

# PHOTOPHYSICAL PROPERTIES OF PYRIMIDINE-BASED TADF EMITTERS

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Organic light emitting diodes (OLEDs) are devices of great potential and interest. However, 75% of electrically injected charge in the OLED ends up in non-emissive triplet states. Triplets can be harvested through the mechanism of thermally activated delayed fluorescence (TADF), where thermal energy is exploited to upconvert triplets to emissive singlet state. As a result, it is possible to achieve up to 100% internal efficiency, without the use of any heavy metals as it is usual in efficient phosphorescent devices [1]. To achieve efficient TADF, the energy gap between the lowest singlet and triplet states ( $\Delta E_{ST}$ ) should be minimized, this is usually reached by spatially separating the HOMO and LUMO states in charge transfer compounds, composed of electron donor and acceptor [2].

In this work, photophysical properties of new pyrimidine-based emitters were investigated - a pyrimidine acceptor with a tert-butyl carbazole donor attached to it at different places (fig. 1). Standard photophysical properties analysis was conducted - absorption, emission, time-resolved fluorescence experiments - in air or vacuum and in room temperature as well as 50K. The obtained data revealed that attaching donor at different positions leads to emission wavelength shift from 483 nm in compound CP2 to 437 nm in compound CP6. Moreover, the molecule with donors at the *ortho* and *meta* positions (CP2) shows the smallest  $\Delta E_{ST}$  gap (135meV) while for the other compounds it was above 250meV. This may be the result of sterically crowding of donor units leading to larger twist angles and in turn larger separation of HOMO – LUMO orbitals [3]. The reduced  $\Delta E_{ST}$  led to CP2 having the largest amount of delayed emission – 68% compared to 58% and 20% for compounds CP4 and CP6, respectively. The origin of delayed fluorescence was attributed to TADF emission due to being quenched in low temperature of 50 K (fig 1. decay kinetic).

In conclusion, carefully selecting the point of attachments for donor units can lead to superior TADF emission properties.

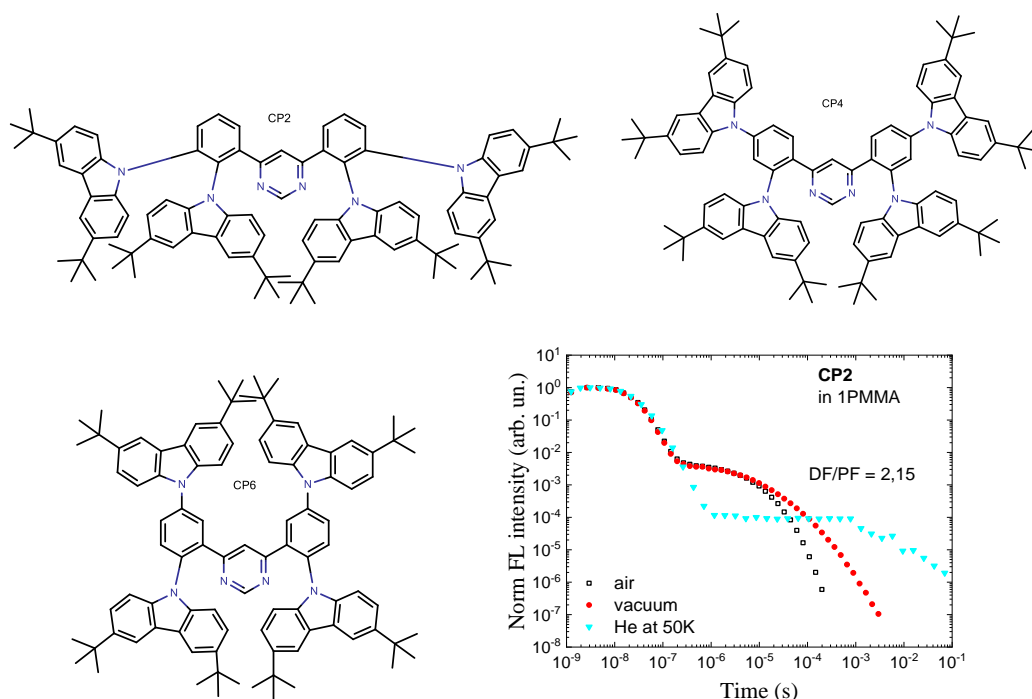


Fig. 1 Pyrimidine – carbazole TADF compounds analyzed in this work and the decay kinetics of compound CP2 in 1 wt% PMMA films at room temperature in air and vacuum ambient and at 50 K temperature.

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[2] F. B. Dias et al., Photophysics of thermally activated delayed fluorescence molecules, *Methods and Applications in Fluorescence* **5**, 012001 (2017).

[3] T. Serevičius, R. Skaisgiris, J. Dodonova, L. Jagintavičius, J. Bucevičius, K. Kazlauskas, S. Juršėnas, S. Tumkevičius, Emission wavelength dependence on the rISC rate in TADF compounds with large conformational disorder, *Chemical Communications* **55**, 1975-1978 (2019).