Electronic Supporting Information (ESI)

Perylenemonoimide-based superstable radical anions and dianions with solid-state emission properties

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I. Materials: All the solvents and reagents were purchased from commercial sources and were used as received. Perylene-3,4,9,10-tetracarboxylic dianhydride, 2-ethylhexylamine, sodium sulfate, meta-chloroperoxybenzoic acid (*m*CPBA) and tetrabutylammonium hexafluorophosphate ($TBAPF_6$) were purchased from Sigma. Imidazole and CrO_3 were purchased from Sisco Research Laboratories (SRL). H_2O_2 were purchased from SDFCL. Triethylamine (TEA), diethylamine (DEA) were purchased from Spectrochem. All the spectroscopic grade solvents like dichloromethane (DCM), chloroform and tetrahydrofuran (THF) used for UV-Vis. absorption and fluorescence spectroscopy were obtained from SRL. N, N-Dimethylformamide (DMF) was purchased from Sigma. Thin Layer chromatography (TLC) analyses were carried out by using Merck TLC Silica gel 60 F_{254}. Column chromatography was performed on silica gel (230-400 mesh size), purchased from Rankem. Experimental Steady-state Measurements The stock solutions of 1 mM concentration of compounds were made in Toluene (Tol) and diluted as required in the experiments. Spectroscopic investigations of radical anions were done at 10 μM concentration of compounds in DMF.

1. Instrumentation and methodology:

1.1 Nuclear Magnetic Resonance spectroscopy and Mass Spectrometry:

The ^{1}H NMR spectra were recorded on Bruker 400 MHz, 500 MHz spectrometer and ^{13}C NMR spectra were recorded on Bruker 500MHz, 700 MHz spectrometer in $CDCl_3$ solvent. Chemical shifts were determined in ppm scale with respect to the residual solvent signal (δ = 7.26 ppm). The high-resolution liquid chromatograph mass spectra for all compounds were recorded using quadrupole time-of-flight-electro spray ionization (HRLC-QTOF-ESI) using acetonitrile (ACN) as solvent.

1.2 Steady-state absorption and fluorescence spectroscopy:

All steady-state absorption measurements were carried out using Shimadzu 1800 UV-spectrophotometer using 1 cm path length quartz cuvettes. All steady-state fluorescence measurements were carried out on Jobin Yvon Horiba Model Fluorolog-3-21 equipped with a 450 W Xenon CW lamp as the excitation source. All the acquired fluorescence spectra were corrected with respect to the excitation light intensity and photomultiplier tube (PMT) response using the correction files available in Horiba software. Absolute fluorescence quantum yield measurement was also performed in integrating sphere using HORIBA Jobin Yvonn Fluorolog fluorimeter. Fluorescence spectra were recorded using a 1 cm path length quartz cuvette and keeping both excitation and emission slit at 2 nm. All the experiments were carried out at ambient temperature (298K). For the powder sample,

fluorescence measurements were carried out using front face excitation by placing the powder sample in a solid-state holder oriented at an angle of 45^{O}.

1.3 Time resolved fluorescence spectroscopy:

Time-resolved fluorescence measurements were carried out using time-correlated single photon counting (TCSPC) spectrometer (Delta Flex-01-DD/ HORIBA). Picosecond photon detection module equipped with Hamamatsu MCP photomultiplier (R-3809U-50) tube was used as detector. Delta diode laser 468 nm were used as excitation source and the photon-count was set to 10000. The instrument response function (IRF) was recorded using an aqueous solution of colloidal silica (Ludox). Decay curves were analyzed by nonlinear least-squares iteration using inbuilt Eztime decay analysis software. The quality of the fitting was then assessed by taking a note of the fitting parameter (χ^2).

1.4 Commission Internationale de L`Eclairage (CIE) chromaticity index calculation:

The CIE chromaticity index was calculated by using the following equations:

$$X = \Sigma_{K=1} \Phi_K(\lambda) B_K(\lambda)$$

$$Y = \Sigma_{K=1} \Phi_K(\lambda) G_K(\lambda)$$

$$Z = \Sigma_{K=1} \Phi_K(\lambda) R_K(\lambda)$$

Where the Tristimulus values X, Y, Z represent a specific color coordinates. $B_k(\lambda)$, $G_k(\lambda)$, $R_k(\lambda)$ are defined as color matching functions of a standard colorimetric observer. $\Phi_K(\lambda)$, spectral distribution of color stimulus obtained from the emission spectra of species, The CIE co-ordinates (x, y, z) was calculated by considering the equations: x = X/ (X+Y+Z), y = Y/ (X+Y+Z), z = Z/ (X+Y+Z).

1.5 Photo-irradiation:

Photo-irradiation technique was carried out in a Luzchem photoreactor (LZC-ORG). The LZC-ORG photoreactor houses 10 lamps providing side irradiation to samples. For the present work, visible cool white fluorescence lamps (8 W, 390 lumen) were used for irradiation. Illuminance, which is a measure of how much incident light illuminates a surface was measured by an illuminance meter (Lutron LX 101 luxmeter). The SI unit for illuminance is lux (lx). In this case, illuminance was found to be ~ 970 lx.

1.6 Electron paramagnetic resonance spectroscopy:

The samples required for EPR spectroscopy were prepared in DMF with and/ or without reducing agent *i.e.*, TEA at 10 μM concentration of compounds. The measurements were recorded at a temperature of 150 K. Modulation amplitude was set to 1. Time constant was set to 24. All the EPR spectra was

measured in Microwave frequency of 9.4 GHz at the X-band on a Bruker Biospin GmbH spectrometer. The Lande factor, g was calculated using:

$$g = \frac{h.\nu}{H_{\circ}.\beta}$$

h being Planck's constant

ν is the operating frequency (9.4 GHz for X-band)

$H_{\circ}$ is magnetic field (Gauss)

β is the Bohr Magneton

1.7 Density functional theory calculations:

The structures of the molecules were optimized by DFT using the B3LYP density functional with basis set 6-311G+dp. Quantum chemical calculation was performed with the Gaussian 16 package. Optimization and calculation of frontier orbital energies were carried out using DCM as solvent. Structures were visualized using Mercury 3.8 software.

1.8 Fourier transform infrared spectroscopy (FTIR):

FTIR measurements were done on Perkin-Elmer Model 2000 FTIR using pellets made with KBR as a binder. Thirty scans were signal averaged, with a resolution of 8 cm^{-1} at ambient temperatures.

1.9 Single crystal X-ray diffraction (SC-XRD):

Single Crystal X-ray Diffraction data were collected on a Bruker D8 Venture diffractometer equipped with a Photon-III detector using S4 monochromated Mo Kα radiation (λ = 0.71073 Å) at 100 K using an Oxford cryostream low temperature device. Unit cell measurement, data integration, scaling and absorption corrections for the crystal were done with Bruker APEX II software. Data reduction was carried out with Bruker SAINT suite. Absorption correction was performed by the multi-scan method implemented in SADABS. The crystal structure solutions and refinements were done using SHELXS and SHELXL implemented in OLEX2. Bright plate shape crystals of the orange solid were obtained from mixture of dichloromethane and toluene under ambient conditions after 10 to 15 days by solvent evaporation. Growing quality diffraction quality crystals for the material was challenging even after making changes in the solvents of crystallization. The solvent of crystallisation in the lattice could not be modelled from the diffraction data, and the electron density due to the same was treated with SQUEEZE routine of PLATON. The CIF file containing complete information on TT-PMI-8O

(CCDC No. 2313796) were deposited with CCDC and are freely available upon request from the following web site: www.ccdc.cam.ac.Uk/data_request/cif.

2 Electrochemical measurements:

2.1 Cyclic voltametric (CV) studies:

Cyclic voltammetry experiments were carried out using a BioLogic SP-300 potentiostat in a three-electrode setup at room temperature (25 ^{O}C). Working, counter and reference electrodes were glassy carbon disc (3 mm in diameter), platinum wire, and saturated Ag/AgCl (0.022 V vs SHE) respectively. 1 mM of each sample was taken in DCM solution (5.0 ml) and 0.1 M of nBu_4PF_6 electrochemical solution. The CVs were recorded at the scan rate of 100 mVs^{-1}.

2.2 Spectroelectrochemistry experiment:

Absorption spectra were taken using an HR 4000 spectrophotometer developed by Ocean Optics along with a 1 cm cuvette holder and a DT-MINI-2-GS UV-vis-NIR light source. A CH electrochemical analyzer was used to hold the samples at desired potentials. A pt working electrode, Ag/AgCl as reference electrode, and a Pt counter electrode were also used in this measurement. Supporting electrolyte used was 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in dry DCM solvent.

II. Synthesis and characterization:

The PMI was synthesized as the reported procedure.[1, 2]

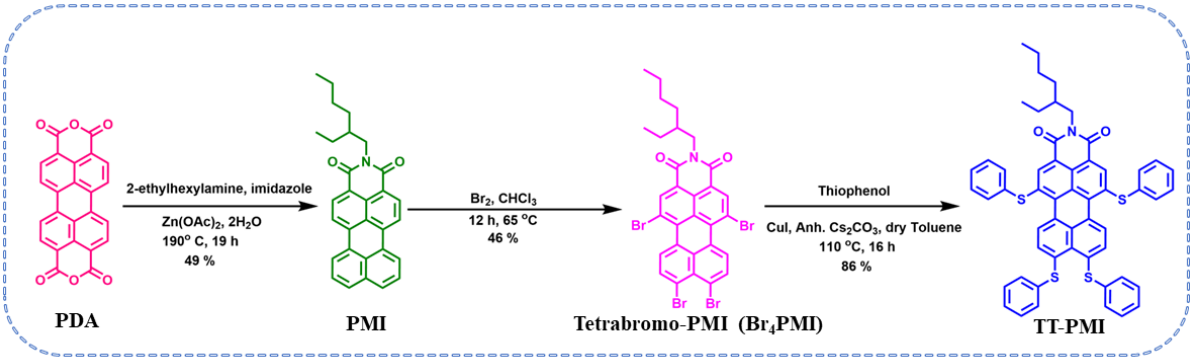
In the next step, Br_2 was introduced to activate the *bay* and *peri* position of perylenemonoimide, as reported.[3] To a solution of PMI (200 mg, 0.46 mmol) in chloroform (21 mL) Br_2 (4.7 mL, 92.3 mmol) was added slowly. The reaction mixture was refluxed at 70 ^{o}C. After cooling down the reaction mixture to room temperature excess bromine was removed by flow of nitrogen. The reaction mixture was washed with saturated sodium thiosulfite solution (3x100 mL) followed by water (2x100 mL). The organic phase was dried over Na_2SO_4, and the solvent was evaporated on a rotary evaporator until free-flowing precipitates came out and filtered. The obtained solids were dried in high vacuum to obtain tetrabromo PMI as desired compound. This process yielded 158 mg of the product, representing 46 % yielded.

Synthesis of TT-PMI: TT-PMI was synthesized according to our previously reported procedure. First, tetrabromo PMI (24 mg, 0.032 mmol) was dissolved in dry toluene (2 mL) with the subsequent addition of thiophenol (34.13 mg, 0.31 mmol) under inert atmosphere. Following this, CuI (1.8 mg, 0.009 mmol) and Cs_2CO_3 (114.27 mg, 0.351 mmol) were introduced. The reaction mixture was then refluxed for a

duration of 14 hours. Once the reaction had concluded, the mixture was thinned with $CHCl_3$ and subjected to a water wash. The resulting crude product was subsequently dehydrated and subjected to purification through column chromatography utilizing a 2:1 mixture of $CHCl_3$ and n- hexane as the elution solvent. This process yielded 24 mg of the product, representing an 86 % yield.

^{1}H NMR (400 MHz, $CDCl_3$):

δ 8.40 (s, 2H), 8.30 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 6.9 Hz, 4H), 7.43 – 7.32 (m, 16H), 4.00 (dd, *J* = 7.1, 4.1 Hz, 2H), 1.86 (d, *J* = 5.9 Hz, 1H), 1.38 – 1.17 (m, 8H), 0.89 (d, *J* = 7.3 Hz, 3H), 0.87 – 0.82 (m, 3H).



Scheme S1: Synthesis of TT-PMI

Synthesis of TT-PMI-2O (1): Under inert conditions, a solution of TT-PMI (10 mg, 0.011 mmol) was dissolved in 2 mL of dichloromethane (DCM) and cooled to 0 °C. Subsequently, *m*CPBA (3.98 mg, 0.023 mmol) was added and allowed to stir for 1 hour. The resulting reaction mixture was then subjected to extraction with water. The organic phase was dehydrated using sodium sulphate (Na_2SO_4), removed *in vacuo* and the resultant residue was purified by column chromatography using a mixture of DCM and n-hexane (3:1 ratio) as the eluting solvent. This process yielded 3 mg of the product, representing a 29 % yield.

^{1}H NMR (500 MHz, $CDCl_3$):

δ 9.01 (d, *J* = 8.2 Hz, 1H), 8.80 (d, *J* = 8.2 Hz, 1H), 8.48 (d, *J* = 1.2 Hz, 1H), 8.46 (s, 1H), 8.43 (s, 1H), 7.90 – 7.87 (m, 1H), 7.67 – 7.61 (m, 2H), 7.46 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.38 (tdd, *J* = 9.8, 6.9, 3.0 Hz, 11H), 7.25 (t, *J* = 7.8 Hz, 3H), 7.06 (d, *J* = 6.6 Hz, 2H), 4.06 – 3.97 (m, 2H), 1.91 – 1.84 (m, 1H), 1.35 – 1.25 (m, 8H), 0.90 (t, *J* = 7.4 Hz, 3H), 0.87 – 0.85 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$):

δ 163.5, 137.1, 136.7, 136.3, 135.1, 134.2, 133.9, 133.8, 133.7, 133.2, 132.9, 130.5, 129.9, 129.5, 129.3, 129.2, 127.2, 125.7, 124.1, 120.9, 120.7, 44.4, 37.8, 30.6, 28.6, 24.00, 23.1, 14.1, 10.6.

Synthesis of TT-PMI-2IO (2): Under an inert atmosphere, a solution of TT-PMI (10 mg, 0.011 mmol) was dissolved in 1.5 mL of dichloromethane (DCM) and cooled to 0 ^{o}C temperature. After that solution of *m*CPBA (7.96mg, 0.046 mmol) in DCM of 1.5 mL was added dropwise for 30 min with stirring. Then the reaction mixture was continued for 1.30 hours at 0 ^{o}C temperature. The resulting reaction mixture was then subjected to extraction with a saturated aqueous solution of sodium bicarbonate ($NaHCO_3$) and concentrated under vacuo. The crude product was further purified through column chromatography using a mixture of DCM and n-hexane in a 4:1 ratio as the eluting solvent. This process yielded 2.1 mg of the product, representing a 20 % yield.

^{1}H NMR (500 MHz, $CDCl_3$):

δ 9.11 (s, 1H), 9.06 (d, *J* = 8.1 Hz, 1H), 8.82 (d, *J* = 8.0 Hz, 1H), 8.55 (s, 1H), 8.13 (dd, *J* = 14.8, 8.2 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.60 (s, 4H), 7.47 (s, 6H), 7.43 (s, 3H), 7.38 (s, 3H), 7.07 (s, 2H), 4.06 (s, 2H), 1.89 (s, 1H), 1.43 – 1.15 (m, 8H), 0.94 – 0.82 (m, 6H).

^{13}C NMR (176 MHz, $CDCl_3$):

δ 162.9, 147.0, 145.4, 144.2, 138.1, 135.5, 133.6, 131.5, 131.0, 130.8, 130.3, 130.1, 129.7, 129.6, 129.6, 129.5, 129.4, 127.9, 127.3, 126.2, 126.1, 126.1, 37.8, 31.9, 29.4, 28.7, 23.1, 22.7, 14.1, 10.6.

Synthesis of TT-PMI-4O (3): Under an inert condition, a solution of TT-PMI (10 mg, 0.011 mmol) was dissolved in 2 mL of dichloromethane (DCM) and cooled to 0 ^{o}C. Subsequently, *m*CPBA (5.97 mg, 0.034 mmol) was added and allowed to stir for 2 hours at 0 ^{o}C. The resulting reaction mixture was then subjected to extraction with a saturated aqueous solution of sodium bicarbonate ($NaHCO_3$) and concentrated under vacuo. The crude product was further purified through column chromatography using a mixture of dichloromethane (DCM) and acetonitrile (ACN) in a 99:1 ratio as the eluting solvent. This purification process yielded 1.9 mg of the product, corresponding to an 18 % yield.

^{1}H NMR (500 MHz, $CDCl_3$):

δ 8.76 (q, *J* = 8.1 Hz, 4H), 8.40 (s, 2H), 7.74 (d, *J* = 6.9 Hz, 4H), 7.46 (d, *J* = 6.9 Hz,6H), 7.40 (s, 4H), 7.36 (s, 6H), 3.99 (d, *J* = 6.8 Hz, 2H), 1.84 (s, 1H), 1.37 – 1.18 (m, 8H), 0.87 (d, *J* = 6.9 Hz, 3H), 0.88 – 0.79 (m, 3H).

^{13}C NMR (176 MHz, $CDCl_3$):

δ 163.4, 145.1, 138.2, 133.7, 133.5, 133.3, 132.9, 132.1, 131.3, 130.6, 130.0, 129.7, 129.4, 129.0, 127.2, 126.3, 126.1, 121.4, 37.8, 33.3, 29.4, 24.0, 23.1, 22.7, 14.1, 10.6.

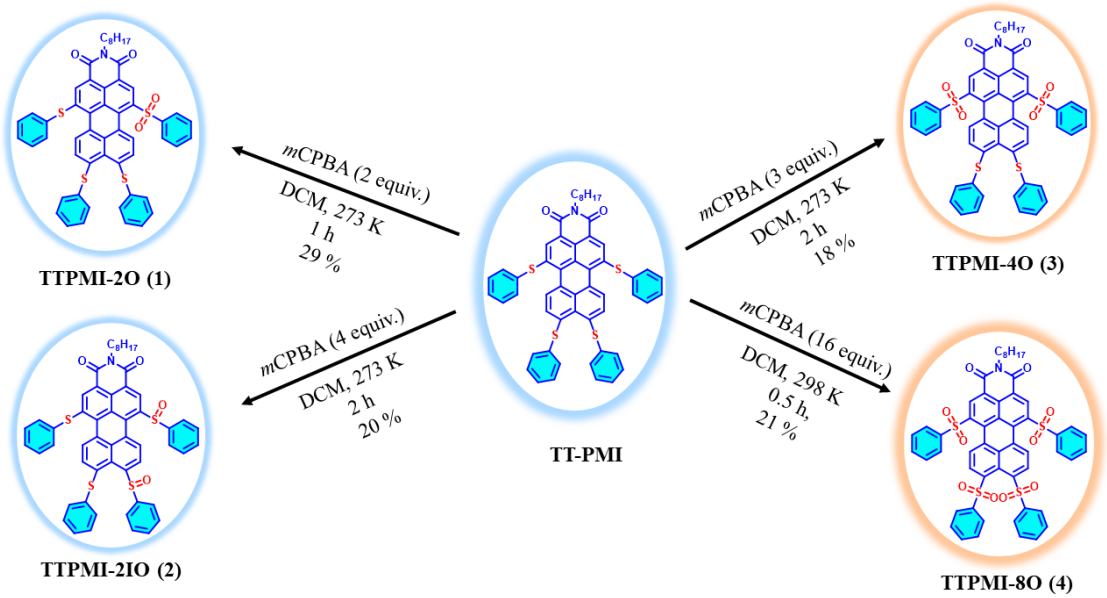
Synthesis of TT-PMI-8O (4): Under an inert atmosphere, TT-PMI (10 mg, 0.011 mmol) and *m*CPBA (31.88 mg, 0.1847 mmol) were dissolved in 3 mL of dichloromethane (DCM). The resulting reaction mixture was stirred at 25 ^{O}C for 30 minutes, followed by the evaluation of its progress using TLC. Subsequently, the reaction mixture was subjected to extraction with a saturated aqueous solution of sodium bicarbonate ($NaHCO_3$). The resulting solution was then dehydrated by passing it over sodium sulfate (Na_2SO_4) and concentrated *under vacuo*. The crude product obtained was further purified through column chromatography using a mixture of DCM and acetonitrile (ACN) in a 97:3 ratio as the eluting solvent. This purification process yielded 2.5 mg of the product, corresponding to a 21 % yield.

^{1}H NMR (500 MHz, $CDCl_3$):

δ 9.05 (s, 2H), 8.98 (d, *J* = 7.8 Hz, 2H), 8.20 (d, *J* = 7.9 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 4H), 7.75 (d, *J* = 7.9 Hz, 4H), 7.63 (t, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 2H), 7.48 (dd, *J* = 15.6, 7.9 Hz, 8H), 4.13 – 4.00 (m, 2H), 1.92 – 1.79 (m, 1H), 1.40 – 1.20 (m, 8H), 0.92 (t, *J* = 7.4 Hz, 3H), 0.87 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$):

δ 162.1, 143.8, 142.5, 141.3, 138.3, 135.4, 134.7, 133.3, 133.2, 133.0, 132.7, 129.3, 129.0, 128.5, 127.5, 121.2, 44.8, 37.8, 30.6, 28.5, 24.0, 23.0, 14.1, 10.6.



Scheme S2: Synthetic scheme of **TT-PMI-2O** (**1**), **TT-PMI-2IO** (**2**), **TT-PMI-4O** (**3**), and **TT-PMI-8O** (**4**).

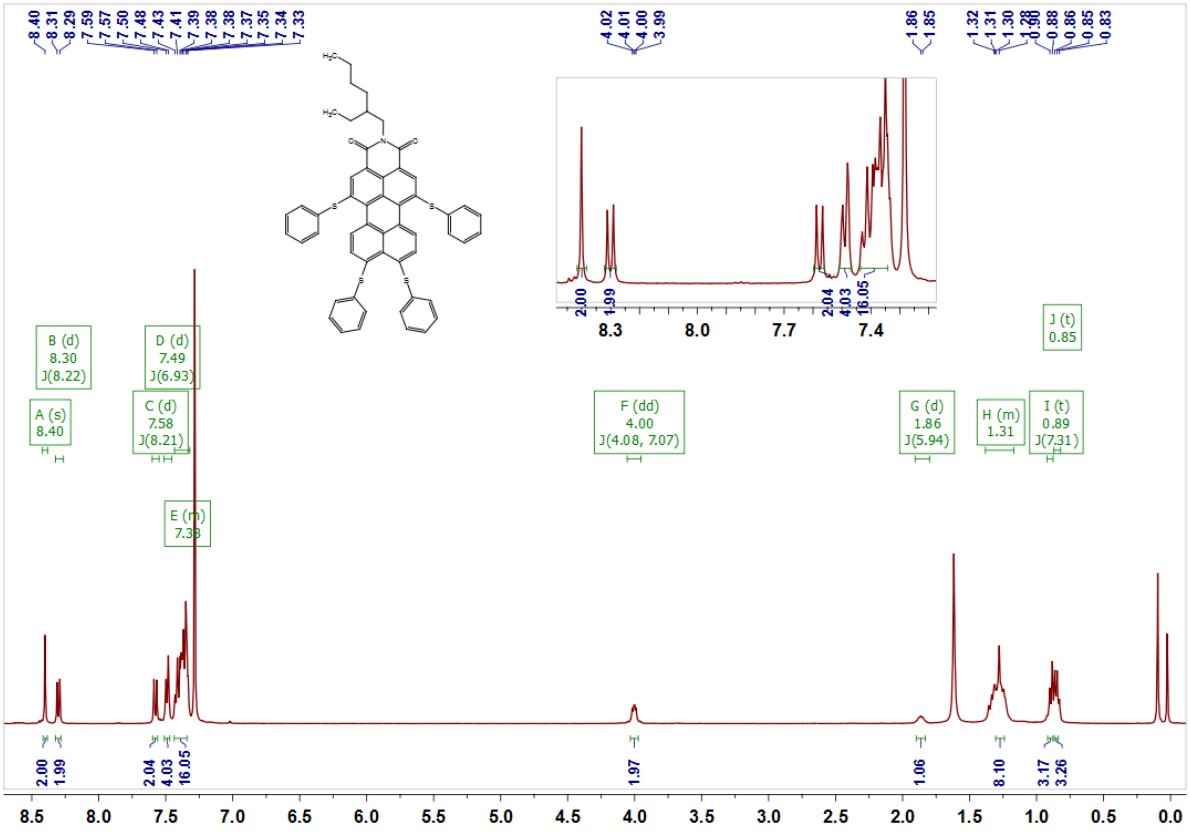


Fig. S1: ^{1}H NMR of **TT-PMI** recorded in $CDCl_3$ at 400 MHz

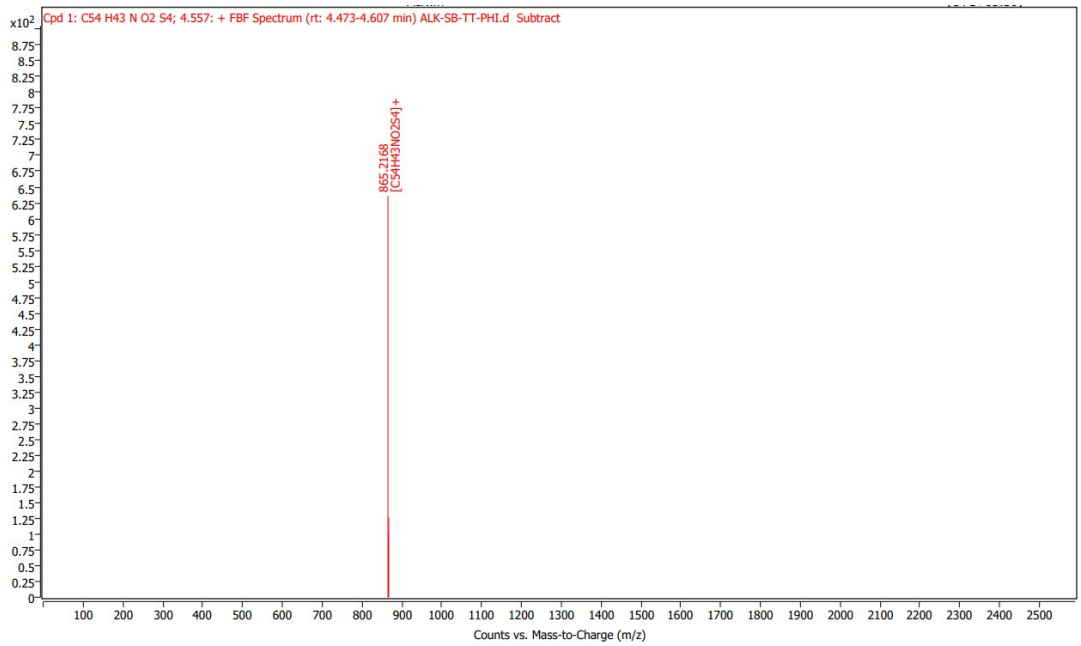


Fig. S2: HRLC-QTOF ESI of **TT-PMI**; Calculated mass – 865.2177 Da and Obtained mass- m/z 865.2168 Da $[M+H]^+$

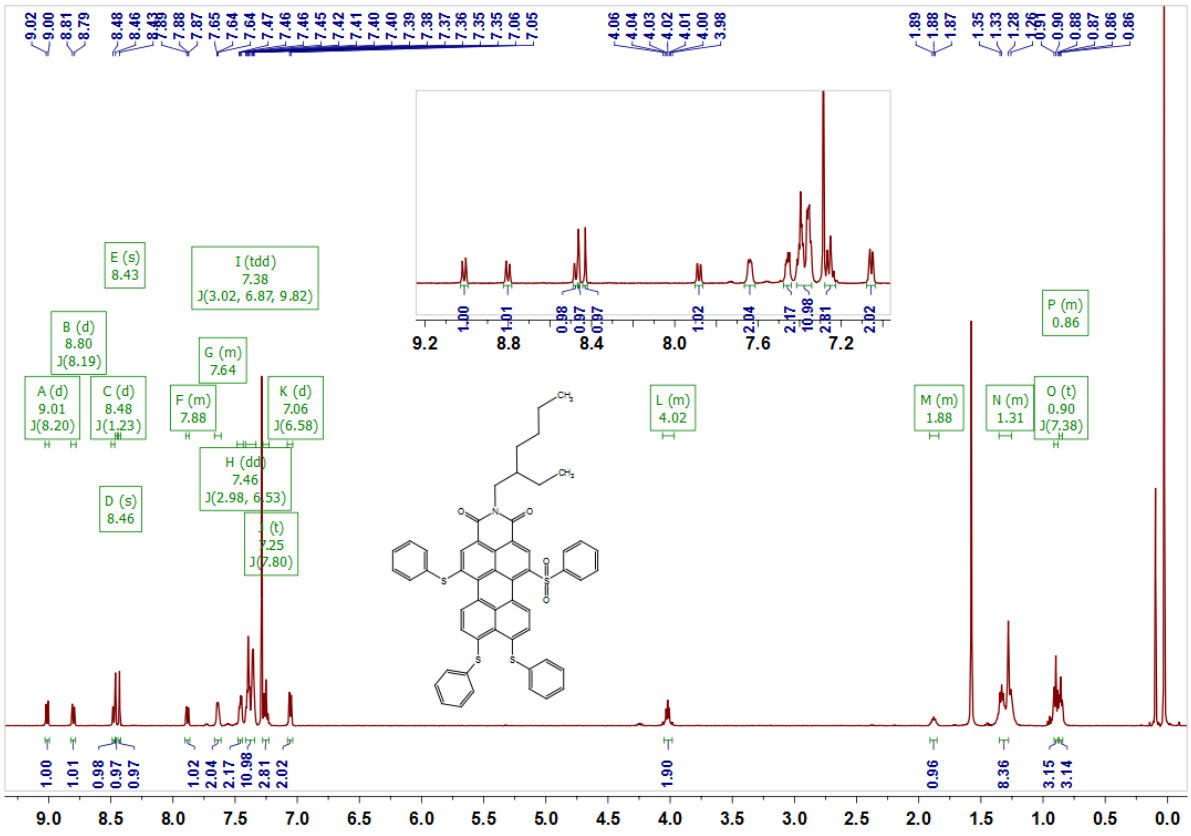


Fig. S3: ^{1}H NMR of **1** recorded in $CDCl_3$ at 500 MHz

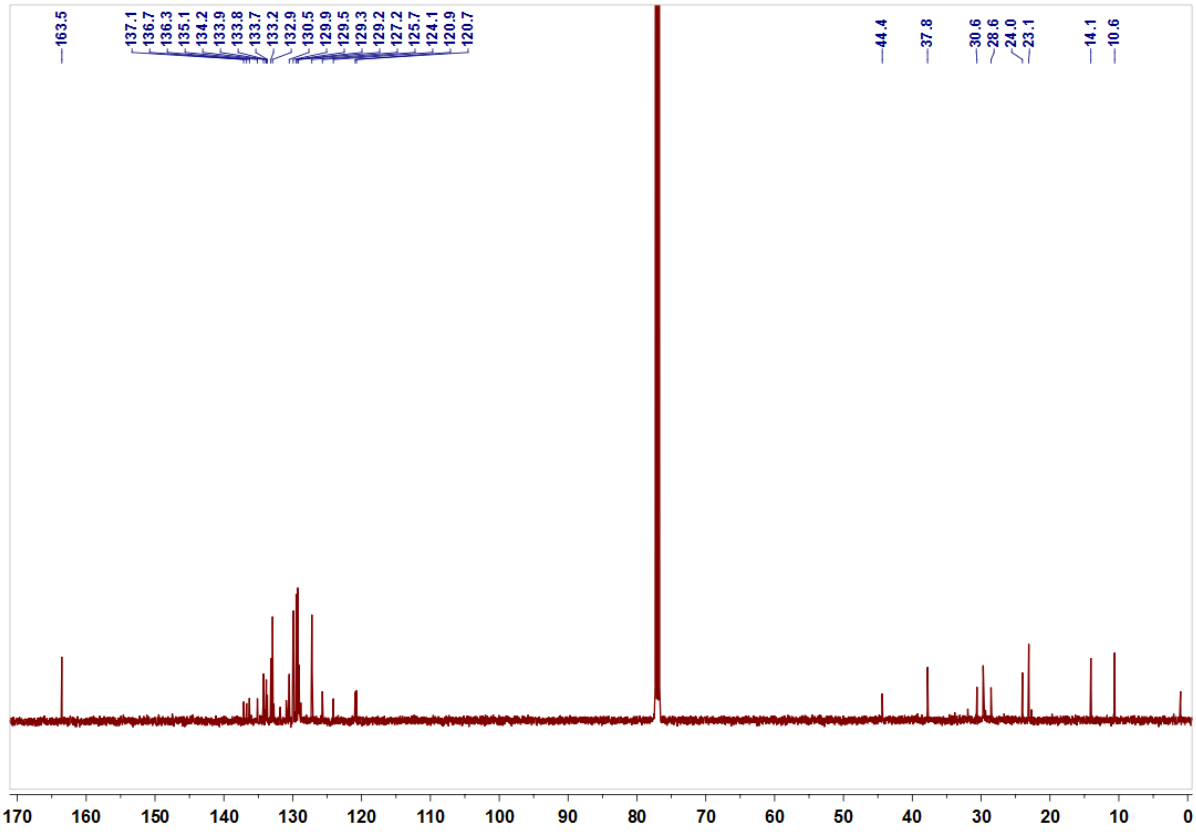


Fig. S4: ^{13}C NMR of **1** recorded in $CDCl_3$ at 126 MHz

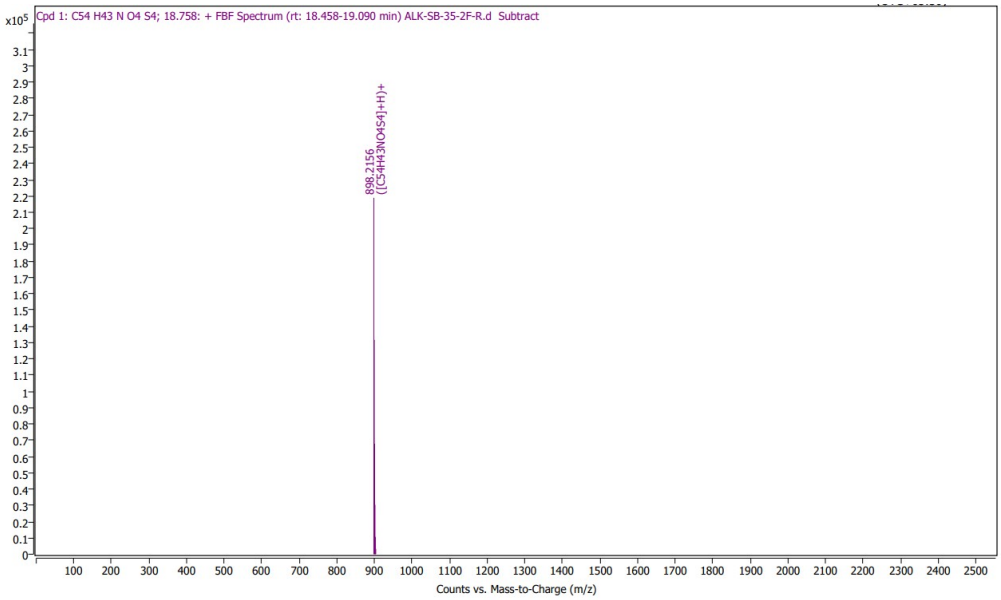


Fig. S5: HRLC-QTOF ESI of **1**; Calculated mass – 898.2148 Da and Obtained mass- m/z 898.2156 Da $[M+H]^+$

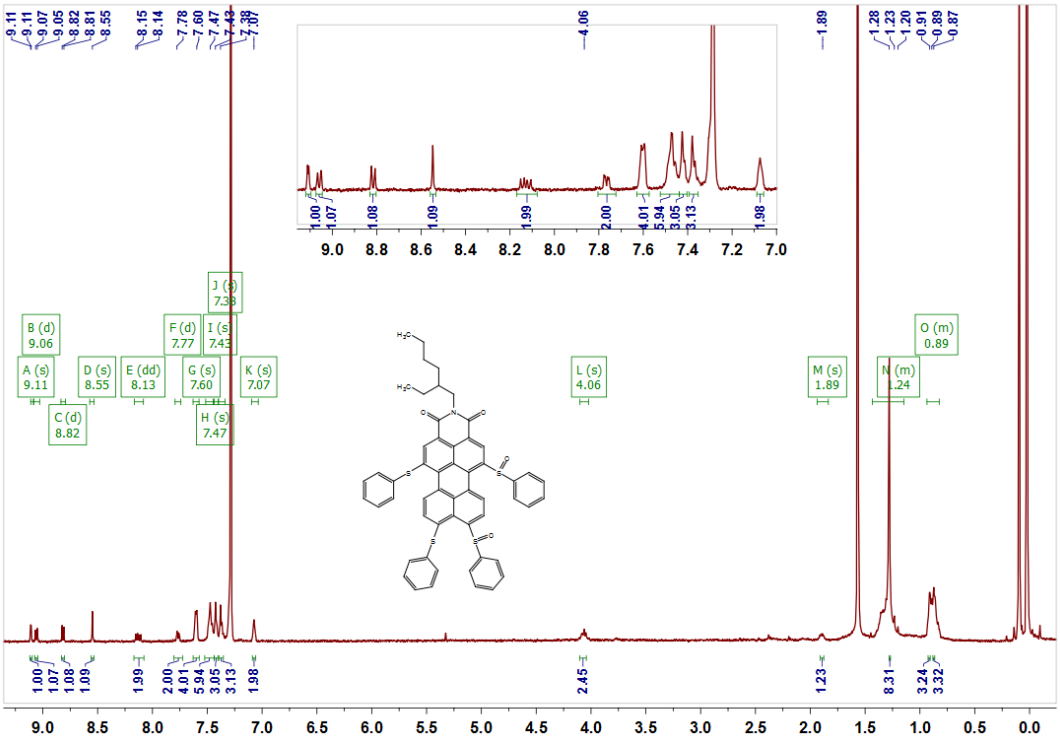


Fig. S6: ^{1}H NMR of **2** recorded in $CDCl_3$ at 500 MHz

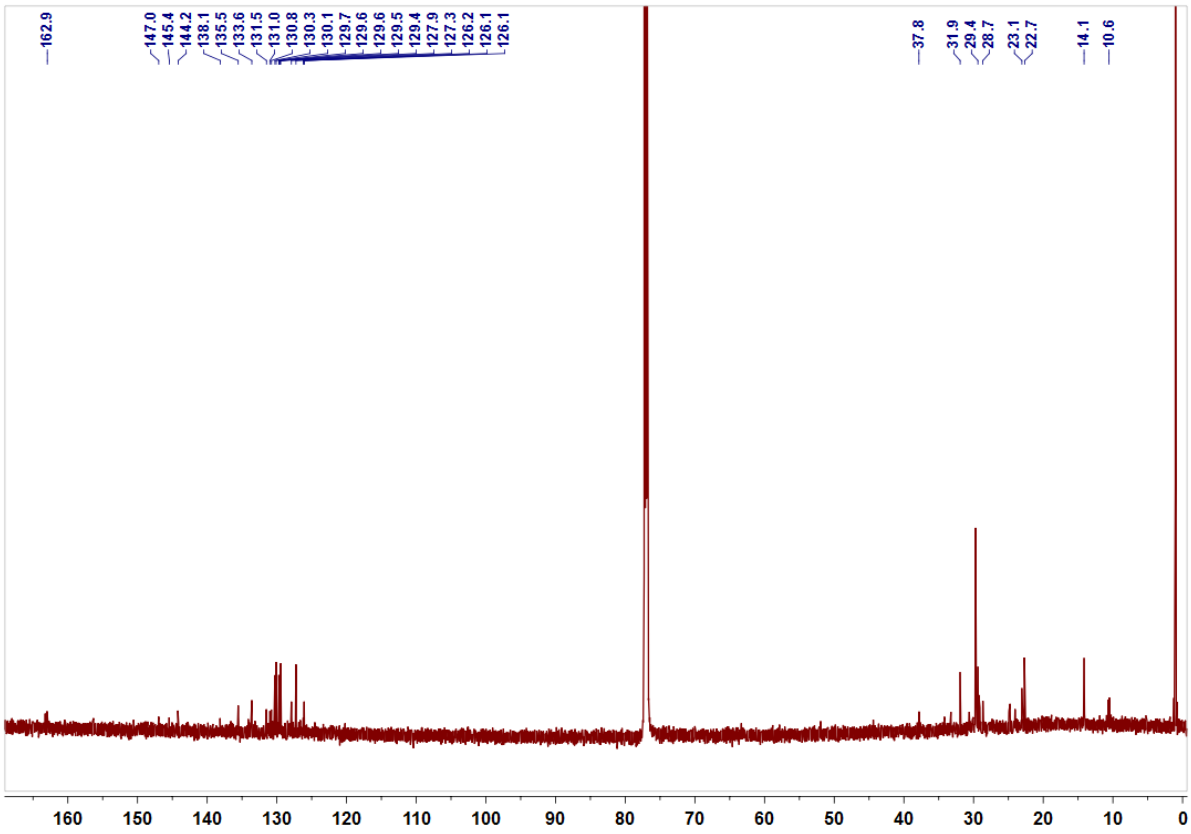


Fig. S7: ^{13}C NMR of **2** recorded in $CDCl_3$ at 176 MHz

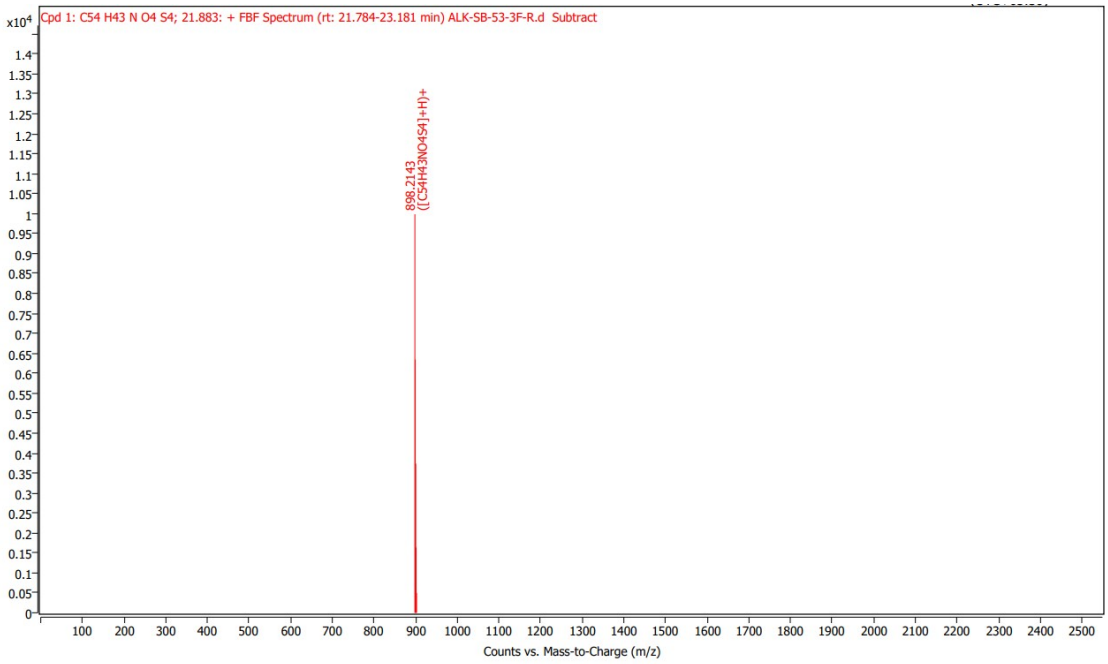


Fig. S8: HRLC-QTOF ESI of **2**; Calculated mass – 898.2148 Da and Obtained mass- m/z 898.2143 Da $[M+H]^+$

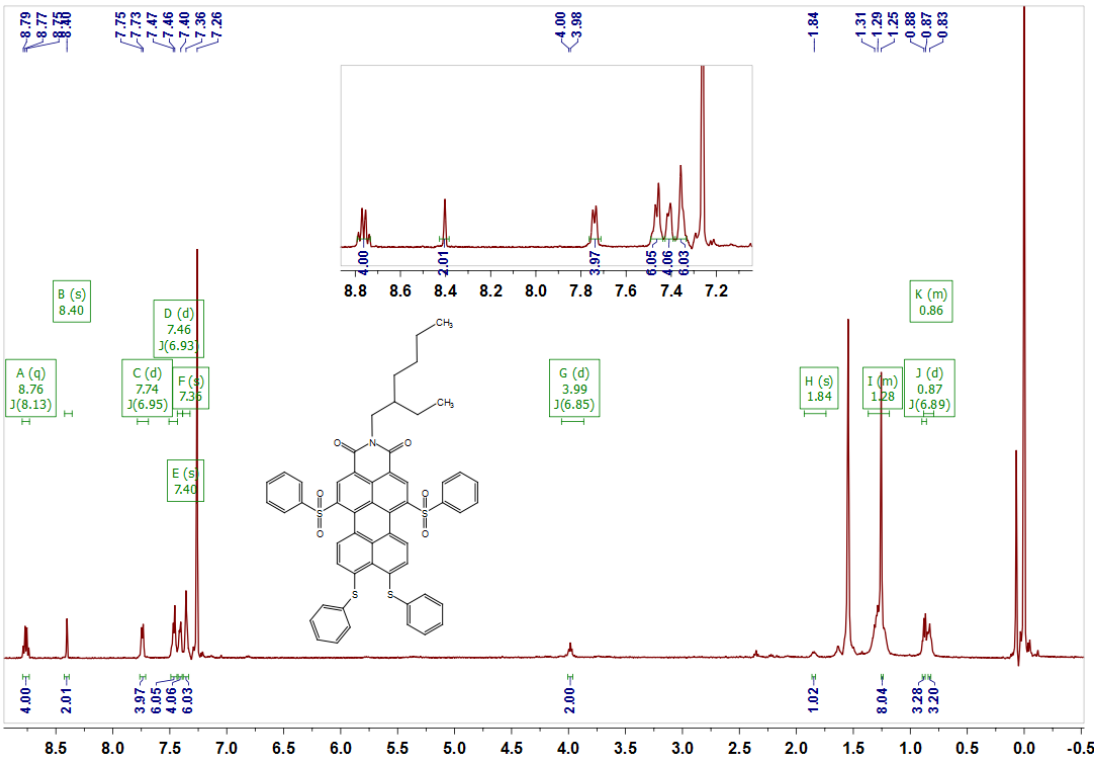


Fig. S9: ^{1}H NMR of **3** recorded in $CDCl_3$ at 500 MHz

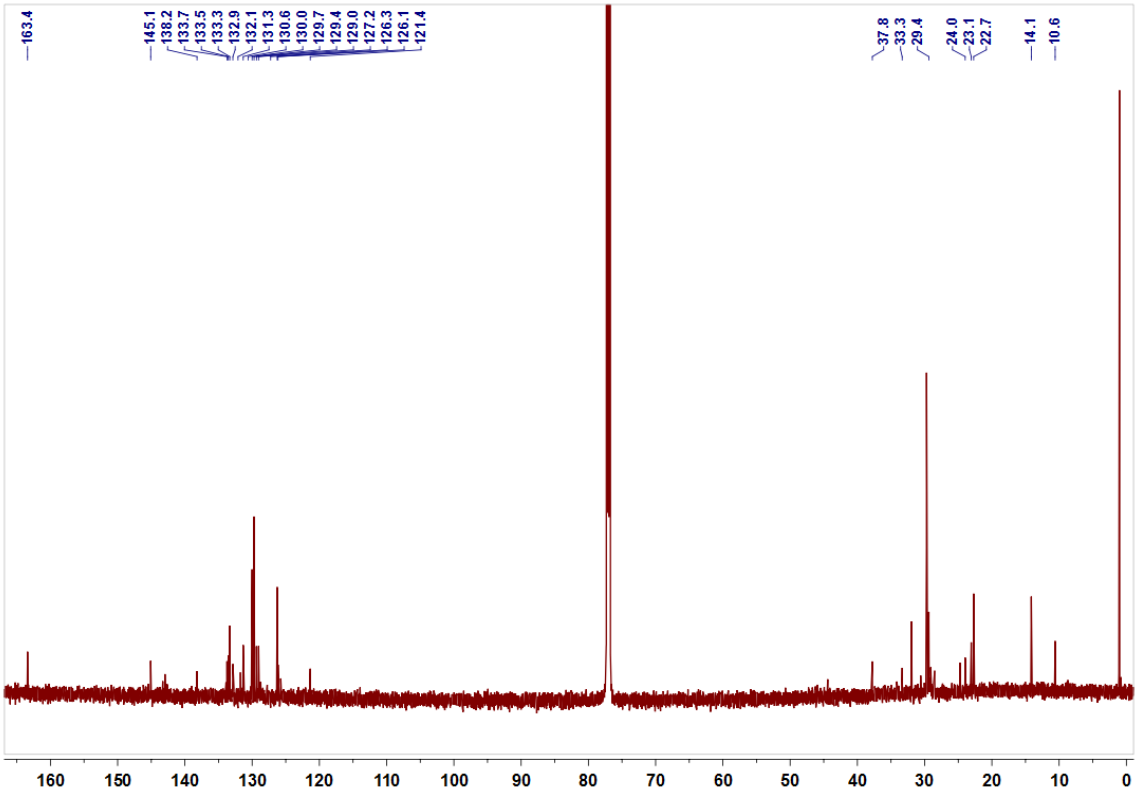


Fig. S10: ^{13}C NMR of **3** recorded in $CDCl_3$ at 176 MHz

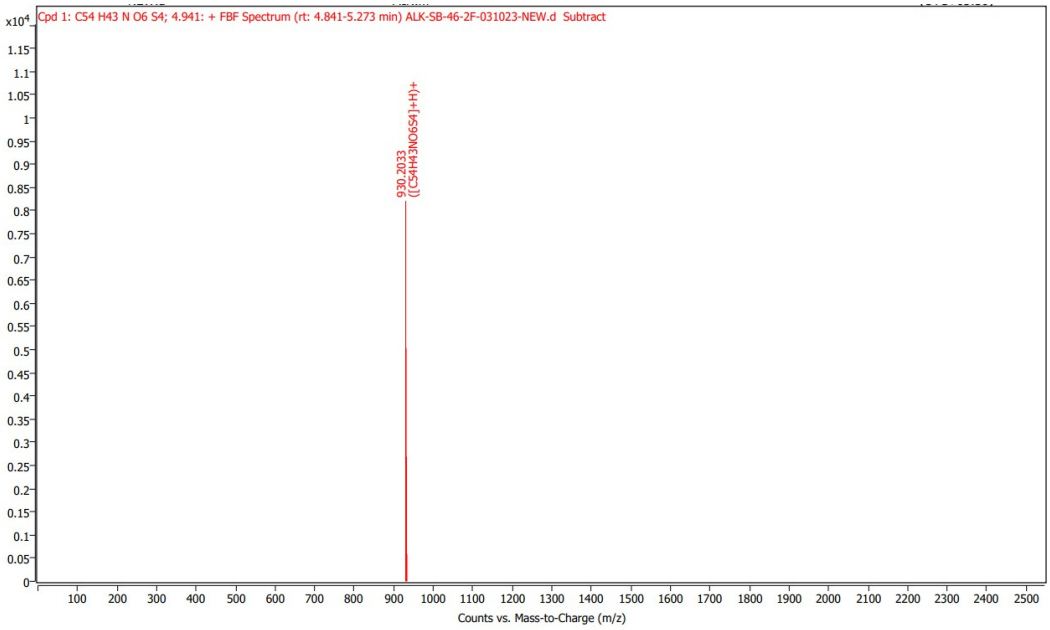


Fig. S11: HRLC-QTOF ESI of **3**; Calculated mass – 930.2007 Da and Obtained mass- m/z 930.2033 Da $[M+H]^+$

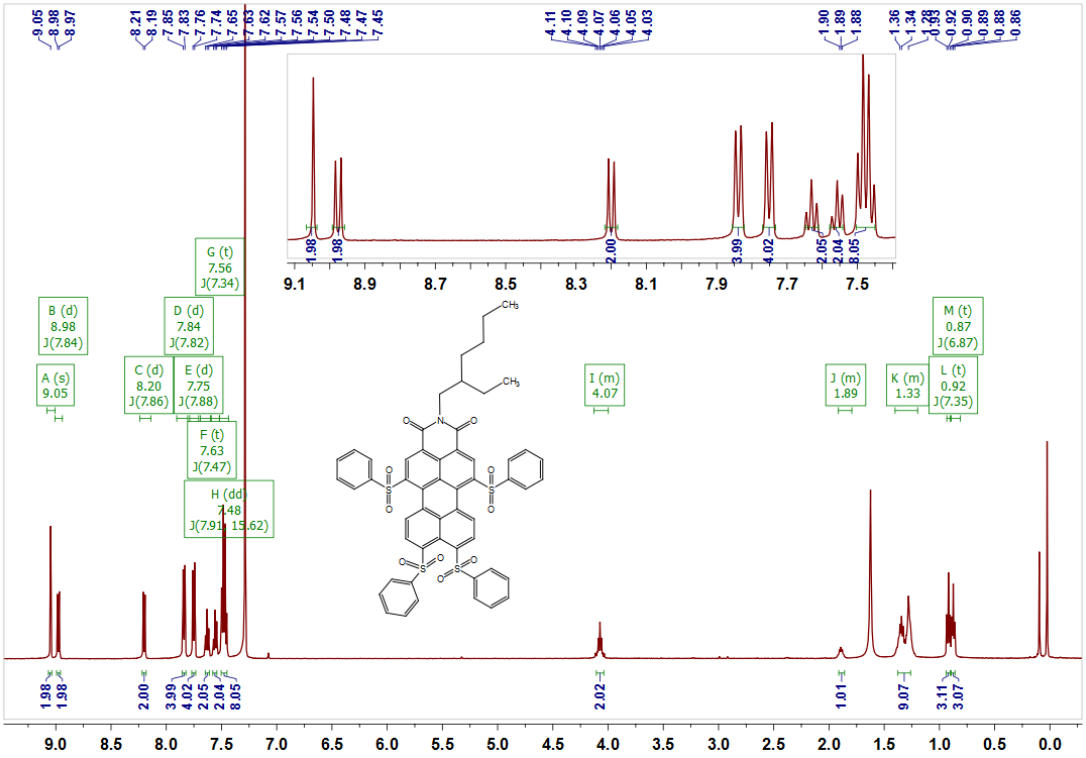


Fig. S12: ^{1}H NMR of **4** recorded in $CDCl_3$ at 500 MHz

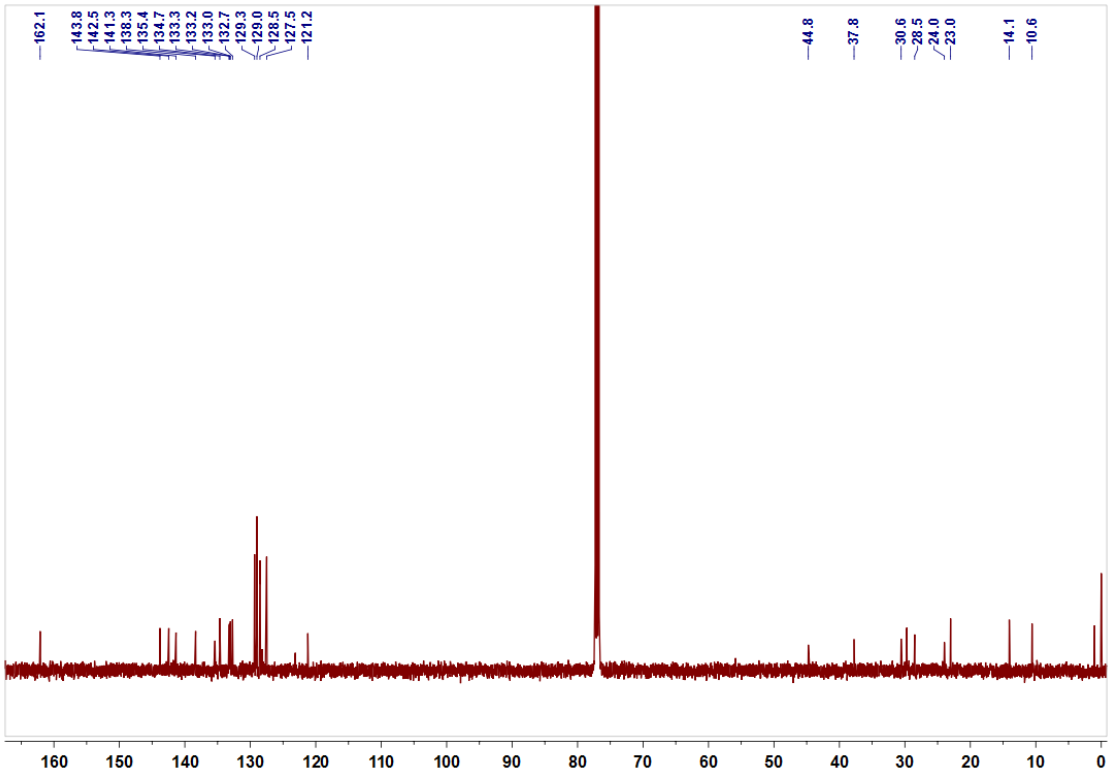


Fig. S13: ^{13}C NMR of **4** recorded in $CDCl_3$ at 126 MHz

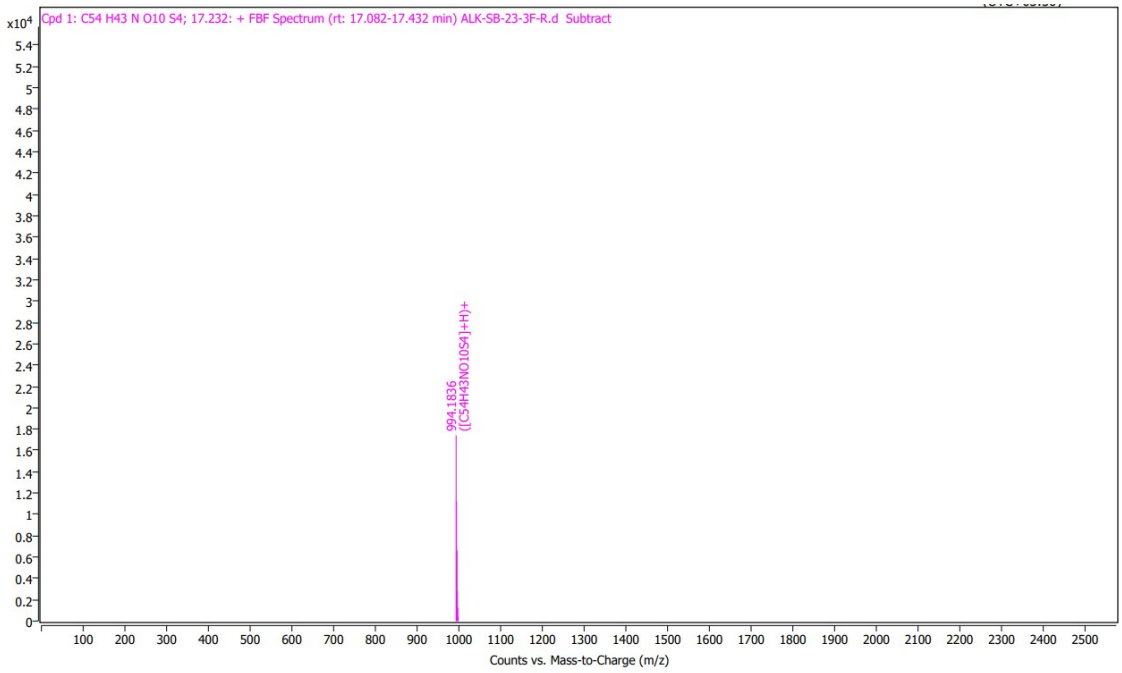


Fig. S14: HRLC-QTOF ESI of **4**; Calculated mass – 994.1803 Da and Obtained mass- m/z 994.1836 Da $[M+H]^+$

III Optical properties:

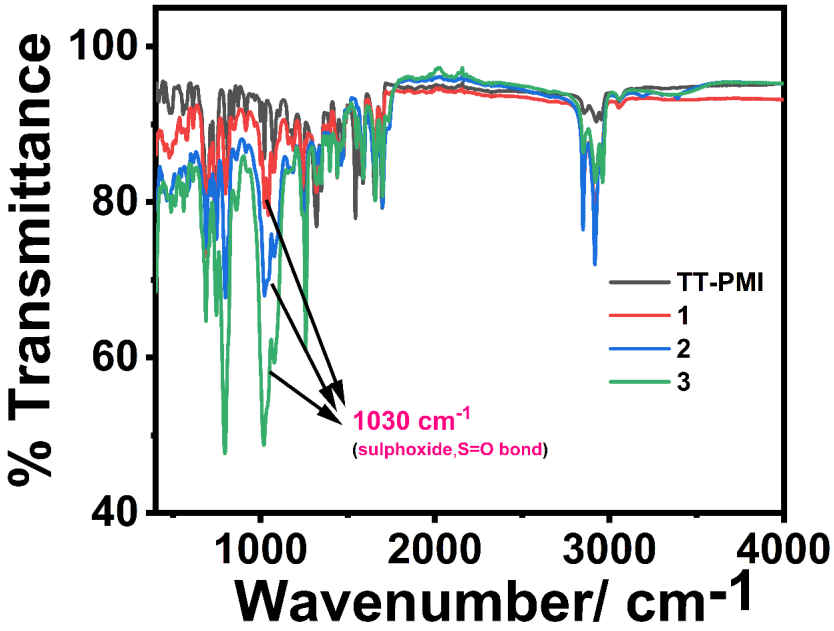


Fig. S15: Merged IR spectra of **TT-PMI**, **1**, **2**, and **3** for confirmation of oxidized species

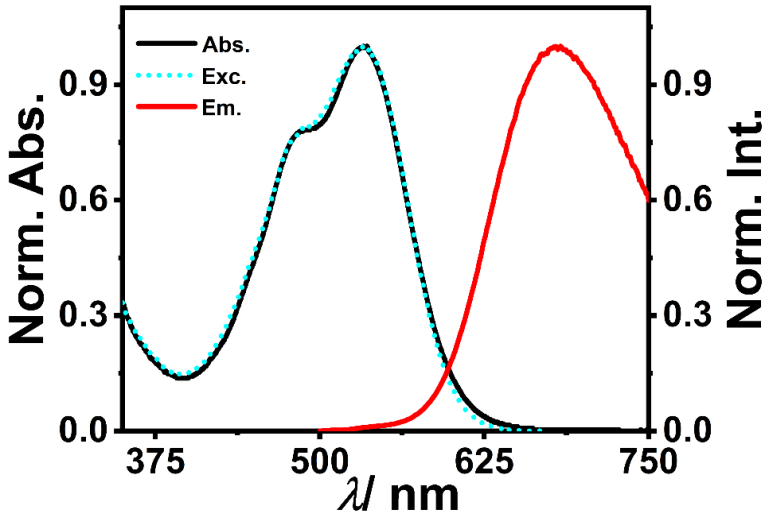


Fig. S16: Absorption, excitation, and emission spectra of **1** in DCM solvent

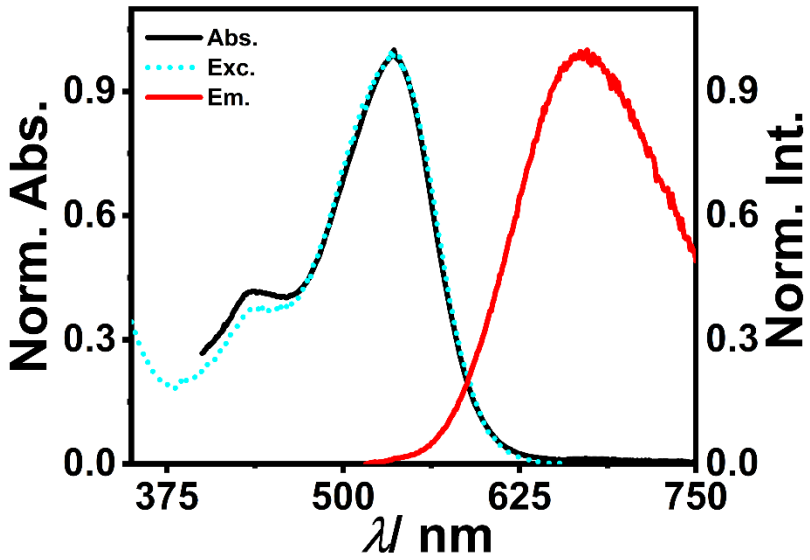


Fig. S17: Absorption, excitation, and emission spectra of **2** in DCM solvent

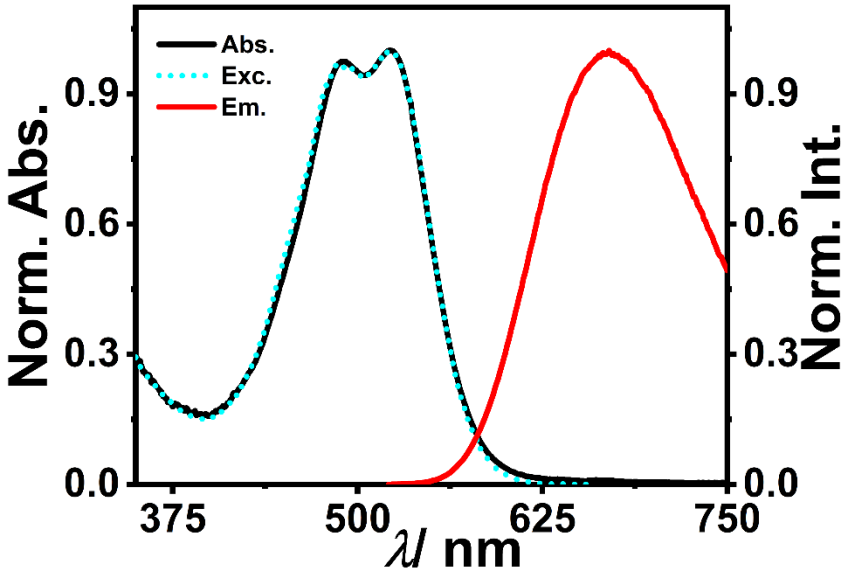


Fig. S18: Absorption, excitation, and emission spectra of **3** in DCM solvent

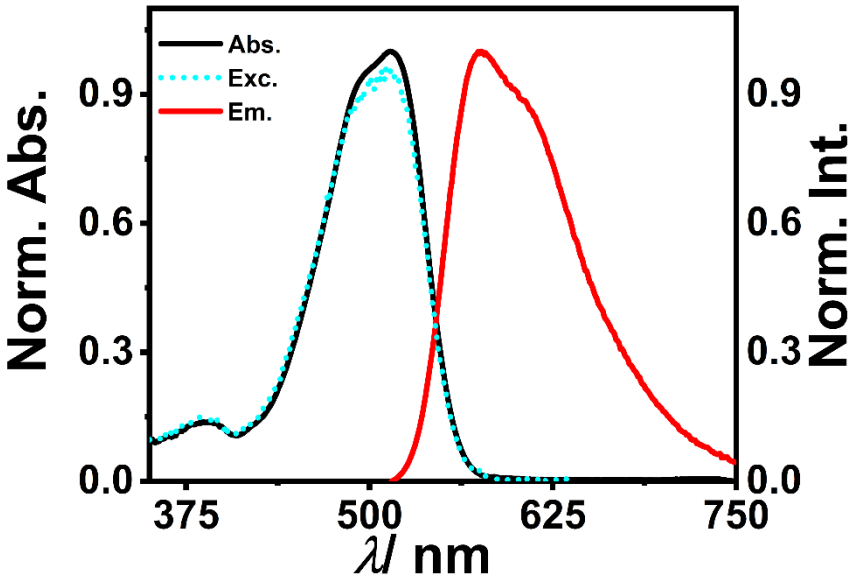


Fig. S19: Absorption, excitation, and emission spectra of **4** in DCM solvent

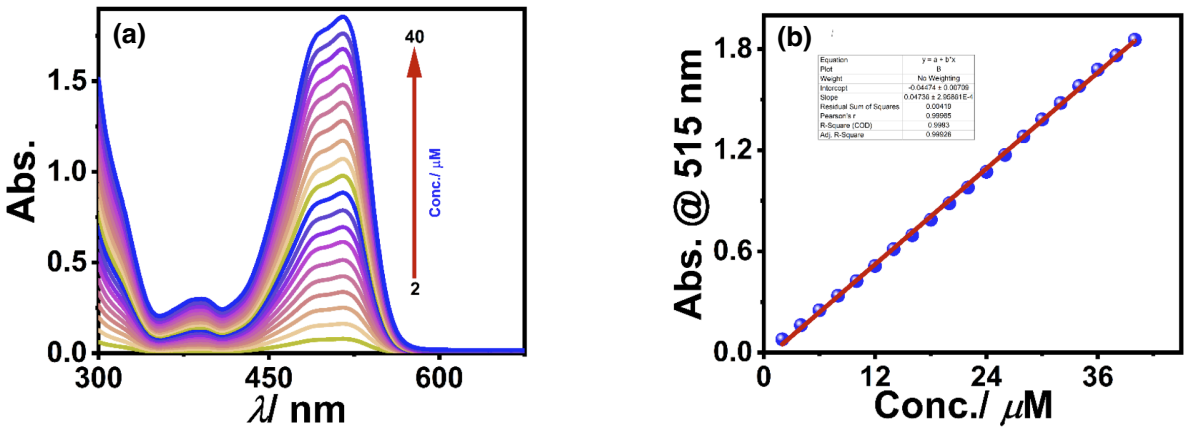


Fig. S20: Concentration-dependent UV-vis. absorption spectra (a) and respective Abs. vs concentration plot (b) for compound **4** in DCM solvent

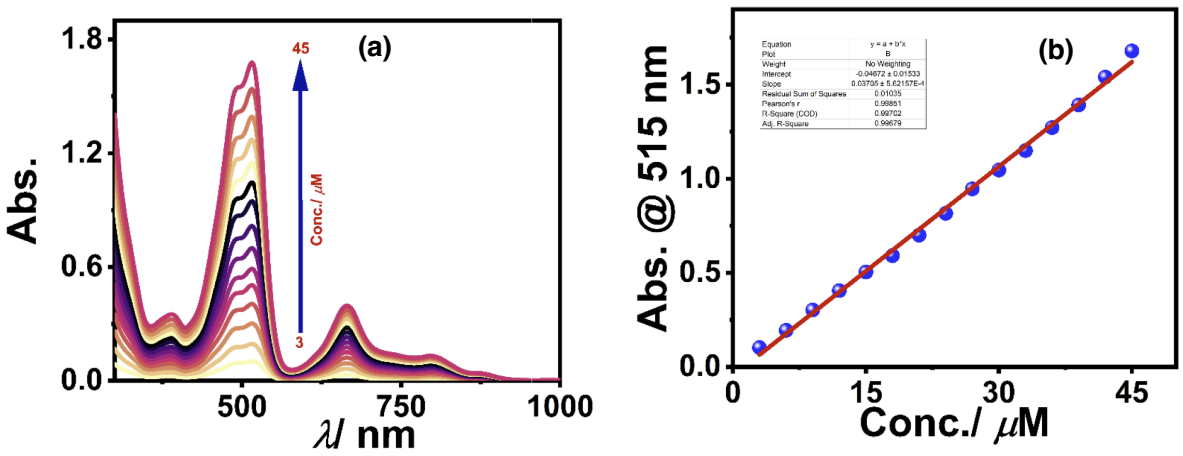


Fig. S21: Concentration-dependent UV-vis. absorption spectra (a) and respective Abs. vs concentration plot (b) for compound **4** in DMF solvent

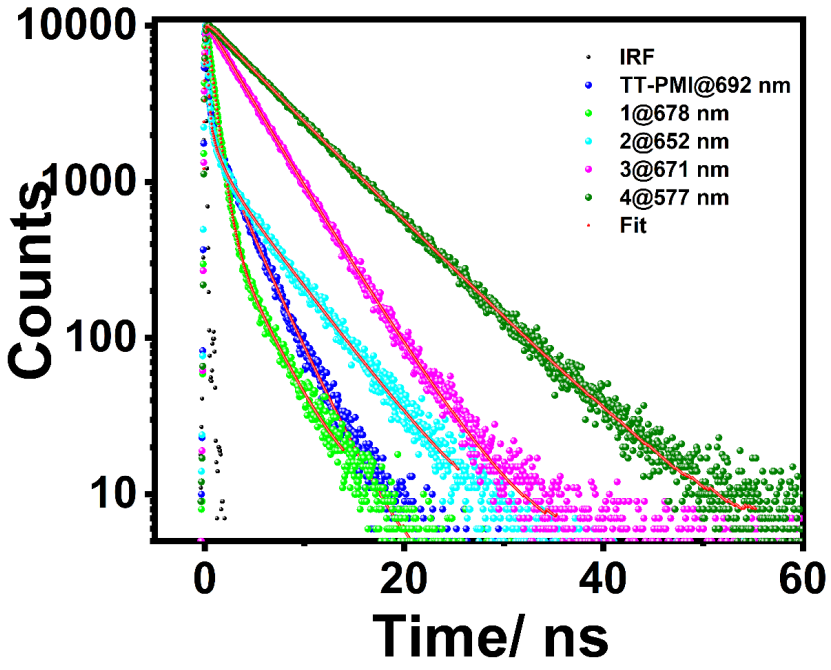


Fig. S22: Fluorescence lifetime plot of **TT-PMI**, **1**, **2**, **3**, and **4** in DCM solvent

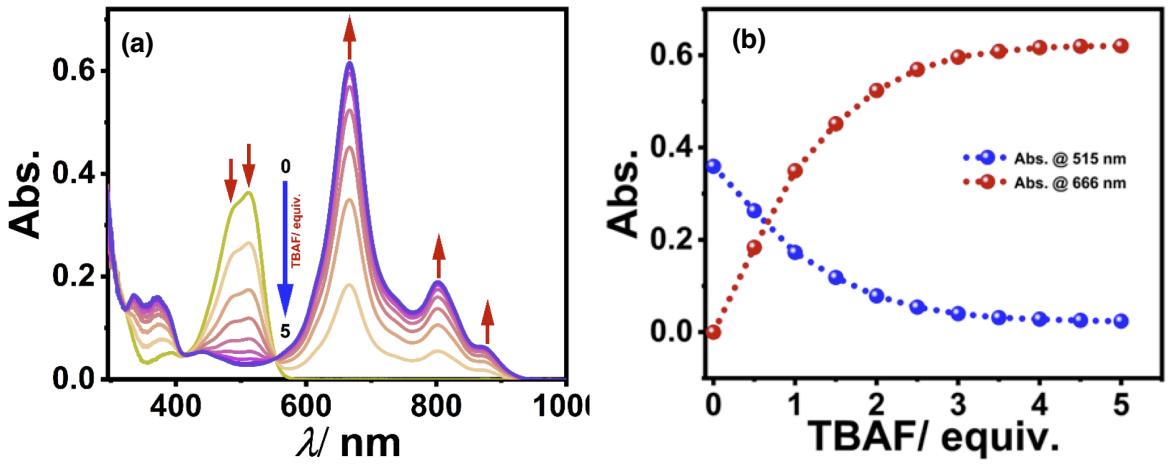


Fig. S23: Radical anion generation monitored using UV-vis.-NIR absorption spectroscopy in THF (20 μM) of **4**.

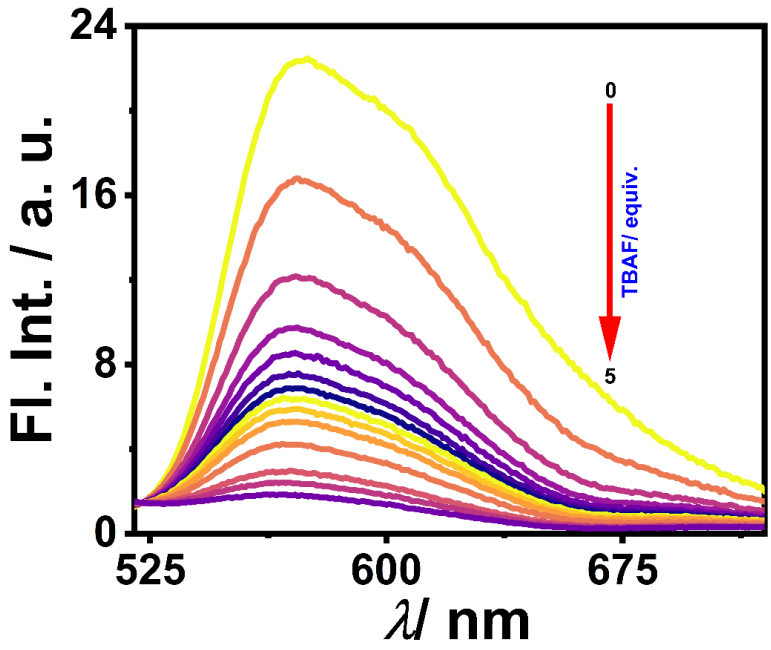


Fig. S24: Radical anion generation monitored using fluorescence spectroscopy in THF of **4**.

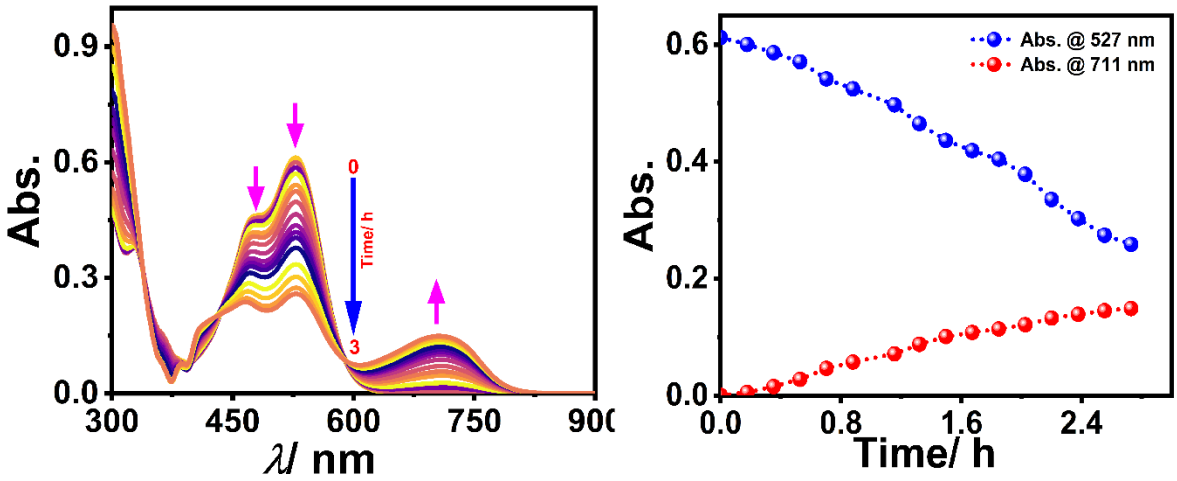


Fig. S25: Radical anion generation monitored using UV-vis.-NIR absorption spectroscopy in THF (20 μM) with 5 equivalents of TBAF of **1.**

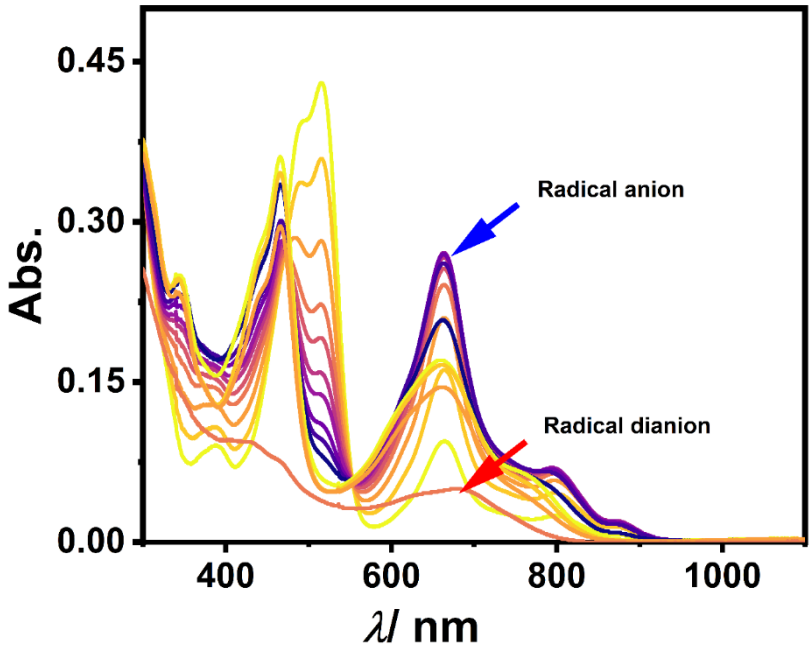


Fig. S26: UV-Vis. NIR absorption spectra in DMF of **4**

Notes: Upon initial visible light exposure, at first radical anions formed but with prolonged irradiation, which subsequently transformed into radical dianions.

IV. Theoretical calculation:

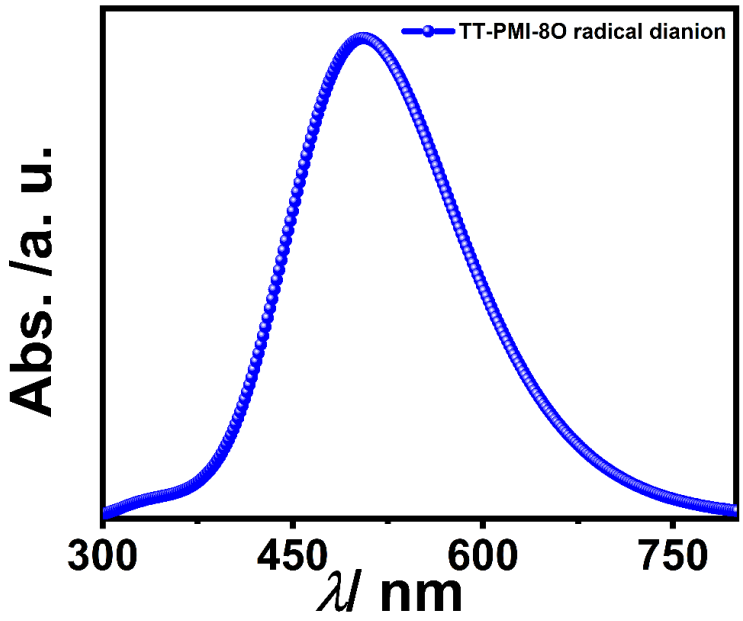


Fig. S27: Calculated absorption spectrum of **TT-PMI-8O (4)** radical dianion.

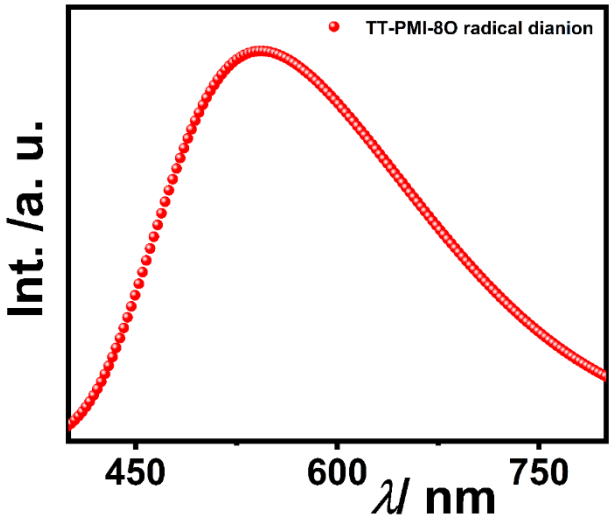


Fig. S28: Calculated emission spectrum of **TT-PMI-8O (4)** radical dianion.

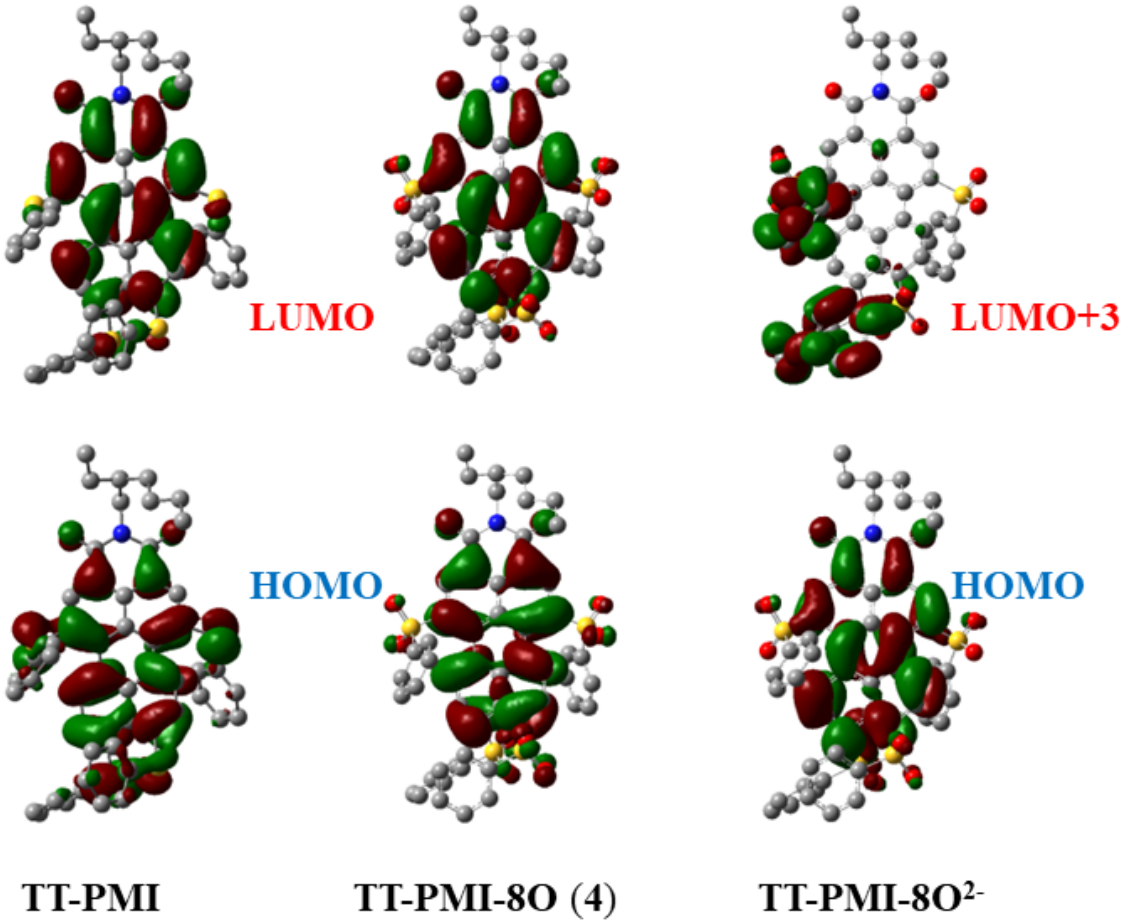


Fig. S29: Energy optimized Kohn-Sham HOMO and LUMO of **TT-PMI**, **TT-PMI-8O** (**4**) and **TT-PMI-8O**$^{2-}$.

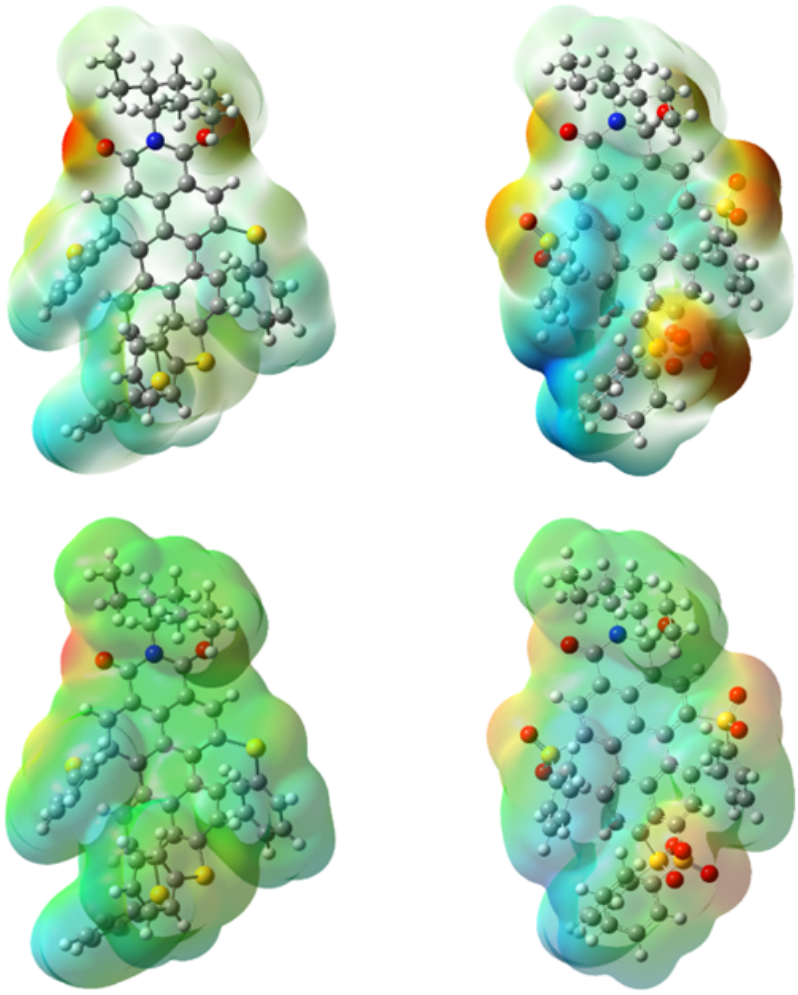


Fig. S30: Calculated electrostatic potential surfaces for **TT-PMI**, **TT-PMI-8O** (**4**). Red and blue surfaces indicate extreme electrophilic and nucleophilic centre respectively.

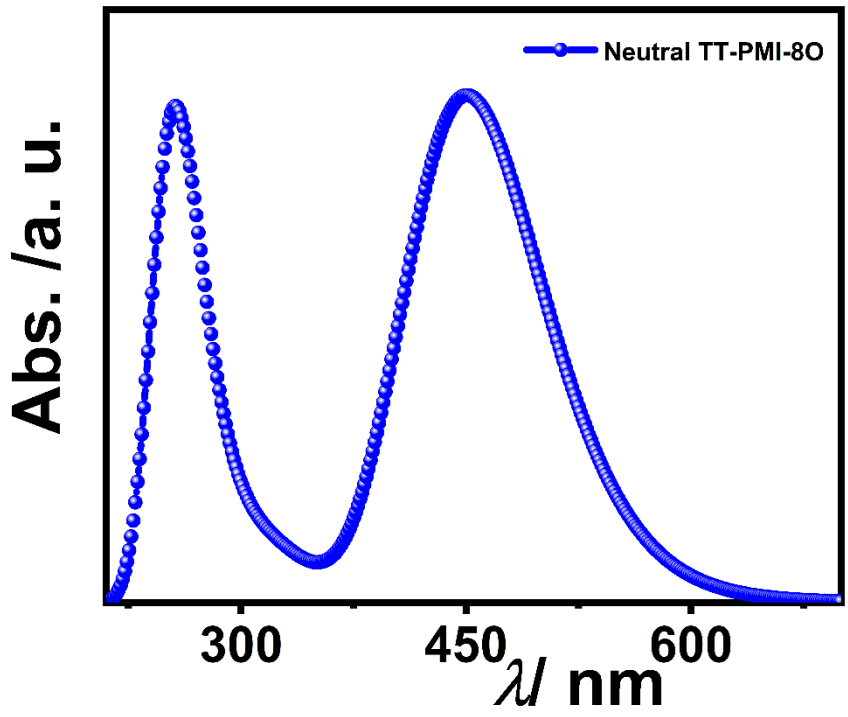


Fig. S31: Calculated absorption spectra of neutral **TT-PMI-8O (4)**.

Coordinates of optimized geometries of some studied systems using B3LYP/6-311+G (d, p) level of theory.

TT-PMI

0 1	(charge, spin multiplicity, respectively)		
C	-1.25629200	1.06994800	-1.38546100
C	-0.92716300	-0.25614500	-1.05893900
C	0.31421200	-0.56452100	-0.45522800
C	1.12981400	0.53637800	-0.01822900
C	0.79368800	1.86431500	-0.41361300
C	-0.40019800	2.11706000	-1.11733100
C	2.28471800	0.31630900	0.80557600
C	3.19001900	1.38776300	0.97141600
C	2.86092600	2.67526500	0.51265500
C	1.66284500	2.93360400	-0.11688700
C	0.85162100	-1.91594600	-0.25070100
C	1.81115800	-2.13787600	0.78361400
C	2.42636000	-1.01386500	1.41918100
C	0.49235500	-3.00198200	-1.03484300
C	1.01898900	-4.27131000	-0.81045300
C	1.82979000	-4.55228700	0.27753400
C	2.17106900	-3.48136800	1.18139900
C	2.84093900	-3.61971600	2.44227700
C	3.25482800	-2.49727600	3.13638400

C	3.11350700	-1.21535100	2.60474500
C	1.33735800	4.32088700	-0.52429300
N	0.09014400	4.52852100	-1.13527400
C	-0.77046000	3.48918900	-1.53183600
S	4.81495200	1.32768200	1.75192600
S	-2.22549700	-1.42993100	-1.49824900
S	2.50282300	-6.20733700	0.46822600
S	3.23215700	-5.17228300	3.24910300
C	-0.24119500	5.90672800	-1.57251400
C	-1.08412400	6.78243800	-0.61498500
C	-0.37833600	7.14639900	0.71612500
C	-0.45997500	6.12846100	1.86368700
C	0.33085000	6.57680300	3.09889800
C	0.24022200	5.59007800	4.26666500
C	-2.53025600	6.27802000	-0.44383000
C	-3.46562400	7.29713500	0.21698100
C	5.67604800	0.01160500	0.88575600
C	-2.71521000	-2.13679500	0.07814800
C	2.03489500	-7.01365000	-1.07453900
C	1.64525100	-5.80342100	3.80253500
C	0.49679100	-5.01994300	3.92916300
C	-0.67777900	-5.59034200	4.41682000
C	-0.71349700	-6.93083900	4.79525000
C	0.43792900	-7.70805800	4.67296400
C	1.61139600	-7.15330000	4.17039800
C	6.60910000	-0.73302600	1.61254800
C	7.37867800	-1.70201600	0.97088000
C	7.20798500	-1.94722900	-0.38944600
C	6.27046600	-1.20719600	-1.11045400
C	5.51265100	-0.22280500	-0.48246200
C	-3.24581400	-3.43036700	0.05982500
C	-3.74598200	-3.99503500	1.23130700
C	-3.70239900	-3.28464900	2.42898900
C	-3.15965600	-1.99992200	2.44698100
C	-2.67422800	-1.42035700	1.27753900
C	0.92517600	-7.86290200	-1.09984700
C	0.62079100	-8.57573700	-2.25921300
C	1.42281200	-8.44518400	-3.39159600
C	2.53528700	-7.60387200	-3.36400800
C	2.84607200	-6.89246300	-2.20728500
O	2.10617600	5.24762000	-0.33075300
O	-1.77473600	3.72092800	-2.18258400
H	-2.20480000	1.28283800	-1.86153700
H	3.55903100	3.49038500	0.65534900
H	-0.19646200	-2.87437500	-1.85526800
H	0.76008700	-5.05854500	-1.50324600

H	3.72268100	-2.62563400	4.10410900
H	3.53397200	-0.37767500	3.13994600
H	-0.77632500	5.80316800	-2.51589200
H	0.71269900	6.39923100	-1.75476900
H	-1.15367600	7.72637400	-1.17619500
H	-0.80481400	8.08978200	1.07705100
H	0.67463200	7.35419200	0.50184000
H	-0.08584100	5.15147300	1.54307800
H	-1.50607800	5.97086400	2.15141500
H	-0.03360500	7.55967800	3.42298300
H	1.38113500	6.71800200	2.81901100
H	0.81481300	5.93787400	5.12992400
H	-0.79648400	5.45347300	4.59138500
H	0.62996000	4.60682000	3.98409700
H	-2.92456700	6.01484100	-1.42891100
H	-4.48951800	6.91482700	0.25464400
H	-3.48526600	8.23663900	-0.34564600
H	-3.16653700	7.53332600	1.24175800
H	0.51224400	-3.97404500	3.65047400
H	-1.56645400	-4.97540700	4.50282900
H	-1.62825400	-7.36650100	5.18018100
H	0.42316900	-8.75374200	4.95977300
H	2.49847500	-7.76714700	4.06006000
H	6.73094900	-0.55756300	2.67539700
H	8.10122400	-2.27419700	1.54184200
H	7.79945300	-2.70835900	-0.88488500
H	6.13557700	-1.38671400	-2.17130100
H	4.80168100	0.36083400	-1.05424200
H	-3.26751500	-3.99243900	-0.86702300
H	-4.15908900	-4.99717700	1.20644400
H	-4.09082100	-3.72584500	3.33968900
H	-3.12609300	-1.43645800	3.37300700
H	-2.27475700	-0.41405000	1.29811700
H	0.30786800	-7.96204500	-0.21481600
H	-0.24059000	-9.23396000	-2.27503500
H	1.18593000	-9.00144400	-4.29144100
H	3.16558400	-7.50665000	-4.24080200
H	3.71464300	-6.24533200	-2.17685500
H	-2.53930200	5.34682100	0.13186800

TT-PMI-2O (1)

0 1

C	-1.16418000	1.08247400	-1.43771900
C	-0.82882600	-0.24161600	-1.10818200
C	0.38936800	-0.53508800	-0.45200100

C	1.17320500	0.57944300	0.00929400
C	0.83857900	1.90424200	-0.39485500
C	-0.33642100	2.14251800	-1.13289000
C	2.31054200	0.37312700	0.85889700
C	3.20628100	1.45028800	1.01537500
C	2.88688100	2.73768500	0.56101600
C	1.69005200	2.98267400	-0.07612200
C	0.93535300	-1.87806300	-0.21567600
C	1.85454900	-2.07574200	0.85792500
C	2.42690700	-0.93669800	1.50636000
C	0.61704800	-2.98286900	-0.99348500
C	1.15547900	-4.23928200	-0.73095100
C	1.92895400	-4.49295500	0.39207500
C	2.21258700	-3.40534800	1.29474000
C	2.81644700	-3.51214000	2.59344600
C	3.16474700	-2.37360000	3.29710900
C	3.03143400	-1.09876800	2.74158300
C	1.35091500	4.36903800	-0.48018900
N	0.11517300	4.56064900	-1.12167800
C	-0.71586100	3.51227200	-1.55057300
S	4.94554600	1.36517400	1.62853700
S	-2.08534600	-1.43026500	-1.61960800
S	2.62434100	-6.13057900	0.63100700
S	3.19018300	-5.04623100	3.44264700
C	-0.22808200	5.93822800	-1.55331100
C	-1.10937300	6.78854300	-0.60772800
C	-0.44296400	7.15057000	0.74407100
C	-0.53463200	6.12024500	1.87981100
C	0.21552000	6.57158900	3.13913500
C	0.11455500	5.57184600	4.29481500
C	-2.55004600	6.25672300	-0.47803600
C	-3.51976000	7.25215200	0.16917500
C	5.66608100	-0.05901100	0.78452900
C	-2.63540000	-2.16716600	-0.07694000
C	2.23287600	-6.96686400	-0.91679000
C	1.58568400	-5.71988500	3.88534000
C	0.41789000	-4.95864500	3.95859500
C	-0.77169400	-5.55842000	4.36800600
C	-0.80318000	-6.90559700	4.72253300
C	0.36765200	-7.65993200	4.65495100
C	1.55729200	-7.07588100	4.22915200
C	6.23095700	-1.07939400	1.54239100
C	6.86048800	-2.13559200	0.88518100
C	6.91347000	-2.16090600	-0.50675300
C	6.34814700	-1.12523700	-1.25287500
C	5.72594400	-0.06056500	-0.60863300

C	-3.14612900	-3.46732700	-0.13871600
C	-3.69320600	-4.05553900	0.99978100
C	-3.71603100	-3.36204300	2.20785700
C	-3.19294000	-2.07058500	2.26955200
C	-2.66105600	-1.46754300	1.13262000
C	1.14339800	-7.84057300	-0.97093200
C	0.89753100	-8.57424300	-2.13114700
C	1.73781000	-8.44015600	-3.23500000
C	2.83012300	-7.57429600	-3.17810100
C	3.08257200	-6.84172100	-2.02043400
O	2.09814100	5.30525000	-0.26018900
O	-1.70491500	3.72951300	-2.22862400
H	-2.09723800	1.28425300	-1.94816100
H	3.58959000	3.54931900	0.69746900
H	-0.04608900	-2.87867100	-1.83820600
H	0.93480800	-5.04102700	-1.42037600
H	3.56817300	-2.47902100	4.29610800
H	3.38635100	-0.24544900	3.29913500
H	-0.73721300	5.83568500	-2.51106500
H	0.72180800	6.44806000	-1.70618000
H	-1.18180200	7.73692200	-1.16096300
H	-0.89485800	8.08260500	1.10337600
H	0.61102700	7.37935900	0.55823600
H	-0.13344800	5.15346700	1.56060400
H	-1.58460600	5.93993200	2.13885000
H	-0.17663800	7.54395800	3.46259700
H	1.26963000	6.73570400	2.88810800
H	0.65844100	5.92341500	5.17606200
H	-0.92741900	5.41016400	4.59015100
H	0.53392400	4.60026600	4.01459400
H	-2.91504100	5.99695800	-1.47533500
H	-4.53724100	6.85138800	0.17740200
H	-3.54223600	8.19687200	-0.38447500
H	-3.25038100	7.48292000	1.20332600
H	0.42989300	-3.90739800	3.70034000
H	-1.67523000	-4.96120400	4.41341600
H	-1.72991800	-7.36388300	5.04785500
H	0.35633200	-8.71012000	4.92475800
H	2.46074600	-7.67148200	4.16022100
H	6.18307800	-1.03588100	2.62251800
H	7.30709800	-2.93640900	1.46273800
H	7.40237100	-2.98533200	-1.01318800
H	6.40086600	-1.14107600	-2.33519600
H	5.30648300	0.76011100	-1.17790600
H	-3.11763000	-4.01566700	-1.07360900
H	-4.09162500	-5.06219000	0.94121700

H	-4.14159700	-3.82123600	3.09265000
H	-3.21178400	-1.51994200	3.20363400
H	-2.27871100	-0.45578800	1.18620100
H	0.49628000	-7.94252200	-0.10782400
H	0.05184500	-9.25152500	-2.16972100
H	1.54641400	-9.01281600	-4.13533800
H	3.48999900	-7.47434400	-4.03250000
H	3.93515700	-6.17516000	-1.96711400
H	-2.55669000	5.31979000	0.08846700
O	5.00502100	1.12652900	3.07747600
O	5.59536500	2.56319900	1.08566500

TT-PMI-2IO (2)

0 1

C	-1.05891000	1.09967500	-1.47473500
C	-0.71292700	-0.22215500	-1.14619800
C	0.50402600	-0.50525600	-0.48390500
C	1.26168600	0.61498800	0.00835200
C	0.91206700	1.94061300	-0.38665200
C	-0.24855200	2.16797500	-1.15187900
C	2.37265100	0.41578900	0.88945600
C	3.22537500	1.51432500	1.13391500
C	2.88807800	2.79950200	0.68663000
C	1.72710400	3.03078500	-0.02251500
C	1.07217200	-1.84131500	-0.26991900
C	1.99309200	-2.04669000	0.79990500
C	2.53079100	-0.91064600	1.48708800
C	0.78721200	-2.92548300	-1.09356400
C	1.36379300	-4.17027100	-0.87694600
C	2.13976100	-4.43435700	0.24345000
C	2.39286600	-3.38107000	1.18708500
C	3.00646500	-3.51210900	2.48242000
C	3.34167400	-2.38637100	3.20784100
C	3.16879400	-1.09374900	2.69955900
C	1.38191000	4.41378800	-0.42744600
N	0.16806800	4.59296100	-1.10943600
C	-0.63576100	3.53476100	-1.56970100
S	4.93174100	1.56390600	1.85489300
S	-1.95717800	-1.42562800	-1.65367500
S	2.94453400	-6.00939300	0.42887400
S	3.36500900	-4.97883500	3.57981200
C	-0.17897400	5.96772600	-1.54734200
C	-1.10459200	6.80290700	-0.63104200
C	-0.49260200	7.16733900	0.74556100
C	-0.61205000	6.13076100	1.87295500
C	0.08132600	6.58828200	3.16225600

C	-0.04865800	5.58232300	4.30962100
C	-2.54263800	6.25372800	-0.55585800
C	-3.54656700	7.23483800	0.06028700
C	5.70161600	0.17989400	0.93822000
C	-2.51973000	-2.13944600	-0.10477500
C	2.03303000	-7.07531100	-0.69513800
C	1.74938200	-5.84213700	3.56800000
C	0.55314300	-5.14916900	3.74652900
C	-0.63124600	-5.86802300	3.89742300
C	-0.61208800	-7.26305400	3.89171200
C	0.59472600	-7.94311700	3.73053100
C	1.78390800	-7.23367800	3.57133200
C	6.39682300	-0.77702300	1.66812400
C	7.08515700	-1.78177800	0.98743800
C	7.08652100	-1.80955100	-0.40512200
C	6.40467500	-0.82723400	-1.12597200
C	5.71403600	0.17930600	-0.45662400
C	-3.06760900	-3.42495300	-0.16229900
C	-3.62421200	-3.99666200	0.97975800
C	-3.62037500	-3.30263700	2.18807500
C	-3.05955400	-2.02706600	2.24557800
C	-2.51774800	-1.43966000	1.10492500
C	0.75130600	-7.53207900	-0.36825600
C	0.09930100	-8.42445000	-1.21472200
C	0.72640500	-8.87992300	-2.37562500
C	2.00895700	-8.43787000	-2.69122900
C	2.66339900	-7.53300200	-1.85489300
O	2.11090000	5.35825900	-0.17559200
O	-1.60661900	3.74452000	-2.27552700
H	-1.98723500	1.29279100	-1.99712000
H	3.54321200	3.63815500	0.89218900
H	0.13739700	-2.80189900	-1.94578400
H	1.19178800	-4.95357000	-1.60182400
H	3.76933500	-2.50185700	4.19697700
H	3.53378200	-0.25384400	3.27649300
H	-0.65251000	5.86226000	-2.52288700
H	0.76871000	6.49095600	-1.66470400
H	-1.16832300	7.75270100	-1.18292100
H	-0.96981600	8.09161500	1.09182500
H	0.56435600	7.41102300	0.59935900
H	-0.18388400	5.17165600	1.56581600
H	-1.66824500	5.93315500	2.09045700
H	-0.33836900	7.55302200	3.47367300
H	1.14170800	6.77042700	2.95300600
H	0.45519000	5.93842000	5.21257400
H	-1.09864200	5.40389800	4.56385500

H	0.39560300	4.61810500	4.04265500
H	-2.86827100	5.99460800	-1.56681300
H	-4.55897700	6.82261300	0.02923600
H	-3.55959100	8.18217700	-0.48915900
H	-3.31796500	7.46308100	1.10477000
H	0.53392300	-4.06550800	3.75451200
H	-1.56731700	-5.33489700	4.01636800
H	-1.53506700	-7.81783500	4.01744700
H	0.61309500	-9.02718500	3.72817600
H	2.73195000	-7.73994200	3.43370700
H	6.38733200	-0.72900500	2.75037200
H	7.61618600	-2.54237800	1.54801300
H	7.62123900	-2.59233000	-0.93060400
H	6.41154000	-0.84373800	-2.20986300
H	5.18823500	0.94464300	-1.01682900
H	-3.06060700	-3.97448100	-1.09692400
H	-4.05340000	-4.99078400	0.92295500
H	-4.05511200	-3.74792900	3.07561500
H	-3.05669800	-1.47557800	3.17934200
H	-2.10615900	-0.43947900	1.15671500
H	0.27480200	-7.19275400	0.54346600
H	-0.89493500	-8.77498200	-0.96119300
H	0.21785400	-9.58101000	-3.02755500
H	2.50218500	-8.79189200	-3.58935900
H	3.65889600	-7.18126900	-2.09818600
H	-2.55880800	5.31401400	0.00575600
O	4.97585200	1.19563100	3.32605000
O	4.39722000	-5.93520300	3.03331000

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C	-1.10500000	1.11999000	-1.55014900
C	-0.80040200	-0.20322000	-1.20084300
C	0.39685300	-0.53088300	-0.52580100
C	1.17666400	0.56796700	-0.02145000
C	0.87540400	1.89866000	-0.42867900
C	-0.26027900	2.15775200	-1.22100300
C	2.26825600	0.33355100	0.87964400
C	3.16012400	1.40258000	1.10309500
C	2.87718000	2.69718600	0.64527800
C	1.72183900	2.96268100	-0.05704900
C	0.94320800	-1.87317900	-0.32331800
C	1.80820700	-2.11121400	0.78691500
C	2.34802700	-0.99436100	1.49714400
C	0.70038600	-2.92955900	-1.18934600
C	1.21986200	-4.19821500	-0.94379100

C	1.90705200	-4.50727900	0.22084500
C	2.15345800	-3.45667700	1.18221100
C	2.72543800	-3.61035600	2.49005400
C	3.03644500	-2.49726600	3.25135300
C	2.90499800	-1.20133600	2.74815700
C	1.42434800	4.35717800	-0.46962600
N	0.23274200	4.56920000	-1.18099200
C	-0.59049900	3.53504000	-1.65983400
S	4.85828100	1.30378700	1.82316300
S	-2.21814200	-1.33011300	-1.56824100
S	2.55079800	-6.16720000	0.44204000
S	3.13540600	-5.17435300	3.27100200
C	-0.06321300	5.95279000	-1.62981200
C	-0.98608900	6.81563400	-0.73685100
C	-0.39270900	7.17331200	0.64965300
C	-0.56006700	6.14715300	1.78051900
C	0.12059900	6.59484300	3.07999300
C	-0.05633200	5.59942400	4.23026700
C	-2.43814800	6.30157800	-0.68760700
C	-3.43032700	7.31001700	-0.09715000
C	5.63132000	-0.10619300	1.00274900
C	-2.57356600	-2.14342000	0.00287800
C	2.16988000	-6.96830600	-1.12739300
C	1.54968900	-5.84975100	3.77767000
C	0.44387500	-5.05770000	4.09325300
C	-0.72058700	-5.65783600	4.56811800
C	-0.78809300	-7.03905600	4.74341800
C	0.31940700	-7.82528900	4.42909100
C	1.48294400	-7.23761100	3.93916400
C	6.18538400	-1.11712900	1.78110600
C	6.86053000	-2.15962800	1.14788400
C	6.96833500	-2.18137800	-0.24097500
C	6.41308500	-1.15521700	-1.00749800
C	5.74639500	-0.10347800	-0.38692500
C	-2.46315100	-3.52681300	0.09679200
C	-2.82913700	-4.15046200	1.28885000
C	-3.29544600	-3.39158300	2.35987500
C	-3.40431900	-2.00435700	2.24876700
C	-3.04837700	-1.37077500	1.06266700
C	1.03044600	-7.77046600	-1.23524500
C	0.78661600	-8.47659000	-2.41240800
C	1.68000500	-8.38844700	-3.47871100
C	2.82278400	-7.59673800	-3.36701500
C	3.07240300	-6.89015400	-2.19246500
O	2.17160300	5.27961800	-0.19864600
O	-1.53297000	3.76893500	-2.39349400

H	-2.02510200	1.33748100	-2.07666300
H	3.57849300	3.50048700	0.83037000
H	0.11950400	-2.78130500	-2.08654500
H	1.05398700	-4.96418000	-1.68695000
H	3.42280400	-2.64162900	4.25219800
H	3.23627900	-0.36955900	3.35108700
H	-0.51626800	5.85821700	-2.61607600
H	0.90186300	6.44783800	-1.72567000
H	-1.01542900	7.76332000	-1.29512800
H	-0.85370200	8.11115800	0.98103000
H	0.67265400	7.39001100	0.52342400
H	-0.15043200	5.17567700	1.48726200
H	-1.62494600	5.97773100	1.97877800
H	-0.28027300	7.57169100	3.37814200
H	1.18894500	6.74841000	2.88982300
H	0.43903900	5.94845800	5.14064700
H	-1.11511700	5.44837800	4.46527400
H	0.36932100	4.62311700	3.97705600
H	-2.75017400	6.04403100	-1.70318700
H	-4.45133200	6.92152300	-0.14610600
H	-3.40999000	8.25380900	-0.65241700
H	-3.21690200	7.53951500	0.95029900
H	0.48986700	-3.98195600	3.97802100
H	-1.57318400	-5.03586000	4.81652800
H	-1.69334500	-7.49819500	5.12350000
H	0.27832000	-8.90121900	4.55698300
H	2.33644600	-7.85386300	3.68063000
H	6.09370200	-1.07716900	2.85862200
H	7.29980000	-2.95264000	1.74161900
H	7.49206600	-2.99546200	-0.72889600
H	6.50812100	-1.16816200	-2.08692200
H	5.33456500	0.70989000	-0.97210000
H	-2.11304200	-4.09765200	-0.75289500
H	-2.74993900	-5.22732100	1.37799900
H	-3.58546200	-3.88176500	3.28213600
H	-3.77859900	-1.41797300	3.07974500
H	-3.15679000	-0.29851600	0.95450400
H	0.34308400	-7.83952900	-0.40041300
H	-0.09908400	-9.09631200	-2.49416400
H	1.48922400	-8.93885900	-4.39284100
H	3.52279300	-7.53250300	-4.19230700
H	3.96242600	-6.27950700	-2.09744500
H	-2.48802800	5.36606100	-0.12086300
O	5.54142800	2.51079500	1.34633100
O	4.82127700	1.03974100	3.26847400
O	-3.34873100	-0.44005200	-1.85301500

O	-1.86561000	-2.35854400	-2.55656700

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C	-1.24454700	1.24651300	-1.40321700
C	-0.93042300	-0.06778300	-1.02234500
C	0.28853900	-0.38045400	-0.39040900
C	1.10495900	0.72488500	0.02816500
C	0.80551600	2.03920200	-0.42677100
C	-0.36977700	2.28218100	-1.16372100
C	2.23037400	0.52047900	0.89519900
C	3.14956400	1.57561000	1.02186300
C	2.87418900	2.84972400	0.50079100
C	1.69119900	3.10273300	-0.15728400
C	0.84018000	-1.72740000	-0.16368100
C	1.75100600	-1.91254100	0.92623100
C	2.31040700	-0.77518600	1.57760500
C	0.56479300	-2.80395300	-0.98845900
C	1.23082600	-4.01983900	-0.78447000
C	1.98664200	-4.24979200	0.34234100
C	2.11608800	-3.23971700	1.35811600
C	2.57191300	-3.34862400	2.71434000
C	2.91153500	-2.20755500	3.41475500
C	2.88808800	-0.94198900	2.82356500
C	1.39537600	4.48132900	-0.62635400
N	0.16322700	4.68476600	-1.27023400
C	-0.70517400	3.64849100	-1.64507000
S	4.86297100	1.48189800	1.71790000
S	-2.34990400	-1.20448600	-1.33849400
S	3.24072600	-5.56794400	0.16121100
S	2.53937600	-4.76174500	3.94384800
C	-0.13841800	6.05367500	-1.76174400
C	-0.98850800	6.97038900	-0.85061800
C	-0.30559000	7.36753900	0.48292700
C	-0.42458700	6.38944100	1.66156900
C	0.33843800	6.87305300	2.90108600
C	0.21288800	5.92527200	4.09733300
C	-2.44516300	6.49135400	-0.69551900
C	-3.37953400	7.54391600	-0.08811200
C	5.56036900	-0.03116200	1.03659600
C	-2.61255300	-2.08227300	0.21596700
C	2.47853900	-6.82148300	-0.89280200
C	1.42267300	-6.08401000	3.42368700
C	0.08510700	-5.80343100	3.15917400
C	-0.79935700	-6.86620000	2.98344700
C	-0.35017700	-8.18114000	3.10505700

C	0.99175200	-8.44133400	3.38370500
C	1.89153400	-7.38948700	3.53796900
C	6.05750600	-0.99657600	1.90724900
C	6.62404200	-2.15321500	1.37435600
C	6.68228000	-2.33111000	-0.00585200
C	6.19915900	-1.34308300	-0.86535700
C	5.64065900	-0.17879800	-0.34816300
C	-2.80851400	-3.45861200	0.16752700
C	-3.15931900	-4.12696700	1.33942000
C	-3.29325000	-3.42417000	2.53524200
C	-3.08856000	-2.04360900	2.56689600
C	-2.76033200	-1.36069900	1.39989400
C	1.50578200	-7.66759700	-0.36389200
C	0.96090000	-8.65456300	-1.18055000
C	1.39237600	-8.79011500	-2.50092300
C	2.37341000	-7.94192800	-3.01170900
C	2.92398400	-6.94584300	-2.20693800
O	2.17669300	5.39705000	-0.45299600
O	-1.68955800	3.86079100	-2.32678300
H	-2.18911200	1.45420000	-1.88902000
H	3.60074500	3.64470300	0.61075800
H	-0.08187400	-2.70025400	-1.84609100
H	1.17262300	-4.77391800	-1.55862500
H	3.19009100	-2.28617700	4.45745200
H	3.26812600	-0.09711800	3.37872500
H	-0.65378300	5.92478000	-2.71288800
H	0.82682900	6.52480500	-1.93968800
H	-1.03206700	7.89598200	-1.44374100
H	-0.72777900	8.32692100	0.80370100
H	0.75405300	7.55739400	0.28527100
H	-0.05049100	5.39873200	1.38456300
H	-1.47885900	6.24910200	1.92735600
H	-0.02857500	7.86760100	3.18355600
H	1.39619900	7.00005200	2.64385900
H	0.76559200	6.29971900	4.96335700
H	-0.83262000	5.80217900	4.39851700
H	0.60821600	4.93260800	3.85891800
H	-2.82273700	6.20276300	-1.68013100
H	-4.40922900	7.17699800	-0.06162600
H	-3.37308700	8.46499000	-0.68047600
H	-3.09949400	7.80819800	0.93507500
H	-0.26982000	-4.78117400	3.11301100
H	-1.84339500	-6.66571900	2.77578900
H	-1.04837100	-9.00273300	2.99054600
H	1.34084200	-9.46265800	3.48165200
H	2.93939400	-7.56360500	3.74240400

H	5.99858000	-0.84067300	2.97646000
H	7.00257800	-2.92007600	2.03941500
H	7.09720100	-3.24437400	-0.41413800
H	6.25638700	-1.48075400	-1.93859200
H	5.27820800	0.60032400	-1.00811800
H	-2.70023300	-3.98536400	-0.77197900
H	-3.33439400	-5.19596500	1.31065200
H	-3.56572300	-3.94751000	3.44468800
H	-3.19877100	-1.49783800	3.49637100
H	-2.63226100	-0.28499900	1.41162600
H	1.18880300	-7.56810100	0.66606000
H	0.20496200	-9.32205600	-0.78380500
H	0.96600000	-9.56258000	-3.13060800
H	2.71281500	-8.05413400	-4.03466500
H	3.69201600	-6.27884000	-2.57742400
H	-2.48055800	5.57968300	-0.09005700
O	3.88292300	-5.29717700	4.14534100
O	1.85369200	-4.14338400	5.09049100
O	3.53362200	-6.15963200	1.46489800
O	4.32431400	-4.95345800	-0.61581900
O	-2.02584900	-2.18908200	-2.38078400
O	-3.50625700	-0.32680100	-1.53978300
O	4.81892600	1.36705600	3.18189800
O	5.56685700	2.61715100	1.11367400

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C	-1.12516000	1.21541400	-1.46991300
C	-0.83082600	-0.08489000	-1.08693200
C	0.38147600	-0.40459900	-0.38605000
C	1.16977400	0.70669400	0.07546500
C	0.87256700	2.03322700	-0.37657000
C	-0.26169300	2.26751100	-1.18196100
C	2.26306700	0.50068000	0.97816500
C	3.17339300	1.58831500	1.16743900
C	2.89583900	2.85288600	0.67377800
C	1.72089700	3.10516900	-0.03065000
C	0.91055100	-1.73090100	-0.14816500
C	1.80492500	-1.92528700	0.95633100
C	2.34752400	-0.79015900	1.62797700
C	0.63300400	-2.82623800	-0.98227300
C	1.26829900	-4.03559600	-0.76465200
C	2.02108600	-4.28381200	0.38149200
C	2.16288600	-3.26428300	1.39139800
C	2.60664600	-3.37503200	2.74602200
C	2.94269200	-2.22781700	3.46761300

C	2.90859900	-0.96957600	2.89891400
C	1.43259500	4.47204300	-0.47920800
N	0.24306900	4.66161800	-1.21047200
C	-0.58753200	3.61486000	-1.65951100
S	4.89007400	1.45487900	1.79650300
S	-2.25267800	-1.19461300	-1.35787500
S	3.26040800	-5.57518900	0.16988100
S	2.57445700	-4.78674600	3.93405100
C	-0.03762200	6.02268800	-1.71396600
C	-0.95752600	6.93420700	-0.86525800
C	-0.36639200	7.34717800	0.50690100
C	-0.54469200	6.36865800	1.67730900
C	0.15645000	6.85188800	2.95269100
C	-0.03510700	5.90777300	4.14346900
C	-2.41305200	6.43291100	-0.79695500
C	-3.40091100	7.47309200	-0.25545600
C	5.54801100	-0.01860900	0.98433400
C	-2.52373600	-2.01142700	0.23653900
C	2.45887200	-6.83866700	-0.86345400
C	1.42747600	-6.08029900	3.38895400
C	0.10339800	-5.76608500	3.09792400
C	-0.80873600	-6.80408500	2.91260500
C	-0.40009500	-8.13105400	3.04650000
C	0.93037300	-8.42681700	3.34478600
C	1.85556700	-7.39869600	3.50993600
C	6.01444000	-1.07452200	1.76022500
C	6.51548700	-2.20928000	1.12418800
C	6.54226700	-2.27643300	-0.26673900
C	6.09193800	-1.19928100	-1.03144600
C	5.59429300	-0.05894600	-0.40843700
C	-2.81017900	-3.37212200	0.23776600
C	-3.15967700	-3.98610700	1.43941600
C	-3.19981000	-3.24653900	2.62013800
C	-2.90030400	-1.88353500	2.60387900
C	-2.57237200	-1.25522700	1.40580800
C	1.42327100	-7.60972800	-0.34160100
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C	1.33512700	-8.83109400	-2.42538200
C	2.37707500	-8.05648900	-2.93212000
C	2.94458500	-7.05062300	-2.15060200
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O	-1.53229900	3.84792600	-2.40478700
H	-2.05683000	1.43471700	-1.97380300
H	3.61052500	3.65542300	0.79850900
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H	1.19424400	-4.79798700	-1.52959500

H	3.22266000	-2.32210200	4.50836300
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H	-0.49003200	5.89449600	-2.69722200
H	0.93106500	6.50898400	-1.82253200
H	-0.97944400	7.85840600	-1.46366500
H	-0.81866200	8.30369800	0.79836100
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H	-0.15527300	5.38136700	1.41541900
H	-1.61131400	6.22806800	1.89072500
H	-0.21679000	7.85093100	3.21437200
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H	0.47722000	6.27923900	5.03609500
H	-1.09566800	5.79233700	4.39192800
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H	-2.72252900	6.12831600	-1.79994100
H	-4.42479000	7.08873200	-0.28760700
H	-3.37409100	8.39120200	-0.85332800
H	-3.18706300	7.74958000	0.78089700
H	-0.21824900	-4.73414700	3.03050800
H	-1.84094900	-6.57288400	2.67849100
H	-1.11882600	-8.93345000	2.91920400
H	1.25125200	-9.45776500	3.44352800
H	2.89710900	-7.59749900	3.72457100
H	5.96707500	-1.00824700	2.83899500
H	6.85509700	-3.05061300	1.71651700
H	6.89255500	-3.17757400	-0.75505400
H	6.11413000	-1.25352700	-2.11385700
H	5.24007000	0.78222300	-0.99224900
H	-2.75841700	-3.92906100	-0.68918600
H	-3.39916200	-5.04340500	1.44886100
H	-3.46235500	-3.72937000	3.55492600
H	-2.92521000	-1.30922000	3.52264900
H	-2.35575900	-0.19408500	1.38183800
H	1.06374000	-7.43722000	0.66400600
H	0.05161500	-9.21254600	-0.73674500
H	0.89230300	-9.60936800	-3.03712700
H	2.74722000	-8.23002000	-3.93624500
H	3.75360900	-6.43254500	-2.51897700
H	-2.46937800	5.52397200	-0.19014200
O	3.90101800	-5.37436200	4.13753600
O	1.90543900	-4.21636000	5.12096900
O	3.59913900	-6.19133700	1.45648500
O	4.35389200	-5.02430900	-0.64938100
O	-1.98620600	-2.24502100	-2.35708700
O	-3.42135000	-0.33189900	-1.59114800
O	4.93772300	1.23646000	3.25234800

O	5.60949700	2.61868200	1.25558900

TT-PMI-8O-radical dianion

-2 1

C	-1.03991700	1.22015700	-1.51801000
C	-0.75564400	-0.07272300	-1.14558000
C	0.44683100	-0.40267700	-0.38791400
C	1.21310400	0.71240900	0.10887100
C	0.91567400	2.05049700	-0.33225200
C	-0.18481700	2.28427500	-1.18739000
C	2.28091500	0.50072700	1.03698300
C	3.18374700	1.61209700	1.27914000
C	2.90470100	2.87237400	0.81051300
C	1.72999700	3.12867400	0.07988000
C	0.95379200	-1.71455900	-0.14149100
C	1.83232100	-1.91930100	0.97644800
C	2.36652000	-0.78549200	1.66135900
C	0.67059900	-2.82748400	-0.98655300
C	1.27412700	-4.02970000	-0.75659900
C	2.02050900	-4.30724000	0.41626800
C	2.18020700	-3.27116500	1.41604700
C	2.61598400	-3.37997400	2.76780700
C	2.95739100	-2.22298500	3.50599900
C	2.91890300	-0.97390400	2.95347300
C	1.44528600	4.48682500	-0.34542100
N	0.29130100	4.67068400	-1.13966400
C	-0.50731500	3.61964000	-1.65017600
S	4.91503100	1.44434800	1.82532000
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S	3.26664700	-5.53105700	0.15111900
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C	0.02770100	6.02833600	-1.64407800
C	-0.93653700	6.93419100	-0.83681000
C	-0.40239500	7.36114100	0.55440800
C	-0.60788300	6.38060900	1.71826400
C	0.06829400	6.85947700	3.00835800
C	-0.15341300	5.91511000	4.19404400
C	-2.38505600	6.40987300	-0.81763700
C	-3.41040400	7.43696100	-0.32126200
C	5.51794800	0.01072200	0.89697200
C	-2.44292600	-1.99533000	0.18124500
C	2.42638500	-6.85559300	-0.79731000
C	1.44997300	-6.07350700	3.34704200
C	0.11879200	-5.75784700	3.09126400
C	-0.79929800	-6.79245200	2.91610900
C	-0.38788900	-8.12237300	3.01735400

C	0.95123600	-8.42125300	3.26873300
C	1.87984900	-7.39387700	3.42682400
C	5.88881800	-1.14504200	1.57522700
C	6.29543300	-2.25926800	0.84215300
C	6.32958800	-2.20599100	-0.54928700
C	5.98207000	-1.02951200	-1.21513900
C	5.57182500	0.08782300	-0.49357400
C	-2.76986400	-3.34641200	0.17275600
C	-3.11071600	-3.96792200	1.37306500
C	-3.09885500	-3.24516400	2.56535000
C	-2.75273900	-1.89338100	2.56036400
C	-2.43276800	-1.25837700	1.36286600
C	1.28646600	-7.47432400	-0.29233600
C	0.71403600	-8.53092200	-0.99699700
C	1.28212100	-8.96604700	-2.19526200
C	2.42527600	-8.34059100	-2.69085500
C	3.00015900	-7.27830100	-1.99287500
O	2.14104200	5.46365200	-0.04358700
O	-1.42461400	3.87680700	-2.43751300
H	-1.96548400	1.45240700	-2.02653500
H	3.61619000	3.67694100	0.93653800
H	0.07413800	-2.69695600	-1.87433100
H	1.18256300	-4.80042700	-1.51326400
H	3.24561300	-2.33043300	4.54343500
H	3.24248100	-0.12387800	3.53325300
H	-0.38261500	5.90548700	-2.64691600
H	0.99634700	6.52496200	-1.70244300
H	-0.95143800	7.85716100	-1.43956400
H	-0.87557500	8.31446400	0.82826800
H	0.66873600	7.56172400	0.45750500
H	-0.21159700	5.39643700	1.45925000
H	-1.67947400	6.24068600	1.90916300
H	-0.30278600	7.86221700	3.26371900
H	1.14302300	6.96441200	2.82302200
H	0.34402400	6.28089600	5.09827400
H	-1.21997600	5.80578700	4.42059100
H	0.24250600	4.91841900	3.97932900
H	-2.65033400	6.08754600	-1.82740500
H	-4.42636500	7.03379500	-0.38409000
H	-3.37937800	8.35061700	-0.92730200
H	-3.23686400	7.72789400	0.71919600
H	-0.19860100	-4.72375800	3.03981100
H	-1.83659800	-6.55647400	2.70816600
H	-1.10980000	-8.92336300	2.89350900
H	1.27686600	-9.45417500	3.33207700
H	2.92866800	-7.59042000	3.60551800

H	5.82284100	-1.17493100	2.65426300
H	6.53966100	-3.18119700	1.35642400
H	6.58870100	-3.09438100	-1.11249000
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H	-3.37223600	-5.02057600	1.37507200
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H	-2.16742200	-0.20826600	1.34717900
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H	-0.17853900	-9.01072500	-0.61010700
H	0.83075300	-9.78682500	-2.74327000
H	2.86563500	-8.67133900	-3.62577500
H	3.87959100	-6.76355200	-2.35946800
H	-2.44627100	5.50479700	-0.20635400
O	3.91663500	-5.40790800	4.12960400
O	1.93550200	-4.27060900	5.13626200
O	3.72576800	-6.12647400	1.41815600
O	4.32530300	-5.05054600	-0.76869700
O	-1.95628700	-2.21616100	-2.42210000
O	-3.36538400	-0.30936100	-1.62672500
O	5.05573500	1.14094500	3.26294200
O	5.64360300	2.62812600	1.32633700

V. Band gap Energy Calculation:

To determine the LUMO and HOMO energy levels of the molecules, and the potential difference can be used to estimate the energy gap of the molecules.[4] E_{LUMO} =-(E_{red}^{onset}+4.4) eV, E_{HOMO}= E_{LUMO}-E_g(optical) eV, where E_{LUMO} is the LUMO energy level, E_{HOMO} is the HOMO energy level, and all electrode potential values are vs. SCE as the reference electrode.

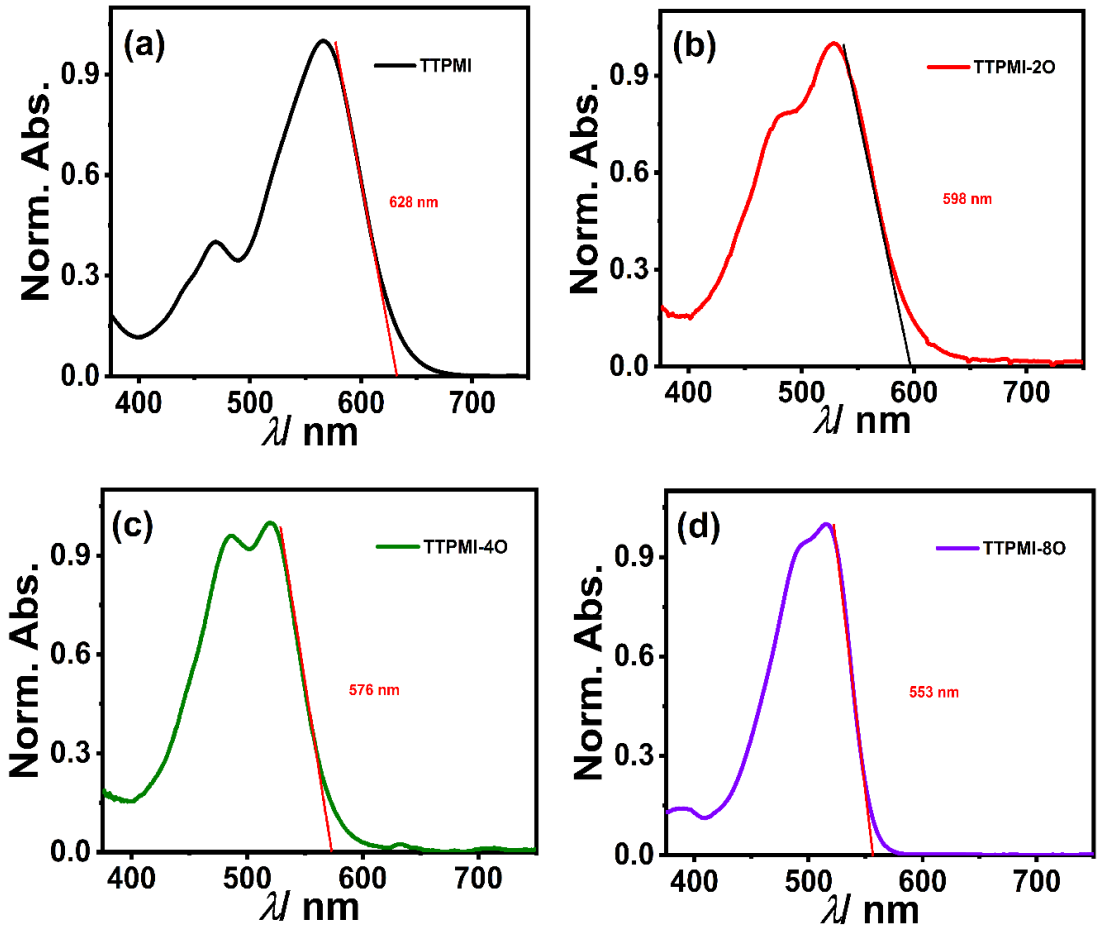


Fig. S32: Onset determination of λ_{onset} absorption for (a) **TT-PMI**, (b) **TT-PMI-2O**, (c) **TT-PMI-4O**, (d) **TT-PMI-8O**.

Additionally, we calculated the optical gap energy, E_g, using the equation: E_g = 1242/λ_{onset} of the absorption spectra. Subsequently, we derived the HOMO energy level from these calculations.

TT-PMI: E_{LUMO} = -(E_{red}^{onset}+4.4) eV, where E_{red}^{onset} = -0.73 V, E_{LUMO}= -3.65 eV; E_{HOMO}= E_{LUMO}-E_g(optical) eV, where E_g= 1242/628= 1.98; E_{HOMO}= (-3.65-1.98) eV= -5.63 eV

TT-PMI-2O: E_{LUMO} = -(E_{red}^{onset}+4.4) eV, where E_{red}^{onset} = -0.66 V, E_{LUMO}= -3.72 eV; E_{HOMO}= E_{LUMO}-E_g(optical) eV, where E_g= 1242/598= 2.07; E_{HOMO}= (-3.72-2.07) eV= -5.79 eV

TT-PMI-4O: E_{LUMO} = -(E_{red}^{onset}+4.4) eV, where E_{red}^{onset} = -0.55 V, E_{LUMO}= -3.83 eV; E_{HOMO}= E_{LUMO}-E_g(optical) eV, where E_g= 1242/577= 2.19; E_{HOMO}= (-3.83-2.19) eV= -6.02 eV

TT-PMI-8O: E_{LUMO} = -(E_{red}^{onset}+4.4) eV, where E_{red}^{onset} = -0.045 V, E_{LUMO}= -4.33 eV; E_{HOMO}= E_{LUMO}-E_g(optical) eV, where E_g= 1242/553= 2.24; E_{HOMO}= (-4.33-2.24) eV= -6.57 eV

Table S1. Calculated HOMO and LUMO energy levels of the molecules.

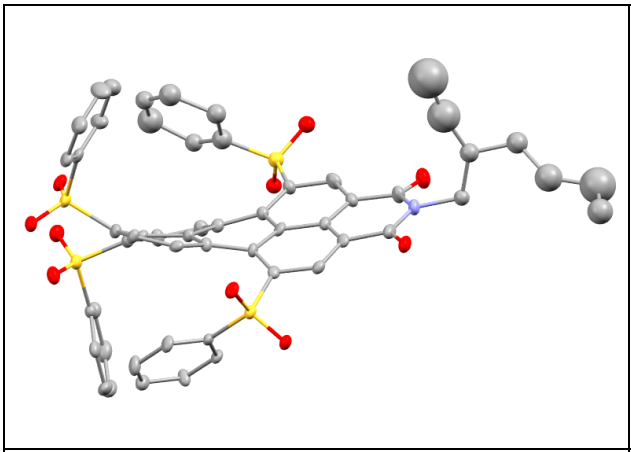
Compound	Energy Level/eV		Band Gap/eV
	HOMO	LUMO	
TT-PMI	-5.66	-3.65	2.01
1	-5.84	-3.72	2.12
3	-6.02	-3.83	2.19
4	-6.57	-4.33	2.24

VI. Single-crystal X-ray diffraction studies:

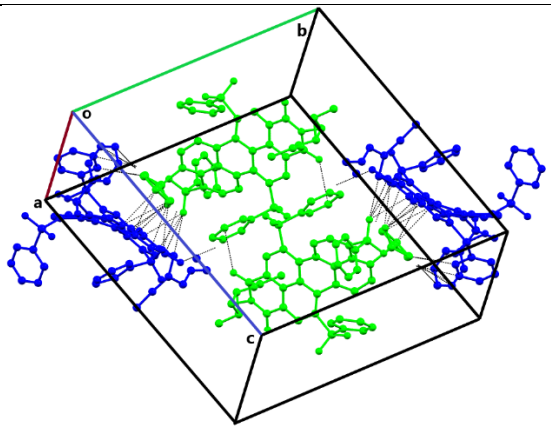
Table S2: Crystallographic parameters for **TT-PMI-8O**	
Identification code	TT-PMI-8O
Empirical formula	$C_{54}H_{25.73}NO_{9.96}S_4$
Formula weight	976.05
Temperature/K	140.0
Crystal system	triclinic
Space group	P-1
a/Å	14.270(5)
b/Å	18.590(6)
c/Å	19.695(7)
α/°	76.026(13)
β/°	83.735(15)
γ/°	89.836(13)
Volume/Å^3	5038(3)
Z	4
ρ_{calc}g/cm^3	1.287
μ/mm^{-1}	0.247
F(000)	2002.0
Crystal size/mm^3	0.18 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.48 to 50.06
Index ranges	-16 ≤ h ≤ 16

	$-22 \leq k \leq 22$ $-23 \leq l \leq 23$
Reflections collected	86383
Independent reflections	17775 $R_{int} = 0.2271$ $R_{sigma} = 0.1906$
Data/restraints/parameters	17775/46/1213
Goodness-of-fit on F^2	1.177
Final R indexes [I>=2σ (I)]	$R_1 = 0.1402$ $wR_2 = 0.3498$
Final R indexes [all data]	$R_1 = 0.2508$ $wR_2 = 0.4244$
Largest diff. peak/hole / e $Å^{-3}$	1.64/-0.60

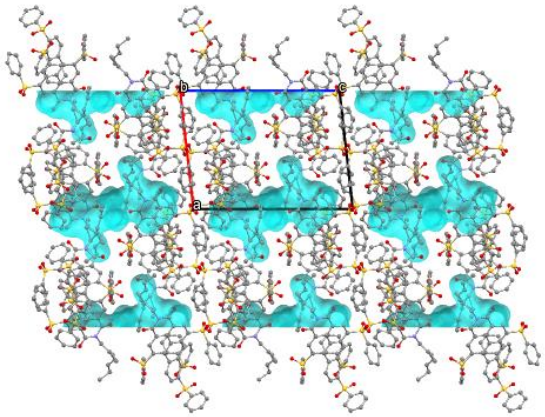
Table S3: Intermolecular interaction geometry for selected interactions in **TT-PMI-8O**.		
1	C94─H94···O1	3.20(1)
2	O9···C92 (O···π)	4.16(2)
3	C5─H5···O6	3.40(2)
4	C6─H6···O6	3.39(2)
5	C9─H9···O5	3.40(1)
6	C8─H8···O5	3.29(1)
7	C36─H36···O5	3.35(1)
11	C64─H64···C40	3.70(2)
12	O6···C63 (O···π)	3.35(1)
13	C93─H96···O6	3.58(1)
15	C5─H5···C63 (C─H···π)	3.96(2)
16	C4···C69 (π···π)	3.36(2)
17	C3···C69 (π···π)	3.52(2)
18	O18A···C3 (O···π)	3.25(2)
19	O2···C88 (O···π)	3.03(1)
20	C80···O2 (O···π)	3.11(1)
21	O4···C81 (O···π)	3.32(1)
22	O4···C82 (O···π)	3.09(1)



(a)



(b)



(c)

Fig. S33: **(a)** Structure of TT-PMI-8O (only the ordered part of one of the molecules forming the asymmetric unit is shown for clarity to confirm and establish the structural connectivity; Thermal ellipsoid probability set at 30%) **(b)** The crystal packing of TT-PMI-8O sustained by $\pi\cdots\pi$, O$\cdots\pi$, and C—H$\cdots\pi$ interactions. **(c)** The voids in the crystal structure (shown in turquoise) along the crystallographic *c* axis occupied by the solvent of crystallization (could not be modelled due to poor data quality; treated with SQUEEZE routine of PLATON).

VII. References:

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