## Monopyridyl-linked unsymmetrical anthracenyl $\pi$ -conjugate as a platform for acid-pen base-eraser platform

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## Information on the experiments performed:

Solid state Fluorescence: For a solid-state emission, **AT2P** is placed in a quartz grooved plate and both absorption and emission spectra were recorded. The same sample was exposed to acid vapours and neutralized back to **AT2P** and both absorption and emission spectrum were recorded.  $\lambda ex = 405$  nm.

**DLS studies**: An aggregate solution of AT2P ( $10^{-5}$  M) at  $f_w$  90% was prepared and subjected to average particle size determination.

**AIE-studies:** Preparation of AT2P ( $10^{-5}$  M)  $f_w$  20% in MeCN: Take 1580 µL of acetonitrile solvent in a quartz cuvette, 20 µL of **AT2P** ( $10^{-3}$  M) was added and the solution was made homogenous and then injected 400 µL of water to make a solution of 20%  $f_w$ . Similarly, other fractions from 0-99% were made.

Pristine sample: Pure AT2P crystals were crushed and spread over the glass slide.

**Acidified sample in solid crystalline state (drop method)**: 2 μL of HCl (6M) was added to the pure **AT2P** solid.

**Neutralized sample in solid crystalline state**: 2  $\mu$ L of Triethylamine (TEA) or ammonia (NH<sub>3</sub>) was added to the acidified **AT2P** sample.

**AT2P on filter paper (solid state)**: AT2P (10<sup>-3</sup> M) in MeCN was dropped on the filter paper and dried (evaporate MeCN).

Acidified sample on filter paper (via vaporization): The AT2P absorbed on filter paper was kept in a chamber containing HCl gas.

**Neutralized sample on filter paper (via vaporization)**: The acidified **AT2P** sample absorbed on filter paper was placed in a chamber containing vapor of triethylamine (TEA) or ammonia ( $NH_3$ ).

Acid-base titration studies using <sup>1</sup>H NMR: 5 mg pure AT2P was dissolved in CDCl<sub>3</sub> (0.5 mL) and the spectrum was recorded. 0.5 equivalent of methane sulfonic acid (MSA) was added, homogenized and recorded. 0.75 equivalent: More 0.25 equiv. of MSA was added to the above 0.5 equiv. solution, and is homogenized and recorded. 1 equiv.: More 0.25 equiv. of MSA was added to the 0.75 equiv. solution, and is homogenized and recorded. In a manner similar to the addition of MSA, TEA was added gradually in different portions.

**Formation of AT2P.HCl crystals:** 5 μL of conc. HCl (12 M) was added to 20 mg **AT2P**, dissolved in toluene and acetonitrile (9:1) mixture in a 5mL glass vial and allowed it for slow evaporation.

**Density Functional Theory (DFT)-studies**: The DFT calculations were performed using GAUSSIAN 09 software with the basis set B3LYP-6-31G(d,p).

Synthesis of AT2P:



Scheme S1: Synthesis of AT2P

(E)-2-(2-(10-(p-tolyl)anthracen-9-yl)vinyl)pyridine: ((10-(aryl)anthracen-9-yl)methyl)phosphonate (0.3 g, 0.716 mmol) was taken in a 25 mL round bottomed flask and was dissolved in dry THF under inert atmosphere. Potassium tert-butoxide (0.321 g, 2.867 mmol), was added to the above solution under nitrogen atmosphere. The solution was allowed to stir for 2-3 minutes. Then pyridine-2-carboxaldehyde (0.076 g, 0.716 mmol) was added and the reaction was allowed to stir for 2-3 hours. Completion of the reaction was monitored by TLC. The reaction mixture was quenched with water, washed with brine and extracted with ethyl acetate (20 mL x 2). The resulting organic layer was dried over anhydrous sodium sulphate and concentrated. And the resulting compound was purified by column chromatography using fractions of ethyl acetate in hexane (25/75: EtOAc/Hexane). The product was obtained as crystals with yield of 78% (0.207 g); mp. 192-196 °C; IR (v cm<sup>-1</sup>, in KBr): 3564, 2923, 2851, 1731, 1583, 1508, 1464, 1431, 1386, 1262, 1021, 972, 812, 762; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.79 (d, J = 4.8 Hz, 1H), 8.63 (d, J = 16.3 Hz, 1H), 8.49 (d, J = 8.8 Hz, 2H), 7.77 (dd, J = 8.3, 2.6 Hz, 3H), 7.54 – 7.46 (m, 3H), 7.44 (d, J = 7.7 Hz, 2H), 7.41 – 7.35 (m, 4H), 7.29 (ddd, J = 7.5, 4.7, 1.0 Hz, 1H), 7.11 (d, J = 16.3 Hz, 1H), 2.57 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 155.39, 149.92, 137.43, 137.10, 136.74, 136.67, 135.95, 132.21, 131.18, 130.19, 129.89, 129.39, 129.12, 127.44, 126.12, 125.27, 125.05, 122.50, 122.45, 77.31, 77.05, 76.80, 21.42; ESI-MS: 372 [MH]<sup>+</sup>; X-ray structure is determined for this sample.



**Figure S1**. Absorption spectra of **AT2P** in MeCN ( $10^{-5}$  M) with acidified spectra using HCl (A) and neutralized spectra using TEA (B).



**Figure S2**. AT2P (10-5 M) in MeCN. On addition of acid (HCI) the fluorescence quenched. And on addition of base (TEA or NH<sub>3</sub>) to the acidic solution, the fluorescence was regained. In visible light, on addition of acid, the color got changed to bright yellow and on addition of base the color was restored to pale greenish yellow. Under UV 365 nm light, on addition of acid, the fluorescence was quenched and on further base addition, the fluorescence was restored.



**Fig S3.** Acid-base reversible (a) emission spectra and (b) fluorescence intensity point spectra of compound **AT2P** aggregates.  $\lambda_{ex}$  = 405 nm. Temp 25 °C.



Fig S4. Emission spectra of AT2P in solid state before and after fuming with acid (A) and base (B)



Fig S5: The crystal packing diagram with supramolecular interactions. The distances are given in Å.

N-	NCl-	=C-HCl	ClHAnth	ClC py	ClHpy	СН	НН
HCl-							
2.147	2.965	2.779	2.675	3.435	2.649	2.898,	2.293
						2.865,	
						2.872, 2.732	

 Table S2: Crystal data for the compounds

Compound	AT2P	AT2P HCI
Emp. Formula	$C_{28}H_{21}N$	C <sub>28</sub> H <sub>22</sub> NCI
Formula weight	371.49	407.91
Crystal system	monoclinic	triclinic
Space group	P 21/c	P -1
a /Å	24.1517(6)	6.0496(4)
b/Å	9.13490(17)	7.4880(4)
c/Å	19.4787(5)	23.2847(9)
α/deg	90	88.896(4)
$\beta$ /deg	112.160(3)	88.491(4)

∕∕/deg	90	81.556(5)
V/Å <sup>3</sup>	3980(17)	1042.86(10)
Ζ	8	2
$D_{calc} / g \text{ cm}^{-3}$ ]	1.240	1.299
$\mu$ /mm <sup>-1</sup>	0.544	0.198
F(000)	1568	428.44
Data/ restraints/ parameters	7720/0/690	5317/0/272
S	1.052	1.080
R1 [I>2σ(I)]	0.0608	0.0385
wR2 [all data]	0.1694	0.1327
Max./min. residual electron dens. [eÅ-3]	0.7133/-0.3266	0.471/-0.287



**Fig S6:** (a) HOMO (Highest Occupied Molecular Orbital) of **AT2P** (b) LUMO (Lowest Unoccupied Molecular Orbital) of **AT2P** (c) HOMO of **AT2P.HCI** (d) LUMO of **AT2P.HCI** 

 Table S3: The energy values of HOMO and LUMO obtained from DFT-studies

Molecules	HOMO (ev)	LUMO (ev)	Gap (in ev)
AT2P	-5.2515	-2.1077	3.1438
AT2P. HCI	-5.5492	-2.8507	2.6985







Fig S9. <sup>1</sup>H NMR spectra of AT2P by progressive addition of acid (MSA)



**Fig S10**. <sup>1</sup>H-NMR titration spectra of **AT2P** after the addition of acid (MSA) and base (TEA) (reversible nature)

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