

References:

- [1] Williams, J. H., Cockcroft, J. K. & Fitch, A. N. (1992) *Angew. Chem. Int. Ed. Engl.* 31, 1655-1657.
- [2] Cockcroft, J. K., Rosu-Finsen, A., Fitch, A. N. & Williams, J. H. (2018) for submission in May.
- [3] Cockcroft, J. K., Ghosh, R. E., Shephard, J.J., Singh, A. & Williams, J.H. (2017) *CrystEngComm*, 2017, 19, 1019-1023.

Keywords: Variable temperature powder diffraction, C-H...F-C Interactions, Co-crystals

MS31-P14**Co-crystallisation of energetic materials with reduced sensitivity**

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Insensitive explosives have attracted significant interest in the past three decades owing to their potential application in numerous energetic materials. Research of the explosive of low impact sensitivity and high explosive performance is the vital problem in the energetic materials, which has not been solved yet **(1-4)**. Efforts have been made to diminish this through synthesis of new molecules, however this is usually a complex, need to time consuming process cost-effective production methods, extensive validation, and requirements to meet increasing challenging performance target **(5)**. Co-crystallisation is new an effective technique to improve the solubility, bioavailability physical and chemical stability properties of drugs without altering their chemical structure, and it is extensively used for the pharmaceutical industry **(6-9)**. Therefore, co-crystallization may supply a new method to possibility of tuning the performance and sensitivity of an energetic material without requiring complex preparation or synthesis of novel compounds **(10-13)**. To modify and improve the properties of energetic materials, via co-crystallisation between TNT, Picric Acid with non-energetic materials were studied. Co-crystallisation studies including characterization (single crystal X-ray data, Powder X Ray diffraction), thermal behavior (Differential Scanning Calorimetry), impact sensitivity (BAM Fall Hammer), and intermolecular interactions were carried out in detail. And also we analysed the crystal packing and show how this may influence sensitivity to impact.

References:

1. Becuwe, A.; Delclos, A. *Propellants, Explosives, Pyrotechnics*. (1993)18, 1–10.
2. Van der Heijden, A. E. D. M.; Bouma, R. H. B.; Van der Steen, A. C. *Propellants, Explosives, Pyrotechnics*. (2004) 29, 304–313.
3. Millar, R. W.; Philbin, S. P.; Claridge, R. P.; Hamid, J. *Propellants, Explosives, Pyrotechnics*. (2004) 29, 81–92.
4. Zhurova, E. A.; Zhurov, V. V.; Pinkerton, A. A. *J. Am. Chem. Soc.* (2007) 129, 13887–13893.
5. Sikder, A.K.; Sikder, N. *J. Haz. Mat.* (2004) 112, 15.
6. Shen, J. P.; Duan, X. H.; Luo, Q. P.; Zhou, Y.; Bao, Q.; Ma, Y. J.; Pei, C. H. *Cryst. Growth Des.* (2011), 11, 1759–1765.
7. Remenar, J. F.; Morissette, S. L.; Peterson, M. L.; Moulton, B.; MacPhee, J. M.; Guzman, H. R.; Almarsson, O. *J. Am. Chem. Soc.* (2003) 125, 8456–8457.
8. Weyna, D. R.; Shattock, T.; Vishweshwar, P.; Zaworotko, M. J. *Cryst. Growth Des.* (2009), 9, 1106–1123.
9. Almarsson, Ö.; Zaworotko, M. J. *Chem. Commun.* (2004), 1889–1896.
10. Zhu, W.; Xiao, J.; Zhao, F.; Ji, G.; Ma, X.; Xiao, H. *Acta Ch*

Keywords: Sensitivity, Inter molecular interaction, Co-crystallisation