Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Examination of Aggregation Induced Enhanced Emission in a Propeller Shaped Chiral- Nonconjugated Blue Emitter from Restricted Intramolecular Rotation and *J Type* $\pi \cdots \pi$ Stacking Interactions

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1. Thermogravimetric Analysis

According to thermogravimetric analysis (Figure S1), thermal decomposition onset and offset temperature of the molecule was measured approximately at 200 °C and 305 °C, respectively. Maximum degredation temperature and maximum degradation rate of the molecule were at 300°C and approximately 2.5%/°C, respectively. The molecule has single and clear degradation step like pure organic samples. According to DTG thermogram, at 98°C weight change could be melting point of the molecule. Weight loss of samples at 600ºC, under nitrogen atmosphere were measured as %98.7 that residue of sample does not contain any inorganic impurities like catalyst.

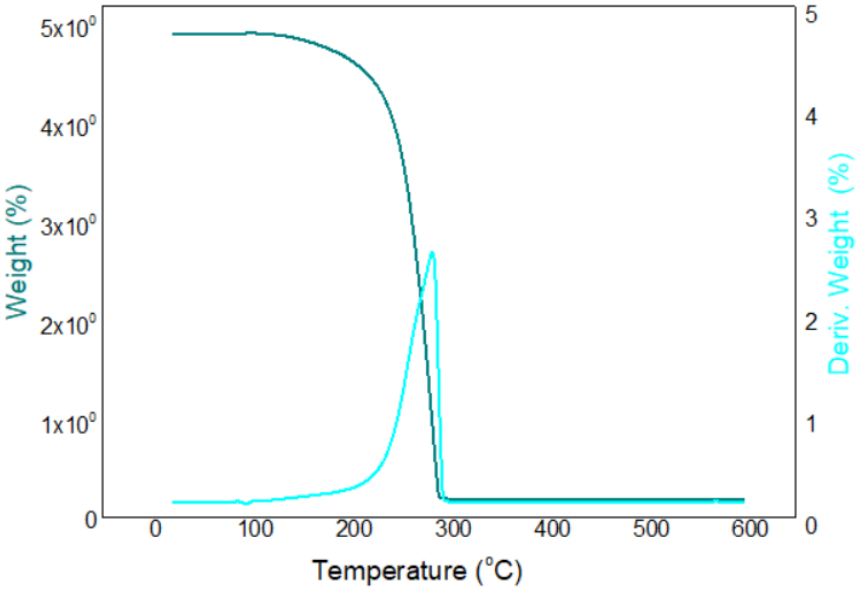

Figure S1. TGA (green) and DTG (blue) curves of the molecule.

3.6 Electrochemical Studies of the Molecule

To understand the electrochemical properties of the molecule, the cyclic voltammetry (CV) analysis (Figure S2) was performed in tetrabuthylamonium hexaflourophosphate supporting electrolit at room temperature. In this study, counter, reference and working electrode are platinum wire, silver wire and glassy-carbon electrodes, respectively. The onset oxidation (E_{ox}^{onset}), reduction (E_{red}^{onset}), HOMO, LUMO and E_{gap} values of the molecule were calculated from the CV curves and are given in Table S5. The HOMO and LUMO energy level of the molecule were estimated as -6.0 eV and -1.90 eV, respectively. The LUMO energy level of the molecule was determined by using its optical band gap (E_g^{opt}). One of the most common approaches used in the determination of the optical band gap of semiconductors in literature is the wavelength corresponding to the maximum absorption band edge[58,59]. The optical band gap of the molecule is 4.1 eV. All results was obtained from the given equations. These results show that the theoretical results are good agreement with the experimental electrochemical studies.

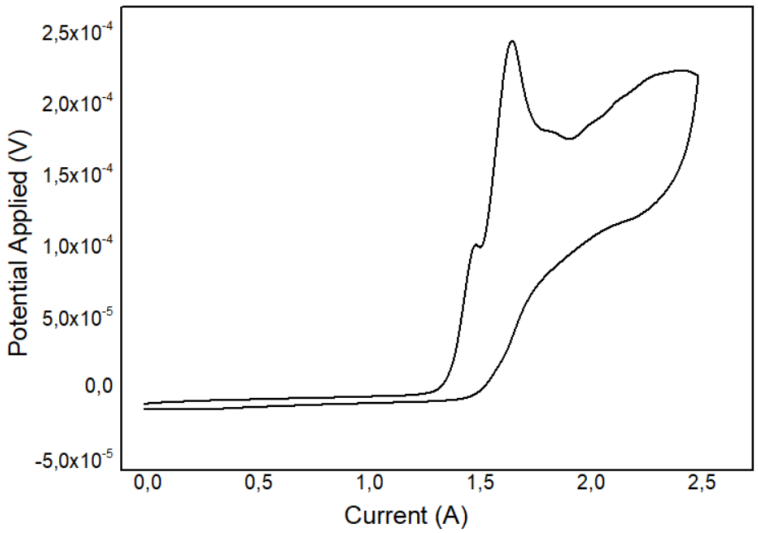

Figure S2. Cyclic voltammograms of the compound: working electrode, glassy carbon; auxiliary electrode, Pt wire; reference electrode, Ag wire.

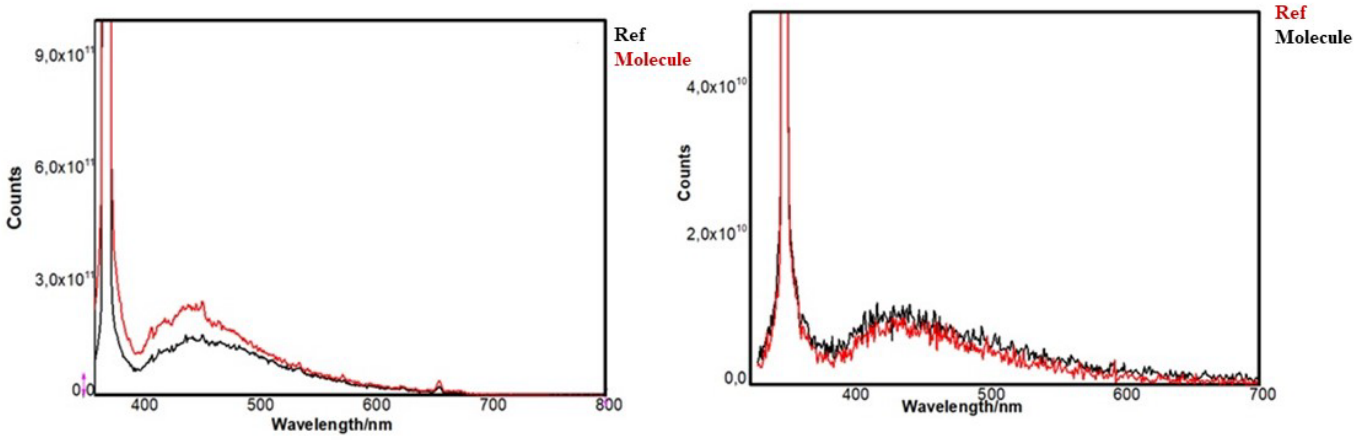

Figure S3. Solution (left) and solid phase (right) PLQY results of the molecule.

Table S1. Crystallographic details for the compound.

Crystal Data	
Empirical Formula	$C_{22}H_{20}O_2S$
Formula Weight (g/mol)	348.47
Cell setting / Space group	monoclinic/ $P2_1/c$
Unit cell dimensions (Å, °)	a= 18.7765(12)
	b= 5.7331(4)
	c= 17.6642(10)
	β=107.791(7)
Unit cell volume ($Å^3$)	1810.6(2)
Temperature (K)	298 (2)
Absorption coefficient (mm^{-1})	0.191
Z / Density [g/cm^3]	4/ 1.2783
F(000)	736.8
Crystal size (mm^3)	0.512 × 0.283 × 0.218
2θ range (°)	6.48-52.74
h range	$\mathbf{-23 \rightarrow 18}$
k range	$\mathbf{-3 \rightarrow 7}$
l range	$\mathbf{-22 \rightarrow 18}$
Reflections collected / unique	6146/3674
Data / restrains / parameters	3674/0/227
Goodness-of-fit on F^2	1.034
Final R indices [I > 2σ(I)]	R_1 = 0.0416
	wR_2 = 0.0861
R indicesall data	R_1 = 0.0588
wR_2 = 0.0962	
Large diff. peak and hole	0.35/-0.40

Table S2. Selected interatomic distances (Å), angles and torsion angles (°) for the compound.

Parameter	Experimental	Theoretical
Bond length (Å)		
S1-C8	1.8417(18)	1.874
S1-C17	1.7801(17)	1.796
O1-C1	1.430(2)	1.419
O1-C2	1.373(2)	1.363
O2-C10	1.217(2)	1.215
C5-C8	1.512(2)	1.513
Bond Angle (^{0})		
C17-S1-C8	100.88(8)	101.878
C2-O1-C1	117.22(16)	118.485
C9-C10-O2	121.34(17)	120.912
O2-C10-C11	120.22(17)	120.424
S1-C8-C5	106.87(11)	107.307
S1-C8-C9	110.65(12)	111.469
C5-C8-C9	114.36(14)	113.925
O1-C2-C7	114.95(16)	115.862
Torsion Angle (^{0})		
S1-C8-C5-C4	74.50(18)	63.215
C8-S1-C17-C18	103.29(15)	116.291
C1-O1-C2-C3	-1.7(3)	-0.856
O2-C10-C11-C16	-161.21(18)	-175.612

Table S3. Detailed interactions geometry of the compound. (Å , °)*.

Rings i-j		R_c^a	R1v^b	R2v^c	α^d	β^e	γ^f	Symmetry
Molecule	Cg1…Cg3	4.7688 (11)	-1.8445(7)	4.4133(8)	50.19(9)	22.3	67.2	x, 3/2-y,1/2+z
	Cg2…Cg2	4.1175(12)	3.4422(8)	3.4422(8)	0.03(10)	33.3	33.3	1-x,-1-y,1-z
	Cg3…Cg1	4.6210(10)	2.1719(8)	-4.4506(7)	50.19(9)	15.6	62	x.1/2-y, -1/2+z
	Cg3…Cg2	4.9930(12)	1.4286(8)	4.7652(8)	76.69(9)	17.4	73.4	1-x,1-y,1-z
	C-H…π interactions							
Molecule	**X-H…Cg**	**H…Cg**	**X-H…Cg**	**X…Cg**				
	C1-H1A…Cg1	2.922(9)	131.7(7)	3.632(2)				
	C21-H21…Cg1^{ii}	2.953(2)	129.31(19)	3.614(2)				

Cg1 is the centoid of (C2/C7); Cg2 is the centrois of (C11-C16); Cg3 is the centroid of (C17-C22)

[a] Centroid distance between ring i and ring j; [b] Vertical distance from ring centroid i to ring j; [c] Vertical distance from ring centroid j to ring i; [d] Dihedral angle between the first ring mean plane and the second ring mean plane of the partner molecule; [e] Angle between centroids of first ring and second ring mean planes; [f] Angle between the centroid of the first ring and the normal to the second ring mean plane of the partner molecule; [g] Distance between centroid of ring i and perpendicular projection of centroid of ring j on ring i.

Table S4. Crystallographic stacking data of the compound.

Stacking parameters	Cg1···Cg3	Cg2···Cg2	Cg3···Cg1	Cg3···Cg2
Pitch angle (P:°)	50.19	0.03	50.19	76.69
Roll angle (R:°)	67.2	33.3	62	73.4
Pitch distance(d_p: Å)	5.71	0.02	5.54	21.05
Roll distance (d_r: Å)	11.3	2.70	8.68	16.7
Slipping angle (β: °)	22.3	33.3	15.6	17.4
Interplanar distance ($d_{\pi\pi}$: Å)	4.76	4.11	4.62	4.99

Table S5. Electronic properties of the compound.

Cyclic Voltammeter		**Absorption**		**Theoretical Calculations**		
$\boldsymbol{E_{ox}^{onset}}$**(V)**	**HOMO (eV)**	**LUMO (eV)**	**Optical Band gap (eV)**	**HOMO (eV)**	**LUMO (eV)**	**ΔE (eV)**
1.65	-6.0	-1.90	4.1	-5.97	-1.76	4.15

$$I_p = -e(E_{1/2(ox,dye)} + 4.4)\ eV \quad (1)$$

$$E_a = -e(E_{1/2(red,dye)} + 4.4)\ eV \quad (2)$$

$$E_g = I_p - E_a \quad (3)$$

$$E_g^{opt} = \frac{1241}{\lambda(nm)} \quad (4)$$