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Star-shaped Blue Emitting Truxene-based Discotic Liquid Crystalline Molecules: Synthesis, Self-assembly, and Electroluminescence Studies

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Abstract

Two new C₃ symmetrical star-shaped truxene-based discotic liquid crystals have been designed to study their optoelectronic properties. Both the truxene derivatives exhibited columnar hexagonal self-assembly, confirmed by a thorough analysis using POM, DSC, and XRD. A multilayered OLED device was structured using these mesogens as blue emitters for electroluminescent studies. The best-performing configuration was perceived for devices based on emitter **1b** at a dopant concentration of 1 wt% in a well-aligned CBP host, giving a maximum EQE of 2.9%.

Keywords: Discotic liquid crystal, truxene, columnar hexagonal mesophase, blue emitter, OLED, EQE

1. Introduction

Discotic liquid crystals (DLCs), in columnar self-assembly, are emerging candidates for their fabrication in organic lightemitting diodes (OLEDs) as emitters because of their selfhealing and substantial charge transport properties.¹ Also, the present fluidic alkyl chains in the molecular design of DLCs improve the solubility, thus, escalating the solution processability and making device manufacturing easy and affordable.² Concerning a full digital display palette, red^{3.} and green⁴ emitters with improved efficiencies have been widely known in contrast to blue emitters⁵ in the literature. So, there is a need to design new DLC-based blue emitters in guiding the improvisation required for future research.

The π -conjugated organic DLC core is chosen such that it should have an intrinsic blue-emitting property and can easily be tailored. Novel designs based on triphenylene,⁶ pentaalkynylbenzene,⁷ heptazine,⁸ phenylenevinylene,⁹ and many more have been presented in this thriving field since the discovery of DLCs. However, star-shaped cores are emerging candidates due to their better thermal and physical characteristics.¹⁰ In this context, truxene (Figure 1) derivatives have been proven to be a potential material for various organic devices, including photovoltaic solar cells, organic lasers, organic field emitting transistors (OFETs), and many more, after functionalization at reactive sites.¹¹ But due to the challenging synthesis and purification, not many Truxene-based hexagonal columnar DLC as a blue emitter in OLED



reports exist for truxene-based DLCs.¹² Mesomorphism in the systems arises when the truxene core is attached to six¹³ or three¹⁴ flexible chains (straight,¹⁴ branched,¹³ or substituted¹⁵) *via* ether or ester bonds.¹⁶ However, only the hexaesters of truxene moiety are reported to emit in the blue region.^{13, 15} The modulation of electronic and redox properties of truxene-based LC has been carried out in the literature by altering either side chains or the π -conjugated truxene core.¹⁷ So, herein, we have developed a novel design for truxene-based DLCs, employed in OLED devices as a blue emitter for the first time.

The columnar phases of the truxene-based system are revealed to have high mobility,18 making it an appropriate contender for optoelectronic applications. The introduction of flexible fluidic alkyl chains at C-2, C-7, and C-12 positions can enhance the solubility of planar C3 symmetric truxene derivatives.¹⁹ In this regard, the trialkoxybenzene unit is attached to the central truxene core to augment the columnar stacking and solubility, forming star-shaped DLCs. Molecular design in the present work uses an alkynyl linker between truxene core and trialkoxybenzene moiety for two reasons. The first reason is to reduce the stacking distance between molecules, increasing the intracolumnar order.²⁰ The second reason is that they tend to show luminescence in the blue region.²¹ Additionally, the C-5, C-10, and C-15 positions are methylated to avoid aggregation so that the emission is retained, leading to color purity.22 Considering all this, we

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have rationally designed and produced two novel solutionprocessable mesogens, **1a** and **1b** (Figure 1), with a proper balance of stacking without luminescence quenching. These mesogens were observed to have a columnar assembly with high thermal stability and emission in the blue region. These blue fluorescent mesogens were fabricated in five-layered OLED structures as emitters using 4,4'-bis(N-carbazolyl)-1,1'biphenyl (CBP) as host and optimized at varying doping concentrations to get the finest device. Amongst all the configurations, the emitter **1b** resulted in the best-performing device perceived at 1 wt% dopant concentration using the CBP host matrix, giving a maximum external quantum efficiency (EQE) of 2.9%.



Figure 1. Chemical structure of truxene (left) and truxenebased DLC (right).

2. Experimental

Materials

The chemicals were used as received commercially. 3,4,5trihydroxybenzaldehyde monohydrate, 1-bromododecane, 1bromotetradecane, tetrabromomethane (CBr₄), (PPh₃), triphenylphosphine 1-indanone, acetic acid, potassium tert-butoxide (t-BuOK), tetrakis(triphenylphosphine)palladium(0) (Pd(PPh₃)₄), potassium iodide (KI), bromine, concentrated HCI, iodomethane (CH₃I), potassium carbonate (K₂CO₃), copper lodide (Cul), and n-Butyl Lithium (n-BuLi) were commercially available from Sigma-Aldrich. The solvents used for reactions, such as dichloromethane (DCM), triethylamine (Et₃N), N,N-dimethylformamide (DMF), and tetrahydrofuran (THF), were purchased from Sigma-Aldrich. THF solvent was dried using refluxing over sodium wire and benzophenone (as an indicator) using distillation apparatus. Et₃N was dried by refluxing over phosphorus pentoxide.

For column chromatography, silica gel and neutral alumina gel were used. For thin layer chromatography, silica gel coated alumina sheets (Merck, Kieselgel 60, F254) were used.

Instrumentation

Structural characterization for all the compounds was done using ¹H (400 MHz) and ¹³C NMR (100 MHz) in Bruker Biospin, Switzerland, Avance-iii spectrometer using CDCl₃ solvent, infrared spectroscopy (attenuated total reflection, Bruker-Alpha), and mass spectrometry (MALDI ion source, Water Synapt G-2-s QTOF). Thermal studies were carried out utilizing differential scanning calorimetry (DSC, Perkin Elmer DSC 8000 with controlled liquid nitrogen accessory), thermogravimetric analysis (TGA, Shimadzu DTG-60 instrument), polarizing optical microscope (POM, Nikon Eclipse LV100POL with LTS 420), and X-ray diffraction (XRD, Xenocs, GeniX 3D and Pilatus 200 hybrid pixel Dectris detector).

Photophysical studies were performed by UV-vis absorption (Agilent UV-vis-NIR spectrophotometers), emission spectra (Horiba Scientific Fluoromax spectrofluorometer), and time-correlated single photon counter (TCSPC, Horiba Jobin Yvon).

Electrochemical studies were performed using cyclic voltammetry (Princeton Applied Research VersaSTAT). Electroluminescent studies were performed in a complete darkroom under an ambient atmosphere using a CS-100A luminance meter and PR-655 spectrophotometer.

Synthesis

Scheme 1 outlines the synthesis carried out by employing a Sonogashira²³ cross-coupling reaction of compound **4** with terminal alkynes **7a** and **7b**, resulting in target compounds **1a** and **1b**. Their NMR and HRMS data are provided in Figures S1-S6, Supporting Information. A brief synthetic details of intermediates and a detailed synthesis of target molecules is provided below:

Synthesis of compounds 2, 3, and 4 is similar to the previous report.²⁴ Briefly, 1-indanone (3.0 g, 22.7 mmol) solution in a 1:2 (v:v) mixture of concentrated HCl and acetic acid was refluxed for 16 h. The resulting yellow suspension was poured over ice to get compound 2 as precipitate (2.6 g, 34%), which was filtered and washed with different organic solvents. Compound 2 (2.8 g, 8.1 mmol) in 150 mL dry THF was placed in an ice bath in a nitrogen atmosphere. Then, the addition of t-BuOK (13.7 g, 122.1 mmol) was done, followed by the slow addition of CH₃I (13.7 g, 6.2 mL, 96.5 mmol) after 15 min. of stirring. The final mixture was refluxed for 16 h. The suspension was then filtered. For the purification of concentrated filtrate, a column chromatography packed with silica gel (100-200 mesh) was run using hexane to give compound 3 as a white solid (2.35 g, 68%). To the ice-cooled DCM solution of 3 (2.35 g, 5.5 mmol) in DCM (50 mL), the gradual addition of bromine (1.2 mL, 46.5 mmol) was done and stirred overnight for 16 h. The product was extracted using DCM and saturated Na₂SO₃ aqueous solution. Compound 4 was recrystallized from ethanol as offwhite crystals (3.36 g, 92%).

Compounds **5**, **6**, and **7** were synthesized as reported in the earlier report.²⁵ In summary, to the solution of 3,4,5-trihydroxybenzaldehyde monohydrate (2 g, 12.97 mmol) in dry DMF (30 mL), the addition of K_2CO_3 (8.9 g, 64.88 mmol) was done. After 15 minutes, 1-bromoalkane was added (38.93 mmol) with a pinch of KI, and the reaction was refluxed for 12 h. The crude product was obtained using extraction with diethyl ether, and purification was carried out using column chromatography packed with 100-200 mesh

silica gel to get compound **5** as a white solid (yield - **5a**: 91%, **5b**: 93%) in hexane. To the cooled DCM solution of compound **5** (1 g, 1 equiv.), the addition of CBr₄ (2 equiv.) and PPh₃ (4 equiv.) was done in portions and stirred for half an hour. The purification of crude suspension was done over silica gel-packed column chromatography to get compound **6** (yield - **6a**: 79%, **6b**: 81%) in hexane. To the -78 °C cooled solution of compound **6** (1 equiv.) in dry THF, *n*-BuLi (1.6M in hexane) (2.5 equiv.) was added gradually and stirred at room temperature for 24 h. After extraction using DCM and purification using column chromatography (100-200 mesh silica gel), compound **7** (white solid, yield - **7a**: 59%, **7b**: 63%) was obtained in hexane.

5,5,10,10,15,15-hexamethyl-2,7,12-tris((3,4,5tris(dodecyloxy)phenyl)ethynyl)-10,15-dihydro-5Hdiindeno[1,2-a:1',2'-c]fluorene (1a)

In a dried two-necked round-bottomed flask, 10 mL dry DMF and 20 mL Et₃N were taken, and nitrogen was purged for half an hour. Then, compound **4** (75.00 mg, 0.11 mmol), Pd(PPh₃)₄ (13.00 mg, 0.011 mmol), and Cul (4.30 mg, 0.022 mmol) were added. Lastly, after purging for another 15 min, the addition of compound **7a** (444.45 mg, 0.66 mmol) was done and left for refluxing for 72 h at 110 °C. The crude product was extracted using diethyl ether and dilute HCl solution followed by purification using alumina-gel packed column chromatography to yield **1a** (116.12 mg, 43%) as a semi-solid brown-colored product.

¹H NMR (400 MHz, ppm): δ 8.25 (d, 3H), 7.70 (s, 3H), 7.58 (dd, 3H), 6.81 (s, 6H), 4.04-3.98 (m, 18H), 1.89-1.73 (m, 36H), 1.51-1.47 (m, 18H), 1.31-1.25 (m, 144H), 0.90-0.87 (m, 27H).

IR (ATR, cm⁻¹): 2922, 2852, 2206, 1744, 1657, 1572, 1501, 1467, 1420, 1379, 1352, 1282, 1234, 1167, 1115, 1006, 967, 907, 889, 837, 807, 754, 739, 690, 660, 630, 604.

MALDI-MS (m/z): $[M+H]^+$ - 2384.9636 (theoretical value for M-C₁₆₅H₂₅₈O₉, $[M+H]^+$ - 2384.9809).

5,5,10,10,15,15-hexamethyl-2,7,12-tris((3,4,5tris(tetradecyloxy)phenyl)ethynyl)-10,15-dihydro-5Hdiindeno[1,2-a:1',2'-c]fluorene (1b)

In a dried two-necked round-bottomed flask, 10 mL dry DMF and 20 mL Et₃N were taken, and nitrogen was purged for half an hour. Then, compound **4** (80.00 mg, 0.12 mmol), Pd(PPh₃)₄ (13.94 mg, 0.012 mmol), and Cul (4.59 mg, 0.024 mmol) were added. Lastly, after purging for another 15 min, the addition of compound **7b** (534.98 mg, 0.72 mmol) was done and left for refluxing for 72 h at 110 °C. The crude product was extracted using diethyl ether and dilute HCl solution followed by purification using alumina-gel packed column chromatography to yield **1b** (155.91 mg, 49%) as a semi-solid brown-colored product.

 ^1H NMR (400 MHz, ppm): δ 8.25 (d, 3H), 7.70 (d, 3H), 7.58 (dd, 3H), 6.80 (s, 6H), 4.03-3.98 (m, 18H), 1.89-1.74 (m, 36H), 1.51-1.47 (m, 18H), 1.30-1.27 (m, 180H), 0.90-0.86 (m, 27H).

IR (ATR, cm⁻¹): 2921, 2852, 2202, 1743, 1651, 1573, 1501, 1467, 1419, 1379, 1352, 1282, 1234, 1116, 1027, 973, 907, 889, 838, 807, 753, 739, 721, 655, 632, 606.

MALDI-MS (m/z): $[M+H]^{+}$ 2637.2417 (theoretical value for M-C₁₈₃H₂₉₄O₉, $[M+H]^{+}$ 2637.2626).

3. Result and discussion

POM, XRD, and DSC analyses were coupled to thoroughly analyze compounds **1a** and **1b**'s mesogenic thermal behavior and found columnar hexagonal self-assembly stable at room temperature. The optical textures for compounds were obtained using POM by sandwiching the compounds between the coverslip and glass slide during heating as well as a cooling cycle with a 1 °C/min scan rate. Under POM, shearable birefringent textures started to appear on heating, shown in Figure 2a (photomicrograph taken at 46.8 °C) for compound **1a** and Figure 2b (photomicrograph taken at 52.5 °C) for compound **1b**. Furthermore, after cooling from the isotropic melt, both compounds maintain their optical



Scheme 1. Reaction details: (i) Acetic acid, conc. HCI, 100 °C, 16 h, yield - 34%; (ii) a. t-BuOK, THF, 0 °C, 15 min; b. CH₃I, reflux, 16 h, yield - 68%; (iii) Br₂, DCM, 16 h, yield - 92%; (iv) RBr, K₂CO₃, DMF, 80 °C, 12 h, yield - **5a**: 91%, **5b**: 93%; (v) PPh₃, CBr₄, DCM, 30 min, yield - **6a**: 79%, **6b**: 81%; (vi) n-BuLi, -78 °C, THF, 24 h, yield - **7a**: 59%, **7b**: 63%; (vii) Pd(PPh₃)₄, Cul, Et₃N, DMF, 110 °C, 72 h, yield - **1a**: 43%, **1b**: 49%.

isotropy. The DSC thermogram of compounds did not show a peak during the heating and cooling cycles. Thermogravimetric analysis (TGA) plots show that both compounds have high thermal stability (Figures 2c and 2d).



Figure 2. POM textures exhibited by compounds (a) **1a** at 46.8 °C, (b) **1b** at 52.5 °C on heating under crossed polarizers and X 100 magnification (scan rate of 1 °C min⁻¹). TGA curve of compounds (c) **1a** and (d) **1b** obtained at 10 °C/min scan rate under nitrogen atmosphere (Temperature highlighted in red corresponds to 5% weight loss).

To determine the precise assembly structure of compounds 1a and 1b, small-angle X-ray scattering (SAXS) and wideangle X-ray scattering (WAXS) studies were conducted. Four narrow peaks were found in the small-angle region from the XRD pattern of compound 1a in the mesophase temperature range (Figure 3a, Table 1). The indexing of peaks resulted in a 2-D hexagonal lattice. The calculation for d-spacings was performed using the formula $d_{\rm cal} = \frac{\sqrt{3} \, {\rm a}}{2\sqrt{h^2 + {\rm h} \, {\rm k} + {\rm k}^2}},$ where the calculated *d*-spacing is represented as *d*_{cal}, and the hexagonal lattice parameter is represented by a. The indexed peaks correspond to the reflections originating from lattice planes (10), (11), (22), and (50). At a temperature of 40 °C, the lattice parameter was estimated to be a = 41.61 Å. Moreover, the correlation between fluidic alkyl chains causes one broad peak, designated as ha, to occur in a wide-angle region with a d-spacing of 4.92 Å. As a result, the assembly in the mesophase has a columnar hexagonal structure, which is indicated by Colh. Similar results were reported for compound **1b**, which showed a Col_h phase in its mesophase region. Moreover, the computed lattice parameter at 30 °C was a = 43.23 Å (Figure 3b, Table 1). Figures 3c and 3d, respectively, display variations in the correlation length and the number of correlated units with temperature for compounds 1a and 1b. It is clear that the structure is shortrange correlated because there are only roughly two correlated units for each of the two compounds in their mesophase region. Furthermore, a short-range correlation between flexible alkyl chains may be seen in the diffuse peak in the wide-angle area. Six methyl units at the truxene's methylene locations were sufficient for preventing π-stacking

aggregation, which produced short-range 2D order and could be a credible explanation for the isotropic behavior observed during cooling under POM.

The information on the peak intensities and peaks indexes was used to create electron density maps (EDMs), which helped further understand the molecule's arrangement in the hexagonal lattice. Figures 4a and 4b display the EDMs for compounds **1a** and **1b**, respectively. The compounds can be viewed as columns of constructed discotic moieties (Figure 4c), which are then stacked on two-dimensional hexagonal lattices, as seen in Figure 4d.



Figure 3. XRD pattern of compound (a) **1a** at temperature 40 °C and (in set) corresponding 2D pattern. (b) **1b** at temperature 30 °C and (in set) corresponding 2D pattern. (c) Variation of correlation length for compound **1a** (half-filled diamond in blue color) and compound **1b** (half-filled diamond in red color). (d) Variation of the number of correlated units for compound **1a** (half-filled diamond in blue color) and compound **1b** (half-filled diamond in blue color) and compound **1b** (half-filled diamond in blue color) and compound **1b** (half-filled diamond in red color).

	(<i>hk</i>)	d _{obs} (Å)	d _{cal} (Å)	l(<i>hk</i>)	М	Φ(<i>hk</i>)
Å Sol	10	36.03	36.03	100.00	6	0
(40 °C), C i = 41.61	11	20.74	20.80	29.69	6	0
	22	10.45	10.40	22.38	6	π
1a 8	50	7.39	7.20	21.91	6	0
	ha	4.92	Fluid alk	yl chain		
_	10	37.44	37.44	100.00	6	0
³ Å	11	21.58	21.62	28.01	6	0
0 °C), 43.2;	22	10.80	10.81	21.13	6	π
b (3(a =	50	7.50	7.49	20.27	6	0
~	h _a	4.93	Fluid alk	yl chain		
bbreviati	ons- d _{ot}	s: experim	entally of	oserved d-	spaci	ng, <i>d_{cal}</i>

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Figure 4. EDMs in the Col_h assembly of (a) **1a** at temperature 40 °C, (b) **1b** at temperature 30 °C. The conventional unit cell of the Col_h lattice is marked by a hexagon and has three primitive unit cells. The lattice parameter is denoted by a. The deep red color indicates the maximum electron density, and the deep blue color represents the minimum electron density. (c) The starshaped molecular design of the mesogen is described as a disc. (d) The cross-section of the column is made up of molecular discs arranged on 2-D hexagonal lattices.



Figure 5. UV-vis absorption and fluorescence emission spectra of compound **1a** in (a) solution state (inset shows the photograph of **1a** under UV light in THF solvent) and (b) thinfilm state (inset shows the photograph of **1a** under UV light in a thin film). (c) TCSPC plots of **1a** and **1b** in solution state at 25 °C.

The UV-vis absorption and emission spectra for derivatives 1a and 1b were recorded; data is given in Table 2. Figures 5a and 5b describe the photophysical properties of 1a in the solution (10⁻⁵ M THF) and thin film states, respectively. It can be noted that in both states, compounds are blue-emitting, evident from inset photographs. Compound 1b exhibited a similar spectrum profile (data in Table 2), suggesting that optical properties are independent of chain length. The solidstate fluorescence quantum yield (QY) was calculated to be 35.08% for compound 1a and 37.44% for compound 1b. The TCSPC technique was used to find the fluorescence lifetime, which was found to be 3.39 ns for compound 1a and 3.32 ns for compound 1b (Figure 5c). To understand the electrochemical behavior mesogens, of cvclic voltammograms (CV) were recorded in DCM solution using 0.1 M TBAHFP as an electrolyte (CV for compound 1b is

revealed in Figure 6a, scan rate: 0.5 mV s^{-1}). The cell setup consists of three electrodes: Ag/AgNO₃ electrode as the reference electrode, platinum wire as a counter electrode, and glassy carbon as the working electrode. The calculated HOMO and LUMO energy levels of **1a** and **1b** are provided in Table 2, and the electrochemical band gap was lower in compound **1b**.

Table 2: Physical data of compounds 1a and 1b

	Solution state ^a		Thin-film state		E _{LUMO} ^b /	Δ E a ^d	
	λ _{abs} (nm)	λ _{em} (nm)	λ _{abs} (nm)	λ _{em} (nm)	Еномо ^т (eV)	(eV)	
1a	269, 311, 340, 357	378, 393	238, 313, 344, 362	402, 425	-3.41/-5.51	2.10	
1b	269, 311, 340, 357	378, 392	238, 313, 343, 361	400, 425	-3.42/-5.50	2.08	

^aIn 10⁻⁵ M THF solution. ^bEstimated from CV using E_{LUMO} = - (4.8 - E_{1/2,Fc,Fc+} + E_{red,onset}) eV. ^cE_{HOMO} = -(4.8 - E_{1/2,Fc,Fc+} + E_{oxd,onset}) eV. ^dElectrochemical band gap: ΔE_g = E_{LUMO} - E_{HOMO}. Abbreviations- λ_{abs}: absorbance peaks, λ_{em}: emission peaks.



Figure 6. (a) Cyclic voltammogram of compound **1b** using 0.1M tetrabutylammonium hexafluorophosphate (TBAHFP) as an electrolyte. (b) Schematic of a five-layered OLED device using solution-processable blue emitters **1a** and **1b** in CBP host.

Both solution-processable compounds exhibiting blue luminescence were employed as emitters using CBP as a host in an OLED device (energy level schematic diagram shown in Figure 6b), as CBP is well aligned with emitter energy levels. The pre-sputtered glass substrates with indium tin oxide (ITO, anode) were spin-coated with poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT PSS) acting as a hole-transport layer: (HTL) and hole-injection layer (HIL). 2,2'2"-(1,3,5-benzinetriyl)tris(1-phenyl-1-H-benzimidazole) (TPBi) acts as an electron-transport layer (ETL) and lithium fluoride (LiF) acts as an electron-injection layer using aluminium as a cathode. Between ETL and HTL, there is an emissive layer consisting of host CBP and emitters **1a** and **1b** (dopant) at doping concentrations of 0.5,



Figure 7. Electroluminescence spectra, *J-V-L*, and CE-*L*-PE plots obtained for OLED devices based on emitter **1a**, shown in Figures (a), (c), (e), respectively, and for emitter **1b**, shown in Figures (b), (d), (f) respectively at mentioned doping concentration in the CBP host matrix.

1, and 3 wt%. The electroluminescent (EL) spectra obtained from the solution-processed device are presented in Figures 7a and 7b for emitters **1a** and **1b**, respectively. The EL peak maxima shifted from 420 nm to 428 nm on increasing the dopant concentration from 0.5 to 3 wt%, close to the emitter emission peak in the thin film, in both the emitters **1a** and **1b**. The narrow and single peak in the EL spectra suggests the favorable and comprehensive transfer of excitons formed at CBP molecules (host) to emitter molecules (guest).²⁶

The current density-voltage-luminance (J-V-L) plots recorded can be visualized in Figure 7c for emitter **1a** and in Figure 7d for **1b**. The current efficiency-luminance-power efficiency concentrations in the CBP host. The summary of EL properties is given in Table 3. The enhanced device's performance was observed after doping the devices in a host matrix, credited to the effective transfer of excitons. It can be noted that EL characteristics are highly dependent on dopant concentration.²⁷ Increasing the dopant concentration improved the CE, PE, and EQE values. This is a result of the rise in the number of emitting molecules leading to an escalation in the energy transfer process. However, the devices were optimized for balanced charge recombination at their finest doping concentration. The devices based on **1a** emitter yielded the best result at 1 wt% doping concentration

Emitter	Doping concentration (wt%)	Driving Voltage (V)	CE _{max} / PE _{max} / EQE _{max} (cd A ⁻¹ / Im W ⁻¹ / %)	CE ₁₀₀ / PE ₁₀₀ / EQE ₁₀₀ (cd A ⁻¹ / Im W ⁻¹ / %) ^a	CIE _{xy} Coordinates (@L ₁₀₀ /L _{max}) ^b	L _{max} (cd m ⁻²)
1a	0.5	3.0	1.0/0.9/0.9	0.5/0.2/0.9	(0.17,0.10)/(0.20,0.15)	646
	1	3.5	1.4/1.0/2.0	0.8/0.4/1.2	(0.17,0.11)/(0.20,0.16)	628
	3	3.5	1.4/1.0/1.7	1.1//0.5/1.5	(0.18,0.13)/(0.18,0.13)	661
	Neat	4.0	-/-/-	-/-/-	-/-	3
1b	0.5	3.5	1.1/1.0/1.7	07/0.3/1.2	(0.17,0.10)/(0.26,0.25)	705
	1	3.0	1.7/0.9/2.9	0.8/0.4/1.2	(0.18,0.11),(0.23,0.19)	658
	3	3.5	1.6/1.0/2.1	1.0/0.5/1.3	(0.17,0.11),(0.22,0.18)	653
	Neat	4.0	-/-/-	-/-/-	-/-	3

Table 3. Electroluminescence data obtained from devices fabricated with 1a and 1b as emitters and CBP as a host

^aPE, CE, EQE at 100 cd m⁻² luminance. ^bClE_{xy} coordinates at 100 cd m⁻² luminance (L_{100})/ L_{max} . Abbreviations- CE_{max}: maximum current efficiency, PE_{max}: maximum power efficiency, EQE_{max}: maximum external quantum efficiency, L_{max} : maximum luminance.

(CE-*L*-PE) curves of emitter **1a** and **1b** are illustrated in Figures 7e and 7f, respectively, at three different doping

with a maximum CE of 1.4 cd A^{-1} , and EQE of 2.0%, emitting in the blue region corresponding to the CIE (Commission

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Internationale de L'Eclairage, 1931) chromatogram coordinates of (0.17,0.11). However, this result was surpassed by devices based on **1b** emitter at 1 wt% doping concentration with a maximum CE of 1.7 cd A⁻¹, EQE of 2.9%, and CIE coordinates of (0.18,0.11). The further increase of doping concentration deteriorated the performance (decrease in EQE) owing to the exciton quenching.²⁸ A high QY, short fluorescence lifetime (ns), and small band gap have contributed to the improved performance of the emitter **1b**.

4. Conclusions

We have synthesized and characterized two truxene-based discotic liquid crystals exhibiting different chain lengths. The mesogens 1a and 1b possess six methyl units at methylene positions of the truxene core resulting in short-range correlation. Further, the detailed POM, DSC, and XRD analysis confirmed columnar hexagonal self-assembly at room temperature. These molecules are thermally stable and emit blue light, which led to their optoelectronic studies. From EL data recorded for various OLED configurations, the best result was observed for emitter 1b at a dopant concentration of 1 wt% in the CBP host, with a maximum EQE of 2.9%. The present work has resulted in the blue-emitting OLED devices exhibiting CIE coordinates ranging between (0.17, 0.10) and (0.18,0.13) at a luminescence of 100 cd m⁻². These results will help guide the design of new blue fluorescent mesogens to improve the device's efficiencies further.

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6. References

- Wöhrle, T.; Wurzbach, I.; Kirres, J.; Kostidou, A.; Kapernaum, N.; Litterscheidt, J.; Haenle, J. C.; Staffeld, P.; Baro, A.; Giesselmann, F.; Laschat, S., Discotic liquid crystals. *Chem. Rev.* 2016, **2016**, *116*(3), 1139-1241.
- Kaafarani, B. R., Discotic liquid crystals for opto-electronic applications. *Chem. Mater.* 2011, 23(3), 378-396.
- Kozma, E.; Mróz, W.; Villafiorita-Monteleone, F.; Galeotti, F.; Andicsová-Eckstein, A.; Catellani, M.; Botta, C., Perylene diimide derivatives as red and deep red-emitters for fully solution processable OLEDs. *RSC Adv.* **2016**, *6*(66), 61175-61179.
- Dhingra, S.; Siddiqui, I.; Gupta, S. P.; Jayakumar, J.; Jou, J.-H.; Pal, S. K., Solution-processable organic light-emitting diodes utilizing electroluminescent perylene tetraester-based columnar liquid crystals. *Soft Matter* **2022**, *18*(46), 8850-8855.
- Zhu, M.; Yang, C., Blue fluorescent emitters: design tactics and applications in organic light-emitting diodes. *Chem. Soc. Rev.* 2013, 42(12), 4963-4976.
- Gupta, M; Pal, S. K., Triphenylene-based room-temperature discotic liquid crystals: a new class of blue-light-emitting materials with long-range columnar self-assembly. *Langmuir* 2016, 32(4), 1120-1126.

- Bala, I.; Yang, W.Y.; Gupta, S. P.; De, J.; Yadav, R. A.; Singh, D. P.; Dubey, D. K.; Jou, J.-H.; Douali, R.; Pal, S. K., Room temperature discotic liquid crystalline triphenylenepentaalkynylbenzene dyads as an emitter in blue OLEDs and their charge transfer complexes with ambipolar charge transport behaviour. *J. Mater. Chem. C* **2019**, 7(19), 5724-5738.
- Bala, I.; Ming, L.; Yadav, R. A.; De, J.; Dubey, D. K.; Kumar, S.; Singh, H.; Jou, J.-H.; Kailasam, K.; Pal, S. K., Deep-Blue OLED Fabrication from Heptazine Columnar Liquid Crystal Based AIE-Active Sky-Blue Emitter. *ChemistrySelect* 2018, 3(27), 7771-7777.
- De, J.; Yang, W. Y.; Bala, I.; Gupta, S.P.; Yadav, R. A.; Dubey, D. K.; Chowdhury, A.; Jou, J.-H; Pal, S. K., Roomtemperature columnar liquid crystals as efficient pure deepblue emitters in organic light-emitting diodes with an external quantum efficiency of 4.0%. ACS Appl. Mater. Interfaces 2019, 11(8), 8291-8300.
- Jarosz, T.; Lapkowski, M.; Ledwon, P., Advances in starshaped π-conjugated systems: properties and applications. *Macromol. Rapid Commun.* **2014**, *35*(11), 1006-1032.
- Wagay, S. A.; Rather, I. A.; Ali, R., Functionalized truxene scaffold: a promising advanced organic material for digital era. *ChemistrySelect*, **2019**, *4*(42), 12272-12288.
- Cheng, X. P.; Xiong, X. P.; He, J. W.; Yu, W. H.; Feng, C.; Ni, H. L.; Hu, P. C., 3-symmetric truxene discotic liquid crystals with mixed ether chains: synthesis, mesomorphism, and selfassembly properties. *Soft Mater.* **2022**, *20*(4), 394-404.
- Vinayakumara, D. R.; Kumar, M.; Sreekanth, P.; Philip, R.; Kumar, S., Synthesis, characterization and nonlinear optical studies of novel blue-light emitting room temperature truxene discotic liquid crystals. *RSC Adv.* **2015**, *5*(34), 26596-26603.
- Zhao, K. Q.; Chen, C.; Monobe, H.; Hu, P.; Wang, B. Q.; Shimizu, Y., Three-chain truxene discotic liquid crystal showing high charged carrier mobility. *Chem. Commun.* 2011, 47(22), 6290-6292.
- Bala, I.; Pal, S. K., Rod-disc oligomeric liquid crystal based on 4-cyanobiphenyl and truxene core. *Liq. Cryst.* **2016**, *43*(7), 963-971.
- Li, L. L.; Hu, P.; Wang, B. Q.; Yu, W. H.; Shimizu, Y.; Zhao, K. Q., Synthesis and mesomorphism of ether–ester mixed tail C3-symmetrical truxene discotic liquid crystals. *Liq. Cryst.* 2010, 37(5), 499-506.
- Huang, J.; Xu, B.; Su, J. H.; Chen, C. H.; Tian, H., Efficient blue lighting materials based on truxene-cored anthracene derivatives for electroluminescent devices. *Tetrahedron* 2010, 66(38), 7577-7582.
- Ni, H. L.; Monobe, H.; Hu, P.; Wang, B. Q.; Shimizu, Y.; Zhao, K. Q., Truxene discotic liquid crystals with two different ring substituents: synthesis, mesomorphism and high charged carrier mobility. *Liq. Cryst.* **2013**, *40*(3), 411-420.
- Orofino, C.; Klimash, A.; Kanibolotsky, A. L.; Skabara, P. J., Synthesis and Analysis of Hyperbranched Oligofluorenes for Optoelectronic Applications. *Display and Imaging* **2017**, *2*, 175-196.
- García-Frutos, E. M.; Pandey, U. K.; Termine, R.; Omenat, A.; Barberá J.; Serrano J. L.; Golemme A.; Gómez-Lor, B., High Charge Mobility in Discotic Liquid-Crystalline Triindoles: Just a Core Business?. *Angew. Chem., Int. Ed.* 2011, 123(32), 7537-7540.
- De, J.; Yadav, R. A.; Yadav, R. S.; Gupta, S. P.; Joshi, M.; Choudhury, A. R.; Jayakumar, J.; Jou, J.-H; Cheng, C. H.; Pal, S. K., Molecular Engineering for the Development of a Discotic Nematic Mesophase and Solid-State Emitter in Deep-Blue OLEDs. J. Org. Chem. **2021**, 86(10), 7256-7262.

https://doi.org/10.53023/p.rasayan-20230608

- 22. Wu, Y.; Hao, X.; Wu, J.; Jin, J.; Ba, X., Pure blue-lightemitting materials: hyperbranched ladder-type poly (pphenylene) s containing truxene units. Macromolecules 2010, 43(2), 731-738.
- 23. Horbaczewskyj, C. S.; Fairlamb, I. J., Pd-Catalyzed Cross-Couplings: On the Importance of the Catalyst Quantity Descriptors, mol% and ppm. Org. Process Res. Dev. 2022, 26(8), 2240-2269.
- 24. Nailwal, Y.; Wonanke, A. D.; Addicoat, M. A.; Pal, S. K., A Dual-Function Highly Crystalline Covalent Organic Framework for HCI Sensing and Visible-Light Heterogeneous Photocatalysis. Macromolecules 2021, 54(13), 6595-6604.
- 25. Bala, I.; De, J.; Gupta, S. P.; Singh, H.; Pandey, U. K.; Pal, S. K., High hole mobility in room temperature discotic liquid

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- 26. Li, G.; Zhu, D.; Peng, T.; Liu, Y.; Wang, Y.; Bryce, M.R., Very High Efficiency Orange-Red Light-Emitting Devices with Low Roll-Off at High Luminance Based on an Ideal Host-Guest System Consisting of Two Novel Phosphorescent Iridium Complexes with Bipolar Transport. Adv. Funct. Mater. 2014, 24(47), 7420-7426.
- 27. Tang, C. W.; VanSlyke, S. A.; Chen, C. H., Electroluminescence of doped organic thin films. J. Appl. Phys. 1989, 65(9), 3610-3616.
- 28. Murawski, C.; Leo, K.; Gather, M. C., Efficiency roll-off in organic light-emitting diodes. Adv. Mater. 2013, 25(47), 6801-6827.

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