

## Poster Presentation

MS115.P18

### *Crystal doping of an energetic material to control its polymorphism*

Daniel W. Ward<sup>1</sup>, Paul L. Coster<sup>1</sup>, Colin R. Pulham<sup>1</sup>

<sup>1</sup>School Of Chemistry, University Of Edinburgh, Edinburgh, United Kingdom  
E-mail: dan.ward@ed.ac.uk

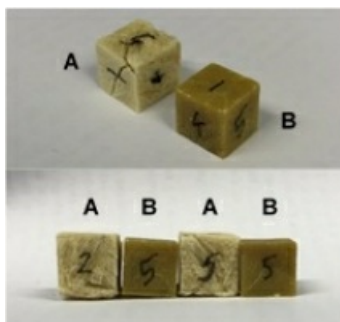
Up to 15 % irreversible growth of 2,4-dinitroanisole (DNAN) has been previously observed when the material is temperature cycled from 219 K to 344 K (-54 °C to +71 °C), whereby less than 1% is considered acceptable. We have discovered a complex system of polymorphism in DNAN, with one notable phase transition occurring within the temperature cycling regime at 266 K. This disorder-order phase transition from DNAN-II to III involves a notable ~4 % jump in the unit cell volume and has been found to be the major cause of the growth experienced with DNAN.

Doping the crystal structure of DNAN with molecularly similar materials is able to suppress this II-III transition to outside the temperature cycling regime. With dopants such as 2,4-dinitrotoluene (10 %) suppressing the transition to below 220 K. Additional dopants, termed EDX-1 and EDX-2, are able to even more significantly suppress the transition to below 150 K. When samples of DNAN doped with EDX-1 are temperature cycled, the II-III transition is no longer encountered and more importantly, irreversible growth is no longer observed.

Through these studies we have developed further understanding of DNAN which has the potential to help enable DNAN to be used as a less sensitive replacement for TNT in melt-cast formulations.

[1] Samuels, P. (2012). Proceedings of NDIA IM/EM, Las Vegas, Nevada, USA.

[2] Provatas, A. & Davies, P. J. (2013). Report, Australian Defence Science and Technology Organisation.



**Keywords:** [crystal doping](#), [polymorphism](#), [DNAN](#).