Molecular dynamics and kinetics of isothermal cold crystallization in the chiral smectogenic 3F7FPhH6 glassformer

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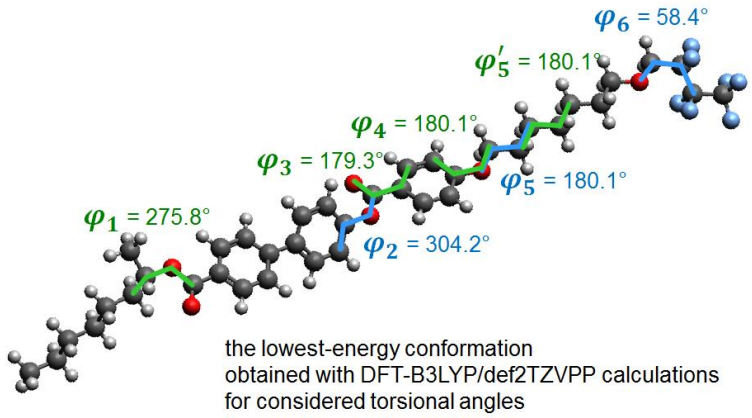
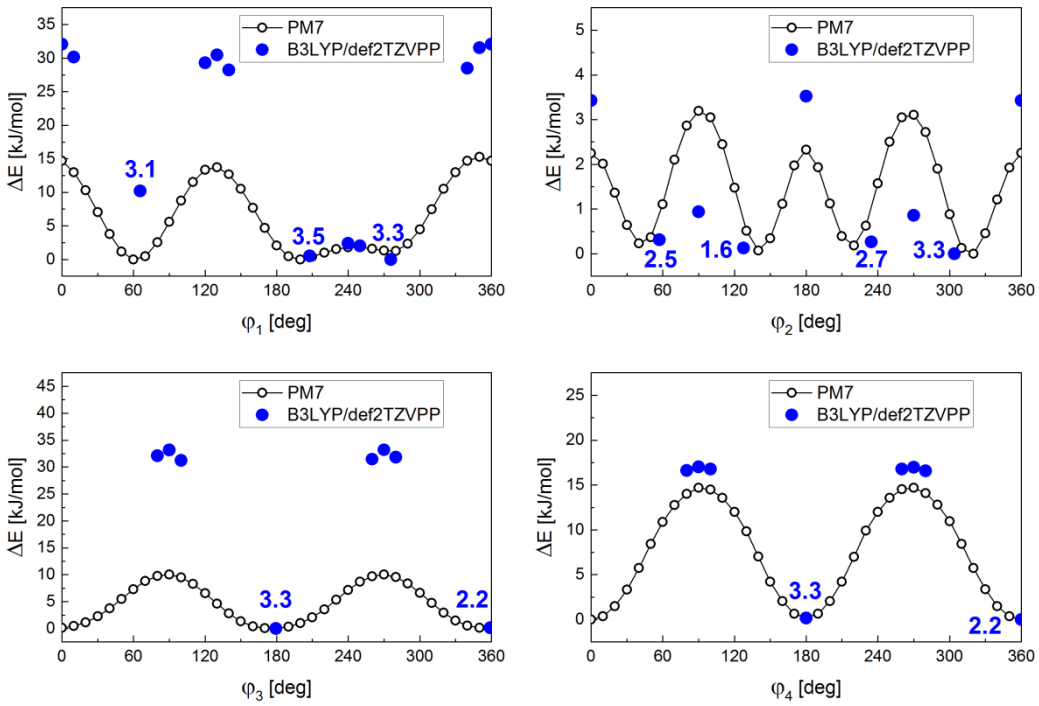
Supplementary Materials



the lowest-energy conformation
obtained with DFT-B3LYP/def2TZVPP calculations
for considered torsional angles



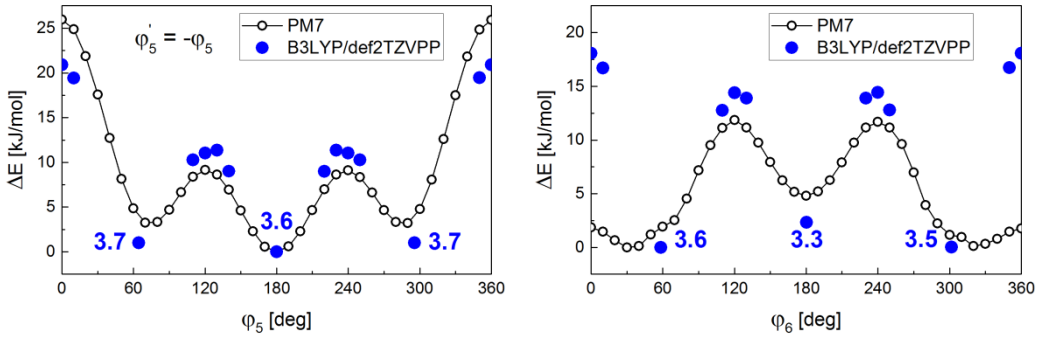


Figure S1. Relative conformational energy calculated with PM7 and DFT-B3LYP/def2TZVPP methods for selected torsional angles within the isolated 3F7HPhH6 molecule. For each energy minimum, the total dipole moment (in Debye) is shown as calculated with DFT-B3LYP/def2TZVPP.

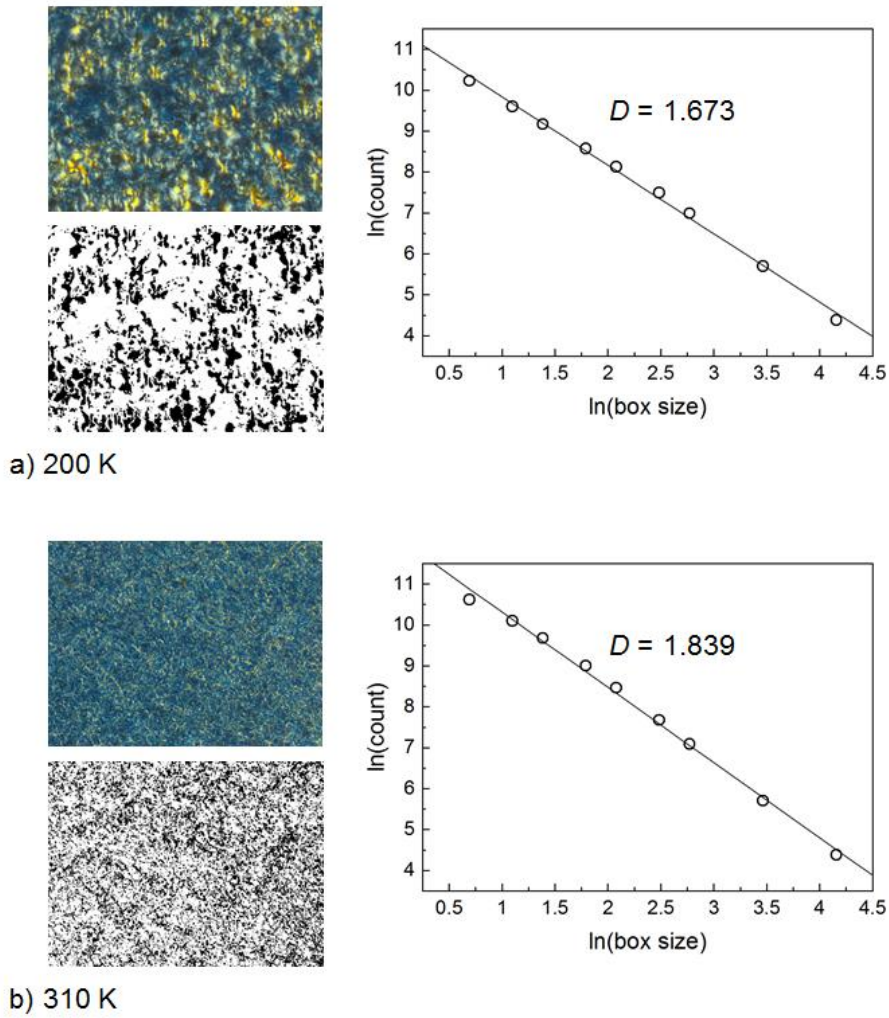


Figure S2. Textures of 3F7FPhH6 registered during heating from 173 K with 2 K/min rate at 200 K (a) and 310 K (b), analysed with the fractal box count method. The fractal dimension D is determined as the slope of the $\ln L$ vs. $\ln N$ plot, where L is the box size and N is the number of boxes necessary to cover the whole pattern in the binary version of the texture (black area in this case).

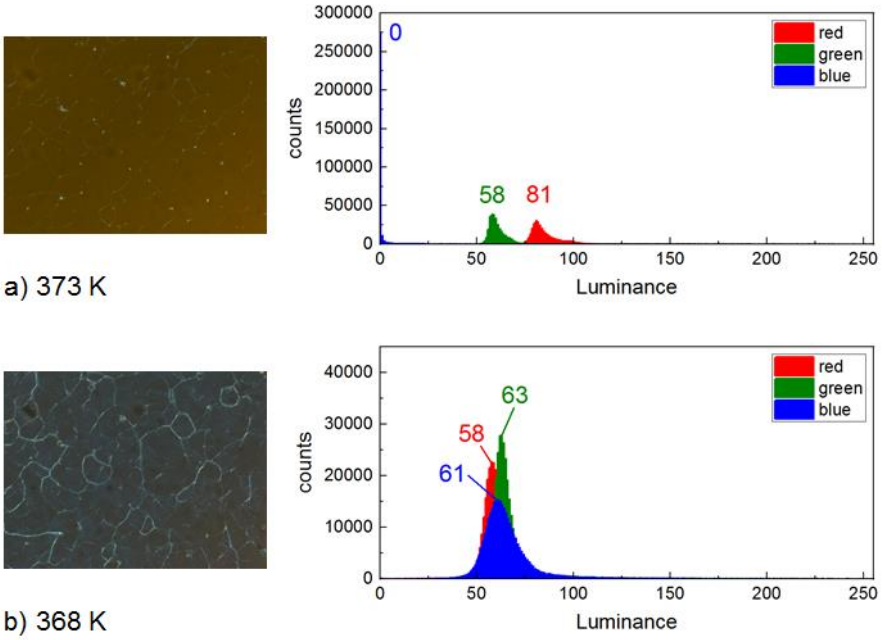


Figure S3. Textures of 3F7FPhH6 registered on cooling with 2 K/min rate at 373 K (a) and 368 K (b) with histograms of luminance of red, green and blue components. The modal luminance of (red, green, blue) component is (81, 58, 0) for 373 K and (58, 63, 61) for 368 K.

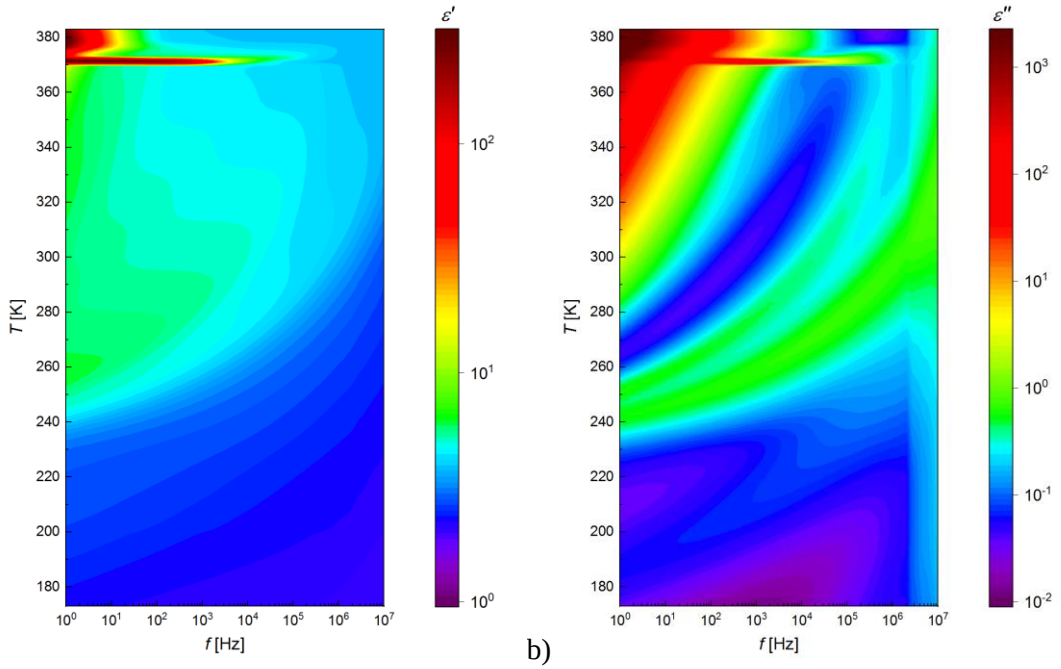
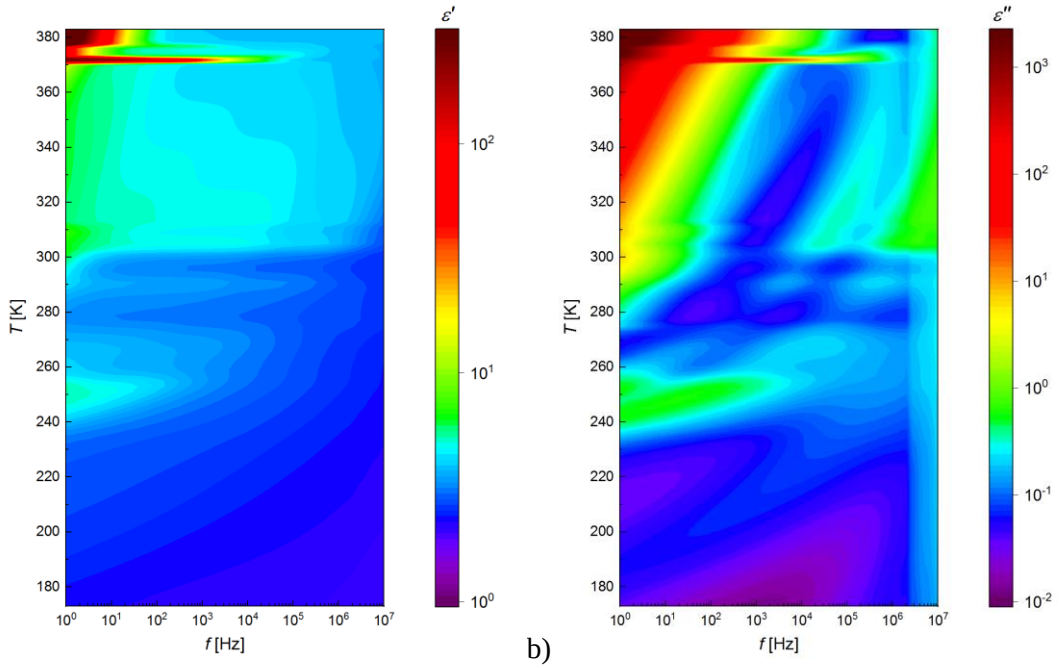
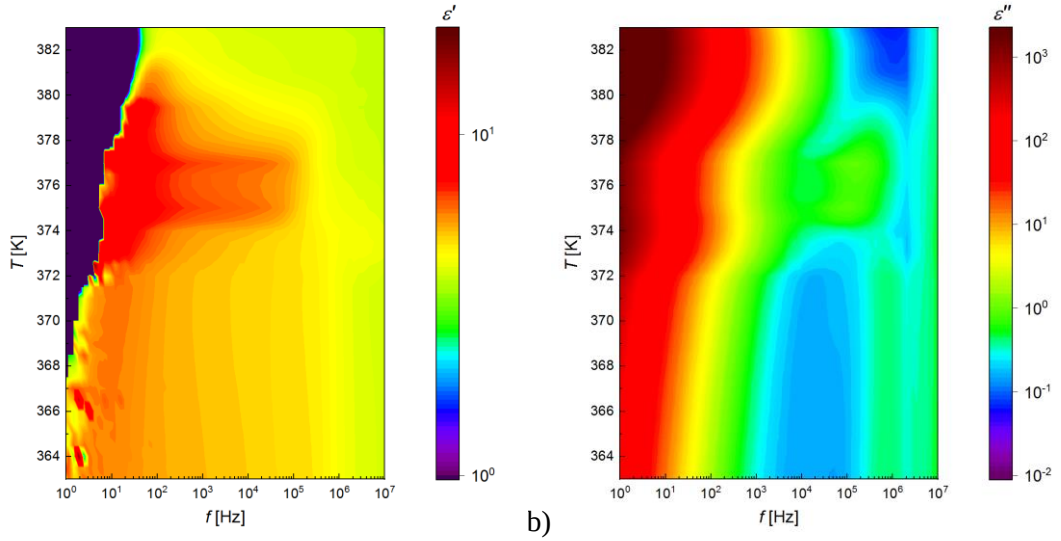


Figure S4. Real (a) and imaginary (b) part of the dielectric spectra of 3F7FPhH6 registered on cooling without application of the bias field.



a) b)

Figure S5. Real (a) and imaginary (b) part of the dielectric spectra of 3F7FPhH6 registered on heating without application of the bias field.



a) b)

Figure S6. Real (a) and imaginary (b) part of the dielectric spectra of 3F7FPhH6 registered on cooling in the 40 V bias field.