Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

On relaxation and vibrational dynamics in the thermodynamic states of a chiral smectogenic glass-former

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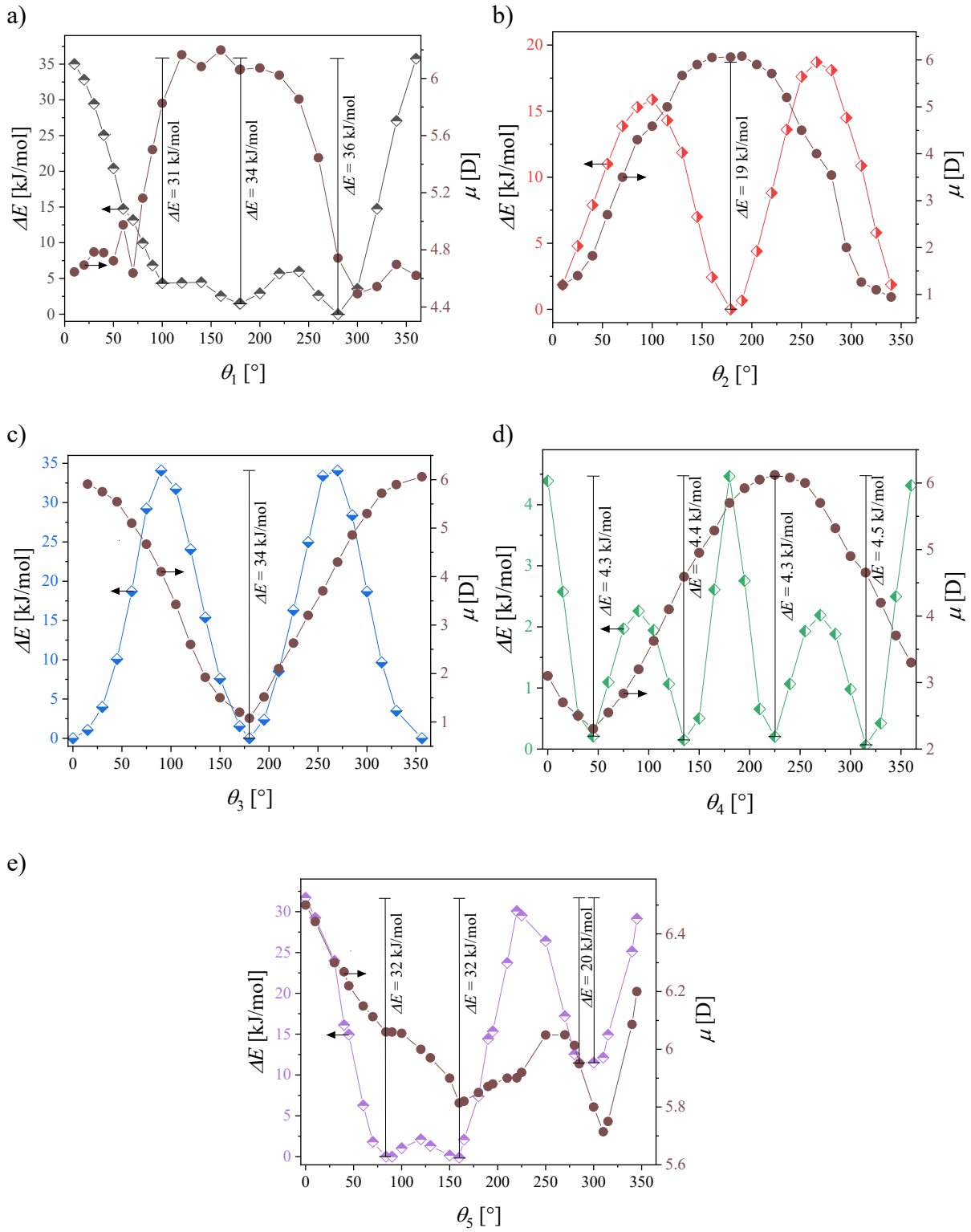

Fig. S1. The relative conformational energy ΔE and the dipole moment μ with respect to the optimized structure of 3F5HPhH7 vs. the torsional angles: a) θ_1, b) θ_2, c) θ_3, d) θ_4 and e) θ_5 obtained by DFT calculations.

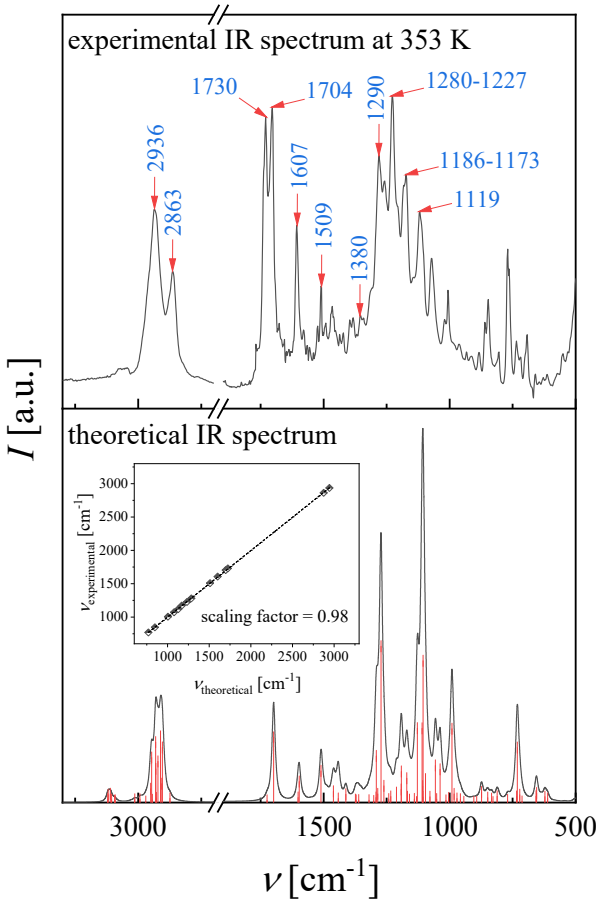

Fig. S2. Measured (upper plot) and calculated (lower plot) infrared spectra of 3F5HPhH7. The inset presents the determination of a scaling factor.

$\nu_{experimental}\,[cm^{-1}]$	$\nu_{theoretical}\,[cm^{-1}]$	**Assignment**
776	785	ρ(C-H)
1024	1030	ν(C-C-O)$_{sym}$
1119	1128	ρ(C-H)
1165-1195	1170-1192	ν(C-O-C)$_{sym}$
1207-1280	1203-1282	ν(C-O-C)$_{asym}$
1510-1290	1509-1287	γ(C-H) + ω(C-H) + β(C-H)$_{sym}$
1607	1601	ν(C=O)
1704	1698	ν(C=O)$_{chiral\_c.}$
1730	1724	ν(C=O)$_{core}$
2853	2864	ν(CH$_2$)$_{sym}$
2872	2883	ν(CH$_3$)$_{sym}$
2928	2935	ν(CH$_2$)$_{asym}$
2953	2963	ν(CH$_3$)$_{asym}$

Fig. S3. Assignment of the most representative vibration modes observed on experimental $(\nu_{experimental})$ and theoretical $(\nu_{theoretical})$ FTIR spectra. Abbreviations: ρ-rocking, ν-stretching, γ- bending out-of-plane, ω-wagging, β-bending in-plane, asym-asymmetric, sym-symmetric.

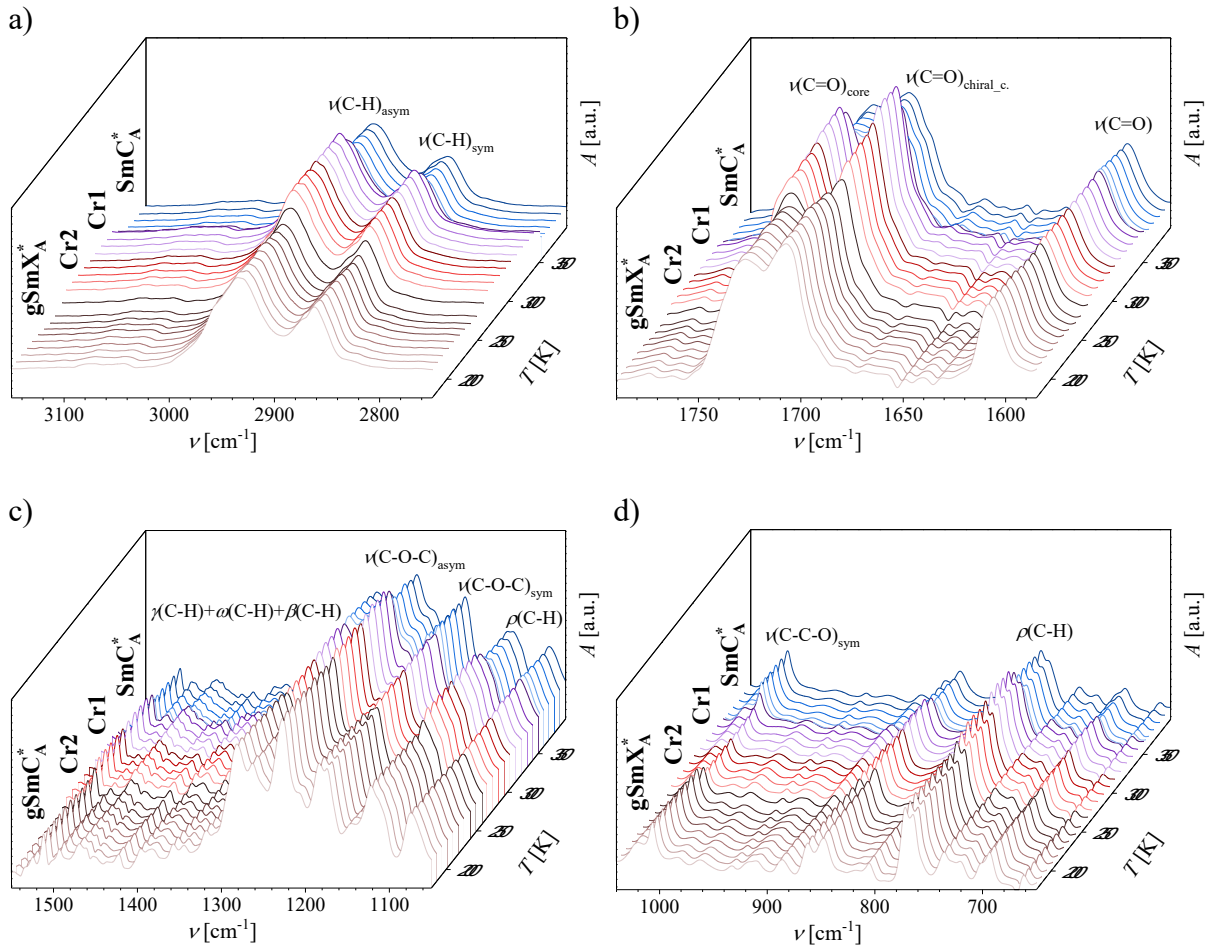

Fig. S4. Infrared spectra obtained upon heating after fast cooling from 173 to 400 K in the wavenumber ν regions of: a) 3150-2750 cm^{-1}; b) 1800-1580 cm^{-1}, c) 1550-1050 cm^{-1}, d) 1000-680 cm^{-1}.

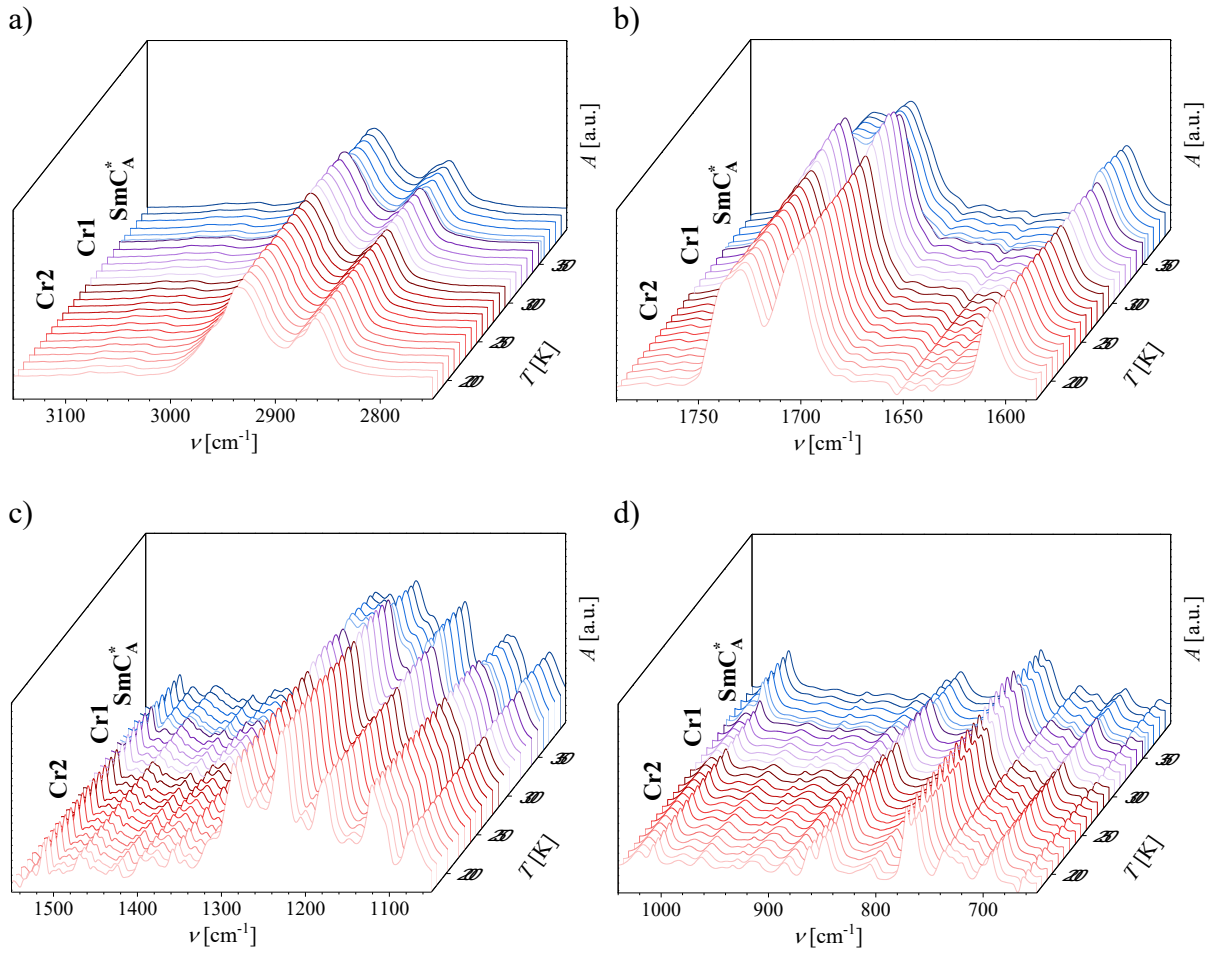

Fig. S5. Infrared spectra obtained upon heating after slow cooling from 173 to 400 K in the wavenumber ν regions of: a) 3150-2750 cm^{-1}; b) 1800-1580 cm^{-1}, c) 1550-1050 cm^{-1}, d) 1000-680 cm^{-1}.