

Electronic Supporting Information

In search of a new design strategy for solid single-component organic ferroelectrics: Polar crystalline phases formed by bent-core molecules

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Fig. ESI 1: Microphotograph of compound **2 (2676)** showing two different crystalline modifications at 146 °C on cooling: grey: CrI; brownish-orange: CrII

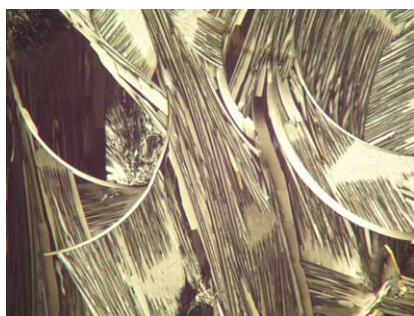


Fig. ESI 2: Micrograph of the crystalline texture of compound **3 (2678)** on cooling the isotropic liquid, cooling rate 2K/min

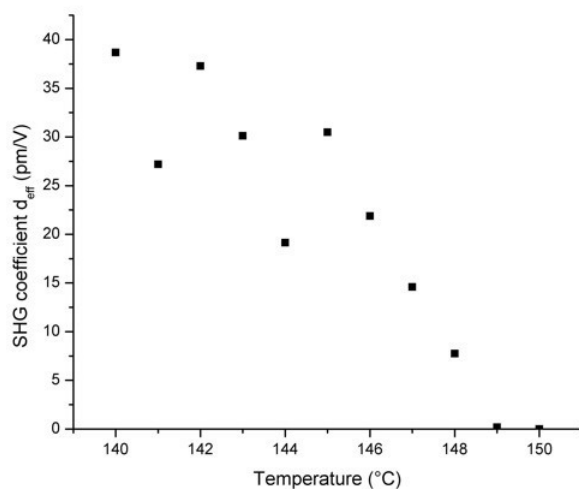


Fig. ESI 3: SHG signal found on compound **21** (**SM 13**) after the sample was cooled down from the isotropic liquid without electric field



Fig. ESI 4: Texture of the crystalline phase CrIII of compound **31**/KB 70/11e at 135 °C



a)



b)

Fig. ESI 5: Textures of the crystalline phase of compound **28**/KB93/11c in a 6 μm cell at 162 °C. By de-crossing of one polarizer from the 90° state chiral domains become apparent: a) decrossing by + 15°; b) decrossing by -15°.

X-ray studies on compound **28**:

Guinier powder patterns for the high temperature phase of compound **28** indicate a layer structure with a layer spacing of 4.7 nm (at 155 °C) (Fig. ESI 6). The diffuse outer scattering characteristic for a liquid-like order of parts of the structure is superimposed by a comparatively sharp and strong reflection at $2\theta = 15.74^\circ$ ($d = 5.6 \text{ \AA}$) (see interpretation of the X-ray measurements for compound **30**).

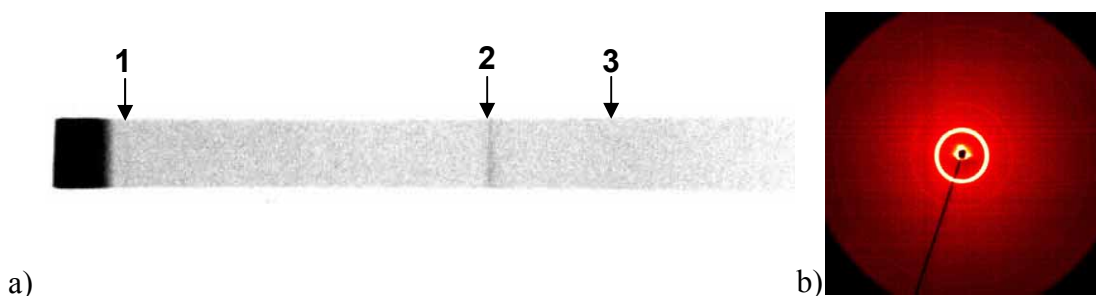


Fig. ESI 6: XRD patterns of powder-like samples of compound **28**/KB93 at 155 °C on cooling: a) Guinier film pattern for the wide-angle region showing one reflection (2) and the outer diffuse scattering (3) along with the second order layer reflection (1), b) 2D pattern showing the 1st, 2nd, 3rd (very weak), and 5th order of the layer reflection.

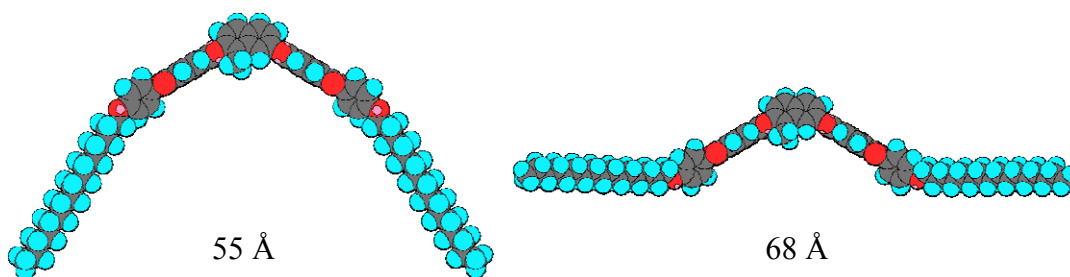


Fig. ESI 7 Molecular length of compound **34** estimated for two extreme chain conformations (measurement as in Fig. 15 for compound **23**, Chem3D, Cambridge Soft.Com, 2000; energy minimized by MM2 starting from all-trans conformations of the chains)