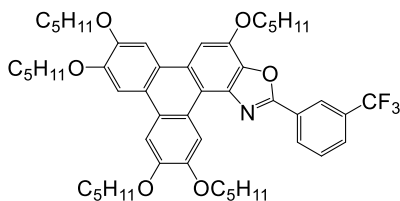


TpOx-Ph-*m*-CF₃

TpOx-Ph-*m*-CF₃ 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 (3-trifluoromethyl-phenyl) act as the acceptor group. The push-pull, donor-acceptor, structure facilitates intramolecular charge transfer in the excited state that results in a 232 nm emission Stokes Shift. TpOx-Ph-*m*-CF₃ is also a photo-conducting Discotic Liquid Crystalline (DLC) material with mesophase transition onset temperature of 132°C. TpOx-Ph-*m*-CF₃ is designed for 355 nm and 405 nm excitation with emission at 503 nm with quantum yield of 0.48, high thermal, chemical and photostability. TpOx-Ph-*m*-CF₃ has potential uses in fluorescent dye staining, organic electronics and photonics, and imaging applications.

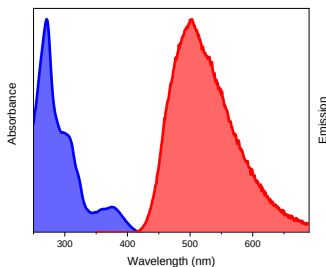
Chemical Structure



Chemical Data

- Catalogue Number: 922854
- Other Name: TpOxPh-*m*-CF₃, CT 503 11 055 01 01
- CAS #: 2612025-76-8
- Molecular Formula: C₅₁H₆₄F₃NO₆
- Molecular Weight: 844.07

Absorbance and Emission spectra in Ethyl Acetate



Photophysical Data

- In Solvent: EtOAc
- Abs λ_{max} (nm) = 271
- Emis λ_{max} (nm) = 503
- pSS (nm) = 232
- ε (M⁻¹ cm⁻¹) at Abs λ_{max} = 73,000
- Quantum Yield (Φ) = 0.48
- Fluorescence Lifetime (ns) = 7.07
- Band Gap (Optical, Solution state) = 2.94 eV
- HOMO_{CV} = -5.47 eV
- LUMO = -2.52 eV

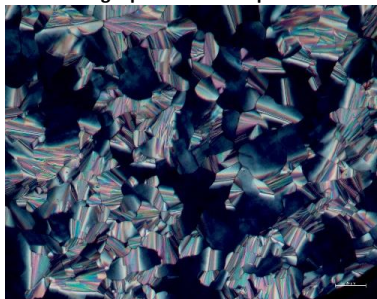
Fluorescence Emission



Material Data

- Physical State: Crystal Powder
- Appearance (Colour): Pale yellow
- Polymorph crystalline phase: Solid, Discotic Liquid Crystal, Isotropic
- Solubility: THF > 1 mg/mL, MeCN < 0.4 mg/mL, DMSO < 0.27 mg/mL, DCM > 1 mg/mL

Polarising Optical Microscope Picture



Phase Transition Data

Phase transition temperature:

- Heating Crys - Col_h – 132°C, Col_h - Iso – 243°C
- Cooling Iso - Col_h – 238°C, Col_h - Crys – <22°C