ESRF	**Experiment title:** Structural study of LiH in the range 100 GPa - 200 GPa: search for the B1-B2 phase transition.	**Experiment number**: HS 2866
Beamline: ID27	**Date of experiment**: from: 17 November 2005 to: 21 November 2005	**Date of report**: September 14, 2006
Shifts: 12	**Local contact(s)**: Mohamed MEZOUAR	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Paul LOUBEYRE* and Florent OCCELLI*

CEA-DPTA

B.P. 12

91680 Bruyères-le-Châtel

FRANCE

Report:

The aim of the proposal was to extend previous single crystal structural determinations of LiH in the 100 GPa – 250 GPa range. Apart from constraining better the EOS of this compound the main goal was to look for two structural transitions, namely: the rocksalt (B1) structure to the cesium-chloride (B2) structure; the metallisation predicted in the range 85 GPa to 450 GPa [1,2].

The proposal was allocated 12 shifts of beamtime on ID27. 3 diamond anvils cells (DAC) were brought loaded with single-crystals of LiH compressed in a ring of gold. 75 μm and 50 μm culets were used, the typical size needed to reach the 200 GPa range. The LiH single crystals were smaller than 12 μm. The breakage of the single crystal was observed under pressure, leading to a 6° width for the rocking curve.

The maximal pressure attained during this run was 200 GPa at room temperature, the pressure being measured using the diffraction pattern of the gold ring. Five gold diffraction peaks were recorded. Only the (200) peak of the B1 phase of LiH could be followed up to the maximum pressure.

Figure 1 displays the first analysis of the data. It is seen that the extension of the EOS above 100 GPa is in good agreement with the previous determinations by using He as a pressure hydrostatic medium. The pressure inverted from the gold diffraction pattern has not been corrected yet for uniaxial stress. That can explain the slight deviation from the extrapolation of previous measurements up to 100 GPa under hydrostatic condition and the dispersion of the data points.

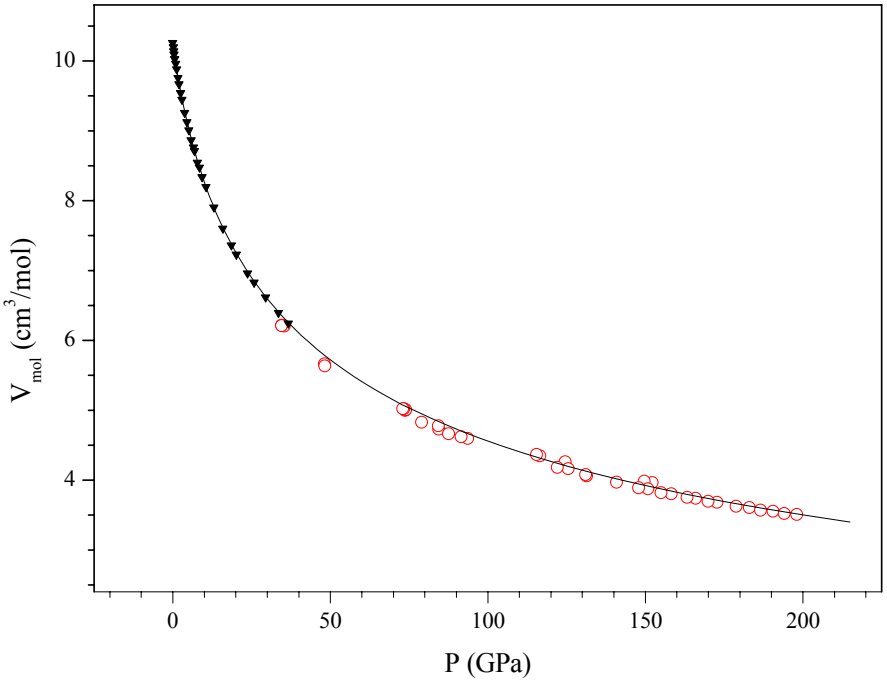

Fig. 1: LiH Equation of State up to 200 GPa. The symbols are: ○ Dataset collected during this experiment, ▼ published data [2] with pressures corrected according to the new scale, — Vinet fit to the full experimental dataset.

A first look at this curve shows that:

1- no phase transformation occurs in the 200 GPa range;
2- the LiH bulk parameters (V_0, K_0, and K_0') derived from a Vinet fit to the full dataset (that is this run data + the lower-pressure results[2]) are close to those published[3];

Furthermore, around the maximum pressure, the LiH sample was optically observed to turn orange. That could indicate a closure of the electronic gap. Hence, metallization could occur in the 200-300 GPa range, which is within the reach of spectroscopic measurements performed in a diamond anvils cell[4], but yet out of the reach of x-ray measurements.

References:

[1] S. Duclos et al, Phys.Rev.B **36:**7664 (1987).

[1] Q. Gou et al, High Press. Res. **6**:141 (1991).

[2] J.L. Martins, Phys. Rev. B **41**:7883 (1990).

[3] P. Loubeyre *et al.*, Phys. Rev. B **57**:10403 (1998).

[4] P. Loubeyre *et al.*, Nature **416**:613 (2002).