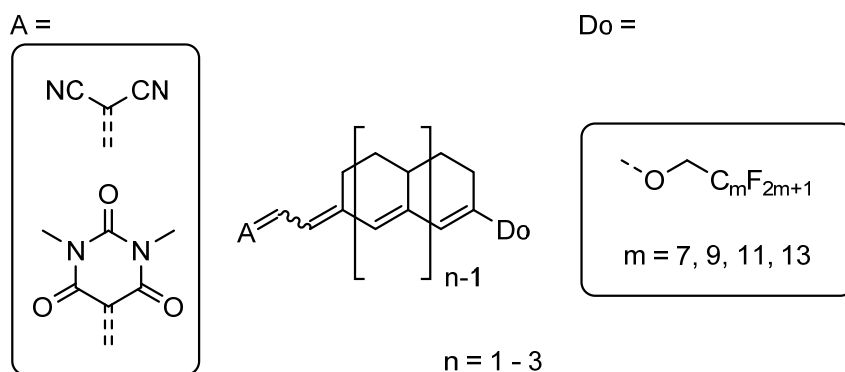


FLUOROPHOBIC EFFECT LEADS TO NOVEL LIQUID CRYSTALLINE DONOR ACCEPTOR DYES

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Liquid crystalline and linear optical properties were combined in a single molecule by exploiting the fluorophobic effect. A series of merocyanines with 1*H*,1*H*-perfluorinated alkyl chains of different lengths was successfully synthesized in 5 steps with overall yields of 1.4 - 6.6% [1]. Malononitrile (mal) and *N,N*-dimethylbarbiturate (barb) acceptors were combined with mono-, bi-, and tricyclic chromophores. UV/Vis and fluorescence spectroscopy, cyclic voltammetry and DFT calculations were performed to determine absorbance and emission maxima, Stokes shifts, and LUMO energies. The perfluorinated chain did not affect the electronic properties of the chromophore and therefore, dye properties were mainly regulated by acceptor strength and chromophore size. A larger conjugated system induced a bathochromic shift of the absorption and emission maxima. In contrast to the barbiturate based derivatives, malononitriles showed a hypsochromic shift of about $\lambda = 30$ nm. In comparison with alkoxy substituted donors, perfluorinated alkoxy chains induced a self-assembly of partially interdigitated SmA bilayers pursuant to differential scanning calorimetry, polarization microscopy, X-ray diffraction experiments (WAXS, SAXS) and density profile calculations. Variation of the chain length identified the most stable mesophases for derivatives with C₁₂ chains. Phase widths increased with larger chromophores. While the merocyanines with only one cyclohexene unit only formed small mesophases of 4 K (mal) and 12 K (barb), the phase widths increased to 112 K (mal) and 91 K (barb) for the tricyclic derivatives.



[1] J. C. Haenle, Y. Stöckl, R. Forschner, E. Haenle, S. Laschat, *ChemPhysChem* **2018**, *19*, 2758–2767.