Poster Presentation

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Uncovering Charge Transfer Interactions of Energetic Molecules

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Energetic materials are systems that store a large amount of chemical energy, which can be converted into mechanical energy though molecular decomposition, e.g. explosives, propellants and fuels. Co-crystallization of energetic materials with desirable co-crystal formers provides a novel way of tailoring existing energetic materials without structural manipulation. Examples include trinitrotoluene (TNT) with electron rich aromatics along with other energetic materials (CL-20, DADP) [1-3]. In order to take advantage of this methodology it is necessary to develop an understanding of the synthons involved in non-covalent interactions. The interpretation of non-covalent interactions has been highlighted in many recent publications, notably the publications by Gilli et al. which classifies short contacts as interactions, where the distance between atoms is less than the sum of their van der Waals radii. Depending on the type of interactions, the complexes can be divided into different categories, the most well known and studied are: H-bond theory and charge transfer (CT). In this study, a systematic series of crystal structures of organic CT complexes were determined to allow for the identification of structural packing trends, variations in aromaticity, decomposition temperatures and enthalpies along with non-covalent interactions, focusing mainly on the π•••π interactions. The complexes investigated were of the electron donor acceptor type, with polycyclic hydrocarbons acting as the donor (D) molecules, whilst 1,3,5-trinitrobenzene was selected as the energetic acceptor (A) molecule, due to its similarity with TNT. The CT complexes were observed to exhibit strong colours in the yellow to red regions of visible light with the co-crystals forming alternating DA stacks.

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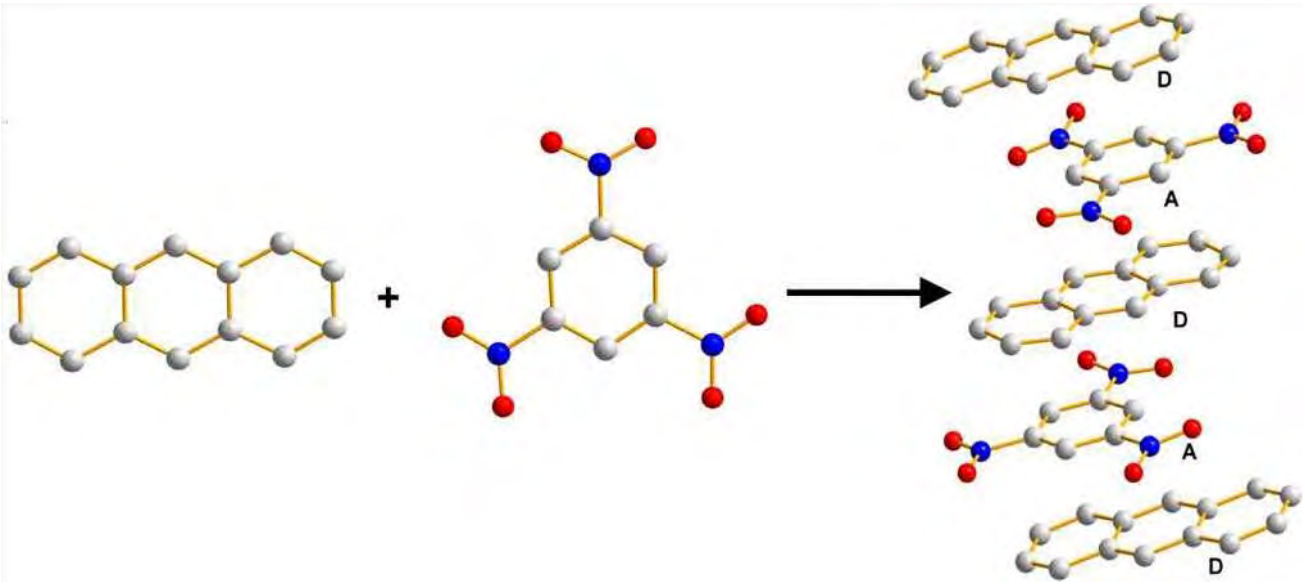

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