MS21-O3 **Diffuse scattering resulting from macromolecular frustration.** T.R. Welberry, A.P.Heerdegen, P.D. Carr, *Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia,* E-mail: welberry@rsc.anu.edu.au

Distinctive diffuse scattering in the form of diffuse rings around Bragg positions has been observed in the diffraction patterns of a crystal of the N-terminal fragment of the Gag protein from Feline Foamy Virus. It has been shown that these are caused by geometric frustration as molecules try to pack on the triangular b–c mesh of the space group $P6_122$ [1]. In order to explain the strong diffuse scattering it is necessary for the crystal to contain occupational disorder such that each unit cell contains one or other of two different molecular arrangements, **A** and **B**. The frustration arises because the nearest-neighbour packing prefers neighbouring cells to be **AB** or **BA**, which cannot be achieved on all three sides of a triangle simultaneously. To explain the observation that reciprocal sections $h\,k\,5n$, where n = integer, contain only Bragg peaks it is necessary that **A** and **B** are identical molecular arrangements differing only by a translation of $0.2c$. The presence of the disorder has so far prevented the solution of the protein structure by conventional techniques. Consequently in the present work we are attempting additionally to make use of the detailed and very extensive diffuse scattering data to aid the solution of the molecular structure. Reverse Monte Carlo (RMC) simulation [2] has been used to obtain a low-resolution (~4Å) scattering model that fits both the Bragg intensities as well as the diffuse scattering data. In this paper we report on the latest progress that has been made in using this to solve the protein structure.

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MS21-O4 **Complex ordering in Metal Organic Framework.** Olivier Pérez, [a] Florence Porcher,[b] Joël Jaud,[c] Jean-Michel Rueff,[a]*CRISMAT/ENSICAEN, Caen, France,*[b] *LLB, Saclay, France,* [c]*CEMES, Toulouse, France.* E-mail: Olivier.perez@ensicaen.fr

The coordination polymers, also called metal–organic frameworks (MOFs), have been extensively studied the last decades. These hybrids materials, synthesized from metal and polyfunctional organic precursors, lead to 1D, 2D or 3D structures and could be used for their properties in diverse fields including magnetism, luminescence, catalysis, gas storage or drug release. The observed crystalline edifices present usually "classical orderings" but complex structural arrangements, consequence of the relative flexibility of the organic part, can be observed. Thus, an accurate analysis of diffraction patterns of some coordination polymers reveals weak additional reflections related to the existence of commensurate or incommensurate modulations. Most of the time these reflections can be easily forgotten: the structure of the MOF is then globally correct but some details are missing … and this feature is attributed to disorder. The collection of the weak reflection and their use sometimes via the superspace formalism [1] is essential for revealing the fine structure of these MOFs. Our purpose is to show that these complex ordering are not so anecdotal; in this aim three examples of coordination polymers exhibiting different degrees of ordering will be described. In the first chosen MOF, $Mn_2(O_3P-C_4H_2S-O_3P).2H_2O$, the possible rotation of the thiophene heterocycle around the direction defined by the two P atoms prevents the location of the cycles. But weak diffraction phenomena leading to a cell distortion provide a key for deciphering the apparent disorder. In the second example, the $LaC_{14}H_{12}N_2O_{10}$ compound [2] crystallizes in a triclinic symmetry and exhibits an incommensurate modulated structure. The modulation is characterized by a modulation vector with three irrational components (-0.184, -0.439, 0.415) respectively along $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$. The satellite reflections associated to this vector are relatively difficult to locate since both weak and apparently "lost" in the diffraction patterns. But the use of these reflections and of the superspace formalism is the only to reveal the true structure of this coordination polymer. Finally, a complex incommensurate host-guest system based on gallium and terephthalate group (BDC) will be described [3]. H2BDC molecules are inserted in the framework built from Ga and BDC. The mismatch observed between the **a** parameters of the two orthorhombic sub lattices (a_1=6.76Å, b_1=17.53Å, c_1=12.19Å for the host and a_2=4.74Å, b_2= b_1, c_2= c_1 for the guest) is characteristic of a composite structure; satellite reflections relating to their mutual interaction are clearly visible. The reveal the existence of an intrinsic incommensurate modulation revealed by the existence of additional reflections located at $\mathbf{q_2}$=0.119$\mathbf{a_1}^*$ is in agreement with a breathing phenomena of the host framework. The analysis of such structure requires five dimensional approach.

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Metal-organic Framework; aperiodicity; complex ordering