

Supporting Information

A novel biomass-based reusable AIE material: The AIE properties and potential applications in amine/ammonia vapors sensing and information storage

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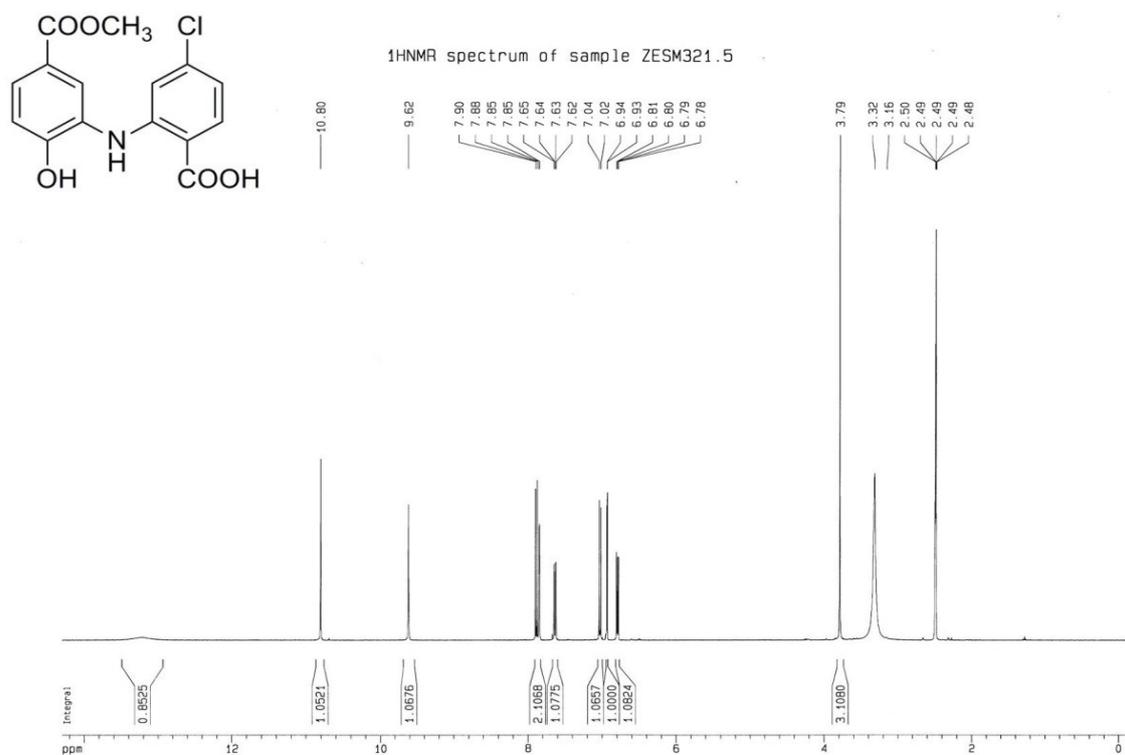


Fig. S1 ¹H NMR of CHMPBA in DMSO-*d*₆ (400 MHz)

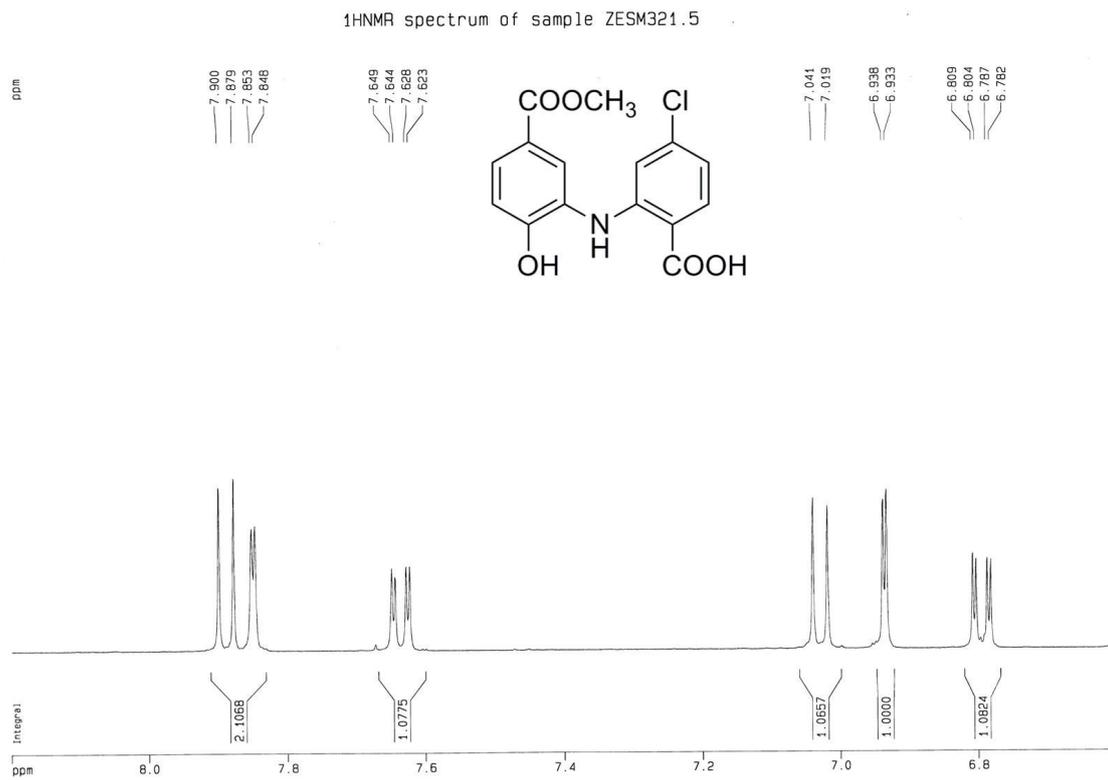


Fig. S2 ^1H NMR of CHMPBA in $\text{DMSO-}d_6$ (400 MHz)

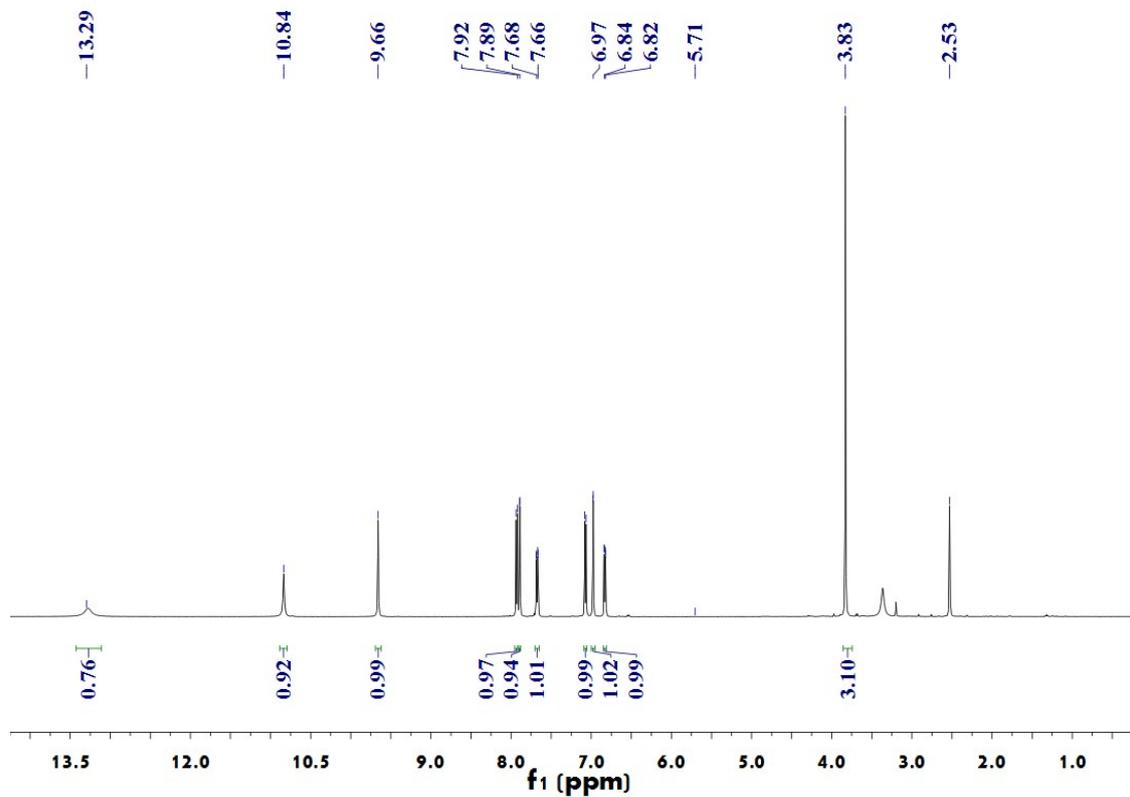


Fig. S3 ^1H NMR of CHMPBA in $\text{DMSO-}d_6$ (500 MHz)

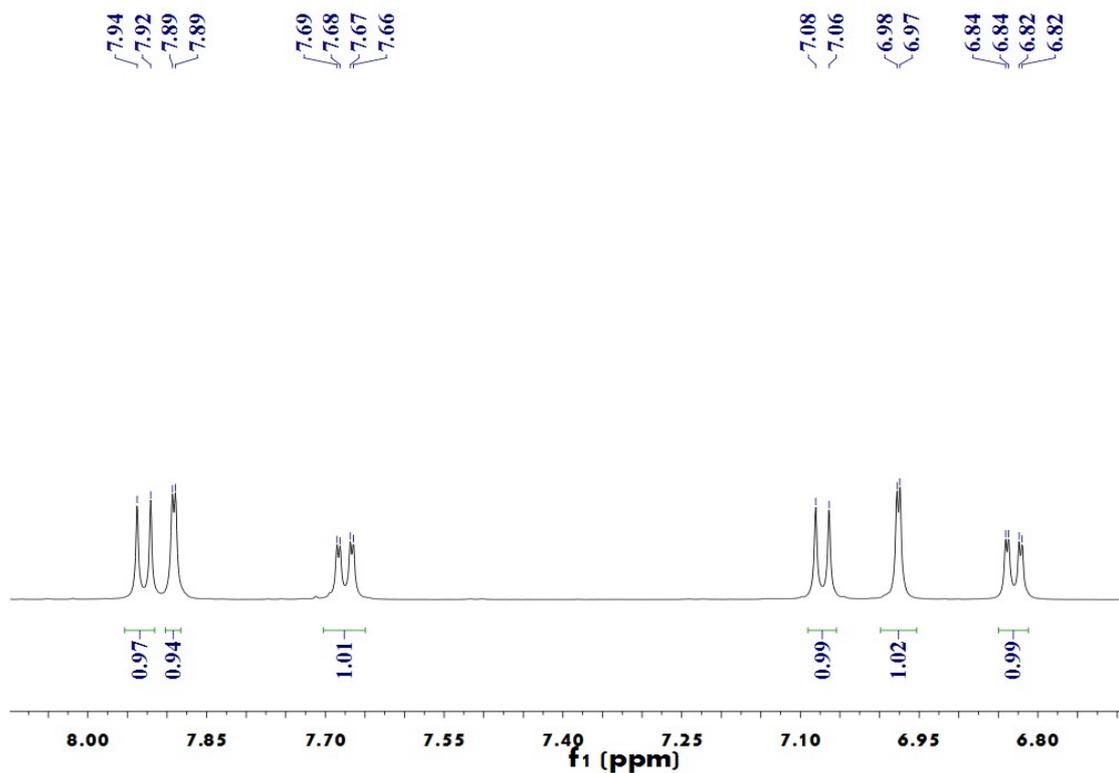


Fig. S4 ^1H NMR of CHMPBA in $\text{DMSO-}d_6$ (500 MHz)

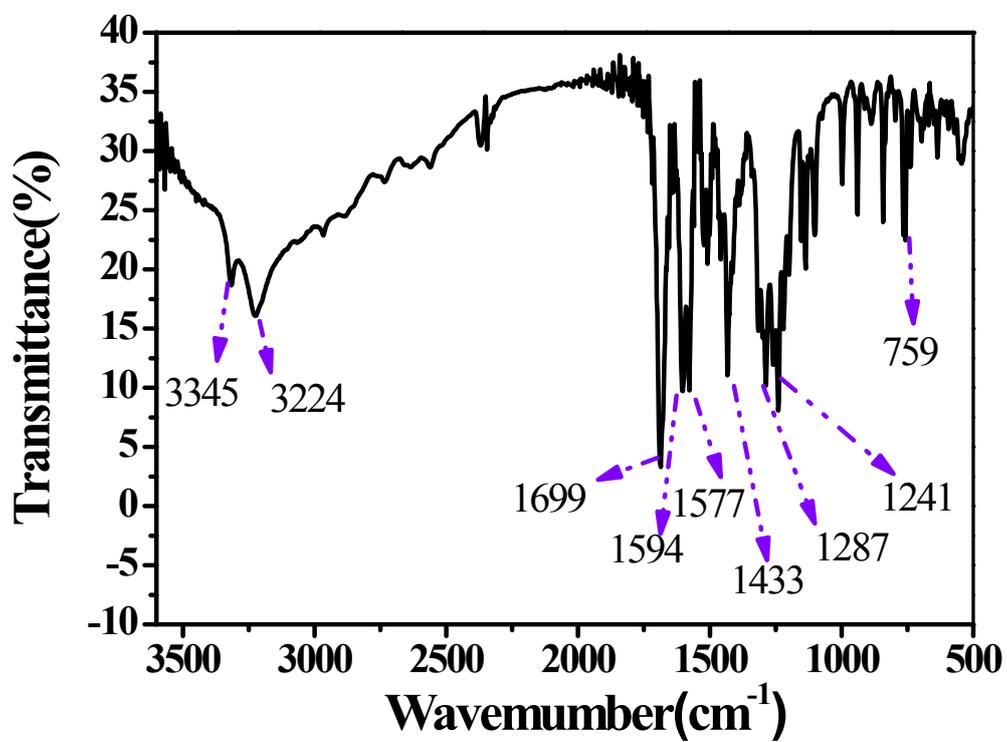


Fig. S5 FT-IR spectrum of CHMPBA

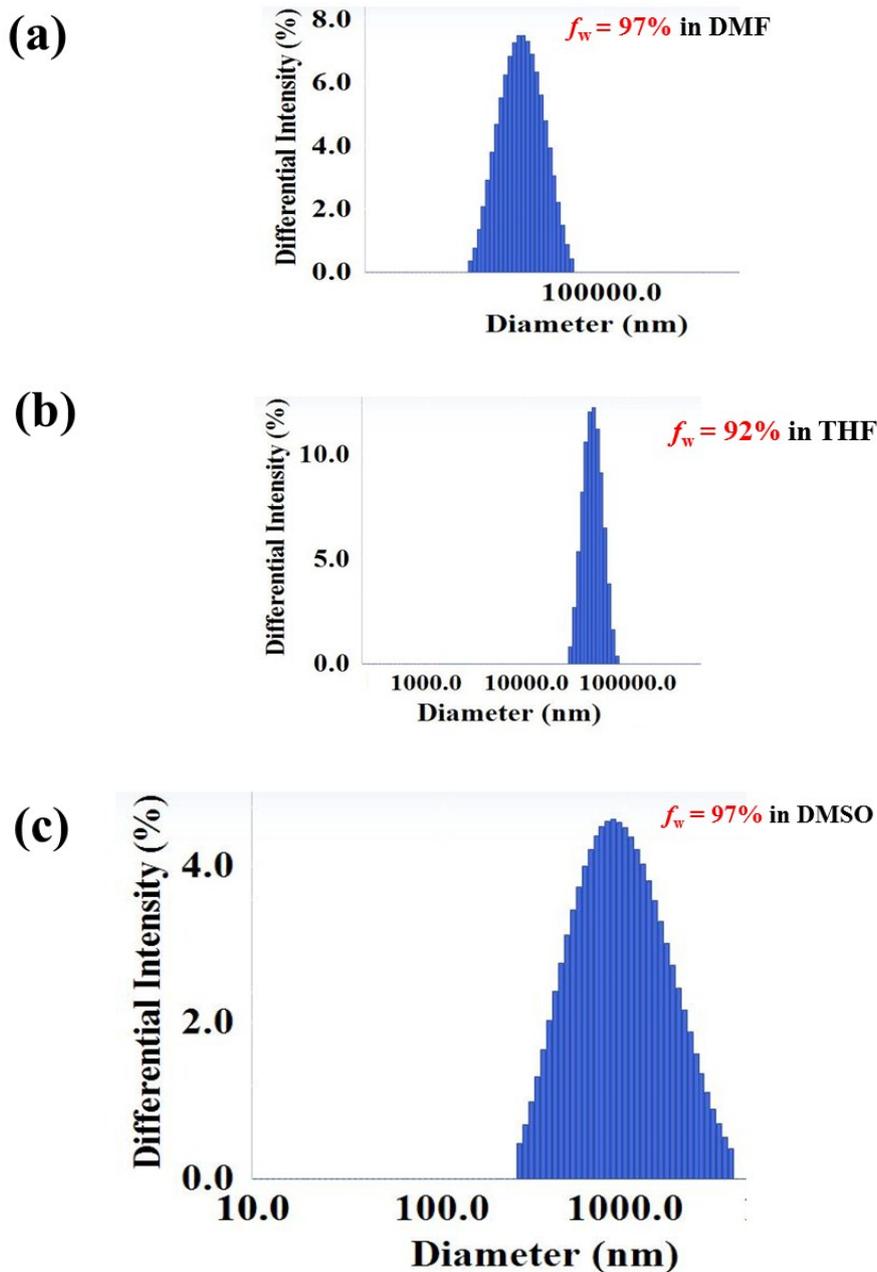


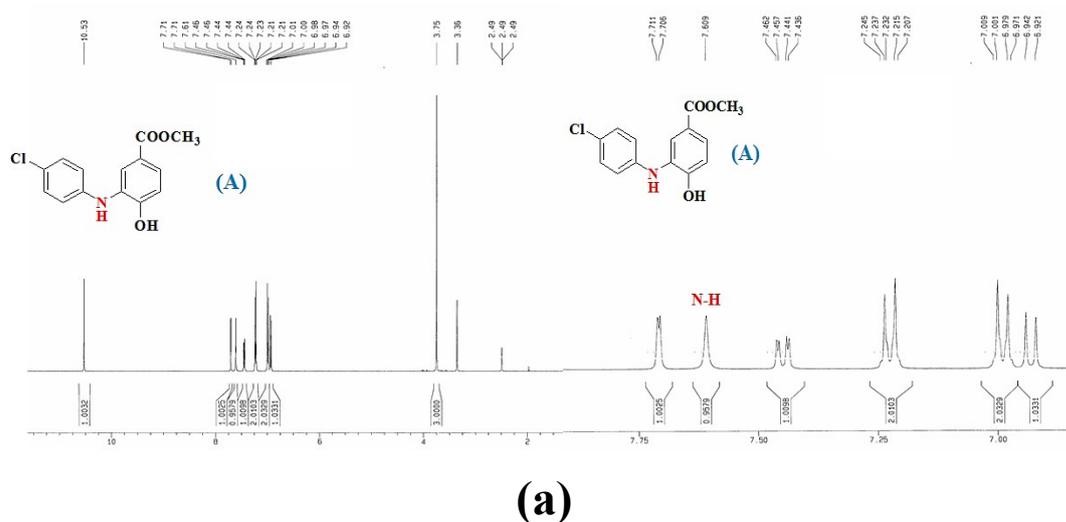
Fig. S6 Particle size analysis of CHMPBA in mixed-solvents DMF-H₂O (a), THF-H₂O (b) and DMSO-H₂O (c) with different f_w .

AIE Mechanism study

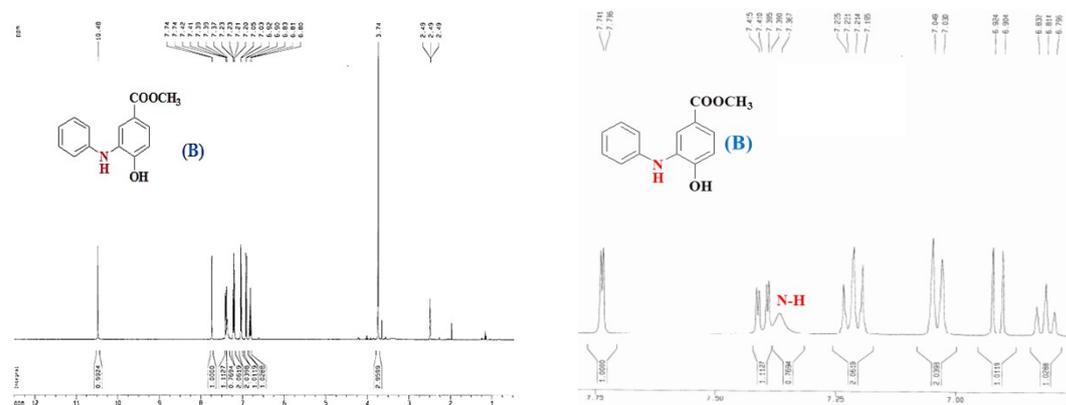
According to the previous literatures, there are several accessible mechanisms for the AIE phenomenon such as the restricted intramolecular rotation (RIR), intramolecular co-planarization, *J*-aggregate formation and special excimer formation.^[1] With the experimental results in hand, we believe that the restricted intramolecular rotation (RIR) mechanisms could explain the AIE phenomenon of

CHMPBA.

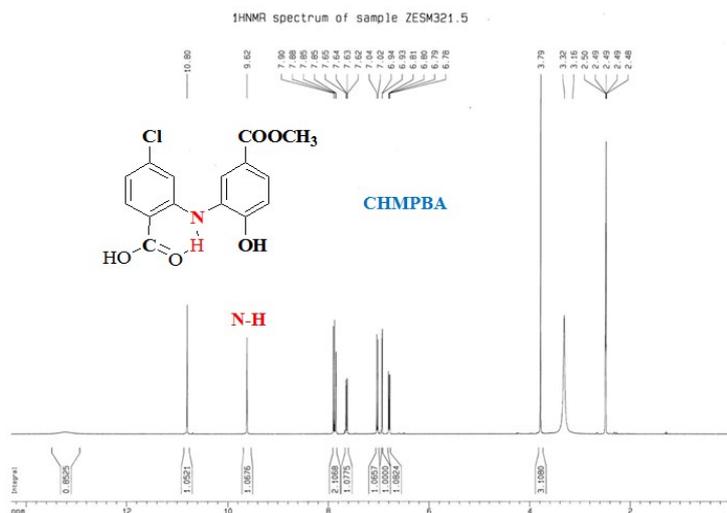
Firstly, in order to reveal the influence of the intra-molecular hydrogen bond between carboxyl oxygen and H_g (N-H) on the AIE phenomenon of CHMPBA, two structural analogues of CHMPBA (compound **A** and **B**) were synthesized and their ¹HNMR spectra were displayed in Fig. S7 (a and b). The chemical shifts of N-H in compound A (Fig. S7a) and B (Fig. S7b) were 7.61 ppm and 7.37 ppm, respectively. Compared with compound A (Fig. S7a) and B (Fig. S7b), the chemical shifts of N-H in CHMPBA greatly shifted to the low field ($\delta = 9.62$ ppm), which was caused by the intra-molecular hydrogen bond between carboxyl oxygen and N-H (Fig. 7Sc). In addition, no AIE phenomenon was observed for compound A and B. The results revealed that the intra-molecular hydrogen bond between carboxyl oxygen and N-H in CHMPBA is necessary for the AIE phenomenon.[2]



(a)



(b)



(c)

Fig. S7 ^1H NMR of A, B and CHMPBA in $\text{DMSO-}d_6$ (400 MHz)

As displayed in Fig. 9 (in the manuscript), the intra-molecular hydrogen bond between carboxyl oxygen and H_g (N-H) restrict the intra-molecular rotation (RIR) of the C-N bond leading to a relative rigid intra-molecular co-planarization configuration (Fig. 9 ring A and ring B). Upon restriction of intra-molecular rotation (RIR) of CHMPBA, the radiative decay channel is activated, which leads to the high fluorescent emission.^[3] After treated with NH_3 , the intra-molecular hydrogen bond between carboxyl oxygen and H_g (N-H) was destroyed and the rotation of C-N single bond was activated, which would result in the nonradiative decay of CHMPBA (“Fluorescent OFF”).^[3]

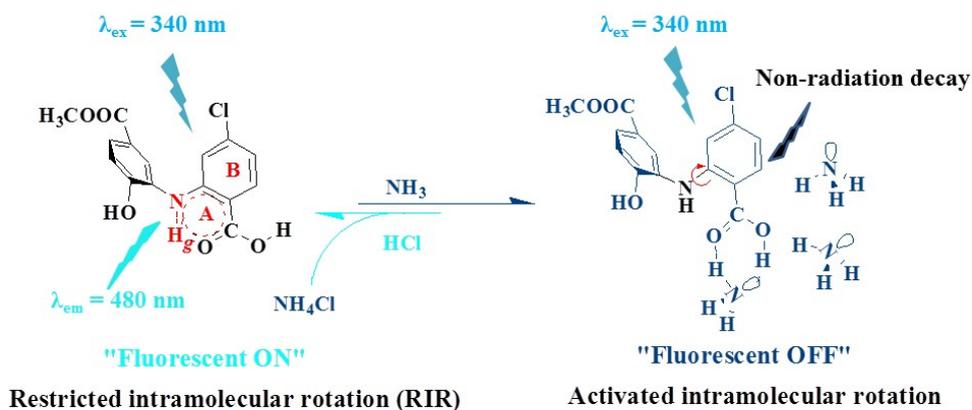


Fig. 9 Plausible reaction mechanism for the “Fluorescent ON” and “Fluorescent OFF” phenomena.

In addition, according to the previous reports, the fluorescence intensity of these AIE molecules adopting RIR mechanism will be enhanced with the decreasing of temperature or increasing of solvent viscosity.^[4] In order to confirm the RIR mechanism, the fluorescence intensity of CHMPBA were recorded with increasing and decreasing temperatures, respectively. As displayed in Fig. S8a, the fluorescent intensities of CHMPBA decreased with increasing temperature. In the contrary, the decrease of temperature resulted in the enhancement of fluorescent intensities (Fig. S8b). Furthermore, the fluorescent intensities of CHMPBA were enhanced with the increasing of solvent viscosity. As shown in Fig. S8c, the fluorescent intensities of CHMPBA gradually enhanced when the solvent were changed from ethanol to PEG-400 (Ethanol, Glycol and PEG-400).

In conclusion, with our previous and the above experiments in hand we believe that the restricted intra-molecular rotation (RIR) mechanisms could responsible for the AIE phenomenon of CHMPBA.

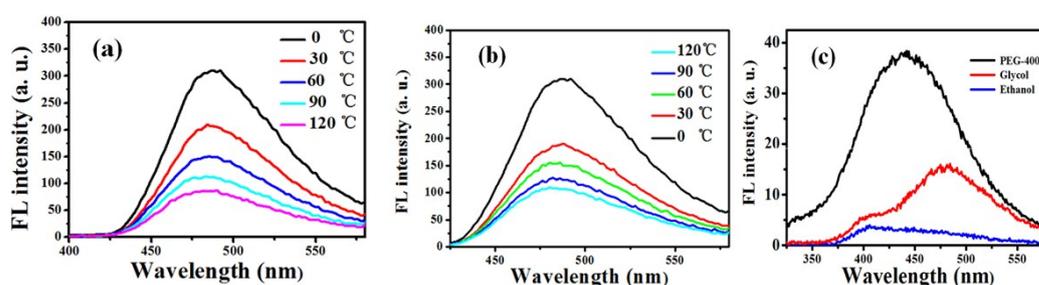


Fig. S8 Fluorescent intensities of CHMPBA with the increase (a) and decrease of temperatures (b); Fluorescent intensities of CHMPBA in solvents with different viscosities (c).

References:

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