Supplementary Materials

Molecular dynamics simulation study on the isomerization and molecular orientation of liquid crystals formed by azobenzene and (1-cyclohexenyl)phenyldiazene

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Table I: Atom type, atomic weight, and charges for 5AZCN

Index	Atom Type	Atomic Weight	Charge
1	CA	12.0000	-0.212169
2	CA	12.0000	-0.101706
3	CA	12.0000	-0.101746
4	CA	12.0000	-0.101706
5	CA	12.0000	-0.212169
6	CA	12.0000	0.364609
7	HA	1.00800	0.125335
8	HA	1.00800	0.173231
9	HA	1.00800	0.173231
10	HA	1.00800	0.125335
11	CZ	12.0000	0.401598
12	NZ	14.0070	-0.482531
13	NAT	14.0070	-0.198992
14	NAT	14.0070	-0.173095
15	CA	12.0000	0.332219
16	CA	12.0000	-0.204819
17	CA	12.0000	-0.204819
18	CA	12.0000	-0.173005
19	HA	1.00800	0.120850
20	CA	12.0000	-0.173005
21	HA	1.00800	0.120850
22	CA	12.0000	-0.002102
23	HA	1.00800	0.169450
24	HA	1.00800	0.169450
25	CT	12.0000	-0.048932
26	HC	1.00800	0.035727
27	HC	1.00800	0.035727
28	CT	12.0000	0.027656
29	HC	1.00800	0.001103
30	HC	1.00800	0.001103
31	CT	12.0000	-0.026104
32	HC	1.00800	0.006810
33	HC	1.00800	0.006810
34	CT	12.0000	0.142701
35	HC	1.00800	-0.020558
36	HC	1.00800	-0.020558
37	CT	12.0000	-0.232073
38	HC	1.00800	0.052098
39	HC	1.00800	0.052098
40	HC	1.00800	0.052098

Table II: Atom type, atomic weight, and charges for 5CPDCN

Index	Atom Type	Atomic Weight	Charge
1	CA	12.0000	-0.226215
2	CA	12.0000	-0.093847
3	CA	12.0000	-0.117258
4	CA	12.0000	-0.093847
5	CA	12.0000	-0.226215
6	CA	12.0000	0.397074
7	HA	1.00800	0.123567
8	HA	1.00800	0.173075
9	HA	1.00800	0.173075
10	HA	1.00800	0.123567
11	CZ	12.0000	0.405163
12	NZ	14.0070	-0.484224
13	NAT	14.0070	-0.218358
14	NAT	14.0070	-0.187026
15	CM	12.0000	0.339508
16	CM	12.0000	-0.382356
17	CT	12.0000	-0.140270
18	CT	12.0000	0.109357
19	HC	1.00800	0.145087
20	CT	12.0000	-0.006671
21	HC	1.00800	0.035572
22	CT	12.0000	0.012482
23	HC	1.00800	0.029174
24	HC	1.00800	0.029174
25	HC	1.00800	0.031515
26	HC	1.00800	0.031515
27	HC	1.00800	0.036202
28	CT	12.0000	-0.154842
29	HC	1.00800	0.023619
30	HC	1.00800	0.023619
31	CT	12.0000	0.066939
32	HC	1.00800	-0.012547
33	HC	1.0080	-0.012547
34	CT	12.0000	-0.024309
35	HC	1.00800	0.012287
36	HC	1.00800	0.012287
37	CT	12.0000	0.102826
38	HC	1.00800	-0.012983
39	HC	1.00800	-0.012983
40	CT	12.0000	-0.206554
41	HC	1.00800	0.046932

Index	Atom Type	Atomic Weight	Charge
42	HC	1.0080	0.046932
43	HC	1.0080	0.046932
44	HC	1.0080	0.035572

Table III: Equilibrium bond lengths and force constants used in the OPLS-AA force field. $E_{bond} = \sum_{bonds} \frac{1}{2} k_b (r - r_0)^2$

Atom Type	Atom Type	k_b (kcal/mol/Å^2)	r_0 (Å)
HA	CA	734.00	1.0800
CA	CA	938.00	1.4000
CA	CZ	800.00	1.4510
CA	NAT	854.57	1.4000
CZ	NZ	1300.00	1.1570
NAT	NAT	1098.70	1.3400
CA	CT	634.00	1.5100
HC	CT	680.00	1.0900
CT	CT	536.00	1.5290
CM	NC	966.00	1.4048
CM	CM	1098.00	1.3400
CM	CT	634.00	1.5100
CM	HC	680.00	1.0800

Table IV: Equilibrium angles and force constants used in the OPLS-AA force field.

$$E_{angle} = \sum_{angles} \frac{1}{2} k_\theta (\theta - \theta_0)^2$$

Atom Type	Atom Type	Atom Type	k_θ (kcal/mol/rad^2)	θ_0 (deg)
HA	CA	CA	70.00	120.00
CA	CA	CA	126.0	120.00
CA	CA	CZ	140.0	120.00
CA	CZ	NZ	300.0	180.00
CA	CA	NAT	140.0	124.00
CA	NAT	NAT	239.0	114.30
CA	CA	CT	140.0	120.00
CT	CT	HC	75.0	110.70
CT	CT	CT	116.7	112.70
HC	CT	HC	66.0	107.80
CA	CT	HC	70.0	109.50
CA	CT	CT	126.0	114.00
CM	NAT	NAT	239.0	114.30
CT	CM	NAT	140.0	124.0 0
CM	CM	NAT	140.0	115.00
CM	CM	CT	140.0	124.00
HC	CM	CM	70.0	120.00
HC	CM	CT	70.0	117.00
CT	CT	CM	126.0	113.10
HC	CT	CM	70.0	109.50

Table V: The dihedral angle parameters used in the OPLS-AA force field.

$$E_{dihedrals} = \sum_{dihedrals} \frac{1}{2}V_1(1+\cos\varphi)^2 + \frac{1}{2}V_2(1-\cos 2\varphi)^2 + \frac{1}{2}V_3(1+\cos 3\varphi)^2$$

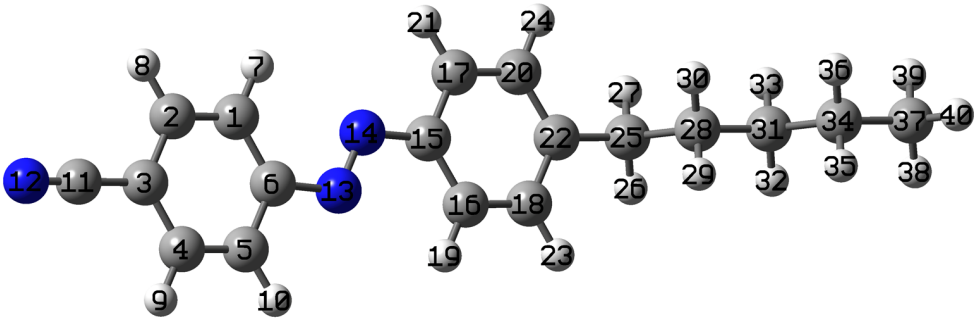
Atom Type	Atom Type	Atom Type	Atom Type	V_1(kcal/mol)	V_2(kcal/mol)	V_3(kcal/mol)
HA	CA	CA	HA	0.000	7.250	0.000
HA	CA	CA	CA	0.000	7.25	0.000
CA	CA	CA	CA	0.000	7.250	0.000
HA	CA	CA	CZ	0.000	7.250	0.000
CA	CA	CA	CZ	0.000	7.250	0.000
CA	CA	CZ	NZ	0.000	0.000	0.000
HA	CA	CA	NAT	0.000	7.250	0.000
CA	CA	NAT	NAT	0.000	7.250	0.000
CA	NAT	NAT	CA	5.200	12.00	0.000
HA	CA	CA	CT	0.000	7.250	0.000
CA	CA	CA	CT	0.000	7.250	0.000
CA	CA	CT	CT	0.000	0.000	0.000
CA	CA	CT	HC	0.000	0.000	0.000
CA	CT	CT	HC	0.000	0.000	0.462
CA	CT	CT	CT	0.000	0.000	0.000
CT	CT	CT	CT	1.300	-0.050	0.200
HC	CT	CT	CT	0.000	0.000	0.300
HC	CT	CT	HC	0.000	0.000	0.300
CA	NAT	NAT	CM	5.200	12.00	0.000
NAT	NAT	CM	CM	0.000	7.250	0.000
NAT	NAT	CM	CT	0.000	7.250	0.000
NAT	CM	CM	CT	0.000	14.00	0.000
NAT	CM	CM	HC	0.000	14.00	0.000
NAT	CM	CT	CT	0.000	0.000	0.000
NAT	CM	CT	HC	0.000	0.000	0.000
CM	CM	CT	CT	0.346	0.405	-0.904
CM	CM	CT	H	0.000	0.000	-0.372
CM	CT	CT	CT	0.000	0.000	0.000
CM	CT	CT	H	0.000	0.000	0.366
HC	CM	CT	CT	0.000	0.000	0.000

HC	**CM**	**CT**	**H**	**0.000**	**0.000**	**0.318**
HC	**CM**	**CM**	**CT**	**0.000**	**14.00**	**0.000**
CT	**CM**	**CM**	**CT**	**0.000**	**14.00**	**0.000**

Table VI: Lennard-Jones parameters used in the OPLS-AA force field.

Atom Type	**ε**	**σ**
HA	**0.0300**	**2.4200**
CA	**0.0700**	**3.5500**
CZ	**0.1500**	**3.6500**
NZ	**0.1700**	**3.2000**
NAT	**0.1701**	**3.2500**
CT	**0.0660**	**3.5000**
HC	**0.0300**	**2.5000**
CM	**0.0760**	**3.5500**

Fig. S1. Molecular structures of 5AZCN and 5CPDC



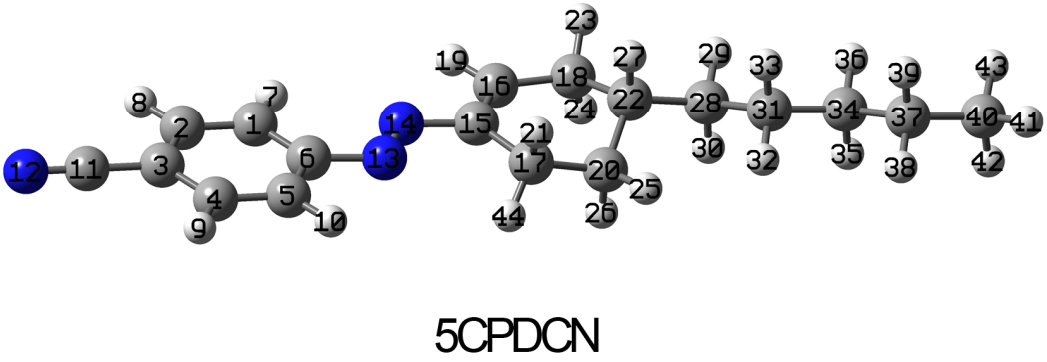


Fig. S2. The instantaneous densities for 5AZCN and 5CPDCN systems within the equilibration stages.