## MS115.P36

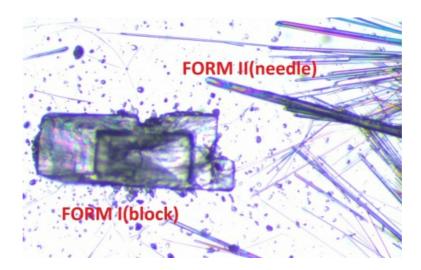
Concomitant dimorphism in diphenyl (3,4-difluorophenyl) phosphoramidates

<u>Avantika Hasija</u><sup>1</sup>, Deepak Chopra<sup>1</sup>

<sup>1</sup>Chemistry, IISER Bhopal, Bhopal, India
E-mail: avantika16@iiserb.ac.in

Polymorphism is a phenomenon where a compound crystallises in more than one crystalline form. [1] Polymorphs are ideal systems to study molecular structure–crystal structure–crystal energy relationships on account of the differences which arise due to different inter-molecular interactions and crystal packing effects. With increasing evidence of this phenomenon, the simultaneous occurrence of crystalline forms, i.e. concomitant polymorphism is found to be significant among the class of polymorphs. [2] The current investigation provides a complete elucidation of the structural diversity which is manifested as prevalence of concomitance in two diverse crystalline forms of Diphenyl (3,4-difluorophenyl) phosphoramidates. Form I (blocks) crystallises in the centrosymmetric P21/c space group (Z'=1), and Form II (needles) crystallises in the non-centrosymmetric Pca21 (Z'=2). The polymorphs were also characterized using DSC, PXRD and HSM. [3] The supra molecular architecture of both the dimorphs is guided by strong N-H···O=P and stabilised in addition via weak C-H···O=P, C-H···F-C, C-H···n hydrogen bonds.

- 1. Bernstein, J. (2002). Polymorphism in Molecular Crystals, Oxford University Press, New York.
- 2. (a) Bernstein, J. et al. (1999). Angew. Chem. Int. Ed. 38, 3440 3461
- (b) Cabeza, A. et al. (2015). Chem. Soc. Rev. 44, 8619-8635
- (c) Panini, P. et al. (2016). Cryst.Growth Des. 16, 2561-2572.
- 3. Threlfall, L. (1995). Analyst. 120, 2435-2460.



Keywords: Polymorphism, Concomitant Polymorphism, Di-fluorinated Phosphoramidates