

Supplementary materials for the article

The influence of the molecular structure of compounds on their properties and the occurrence of chiral smectic phases

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MASS SPECTRA OF MESOGENS

The purity of the liquid crystalline esters was recorded using a Shimadzu prominence chromatograph. The strong molecular ion with a captured sodium atom $[M + Na]^+$ was observed; see Figures S1 and S2.

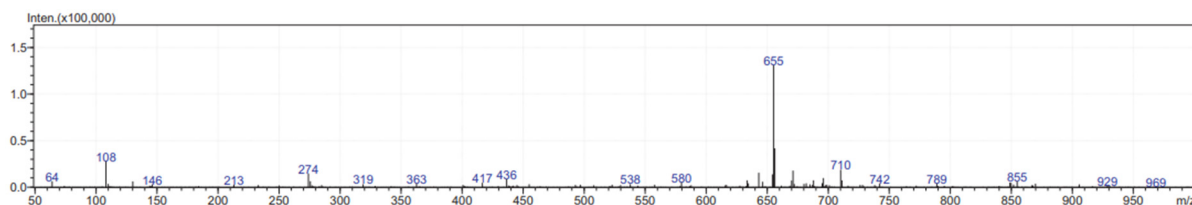


Figure S1. Mass spectrum of the compound 3PhPhCH₂O.

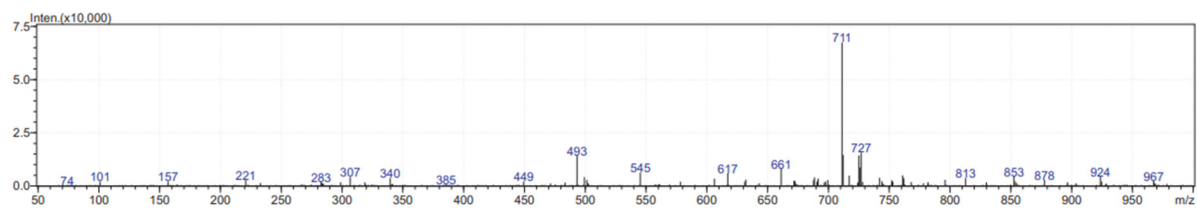


Figure S2. Mass spectrum of the compound 7PhPhCH₂O.

STRUCTURE CONFIRMATION OF MESOGENS

A comparison of NMR spectra confirmed the compliance of real structures with the planned structures; see Figures S3-S6.

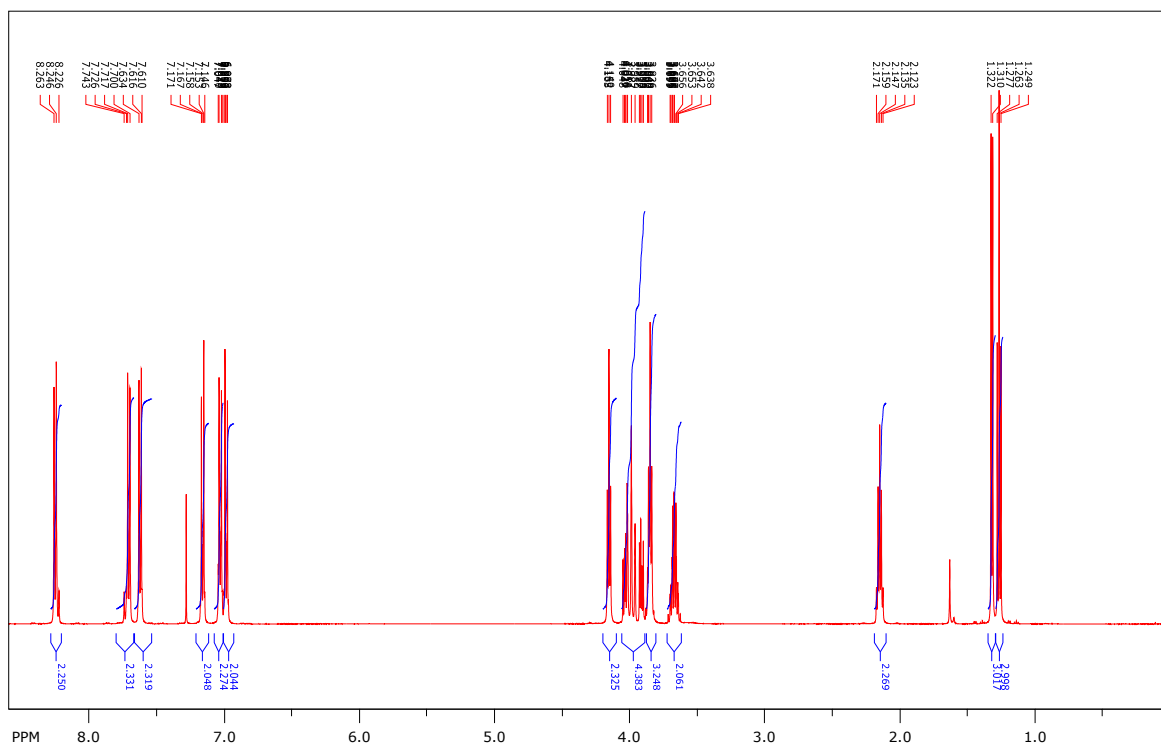


Figure S3. ¹H NMR spectrum of the compound 3PhPhCH₂O in CDCl₃.

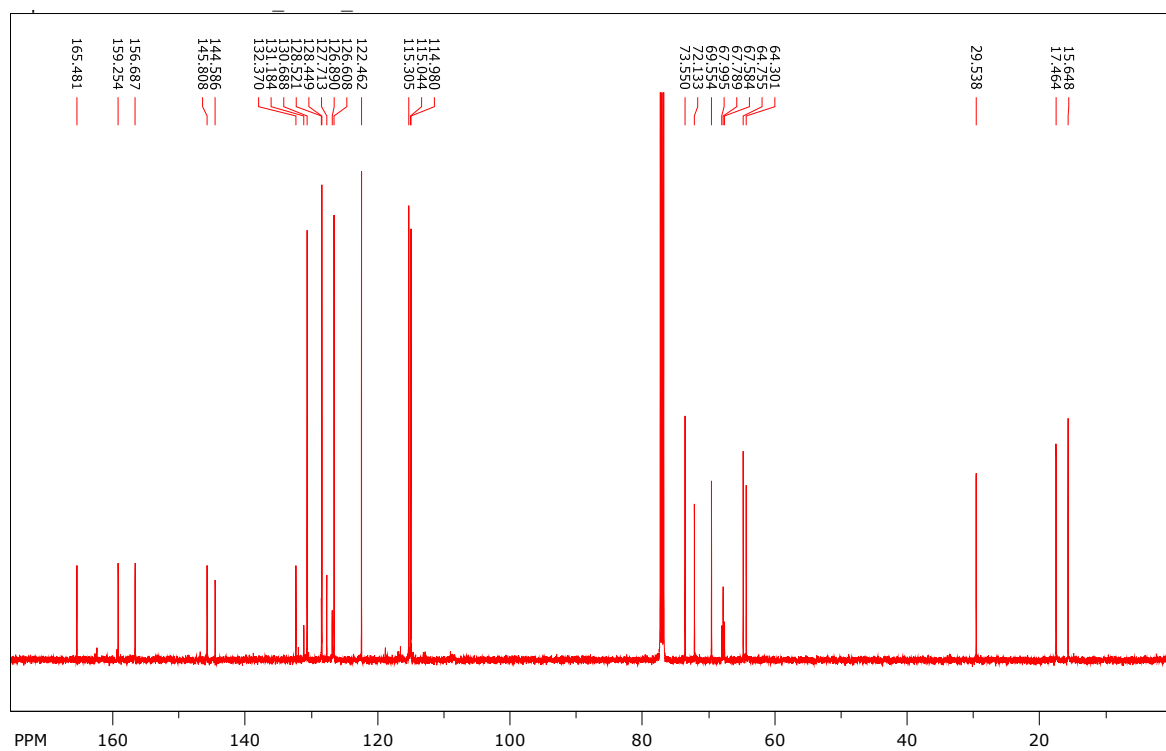


Figure S4. ¹³C NMR spectrum of the compound 3PhPhCH₂O in CDCl₃.

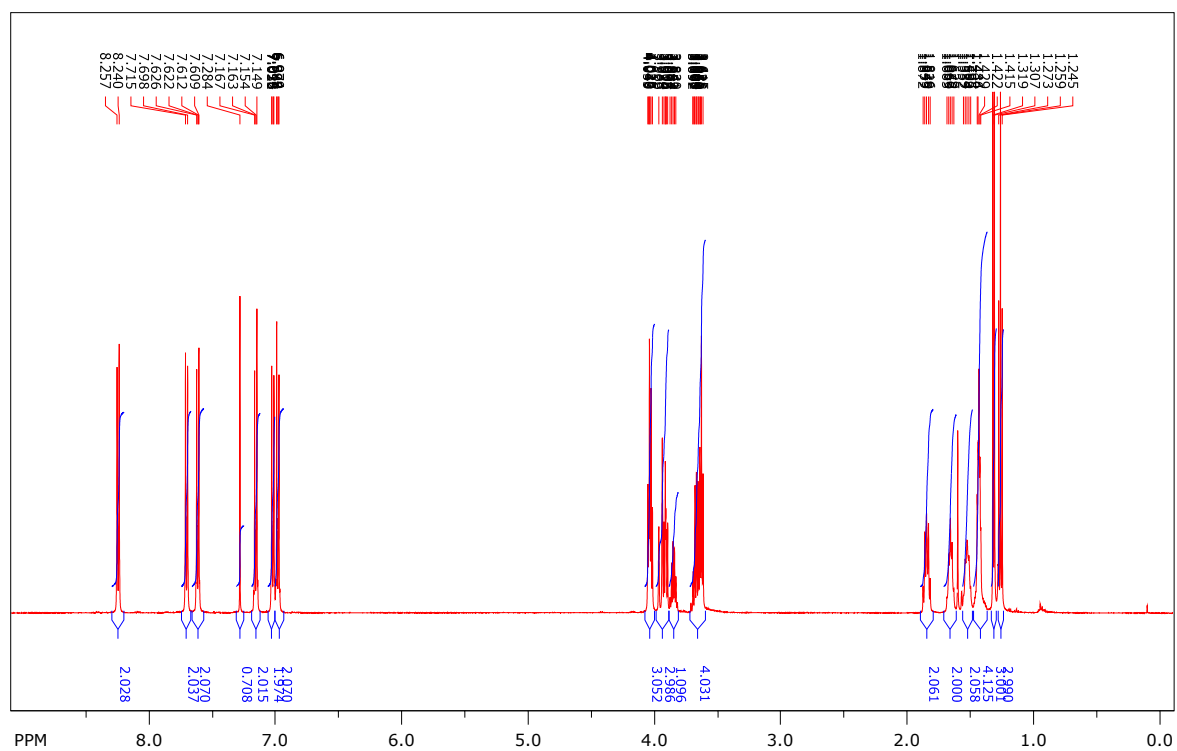


Figure S5. ¹H NMR spectrum of the compound 7PhPhCH₂O in CDCl₃.

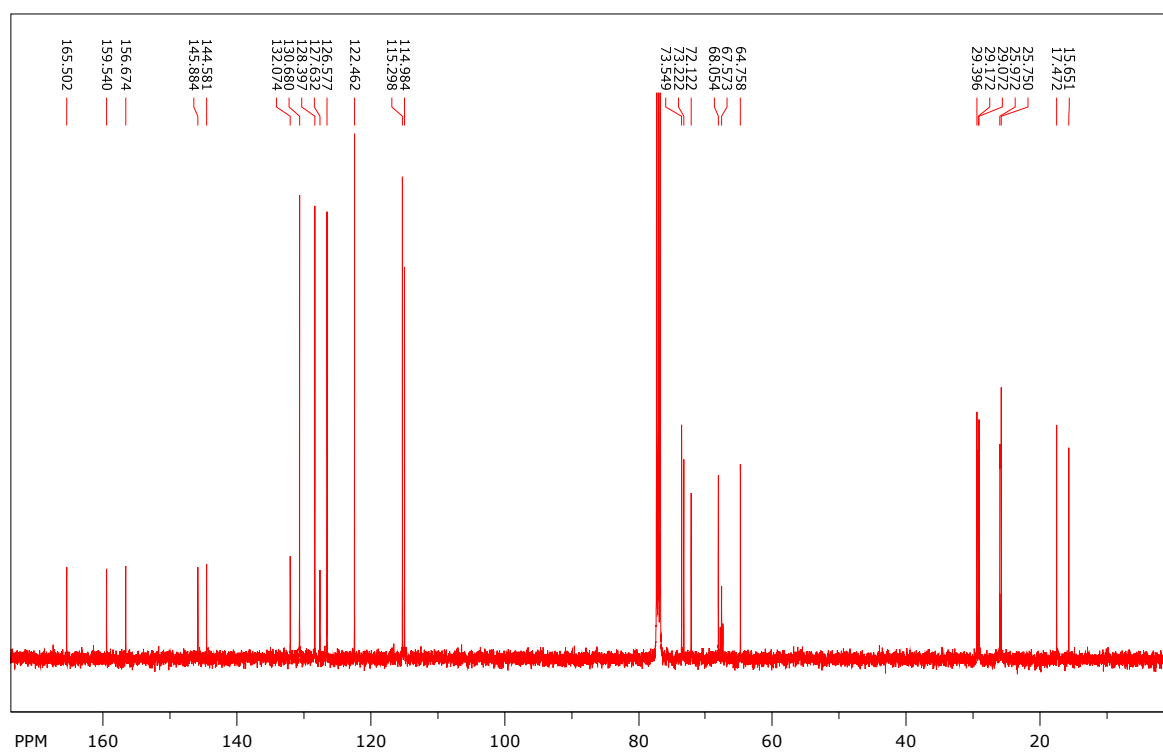
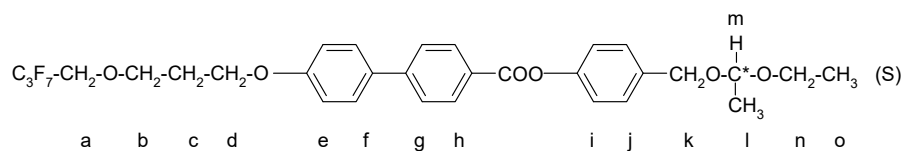


Figure S6. ^{13}C NMR spectrum of the compound 7PhPhCH₂O in CDCl₃.

The chemical shift values for obtained mesogens are given in Tables S1 and S2. Protons are marked as shown below:

A. 3PhPhCH₂O



B. 7PhPhCH₂O

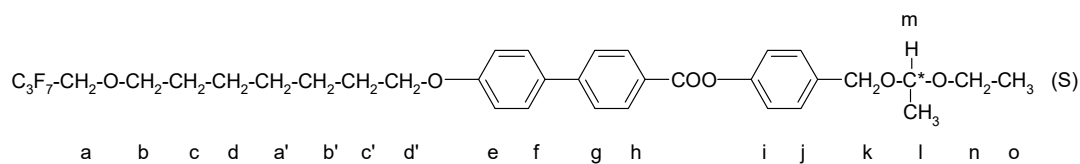


Table S1. ¹H NMR chemical shift data (ppm) for mesogens in CDCl₃ solution.

| Protons | Mesogen A. | Mesogen B. |
|-----------|---------------|----------------------|
| a | 3.917 (2H, t) | 3.914 (2H, t) |
| b | 3.670 (2H, t) | 3.664 (2H, t) |
| c | 2.147 (2H, m) | 1.415-1.872 (10H, m) |
| d | 4.037 (2H, t) | |
| a' | | |
| b' | | |
| c' | | |
| d' | | 3.966 (2H, t) |
| e | 7.023 (2H, d) | 7.028 (2H, d) |
| f | 7.158 (2H, d) | 7.163 (2H, d) |
| g | 7.616 (2H, d) | 7.622 (2H, d) |
| h | 7.726 (2H, d) | 7.715 (2H, d) |
| i | 6.992 (2H, d) | 6.988 (2H, d) |
| j | 8.246 (2H, d) | 8.257 (2H, d) |
| k | 3.860 (2H, t) | 3.853 (2H, t) |
| l | 1.310 (3H, d) | 1.307 (3H, d) |
| m | 4.152 (1H, m) | 4.040 (1H, m) |
| n | 1.322 (2H, m) | 1.319 (2H, m) |
| o | 1.263 (3H, t) | 1.259 (3H, t) |

Table S2. Values of chemical shifts for the chiral center (atoms “m”) of mesogens in ^1H and ^{13}C NMR spectra.

| | | |
|-------------------|-----------------|-----------------------------------------------------|
| Mesogen A. | 4.152 67.789 | ^1H NMR [ppm] ^{13}C NMR [ppm] |
| Mesogen B. | 4.040 68.054 | ^1H NMR [ppm] ^{13}C NMR [ppm] |

3D PLOTS OF IMAGINARY PART ϵ''_{\perp} OF DIELECTRIC PERMITTIVITY VERSUS FREQUENCY AND TEMPERATURE AT COOLING WITH THE 10 V DC FIELD FOR BOTH STUDIED MESOGENS

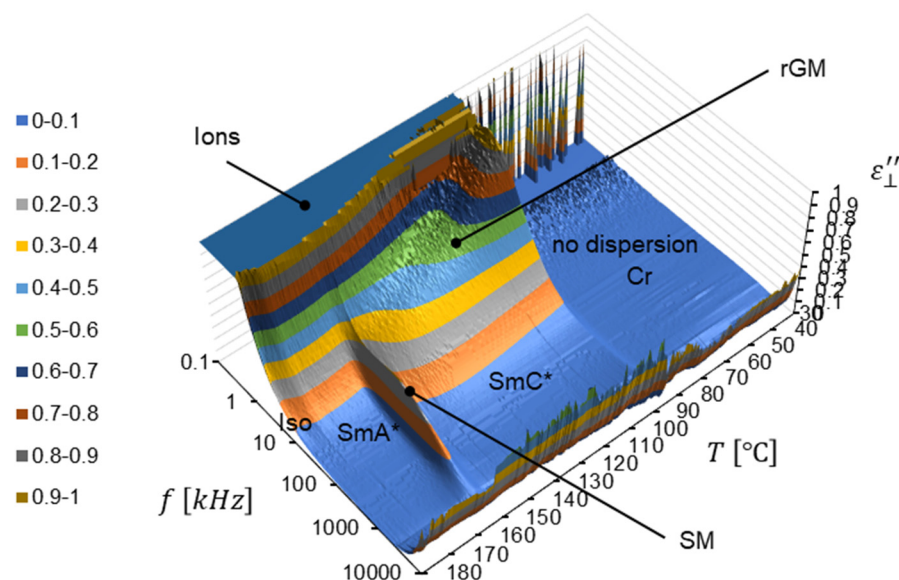


Figure S7. Imaginary part ϵ''_{\perp} of dielectric permittivity for the compound 3PhPhCH₂O. In 5 μm thin cell measurement at cooling, planarly aligned, with gold electrodes. Cooling rate 0.5°C/min. The 10 V DC field. Isotropic liquid, the SmA* (soft mode: SM) and the SmC* (residual Goldstone mode: rGM) phases, and molecular crystal (Cr) are observed.

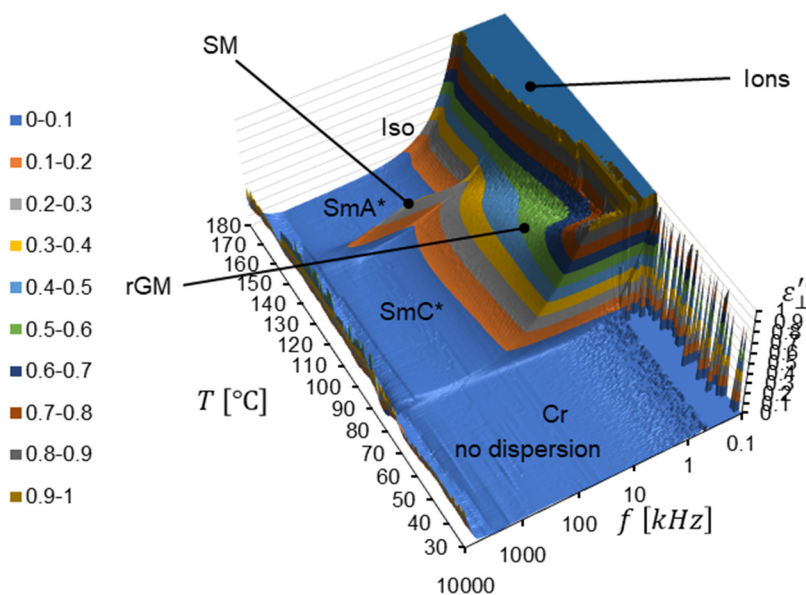


Figure S8. Imaginary part ϵ''_{\perp} of dielectric permittivity for the compound 3PhPhCH₂O. In 5 μm thin cell measurement at cooling, planarly aligned, with gold electrodes. Cooling rate 0.5°C/min. The 10 V DC field. Isotropic liquid, the SmA* (soft mode: SM) and the SmC* (residual Goldstone mode: rGM) phases, and molecular crystal (Cr) are observed.

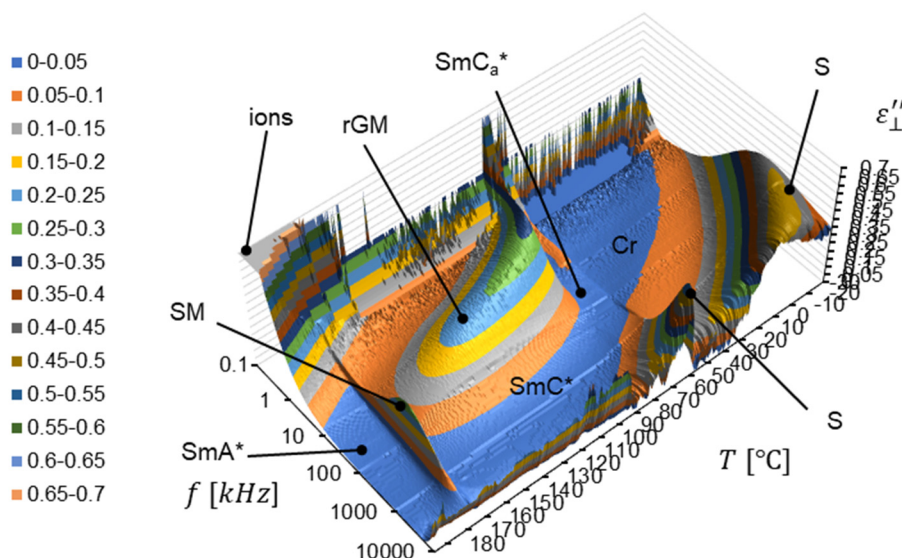


Figure S9. Imaginary part ϵ''_{\perp} of dielectric permittivity for the compound 7PhPhCH₂O. In 5 μm thin cell measurement at cooling, planarly aligned, with gold electrodes. Cooling rate 0.5°C/min. The 10 V DC field. The SmA* (soft mode: SM), the SmC* (residual Goldstone mode: rGM), the SmC_a* (molecular S-mode) phases, and molecular crystal (Cr) (molecular S-mode) are observed.

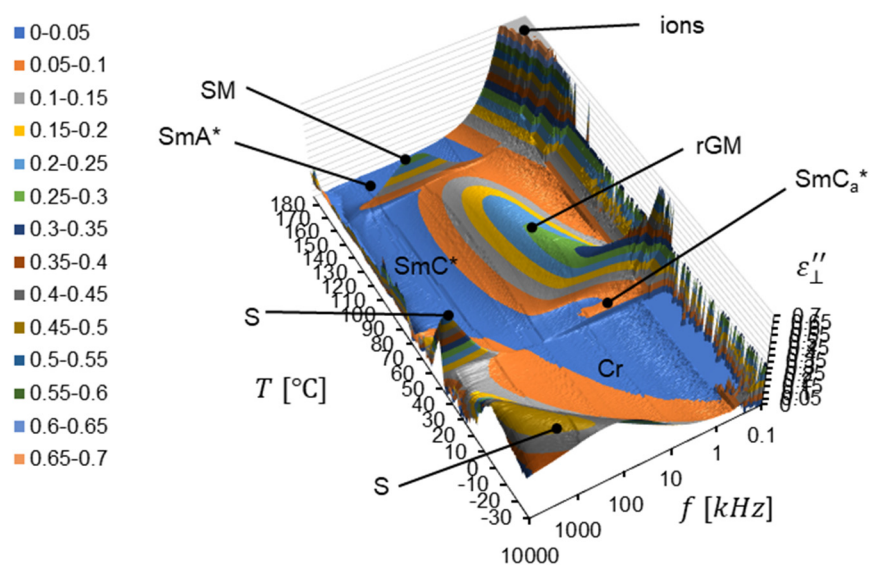


Figure S10. Imaginary part ϵ''_{\perp} of dielectric permittivity for the compound 7PhPhCH₂O. In 5 μm thin cell measurement at cooling, planarly aligned, with gold electrodes. Cooling rate 0.5°C/min. The 10 V DC field. The SmA* (soft mode: SM), the SmC* (residual Goldstone mode: rGM), the SmC_a* (molecular S-mode) phases, and molecular crystal (Cr) (molecular S-mode) are observed.