A STUDY OF INFLUENCING FACTORS OF TADF EMISSION IN ORGANIC MOLECULES

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Organic materials exhibiting thermally activated delayed fluorescence (TADF) are now recognized as next-generation materials for organic light-emitting diodes. TADF is generally known to originate from reverse intersystem crossing (RISC) from the lowest excited triplet state (T_1) to the lowest excited singlet state (S_1). However, the details of TADF emission mechanisms are not fully understood.

Here we study excited-state dynamics of 2,3-di(9*H*-carbazole-9- yl)benzonitrile (2CzBN) in toluene by means of transient spectroscopies. Previously, we found that the 2CzBN system is TADF non-emissive system at room temperature; however, it becomes TADF emissive when the solution is frozen. To understand this phenomenon, we here determined the temperature dependent lifetime of T_1 of the system.

By decreasing temperature, we found that a lifetime of T_1 increases according to Arrhenius law. Especially, we observed that the lifetime suddenly increased when the sample was frozen, and TADF was observed at that temperature. However, further decreasing the temperature resulted in no TADF emission, and near liquid nitrogen temperature only phosphorescence was observed.

In general, the lifetime of T_1 is determined by the following competitive processes; RISC, radiative decay to ground state (S_0), and nonradiative decay to S_0 . Our results indicated that when the solution is frozen, the nonradiative decay of T 1 to S_0 is strongly suppressed because of suppression of molecular collisions to surrounding solvent molecules. In that condition, while RISC also be weakened, molecules can still vibrate effectively to promote thermal activation of T_1 to S_1 for subsequent TADF emission. Further decreasing of the temperature switches off the RISC due to further suppression of the thermal vibration and only the radiative decay path is left for phosphorescence emission. Consequently, we can propose that not only RISC but also suppression of the nonradiative decay from T_1 to S_0 are key factors for the TADF activation and emission efficiency.

Keywords: *Organic light-emitting diodes, TADF, Reverse intersystem crossing, Nonradiative decay*