Supporting Material for the paper:

"Conformational Study of a Bent-core Liquid Crystal: ^{13}C NMR and DFT Computation Approach"

by

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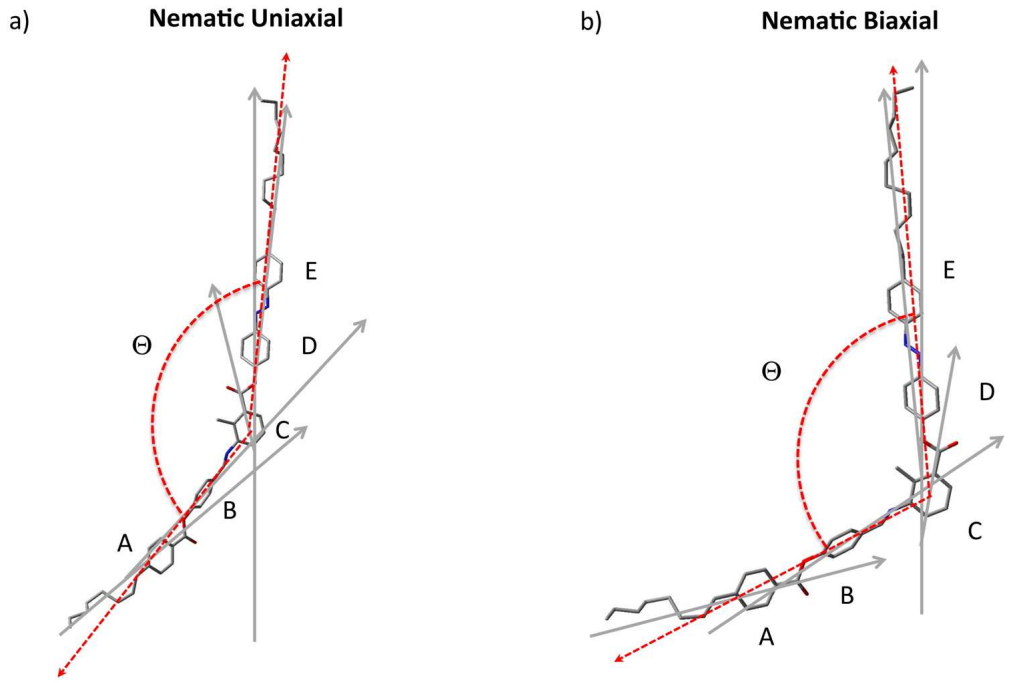
Table S.1: Relative energies (in kcal/mol) and populations in (%) for **ABC$_i$**, **BCD$_i$** and **CDE$_i$** conformers.

Conformation	ψ_2 (°)	ψ_4 (°)	Δ E(Kcal/mol)	P (%)
ABC$_1$	30	60	0.102	13.0
ABC$_2$	-30	60	0.000	16.0
ABC$_3$	150	60	0.212	11.0
ABC$_4$	-150	60	0.263	10.0
ABC$_5$	30	-60	0.000	16.0
ABC$_6$	-30	-60	0.102	13.0
ABC$_7$	150	-60	0.263	10.0
ABC$_8$	-150	-60	0.212	11.0
Conformation	ψ_4 (°)	ψ_5 (°)	Δ E(Kcal/mol)	P (%)
BCD$_1$	45	-165	0.000	30.0
BCD$_2$	45	-15	1.665	1.9
BCD$_3$	45	15	2.315	0.6
BCD$_4$	45	165	0.325	17.5
BCD$_5$	-45	-165	0.325	17.5
BCD$_6$	-45	-15	2.315	0.6
BCD$_7$	-45	15	1.665	1.9
BCD$_8$	-45	165	0.000	30.0
Conformation	ψ_5 (°)	ψ_7 (°)	Δ E(Kcal/mol)	P (%)
CDE$_1$	30	0	0.685	6.0
CDE$_2$	-30	0	0.685	6.0
CDE$_3$	150	0	0	19.0
CDE$_4$	-150	0	0	19.0
CDE$_5$	30	180	0.685	6.0
CDE$_6$	-30	180	0.685	6.0
CDE$_7$	150	180	0	19.0
CDE$_8$	-150	180	0	19.0

Figure S.1: Plot of the relevant fragmental angles (with respect to the *para* axis of ring D) and Cartesian z-axis systems for the two distinct conformational states of A131 in its N_u (a) and N_b (b) phases. For the sake of clarity, only the carbon skeletal has been reported for each conformation, together with the proper formulae for the estimations of the bent angle of A131. UL and LL refer to Upper and Lower Limit (based on fragmental angles that are average values in the respective phases) of the bend angle, respectively.



LL(N_u): Θ=180°-θB+θE-θA=180°-35°+18°-10°=153°

UL(N_u): Θ=180°-θB+θE=180°-35°+18°=163°

LL(N_b): Θ=180°-θB-θE-θA=180°-32°-19°-18°=111°

UL(N_b): Θ=180°-θB-θE=180°-32°-19°=129°