1,3,5-Tris(4'-aminophenyl)benzene as a supramolecular sensor for polynitroaromatics; solid and solution phase studies

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Designing of sensing materials for chemically inert and low vapor pressure polynitroaromatics (PNACs) such as TNT, PA and DNT is a challenging task within the area of chemical sensors. Owing to the unique electron-deficient property of PNACs, these analytes can form π -stacks and produce optically readable signal upon binding with electron rich fluorophores. Using single crystal X-ray diffraction studies, we have investigated the binding of TNT, PA, DNT and m-DNB with a supramolecular fluorophore, 1,3,5-tris(4'-aminophenyl)benzene (TAPB). The crystal structures show that the nitro compounds intercalate TAPB sheets through strong π - π stacking, whereas the NO₂ groups form hydrogen bonds (N-H···O) with the NH₂ groups. The strong binding affinity also enhances markedly the sensing efficiency which is further confirmed by the steady state Stern-Volmer quenching studies where the fluorescence intensity of TAPB quenched increasingly upon systematically titrating with the nitro analytes. Furthermore, vapor phase detection of DNT demonstrates the utility of TAPB as selective and discriminatory real time sensor for nitroaromatic explosives.

