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Blue thermally activated delayed fluorescence materials based on bi/tri-carbazole derivatives

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Three blue thermally activated delayed fluorescence materials (Cy-2Cz, Cy-3Cz and Sf-3Cz) based on bi/tri-carbazole derivatives have been designed and prepared. In Cy-2Cz, one bi-carbazole unit and one cyano group were covalently linked to the 2,2'-positions of one biphenyl motif. The molecular structure of Cy-2Cz is highly twisted due to the steric hindrance, which could efficiently break the π -conjugation within the molecule, thus leading to high triplet energy. The introduction of an additional carbazole unit into Cy-2Cz finished the synthesis of Cy-3Cz. The preparation of Sf-3Cz was accomplished by the replacement of the electron-withdrawing biphenylcarbonitrile group in Cy-3Cz with phenylsulfonylbenzene. Due to the incorporation of big rigid π -system, Cy-3Cz and Sf-3Cz exhibited excellent thermal stability with the glass transition temperature over 180°C. These three carbazole derivatives showed small singlet-triplet energy gaps $(\Delta E_{\rm ST}s)$ in the range of 0.16-0.31 eV. Therefore, thermally activated delayed fluorescence behavior was observed in these compounds with their photoluminescence quantum yields up to 97.2%. These blue TADF materials were applied in typical OLEDs as dopants and demonstrated high device efficiency. The blue OLED device based on Cy-2Cz at the doping level of 8 wt% achieved a maximum efficiency of 11.8 cd/A and external quantum efficiency (EQE) of 11.9% with the Commission Internationale de l'Eclairage (CIE) of (0.16, 0.10). An efficient blue fluorescent OLED based on Sf-3Cz was achieved with current efficiency of 19.2 cd/A and EQE of 15.8% with the CIE of (0.16, 0.14).

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