[MS24-P26] Energetic Co-crystals – Structural Studies of Nitrotriazolone Salts and Co-crystals.

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Energetic materials (explosives and propellants) contain large amounts of stored energy, which can be rapidly released in the form of heat and gaseous products upon stimuli such as shock and impact. Developments in energetic materials are currently focused on the requirements for safer, yet still powerful materials for uses within mining, munitions and rocket propulsion systems [1] One strategy that can be used to achieve these desirable properties is to synthesise new molecules, but this is both time-consuming and resource-intensive. Instead, another strategy is to crystallise energetic molecules with other molecules to form salts or co-crystals. This approach has been used extensively within the pharmaceutical industry in order to enhance desirable properties, e.g. solubility and bioavailability. To date, however, there has been very little research on the co-crystallisation of energetic materials. Examples include trinitrotriazolone (TNT) with pyrene, naphthalene, and CL-20 [2-4]. To start this design process, the relationships between the types and strengths of interactions within a crystal structure and materials properties need to be established. Once these structure-property relationships have been established, the engineering of new and improved energetic materials can be achieved. The main focus of this work is on the energetic material nitrotriazolone (NTO) and the characterisation of a selection of new salts and cocrystals. NTO is an insensitive high explosive that has a similar performance to the more widely used explosive, RDX, (found in compositions such as C4) yet is more stable, less prone to accidental detonation, and more soluble in water. Its high solubility in water is a major issue, as NTO is biologically active and represents a potential risk to the environment. There are only a few known salts of NTO and no published co-crystals, so the design and preparation of the first NTO co-crystals is a key objective [5, 6]. A selection of crystal structures of salts and co-crystals of NTO with nitrogen-rich aromatic systems has been obtained and the results are presented here. Interesting trends between pKa, functional groups, and intermolecular interactions have been observed.

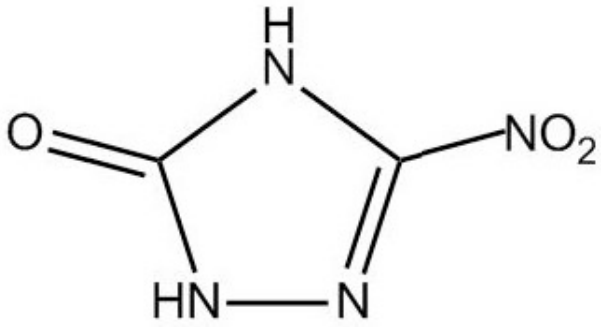

Figure 1. Nitrotriazolone (NTO)

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