ESRF	**Experiment title:** Role of Hydrogen Bonding in the High Frequency Dynamics of CH_4, CH_3OH,NH_3,H_2O and HF	**Experiment number**: HS-1744
Beamline: ID16	**Date of experiment**: from: 06-03-02 to:13-03-02	**Date of report**: 29-8-02
Shifts: 21	**Local contact(s)**: P. Giura	*Received at ESRF:*

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Report:

We performed an experiment at ID16 to assess the detailed shape of the dynamic structure factor S(Q,ω) of liquid hydrogen fluoride (HF) in the momentum transfer region 1-15 nm^{-1} and as a function of the temperature. The temperatures we investigated were T=214K and T=254K. The results were then compared with the already existing measurements done at T=239K and T= 283 K.
Being T_m=193K the melting point of HF and T_b=292K its boiling point the whole liquid range has thus been investigated. A sample of the measured spectra at T=214K is reported in Fig.1 at the indicated momentum transfers. The spectra consist of a band centered at zero energy transfer which becomes broader on increasing Q and with a characteristic asymmetry due to the detailed balance.
A preliminary determination of the frequency of the sound excitations Ω(Q) and of the apparent sound velocity c(Q)=Ω(Q)/Q has been obtained fitting the spectra with a Lorentzian for the central line and a damped harmonic oscillator (DHO) for the inelastic signal. The dispersion curve Ω(Q) vs Q is reported in Fig. 2 as a function of temperature. It shows an increase of c(Q) from the low frequency value c_0 (as measured by Brillouin light scattering) to the high frequency value $c_{\infty\alpha}$ interpreted as due to the α or structural relaxation. To better characterize this relaxation a viscoelastic analysis has been done. In this approach, we take into account the presence of a second relaxation (microscopic) faster than the structural one. The relevant independent parameters coming out from this fit procedure are $c_{\infty\alpha}(Q)$, the infinite frequency limiting value of the sound velocity, $c_0(Q)$ the low frequency limiting value, $\tau_\alpha(Q)$ the structural relaxation time and Γ_μ,(Q) the strength of the microscopic relaxation. In Fig 3 we show the values obtained for $c_{\infty\alpha}(Q)$ and $c_0(Q)$ together with those for c(Q) as deduced from the DHO model. We observe that the positive dispersion found for c(Q) in the DHO analysis takes place between the values of $c_0(Q)$ and $c_{\infty\alpha}(Q)$ derived from the viscoelastic analysis. In Fig. 4 the relaxation times as function of Q are reported at the explored temperatures.

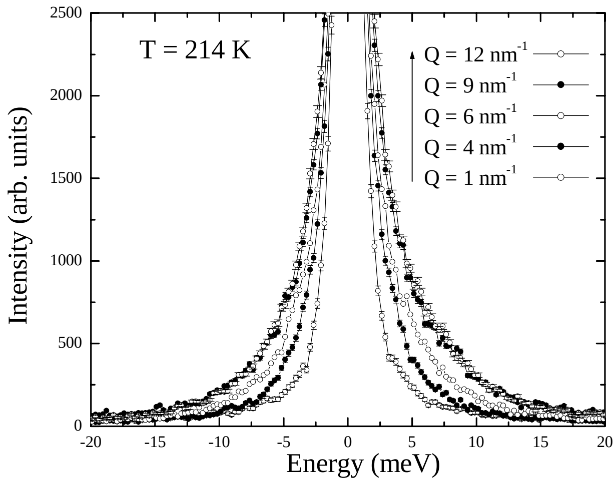

Fig.1: Example of IXS spectra at the indicated Q values and temperature.

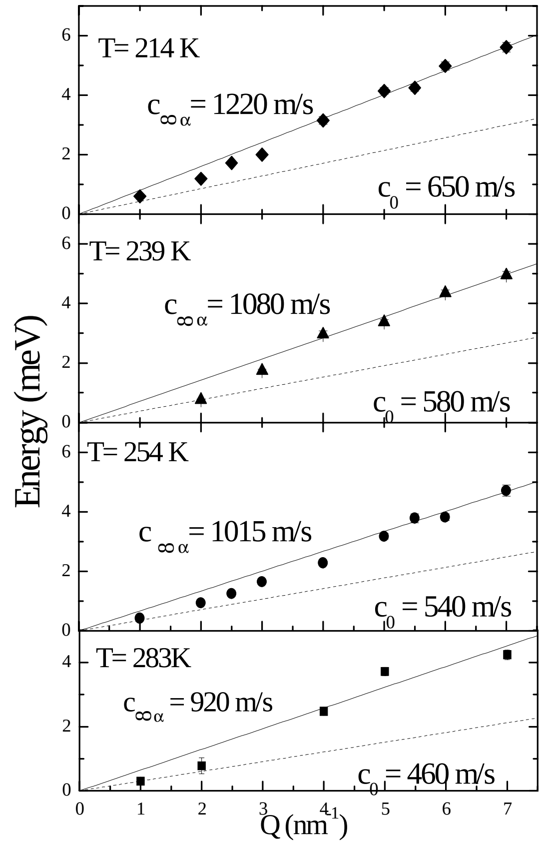

Fig.2: Dispersion curve at the indicated temperatures. The upper full lines are the linear fits to the high-Q data. The lower dashed lines indicate the adiabatic sound velocity as measured by Brillouin light scattering.

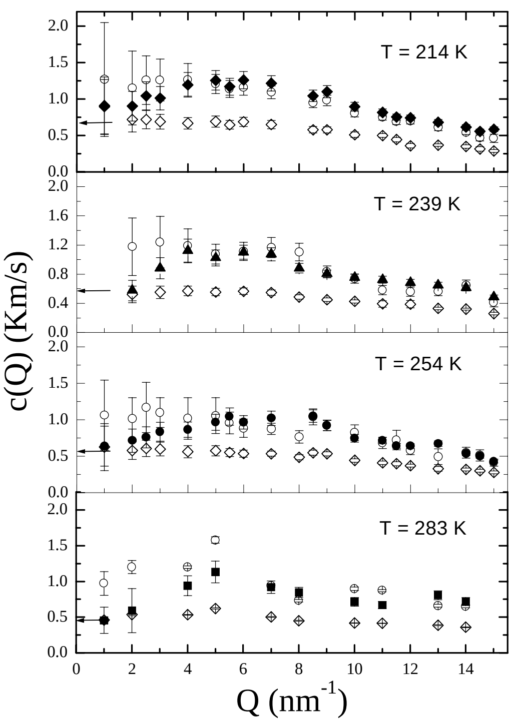

Fig.3: Q dependence of the sound velocity $c_0(Q)$ (open diamonds) and $c_{\infty\alpha}(Q)$ (open circles) from a viscoelastic analysis, together with c(Q) (full symbols) from Fig. 2. The value of the adiabatic sound velocity c_0 is indicated by the arrow.

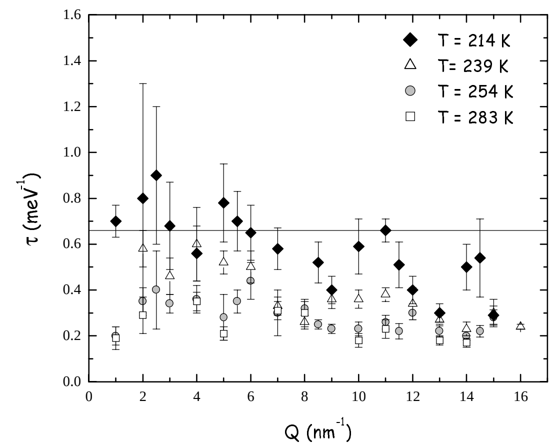

Fig.4: Relaxation time as a function of Q as obtained from the viscoelastic analysis and at the indicated temperatures.