ESRF	**Experiment title:** **Disorder** in Urea Inclusion Compounds	**Experiment number:** **HC-153**
Beamline: **D2AM**	**Date of experiment:** **from:** **26.4.1995** **to:** **29.4.1995** **5.7.1995** **to:** **7.7.1995**	**Date of report:** **28.7.1995**
Shifts: 9+6	**Local contact(s):** J. F. Berar, F. Bley	*Received at ESRF:*

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Report:

Urea inclusion compounds consist of a nearly hexagonal framework of urea molecules forming open channels along the c axis into which various long chain molecules can be embedded. Due to a weak lateral but strong longitudinal correlation between the guest molecules there are layers which are very sharp parallel to c* and diffuse perpendicular to c* with some intensity modulations [1]. There is a further system of (nearly) sharp satellite reflections, which are caused by an interaction of the host and the guest structure [2].

The aim of the experiment was to measure the widths and the exact positions of the layers and the satellites of the example compound urea+$C_{17}H_{36}$ in order to get detailed information about the correlations of the guest molecules and the interaction of the host and the guest lattices.

In the first experiment various experimental problems lead to non-satisfactory refection profiles and weak intensities, such that no diffuse scattering could be observed. Only a diffuse streak-system was observable which showed, that the streaks do not connect

the Bragg reflections in a straight, but in a wavy way. Due to the problems pointed out above no definite conclusions about the exact position of the streaks can be made.

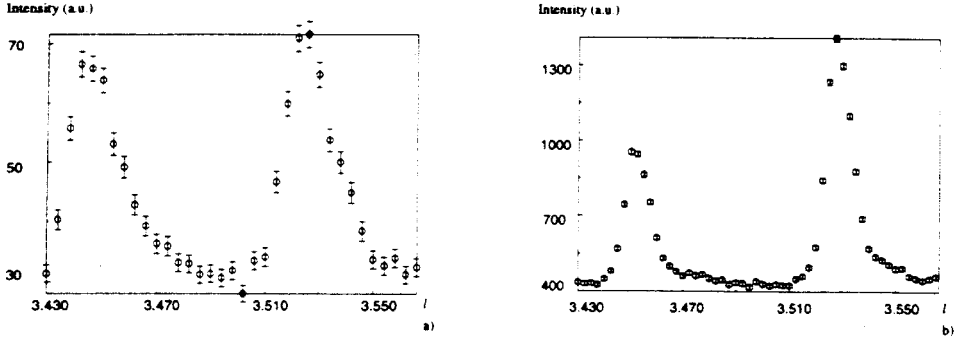

Fig. 1a): Pair of satellites measured in the first part of the experiment (15 sec/point)
Fig. 1b): Same satellites as in Fig. 1a) measured in the second part of the experiment (5 sec/point)

In the second experiment most of these problems were overcome (beamline optics, larger crystal, more suitable orientation, larger wavelength) and both satellites (see Fig. 1) and diffuse layers could be observed. One of the most interesting results was that the widths of the layers increase quadratically parallel 1 (Fig. 2) which was completly unknown so far. In consequence, only a short range order between the included molecules along c can be concluded. The satellites are broadened compared to the Bragg reflections. The satellite vector is the same as the translational vector of the layers. These results confirm, that the satellites are caused by an interaction between the guest and the host lattice. As the widths of very sharp (satellites) and broad diffuse (layers) phenomena can not directly be compared, they have to be analysed taking care of the resolution function of the instrument. This work is in progress.

At low temperature a vibration of the cryostat caused a swinging of the crystal which was mounted on a thin glass capillary (diameter 0.1 mm, side-thickness 0.01 mm) and prevented an exact measurement of the widths.

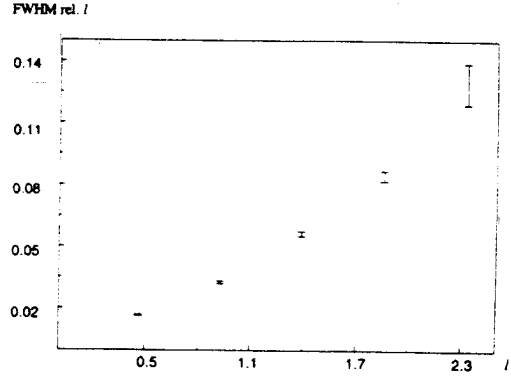

Fig. 2: Widths of diffuse layers parallel to c*

References:

[1] Fukao K. J. Chem. Phys. 101 (9), (1994) 7882-7892

[2 Weber T., Boysen H., Honal M., Frey F. in preparation