TpOx-2-An

TpOx-2-An is a UV excitable fluorescent material with a polycyclic aromatic donor-acceptor structure where the triphenoxazole core acts as a donor and the aromatic group on the two position of the oxazole (2-anthracene) act as the acceptor group. The push-pull, donor-acceptor, structure facilitates intramolecular charge transfer in the excited state that results in a 264 nm emission Stokes Shift. TpOx-2-An is also a photo-conducting Discotic Liquid Crystalline (DLC) material with mesophase transition onset temperature of 162°C. TpOx-2-An is designed for 355 nm and 405 nm excitation with emission at 536 nm with quantum yield of 0.51, high thermal, chemical and photostability. TpOx-2-An has potential uses in fluorescent dye staining, organic electronics and photonics, and imaging applications.

Chemical Structure

Chemical Data

Catalogue Number: 922994

• Other Name: TpOx-2-An, CT 536 11

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CAS #: 2377209-32-8

• Molecular Formula: C₅₈H₆₉NO₆

Molecular Weight: 876.19

Absorbance and Emission spectra in Ethyl Acetate

Photophysical Data

In Solvent: EtOAc

• Abs λmax (nm) = 272

Emis λ max (nm) = 536

pSS (nm) = 264

 ϵ (M⁻¹ cm⁻¹) at Abs λ max = 105,000

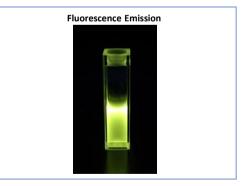
Quantum Yield (Φ) = 0.51

• Fluorescence Lifetime (ns) = 6.54

 Band Gap (Optical, Solution state) = 2.8 eV

HOMO_{CV} = -5.50 eV

• LUMO = -2.55 eV



Wavelength (nm)

Material Data

· Physical State: Solid

Appearance (Colour): Pale yellow

Polymorph crystalline phase: Solid,
Discotic Liquid Crystal, Isotropic

 Solubility: DCM, THF > 1 mg /mL, MeCN, DMSO < 1 mg /mL, Insoluble in aqueous solvents

Polarising Optical Microscope Picture



Phase Transition Data

Phase transition temperature:

Heating Crys - Col_h – 162°C, Col_h - Iso – 172°C

 Cooling Iso - Col_h – 87°C, Col_h - Crys – 151°C