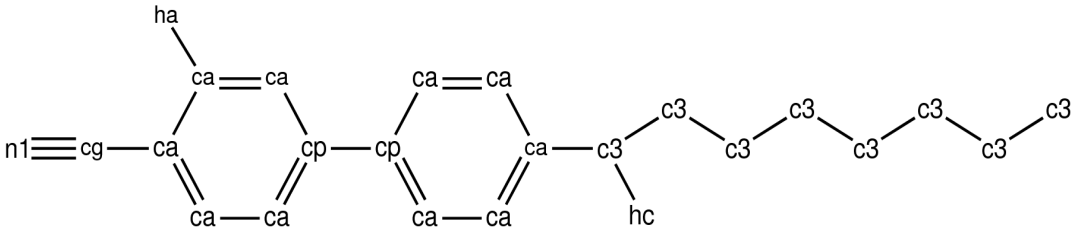
Electronic Supplementary Material (ESI) for Soft Matter

Molecular Dynamics and EPR spectroscopic studies of 8CB liquid crystal

F. Chami, M.R. Wilson and V.S. Oganesyan

Supporting Information

I. Force field parameters and topology for LC molecules:



Atom types for 8CB LC molecule

Table S1. LJ parameters

Atom type	σ (Å)	ε (kcal/mol)
n1	3.648	0.1700
cg	3.816	0.2100
ca	3.816	0.0860
ha	2.918	0.0150
cp	3.816	0.0860
c3	3.816	0.1094
hc	2.974	0.0157

Table S2. Bond-stretching parameters

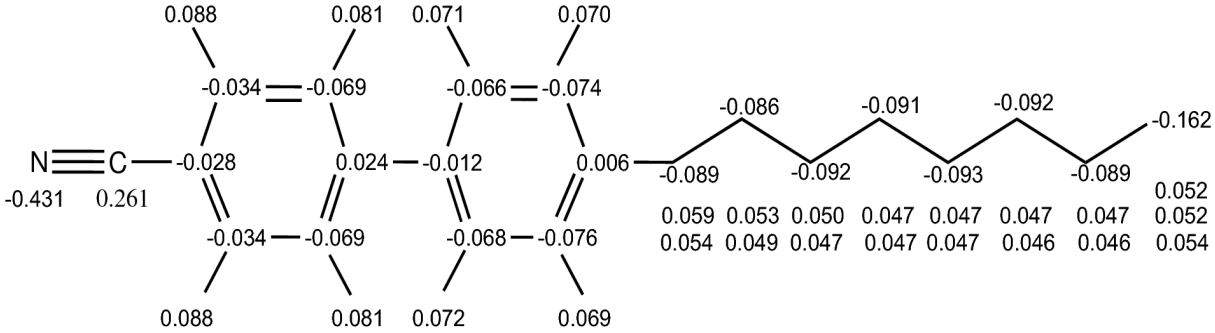
Bond	k_r (kcal mol^{-1} $Å^{-2}$)	r_0 (Å)
n1-cg	994.70	1.143
cg-ca	406.60	1.438
ca-ca	478.40	1.387
ca-ha	344.30	1.087
ca-cp	466.10	1.395
cp-cp	346.50	1.490
ca-c3	323.50	1.513
c3-hc	337.30	1.092
c3-c3	303.10	1.535

Table S3. Bond-angle bending parameters

Bond angle	k_θ (kcal mol^{-1} rad^{-2})	θ_0 (deg.)
n1-cg-ca	58.930	179.420
cg-ca-ca	65.900	120.050
ca-ca-ca	67.180	119.970
ca-ca-ha	48.460	120.010
ca-ca-cp	67.240	119.070
ca-cp-ca	67.250	118.330
ca-cp-cp	64.140	121.140
ha-ca-cp	48.030	121.080
ca-ca-c3	63.840	120.630
ca-c3-hc	46.960	110.150
ca-c3-c3	63.250	112.090
c3-c3-hc	46.370	110.050
c3-c3-c3	63.210	110.630
hc-c3-hc	39.430	108.350

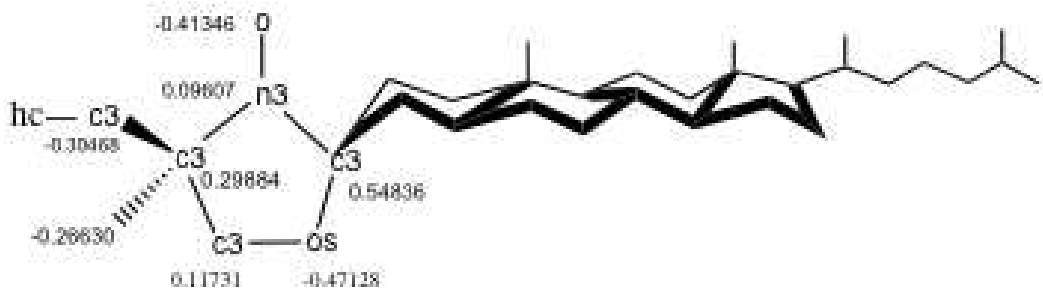
Table S4. Dihedral parameters

Dihedral	pk (kcal mol^{-1})	δ (deg.)	pn
x -ca-ca- x	3.625	180	2
x -ca-cp- x	3.625	180	2
ca-cp-cp-ca	1.000	180	2
ca-c3-c3-x	0.156	0	3
c3-c3-c3-hc	0.160	0	3
c3-c3-c3-c3	0.180	0	3
	0.250	180	2
	0.200	180	1
hc-c3-c3-hc	0.150	0	3



Site partial charges CM4 (in units of the electron charge) for the 8CB model (Hydrogen site charges on each c3 type Carbon are shown under the hydrocarbon tail)

II. Force field parameters and topology for SP molecule:



Atom types for the nitroxide head group and EPS site partial charges (in units of the electron charge) of the SP

Table S5. LJ parameters

Atom type	σ (Å)	ε (kcal/mol)
os	3.367	0.1700
h1	2.774	0.0157
o	3.322	0.2100
n3	3.640	0.1700
c3	3.816	0.1094
hc	2.974	0.0157

Table S6. Bond-stretching parameters

Bond	k_r (kcal mol^{-1} Å^{-2})	r_0 (Å)
c3-hc	337.30	1.092
c3-c3	303.10	1.535
c3-n3	320.60	1.470
n3-o	564.00	1.303
c3-h1	335.90	1.093
c3-os	301.50	1.439

Table S7. Bond-angle bending parameters

Bond angle	k_θ (kcal mol^{-1} rad^{-2})	θ_0 (deg.)
c3-c3-n3	66.180	110.380
c3-c3-c3	63.210	110.630
hc-c3-hc	39.430	108.350
hc-c3-c3	46.370	110.050
c3-n3-o	68.680	113.310
c3-n3-c3	64.010	110.900
c3-c3-h1	46.360	110.070
c3-c3-os	67.780	108.420
n3-c3-os	71.150	108.330
c3-os-c3	62.390	112.450
h1-c3-h1	39.180	109.550
h1-c3-os	50.840	108.820

Table S8. Dihedral parameters

Dihedral	pk (kcal mol^{-1})	δ (deg.)	pn
c3-c3-n3-o	0.300	0	3
c3-c3-n3-c3	0.300	0	3
	0.480	180	2
c3-c3-c3-hc	0.160	0	3
c3-c3-c3-h1	0.156	0	3
c3-c3-c3-os	0.156	0	3
hc-c3-c3-n3	0.156	0	3
c3-n3-c3-os	0.300	0	3
c3-c3-os-c3	0.383	0	3
	0.100	180	2
n3-c3-c3-h1	0.156	0	3
n3-c3-c3-os	0.156	0	3
n3-c3-os-c3	0.383	0	3
n3-c3-c3-c3	0.156	0	3
o -n3-c3-os	0.300	0	3
h1-c3-os-c3	0.383	0	3
os-c3-c3-hc	0.250	0	1
c3-c3-c3-c3	0.180	0	3
	0.250	180	2
	0.200	180	1
hc-c3-c3-hc	0.150	0	3

Additional Figures:

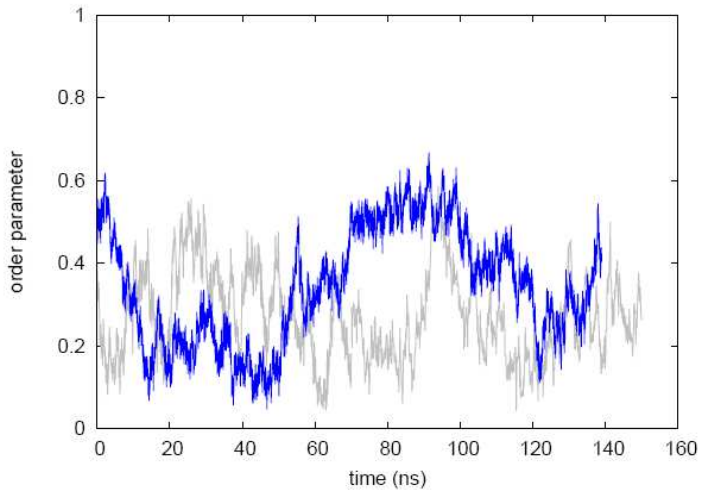


Figure S1. Comparison between the trajectories generated form MD simulations on 8CB carried out with electrostatics interactions included (blue line) and excluded (grey line).

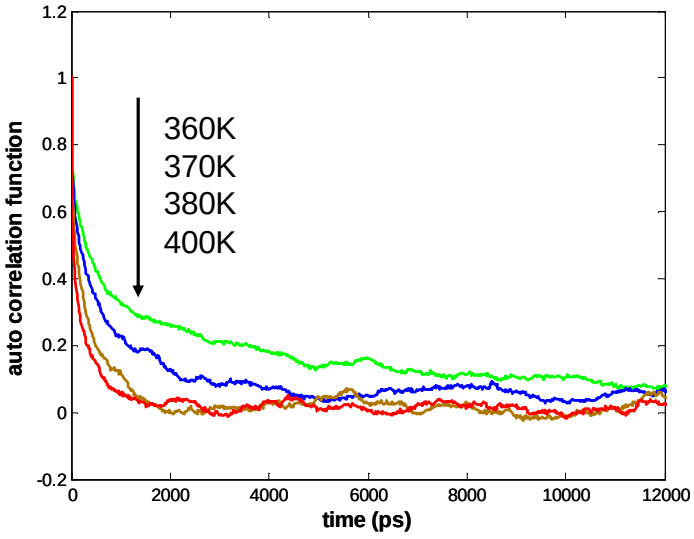


Figure S2. Example of rotation correlation functions of the Z axis of SP calculated from MD trajectories generated at different temperatures.