ESRF	**Experiment title:** Structure of I_2 in the liquid along the coexistence curve up to the critical point and in the super-critical region	**Experiment number:** HS224
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Report:

In the preliminary run of this experiment we have successfully measured x-ray absorption spectra of low density 12 vapors from 423 K to 1100 K. The sample was confined in a sealed quartz cell 30 cm long heated in a specially designed furnace able to generate an homogeneous temperature field. Further measurements have been performed on liquid I_2 just above the I_2 melting point using an ambient pressure cell previously described [l]. Another set of measurements have been collected along the liquid-vapor coexistence curve using a pressurized vessel able to confine the high pressure fluid (up to 100 bar). For these measurements the high flux and stability of the instrument were essential to obtain high quality data due to the non negligible absorption of the sample environment.

Examples of spectra of liquid iodine at different temperatures (423 K, 523 K and 633 K, respectively, from top to bottom) are reported in the figure; they are dominated by the molecular I-I oscillating contribution. The measurements extend up to E=35 keV ($k > 20$ Å^{-1}) and are here truncated for clarity of presentation. The average noise level is in the low 10^{-4} range and this guarantees the possibility to determine the molecular parameters with high accuracy.

In comparison, neutron diffraction data [2] provide a complete information on the inter-molecular atomic distribution, but are less precise in the determination of the molecular parameters due to the limited q range. XAS and ND are therefore highly complementary and an increased insight into the structure of this molecular fluid can be obtained by combining the information available from the two techniques. The interest in a precise determination of the I-I bond-length distribution resides in its sensitivity to the average inter-molecular interactions in the fluid. The bond length of an isolated I_2 molecule expands from $R \approx 2.68$ Å to $R \approx 2.70$ Å in the liquid just above the melting point. The expansion of liquid I_2 on increasing temperature (as clearly seen by the decrease of the x-ray absorption edge jump in the three spectra) produces a modification of these interactions which we are now able to reveal in the changes of the EXAFS spectra.

This experiment is the natural continuation of a research line initiated at ESRF with project HC120 whose results are now included in a comprehensive paper [3].

[l] E. Degiorgi, P. Postorino, and M. Nardone, Meas. Sci. Technol. 6, 8929 (1995).

[2] M. C. Bellissent-Funel, U. Buontempo, M. Nardone, F. P. Ricci, and M. A. Ricci, Phys. Rev. B 50, 6047 (1994).

[3] U. Buontempo, A. Di Cicco, A. Filipponi, M. Nardone, and P. Postorino, 'Deter-***mination of the I_2 bond-length distribution in Liquid, solid, and solution, by EXAFS spectroscopy. ",*** (submitted 1997).