Supplementary Material

A computational study of the intermolecular interactions in the head-to-tail arrangement of the 5CB liquid crystal monomers.

Luis Humberto Mendoza-Huizar, Eduardo García Sánchez, Luis Octavio Solís Sánchez.

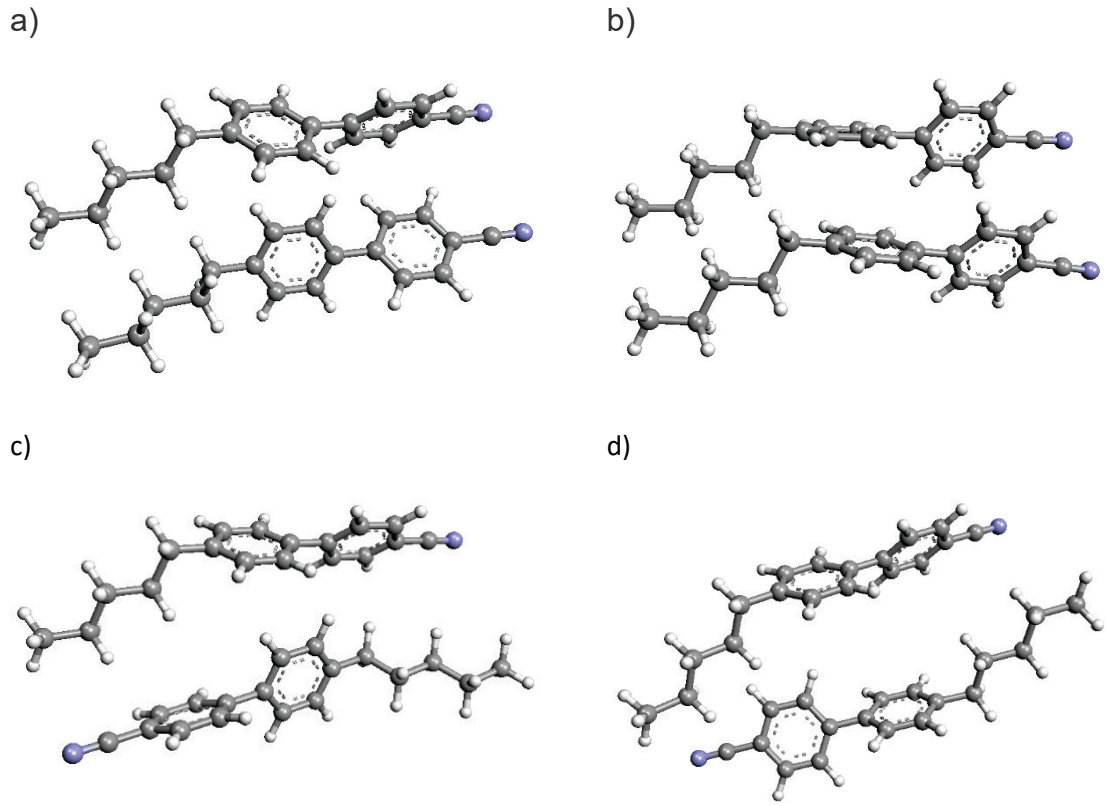

Figure 1. Initial trial structures of 5CB dimer employed to find the conformer more stable. a) head-to-head configuration with the central benzene rings in a close perpendicular position. b) head-to-head configuration with the central benzene rings in a close planar alignment position. c) head-to-tail configuration with the central benzene rings in a close perpendicular position, and d) head-to-tail configuration with the central benzene rings in a close planar alignment position.

Table 1S. xyz coordinates of the 5CB monomer reported in Figure 1 and optimized at the wB97X-D/6-311++G(d,p) level of theory.

Atom	x	y	z
C	-1.112160	1.365664	-0.332069
C	0.252007	-0.491512	1.198651
C	0.252468	1.189318	-0.509721
C	-1.817853	0.624298	0.614774
C	-1.111953	-0.307606	1.374556
C	0.957169	0.257526	0.254786
C	-3.305223	0.795273	0.781802
C	2.417582	0.076483	0.077986
C	-4.113815	-0.129251	-0.136439
C	-5.620328	0.043780	0.031944
C	-6.443227	-0.868180	-0.875026
C	-7.947027	-0.682627	-0.693530
C	5.177302	-0.261078	-0.246555
C	3.260203	1.182126	-0.071480
C	2.984158	-1.201441	0.061661
C	4.348734	-1.375094	-0.097671
C	4.625934	1.021527	-0.233569
C	6.590663	-0.434089	-0.411628
N	7.726411	-0.573272	-0.544077
H	-1.640522	2.092581	-0.941617
H	0.773984	1.769421	-1.263883
H	-1.636527	-0.889614	2.126326
H	0.781875	-1.202889	1.823464
H	-3.581164	0.598995	1.823493
H	-3.579263	1.835745	0.576348
H	-3.835896	-1.170488	0.066730
H	-3.833379	0.064309	-1.178828
H	-5.889113	1.089467	-0.166768
H	-5.891895	-0.146544	1.078461
H	-6.175291	-1.912473	-0.675887
H	-6.173037	-0.677029	-1.920211
H	-8.246595	-0.897417	0.336913
H	-8.244280	0.346822	-0.916180
H	-8.515785	-1.344268	-1.351574
H	2.840992	2.181196	-0.036775
H	2.343314	-2.070969	0.154033
H	4.778177	-2.369474	-0.116388
H	5.271732	1.884823	-0.339941

Table 2S. xyz coordinates of the 5CB dimer reported in Figure 4 and optimized at the wB97X-D/6-311++G(d,p) level of theory.

Atom	x	y	z
C	-3.460999	-2.591999	-0.230000
C	-1.603999	-0.820999	-1.260000
C	-2.135999	-2.667999	0.169000
C	-3.888999	-1.618999	-1.135000
C	-2.933999	-0.743999	-1.648000
C	-1.185999	-1.773999	-0.330000
C	-5.345999	-1.490999	-1.497000
C	0.214001	-1.802999	0.153000
C	-6.209999	-1.071999	-0.301000
C	-7.658999	-0.781999	-0.680000
C	-8.502998	-0.334999	0.511000
C	-9.948998	-0.029999	0.133000
C	2.846001	-1.778999	1.104000
C	1.285001	-1.563999	-0.712000
C	0.491001	-2.038999	1.504000
C	1.789001	-2.028999	1.981000
C	2.588001	-1.548999	-0.247000
C	4.189001	-1.716999	1.601000
N	5.267002	-1.649000	2.002000
C	3.415999	1.586000	1.425000
C	2.019000	1.952000	-0.928000
C	2.035000	1.729000	1.454000
C	4.124999	1.624000	0.226000
C	3.397999	1.815000	-0.950000
C	1.310000	1.911000	0.276000
C	5.625999	1.464000	0.213000
C	-0.165000	2.050000	0.296000
C	6.145999	0.407001	-0.764000
C	7.648999	0.181001	-0.627000
C	8.192999	-0.861999	-1.599000
C	9.693998	-1.088999	-1.443000
C	-2.959000	2.264000	0.283000
C	-0.818000	2.877000	-0.625000
C	-0.943000	1.346001	1.220000
C	-2.324000	1.446001	1.219000
C	-2.197000	2.983000	-0.639000
C	-4.386999	2.359000	0.255000
N	-5.536999	2.434000	0.223000

H	-4.178999	-3.302999	0.168000
H	-1.831999	-3.441999	0.866000
H	-3.239999	0.029001	-2.347000
H	-0.894999	-0.094999	-1.642000
H	-5.455999	-0.748999	-2.295000
H	-5.715999	-2.440999	-1.899000
H	-5.776999	-0.176999	0.154000
H	-6.179999	-1.857999	0.463000
H	-8.108998	-1.672999	-1.138000
H	-7.676999	0.004001	-1.446000
H	-8.041999	0.555001	0.954000
H	-8.480998	-1.114999	1.282000
H	-9.995998	0.768001	-0.614000
H	-10.440998	-0.910999	-0.291000
H	-10.529998	0.292001	1.001000
H	1.095001	-1.391999	-1.765000
H	-0.326999	-2.205999	2.196000
H	1.990001	-2.197999	3.032000
H	3.407001	-1.344999	-0.926000
H	3.953999	1.437000	2.355000
H	1.521000	1.714000	2.408000
H	3.914999	1.848000	-1.904000
H	1.485000	2.068000	-1.865000
H	6.088999	2.430000	-0.026000
H	5.958999	1.201000	1.221000
H	5.913999	0.697001	-1.796000
H	5.628999	-0.539999	-0.578000
H	7.865999	-0.132999	0.401000
H	8.175999	1.132000	-0.780000
H	7.973999	-0.549999	-2.628000
H	7.661999	-1.807999	-1.443000
H	10.249998	-0.161999	-1.615000
H	9.932998	-1.437999	-0.434000
H	10.061998	-1.835999	-2.151000
H	-0.235000	3.461000	-1.328000
H	-0.463000	0.674001	1.921000
H	-2.915999	0.871001	1.920000
H	-2.690000	3.629000	-1.356000