POLIMORPHISM, STRUCTURE AND DYNAMICS INVESTIGATIONS OF 4-N-HEPTYL-2',3'-DIFLUORO-4'-UNDECYLOXYBIPHENYL AND 4-N-HEPTYL-2',3'-DIFLUORO-4'-NONYLOXYBIPHENYL

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4-n-heptyl-2',3'-difluoro-4'-undecyloxybiphenyl (4HFDB) and 4-n-heptyl-2',3'-difluoro-4'-nonyloxybiphenyl (4HFNB) are liquid crystalline compounds of chemical formula C_7H_{15}-C_6H_4-$C_6H_2F_2$-O-$C_{11}H_{23}$ and C_7H_{15}-C_6H_4-$C_6H_2F_2$-O-C_9H_{19}, respectively, i.e. they differ in the length of the alkyl chain. The latter appears to be strongly affecting their physicochemical properties. The crystal phase, when heated, melts to isotropic liquid at 315 K for 4HFDB and 307 K for 4HFNB. Upon cooling, we identify the following sequences (via DSC scans): IL (309.5 K) SmA for 4HFDB, and IL (303.9 K) N (302.5 K) SmA for 4HFNB. More detailed information on the changes in structure and dynamics of 4HFDB and 4HFNB at the phase transitions comes from X-Ray diffraction, polarizing microscopy (Fig. 1) and Fourier absorption infrared spectroscopy (Fig. 2). Both compounds crystallize in orthorhombic structures (space group *Pmmm*) at RT. The *a* lattice parameter, closely related to the molecule length, was 29.9(1) Å for 4HFDB and 27.4(2) Å for 4HFNB. Both liquid mesogens are glass-formers and the glass transition temperature was observed about 210 K and 230 K for 4HFDB and 4HFNB, respectively. The vibration C-F mode is not an easy task to analyse due to a strong influence of other vibrations. Moreover, substitution of original hydrogens with fluorine causes a significant shift of bands towards higher frequencies. In order to interpret the experimental results of dynamics, calculations were carried out using Mopac and Dmol3 contained in the Materials Studio package.

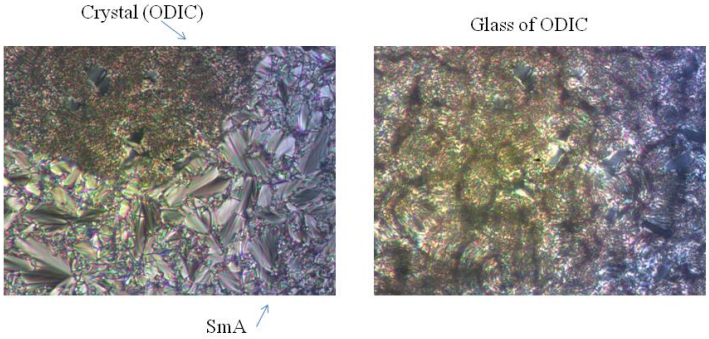

Fig 1 Polarizing microscopy texture observations of 4HFDB SmA to Cr phase ODIC type at 296 K and glass of ODIC at 205 K.

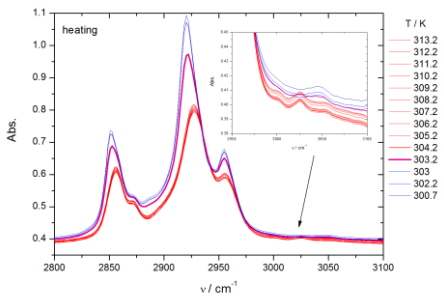

Fig.2. FT-IR spectra for 4HFNB obtained during heating. The melting of the crystal phase (ODIC type) appears at about 303 K.