the home system allows collection of data as soon as the crystals are produced to get the initial solution of novel structures and is invaluable in the quick turnover often required in ligand-binding studies.

We will describe how the combination of the updated Agilent Technologies SuperNova, a highly efficient compact diffractometer, with the new version of fully automated CrysAlisPro data collection and processing software, optimized for macromolecular crystallography, makes an ideal home lab solution complementing synchrotron data collection.

New unique features of CrysAlisPro and several examples of high quality results obtained with the system will be presented.

Keywords: macromolecular, experiment, software

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Fluorine determines the aggregation of pyridines. Experiment vs. theory

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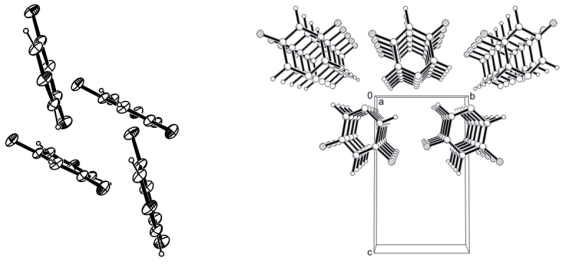
Fluorine is a unique element. The question about the role of Fluorine in intermolecular interactions is discussed controversially. Well known is the influence of fluorine on the electronic structure of aromatic backbones and therefore on the entire molecules. On the other hand, fluorine forms only weak intermolecular interactions and seems to have no influence on the crystal packing. Pauling's definition of the hydrogen bond would imply that fluorine, as the most electronegative atom, should be a stronger hydrogen-bond acceptor then oxygen and nitrogen. But the C-F group, the so-called "organic fluorine", does not form hydrogen bonds commensurate with electronegativity considerations in contrast to the C-O and C-N groups.

We investigated a range of partially fluorinated pyridines and analysed their crystal packings experimentally and theoretically. Low temperature *in situ* crystallisation on the diffraktometer was used to investigate crystal structures of low melting fluorinated pyridines followed by analysis of the crystallisation behavior. Interesting tendencies were observed in crystal packings depending on the fluorination degree.

But still the general question we are interested in, is: what determines the crystal packing in the absence of strong intermolecular interactions? Theoretical study of the energies of weak intermolecular interactions is an innovative method for research of the basic motives in the solid state. The comparison of our experimental and theoretical findings shows how fluorine atoms influence the aggregation of substituted pyridines. The picture below shows the difference between basic structural motives in the experimental (a) and theoretical (b) crystal packing of 3,5-difluoropyridine.



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Keywords: crystal engineering, fluorine, halogen bonding

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TMA alcohol solvates: filling the gaps and increasing the dimensionality

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Benzene-1,3,5-ticarboxylic acid, or trimesic acid (TMA), has been the focus of research interest for many years due to its symmetry, hydrogen bonding ability, ability to form salts and solvates, and use as an organic linker in metal organic frameworks. We have previously reported 1:1 and 1:2 TMA:MeOH solvates that demonstrated the stepwise dissolution of TMA via disruption by methanol of the $R^2_2(8)$ head-to-tail carboxylic acid dimer H-bonding pattern. This common pattern is seen in many pure carboxylic acids including the three-fold interpenetrated honeycomb lattice of pure TMA [1]. The disruption occurs via the insertion of an alcohol OH group into the $R^2_2(8)$ ring to generate an expanded $R^3_3(10)$ motif. More recently, the related structures of the higher alcohol homologues 1-butanol, 1-pentanol, and 1-hexanol were reported by Perepichka and Rosei [2]. This work revealed a structural dependence on the length of the alcohol's alkyl chain.

We are now able to report the intervening 'missing' TMA–alcohol solvate crystal structures with EtOH, 1-propanol, and 2-propanol, two of which are twinned. Their structures are placed in the context of the preceding work and our new findings plug the gap in current knowledge. We also report the structures of two diols which extend the dimensionality from 1D ladders (Fig. 1) to 2D sheets. The diol solvates/co-crystals exhibit further disruption of the $R^2_2(8)$ rings.

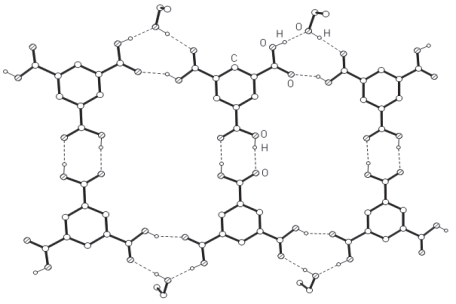

Fig. 1. 1D ladder structure adopted by TMA·EtOH with $R^2_2(8)$ and $R^3_3(10)$ H-binding motifs.

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Keywords: hydrogen bonding, crystal engineering, trimesic acid

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Hydrogen bonding, Z' and stability of diclofenac amine salts

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