Synopsis of Original Research Paper

Development of fluorescent materials for visualization and detection of a trace amount of water in products

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In order to elucidate a detection mechanism of photo-induced electron transfer (PET)-type fluorescent sensor for water, we have designed and developed anthracene-(aminomethyl)-4-cyanophenylboronic acid (AminoMeCNPhenylB$(OH)_2$) **TF-2** by the deprotection of pinacol ester (Pin) of anthracene-AminoMeCNPhenylBPin **OF-2**. For **OF-2** the PET takes place from the nitrogen atom of the Amino moiety to the photoexcited fluorophore (anthracene) skeleton in the absence of water, leading to fluorescence quenching (PET active state). When water was added to **OF-2** solution, a drastic enhancement of the fluorescence emission is observed due to the formation of the PET inactive (florescent) species **OF-2W** or **OF-2WH** by interaction with water molecules which has been determined by ^{1}H NMR spectral measurements. On the other hand, even in the absence of water **TF-2** exhibits intense fluorescence emission and the addition of water to **TF-2** solution shows a negligible change in the fluorescence intensity. The ^{1}H NMR spectrum of **TF-2** solution without the addition of water clearly indicated the formation of PET inactive (florescent) species **TF-2H** by the intramolecular OH···N hydrogen bonding between the hydroxyl group of $B(OH)_2$ moiety and the nitrogen atom of the Amino moiety. For **TF-2** the single-crystal X-ray structural analysis as well as density functional theory (DFT) calculations revealed the existence of the intramolecular OH···N hydrogen bonding, that is, the formation of **TF-2H**. Interestingly, the ^{1}H NMR spectra of **TF-2** solution with the addition of water showed the existence of the PET inactive (florescent) species **TF-2W** or **TF-2WH** by interaction with water molecules, as with the cases of **OF-2**. Consequently, it was found that for the PET-type fluorescent sensor based on anthracene-AminoMeCNPhenylBPin structure, the BPin moiety is essential not only to active the PET in the absence of water, leading to fluorescence quenching, but also to form the PET inactive (florescent) species upon the addition of water. This work provides a direction in molecular design toward creating an effective PET-type fluorescent sensor for water as well as a conclusive detection mechanism of anthracene-AminoMeCNPhenylBPin structure for water.