

Supporting Information

A new strategy towards the synthesis of a room-temperature discotic nematic liquid crystal by employing triphenylene and pentaalkynylbenzene units

Monika Gupta,^a Santosh Prasad Gupta,^a M. V. Rasna,^b Debashis Adhikari,^a Surajit Dhara^b and Santanu Kumar Pal^{*a}

^{a.} *Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Sector-81, Knowledge City, Manauli-140306, India.*

^{b.} *School of Physics, University of Hyderabad, Hyderabad-500046, India*

*Corresponding author: Tel.: +91-172-2240266; fax: +91-172-2240266; E-mail:

skpal@iisermohali.ac.in

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1. Experimental Section

1.1. Materials and Reagents

Chemicals and solvents were all of AR quality and were used without further purification. Pentabromophenol, 1-ethynyl-4-pentylbenzene, copper iodide, bis(triphenylphosphine) palladium(II) dichloride, triphenylphosphine, triethylamine, potassium carbonate, dibromohexane, dibromooctane, dibromodecane, dibromododecane, potassium iodide, catechol, bromohexane, ferric chloride and 2-bromo-1,3,2-benzodioxaborole were all purchased from Sigma–Aldrich (Bangalore, India). Column chromatographic separations were performed on silica gel (60-120 & 230-400 mesh). Thin layer chromatography (TLC) was performed on aluminium sheets pre-coated with silica gel (Merck, Kieselgel 60, F254).

1.2. Synthesis and characterization of target compounds (7a-d)

The synthesis of compounds **2**, **3**, **5** and **6** has been described in the earlier reports. For the synthesis of the target compounds **7**, monohydroxytriphenylene **6** (1 equivalent) was dissolved in *n*-butanone. To that solution, cesium carbonate (3 equivalents) was added & the mixture was stirred for 15 min followed by the addition of compound **3** & a catalytic amount of KI. The mixture was refluxed for 18 h. The solvent was evaporated & the crude was purified through column chromatography to obtain the final compounds **7**. The synthesized compounds were characterized by ¹H NMR, ¹³C NMR, IR, UV-Vis and mass spectrometry as shown below [see supporting information (Figure S1-S8) for full spectroscopic data]:

Compound 7a

FT-IR (cm⁻¹): 3026, 2955, 2930, 2858, 2209, 1616, 1512, 1467, 1433, 1387, 1381, 1347, 1262, 1170, 1115, 1081, 1041, 1021, 986, 929, 866, 839, 769, 658, 645, 625.

UV-Vis (nm): 237, 263, 280, 338, 381, 418.

¹H NMR (400 MHz, CDCl₃, δ in ppm): δ 7.89 (s, 6H), 7.56 (m, 10H), 7.23 (m, 10H), 4.41 (m, 2H), 4.28 (t, 12H, *J* = 8, 4 Hz), 2.67 (m, 10H), 2.00 (m, 14H), 1.66 (m, 16H), 1.40 (m, 50H), 0.97 (m, 30H).

¹³C NMR (400 MHz, CDCl₃, δ in ppm): 160.14, 149.01, 148.94, 148.94, 148.92, 144.03, 143.98, 143.74, 131.78, 131.67, 131.54, 128.78, 128.55, 128.54, 123.62, 123.55, 120.71, 120.48, 120.45, 120.11, 107.29, 99.51, 99.41, 97.34, 87.08, 84.05, 71.92, 69.73, 69.69, 69.53, 50.56, 37.87, 36.01, 35.99, 35.88, 34.67, 31.77, 31.73, 31.70, 31.63, 31.50, 31.47, 31.01, 30.98, 30.89, 30.63, 29.45, 26.94, 26.29, 26.21, 25.89, 22.70, 22.57, 22.52, 14.16, 14.10, 14.08, 14.05, 8.35, 7.46.

MS (MALDI): *m/z* for C₁₂₅H₁₅₈O₇ 1772.2041; found 1772.2258.

Compound 7b

FT-IR (cm⁻¹): 3026, 2955, 2929, 2858, 2208, 1616, 1512, 1467, 1434, 1385, 1347, 1262, 1170, 1115, 1082, 1041, 1021, 976, 963, 929, 898, 769, 752, 727, 667, 645, 625.

UV-Vis (nm): 237, 264, 280, 338, 380, 416.

^1H NMR (400 MHz, CDCl_3 , δ in ppm): δ 7.88 (s, 6H), 7.58 (m, 10H), 7.21 (m, 10H), 4.41 (t, 2H, $J = 8, 4\text{ Hz}$), 4.26 (m, 12H), 2.64 (m, 10H), 1.98 (m, 14H), 1.66 (m, 20H), 1.40 (m, 50H), 0.94 (m, 30H).

^{13}C NMR (400 MHz, CDCl_3 , δ in ppm): 160.22, 149.00, 148.96, 144.04, 143.96, 143.73, 131.80, 131.68, 131.60, 128.79, 128.57, 128.55, 124.11, 123.65, 123.63, 120.73, 120.54, 120.50, 120.13, 107.31, 99.55, 99.39, 97.33, 87.11, 86.63, 84.11, 74.73, 69.70, 36.02, 35.96, 31.74, 31.52, 31.49, 31.01, 30.98, 30.68, 29.71, 29.59, 29.56, 29.47, 26.42, 26.25, 25.92, 25.90, 22.73, 22.72, 22.59, 22.56, 14.11, 14.07.

MS (MALDI): m/z for $\text{C}_{127}\text{H}_{162}\text{O}_7$ 1800.2354; found 1800.2162.

Compound 7c

FT-IR (cm^{-1}): 3026, 2955, 2929, 2857, 2208, 1617, 1512, 1467, 1435, 1386, 1348, 1262, 1171, 1114, 1082, 1042, 1021, 979, 929, 838, 726.

UV-Vis (nm): 239, 262, 280, 335, 370, 414.

^1H NMR (400 MHz, CDCl_3 , δ in ppm): δ 7.88 (s, 6H), 7.56 (m, 10H), 7.21 (m, 10H), 4.41 (t, 2H, $J = 4, 8\text{ Hz}$), 4.27 (t, 12H, $J = 8, 4\text{ Hz}$), 2.66 (m, 10H), 1.98 (m, 14H), 1.65 (m, 24H), 1.42 (m, 50H), 0.96 (m, 30H).

^{13}C NMR (400 MHz, CDCl_3 , δ in ppm): 160.25, 148.97, 144.03, 143.92, 143.73, 131.81, 131.70, 131.69, 131.62, 131.58, 131.52, 128.77, 128.56, 128.55, 124.09, 123.63, 120.75, 120.58, 120.51, 120.13, 107.32, 99.54, 99.38, 87.13, 84.12, 74.78, 69.71, 36.02, 36.00, 31.75, 31.52, 31.50, 31.02, 31.00, 30.69, 29.74, 29.72, 29.64, 29.59, 29.47, 26.95, 26.46, 26.29, 25.91, 22.74, 22.72, 22.59, 14.12, 14.10, 14.08.

MS (MALDI): m/z for $\text{C}_{129}\text{H}_{166}\text{O}_7$ 1828.2667; found 1828.2506.

Compound 7d

FT-IR (cm^{-1}): 3027, 2955, 2929, 2857, 2209, 1617, 1512, 1467, 1456, 1435, 1387, 1381, 1349, 1300, 1262, 1171, 1115, 1042, 1021, 929, 867, 838, 726.

UV-Vis (nm): 238, 261, 280, 336, 380, 417.

^1H NMR (400 MHz, CDCl_3 , δ in ppm): δ 7.85 (s, 6H), 7.53 (m, 10H), 7.19 (m, 10H), 4.37 (t, 2H, $J = 8\text{ Hz}$), 4.25 (t, 12H, $J = 4, 8\text{ Hz}$), 2.65 (m, 10H), 1.96 (m, 14H), 1.61 (m, 28H), 1.36 (m, 50H), 0.94 (m, 30H).

^{13}C NMR (400 MHz, CDCl_3 , δ in ppm): 148.96, 131.79, 131.69, 131.67, 131.61, 131.59, 131.57, 128.55, 123.61, 107.31, 69.71, 35.90, 31.71, 31.48, 30.96, 29.76, 29.74, 29.70, 29.64, 29.56, 29.44, 25.87, 22.69, 22.55, 14.09, 14.06.

MS (MALDI): m/z for $\text{C}_{131}\text{H}_{170}\text{O}_7$ 1856.2980; found 1856.2778.

1.3. Instrumental

Structural characterization. Structural characterization of the compound was carried out through a combination of infrared spectroscopy (Perkin Elmer Spectrum AX3), ^1H NMR and

^{13}C NMR (Bruker Biospin Switzerland Avance-iii 400 MHz and 100 MHz spectrometers respectively), UV-VIS-NIR spectrophotometer (Agilent Technologies UV-Vis-NIR Spectrophotometer) and mass spectrometry (Waters synapt G2s). NMR spectra were recorded using deuterated chloroform (CDCl_3) as solvent and tetramethylsilane (TMS) as an internal standard.

Differential Scanning Calorimetry. DSC measurements were performed on Perkin Elmer DSC 8000 coupled to a Controlled Liquid Nitrogen Accessory (CLN 2) with a scan rate of $5^\circ\text{C}/\text{min}$.

Polarized Optical Microscopy. Textural observations of the mesophase were performed with Nikon Eclipse LV100POL polarising microscope provided with a Linkam heating stage (LTS 420). All images were captured using a Q-imaging camera.

X-ray Diffraction. X-ray diffraction (XRD) was carried out on powder samples using $\text{Cu K}\alpha$ ($\lambda=1.54 \text{ \AA}$) radiation from a source (GeniX 3D, Xenocs) operating at 50 kV and 0.6 mA. The diffraction patterns were collected on a two module Pilatus detector.

2. FT-IR spectra:

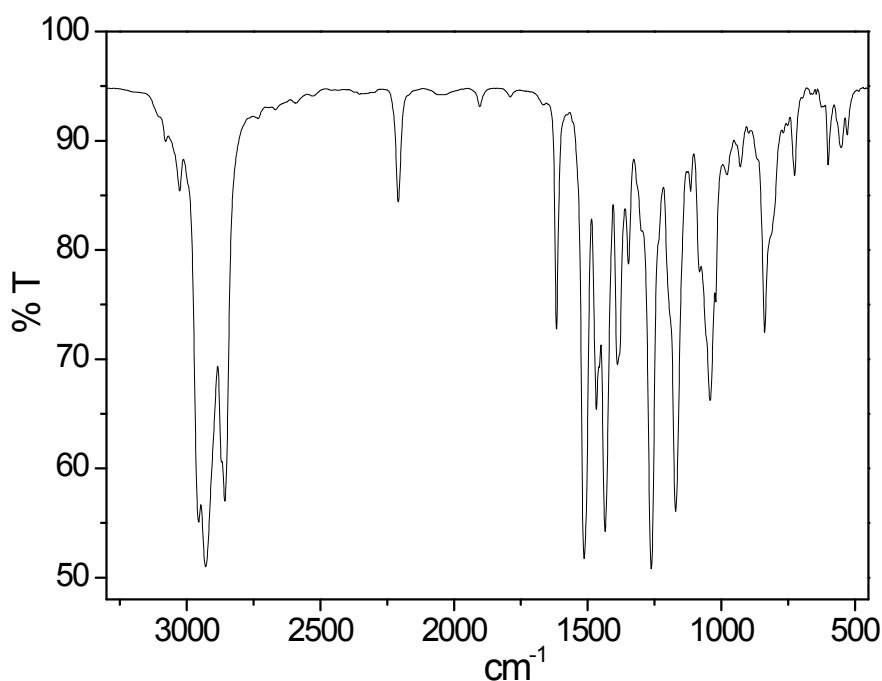


Fig. S1 FT-IR spectrum of compound **7c**. Other Compounds show similar spectra.

3. NMR Spectra

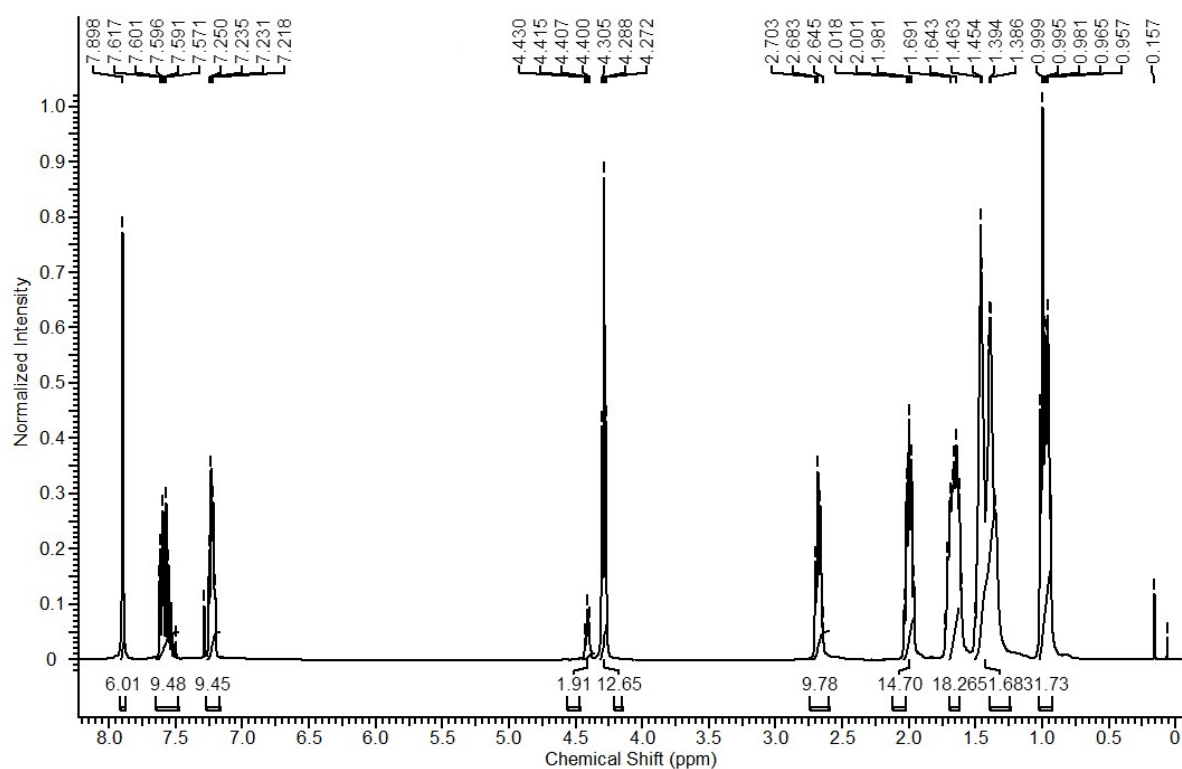


Fig. S2 ¹H NMR spectrum of compound 7a.

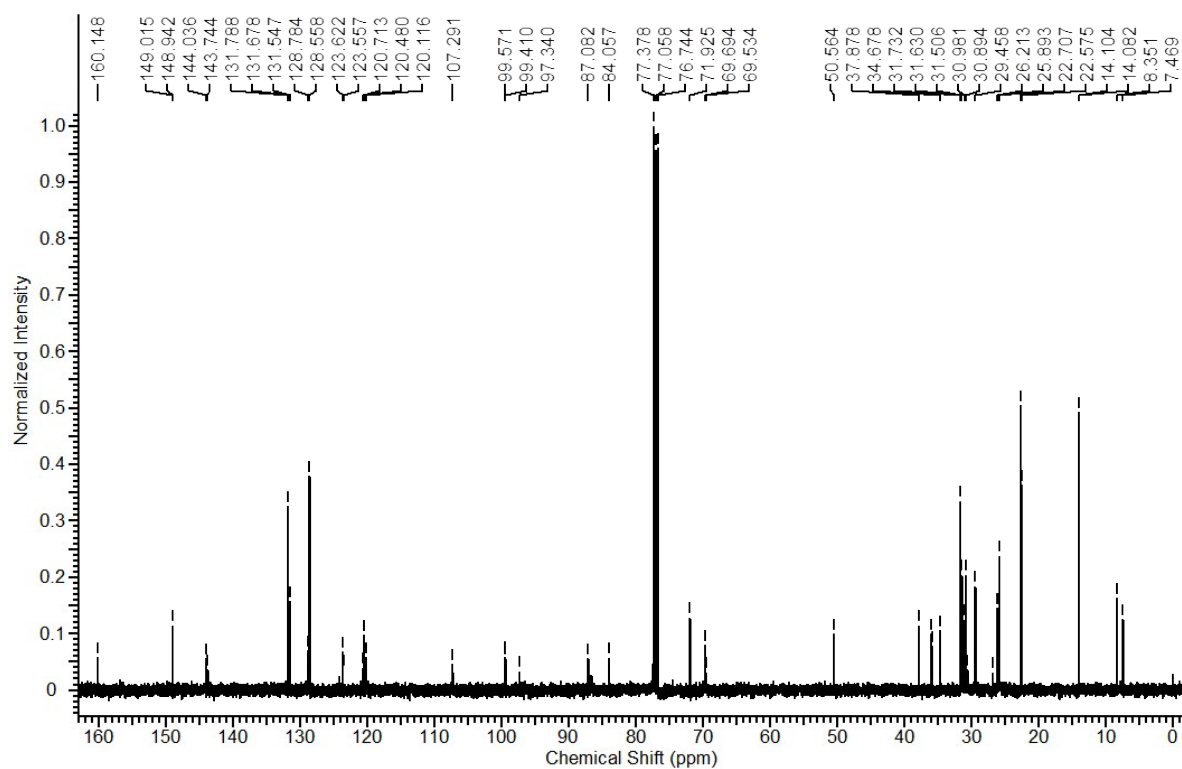


Fig. S3 ¹³C NMR spectrum of compound 7a

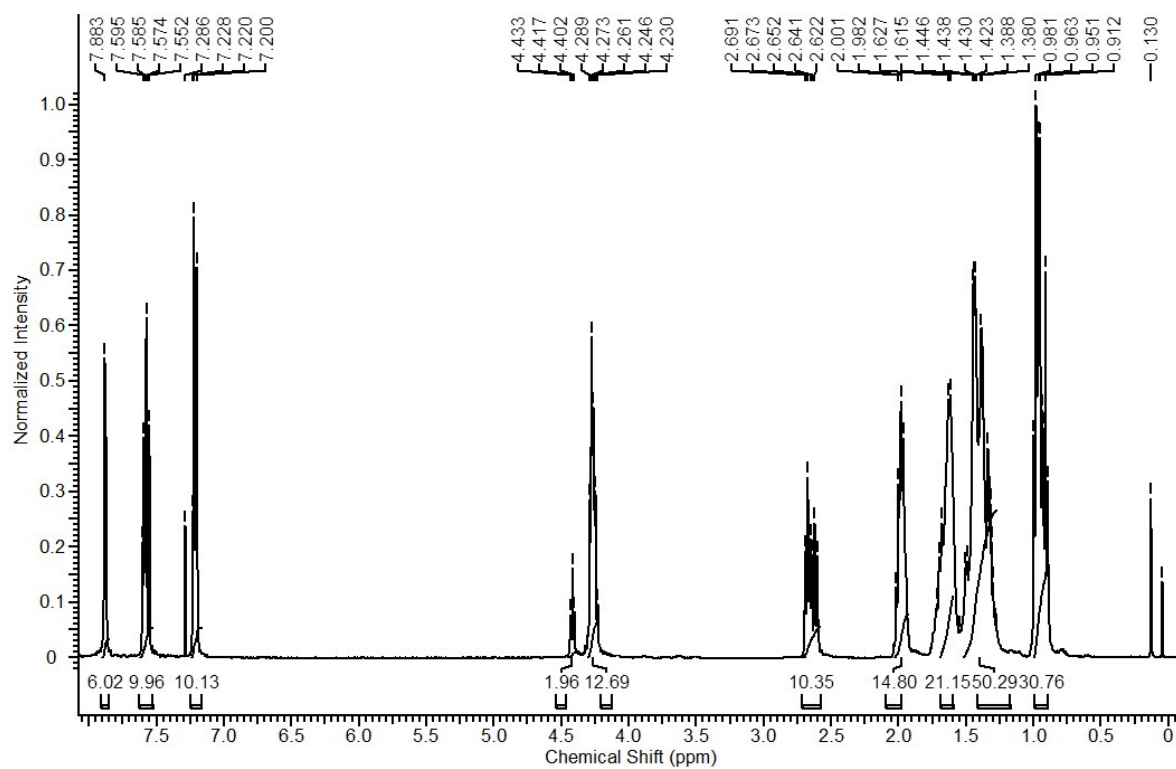


Fig. S4 ¹H NMR spectrum of compound **7b**.

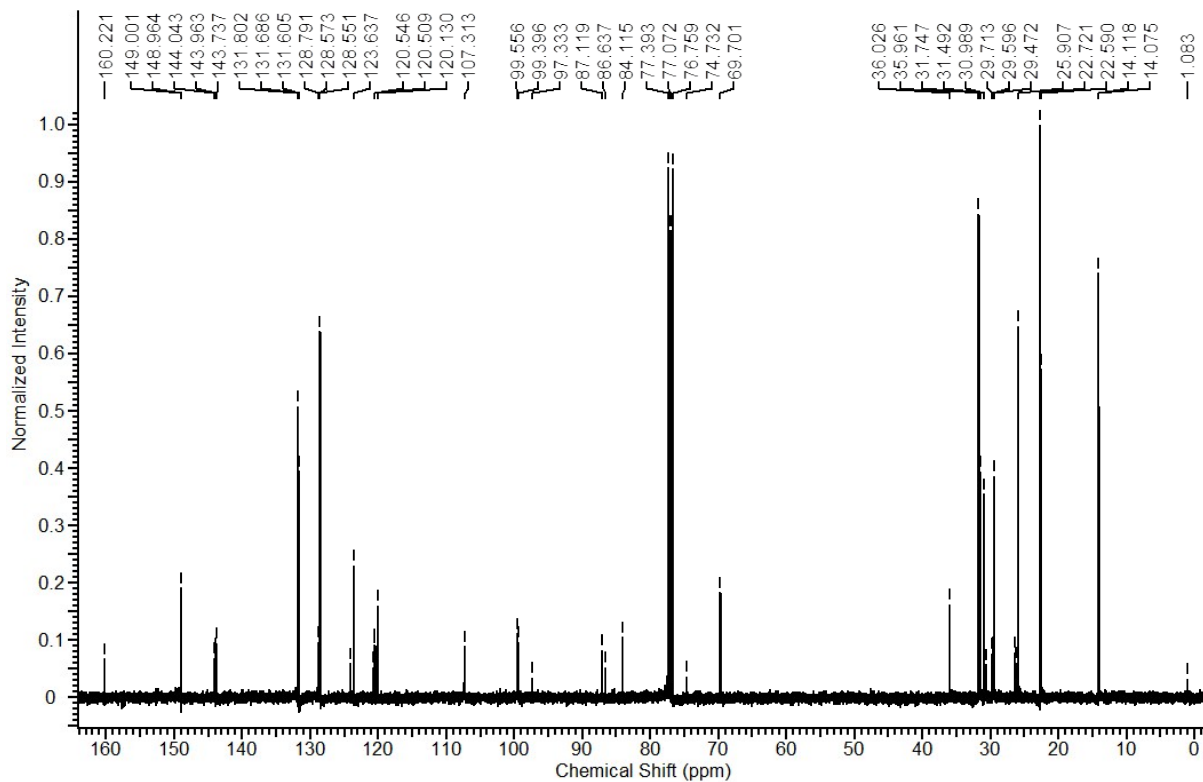


Fig. S5 ¹³C NMR spectrum of compound **7b**.

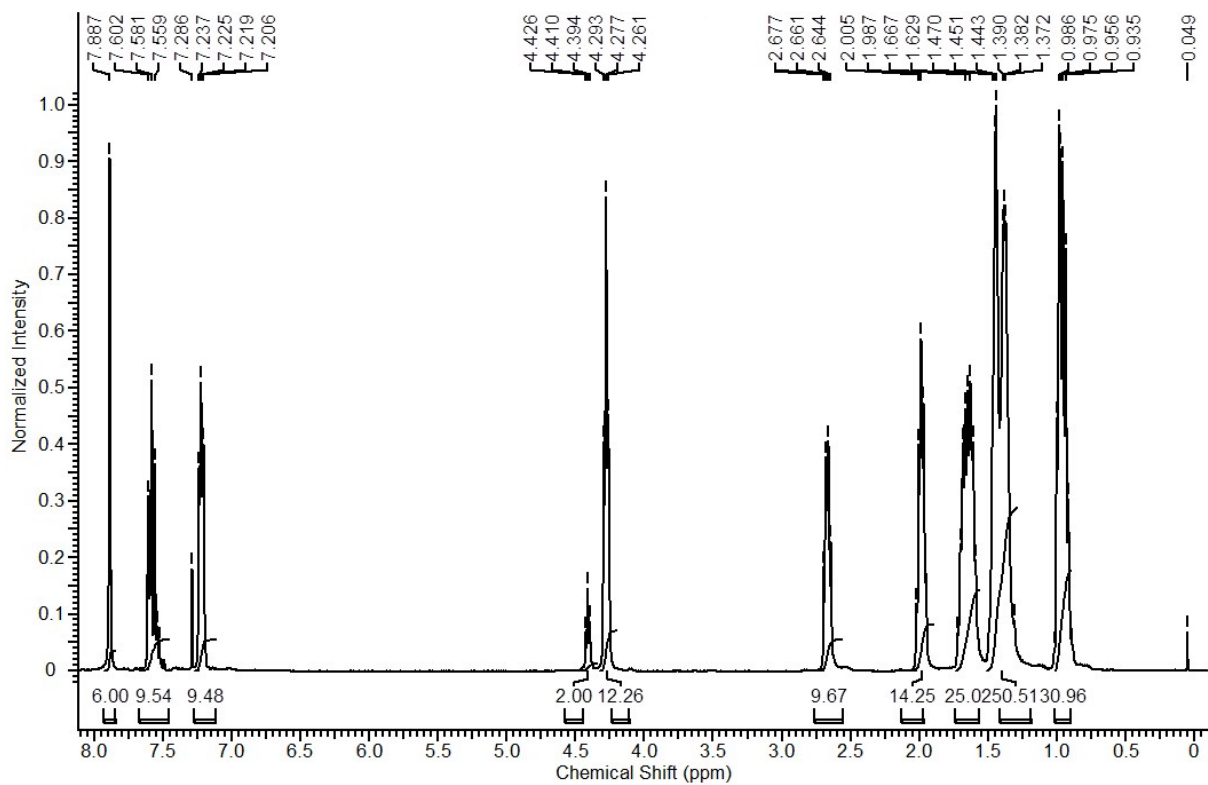


Fig. S6 ^1H NMR spectrum of compound **7c**.

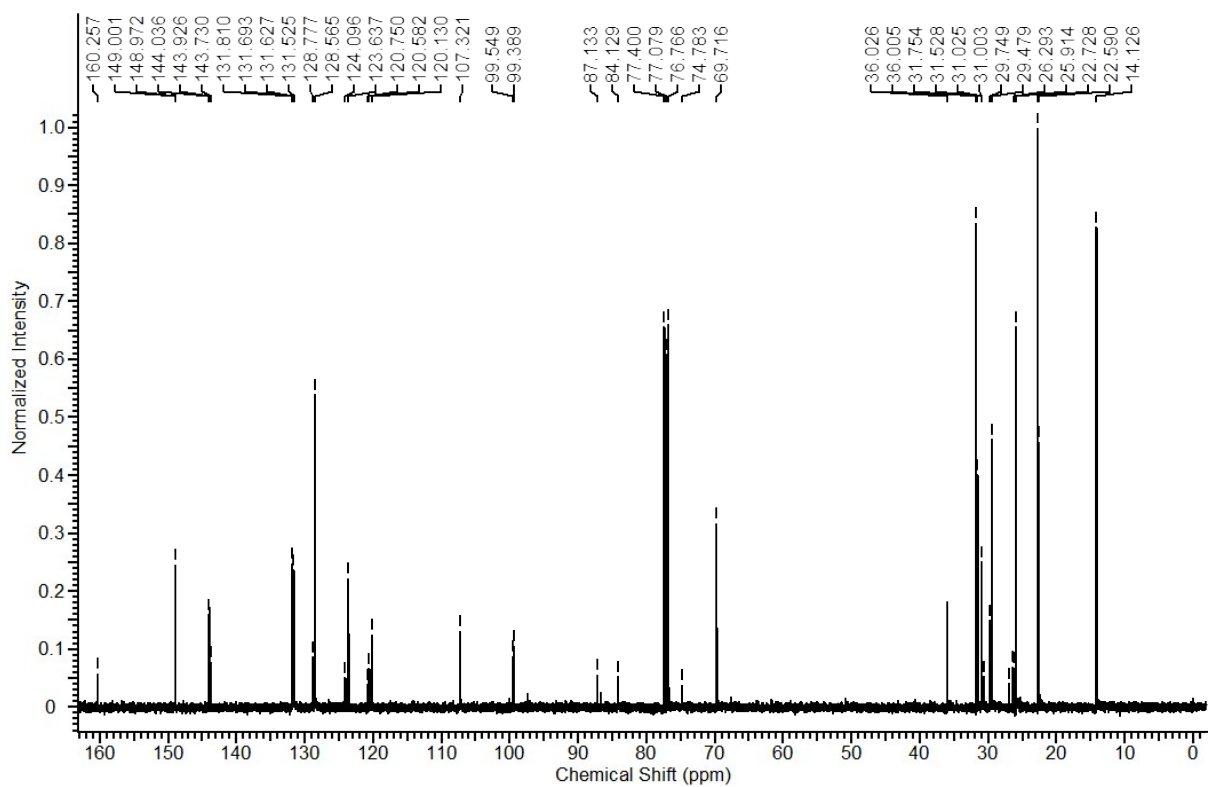


Fig. S7 ^{13}C NMR spectrum of compound **7c**.

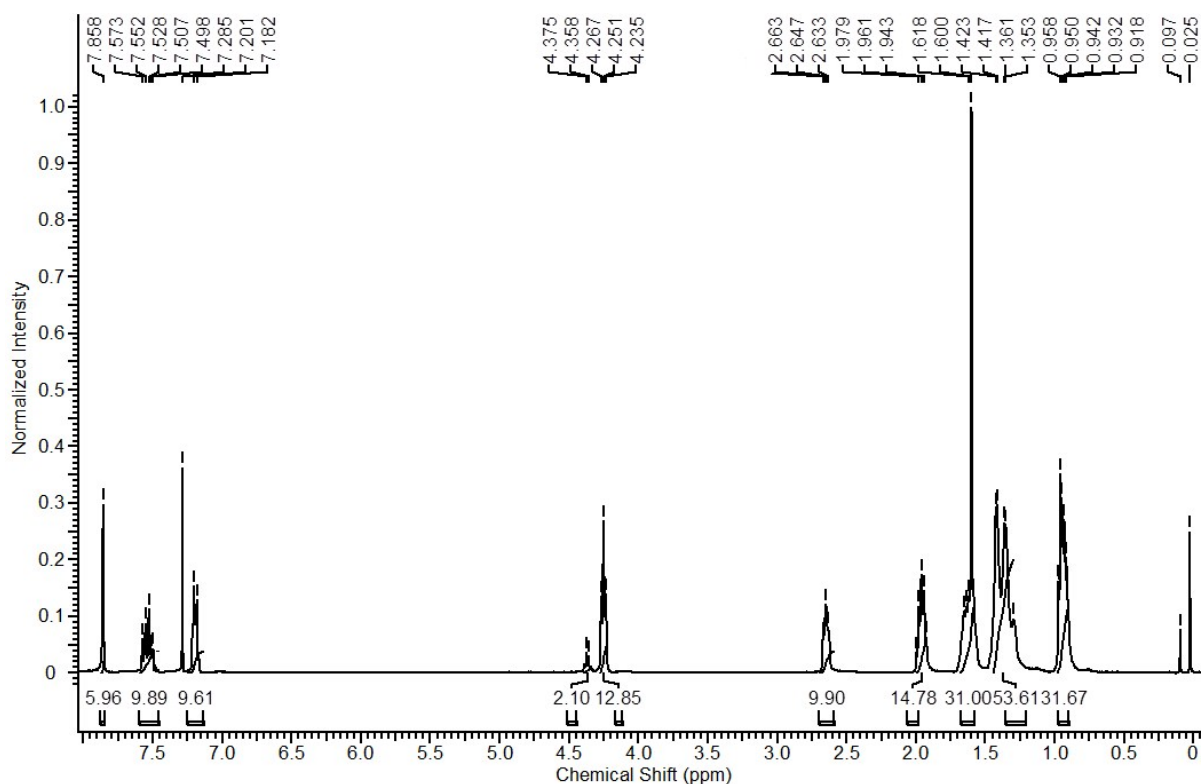


Fig. S8 ^1H NMR spectrum of compound **7d**.

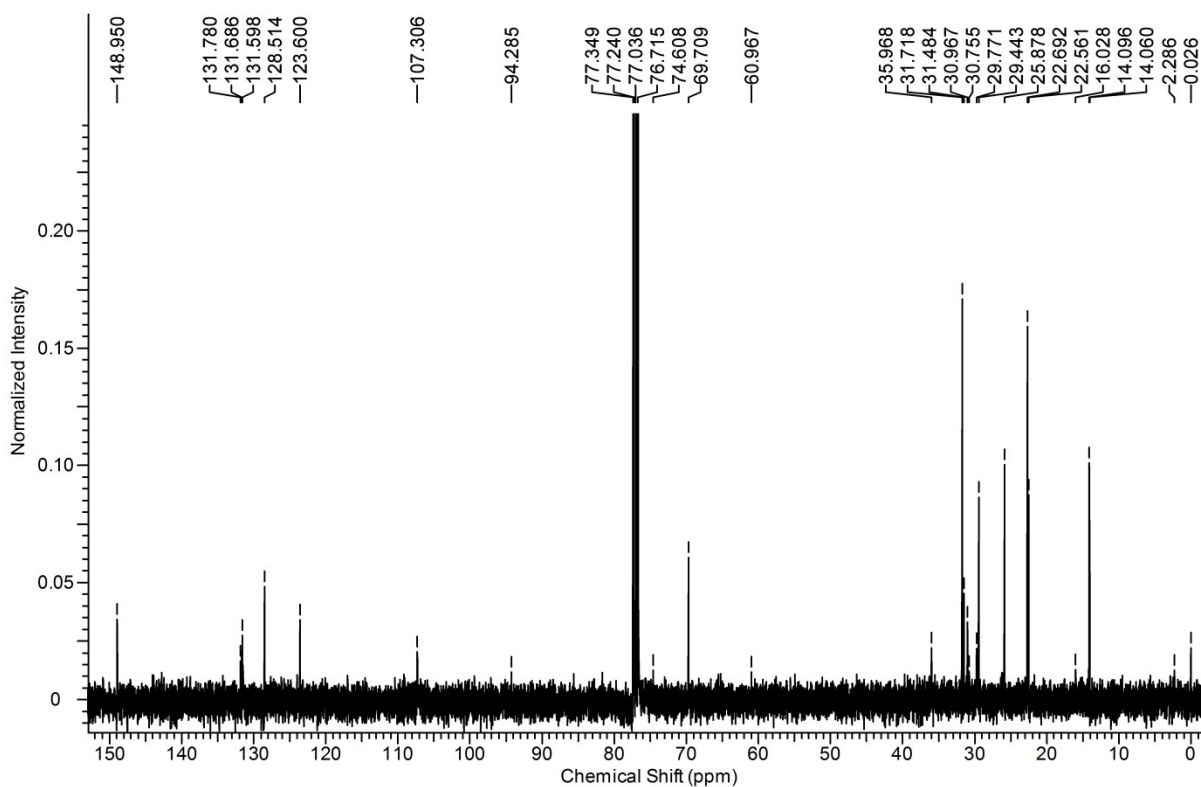


Fig. S9 ^{13}C NMR spectrum of compound **7d**.

4. Photophysical studies

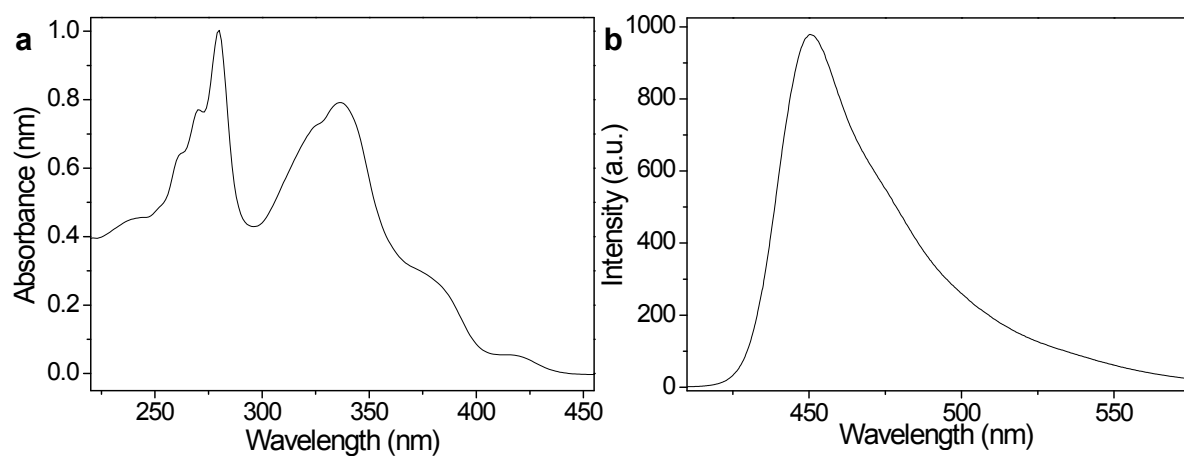


Fig. S10 (a) UV-Vis absorption & (b) emission spectra of compound **7b** in solution (5 μM in dichloromethane)

5. Polarizing Optical Micrograph



Fig. S11 Polarizing optical micrograph of compound **7b** at room temperature on cooling from the isotropic melt between crossed polarizers.

6. 2D diffraction Patterns

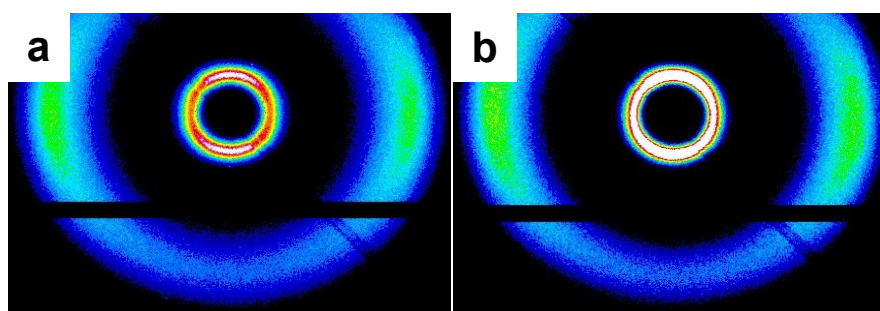


Fig. S12 2D diffraction patterns obtained for (a) **7b** and (b) **7c** at room temperature, on cooling from the isotropic melt.

7. Dielectric constant and birefringence measurement

For the dielectric and electrooptic measurements the liquid crystal cells were made of two indium-tin-oxide (ITO) coated glass plates with patterned electrodes. These plates were cleaned thoroughly and spin coated with polyimide AL-1254. Subsequently they were cured at 180°C for 1 hour and rubbed in an antiparallel way. Such cells usually provide planar alignment of the calamitic liquid crystals. However, it gives uniform and homeotropic alignment of the discotic nematic liquid crystal. A typical cell thickness used in the experiment was about 8 μm . The empty cell was heated by using a temperature controller (Mettler FP 90) and the sample was filled in the isotropic phase. Birefringence was measured using a phase modulation technique.¹⁻⁴ The sample retardation was measured by using two crossed Glan–Thompson polarizers, Helium-Neon laser ($\lambda = 632.8 \text{ nm}$), photoelastic modulator (PEM) and a lock-in amplifier.¹⁻⁴ A photodetector collected the light transmitted through the liquid crystal, lock-in amplifier measured the first and second harmonics of the ac signal. Using a function generator (Tektronix-AFG 3102) and voltage amplifier (TEGAM-2350) a sinusoidal voltage of frequency 1 kHz and amplitude up to 23 V was applied. At this high voltage the director was completely reoriented to the homogeneous or planar state. This was further verified by the optical polarising microscope. The birefringence was measured as a function of temperature and voltage. The dielectric constant as a function of voltage was measured using a LCR meter (Agilent, E4980A). All the instruments were interfaced with a computer and a suitable computer program written in LabView was used to control the experiments.

8. Coordinates for computationally optimized structures

7b_folded

C	-1.39051300	-4.62116900	-1.62512100	H	-1.50300300	-3.72451800	-1.00505600
C	0.09786900	-5.00647400	-1.65216400	H	-1.71171100	-4.34164800	-2.63862200
C	0.93263800	-3.75597100	-1.87493800	H	0.30309800	-5.74969500	-2.43346600
O	2.32540500	-4.08691300	-1.82847800	H	0.40564800	-5.44486300	-0.69755700
C	3.20899700	-3.05781700	-1.70143400	H	0.70661800	-3.03578000	-1.08007700
C	2.85705500	-1.71779000	-1.74877500	H	0.69752300	-3.28685500	-2.84278500
C	3.78055700	-0.67709400	-1.50697200	H	1.82775200	-1.46971100	-1.95463300
C	5.12724000	-1.01569400	-1.22612100	H	6.50124400	-2.70263900	-1.05516300
C	5.48234800	-2.38392600	-1.23963600	H	1.27410700	0.31963800	-1.86917800
C	4.56894900	-3.39326900	-1.47122900	H	4.55819200	3.91237300	-1.14531200
C	3.36746500	0.72536300	-1.52468900	H	6.38571700	3.43251500	-0.75831500
C	4.32402400	1.74624500	-1.29615100	H	7.78533400	-1.28505200	-0.51895900
C	5.71157200	1.39718700	-1.00391000	H	-0.70311000	1.10487900	-1.21012700
C	6.09972300	0.03494500	-0.94305400	H	-0.55679800	1.28797000	-2.98903700
C	2.01917900	1.08940600	-1.73831900	H	10.77877100	1.74310000	-0.96340700
C	1.59935700	2.40783400	-1.72107800	H	10.50652700	0.18090000	-1.79723300
C	2.56046100	3.42974200	-1.52123900	H	5.18774700	-5.11839500	-3.39663500
C	3.87981300	3.08685100	-1.32067600	H	3.70862800	-5.75512400	-2.61372300
C	6.67740900	2.39289700	-0.72924200	C	-2.34849500	-5.67848000	-1.05980900
C	7.97951800	2.07922400	-0.37927200	C	-1.98349100	-6.15480700	0.36296900
C	8.36627400	0.71652900	-0.31226000	H	-1.44076400	-5.35600600	0.87732100
C	7.43687600	-0.26216600	-0.59561000	H	-1.29002000	-7.00189800	0.28935800
O	0.30485600	2.81404900	-1.85620800	C	-3.20191400	-6.55847200	1.22555800
C	-0.69899200	1.81965300	-2.03841700	H	-2.94104800	-7.42176400	1.85136000
O	2.20298100	4.75776300	-1.42850200	H	-4.02302200	-6.89732900	0.57689900
O	8.94433200	2.99223800	-0.05379000	H	-3.35019100	-5.23149200	-1.04776100
C	8.61947300	4.37082200	-0.14674900	H	-2.40860000	-6.54566600	-1.73301000
O	9.62651100	0.34510900	0.09088400	C	-3.72007800	-5.46133300	2.17558500
C	10.67884600	0.66174200	-0.82422600	H	-4.54602900	-5.87275200	2.77327300
O	5.00670100	-4.69012100	-1.35977700	H	-2.92600200	-5.18375300	2.88099500
C	4.77376500	-5.55368600	-2.47705200	C	-4.23977400	-4.17952000	1.53230200

H	-4.70183400	-3.53191200	2.28549500	H	0.50621700	-5.97405300	2.07054800
H	-4.98750900	-4.38978400	0.76011000	H	4.88364000	-3.74816200	1.38954200
O	-3.12623200	-3.48924300	0.92862600	H	2.58790200	-7.31000700	2.08030800
C	-2.99720500	-2.14083100	0.98286100	C	-1.73542000	4.63058300	0.89342300
C	-1.41772100	-0.27252400	1.20564100	C	-0.49339700	5.08788700	0.41155600
C	-2.48185800	0.64656700	1.00246900	C	-2.68632700	5.57779800	1.32116700
C	-3.79235700	0.16223400	0.77025300	C	-0.21487400	6.44930500	0.37340000
C	-4.05406500	-1.24025100	0.73832800	H	0.23642500	4.37838900	0.04419900
C	-1.68478300	-1.66867000	1.21922100	C	-2.39329700	6.93744100	1.26984700
C	-0.62558300	-2.58072800	1.44088900	H	-3.64413300	5.23550100	1.70242300
C	0.33285700	-3.31088200	1.60820500	H	0.75677200	6.77139600	0.00649100
C	-0.10638500	0.21611700	1.41483600	H	-3.13648900	7.65581900	1.60908600
C	0.99864800	0.69563500	1.58976300	C	2.25190000	1.32124700	1.82840700
C	-5.35206600	-1.67051400	0.36642500	C	2.32628800	2.72462700	1.92068300
C	-6.48799600	-1.92983900	0.01877600	C	3.43538200	0.57131900	1.97960400
C	-4.83740600	1.08803600	0.54371400	C	3.54498200	3.34703300	2.16756400
C	-5.70026900	1.92368200	0.35561700	H	1.42410500	3.31409400	1.79411600
C	-2.22992600	2.04130600	0.98995300	C	4.64564700	1.20781300	2.22264300
C	-2.01242100	3.23633300	0.94904300	H	3.39473700	-0.50908900	1.90200100
C	-7.82083800	-2.17343700	-0.40958700	H	3.58267900	4.43215300	2.22856700
C	-8.55655800	-1.14466800	-1.03322600	H	5.55211800	0.61482500	2.31278700
C	-8.44094100	-3.42260300	-0.21802900	C	-6.67361700	2.93488800	0.13875900
C	-9.86672600	-1.36570400	-1.44215300	C	-6.27119400	4.26599700	-0.09547800
H	-8.08463900	-0.17980000	-1.19137700	C	-8.05066100	2.63807400	0.15011600
C	-9.75214600	-3.62859400	-0.63507200	C	-7.22063600	5.25821600	-0.31120400
H	-7.88793400	-4.22239400	0.26588700	H	-5.21164200	4.50415700	-0.11074700
H	-10.41902500	-0.55885300	-1.91878700	C	-8.98744300	3.64303700	-0.06823800
H	-10.21591700	-4.59933800	-0.47512700	H	-8.37264000	1.61754300	0.33424100
C	1.51105800	-4.09770500	1.71190900	H	-6.89208300	6.27889500	-0.49423000
C	2.76709600	-3.48148400	1.53771900	H	-10.04660800	3.39564300	-0.05763100
C	1.46557700	-5.48711400	1.92849100	H	7.81387000	4.64265600	0.54770300
C	3.92907000	-4.23702400	1.55994400	H	5.30171900	-6.48265200	-2.24855200
H	2.80653500	-2.41749900	1.33338200	H	11.59498400	0.26338400	-0.38146100
C	2.64139400	-6.23346400	1.93528500	H	-1.64802400	2.35564600	-2.04706900

H	9.52820400	4.91028200	0.12687800	H	4.97603800	-7.50263000	1.78014000
H	8.32341300	4.64758900	-1.16793600	H	5.66073600	-6.25500900	0.71275700
C	-1.15548300	7.39862800	0.79792600	H	5.86581000	-6.13063600	2.46342000
C	-10.48871200	-2.60894600	-1.25424000	C	-11.90002900	-2.85024200	-1.73324200
C	-8.59335000	4.96856200	-0.29991600	H	-11.90936100	-3.19059900	-2.77755000
C	3.88849100	-5.62740700	1.73893400	H	-12.40153800	-3.61936900	-1.13618200
C	4.72211000	2.60447300	2.32984200	H	-12.50216500	-1.93642400	-1.68504400
C	-0.85559200	8.87652100	0.71971000	C	-9.61671700	6.06020800	-0.50110900
H	0.21218800	9.07637600	0.86106600	H	-9.86705600	6.54639500	0.45153700
H	-1.13532500	9.28577200	-0.26074500	H	-9.24492900	6.83999600	-1.17472700
H	-1.41002600	9.44112800	1.47715100	H	-10.54889100	5.66579800	-0.91948300
C	6.03527800	3.28189000	2.63706800	C	1.66504900	5.33953900	-2.62180400
H	6.23854300	3.27587900	3.71648500	H	1.50661800	6.39677200	-2.39702200
H	6.87133300	2.77689500	2.14333000	H	2.37829200	5.24461600	-3.45159100
H	6.02866200	4.32941200	2.31493300	H	0.71292200	4.87817300	-2.89743900
C	5.16373300	-6.42921400	1.67452700				

7b_linear

C	2.19062400	-3.65475700	-1.07516700	C	-11.09385600	0.28614100	0.88088500
C	1.16131600	-3.37261900	-2.17556800	C	-10.35590500	1.07062100	-0.03993100
C	-0.27886000	-3.69673700	-1.75621600	C	-9.22546000	-2.99963700	0.73548700
C	-1.31551600	-2.96090600	-2.61097600	C	-9.93497400	-3.78580000	1.62699200
C	-2.75392000	-3.13050100	-2.11032900	C	-11.03988900	-3.22021600	2.31342900
C	-3.71617600	-2.14701800	-2.78401500	C	-11.39081700	-1.91173800	2.06043200
C	-5.09700900	-2.14535700	-2.14723300	C	-12.21119300	0.86462000	1.52894200
O	-5.80118100	-1.01373600	-2.66369000	C	-12.60526100	2.17015900	1.28984000
C	-6.92281300	-0.58600600	-2.01599300	C	-11.87690800	2.94936100	0.35409100
C	-7.66436300	-1.34912800	-1.13104100	C	-10.78663200	2.39511600	-0.28141300
C	-8.80356200	-0.83646100	-0.46582500	O	-9.66569900	-5.09549000	1.90465500
C	-9.19227000	0.50482000	-0.71574300	C	-8.58869600	-5.71801400	1.22250900
C	-8.42385200	1.26344300	-1.62837000	O	-11.81022600	-3.96140300	3.17550800
C	-7.31604400	0.75181300	-2.26895900	C	-11.16679100	-4.35423000	4.39147100
C	-9.57270300	-1.65230800	0.47363200	O	-13.65690300	2.79501300	1.89624200
C	-10.69260000	-1.09450800	1.14203000	C	-14.40227700	2.06865100	2.86112700

O	-12.19418200	4.26317000	0.11005100	H	-11.92269200	-4.88525400	4.97493200
C	-13.43064300	4.47822500	-0.57617600	H	-8.56256900	-6.74814700	1.58253300
O	-6.56302400	1.57954700	-3.06842300	H	-15.17185800	2.75389300	3.22129200
C	-6.54742400	1.24652000	-4.46098200	H	-13.50648500	5.55722200	-0.73076600
H	1.88796600	-3.12235600	-0.16791700	H	-6.09282400	0.26630800	-4.63361800
H	2.22605000	-4.72293400	-0.82565200	C	3.57966700	-3.14537000	-1.45229400
H	1.41810200	-3.91034600	-3.09949300	H	3.50093000	-2.22829600	-2.04514000
H	1.21748400	-2.30189000	-2.41526200	H	4.14264700	-3.87983900	-2.04088600
H	-0.41838500	-3.38610200	-0.71145700	O	4.35614200	-2.88056200	-0.26014100
H	-0.45395000	-4.78169500	-1.78150800	C	4.94065500	-1.65867900	-0.13782200
H	-1.24066100	-3.27877100	-3.66101600	C	4.19545500	-0.45977300	-0.15146600
H	-1.07021700	-1.88994500	-2.59289500	C	6.33975800	-1.63421000	0.03994700
H	-2.76678600	-2.94520700	-1.02695400	C	4.87367700	0.78657500	-0.01725600
H	-3.09142100	-4.16698100	-2.25488700	C	7.00907600	-0.39266900	0.22414100
H	-3.80378700	-2.35636200	-3.85781300	C	6.27823400	0.82098500	0.16758900
H	-3.31044000	-1.13345900	-2.68876900	C	7.08821900	-2.83677800	0.01637400
H	-5.01419400	-2.05232800	-1.05481400	C	7.81241800	-3.81243700	-0.01399900
H	-5.64787300	-3.07186700	-2.36726600	C	8.40322900	-0.36390300	0.45946000
H	-7.34681900	-2.36618400	-0.94861000	C	9.59521700	-0.32675100	0.69588300
H	-8.66363600	2.29713300	-1.84468300	C	6.93893300	2.06570400	0.31223800
H	-8.38770200	-3.44141400	0.21570200	C	7.48512500	3.14515200	0.42511000
H	-12.25002000	-1.54325300	2.60724200	C	4.13823500	1.99364200	-0.06953400
H	-12.77456300	0.27588100	2.23829500	C	3.49530700	3.02390900	-0.12455600
H	-10.26734800	3.04020500	-0.97940500	C	2.77913400	-0.44106900	-0.26752600
H	-7.63038900	-5.22966600	1.44771200	C	1.57477800	-0.29157600	-0.35063800
H	-8.74685700	-5.71666600	0.13550500	C	8.70531300	-4.91763500	-0.05651700
H	-10.82617700	-3.47343300	4.95333400	C	8.28115700	-6.21873800	0.27484900
H	-10.31718300	-5.01758000	4.20102900	C	10.05229100	-4.72313300	-0.42497200
H	-13.77108600	1.75519700	3.70358500	C	9.17895500	-7.28097300	0.24259500
H	-14.88055400	1.18301600	2.42069700	H	7.24740900	-6.38069400	0.56458400
H	-14.28439200	4.13109100	0.01457200	C	10.93790300	-5.79501000	-0.45152100
H	-13.42798300	3.97069700	-1.55086100	H	10.38687800	-3.72545500	-0.69248800
H	-5.95030700	2.02056600	-4.94893100	H	8.83418600	-8.27806600	0.50751200
H	-7.56561800	1.25901300	-4.87285100	H	11.97378600	-5.62376300	-0.73605200

C	10.98522100	-0.26721200	0.98044600	H	-0.39111100	-1.47458900	1.06812000
C	11.74485900	-1.44482300	1.12931400	C	-1.67410600	1.21271600	-1.40487100
C	11.63185500	0.97595400	1.13197700	H	0.38681500	1.44920900	-1.98749600
C	13.10537300	-1.37233700	1.40768600	H	-2.80349900	-0.94802400	0.95162500
H	11.25373500	-2.40854100	1.03644100	H	-2.02904800	1.96942500	-2.10080500
C	12.99277000	1.03093500	1.41103900	C	10.52002600	-7.09217400	-0.12075500
H	11.05029800	1.88857300	1.04161500	C	13.75586100	-0.13789900	1.54822400
H	13.67505800	-2.29172700	1.52335500	C	9.33069700	6.95619700	0.82920400
H	13.47434500	1.99913400	1.52880400	C	1.21477200	6.60472600	-0.33192100
C	8.10561500	4.41620300	0.56202900	C	-2.59816500	0.55762800	-0.57426400
C	9.46458400	4.59797900	0.23911800	C	9.99183400	8.30234200	1.00426900
C	7.36831200	5.52746600	1.01771900	H	10.39964200	8.41308800	2.01819500
C	10.05901900	5.84854100	0.37241400	H	10.82292000	8.43629700	0.30346700
H	10.03782900	3.75293200	-0.13075600	H	9.28173500	9.12192700	0.84938600
C	7.97671400	6.77161500	1.14474300	C	15.24022900	-0.06840000	1.81505400
H	6.32082300	5.39764200	1.27331700	H	15.58961400	-0.94369700	2.37321700
H	11.10855800	5.97029800	0.11383000	H	15.80887200	-0.03298800	0.87582700
H	7.39091700	7.61792100	1.49670200	H	15.50402300	0.82725500	2.38783000
C	2.73501800	4.22139300	-0.19434800	C	0.40273400	7.87309300	-0.43855400
C	1.32622300	4.17771300	-0.17391500	H	0.17318300	8.10763600	-1.48687900
C	3.37116200	5.47558100	-0.28364000	H	-0.55239100	7.78419800	0.09029100
C	0.58727900	5.35350700	-0.24050000	H	0.94193500	8.73183900	-0.02439100
H	0.82534200	3.21709200	-0.10079100	C	-4.05997900	0.93296100	-0.60439300
C	2.61664500	6.64201300	-0.34976900	H	-4.21774200	1.91141000	-0.13225500
H	4.45618100	5.51939100	-0.30383400	H	-4.45012700	1.00286100	-1.62448000
H	-0.49903900	5.30100300	-0.21956000	H	-4.67572900	0.20875500	-0.06181600
H	3.12378500	7.60199300	-0.41645500	C	11.47870100	-8.25697700	-0.18446100
C	0.17406700	-0.04755600	-0.44694500	H	11.21330800	-9.03593400	0.53848800
C	-0.75027800	-0.72514400	0.36952200	H	11.47101300	-8.72097600	-1.18010400
C	-0.31485500	0.92303900	-1.34722200	H	12.50797500	-7.94187600	0.01848300
C	-2.10866800	-0.42257900	0.30053200				

References:

- (1) P. Sathyanarayana, VSR. Jampani, M. Skarabot, I. Musevic, Le KV, H. Takezoe and S. Dhara, *Phys. Rev. E.*, 2012, **85**, 011702-1.
- (2) P. Sathyanarayana, B. K. Sadashiva and S. Dhara, *Soft Matter*, 2011, **7**, 8556.
- (3) T. C. Oakberg, D. H. Goldstein and R. A. Chipman, *Proc SPIE.*, 1997, **3121**, 19.
- (4) P. Sathyanarayana, M. C. Varia, A. K. Prajapati, B. Kundu, V. S. S. Sastry, and S. Dhara, *Phys. Rev. E.*, 2010, **82**, 050701(R).