SUPPLEMENTARY INFORMATION

Chemical and physical properties of orthoconic liquid crystals: ^{2}H NMR spectroscopy and Molecular Dynamics simulations

Anna Drzewicz[a], Martina Rossi[b], Mario Cifelli[b], Giacomo Saielli[c,d], Marzena Tykarska[e], Valentina Domenici[b*]

a. Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland.
b. Dipartimento di Chimica e Chimica Industriale, University of Pisa, via Moruzzi 13, Pisa 56124, Italy.
c. CNR, Institute on Membrane Technology Unit of Padova, Via Marzolo, 1 – 35131, Padova, Italy.
d. Department of Chemical Sciences, University of Padova, Via Marzolo, 1 – 35131, Padova, Italy.
e. Institute of Chemistry, Military University of Technology, PL-00908 Warszawa, Poland.

* Corresponding author: valentina.domenici@unipi.it

Computational study:

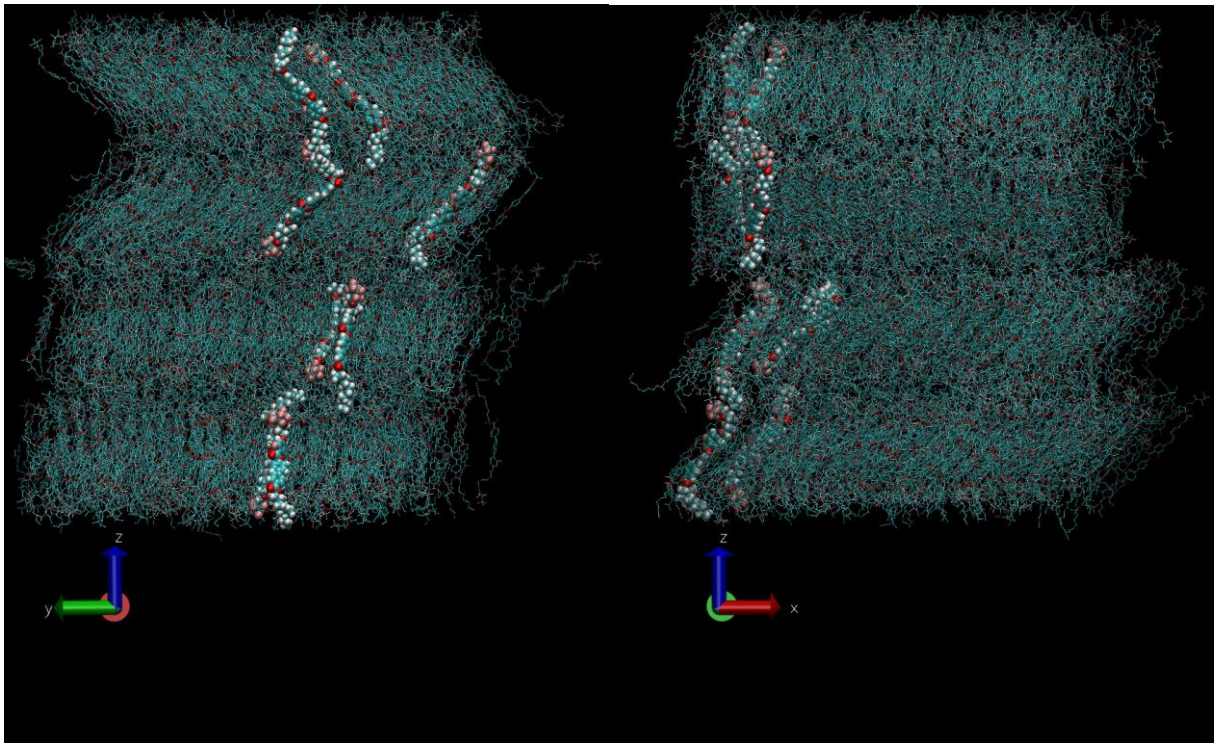

Figure S1. Snapshot of the simulation box after 150 ns at T = 400 K, NpT ensemble with semi-isotropic pressure coupling, (left): view along the *x* axis; (right): view along the *y* axis Molecules show a large tilt with respect to the layer normal, however there is no correlation of the tilt angles of adjacent layers. From top to bottom, molecules in the first layer are tilted approximately along the *zy* diagonal, molecules in the second layer are tilted along the *z*(-*y*) diagonal; molecules in the third and fourth layers are tilted along the *zx* diagonal.

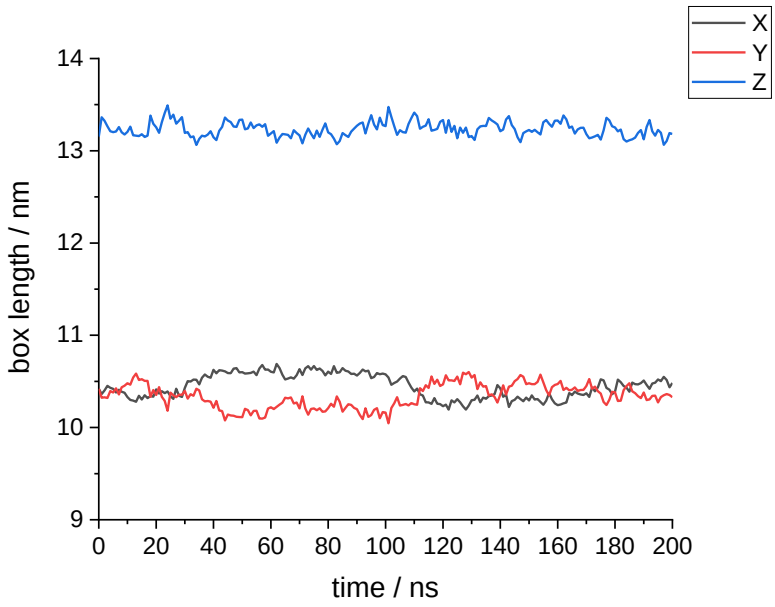

Figure S2. Time dependence of the length of the box sides of the simulation box during the equilibration run with fully anisotropic pressure coupling.

Table S1: Orientation of selected molecular vectors: u_x, u_y, u_z are the unitary components of the given vector in the box frame; θ_z is the angle of the given vector with the director of the phase, that is the normal to the layers (*z* axis of the box).

	Layer	u_x	u_y	u_z	θ_z
	1	-0.0282405	-0.678729	0.733846	42.6545
	2	-0.168539	0.658824	0.733175	42.7108
phenyl	3	-0.347933	-0.575065	0.740435	42.0976
C01-C04	4	0.237812	0.628284	0.740746	42.071
	1	-0.032421	-0.668928	0.74262	41.9116
	2	-0.16388	0.651099	0.74109	42.0419
biphenyl	3	-0.343713	-0.568005	0.747818	41.4663
C0S-C0E	4	0.2354	0.623312	0.745701	41.6481
	1	-0.0326996	-0.676065	0.736116	42.4633
	2	-0.165445	0.657079	0.735442	42.5201
core	3	-0.346887	-0.573589	0.742068	41.9586
C0S-C04	4	0.237121	0.629068	0.740302	42.1088
	1	0.0228838	0.506763	-0.861782	149.043
	2	0.125012	-0.484758	-0.865668	149.483
head2tail	3	0.261362	0.436124	-0.861095	148.966
C1O-C2P	4	-0.173703	-0.468593	-0.866168	149.54
	1	0.0228838	0.506763	-0.861782	149.043
	2	0.125012	-0.484758	-0.865668	149.483
C-chain	3	0.261362	0.436124	-0.861095	148.966
C1W-C2P	4	-0.173703	-0.468593	-0.866168	149.54
	1	0.0227049	0.50334	-0.86379	149.27
	2	0.129351	-0.477743	-0.868925	149.857
F-chain	3	0.254393	0.432335	-0.865084	149.417
C1O-C04	4	-0.17493	-0.45485	-0.873219	150.356

DSC CURVES

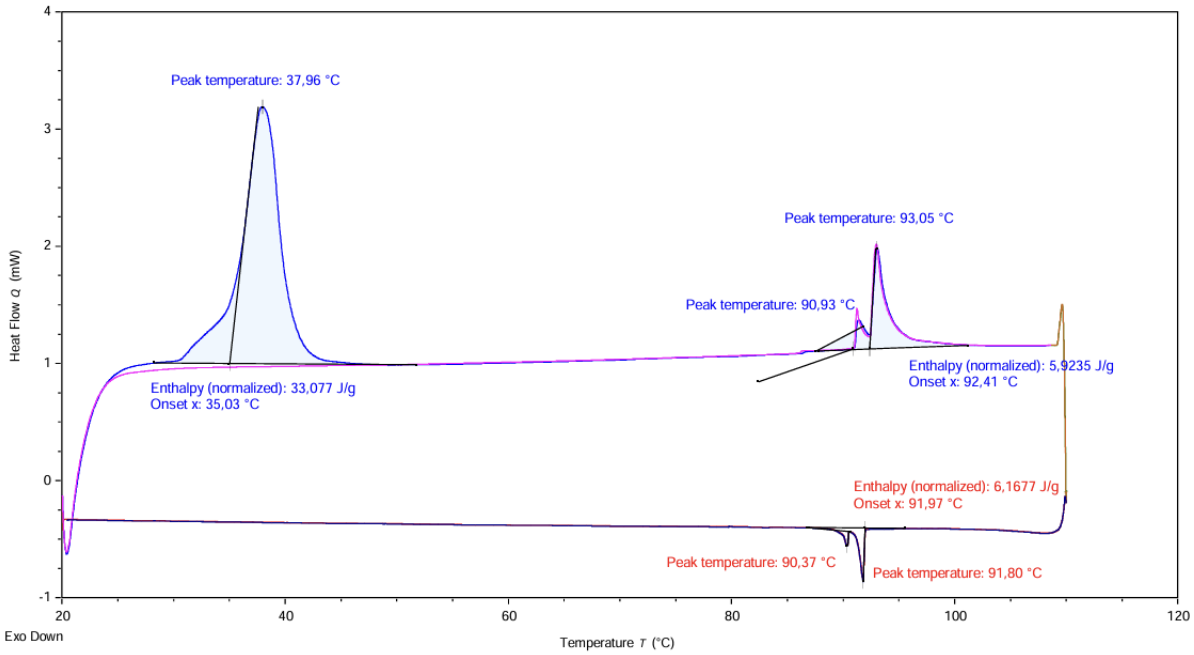

Figure S3. DSC of the mixture **3F7HPhF8 + probe-d_4**. See the main text for explanation.

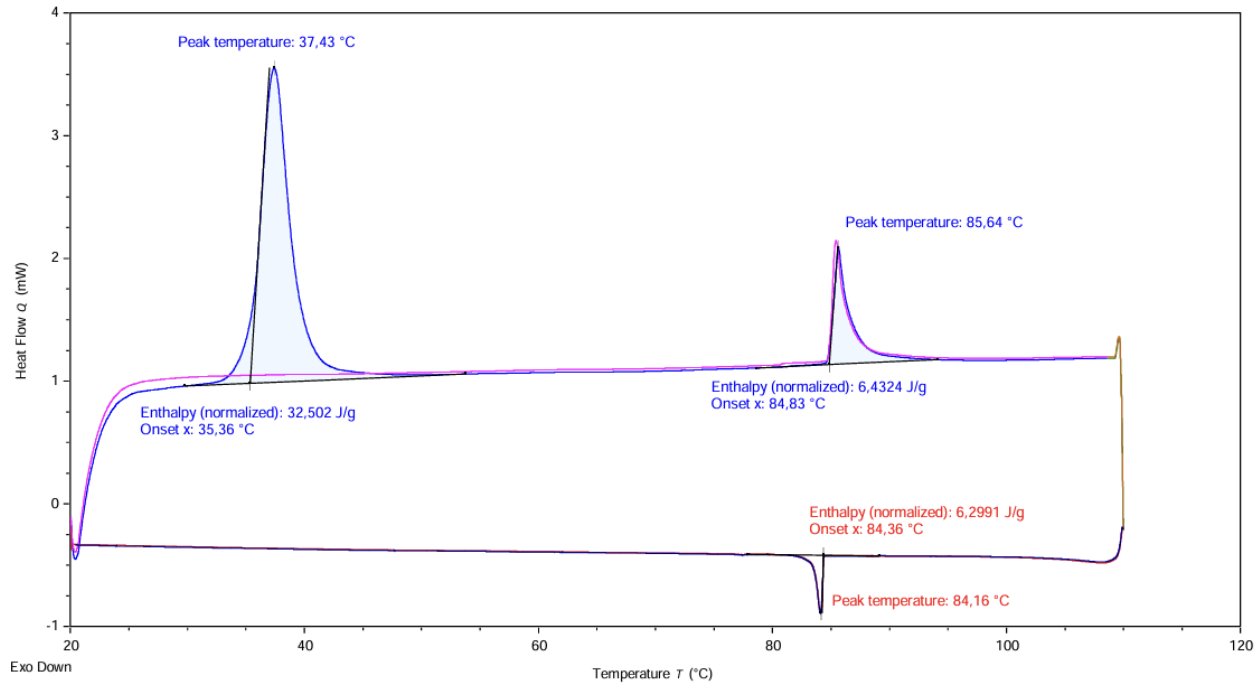

Figure S4. DSC of the mixture **3F5HPhF9 + probe-d_4**. See the main text for explanation.