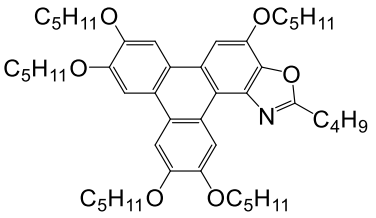
TpOx-*n*-Bu

TpOx-*n*-Bu is a UV excitable fluorescent material with a polycyclic aromatic donor-acceptor structure where the triphenoxazole core acts as a donor and the butyl group on the two position of the oxazole as the acceptor group. TpOx-*n*-Bu is also a photo-conducting Discotic Liquid Crystalline (DLC) material with mesophase transition onset temperature of 90°C. TpOx-*n*-Bu is designed for 355 nm excitation with emission at 366 nm with quantum yield of 0.16, high thermal, chemical and photostability. TpOx-*n*-Bu has potential uses in fluorescent dye staining, organic electronics and photonic applications.

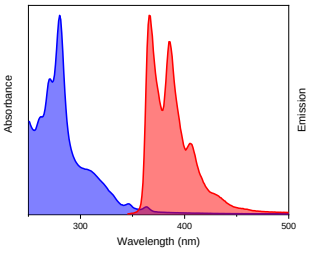
Chemical Structure



Chemical Data

- Catalogue Number: 922978
- Other Name: TpOx-*n*-Bu, CT 366 11 002 01 01
- CAS #: 2377209-24-8
- Molecular Formula: $C_{48}H_{69}NO_6$
- Molecular Weight: 756.08

Absorbance and Emission spectra in Ethyl Acetate



Photophysical Data

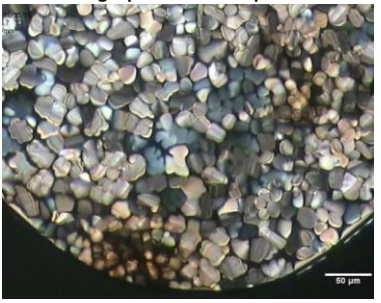
- In Solvent: EtOAc
- Abs λmax (nm) = 280
- Emis λmax (nm) = 366
- pSS (nm) = 86
- ϵ (M^{-1} cm^{-1}) at Abs λmax = 140,000
- Quantum Yield (Φ) = 0.16
- Fluorescence Lifetime (ns) = 5.8
- Band Gap (Optical, Solution state) = 3.43 eV
- $HOMO_{CV}$ = -5.45 eV
- LUMO = -2 eV
- Thermal degradation onset = ~380°C

Fluorescence Emission

Material Data

- Physical State: Crystal Powder
- Appearance (Colour): Pale yellow
- Polymorph crystalline phase: Solid, Discotic Liquid Crystal, Isotropic
- Solubility: THF > 1 mg /mL, MeCN < 0.37 mg / mL, DMSO < 0.03 mg / mL, DCM > 1 mg /mL

Polarising Optical Microscope Picture



Phase Transition Data

Phase transition temperature:

- Heating Crys - Col_h – 90°C, Col_h - Iso – 141°C
- Cooling Iso - Col_h – 137°C, Col_h - Crys – 61°C