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Design and Synthesis of Bio-inspired Energetic Nucleobase Derivatives

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Energetic materials are essential components of modern technological applications. They are used for military, mining, construction, and aviation purposes. In recent years, research in energetic materials has been related to obtaining safer, environmentally friendly, and efficient materials. Insensitive high-energy density materials (IHEMDs) are a subcategory of secondary explosives presenting high performance and immense stability to external stimuli. In recent years, a trend of using H-bonding to increase the stability of high-energy materials has become ubiquitous in the design of new IHEDMs.[1] Incorporating H-bond donors and acceptors to form both intramolecular and intermolecular bonds increases both density and stability of the material.[2] Although nucleobases are highly efficient at forming H-bonds, they have been scarcely explored in the design of IHEDMs.

We will discuss the design and synthesis of adenine and uracil-based energetic materials and their energetic properties (**Figure 1**). We will use the combinations of the different explosophoric groups, such as azido, nitro, amino, hydroxylamino, and tetrazolyl amino, in the design of new IHEDMs and find the optimal conditions towards the proposed structures.

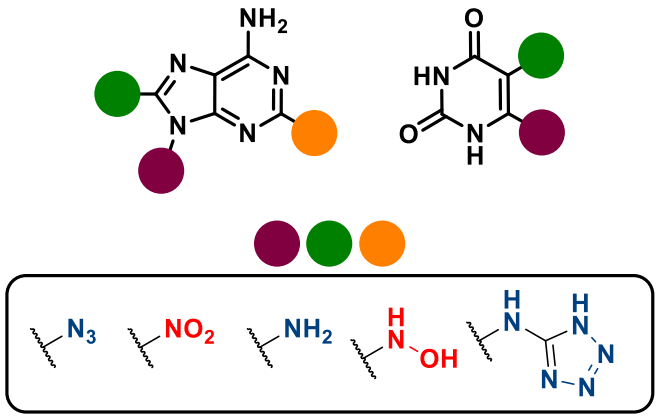

Figure 1: Adenine and uracil derivatives modified with explosophoric groups.

Acknowledgements:

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References:

1. Klapötke, M. *Chemistry of High-Energy Materials. De Gruyter*: Berlin **2022**.
2. Pagoria, P. *Propellants Explos. Pyrotech.*, **2016**, *41*, 452–469.

Development of Co-crystals of Bio-inspired Insensitive Energetic Materials

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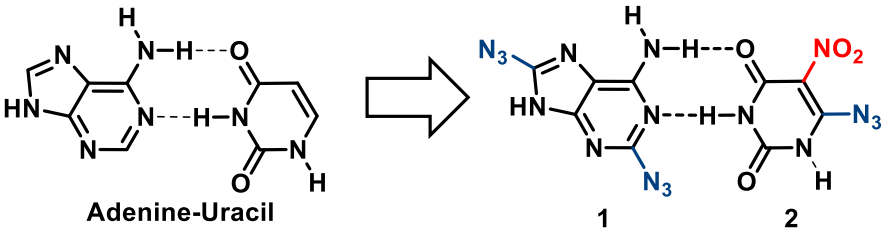
Although energetic materials are some of the most influential materials in human history their modern evolution has been relatively slow. Energetic materials must achieve a challenging combination of properties including high explosive power, high stability and low cost, therefore new strategies for their synthesis are required.[1] Recently co-crystallization has emerged as a new method for generating novel forms of energetic materials. Co-crystallization can increase density, improve thermal stability and decrease the sensitivity of energetic materials.[2] Co-crystals of many energetic materials have been reported, however little to no work has been done on designed intermolecular bonding for these materials.
We will discuss the use of energetically modified nucleobases such as adenine and uracil derivatives in the formation of Watson-Crick type bonded insensitive energetic materials co-crystals and study their properties (**Scheme 1**).



Scheme 1: Watson-Crick base paired adenine and uracil derivatives.

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References:

1. Klapötke, M., *Chemistry of High-Energy Materials. De Gruyter*: Berlin **2022**.
2. Bolton, O. and Matzger, A.J. *Angew. Chem. Int. Ed*. **2011**, *50,* 8960.