formula \( \text{C}_6\text{H}_7\text{F} \text{N}_2 \text{O}_6 \cdot 6(\text{H}_2\text{O}) \) which crystallizes in a triclinic crystal system with space group \( P-1 \). Water molecules of the network array of hydrogen bonding interactions of the type O-H⋯H with distances that are within the range of 1.93 a 2.23 Å and as a few examples, in this case shows that some water molecules have three hydrogen bonds at the same time, which favors a two-dimensional crystal growth with the motif \( R_2(8) \), giving rise to the supramolecular arrangement in a laminar.

In the dimeric complex of copper acetate (II) with molecular formula \( \text{C}_6\text{H}_5\text{Cu}_2\text{O}_4 \), have a monoclinic crystal system with space group \( C 2/c \), in this compound the water molecules establish three hydrogen bonds in the range of 2.03 to 2.58 Å, giving rise to motif \( R_2(8) \) mainly. While for crystals of \( \text{Fe}(\text{H}_2\text{O})_4\text{SO}_2\text{H}_2\text{O} \) (II) with molecular formula \( \text{FeH}_2\text{O}_4\cdot\text{SO}_2\cdot\text{H}_2\text{O} \) crystallizing in a monoclinic crystal system with space group \( P 21/n \), the large number of water molecules present in this complex supports a large number of such interactions O-H⋯H with hydrogen bond lengths are in the range of 1.85 to 2.19 Å.

In a global analysis of data from X-ray diffraction, is that the magnitude of the hydrogen bonds are present in the energy range of 4 to 15 Kcal, being strong bonds with weak covalence and dominant electrostatic contribution, these properties are required for the design and application engineering of crystals and / or molecular devices

**Keywords:** hydrogen-bond, motif, engineering-crystals

**MS73.P14**


**Structural analysis of azidine-2-methanol derivatives**

Aurelia Falcicchio, Angela Altomare, Corrado Cuoci, Renzo Luisi, Anna Moliterni, Rossana Rizzi; "Istituto di Cristallografia IC-CNR, Via Amendola 122/a 70126 Bari (Italy). Dipartimento Farmaco – Chimico, Università degli Studi di Bari “Aldo Moro”, Consorzio C.I.N.M.P.I.S., Via E. Orabona 4, Bari (Italy). E-mail: aurelia.falcicchio@ic.cnr.it

Aziridines are widely used as versatile building blocks for the synthesis of a variety of biologically and pharmaceutically important molecules [1]. Among the available methodologies for the preparation of functionalised aziridines, the lithiation/trapping sequence of simple aziridines is growing in importance [2]. Present work reports the results concerning the structural study of aziridine-2-methanol derivatives by dynamic nuclear magnetic resonance (DMNR) [3] and single crystal X-ray diffraction. A careful examination of the aziridine 2 (see figure 1) by NMR data, shows that at room temperature the meta protons and the protons of the two ortho methyl groups of the mesityl ring gives featureless lumps, likely as consequence of a restricted rotation around the Csp\(^3\)-Csp\(^3\) bond between the carbinoic carbon and the ipso carbon of the mesityl ring. Also in the solid state, an almost identical arrangement of the mesityl ring, with respect to the other two phenyl rings, has been observed. In this case, the aziridine nitrogen substituent was found in a syn relationship with respect to the carbinoic group so preventing the possibility of forming a hydrogen bond with the hydroxyl group. This evidence underlines a slow rotation of the mesityl group instead of a nitrogen inversion as usually is expected.

Figure 1


**Keys:words:** NMR, organic synthesis, structural solution.

**MS73.P15**


Proton migration in molecular complexes of urea and its derivatives

Andrew O. F. Jones, L. H. Thomas, C. C. Wilson; Department of Chemistry, University of Glasgow, Glasgow (UK).

Istituto Laue-Langevin, Grenoble (France). Department of Chemistry, University of Bath, Bath (UK). Bragg Institute, ANSTO, Sydney (Australia). E-mail: anjone@chem.gla.ac.uk

Systems showing proton disorder, transfer and migration are an area of much interest in recent times with widespread implications for areas such as ferroelectrics and enzyme action. These often subtle processes can affect the properties of systems and are often observed in materials containing short strong hydrogen bonds. They can be probed using variable temperature diffraction experiments. We aim to identify and characterise systems that show such effects, with a view to predicting and controlling this potentially "tunable" behaviour. These processes have previously been observed in complexes of urea [1].

Single crystal X-ray and neutron diffraction have been used to study molecular complexes of urea and its derivatives with a particular focus on characterising the hydrogen atom behaviour. The proton behaviour is monitored over variable temperatures, with the aim of observing movement of the proton with changing temperature. A limited number of such mobile proton effects have been observed using variable temperature diffraction measurements, and this project aims to build on these observations by extending these investigations to further, related, systems. The instrument used for the neutron studies is the single crystal Laue diffractometer VIVALDI at the ILL in Grenoble which is ideal for use here due to its potential for high throughput single crystal diffraction of small samples.

Temperature dependent proton migration in the 2:1 complex of N,N-dimethylurea and oxalic acid has been observed by single crystal X-ray and neutron diffraction data confirming the existence of this phenomenon. Accurate determination of the hydrogen atom parameters in this system is vital in understanding this phenomenon and also in explaining a single-crystal to single-crystal phase transition.