Supplementary Information for:

Estimation of the helical twisting power of chiral inducers by time-dependent density functional theory (TD-DFT) for electrochemical polymerization in cholesteric liquid crystals

Haoyue Shen and Hiromasa Goto*

Department of Materials Science, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki, 305-8573, Japan
*Correspondence to H. Goto, e-mail:gotoh@ims.tsukuba.ac.jp

Content：

1. Synthesis and chemical structure confirmation of models

Chemicals were purchased from Tokyo Chemical Industry Co., Ltd. Tetrahydrofuran (THF, 500 mL) was dried by refluxing with sodium strip (2 g). In this treatment, benzophenone (0.5 g) was used as an indicator. When this mixture became purple, the purified THF was collected by distillation.

(*S*)-3,7-dimethyloctan-1-ol [a], 4-octoxy-4'-cyanobiphenyl (8OCB) [b], (bisEDOT) [c] were synthesized, according to the references.

References.

[a] Eleftheriadis, N., Thee, S., Biesebeek, J., Wouden, P., Baas, & B., Dekker, F.J. (2015). *Eur. J. Med. Chem.*, 94, 265.

[b] Schneider, J.M.F.M., Sales, E.S., Livotto, P.R., Schneider, P.H., & Merlo, A.A. (2014). *J. Braz. Chem. Soc.*, 25, 1493-1503

[c] Kawabata, K., Takeguchi, M., & Goto, H. (2013). *Macromolecules*, 46, 2078.

Inducers was synthesized as followed:

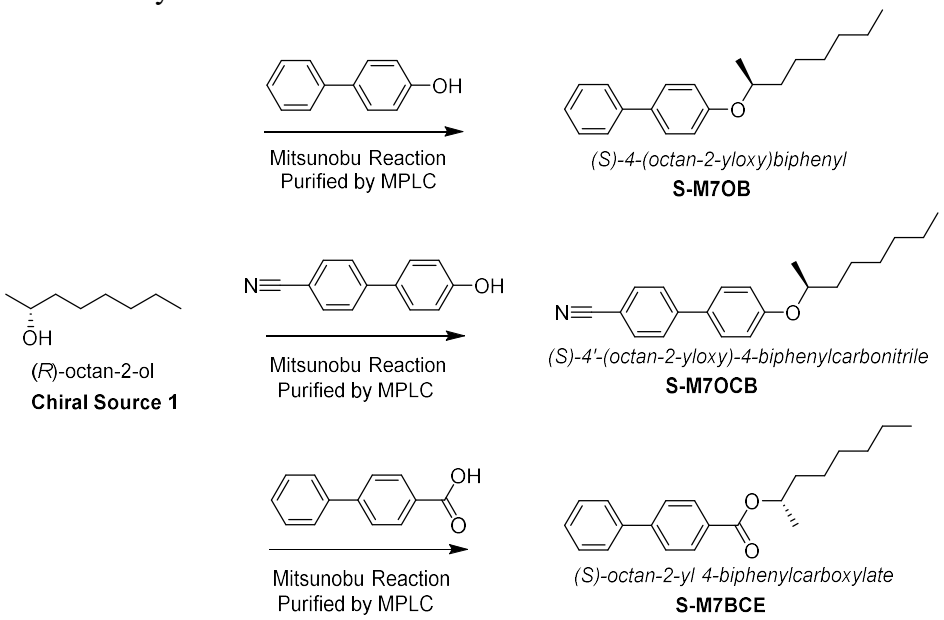

Figure S1.1. Synthetic route for inducers modified by chiral source 1

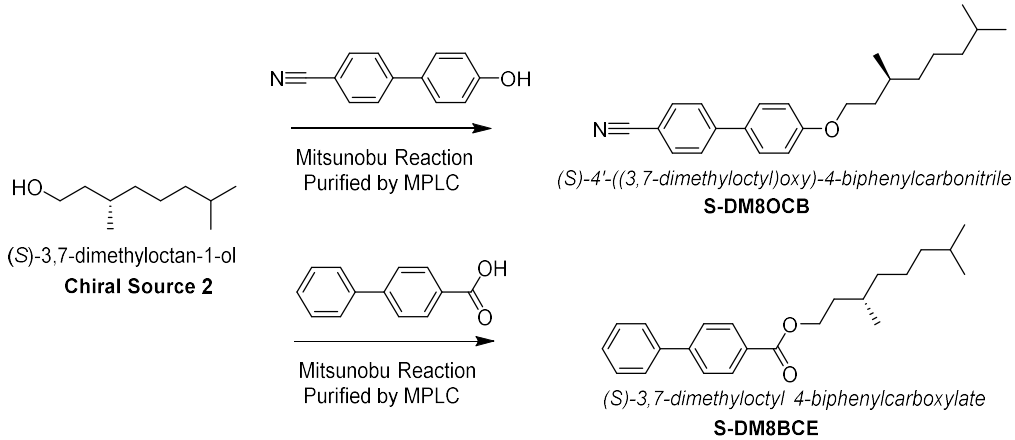

Figure S1.2. Synthetic for inducers modified by chiral source 2

Under an argon atmosphere, triphenylphosphine (5 mmol) in THF (solvent, 3 mL) was stirred and cooled to 0 ^{o}C. Alcohol (chiral source, 5 mmol) was added at this temperature. Then, diethyl azodicarboxylate (DEAD, 5 mmol, 1.9 M in toluene) diluted by THF (3 mL) was added dropwise. The yellow color and the insoluble substance were immediately disappeared after addition of the aromatic acid (5 mmol). The solution was warmed up to room temperature and stirred overnight. The solution was concentrated by rotary evaporator at 50 ^{o}C. The product was purified by medium pressure liquid chromatography with silica gel column. S-M7OB (colorless liquid): Y = 45%, S-M7OCB (colorless liquid): Y = 43%, S-M7BCE (colorless liquid): Y = 63%, S-DM8OCB (white crystal, recrystallized from methanol, melting point is ca. 36 ^{o}C): Y = 55%, S-DM8BCE (colorless liquid): Y = 65%.

^{1}H, ^{13}C or HMBC (^{1}H detected heteronuclear multiple bond correlation) NMR (nuclear magnetic resonance) spectra of each synthesized compound are shown as follow.

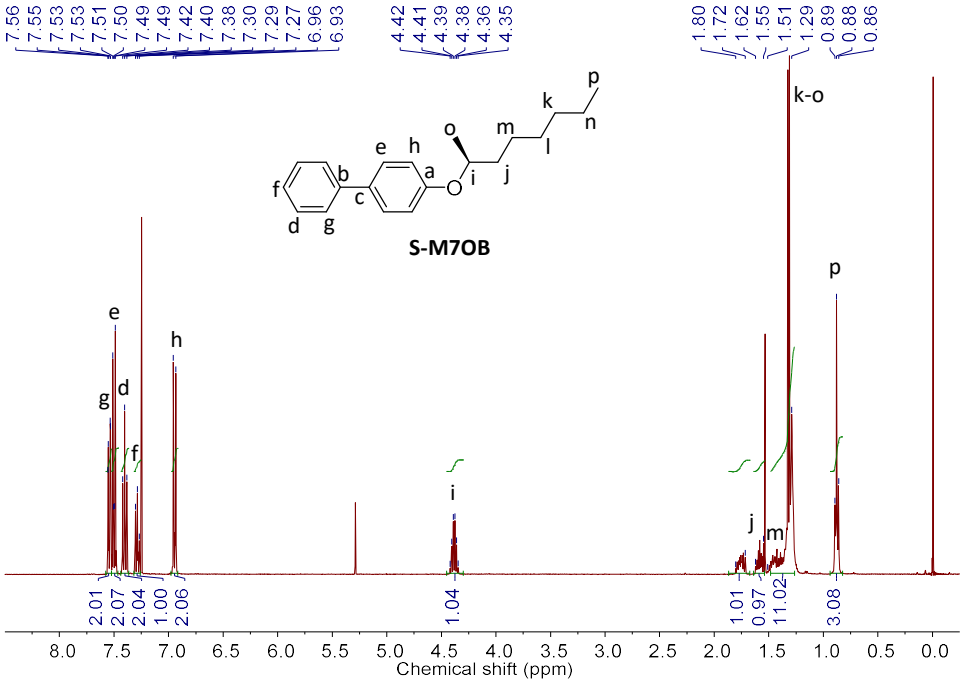

Figure S1.3. ^{1}H NMR spectrum of S-M7OB.

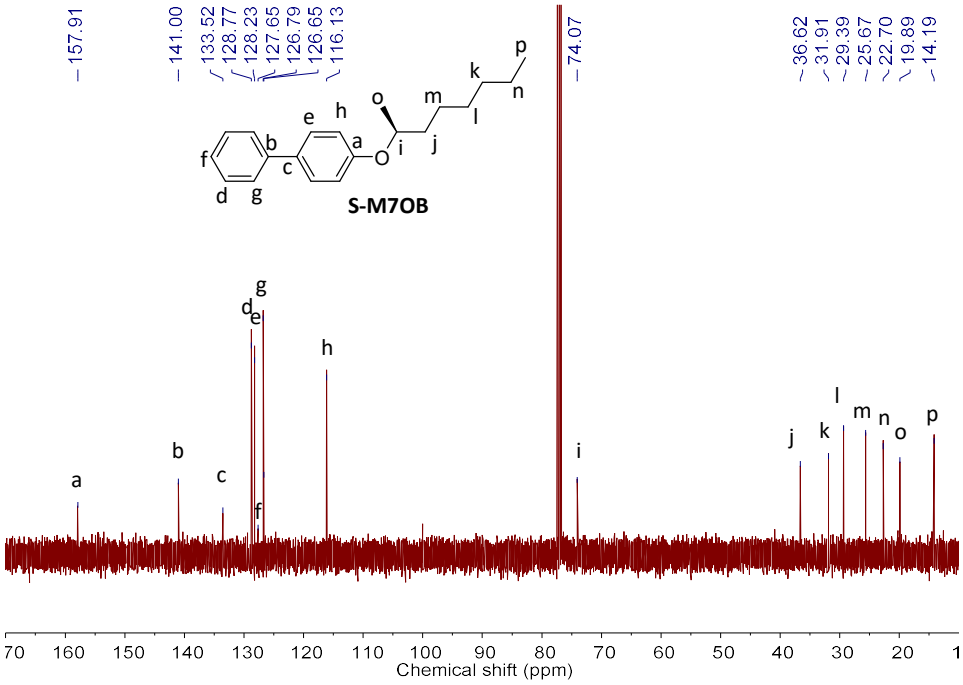

Figure S1.4. ^{13}C NMR spectrum of S-M7OB.

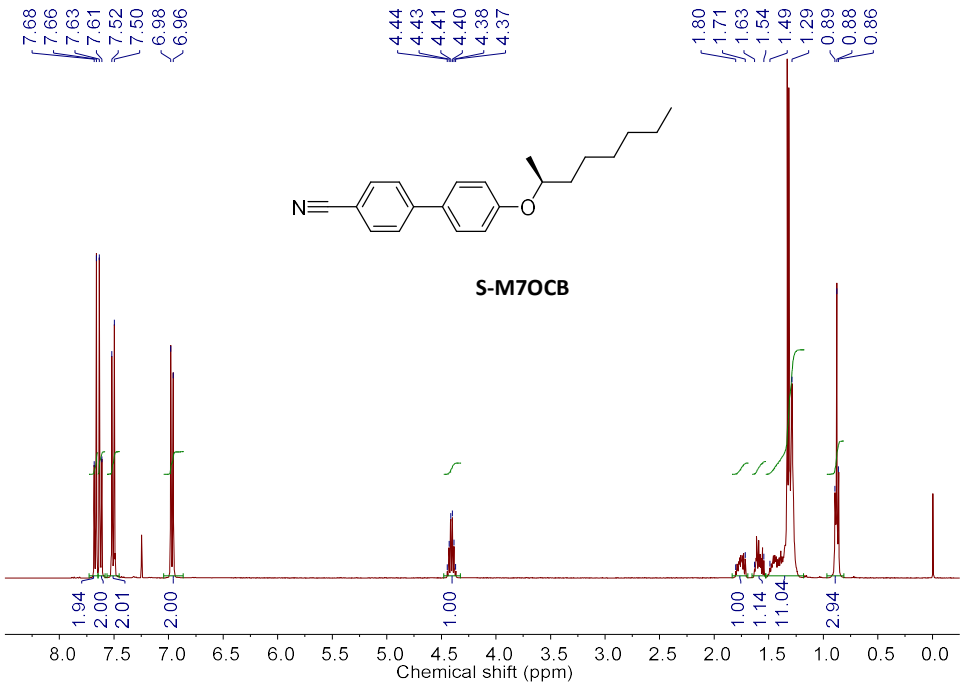

Figure S1.5. ^{1}H NMR spectrum of S-M7OB.

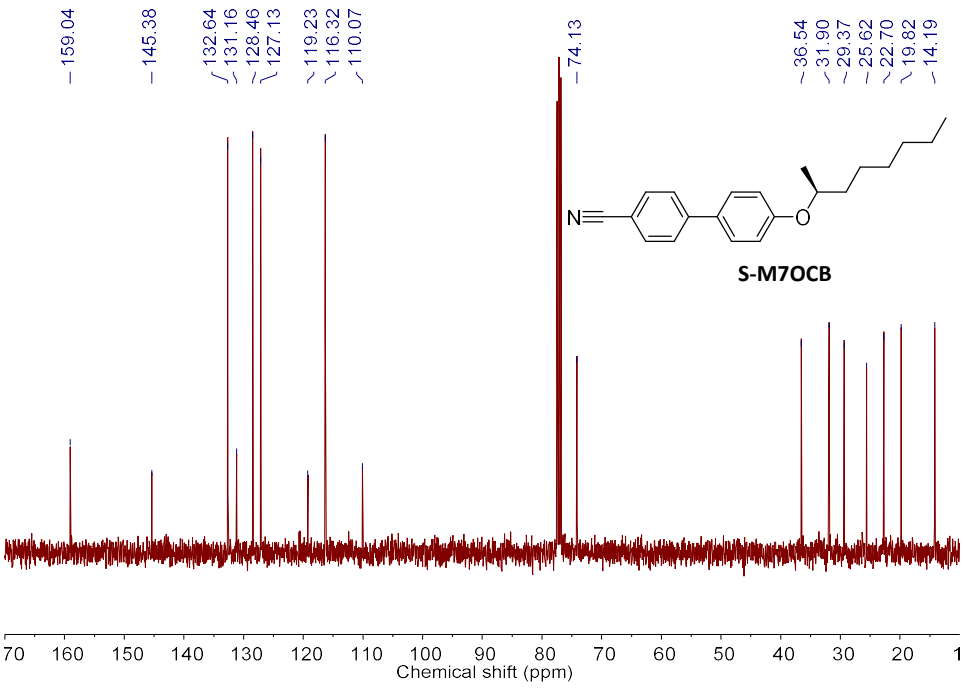

Figure S1.6. ^{13}C NMR spectrum of S-M7OB.

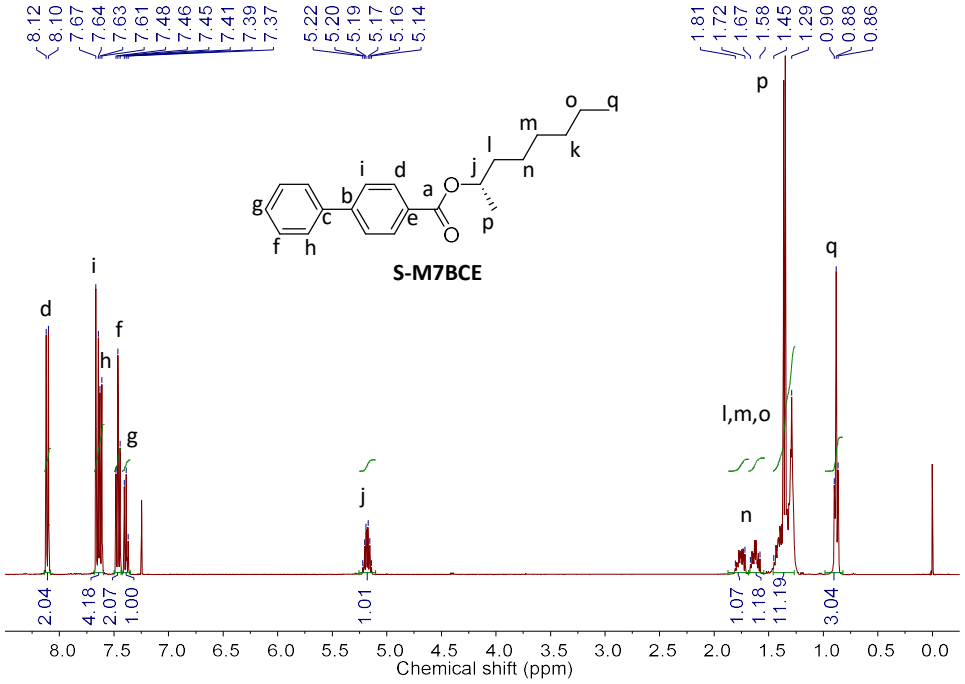

Figure S1.7. ^{1}H NMR spectrum of S-M7BCE.

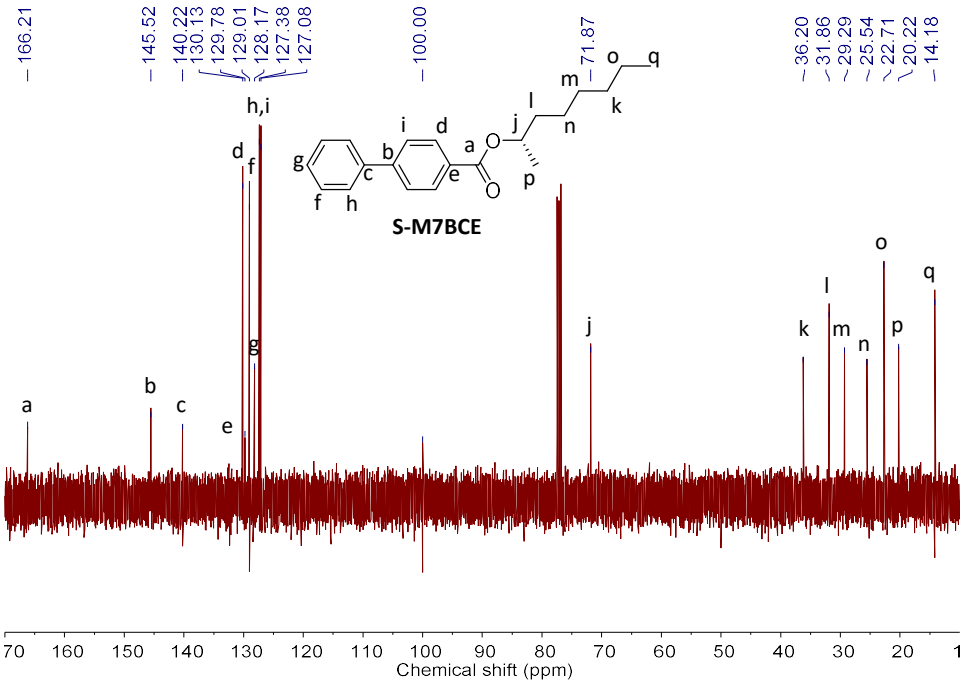

Figure S1.8. ^{13}C NMR spectrum of S-M7BCE.

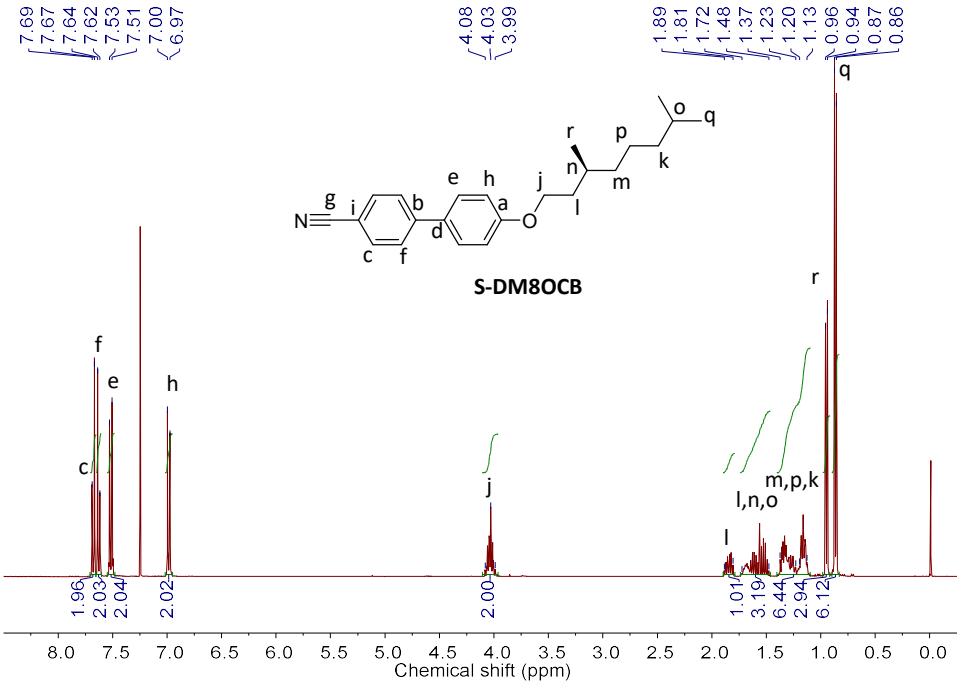

Figure S1.9. ^{1}H NMR spectrum of S-DM8OCB.

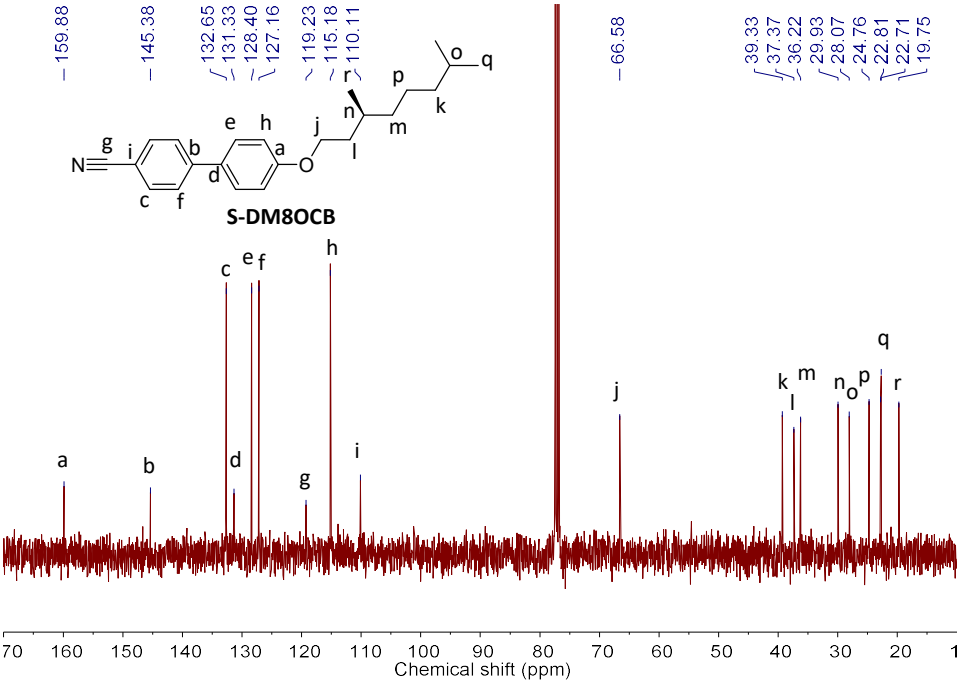

Figure S1.10. ^{13}C NMR spectrum of S-DM8OCB.

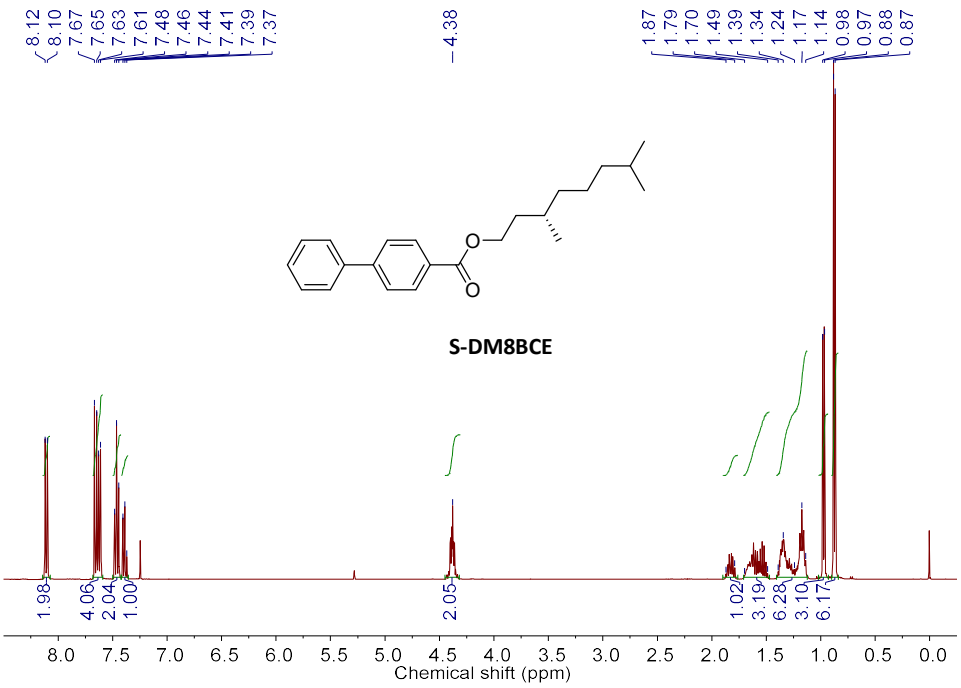

Figure S1.11. ^{13}C NMR spectrum of S-DM8BCE.

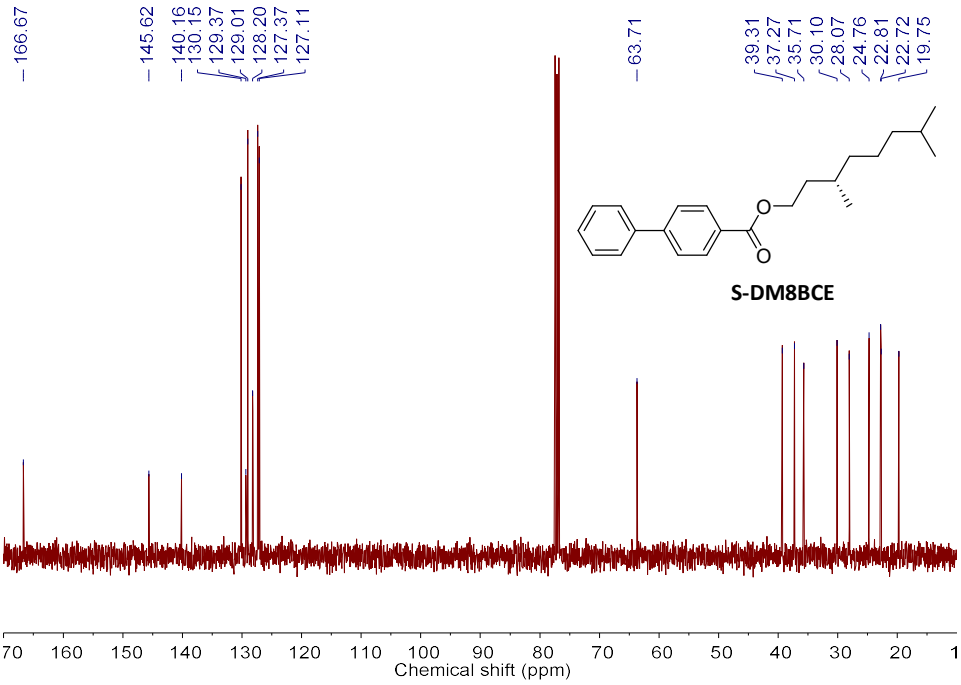

Figure S1.12. ^{13}C NMR spectrum of S-DM8BCE.

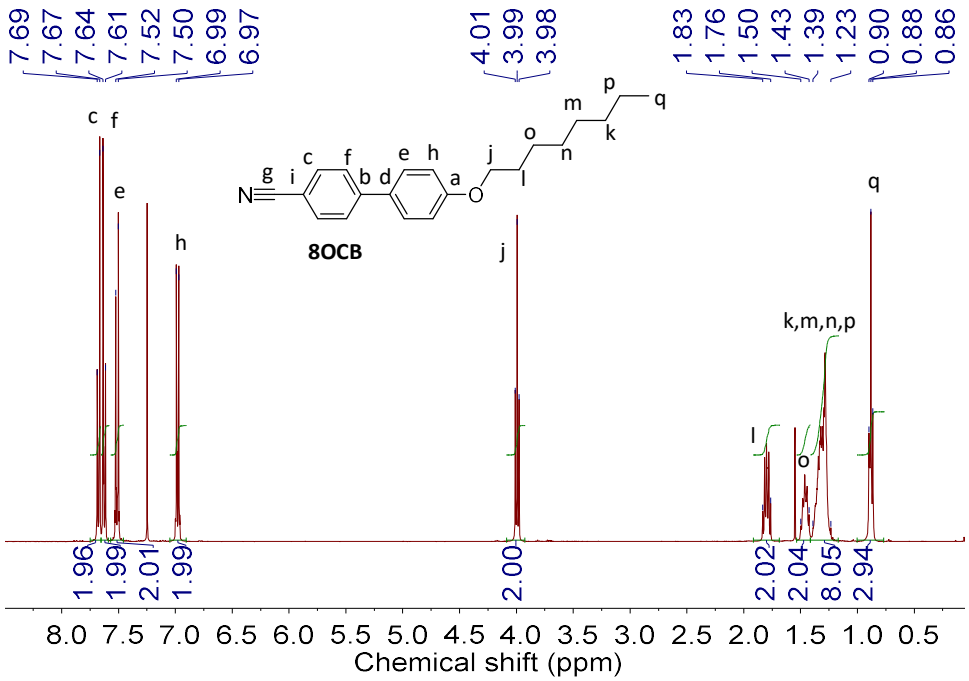

Figure S1.13. ^{1}H NMR spectrum of 8OCB.

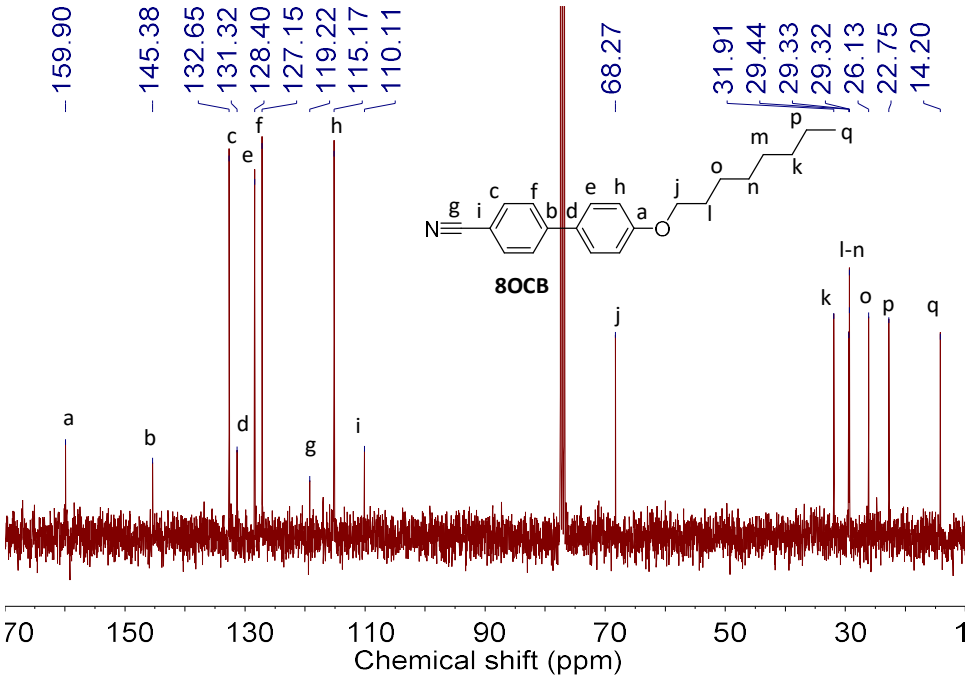

Figure S1.14. ^{13}C NMR spectrum of 8OCB.

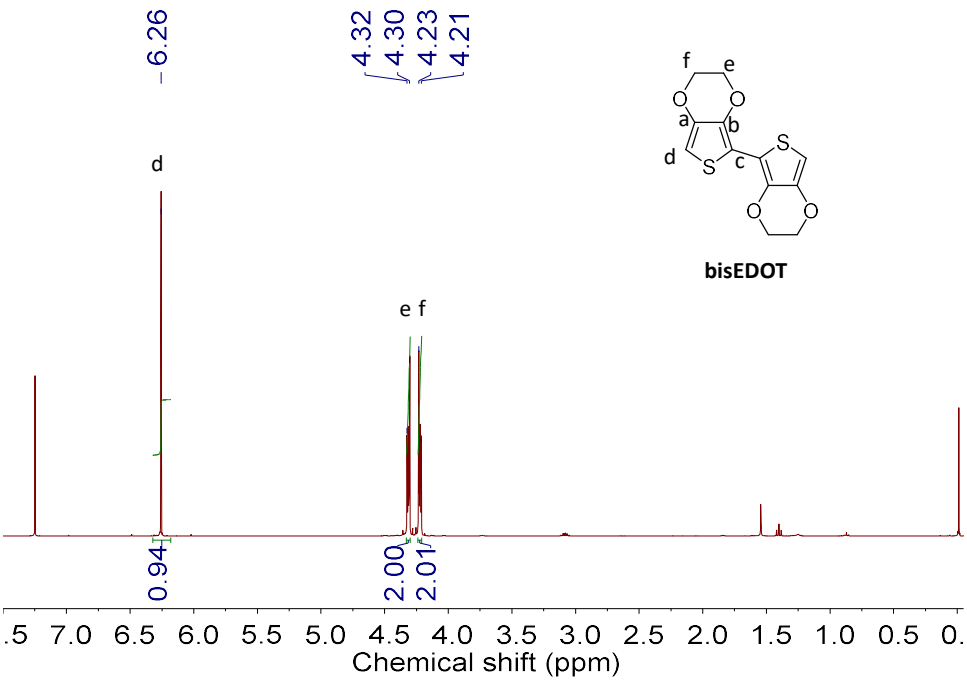

Figure S1.15. ^{1}H NMR spectrum of bisEDOT.

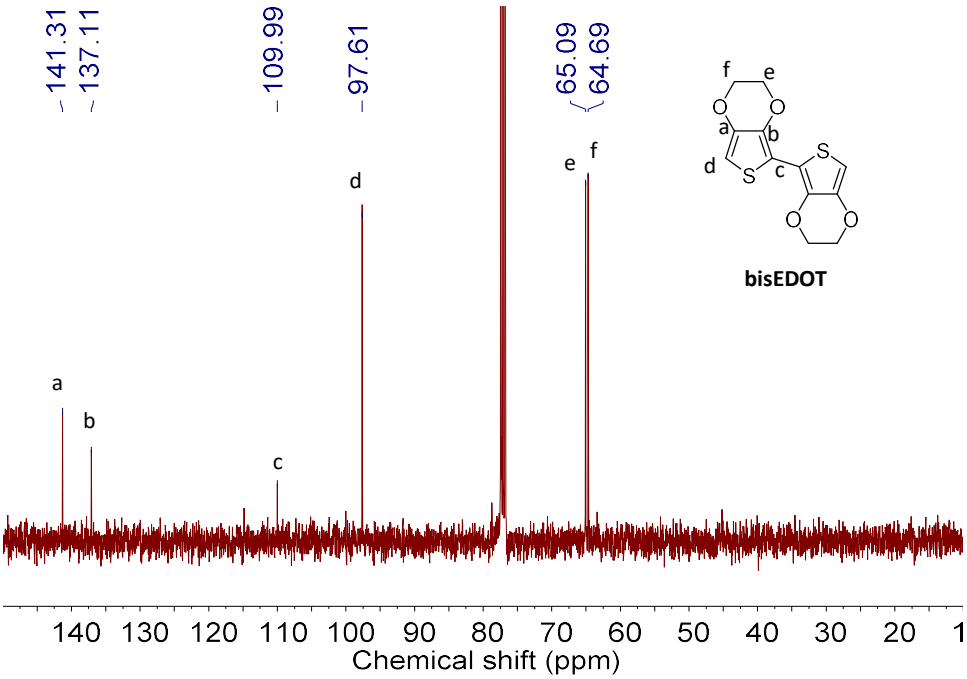

Figure S1.16. ^{13}C NMR spectrum of bisEDOT.

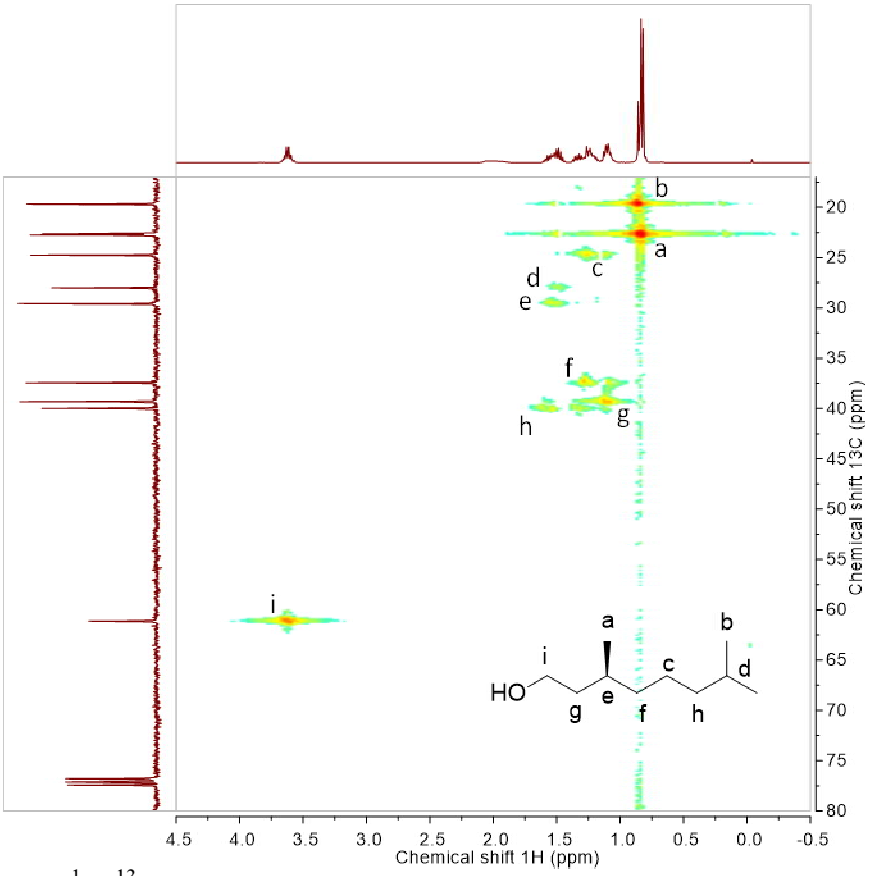

Figure S1.17. ^{1}H-^{13}C Heteronuclear multiple quantum correlation (HMQC) spectrum of (S)-3,7-dimethyloctan-1-ol.

S-M7OB

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 7.56-7.53, 7.42-7.38, 7.30-7.27 (AB_2C_2 system, 5H; Ph-H), 7.51-7.49, 6.96-6.93 (AA'BB' system, 4H; Ph-H), 4.42-4.35 (sext, 1H; C^*-H), 1.80-1.72, 1.62-1.55 (m, 2H; C^*-CH_2), 1.51-1.29 (m, 11H; -CH_2-, C^*-CH_3), 0.89, 0.88, 0.86 (t, 3H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 157.91, 141.00, 133.52, 128.77, 128.23, 127.65, 126.79, 126.65, 116.13 (12C; Ar), 74.07 (1C; C^*), 36.62, 31.91, 29.39, 25.67, 22.70, 19.89, 14.19 (7C; -CH_2-, -CH_3).

S-M7OCB

^{1}H NMR (400 MHz, CDCl3, δ from TMS, ppm): 7.68, 7.66, 7.63, 7.61 (AA'BB' system, 4H; Ph-CN), 7.52, 7.50, 6.98, 6.96 (AA'BB' system, 4H; Ph-O), 4.44-4.37 (sext, 1H; C*-H), 1.80-1.71, 1.63-1.54 (m, 2H; C*-CH_2), 1.49-1.29 (m, 11H; -CH_2-, C*-CH_3), 0.89, 0.88, 0.86 (t, 3H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 159.04, 145.38, 132.64, 131.16, 128.46, 127.13, 116.32, 110.07 (12C; Ar), 119.23 (1C; -CN), 74.13 (1C; C*), 36.54, 31.90, 29.37, 25.62, 22.70, 19.82, 14.19 (7C; -CH_2-, -CH_3).

S-M7BCE

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 8.12, 8.10, 7.67, 7.64 (AA'BB' system, 4H; Ph-H), 7.63, 7.61, 7.48, 7.46, 7.45, 7.41, 7.39, 7. 37 (AB_2C_2 system, 5H; Ph-H), 5.22-5.14 (sext, 1H; C^*-H), 1.80-1.72, 1.67-1.58 (m, 2H; C^*-CH_2), 1.45-1.29 (m, 11H; -CH_2-, C^*-CH_3), 0.90, 0.88, 0.86 (t, 3H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 166.21 (1C; -COO-) 145.52, 140.22, 130.13, 129.78, 129.01, 127.38, 127.08 (12C; Ar), 71.87 (1C; C^*), 36.20, 31.86, 29.29, 25.54, 22.71, 20.22, 14.18 (7C; -CH_2-, -CH_3).

S-DM8OCB

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 7.69, 7.67, 7.64, 7.62 (AA'BB' system, 4H; Ph-CN), 7.53, 7.51, 7.00, 6.97 (AA'BB' system, 4H; Ph-O), 4.08-3.99 (m, 2H; -CH_2), 1.89-1.81, 1.72-1.48 (m, 4H; O-C-CH_2, CH), 1.37-1.13 (m, 6H; -CH_2-), 0.96, 0.94 (d, 3H; C^*-CH_3), 0.87, 0.86 (d, 6H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 159.88, 145.38, 132.65, 131.33, 128.40, 127.16, 115.18, 110.11 (12C; Ar), 119.23 (1C; -CN), 66.58 (1C; C^*), 39.33, 37.37, 36.22, 29.93, 28.07, 24.76, 22.81, 22.71, 19.75 (7C; -CH(-)-, -CH_2-, -CH_3).

S-DM8BCE

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 8.12, 8.10, 7.67, 7.65 (AA'BB' system, 4H; Ph-H), 7.63, 7.61, 7.48, 7.46, 7.44, 7.41, 7.39, 7. 37 (AB_2C_2 system, 5H; Ph-H), 4.38 (m, 2H; -CH_2), 1.87-1.79, 1.70-1.49 (m, 4H; O-C-CH_2, CH), 1.49-1.14 (m, 6H; -CH_2-), 0.98, 0.97 (d, 3H; C^*-CH_3), 0.88, 0.87 (d, 6H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 166.67 (1C; -COO-) 145.62, 140.16, 130.15, 129.37, 129.01, 128.20, 127.37, 127.11 (12C; Ar), 63.71 (1C; C^*), 39.31, 37.27, 35.71, 30.10, 28.07, 24.76, 22.81, 22.72, 19.75 (7C; -CH(-)-, -CH_2-, -CH_3).

8OCB

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 7.69, 7.67, 7.64, 7.61 (AA'BB' system, 4H; Ph-CN), 7.52, 7.50, 9.66, 6.97 (AA'BB' system, 4H; Ph-O), 4.01-3.98 (m, 2H; -CH_2), 1.83-1.76, 1.50-1.43 (m, 2H; O-C-CH_2), 1.39-1.23 (m, 8H; -CH_2-), 0.90, 0.0.88, 0.86 (t, 3H; -CH_3).

^{13}C NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 159.90, 145.38, 132.65, 131.32, 128.40, 127.15, 115.17, 110.11 (12C; Ar), 119.22 (1C; -CN), 68.27 (1C; -O-C), 31.91, 29.44, 29.33, 29.92, 26.13, 22.75, 14.20 (7C; -CH_2-, -CH_3).

BisEDOT

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 6.26 (s, 2H; H-Th), 4.32-4.30, 4.23-4.21 (A_2B_2 system, 8H; -CH_2-).

^{13}C NMR (400 MHz, CDCl3, δ): 141.31, 137.11, 109.99, 97.61 (8C; Ar), 65.09, 64.69 (4C; -CH_2-).

(*S*)-3,7-dimethyloctan-1-ol

^{1}H NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 3.69-3.59 (m, 2H; O-CH_2), 1.71 (s, 1H, -OH), 1.61-1.44 (m, 3H; O-C-CH_2-C*H), 1.38-1.18 (m, 4H; C*-CH_2-CH_2-C), 1.16-1.05 (m, 3H; C-CH_2-$CHMe_2$), 0.86 (d, J = 6.5 Hz, 3H; C*-CH_3), 0.83 (d, J = 6.6 Hz, 6H; $C(CH_3)_2$).

^{13}C NMR (400 MHz, $CDCl_3$, δ from TMS, ppm): 61.23 (1C; O-C), 40.03 (1C; Me_2CH-C), 39.32 (1C; O-CH_2-C), 37.44 (1C; O-C_2H_4-C*HMe-C), 29.57 (1C; C*), 28.03 (1C, Me_2C), 24.75 (Me_2CHCH_2-C), 22.66-22.76 (2C; Me), 19.70 (1C: Me(-C*)).

2. Setting for optical measurements of UV-vis and circular dichroism (CD) optical absorption spectra

UV-vis and CD spectra measurements of inducers were set as followed:
Solvent: hexane
Concentration: 3 x 10^{-5} M
Cuvette: quartz, 1 cm
Machine: JASCO V-630 for UV-vis, JASCO J-720 for CD

CD spectra measurements of inducers were set as followed:
Sensitivity: Low (1000 mdeg)
Scanning speed: 100 nm/min
Response: 4 s
Cumulative number: 5

3. Setting for electrochemical polymerization

All the polymerization was processed between two Indium-Tin Oxide (ITO) glass (10 Ω/cm^2, act as two electrode) in 0.20 mm thickness. A detected 3.0 V direct current (dc) was processed on two ITO for 5 min.

Constituents of the LC electrolyte solution.
Matrix liquid crystal: 8OCB
Supporting salt: tetrabutylammonium perchlorate (TBAP), ca. 0.5 wt%
Inducer: S-M7OB/S-M7OCB/S-M7BCE/S-DM8OCB/S-DM8BCE, ca. 5 wt%
Monomer: BisEDOT, ca. 5 wt%
Temperature: cholesteric phase [c], ca. 65 ^{o}C
Table S3.2 displays details.

Differential scanning calorimetry (DSC) measurement and polarizing optical microscopy (POM) image of 8OCB and the LC electrolyte solution (using S-DM8OCB) are shown as follow.

Table S3.1 Phase transition temperatures obtained with DSC measurements.

Sample and process	Solid-Smectic	Smectic-Nematic	Nematic-Isotropic
8COB, heating	47.01 ^{o}C	66.16 ^{o}C	79.99 ^{o}C
8COB, cooling	19.93 ^{o}C	67.84 ^{o}C	80.43 ^{o}C
LC electrolyte*, heating	38.26 ^{o}C	58.05 ^{o}C	68.94 ^{o}C
LC electrolyte*, cooling	9.86 ^{o}C	52.92 ^{o}C	69.43 ^{o}C

* LC electrolyte solution containing monomer. S-DM8OCB was used for chiral inducer.

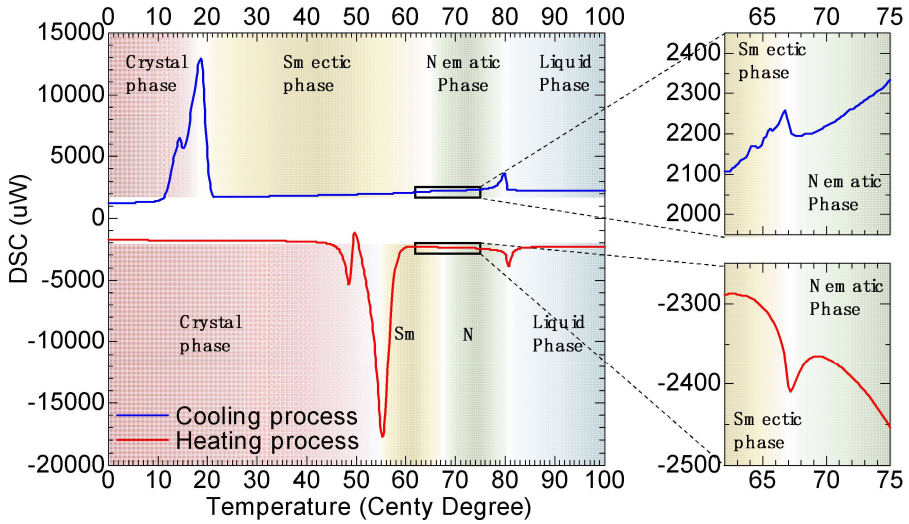

Figure S3.1. DSC result of 8OCB.

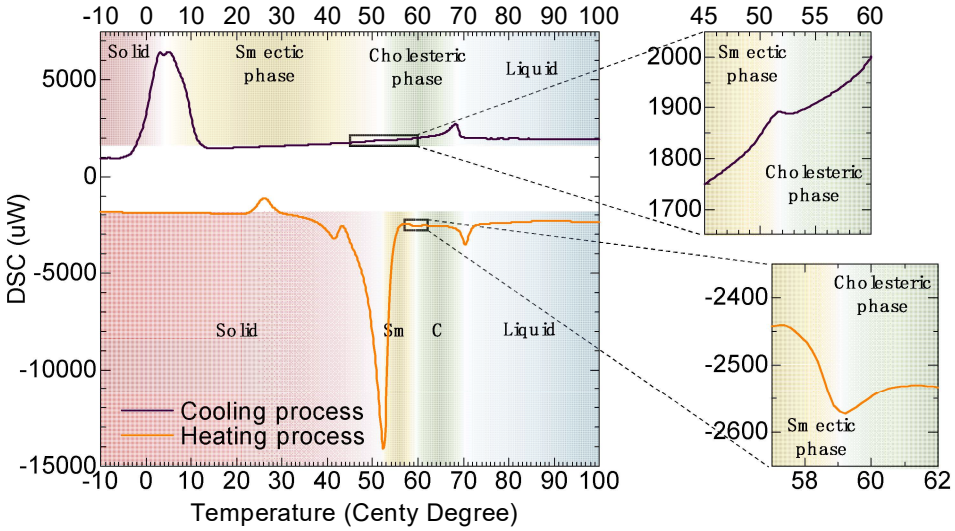

Figure S3.2. DSC result of LC electrolyte solution (using S-DM8OCB).

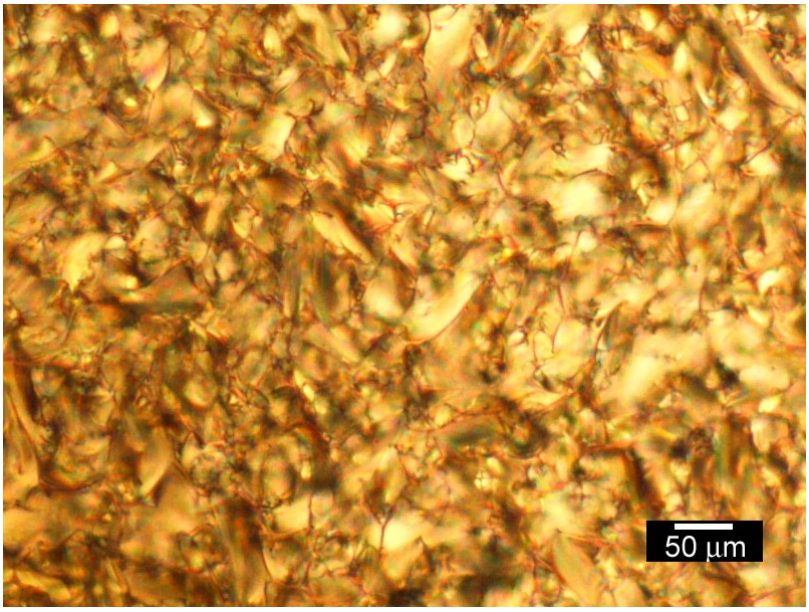

Figure S3.3. POM image of LC electrolyte solution containing monomer, S-DM8OCB in smectic phase.

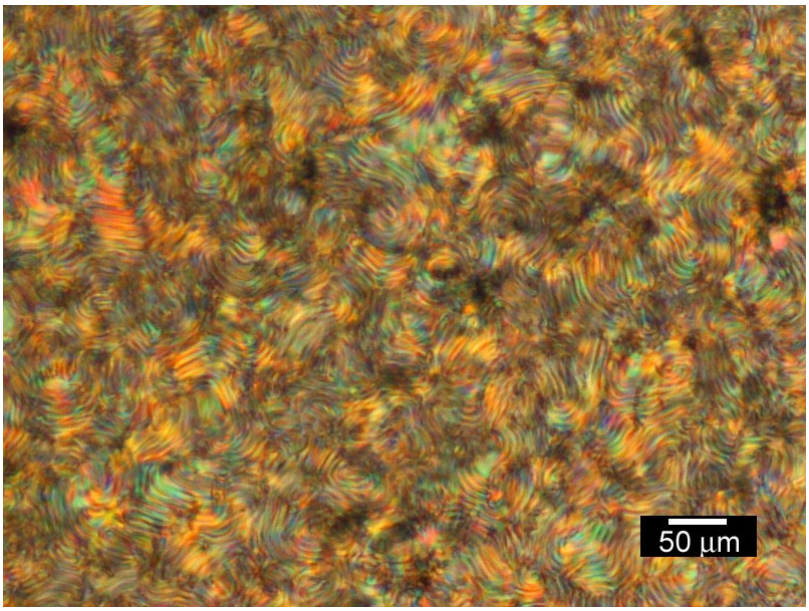

Figure S3.4. POM image of LC electrolyte containing monomer, S-DM8OCB in cholesteric phase

Table S3.2. Components of liquid crystal electrolyte solutions[1].

LC electrolyte solution[2]	Chiral inducer (mg)	BisEDOT (mg)	TBAP (mg)	8OCB (mg)
S-M7OB- based LC	5.1 (5.96wt%, 6.42 mol%)	5.0	0.5	75.0
S-M7OCB- based LC	8.3 (4.75wt%, 4.73%)	8.1	0.8	157.6
S-M7BC- based LC	5.0 (5.89wt%, 5.81mol%)	5.0	0.5	75.0
S-DM8OCB- based LC	5.5g (4.94wt%, 4.53mol%)	5.3	0.5	100.0
S-DM8BCE- based LC	10.1 (4.94wt%, 4.49mol%)	10.0	1.0	183.0

[1]Chiral inducer: S-M7OB, S-M7OCB, S-M7BCE, S-DM8OCB and S-DM8BCE.
[2]Chiral inducer based LC electrolyte solution containing monomer.

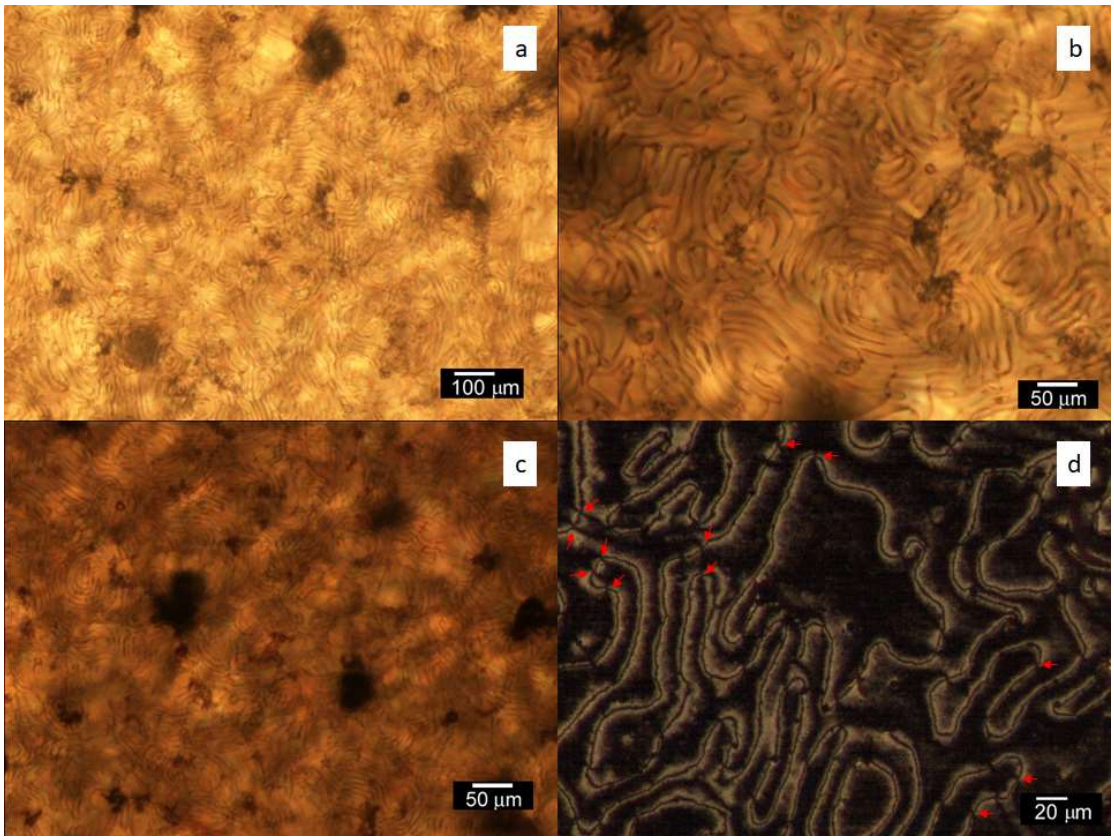

Figure S3.5 POM image of a: LC electrolyte solution containing monomer, S-M7OB; b: Magnification image of LC electrolyte solution containing monomer, S-M7OB); c: LC electrolyte solution containing monomer, S-M7OB at the half-time of the polymerization process; d: Magnification image of polymer film comparing to Figure 4 left top. Red arrows: center of Schlieren brush.

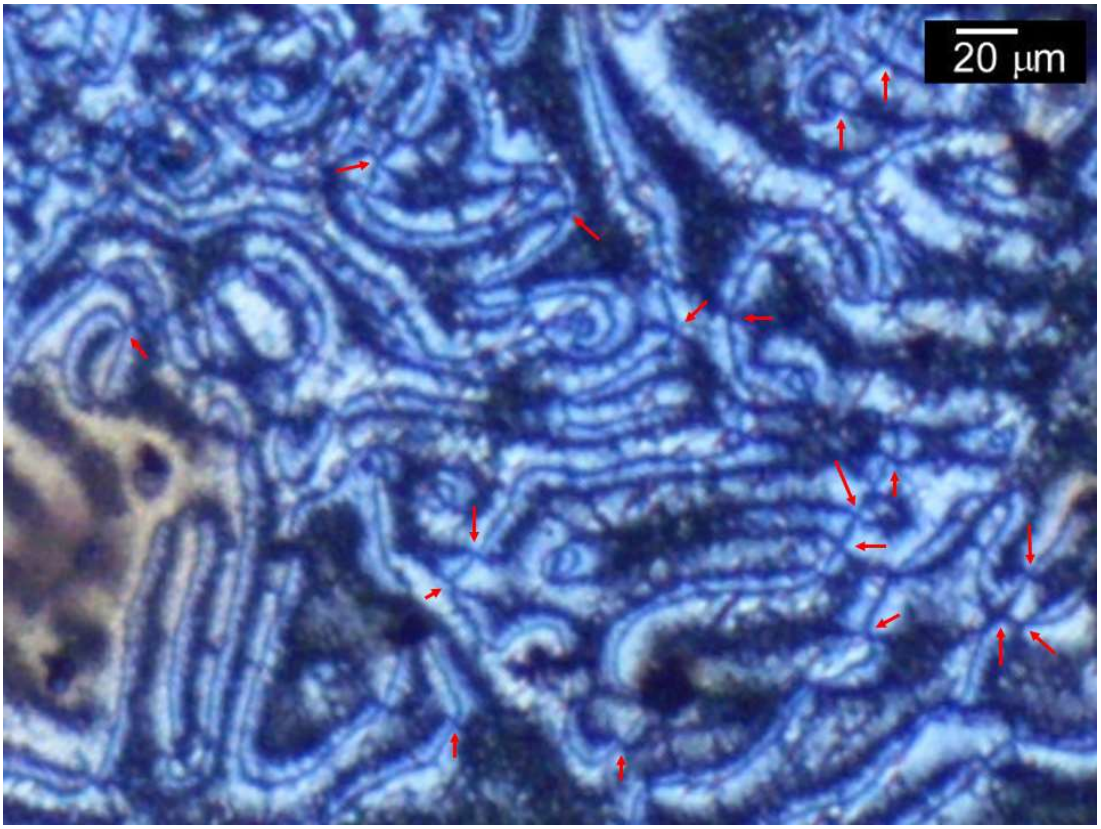

Figure S3.6 Magnification image of Figure 4 right top (polyEDOT film using S-M7OCB). Red arrows: center of Schlieren brush.

4. Models used in time-dependent self-consistent field density functional theory (TD-SCF-DFT) calculation

These models are optimized to minimum energy by TD-SCF-DFT calculation using the soft or parameters as followed.

Operation system:
Windows 10 professional 64-bit (DirectX 12)

Soft:
Gaussian 09 revision D.01 WIN64 Version 9.5

Hard hardware:
CPU: Intel Core i5-2500K 3.30GHz, RAM: 16 G ADATA DDR3 1600 MHz, SSD: 480 GB CT480BX200SSD1

Keywords example in Gaussian 09:
%nprocshared = 4
%mem = 15000MB
%chk = C: \
# opt td = (nstates = 24) b3lyp/6-311++g(d,p) scrf = (solvent = heptane)
geom = connectivity

Atomic axis of each model whose energy was minimized:

S-M7OB (conformation 1):
Job cpu time: 3 days 23 hours 24 minutes 4.0 seconds.
Total energy: -853.1119 a. u. (Lower)
Dipole moment: 5.3363 Debye (4.8371, 2.2033, -0.4739)

C	-2.7494	-2.39084	0.36541
C	-3.81929	-1.31867	0.55069
H	-2.84486	-2.85968	-0.61683
H	-4.78282	-1.83044	0.6612
H	-3.63383	-0.79814	1.49835
C	-3.90889	-0.30623	-0.59628
H	-4.11413	-0.84044	-1.53277
H	-2.9366	0.18081	-0.72603
C	-4.98811	0.75886	-0.37287
H	-4.77374	1.30015	0.55793
H	-5.95821	0.26728	-0.22147
C	-5.10807	1.76361	-1.5244
H	-5.33054	1.22379	-2.45412
H	-4.13754	2.25189	-1.68216
C	-6.17986	2.83515	-1.29583
H	-5.95456	3.37841	-0.36988
H	-7.14861	2.34687	-1.13353
C	-6.299	3.83038	-2.45405
H	-6.55909	3.32122	-3.38761
H	-7.07046	4.58084	-2.25937
H	-5.35494	4.35951	-2.61921
C	-2.78034	-3.46406	1.44979
H	-1.98441	-4.19415	1.2937
H	-2.65957	-3.01505	2.43979
H	-3.73722	-3.99305	1.42453
O	-1.48568	-1.72243	0.3993
C	-0.53584	-2.45766	-0.37668
C	0.81943	-2.04762	-0.53901
C	-0.95939	-3.6606	-1.01304
C	1.69425	-2.78976	-1.28986
H	1.15373	-1.13844	-0.05814
C	-0.09027	-4.40811	-1.76268
H	-1.98936	-3.96961	-0.8886
C	1.29006	-4.01479	-1.94531
H	2.71325	-2.43987	-1.38152
H	-0.46044	-5.3115	-2.22728
C	2.19865	-4.78864	-2.72458
C	1.80274	-6.02745	-3.35799
C	3.5721	-4.3823	-2.92842
C	2.68912	-6.76764	-4.10658
H	0.79107	-6.38958	-3.24333
C	4.44119	-5.13791	-3.68205

H	3.93174	-3.46451	-2.48575
C	4.01885	-6.33921	-4.28243
H	2.35887	-7.69232	-4.56601
H	5.46357	-4.80288	-3.81541
H	4.70988	-6.92792	-4.87414

S-M7OB (conformation 2):
Job cpu time: 2 days 11 hours 6 minutes 8.0 seconds.
Total energy: -853.1108 a. u. (Higher)
Dipole moment: 5.5616 Debye (5.4886, 0.2912, 0.8496)

C	1.78193	2.09723	-0.16743
C	3.24954	1.77489	0.10415
H	1.30392	1.22685	-0.62969
H	3.75693	2.71782	0.33825
H	3.30548	1.15545	1.00684
C	3.96237	1.07995	-1.06031
H	3.90548	1.71964	-1.95057
H	3.43005	0.1559	-1.30898
C	5.43139	0.75755	-0.76334
H	5.48786	0.11094	0.12178
H	5.96226	1.68182	-0.50007
C	6.15145	0.0775	-1.93285
H	6.09881	0.72671	-2.81664
H	5.61682	-0.84317	-2.20024
C	7.61864	-0.25849	-1.64193
H	7.67148	-0.91129	-0.76209
H	8.1526	0.66067	-1.37121
C	8.32881	-0.93221	-2.81972
H	8.3231	-0.28846	-3.7051
H	9.37157	-1.15924	-2.58085
H	7.83786	-1.872	-3.09174
C	1.58969	3.33514	-1.03997
H	0.53203	3.57474	-1.16596
H	2.08766	4.19815	-0.59101
H	2.02107	3.16175	-2.02942
O	1.16962	2.31466	1.13126
C	-0.15418	2.14476	1.33444
C	-0.60581	2.44798	2.64977
C	-1.08862	1.70088	0.3734
C	-1.92034	2.29299	2.99439
H	0.12289	2.8026	3.36913
C	-2.41589	1.54314	0.71011
H	-0.77779	1.48245	-0.63962
C	-2.90902	1.81449	2.05211
H	-2.21681	2.53474	4.00542
H	-3.10044	1.2119	-0.05707
C	-4.27039	1.62083	2.408
C	-5.24376	1.12636	1.44951
C	-4.77148	1.90677	3.73367

C	-6.56504	0.94851	1.80183
H	-4.93837	0.88342	0.44116
C	-6.09562	1.72219	4.05899
H	-4.09972	2.27709	4.497
C	-7.01908	1.24027	3.10149
H	-7.26602	0.57582	1.06205
H	-6.43448	1.94923	5.06409
H	-8.06039	1.09807	3.36556

S-M7OCB (conformation 0, Checkpoint file before error):
Error termination in NtrErr: NtrErr Called from FileIO
Total energy: -945.3955 a. u. (Lower)
Dipole moment: 9.1866 Debye (8.6454, 3.0848, -0.3678)

C	1.78193	2.09723	-0.16743
C	3.24954	1.77489	0.10415
H	1.53484	1.8034	-1.19327
H	3.85542	2.48531	-0.46993
H	3.45551	1.97011	1.16299
C	3.65186	0.34181	-0.25842
H	3.44892	0.16938	-1.32336
H	3.01981	-0.36091	0.29455
C	5.12623	0.03691	0.03039
H	5.32722	0.20107	1.09687
H	5.75998	0.75028	-0.51264
C	5.5355	-1.39092	-0.34715
H	5.3387	-1.55313	-1.41499
H	4.89743	-2.10395	0.19083
C	7.00592	-1.70902	-0.05245
H	7.20184	-1.55208	1.01529
H	7.64393	-0.99456	-0.58699
C	7.40419	-3.13633	-0.43921
H	7.25245	-3.31271	-1.50889
H	8.45683	-3.33187	-0.21638
H	6.80649	-3.87439	0.10507
C	1.43647	3.56641	0.06252
H	0.37037	3.75322	-0.08053
H	1.70581	3.86612	1.07836
H	1.99066	4.19211	-0.64215
O	1.0116	1.26602	0.74057
C	-0.26578	0.91599	0.47905
C	-0.89813	0.14208	1.49257
C	-0.99246	1.24643	-0.68565
C	-2.1836	-0.29955	1.33994
H	-0.33011	-0.08801	2.38624
C	-2.28901	0.80781	-0.84831
H	-0.54451	1.85042	-1.46353
C	-2.95819	-0.01	0.15229
H	-2.62198	-0.88515	2.13583
H	-2.81383	1.09145	-1.74886

C	-4.28279	-0.48938	-0.02965
C	-5.03765	-0.19806	-1.23628
C	-4.96097	-1.28586	0.96832
C	-6.32594	-0.6614	-1.40107
H	-4.5906	0.38537	-2.02927
C	-6.24801	-1.73446	0.77979
H	-4.45599	-1.54073	1.89088
C	-6.9568	-1.43197	-0.40679
H	-6.8613	-0.42712	-2.31543
H	-6.72421	-2.32862	1.55232
C	-8.39718	-1.93891	-0.60656
N	-9.48215	-2.32075	-0.75704

S-M7OCB (conformation 2):
Job cpu time: 3 days 1 hours 14 minutes 22.0 seconds
Total energy: -945.3944 a. u. (Higher)
Dipole moment: 16.5913 Debye (-16.4446, 1.4262, 1.6773)

C	-2.44798	0.2939	0.7393
C	-3.7271	0.6955	0.00676
H	-2.18967	-0.73523	0.47205
H	-3.9607	1.73654	0.25562
H	-3.5206	0.66526	-1.06809
C	-4.92869	-0.20477	0.31988
H	-5.18196	-0.13931	1.38386
H	-4.66076	-1.25188	0.12916
C	-6.16706	0.15709	-0.50983
H	-5.92012	0.08797	-1.5766
H	-6.43183	1.20591	-0.32493
C	-7.37938	-0.73159	-0.21179
H	-7.62655	-0.66285	0.85562
H	-7.11341	-1.78071	-0.39575
C	-8.61908	-0.37449	-1.03995
H	-8.37148	-0.44112	-2.10627
H	-8.88662	0.6729	-0.85467
C	-9.82473	-1.26965	-0.73943
H	-10.11853	-1.19743	0.31258
H	-10.69055	-0.98971	-1.34578
H	-9.59886	-2.32022	-0.94813
C	-2.5124	0.45534	2.25507
H	-1.54978	0.23526	2.7207
H	-2.79779	1.47744	2.51583
H	-3.25339	-0.22901	2.67413
O	-1.40941	1.17163	0.20691
C	-0.11683	0.81698	0.18337
C	0.76806	1.77787	-0.37277
C	0.41056	-0.4092	0.65012
C	2.11321	1.52517	-0.46447
H	0.34772	2.70981	-0.73118
C	1.76331	-0.65726	0.56072

H	-0.23314	-1.15798	1.09067
C	2.68537	0.29124	-0.00374
H	2.74819	2.27502	-0.91531
H	2.13451	-1.59501	0.94965
C	4.10047	0.01784	-0.10098
C	4.63332	-1.29146	0.15755
C	5.04523	1.03898	-0.45165
C	5.97696	-1.55851	0.06434
H	3.96966	-2.1094	0.40662
C	6.39215	0.7858	-0.53328
H	4.70746	2.05095	-0.63501
C	6.90194	-0.5268	-0.28107
H	6.3469	-2.55967	0.24968
H	7.08161	1.58141	-0.78771
C	8.2799	-0.79522	-0.37094
N	9.42307	-1.01751	-0.44648

S-M7BCE (conformation 1):
Job cpu time: 3 days 22 hours 16 minutes 48.0 seconds
Total energy: -966.5088 a. u. (Lower)
Dipole moment: 5.7819 Debye (3.9548, 3.6777, 2.0651)

C	4.44563	3.78927	4.95825
C	3.94764	3.18405	3.83343
C	2.6046	3.41155	3.41381
C	1.79234	4.28812	4.19053
C	2.28326	4.89585	5.31564
C	3.64104	4.67989	5.76646
H	5.46992	3.58485	5.23776
H	4.57398	2.52212	3.25107
H	0.7735	4.46144	3.86843
H	1.6282	5.55237	5.87134
C	2.02561	2.78822	2.22507
O	0.87517	2.96844	1.83671
O	2.9082	1.96748	1.58582
C	2.45379	1.28599	0.38225
C	3.3571	0.06245	0.23396
H	1.42085	0.97421	0.55361
H	3.09602	-0.46328	-0.69243
H	4.38521	0.42058	0.1127
C	4.15567	5.30562	6.93907
C	3.35101	6.19269	7.7505
C	5.51382	5.09099	7.38887
C	3.85846	6.79138	8.88094
H	2.32713	6.39528	7.47054
C	6.00048	5.70071	8.52267
H	6.16786	4.43845	6.82851
C	5.18644	6.55832	9.28684
H	3.22745	7.45084	9.46582
H	7.02352	5.51746	8.83102

H	5.57788	7.034	10.17831
C	3.29743	-0.90912	1.41964
H	2.29145	-1.33461	1.50711
H	3.4813	-0.35925	2.3516
C	4.31342	-2.05177	1.30059
H	5.32409	-1.62953	1.23243
H	4.14399	-2.58938	0.35864
C	4.258	-3.04525	2.46623
H	3.25011	-3.47605	2.52845
H	4.41704	-2.50672	3.40966
C	5.28399	-4.17901	2.35536
H	6.29089	-3.74831	2.29557
H	5.1267	-4.71641	1.41215
C	5.22112	-5.16854	3.52262
H	4.2355	-5.6405	3.5878
H	5.96362	-5.96407	3.41341
H	5.41004	-4.66625	4.4768
C	2.50579	2.25864	-0.79175
H	1.83835	3.10391	-0.61653
H	3.52346	2.63387	-0.93455
H	2.1866	1.76422	-1.71262

S-M7BCE (conformation 2):
Job cpu time: 8 days 12 hours 36 minutes 19.0 seconds
Total energy: -966.5078 a. u. (Higher)
Dipole moment: 5.6875 Debye (-4.1204, -3.7971, 0.9760)

C	-1.16247	-0.12605	0.
C	0.2327	-0.12605	0.
C	0.93023	1.0817	0.
C	0.23258	2.29021	-0.0012
C	-1.16225	2.29013	-0.00168
C	-1.85985	1.08193	-0.00068
H	-1.71222	-1.07837	0.00045
H	0.7822	-1.07856	0.00132
H	0.78278	3.24235	-0.00126
H	-1.71237	3.24241	-0.00263
C	2.47023	1.08181	0.00089
O	3.26217	2.0233	0.00103
O	2.98512	-0.17369	0.00153
C	4.4145	-0.1315	0.00234
C	4.98629	-1.5185	0.00592
H	4.74733	0.43105	-0.90363
H	4.65318	-2.08077	0.91199
H	4.65425	-2.08502	-0.8979
C	-3.39985	1.08218	-0.00093
C	-4.09717	2.29058	-0.00162
C	-4.09755	-0.12561	-0.00059
C	-5.49188	2.29109	-0.00127
H	-3.54682	3.2426	-0.00111

C	-5.49269	-0.12527	-0.00125
H	-3.54811	-1.0781	-0.00023
C	-6.18991	1.08279	-0.00145
H	-6.04158	3.24352	-0.00118
H	-6.04253	-1.07771	-0.00139
H	-7.28959	1.08345	-0.00124
C	6.52564	-1.47368	0.0067
H	6.86698	-0.95736	0.87951
H	6.86797	-0.96087	-0.86779
C	7.08101	-2.91005	0.0099
H	6.73971	-3.42636	-0.86293
H	6.73865	-3.42288	0.88437
C	8.62036	-2.86523	0.01074
H	8.96167	-2.34895	0.8836
H	8.96272	-2.35236	-0.8637
C	9.17573	-4.30159	0.01389
H	8.83443	-4.81787	-0.85896
H	8.83337	-4.81445	0.88834
C	10.71508	-4.25677	0.01473
H	11.05639	-3.7405	0.88759
H	11.10096	-5.25477	0.01691
H	11.05744	-3.7439	-0.85971
C	4.87172	0.64967	1.24826
H	5.29517	1.58507	0.94724
H	4.0312	0.82745	1.88609
H	5.60645	0.07926	1.77713

S-DM8OCB:
Job cpu time: 6 days 2 hours 2 minutes 30.0 seconds
Total energy: -1024.0378 a. u.
Dipole moment: 15.9858 Debye (-15.9408, 0.7552, 0.9311)

C	0.64655	-0.10051	-0.01744
C	1.45942	0.63037	-0.92349
C	1.23954	-1.11621	0.76785
C	2.79805	0.35718	-1.04482
H	0.98835	1.40096	-1.52179
C	2.58567	-1.38495	0.64594
H	0.65224	-1.6829	1.47722
C	3.43516	-0.66813	-0.26695
H	3.37589	0.91991	-1.7647
H	3.01217	-2.1486	1.28113
C	4.84322	-0.96349	-0.39277
C	5.41588	-2.15117	0.17877
C	5.74064	-0.08485	-1.08629
C	6.75281	-2.44112	0.05774
H	4.78524	-2.86442	0.69391
C	7.08213	-0.35671	-1.19698
H	5.37229	0.83933	-1.5131

C	7.6306	-1.55047	-0.63131
H	7.15212	-3.3536	0.48336
H	7.73721	0.33472	-1.71239
C	9.00256	-1.84031	-0.7499
N	10.14018	-2.08085	-0.84908
O	-0.61018	0.23673	-0.00051
C	-1.31713	-0.58885	0.94927
C	-2.70373	0.00889	1.1316
H	-1.36808	-1.61114	0.56205
H	-0.7451	-0.61487	1.87919
H	-2.60704	1.02589	1.53068
H	-3.1657	0.10076	0.14283
C	-3.63074	-0.81769	2.04556
H	-3.66907	-1.84054	1.64418
C	-5.06102	-0.24434	1.98744
C	-3.0994	-0.8908	3.4861
H	-5.33843	-0.11227	0.93418
H	-5.0592	0.76182	2.42866
C	-6.14049	-1.09626	2.66854
H	-3.02668	0.1127	3.92082
H	-3.75532	-1.4846	4.12646
H	-2.10769	-1.34692	3.53362
H	-5.92999	-1.18616	3.74034
H	-6.09913	-2.11236	2.25955
C	-7.54974	-0.5154	2.49097
H	-7.7962	-0.47559	1.42079
H	-7.54397	0.5255	2.83872
C	-8.67127	-1.26822	3.23163
H	-8.38505	-1.33017	4.29079
C	-8.8629	-2.70013	2.71066
C	-9.99051	-0.48708	3.14949
H	-7.96185	-3.30699	2.82857
H	-9.67166	-3.20569	3.24692
H	-9.12476	-2.6929	1.6463
H	-10.78569	-0.99127	3.70683
H	-9.88235	0.52234	3.55766
H	-10.32331	-0.3923	2.1097

S-DM8BCE:
Job cpu time: 6 days 2 hours 16 minutes 49.0 seconds
Total energy: -1045.15080845 a. u.
Dipole moment: 2.8911 Debye (0.7862, 2.7346, 0.5122)

C	0.96155	0.71885	0.07758
C	1.85217	1.80339	-0.1321
C	1.48481	-0.58555	0.22085
C	3.20597	1.59442	-0.19291
H	1.43197	2.79522	-0.24769
C	2.84611	-0.79224	0.1606
H	0.82648	-1.42838	0.38293

C	3.77921	0.28447	-0.04775
H	3.85001	2.44346	-0.37405
H	3.2151	-1.79915	0.29551
C	5.20256	0.06021	-0.10897
C	5.75254	-1.26634	-0.19315
C	6.14224	1.14544	-0.0842
C	7.10631	-1.48654	-0.25611
H	5.0957	-2.1251	-0.23967
C	7.49786	0.93394	-0.13082
H	5.79054	2.16548	0.00176
C	8.02339	-0.39331	-0.22214
H	7.48975	-2.4965	-0.33487
H	8.1817	1.77294	-0.09522
C	-0.53413	1.08239	0.12657
O	-1.51888	0.36368	0.29175
O	-0.75809	2.48328	-0.05298
C	-2.15208	2.76647	0.09361
C	-2.33313	4.26543	-0.08022
H	-2.7069	2.21014	-0.67047
H	-2.47108	2.42216	1.08131
H	-1.77742	4.7854	0.70822
H	-1.8758	4.55008	-1.03301
C	-3.80606	4.72315	-0.06677
H	-4.34124	4.15125	-0.8383
C	-3.8812	6.21214	-0.46106
C	-4.48128	4.44902	1.28651
H	-3.30094	6.355	-1.38097
H	-3.37814	6.8102	0.3108
C	-5.29491	6.76278	-0.68982
H	-3.96817	4.98778	2.09085
H	-5.52489	4.76956	1.28387
H	-4.47675	3.386	1.54168
H	-5.87282	6.71774	0.2402
H	-5.81491	6.11914	-1.40876
C	-5.28414	8.21223	-1.19391
H	-4.76651	8.25728	-2.16207
H	-4.6848	8.81726	-0.50182
C	-6.6689	8.8711	-1.33959
H	-7.17951	8.78716	-0.37014
C	-7.54342	8.17742	-2.39439
C	-6.52192	10.36484	-1.66217
H	-7.73391	7.1295	-2.14958
H	-8.51368	8.67483	-2.48445
H	-7.06237	8.2094	-3.37877
H	-7.49806	10.8546	-1.72689
H	-5.9368	10.88253	-0.89618
H	-6.01461	10.50818	-2.62277
H	9.07902	-0.56327	-0.26285

For red ball = oxygen, gray ball = carbon, white ball = hydrogen, blue ball = nitrogen

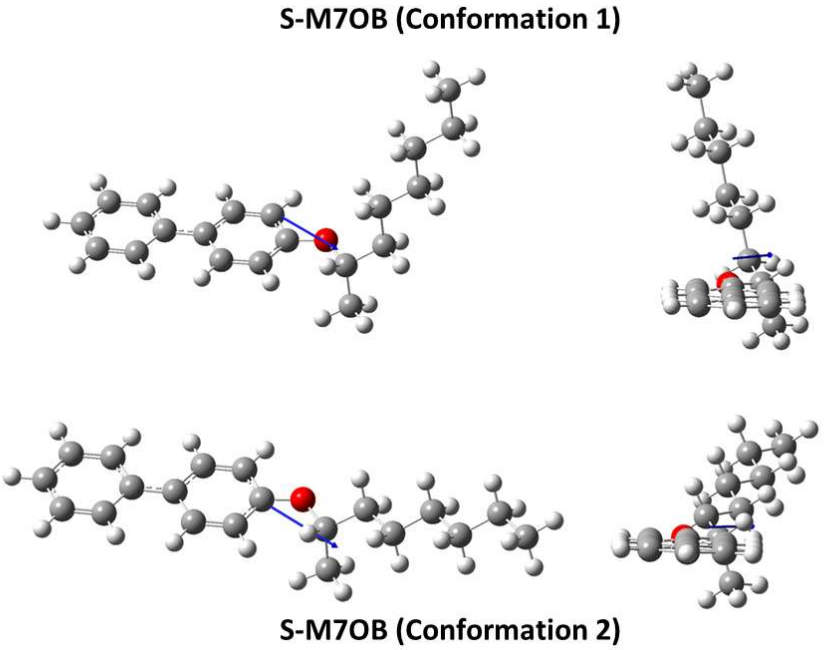

Figure S4.1. Molecular model of S-M7OB. Blue arrow: dipole moment.

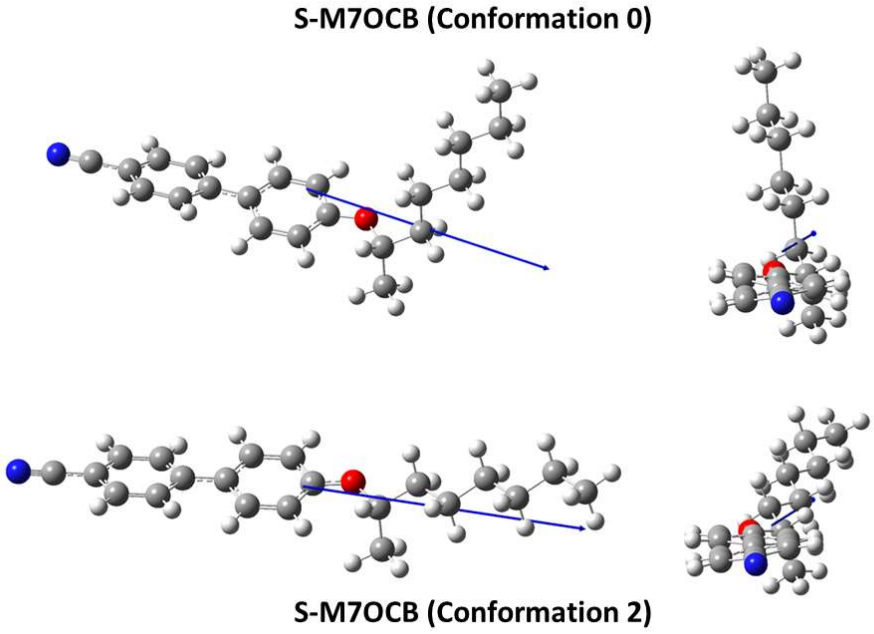

Figure S4.2. Molecular model of S-M7OCB. Blue arrow: dipole moment.

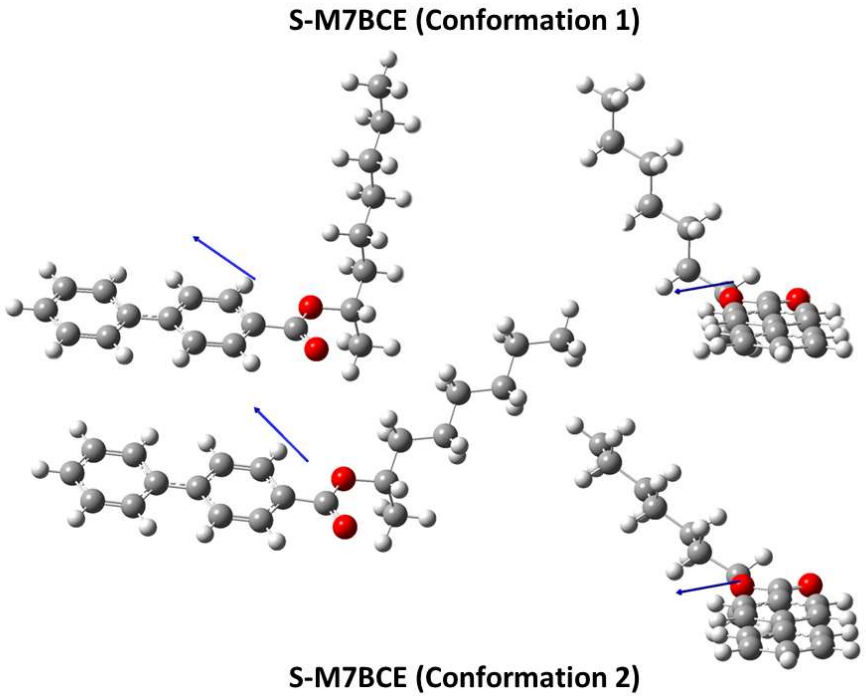

Figure S4.3. Molecular model of S-M7BCE.Blue arrow: dipole moment.

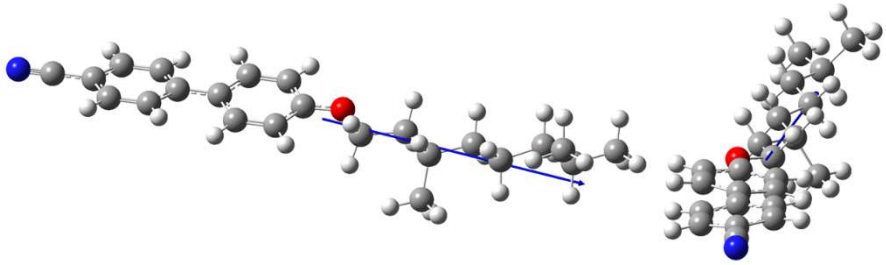

Figure S4.4. Molecular model of S-DM8OCB. Blue arrow: dipole moment.

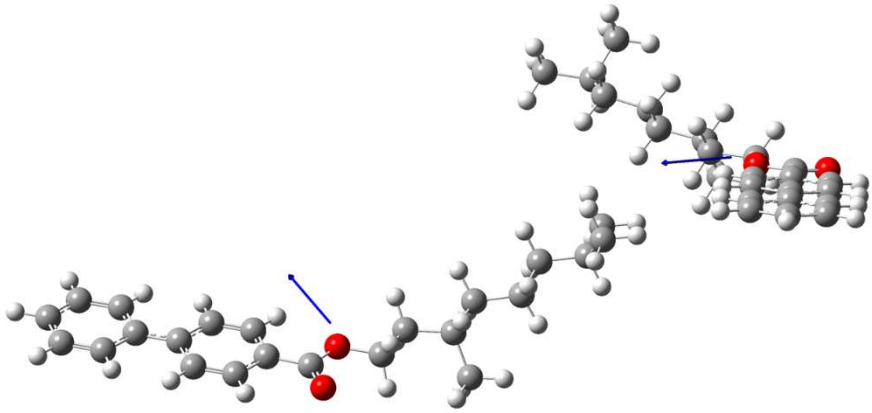

Figure S4.5. Molecular model of S-DM8BCE. Blue arrow: dipole moment.