enantiomeric separation in liquid crystal and soft crystal systems comprised of achiral rod-shaped 4-arylbenzoate esters is described. These systems were found to give rise to spontaneous induced circular dichroism (CD) signals when their homeotropically aligned smectic A (SmA) phase is cooled to room temperature. Negligibly small CD signals are produced in the SmA phases of these substances and the signals were found to increase with increasing smectic order. Since the advent of chirality occurs in freely suspended films, it is not a consequence of surface effects. Both positive and negative CD signals are observed with equal probability at different positions in these films (Fig. 1). An imbalance in the signs of the CD signals is promoted by including small quantities of a chiral analogue of the achiral ester molecule. Vibrational CD spectroscopy (Fig. 2) and theoretical calculations are used to analyze the conformational changes that are associated with the induced chirality of the rod-shaped molecules. The results show that the phenomenon is associated with twisting about the ester moiety in the in 4-arylbenzoate esters.



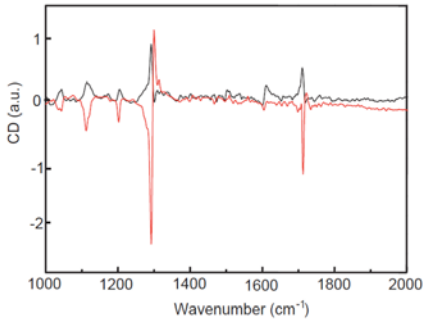


Fig. 1 (left):
CD spectra from + and – domains.

Fig. 2 (right):
VCD spectra from + and – domains.