



	<b>Experiment title:</b> Role of hydrogen bond in the high frequency collective dynamics of liquid systems: the case of HCOOH	<b>Experiment number:</b> HS-1983
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## Report:

We studied the dynamic structure factor  $S(Q,\omega)$  of liquid formic acid (HCOOH) as a function of temperature in the momentum transfer region  $1-15 \text{ nm}^{-1}$ . We investigated four temperatures and exactly  $T= 283\text{K}$ ,  $323\text{K}$ ,  $343\text{K}$  and  $363\text{K}$ ; since  $T_m=281\text{K}$  is the melting point of HCOOH and  $T_b=374\text{K}$  is its boiling point, all the liquid range as been explored.

In Fig.1 we report a sample of the measured spectra at one temperature ( $T = 283 \text{ K}$ ) in the low  $Q$  region and exactly for  $Q$  comprised between  $1$  and  $4 \text{ nm}^{-1}$ . A preliminary analysis of the spectra has been accomplished by fitting the data with a Lorentzian for the central line and a damped harmonic oscillator (DHO) for the inelastic part. The resulting line-shapes are superimposed to the data. The contribution of the central peak and of the inelastic side peaks are individually shown. The main fit parameter  $\Omega(Q)$ , which provides an estimate of the current maxima, has been plotted in Fig.2 as a function of  $Q$  in the range  $1\div 6 \text{ nm}^{-1}$ . The apparent sound velocity  $c(Q)=\Omega(Q)/Q$  is reported in the inset.

A more refined analysis has been performed in terms of viscoelastic model. In presence of a relaxation process it allows to extract the associated relaxation time. We focus our attention on the structural relaxation due to the rearrangements of the hydrogen bond networks in the liquid. The  $Q$  dependence of the relaxation time  $\tau_\alpha(Q)$  is reported in Fig.3 at the four investigated temperature in the range  $Q 1\div 15 \text{ nm}^{-1}$ . A constant fit at low  $Q$  provides, for each temperature,  $Q$  independent values of this parameter. They are plotted on a linear scale in Fig.4 as a function of the temperature. In the explored temperature range, the  $\tau_\alpha$  behavior is well described by the Arrhenius law (full line):

$$\tau_\alpha(T) = \tau_0 e^{E_a/KbT}$$

where  $E_a$  is the activation energy associated to the structural process.

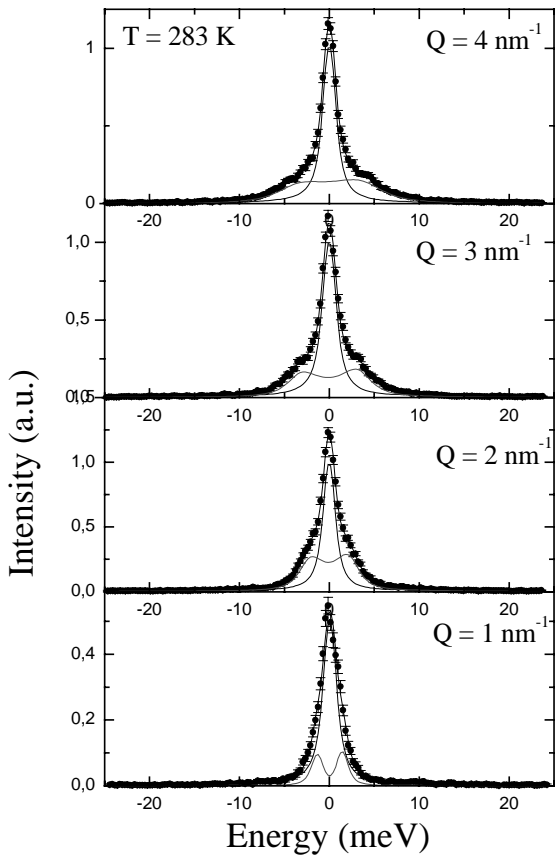


Fig.1: Example of the measured IXS spectra of HCOOH at the indicated  $Q$  values and temperature.

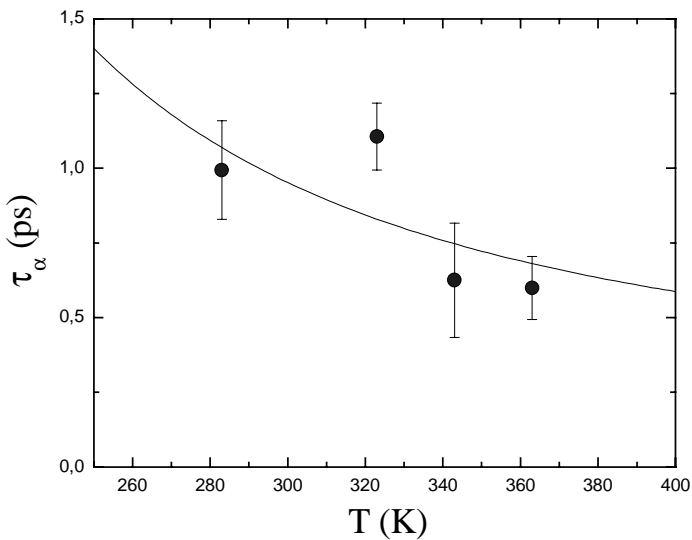


Fig.4:  $T$  dependence of the low- $Q$  extrapolation times of Fig.3 together with the Arrhenius fit (full line) of the equation reported in the text.

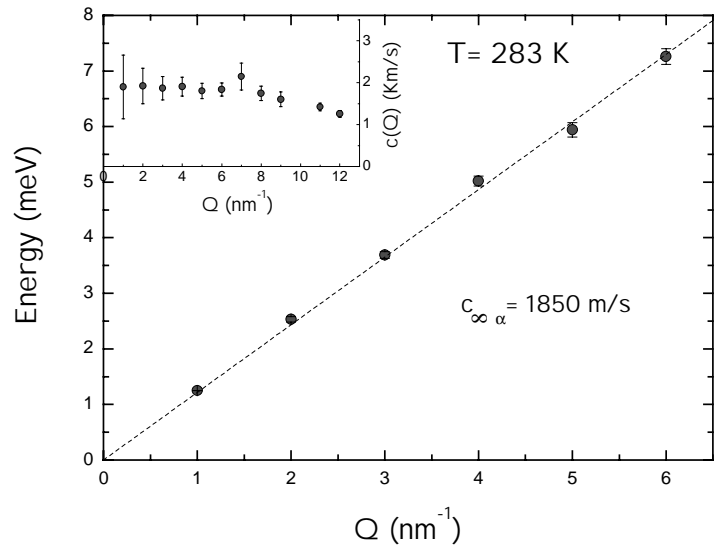


Fig.2: Example of dispersion curve at one of the four investigated temperatures. The dotted line is the linear fit to the data. In the inset the apparent sound velocity  $c(Q)=\Omega(Q)/Q$  is reported as a function  $Q$ .

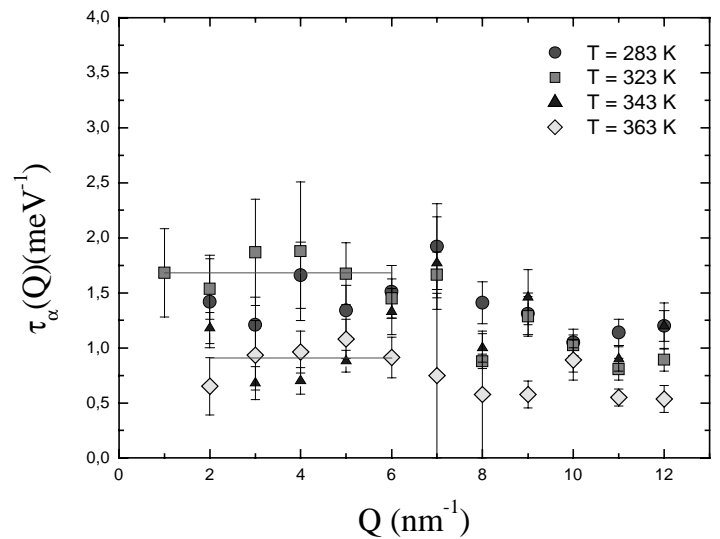


Fig.3:  $Q$ -dependence of the relaxation time  $\tau_\alpha(Q)$  from a viscoelastic analysis in HCOOH at the indicated temperatures.