

## Poster Presentation

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### *Energetic Cocrystals – Structural Studies of Nitrotriazolone Salts & Cocrystals*

H. Lloyd<sup>1</sup>, C. Pulham<sup>1</sup>, P. Coster<sup>1</sup>, C. Henderson<sup>1</sup>, D. Williamson<sup>2</sup>, A. Jardine<sup>2</sup>

<sup>1</sup>University of Edinburgh, Department of Chemistry, Edinburgh, United Kingdom, <sup>2</sup>University of Cambridge, Department of Physics, Cambridge, United Kingdom

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. 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 cocrystals. 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 cocrystallisation of energetic materials. Examples include trinitrotoluene (TNT) with pyrene, naphthalene, and CL-20. 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 3-nitro-1,2,4-triazol-5-one (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, 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 cocrystals, so the design and preparation of the first NTO cocrystals is a key objective. A selection of crystal structures of salts and cocrystals 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.

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