Achieving very fast reverse intersystem crossing by heavy atom effect

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For thermally activated delayed fluorescence (TADF) emitters, acceleration of reverse intersystem crossing (RISC) is of vital importance to boost the performance of organic light-emitting diodes (OLEDs). However, up to now, there are only few TADF molecules possessing rate constant of RISC ($k_{\text{RISC}}$) exceeding $10^7 \text{s}^{-1}$.\(^1\)

In this study, we designed a novel TADF molecule, namely, MCz-TXO (Figure 1, left), using sulfur to enhance spin-orbit coupling (SOC) by heavy atom effect.\(^2\) Our theoretical computation indicated that MCz-TXO possessed a several times larger SOC matrix element values than that of the reference molecule (MCz-XT\(^3\), Figure 1, right, the difference is only sulfur and oxygen atom), demonstrating the importance of the heavy atom effect by sulfur in MCz-TXO. Besides, MCz-TXO achieved a good energy level matching of the three states: charge-transfer (CT) type singlet ($^{1}\text{CT}$), CT-type triplet ($^{3}\text{CT}$) and locally excited type triplet ($^{3}\text{LE}$) states. Owing to the large SOC and good energy level matching, MCz-TXO exhibited an extremely large experimental $k_{\text{RISC}}$ of $\sim 2 \times 10^8 \text{s}^{-1}$, two orders of magnitude larger than that of MCz-XT ($\sim 2 \times 10^6 \text{s}^{-1}$). The $k_{\text{RISC}}$ value of $\sim 2 \times 10^8 \text{s}^{-1}$ is one of the largest values among all reported pure organic materials. A MCz-TXO based OLED achieved a maximum external quantum efficiency of 17.4%, showing blue emission with CIE coordinate of (0.15, 0.21) (the emission peak wavelength at 469 nm).

![Figure 1. The molecular structure of MCz-TXO and MCz-XT.](image)

References