ESRF	**Experiment title:** Structural properties of LiH and LiD at high pressure	**Experiment number:** HC 243
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Report:

The equation of state of LiH has been measured up to 4 GPa by piston-cylinder technique and up to 9 GPa[2] by neutron diffraction in a large volume pressure cell. It has been speculated and calculated that the B_1-B_2 phase transition, observed in other alkali hydrides and alkali halides,[3,4] may occur in LiH at a pressure at the limit of the current DAC capabilities (> 85 GPa -400 GPa), if at all.[4,5] However, the possibility of other structural phase transitions, appearing at lower pressures, cannot be ruled out.

The aim of this work was to measure, for the first time, the structural properties of LiH at a pressure higher than 9 GPa. The method used in this experiment to achieve x-ray diffraction from ultra-light elements under high pressure in a DAC, involves a combination of single crystal and energy-dispersive diffraction techniques with polychromatic radiation, using the high brightness of the wiggler beamline. Two Membrane DAC's were loaded for this experiment, containing each a single crystal of LiH, immersed in He, having dimension approximately of 15 μm (sample 1) and 80 μm (sample 2), respectively. With sample 2, by means of the observation of the diffraction peaks, it has been possible to measure the lattice parameter and to derive the equation of state of LiH in a previously unexplored pressure range, up to about 40 GPa. With sample 2, due probably to the poor quality of the single crystal, no diffraction peaks were detected.

Fig. 1 shows, as a function of pressure, the lattice parameter of LiH (this experiment) and of LiD (ref. 2). The solid lines fit the experimental data by means of the Vinet (LiH) and Birch (LiD) EOS's. The difference between the two compounds, related to the different zero-point energy of the proton to that of the deuteron, evident at low pressure, seems to increase with pressure, if one relies on the extrapolation of the LiD EOS.

Fig. 2 reports the quantity V/V_0 vs. pressure for the two compounds (LiD, thick line, LiH, thin line). The difference between the two compounds is evident only above 30 GPa, where the uncertainty due to the extrapolation of the LiD EOS is of the same order of magnitude. This uncertainty is estimated from the difference between the EOS's of LiH derived considering, in turn, all the experimental points or only those up to 10 GPa. We conclude that, up to the pressure reached in this experiment, no difference is found between LiH and LiD if one is concerned with the ***relative*** volume change.

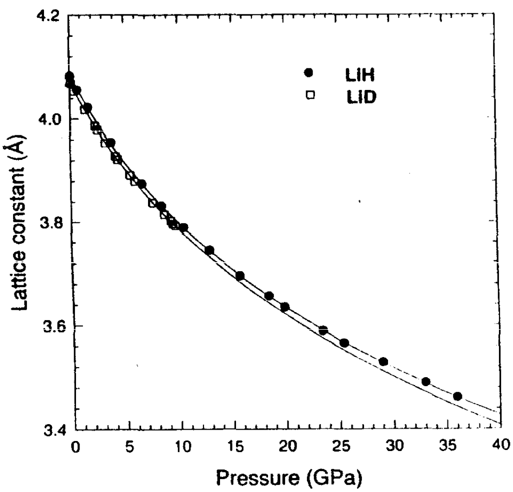

Fig. 1

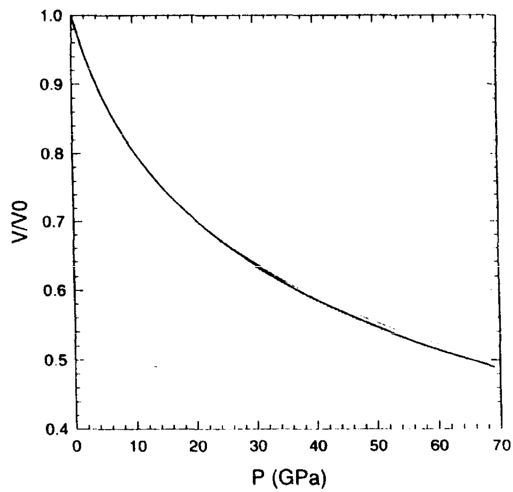

Fig. 2

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