ESRF	**Experiment title:** STUDY OF THE BROMINE METALLIZATION	**Experiment number:** **HS215**
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Report:

The properties of molecular solids are of central interest, both from a theoretical point of view and for applications, in astrophysical problems for example. Among them, those build from diatomic molecules like 1_2, Br2, O_2 are of special interest with respect to the metallization process. They may be used as models for the metallization of hydrogen which, at the present state of theoretical calculation, may happen above 300 GPa at ambient temperature and is therefore out of reach using static compression. The determination of the pressure dependence of the intramolecular distance is of central interest in order to validate the theoretical calculations on metallization. Another one important point to be solved is to determine whether the metallization transition occurs in the molecular solid, or is associated or preceded by the molecular dissociation. It is therefore important to measure the intramolecular distance, and, due to the energetic position of its K edge, bromine is very well adapted for such a measurement.

The present experiment has been performed in a diamond anvil cell with beveled diamonds. The diameter of the diamonds culets was 100 µm, and that of the bevel was 300 pm. The hole in the stainless steel gasket was 50 µm. It was completely filled by the bromine, and therefore, the I_0 was measured for each pressure by completely removing the cell. The pressure was measured using the ruby fluorescence.

The x-ray beam was focused down to 50 µm in the horizontal plane, and limited by a 20 µm wide slit in the vertical plane. Under these conditions, and due to the insufficient stability of the beam on the sample, it was impossible to obtain spectra clean enough to deduce the variation of the intramolecular distances through an analysis of the EXAFS oscillations. On the contrary, the XANES part of the spectra was cleaner, and gives interesting information. Indeed, it has been shown that in diatomic molecular solids, like I_2 or Br_2, the π^* molecular antibonding orbitals gives rise to a strong absorption peak below the absorption edge. It is therefore the fingerprint of the molecular nature of the compound and should disappear I case of molecular dissociation.

In a study by x-ray diffraction up to 88 GPa, Fujii et al[1] claimed that the bromine molecule is dissociated around 80 GPa, when a transition from the low pressure structure Cmca to a Immm structure takes place together with the metallization.

In the present experiment, we could measure the XANES spectra up to pressure above 100 GPa. (due to the gratings of the spectrometer dedicated to the pressure measurement, we were not able to determine pressures above 90 GPa). On the figure are shown spectra taken during the increase of the pressure. At the highest pressure, above 100 GPa, the pre-edge peak is still clearly seen, which definitely proves that far above the claimed crystallographic transition pressure, bromine is still a diatomic molecular solid.

[I] Y. Fujii et al, Phys. Rev. Lett 63, 536 (1989)

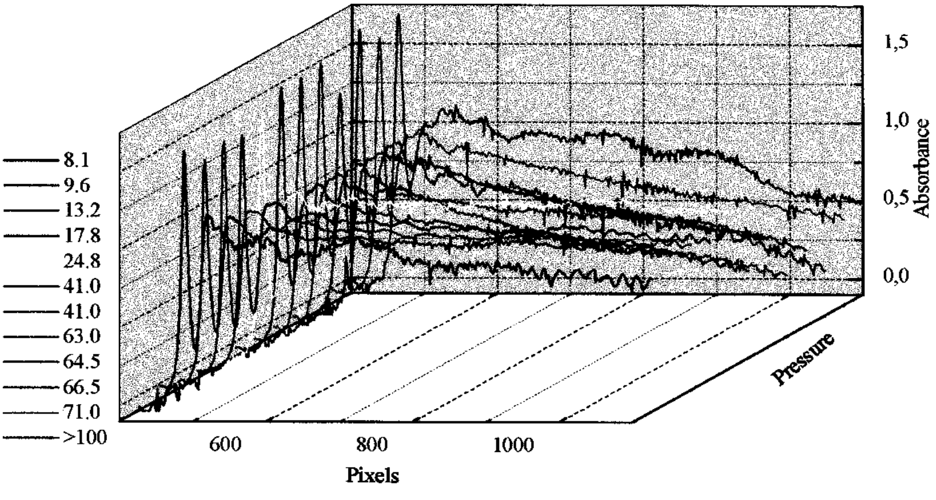

Figure 1 EXAFS spectra of Br_2 at various pressures. The pressures are in GPa.