to control polymorphism in pharmaceuticals. Our compound of interest is pyrazinamide (PZA), a polymorphic API used in the treatment of tuberculosis and is known to exist in 4 different forms. Only two cocrystals of PZA have been reported to date. We identified aminobenzoic acid (ABA) and hydroxybenzoic acid (HBA) as suitable cocystal formers (coformers) for PZA. In addition, we decided to investigate the effect of changing the orientation of the hydrogen bonding groups in ABA and HBA on cocrystal formation by employing the 3 constitutional isomers of each for a total of 6 coformers: *o*-aminobenzoic acid (*o*ABA) commonly known as anthranilic acid, *m*-aminobenzoic acid (*m*ABA), *p*-aminobenzoic acid (*p*ABA), *o*-hydroxybenzoic acid (*o*HBA) commonly known as salicylic acid, *m*-hydroxybenzoic acid (*m*HBA) and *p*-hydroxybenzoic acid (*p*HBA). Our results show that PZA forms a cocrsytal with each of the coformers, repeatedly and consistently suggesting that they are not polymorphic. This presentation will show the synthesis and characterization of 6 new PZA cocrystals, namely PZA•*o*ABA (**1**), PZA•*m*ABA (**2**), PZA•*p*ABA (**3**), PZA•*o*HBA (**4**), PZA•*m*HBA (**5**) and PZA•*p*HBA (**6**). The characterization techniques employed include powder X-ray diffraction (PXRD), differential scanning calorimetery (DSC), melting point, and in some cases ^{1}H NMR and single crystal X-ray crystallography (cocrystals **1** and **3**).

Keywords: cocrystal, polymorphism

MS24.P30

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'Organic' fluorine dictates the molecular conformation and packing

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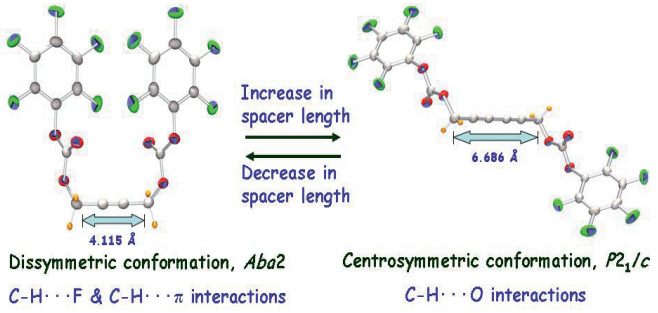
Fluorinated compounds have gained an immense importance because of their role in day-to-day life [1]. The chemical, physical and biological properties of these compounds have been well-recognized in terms of interactions involving fluorine. The robustness of C–F···H, F···F and C–F···π interactions can be exploited in controlling the conformational features and supramolecular structural organization of the conformationally flexible molecules [2]. In this context, the crystal structures of three aryl biscarbonates and an aryl biscarbamate namely, But-2-yne-1,4-diyl bis(2,3,4,5,6-pentafluorophenylcarbonate), 1; But-2-yne-1,4-diyl bis(4-fluorophenylcarbonate), 2: But-2-yne-1,4-diyl bis(2,3,4,5,6-pentafluorophenylcarbamate), 3 and Hexa-2,4-diyne-1,6-diyl bis(2,3,4,5,6-pentafluorophenylcarbonate), 4 with rigid acetylenic unit providing variable spacer lengths have been analysed [3]. Compound 1 adopts a noncentrosymmetric 'twisted' (syn) conformation, whereas 2, 3 and 4 acquire a centrosymmetric 'extended' (anti) conformation, a commonality of such molecules as revealed by Cambridge Crystallographic Database search results. Weak intermolecular interactions and in particular those involving fluorine [C^{sp3}–H···F–C^{sp2}] are found to dictate this conformational variation in the crystal structure of 1. Neutron diffraction study at 90 K was performed on 1 to obtain further insights into these interactions involving 'organic' fluorine. We demonstrate that the conformational preferences and the supramolecular organization in the crystal lattice adopted by aryl biscarbonates 1, 2 and 4 and an aryl biscarbamate, 3 are the consequence of a counterbalance between the molecular symmetry and the weak intermolecular interactions involving the 'organic' fluorine.



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Structural studies of selected photochromic compounds

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Photochromic compounds displaying property changes upon conversion are of interest for potential applications including optical switching devices and memory media. Anils, Schiff bases of salicylaldehyde derivatives with aniline derivatives, exhibit both solid-state thermo- and/or photochromism through an enol-keto tautomerism mechanism. The final thermoproduct is the *cis*-keto form whereas the photoproduct is the *trans*-keto form [1]. These compounds show potential for "crystal engineering" because their properties are greatly influenced by their surroundings. Hence, by altering substituents, adding bulky groups to increase lattice "space" or by making inclusion compounds, thermo- and/or photochromic properties can be enhanced towards specific applications [2].

To examine structure-property relationships various substituted anils have been synthesized and studied using Raman spectroscopy, crystallographic methods and diffuse reflectance spectroscopy [3]. All the compounds investigated display some degree of thermochromism. The strongly thermochromic compounds show a large visible colour change from orange/red at room temperature to yellow in liquid nitrogen but rarely display photochromism. Some of the weakly thermochromic compounds are also photochromic, changing from yellow to orange/red upon UV irradiation and reverting back to their original colour thermally or upon irradiation with visible light ($\lambda > 560$ nm). Molecular planarity is thought to be disfavourable for photochromism but in this study several anil compounds with *inter*planar angles of < 10° have been found to display distinct colour change upon UV irradiation.

It is suggested that the thermo- and/or photochromic properties displayed depend on a complex interplay of factors determined by the type of substituents, the molecular and packing structure, in particular *inter*planar angle, *inter*molecular interactions, void space around the central imine group and possibly other influences.

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