Electronic Supplementary Information (ESI)

Oxadiazole-integrated heterocoronene discotics as ambipolar organic semiconductors

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1) Materials and Methods

Materials. Chemicals and solvents (AR quality) were used as received without any further purification. Column chromatographic separations were performed on silica gel (100-200 & 60-120 mesh). Thin layer chromatography (TLC) was performed on aluminium sheets pre-coated with silica gel (Merck, Kieselgel 60, F254).

Measurements and Characterization. *The detailed specifications of instruments used for the characterization of the synthesized compounds, including NMR, Mass and FT-IR spectroscopy, Polarized Optical Microscopy (POM), Thermogravimetric analysis (TGA), Differential Scanning Calorimetry (DSC), X-Ray diffraction (XRD), photophysical studies (UV-Vis & Fluorescence), electrochemical characterization (Cyclic voltammetry) are similar as mentioned in earlier reports from our group*[1] *and reproduced below for the reader's convenience.*

"Structural characterization of the compounds was carried out through a combination of infrared spectroscopy (IR) (Perkin Elmer Spectrum Two), ^{1}H NMR and ^{13}C NMR (Bruker Biospin Switzerland Avance-iii 400 MHz and 100 MHz spectrometers respectively), UV-vis-NIR spectrophotometers (Agilent Technologies, Cary 5000) and Mass spectrometry (Water Synapt G-2-s QTOF with MALDI ion source and α-cyano-4hydroxy-cinnamic acid as a matrix). IR spectra were recorded in neat form for target compounds. ^{1}H & ^{13}C NMR spectra were recorded using deuterated chloroform ($CDCl_3$) as solvent and tetramethylsilane (TMS) as an internal standard. Cyclic Voltammetry (CV) experiments were performed by using Princeton Applied Research VersaSTAT 3. The transition temperatures and associated enthalpy values were determined using a differential scanning calorimeter (Perkin Elmer DSC 8000 coupled to a controlled liquid nitrogen accessory (CLN 2)) which was operated at a scanning rate of 10 °C min^{-1} both on heating and cooling. Thermogravimetric analysis (TGA) was carried out from 25 to 500 °C (at a heating rate of 10 °C min^{-1}) under nitrogen atmosphere on a Shimadzu DTG-60 instrument. Textural observations of the mesophase were performed with Nikon Eclipse LV100POL polarizing optical microscope (POM) provided with a Linkam heating stage (LTS 420). All images were captured using a Q-imaging camera. X-ray diffraction (XRD) was carried out by filling samples in glass capillaries using Cu-K_α (λ = 1.5418 Å) radiation from Xeuss (Model C HP100 fm) X-ray diffractometer from Xenocs equipped with GeniX 3D source operating at 50 kV and 0.6 mA in conjunction with a multilayer mirror and Pilatus 200 hybrid pixel detector from Dectris."

Thin-film SCLC device fabrication:

ITO-coated pre-patterned glass substrates were first sonicated in 5% Hellmanex III soap solution, subsequently in distilled water, acetone, and then isopropanol (IPA) successively for 20 min each. Then the cleaned substrates were blow-dried with nitrogen gas and lastly treated with UV ozone for 30 min at 50 °C. For electron-only devices, zinc oxide (ZnO) solution was prepared with the previously reported recipe.[2] The ZnO solution was filtered using polytetrafluoroethylene (PTFE) 0.45 µm syringe filter prior to spin coating. Approximately 30-40 nm thick ZnO layer was spin-coated (4000 rpm for 60 s with 2 s acceleration) followed by annealing at 180 °C for an hour in ambient conditions. The compounds **1.1-1.3** were then spin-coated on top of the ZnO layer from 10 mg/ml solution in chloroform, filtered using PTFE 0.22 µm filter. The spin coating parameters were 1000 rpm for 45 s with an acceleration of 2 s. The measured thickness of the spin coated films were ~ 100 nm measured using Dektak Surface Profiler.

Finally, 120 nm aluminium metal was deposited on it using the thermal evaporator at 2×10^{-6} mbar with a deposition rate of ~ 3-4 Å/sec. The active area of the device was 6.6 mm^2, measured using the overlap of bottom patterned ITO and aluminium top contact. Hole-only devices were fabricated in the device architecture of ITO/PEDOT:PSS/Compound **1.1-1.3**/MoO_3/Ag. The PEDOT:PSS solution was first deposited on top of the cleaned ITO-coated glass substrates at 4000 rpm for 65 s fetching a thickness of around 30 nm followed by annealing at 130 °C for 20 min. The filtered solution of compound **1.1-1.3** was then deposited as used for electron-only devices. Finally, a top contact of MoO_3 (6 nm) and Ag (100 nm) was deposited sequentially using a thermal evaporator at 2×10^{-6} mbar pressure. The active area of the device was 6.6 mm^2 in both electron-only as well as hole-only devices. Finally, J-V characteristics were recorded using Keithley 2436B source measure unit to extract charge carrier mobility using the space charge limited current (SCLC) technique. Dielectric constant of **1.1-1.3** compounds were measured using high-frequency LCR meter ZM2376 with an applied oscillation level voltage of 1 V over the frequency range 20 Hz to 1 MHz.

2) Synthesis and characterization details

Experimental Procedure:

The 3,4,5-trialkoxybenzoic acid (**5**) was prepared from the starting material gallic acid monohydrate according to previously reported procedures.[3] The synthetic details of the dodecyloxy derivatives of compounds **7** to **9** are elaborated here (Synthesis is outlined in Scheme 1 in the main manuscript). The decyloxy and the tetradecyloxy derivatives were synthesized in the exact same manner.

Synthesis of 3,4,5-tris(dodecylloxy)-*N*'-(4-nitrobenzoyl)benzohydrazide (7):

To a solution of 3,4,5-tridodecyloxybenzoic acid (**5**) (1 equiv.) in anhydrous dichloromethane (DCM), 8-9 drops of dimethylformamide (DMF) were added, followed by thionyl chloride (2 equiv.), under nitrogen atmosphere. The reaction mixture was allowed to stir for 12 h. Then the excess of thionyl chloride was removed by distillation and the crude product (**6**) was dried in vacuo and used for the next step without further purification. It was then dissolved in THF and 4-nitrobenzohydrazide (2 equiv.) was added, followed by pyridine (2 equiv.). After stirring at 60 °C for 12 h, the reaction mixture was cooled, and THF was removed through distillation. The residue was extracted with ethyl acetate, brine solution, dried over Na_2SO_4 and concentrated. The resulting crude product was recrystallized from ethanol to obtain the pure product in an overall yield of 72%.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.87 (s, 1H), 9.35 (s, 1H), 8.32 (d, J = 12Hz, 2H), 8.06 (d, J = 12Hz, 2H), 7.07 (s, 2H), 4.14-4.05 (m, 6H), 1.91-1.71 (m, 6H), 1.59-1.44 (m, 6H), 1.41-1.21 (m, 48H), 0.92-0.85 (m, 9H).

Synthesis of 2-(4-nitrophenyl)-5-(3,4,5-tris(dodecyloxy)phenyl)-1,3,4-oxadiazole (8):

3,4,5-tris(alkyloxy)-N'-(4-nitrobenzoyl)benzohydrazide (**7**) (1equiv.) in $POCl_3$ (5 equiv.) was refluxed at 100 °C for 24 h. After the reaction, the crude mixture was dropwise added to ice water. Then, it was extracted with DCM. After removal of solvent in vacuo, the crude product was further purified through column chromatography on neutral alumina using hexane/ethyl acetate (95:5) to give the desired product in 60% yield.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.43 (d, J = 8Hz, 2H), 8.36 (d, J = 8Hz, 2H), 7.35 (s, 2H), 4.14-4.05 (m, 6H), 1.91-1.71 (m, 6H), 1.59-1.44 (m, 6H), 1.41-1.21 (m, 48H), 0.92-0.85 (m, 9H). .

Synthesis of 4-(5-(3,4,5-tris(dodecyloxy)phenyl)-1,3,4-oxadiazol-2-yl)aniline (9):

2-(4-nitrophenyl)-5-(3,4,5-tris(alkyloxy)phenyl)-1,3,4-oxadiazole (**8**) was dissolved in dry THF, and Pd on activated charcoal powder (10 weight percent of compound **8**) was added to it, and was carefully fitted with a hydrogen balloon. After 12 h of stirring, the balloon was removed and the reaction mixture was filtered. The filtrate was concentrated to give the required product in nearly quantitative yield.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.94 (d, J = 8Hz, 2H), 7.31 (s, 2H), 6.78 (d, J = 8Hz, 2H), 5.32 (s, 2H), 4.13-4.03 (m, 6H), 1.91-1.71 (m, 6H), 1.59-1.44 (m, 6H), 1.41-1.21 (m, 48H), 0.92-0.85 (m, 9H).

Synthesis of 1,4,5,8-tetrakis((4-(5-(3,4,5-tris(decyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)amino)anthracene-9,10-dione (2.1):

In a round-bottomed flask under nitrogen atmosphere, 1,4,5,8-tetrachloro-9,10-anthracenedione (1 equiv.), 4-(5-(3,4,5-tris(decyloxy)phenyl)-1,3,4-oxadiazol-2-yl)aniline (**9**) (6 equiv.) and Cs_2CO_3 (12 equiv.) were dissolved in 30 ml dry toluene. After purging for 20 min with N_2 gas, Tris(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$, 0.07 equiv.) and 1,1'-Binaphthyl-2,2'-diphenyl phosphine (BINAP, 0.2 equiv.) were added to the solution, followed by refluxing at 110 °C for 72 h. The reaction mixture was subsequently cooled and the solvent was removed under vacuum. The concentrated reaction mixture was then diluted with distilled water and extracted with dichloromethane (DCM), followed by the washing of the combined DCM extracts with brine solution and drying over anhydrous sodium sulfate. After concentrating, it was purified using column chromatography (Silica Gel 60-120 mesh, chloroform/methanol (99:1)) to give a dark green solid as the product (Yield: 78%).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 11.91 (s, 4H), 8.14 (d, J = 12Hz, 8H), 7.75 (s, 4H), 7.44 (d, J = 8Hz, 8H), 7.31 (s, 8H), 4.14-4.00 (m, 24H), 1.90-1.71 (m, 24H), 1.55-1.43 (m, 24H), 1.42-1.20 (m, 144H), 0.92-0.81 (m, 36H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):164.55, 164.17, 153.69, 143.62, 141.43, 140.70, 128.50, 121.43, 118.62, 105.44, 73.73, 69.48, 32.07, 32.04, 30.48, 29.88, 29.81, 29.78, 29.73, 29.56, 29.53, 29.49, 26.24, 26.22, 22.83, 22.81, 14.24.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2923.7, 2853.6, 1729.4, 1599.1, 1491.8, 1327.6, 1258.6, 1214.2, 1179.4, 1117.0, 1010.5, 764.73.

Synthesis of 1,4,5,8-tetrakis((4-(5-(3,4,5-tris(dodecyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)amino)anthracene-9,10-dione (2.2):

Compound **2.2** was synthesized according to a similar procedure to **2.1**. It was purified by column chromatography (Silica Gel 60-120 mesh, chloroform/methanol (99:1)) to give the product as dark green solid in 82% yield.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 11.92 (s, 4H), 8.13 (d, J = 12Hz, 8H), 7.73 (s, 4H), 7.42 (d, J = 8Hz, 8H), 7.30 (s, 8H), 4.12-3.98 (m, 24H), 1.92-1.70 (m, 24H), 1.55-1.44 (m, 24H), 1.42-1.14 (m, 192H), 0.92-0.80 (m, 36H) .

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 164.61, 164.24, 153.74, 143.74, 141.48, 140.80, 128.58, 124.20, 121.54, 118.68, 118.66, 116.15, 105.53, 73.78, 69.54, 37.24, 35.00, 34.66, 32.09, 32.07, 31.57, 30.50, 30.32, 29.90, 29.85, 29.80, 29.74, 29.57, 29.55, 29.51, 29.49, 26.26, 26.23, 22.84, 14.27.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2921.3, 2851.9, 1729.4, 1600.8,1558.0, 1491.6, 1326.6, 1257.6, 1213.2, 1177.8, 1117.4, 979.5,739.2.

Synthesis of 1,4,5,8-tetrakis((4-(5-(3,4,5-tris(tetradecyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)amino)anthracene-9,10-dione (2.3):

Compound **2.3** was synthesized according to a similar procedure to **2.1**. It was purified by column chromatography (Silica Gel 60-120 mesh, chloroform/methanol (99:1)) to give the product as dark green solid in 87% yield.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 11.92 (s, 4H), 8.14 (d, J = 8Hz, 8H), 7.75 (s, 4H), 7.44 (d, J = 12Hz, 8H), 7.31 (s, 8H), 4.12-3.98 (m, 24H), 1.92-1.70 (m, 24H), 1.55-1.44 (m, 24H), 1.42-1.14 (m, 240H), 0.92-0.80 (m, 36H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 186.52, 164.60, 164.24, 153.73, 143.72, 141.47, 140.80, 139.42, 128.57, 124.19, 121.54, 118.67, 118.65, 116.14, 105.51, 73.78, 69.54, 33.97, 32.07, 30.50, 30.43, 29.90, 29.86, 29.84, 29.80, 29.74, 29.57, 29.54, 29.51, 29.49, 29.30, 29.09, 26.26, 26.24, 22.84, 14.27.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2918.7, 2850.5, 1727.4, 1599.1, 1492.8, 1326.6, 1257.6, 1213.2, 1178.4, 1122.0, 973.5, 840.6,737.7.

Synthesis of 1,4,7,10-tetrakis(4-(5-(3,4,5-tris(decyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)-1,4,7,10-tetrahydrobenzo[*lmn*][4,7]phenanthrolino[2,1,10,9-*defgh*][2,9]phenanthroline-2,3,8,9-tetraone (1.1):

Under an inert atmosphere, 1,4,5,8-tetrakis((4-(5-(3,4,5-tris(alkyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)amino)anthracene-9,10-dione (**2**) (1 equiv.), diethyl malonate (20 equiv.), potassium acetate (8 equiv.) and dimethylformamide (DMF) (2 mL) were added in a 10 ml microwave reaction tube. The reaction was irradiated by microwave to a temperature of 172 °C. After 90 min, the crude product was diluted with distilled water and extracted with diethyl ether. The combined organic extracts were washed with brine solution and subsequently dried over anhydrous sodium sulfate. After concentrating, purification was performed by column chromatography (Silica gel 60-120 mesh, ethyl acetate/hexane (5:95)) to give the product. The final product was then precipitated by dissolving in minimum amount of DCM and subsequent dropwise addition of cold methanol. The pure product was obtained in the form of a dark red solid. (Yield: 66%).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.42 (d, J = 12.0 Hz, 8H), 7.58 (d, J = 8.0 Hz, 8H), 7.33 (s, 8H), 7.17 (s, 4H), 4.10-4.02 (m, 24H), 1.90-1.72 (m, 24H), 1.54-1.44 (m, 24H), 1.40-1.20 (m, 144H), 0.90-0.84 (m, 36H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.41, 163.50, 158.29, 153.79, 141.77, 139.77, 137.66, 130.10, 129.16, 125.48, 118.25, 110.55, 105.64, 73.81, 69.57, 32.08, 32.04, 30.48, 29.88, 29.84, 29.81, 29.78, 29.72, 29.54, 29.49, 29.46, 26.23, 26.21, 22.84, 22.82, 14.26.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2955.4, 2925.0, 2854.0, 1738.4, 1704.5,1686.1, 1597.0, 1564.4, 1490.8, 1468.2, 1438.5, 1379.0, 1363.5, 1329.5, 1223.45, 1203.5, 1117.2, 1083.2, 1018.1, 970.0, 903.5,845.7, 828.5, 818.6, 764.8.

MALDI-MS: *m/z* calcd for $C_{196}H_{281}N_{12}O_{20}$ $(M+H)^+$: 3125.1407. Found: 3125.1746.

Synthesis of 1,4,7,10-tetrakis(4-(5-(3,4,5-tris(dodecyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)-1,4,7,10-tetrahydrobenzo[*lmn*][4,7]phenanthrolino[2,1,10,9-*defgh*][2,9]phenanthroline-2,3,8,9-tetraone (1.2):

Compound **1.2** was synthesized according to a similar procedure to **1.1**. It was purified by column chromatography (Silica Gel 60-120 mesh, ethyl acetate/hexane (5:95)) to give the product as dark red solid. The final product was then precipitated by dissolving in minimum amount of DCM and subsequent dropwise addition of cold methanol. (Yield: 63%)

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.43 (d, J = 8.0 Hz, 8H), 7.58 (d, J = 8.0 Hz, 8H), 7.32 (s, 8H), 7.17 (s, 4H), 4.10-4.02 (m, 24H), 1.89-1.72 (m, 24H), 1.55-1.44 (m, 24H), 1.40-1.18 (m, 192H), 0.90-0.82 (m, 36H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):. 165.38, 163.49, 158.27, 153.79, 141.80, 139.79, 137.64, 130.12, 129.12, 125.45, 118.23, 110.52, 105.65, 73.81, 69.59, 32.07, 32.05, 30.49, 29.88, 29.83, 29.78, 29.72, 29.55, 29.53, 29.50, 29.47, 26.24, 26.22, 22.82, 14.24.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2956.2, 2923.6, 2852.8,1730.5 1705.8,1684.7, 1597.0, 1563.7, 1493.2, 1466.0, 1438.7, 1393.0, 1364.5, 1328.6, 1250.7, 1203.5, 1119.5, 1081.2, 1018.1, 967.34, 894.4, 845.7, 825.5, 804.6, 790.4.

MALDI-MS: *m/z* calcd for $C_{220}H_{329}N_{12}O_{20}$ $(M+H)^+$: 3461.5163. Found: 3461.5659.

Synthesis of 1,4,7,10-tetrakis(4-(5-(3,4,5-tris(tetradecyloxy)phenyl)-1,3,4-oxadiazol-2-yl)phenyl)-1,4,7,10-tetrahydrobenzo[*lmn*][4,7]phenanthrolino[2,1,10,9-*defgh*][2,9]phenanthroline-2,3,8,9-tetraone (1.3):

Compound **1.3** was synthesized according to a similar procedure to **1.1**. It was purified by column chromatography (Silica Gel 60-120 mesh, ethyl acetate/hexane (5:95)) to give the product as dark red solid. The final product was then precipitated by dissolving in minimum amount of DCM and subsequent dropwise addition of cold methanol. (Yield: 56%)

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.43 (d, J = 8.0 Hz, 8H), 7.59 (d, J = 8.0 Hz, 8H), 7.31 (s, 8H), 7.16 (s, 4H), 4.12-3.95 (m, 24H), 1.91-1.70 (m, 24H), 1.55-1.47 (m, 24H), 1.44-1.12 (m, 240H), 0.92-0.80 (m, 36H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.40, 163.49, 158.29, 153.79, 141.75, 139.75, 138.71, 137.64, 130.10, 129.14, 125.47, 118.24, 114.47, 110.52, 105.60, 73.80, 69.56, 32.07, 30.49, 29.89, 29.85, 29.84, 29.81, 29.79, 29.73, 29.56, 29.53, 29.51, 29.47, 26.25, 26.22, 22.83, 14.27.

IR (Neat, KBr, ν_{max}/cm^{-1}): 2956.2, 2923.6, 2852.8, 1701.8, 1684.7, 1595.0, 1564.7, 1492.3, 1467.1, 1436.7, 1393.0, 1363.5, 1260.7, 1228.81, 1205.5, 1117.5, 1081.2, 1017.1, 971.1, 900.9, 845.7, 816.5, 803.6, 745.1.

MALDI-MS: *m/z* calcd for $C_{244}H_{377}N_{12}O_{20}$ $(M+H)^+$: 3797.8919. Found: 3797.9404.

3) NMR Spectra:

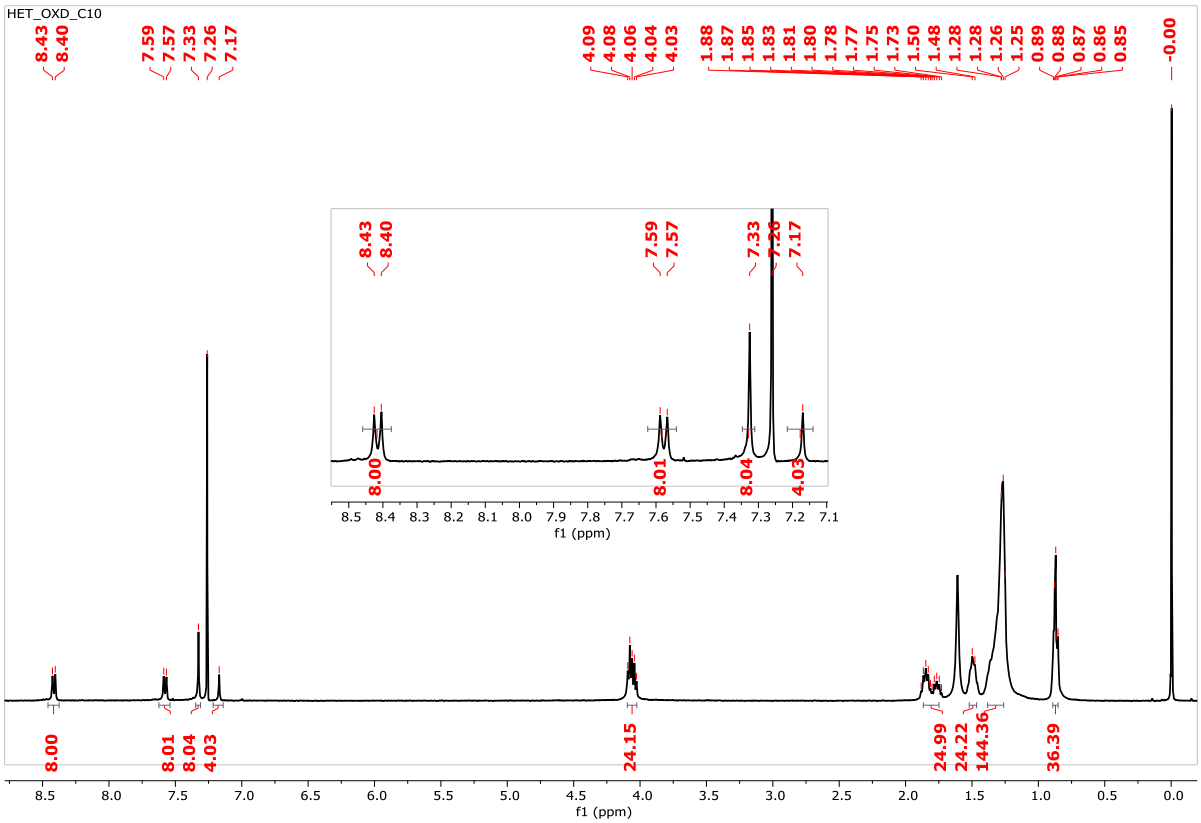

Fig. S1 ^{1}H NMR of Compound **1.1**.

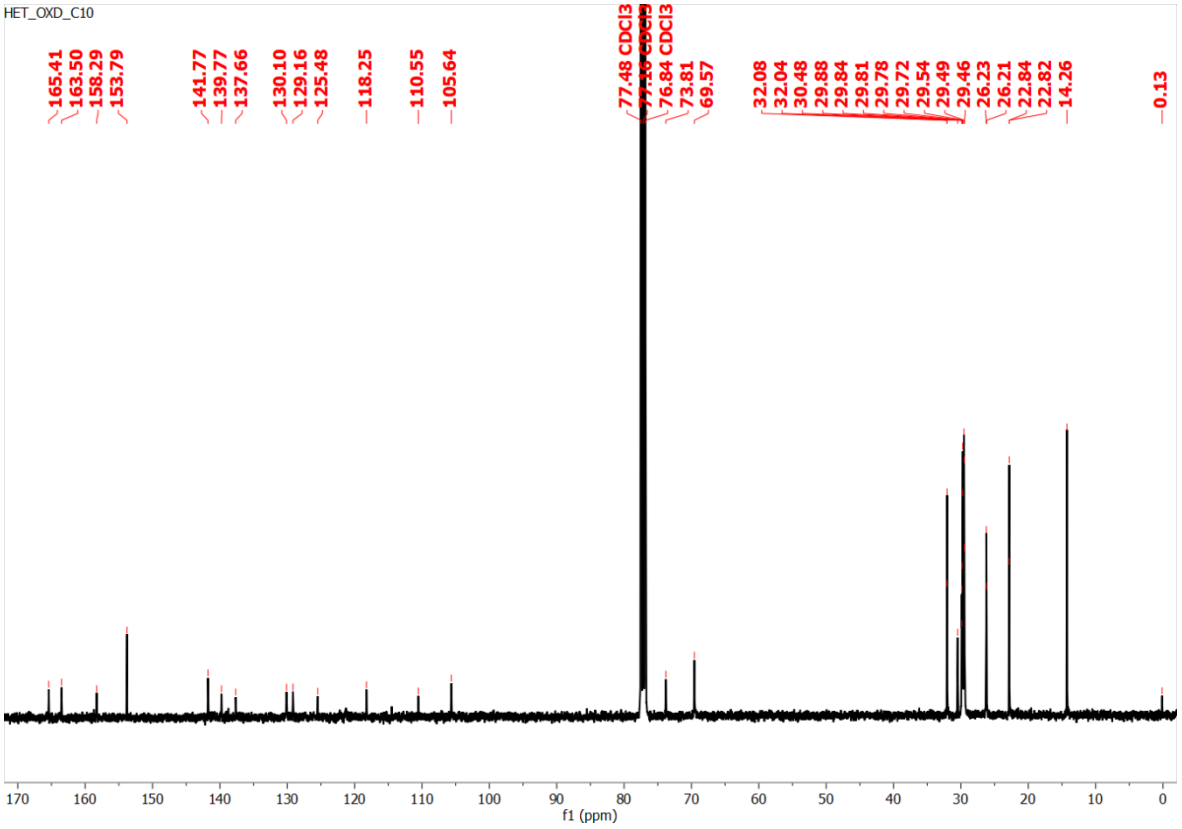

Fig. S2 ^{13}C NMR of Compound **1.1**.

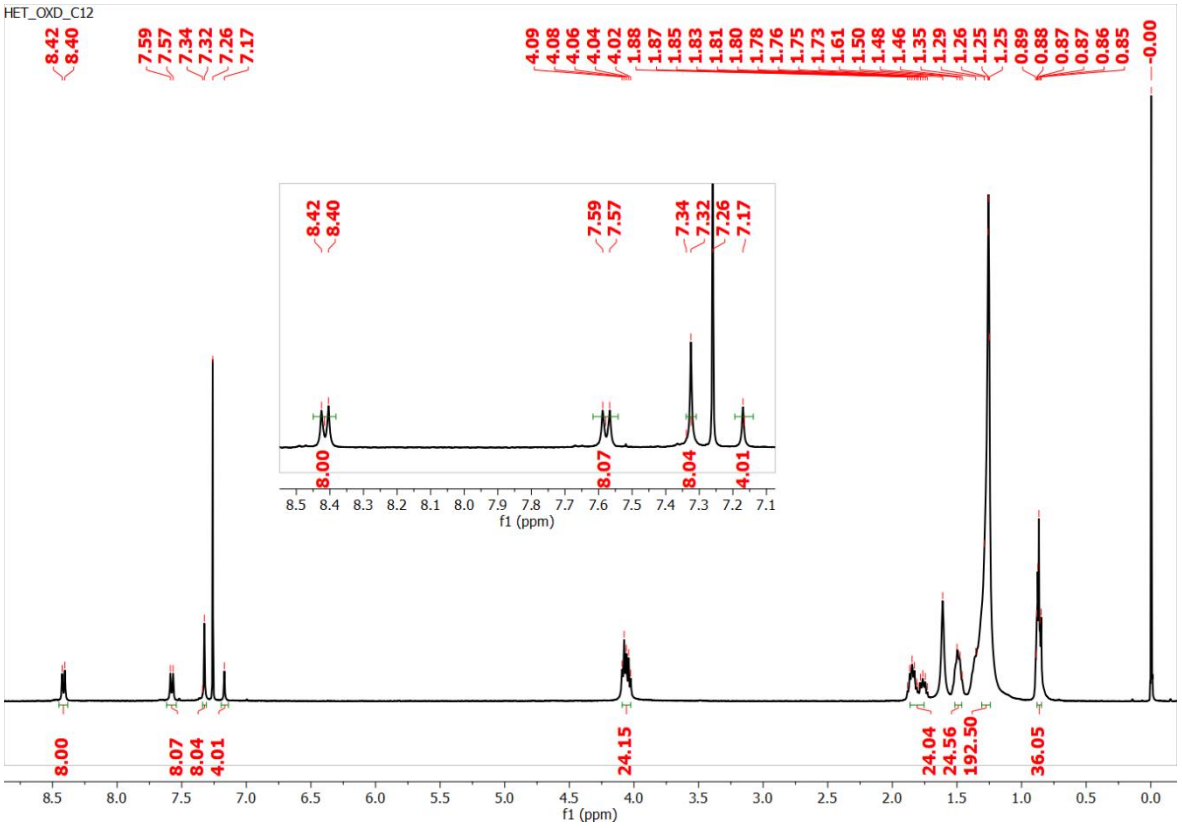

Fig. S3 ^{1}H NMR of Compound **1.2**.

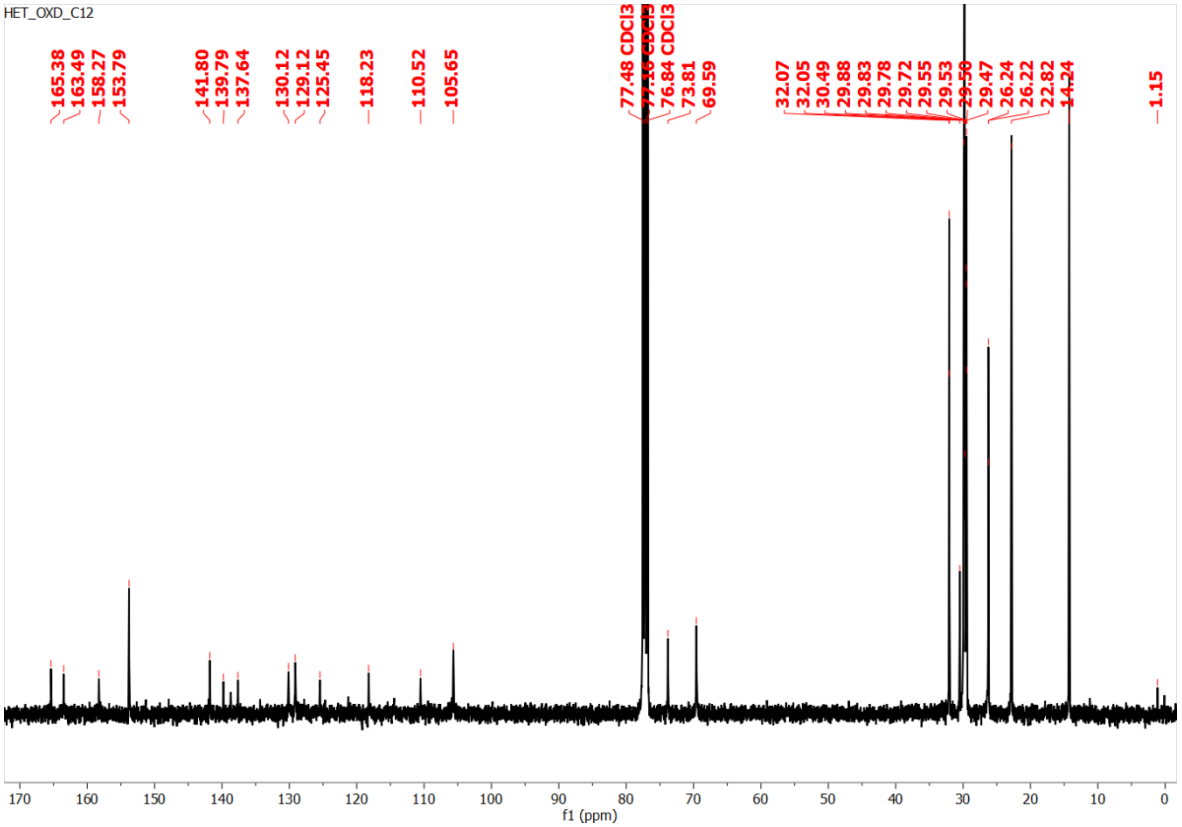

Fig. S4 ^{13}C NMR of Compound **1.2**.

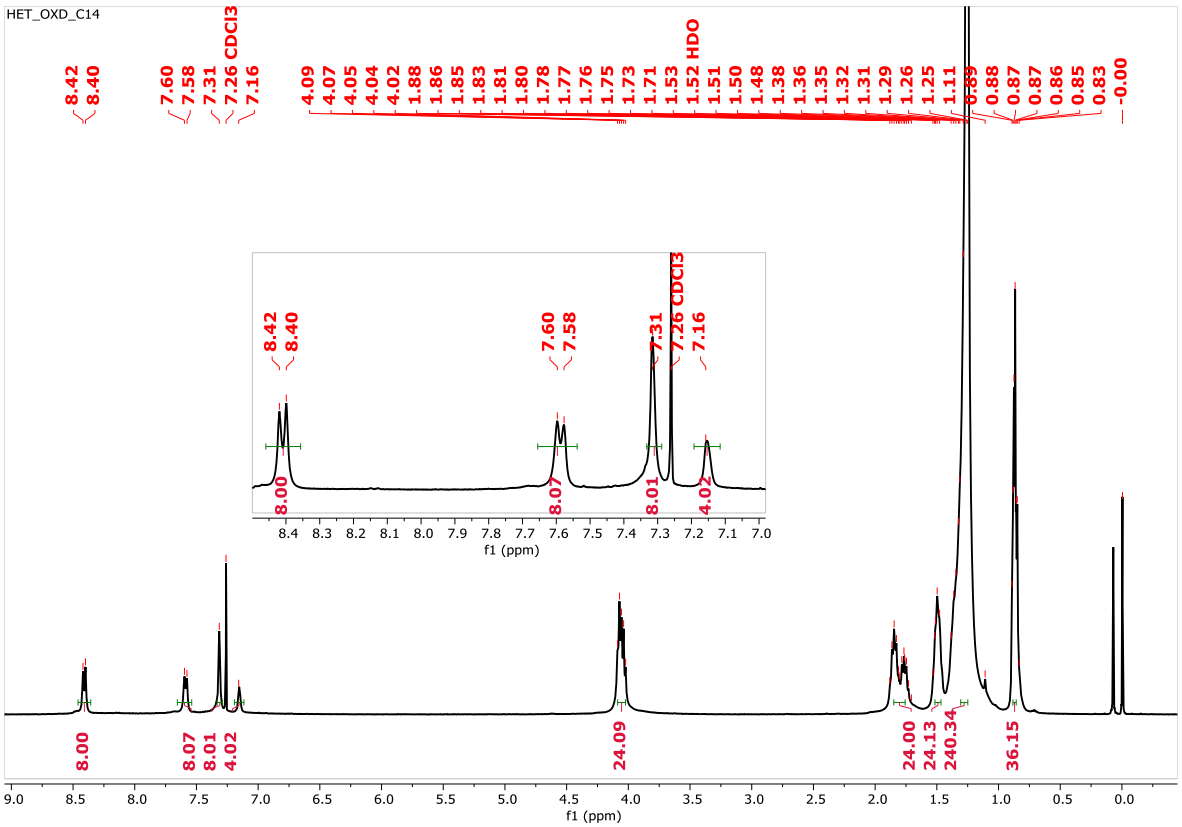

Fig. S5 ^{1}H NMR of Compound **1.3**.

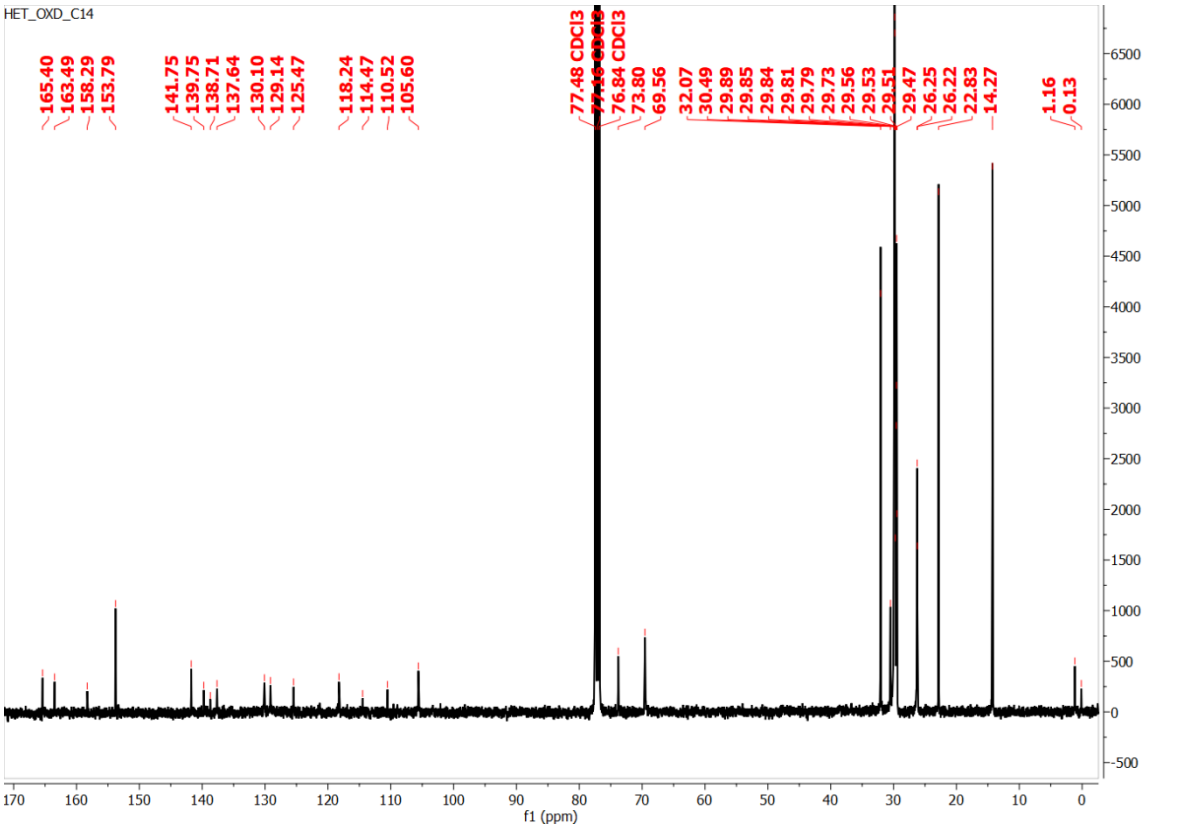

Fig. S6 ^{13}C NMR of Compound **1.3**.

4) HRMS Spectra:

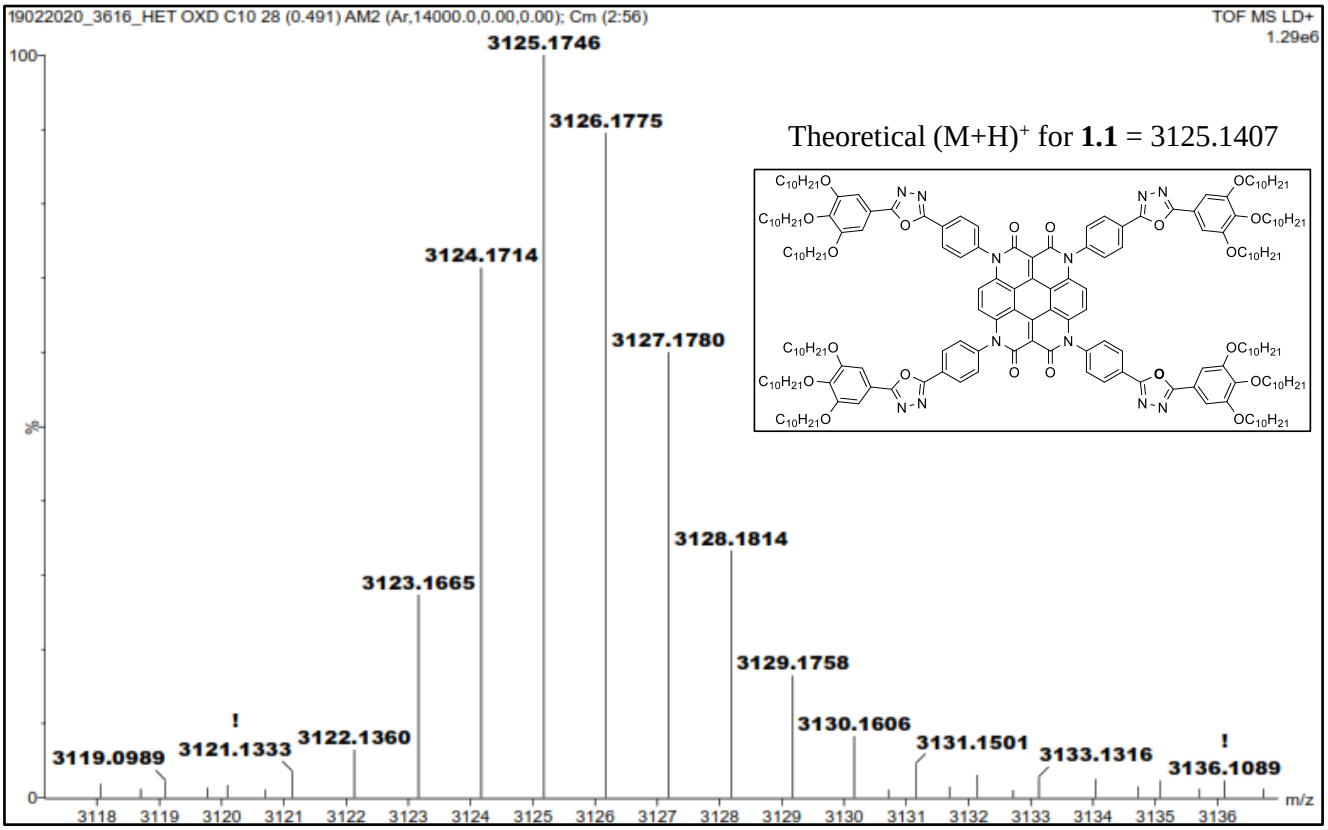

Fig. S7 HRMS spectrum of **1.1**.

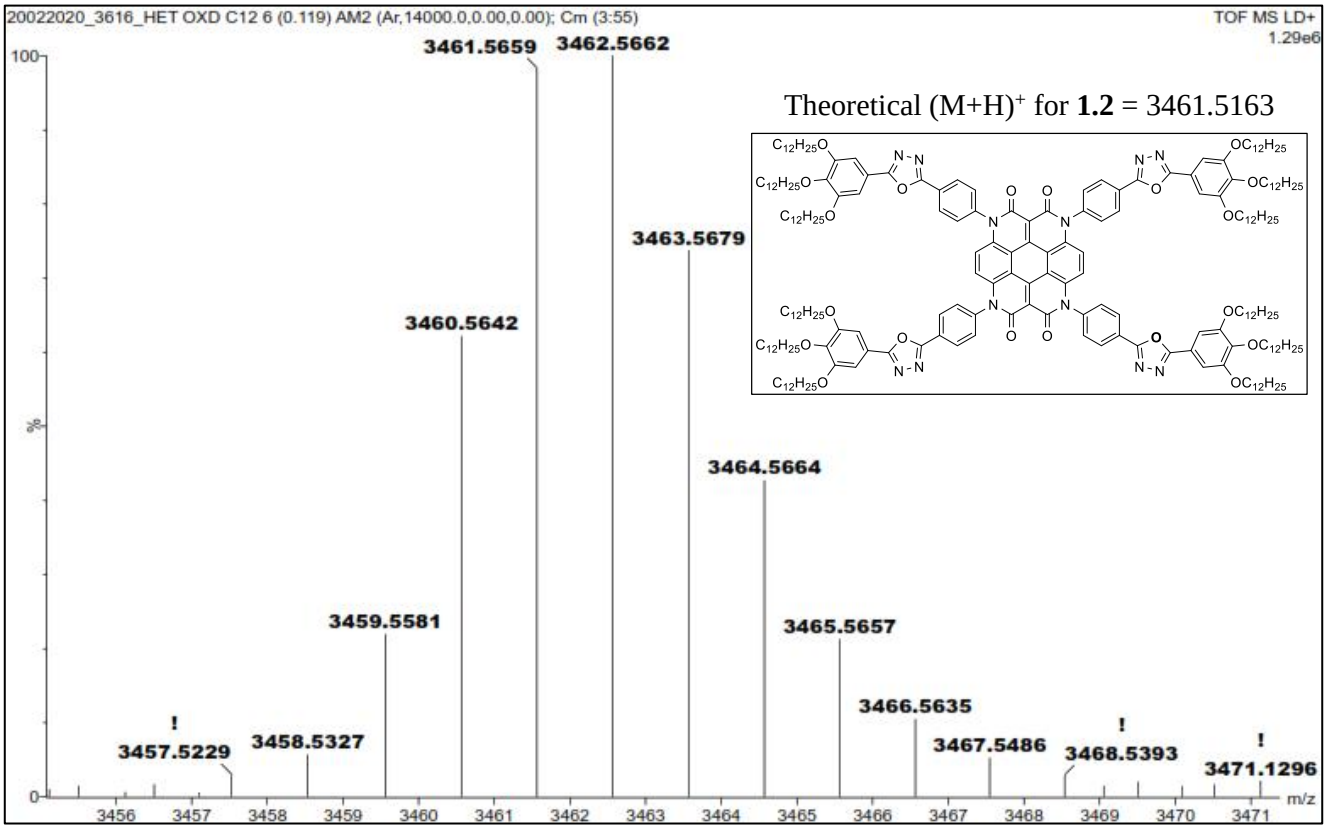

Fig. S8 HRMS spectrum of **1.2**.

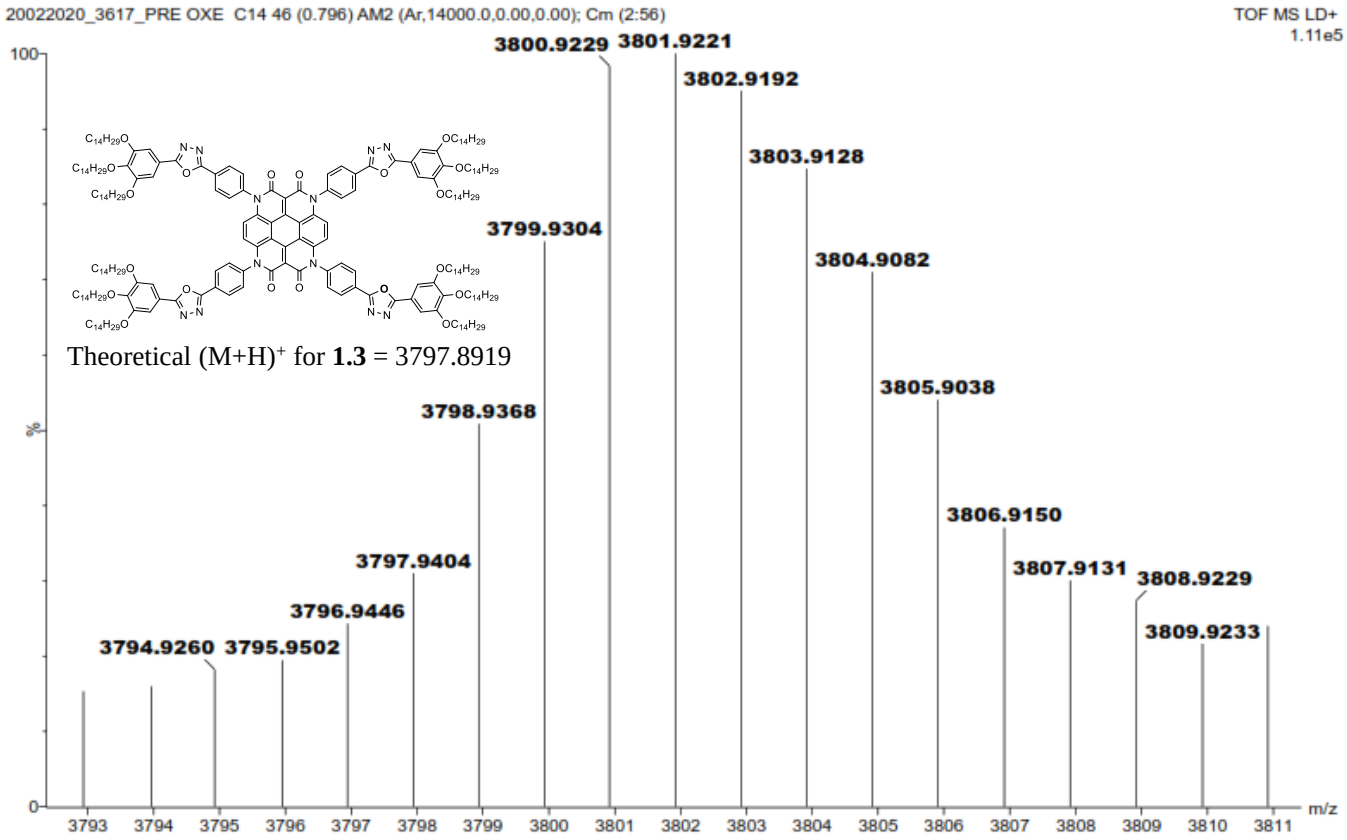

Fig. S9 HRMS spectrum of **1.3**.

5) POM Studies:

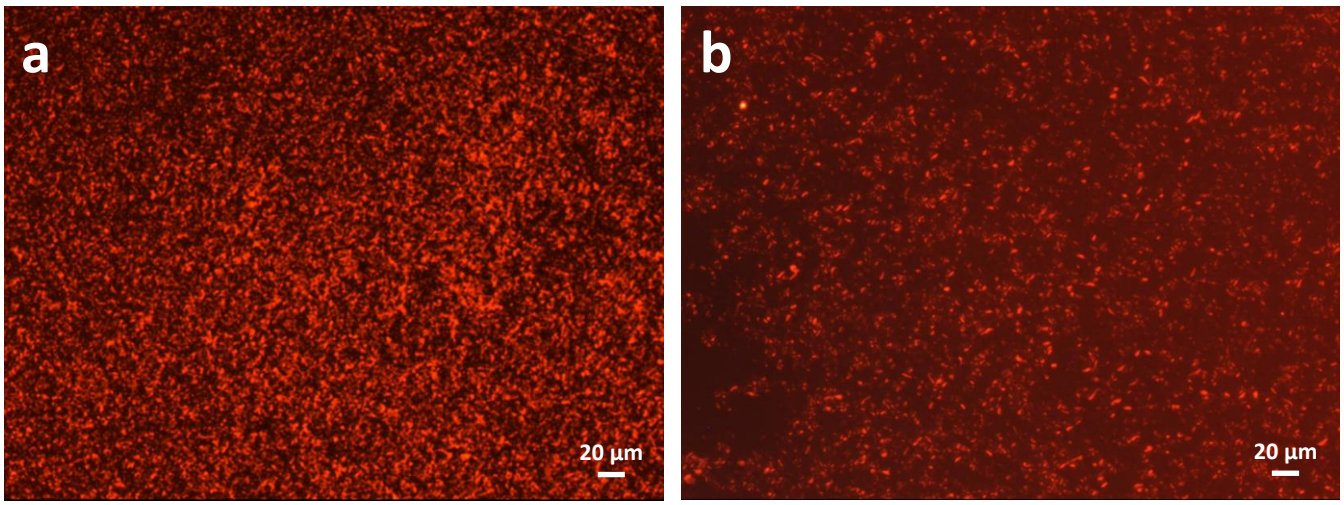

Fig. S10 Polarising optical micrographs (X 100 magnification) of compound (a) **1.2** at 25.8 °C (b) **1.3** at 26.5 °C on cooling from the isotropic phase.

6) DSC Thermograms:

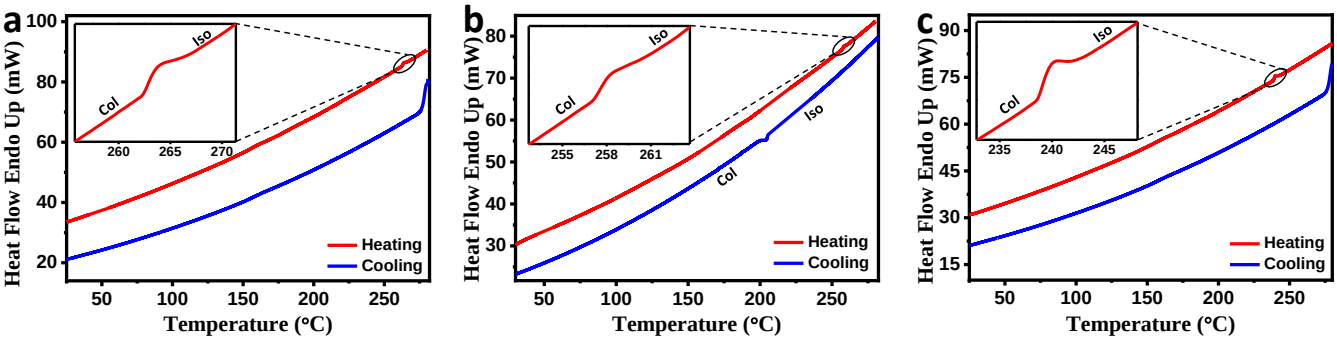

Fig. S11 DSC thermograms of compound (a) **1.1**, (b) **1.2** and (c) **1.3**. All the cooling and heating cycles were measured at 10 °C/min rate.

Table S1. Experimental data of thermal properties of compounds **1.1-1.3**.[a,b]

Mesogen	Heating Scan	Cooling Scan
1.1	Col_h 264.2 (6.22) Iso[a]	Iso 213.1 Col_h[b]
1.2	Col_h 258.0 (5.24) Iso[a]	Iso 204.3 (4.47) Col_h[a]
1.3	Col_h 240.5 (4.54) Iso[a]	Iso 196.3 Col_h[b]

[a] Transition temperatures (peak, in °C) and associated enthalpy changes in brackets in kJ mol^{-1} obtained from DSC. [b] Transition temperatures (in °C) obtained from POM. Abbreviations: Col_h = Columnar hexagonal, Iso = Isotropic liquid.

7) TGA Curves:

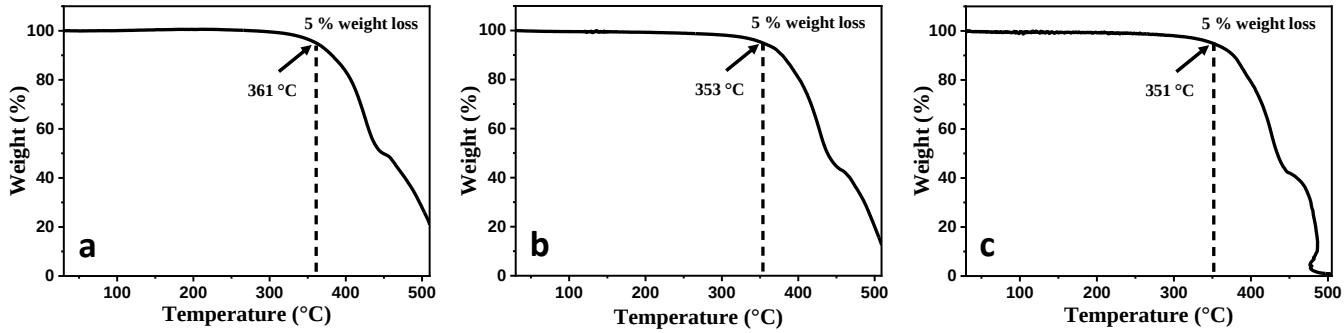

Fig. S12 TGA curves of (a) **1.1**, (b) **1.2** and (c) **1.3**. The measurements were performed under a nitrogen atmosphere, with heating and cooling rates of 10 °C/min.

8) X-ray Diffraction Studies:

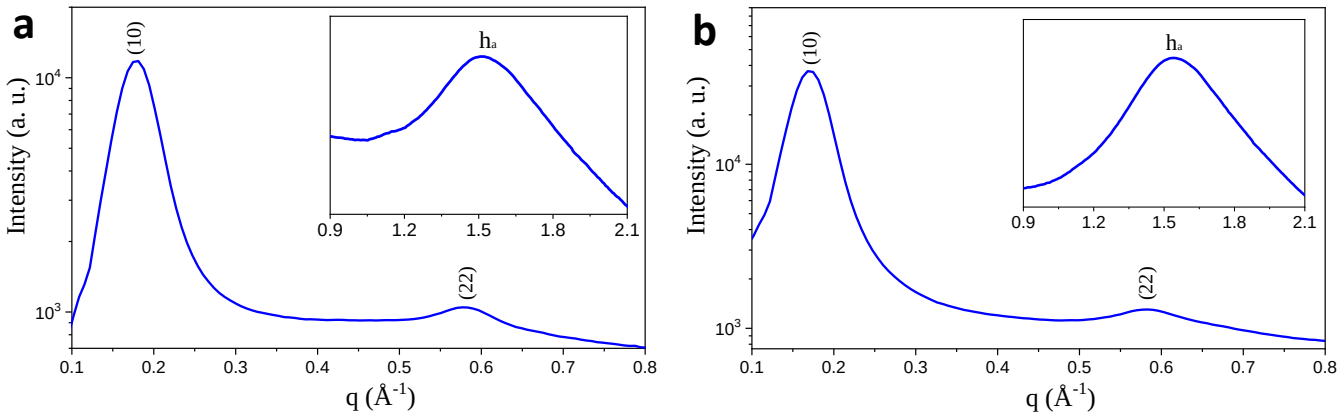

Fig. S13 Small angle and wide angle (inset) X-ray diffraction pattern of compound (a) **1.2** and (b) **1.3** at temperature 25 °C exhibiting columnar hexagonal (Col_h) mesophase.

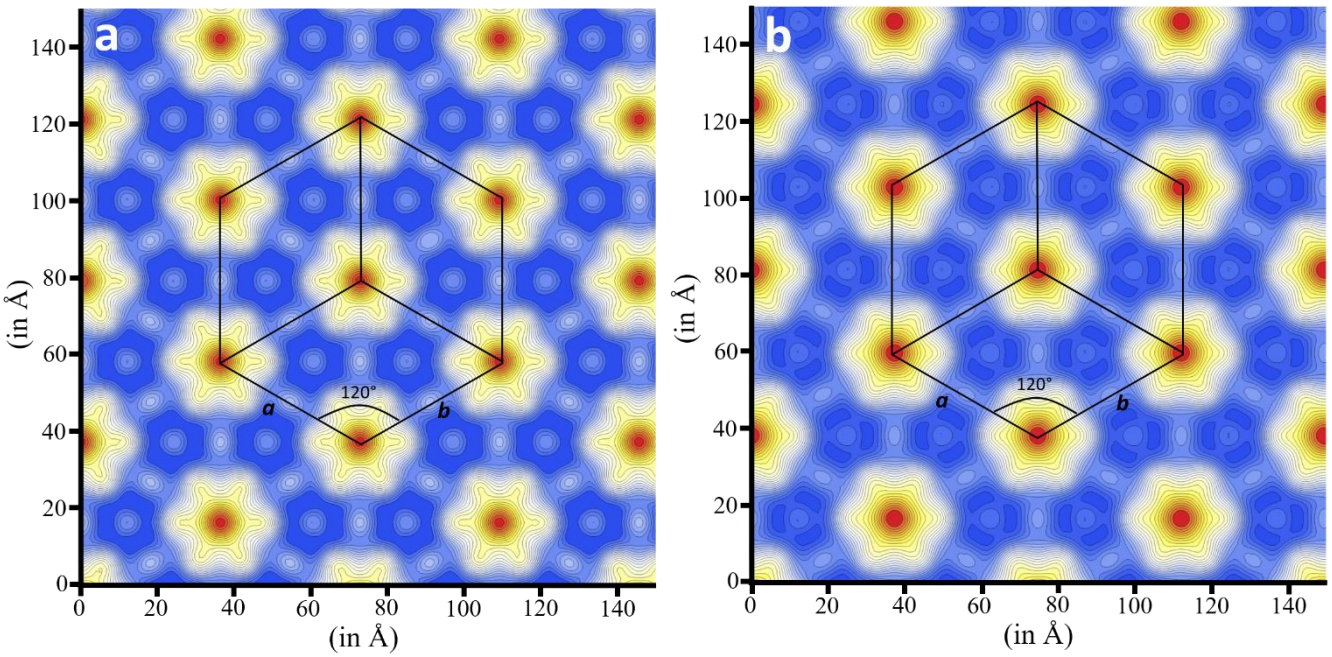

Fig. S14 Electron density maps corresponding to the columnar hexagonal (Col_h) phase of compounds (a) **1.2** and (b) **1.3** at 25 ºC. Hexagon showed the conventional unit cell of the Col_h lattice and there are three primitive unit cells within this conventional unit cell. *a*, *b* are the lattice parameters with *a* = *b* and the angle between them is 120°. Deep red represents the highest electron density and deep blue is the lowest.

Table S2. The Indices observed and calculated *d*-spacings and planes of the diffraction peaks for compound **1.1-1.3**.

Compound	Mesophase	Lattice constants	MI[a] (*hk*)	d_{obs}[b] (Å)	d_{cal}[c] (Å)	RI[d] (hk)	M[e]	Phase Φ(hk)
1.1	Col_h at 25 °C	*a* = 38.20 Å	10	33.08	33.08	100.00	6	0
			30	11.02	11.03	10.91	6	0
			h_a	4.16	--			
			h_c	3.53	--			
1.2	Col_h at 25 °C	*a* = 42.04 Å	10	36.41	36.41	100.00	6	0
			22	10.60	10.51	8.86	6	0
			h_a	4.13	--			
1.3	Col_h at 25 °C	*a* = 43.19 Å	10	37.40	37.40	100.00	6	0
			22	10.79	10.80	3.53	6	0
			h_a	4.10	--			

[a] MI: Miller indices. [b]d_{obs} :experimental *d*-spacing; [c]d_{cal} : calculated *d*-spacing for for Col_h by using the relation: $d_{cal} = \frac{\sqrt{3}\,a}{\sqrt{4\,(h^2+h\,k+k^2)}}$, where *h*, *k* are the Miller indices and *a* is the lattice parameter. [d] RI: Relative Intensity. [e]M: Multiplicity.

9) Photophysical Studies:

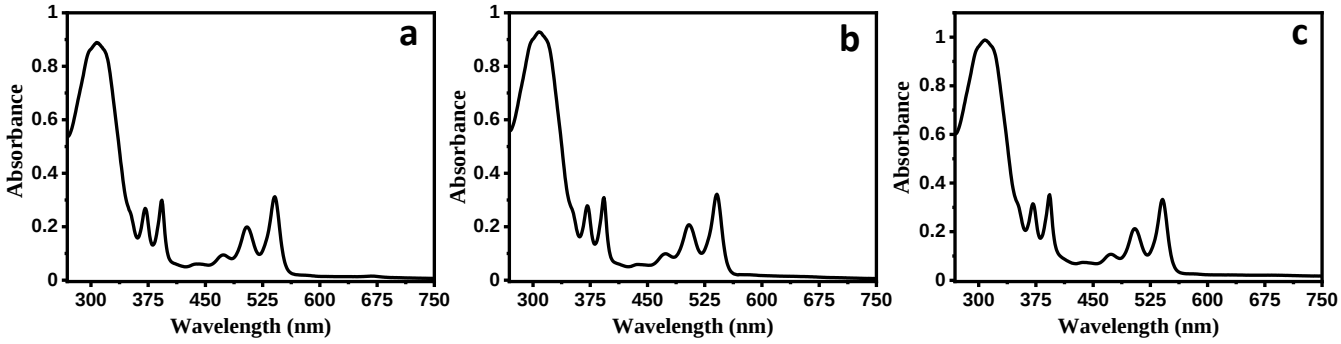

Fig. S15 Absorption spectra of compounds (a) **1.1**, (b) **1.2** and (c) **1.3** in chloroform solvent of 10^{-6} M concentration.

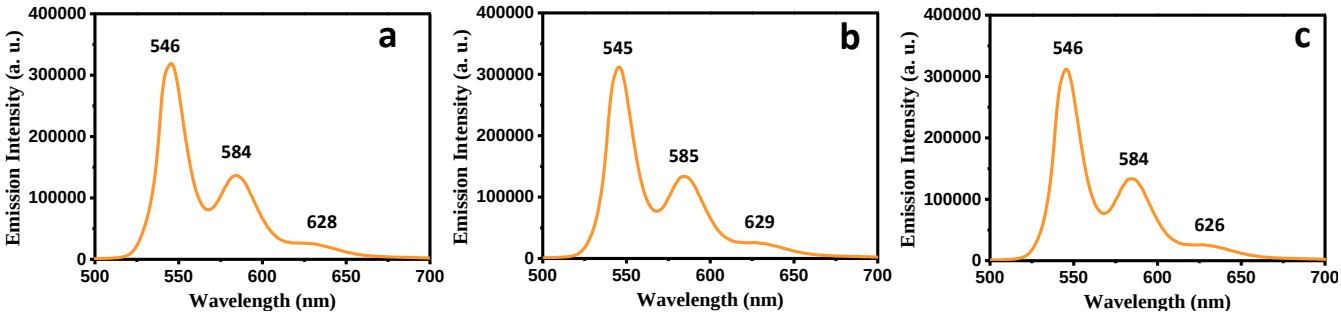

Fig. S16 PL emission spectra of compounds (a) **1.1**, (b) **1.2** and (c) **1.3** in chloroform solvent of 10^{-6} M concentration.

10) Electrochemical Studies:

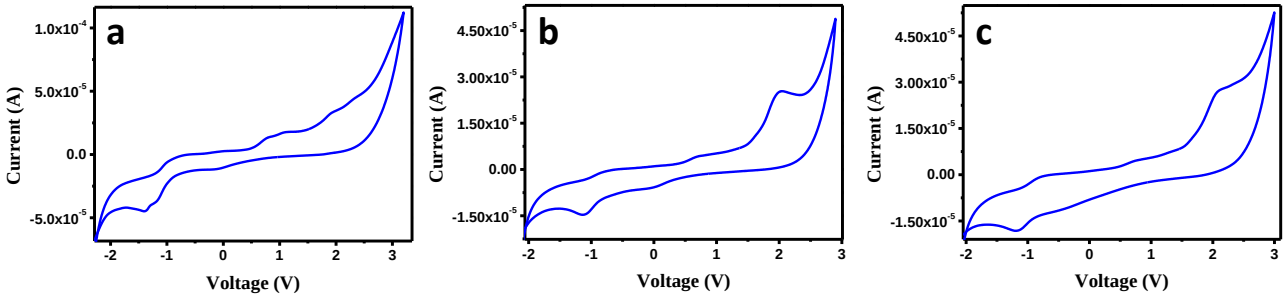

Fig. S17 Cyclic voltammogram of compound (a) **1.1**, (b) **1.2** and (c) **1.3** in HPLC dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) at a scanning rate 50 mVs^{-1}. (Experimental conditions: $Ag/AgNO_3$ as reference electrode, platinum wire as counter electrode, glassy carbon as working electrode, tetrabutylammonium hexafluorophosphate (0.1 M) as supporting electrolyte, room temperature.)

11) Computational Studies:

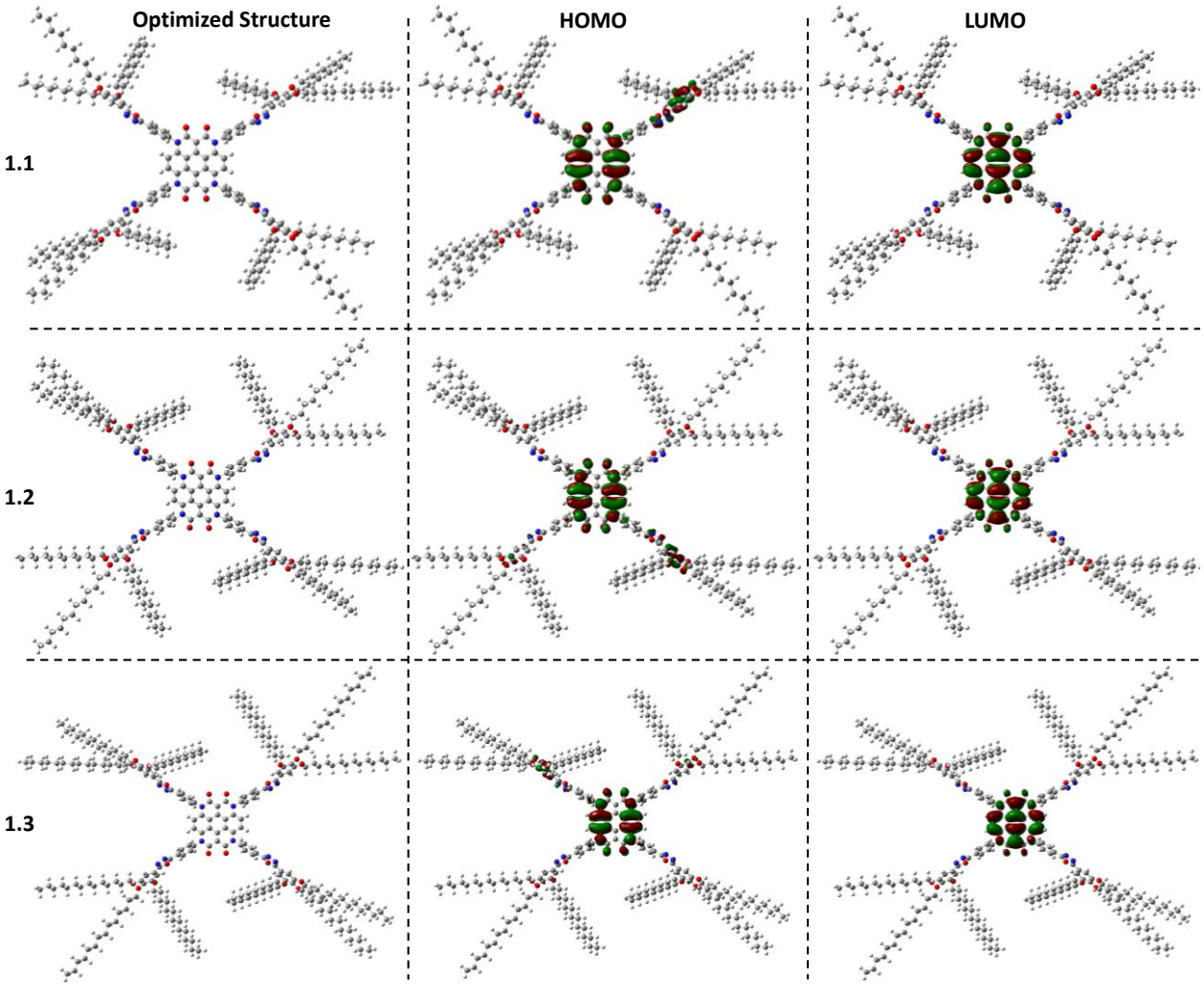

Fig. S18 Optimized geometry and electronic distribution of frontier molecular orbitals (HOMO and LUMO) of compound **1.1-1.3**.

To understand the electronic properties and frontier molecular orbital energy level of compound **1.1-1.3**, theoretical calculations were carried out with the Gaussian 09 suite of packages.[4] A full optimization was carried out using the hybrid functional, Becke's three parameter exchange and the LYP Correlation Functional (B3LYP)[5] at a split valence basis set 6-31G(d,p).

12) SCLC Measurements:

Table S3. Statistic table of all the hole mobility data of compound **1.1-1.3**.[a]

Compound	Hole Mobility (cm^2/Vs)
1.1	3.15×10^{-3}
	6.98×10^{-4}
	2.76×10^{-3}
	3.23×10^{-4}
	1.78×10^{-3}
	Average = 1.74×10^{-3}
	(STD DEV = 1.23×10^{-3})
1.2	3.08×10^{-5}
	3.52×10^{-5}
	4.94×10^{-4}
	2.58×10^{-5}
	1.46×10^{-4}
	Average = 1.46×10^{-4}
	(STD DEV = 2.01×10^{-4})
1.3	2.36×10^{-4}
	7.31×10^{-5}
	3.91×10^{-4}
	1.86×10^{-4}
	1.19×10^{-4}
	Average = 2.01×10^{-4}
	(STD DEV = 1.23×10^{-4})

[a] Avg. value of mobility and Std. Dev. is approximated to two decimal points.

Table S4. Statistic table of all the electron mobility data of compound **1.1-1.3**.[a]

Compound	Electron Mobility (cm^2/Vs)
1.1	1.38×10^{-5}
	2.56×10^{-5}
	5.02×10^{-6}
	2.09×10^{-5}
	1.37×10^{-5}
	Average = 1.58×10^{-5}
	(STD DEV = 7.85×10^{-6})
1.2	3.84×10^{-6}
	1.35×10^{-6}
	1.13×10^{-6}
	7.65×10^{-6}
	1.36×10^{-6}
	Average = 3.07×10^{-6}
	(STD DEV = 2.79×10^{-6})
1.3	2.19×10^{-5}
	7.50×10^{-6}
	7.12×10^{-5}
	9.35×10^{-5}
	3.72×10^{-5}
	Average = 4.63×10^{-5}
	(STD DEV = 3.55×10^{-5})

[a] Avg. value of mobility and Std. Dev. is approximated to two decimal points.

13) References:

1. J. De, I. Bala, S. P. Gupta, U. K. Pandey, S. K. Pal, *J. Am. Chem. Soc.*, 2019, **141**, 18799.
2. I. Bala, H. Kaur, M. Maity, R. A. K. Yadav, J. De, S. P. Gupta, J. H. Jou, U. K. Pandey, S. K. Pal, ACS *Appl. Electron. Mater*., 2022, **4**, 1163.
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4. M. J. Frisch, *et* al. Gaussian 09 (Revision D.01) Gaussian, Inc., Wallingford CT, 2009**.**
5. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.