ESRF	**Experiment title:** Reference equation of state for light alkali halides	**Experiment number**: HS-4328
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Report:

The aims of this proposal were (i) to establish reference ambient temperature equations of state (EoS) for alkali halides which are often used as pressure transmissing media in high pressure devices, but for which the equation of state was poorly constrained above 30 GPa: LiF, KCl, KBr; (ii) to refine the equation of state of NaCl at moderate pressure, by a cross-check with different metals EoS. In fact, it has been suggested that the Decker's NaCl EoS [1], which is at the basis of ruby metrology, underestimates pressure by up to 10 % around 10 GPa [2].

We have prepared several diamond anvil cells, loaded with alkali halides, ruby and metals (both pressure markers) embedded in helium pressure transmitting medium. This pressure medium ensures hydrostatic compression conditions at pressures below freezing (11.6 GPa), and quasi-hydrostatic above this pressure. We have used angle-dispersive X-ray diffraction (λ=0.4155 Å) with a MAR imaging plate. The X-ray diffraction spectra of different samples have been collected separately, by translations of the diamond anvil cell. Pressure was primarily estimated from ruby luminescence signal [3]. The conditions of experimental runs are summarized in **Table 1.** X-ray diffraction signal has been analyzed using Fit2D and Igor softwares.

Cell name	samples	Pressure medium	P domain
CDMX11	NaCl	He	27-155 GPa
CDMX19	LiF+Re	He	14.4-90 GPa
CDMX7	KCl+KBr	He	27.5-154 GPa
CDMX9	NaCl+Cu+Al+W	He	0.36-10.4 GPa
CDMX12	LiF+KCl+KBr+Re	He	0.75-36 GPa
CDMX6	NaCl+LiF+Cu+Al	He	0.9-30 GPa

Table 1: conditions of experimental runs.

The 300K EoS of KCl and KBr have been measured up to 154 GPa; they are presented in **Figures 1** and **2**. They will be complemented by a thermal part calculated with ab initio molecular dynamics to establish a high pressure-high temperature equation of state which will be suitable for analysis of laser-heated diamond anvil cell experiments. The equation of state of LiF has been measured up to 90 GPa.

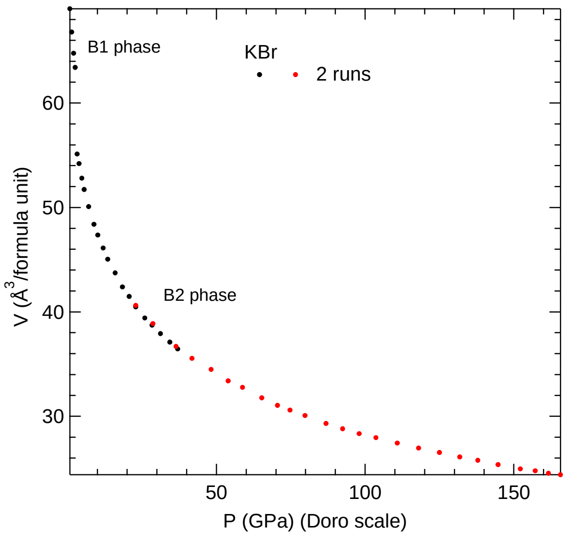

Figure 1: 300K-Equation of state of KBr, compressed in a quasi-hydrostatic pressure medium in a diamond anvil cell. The B2 phase P-V points can be fitted by a Vinet EoS with the following parameters: V_0 =63.74 A^3, K_0 =14.78 GPa, K'_0=5.79.

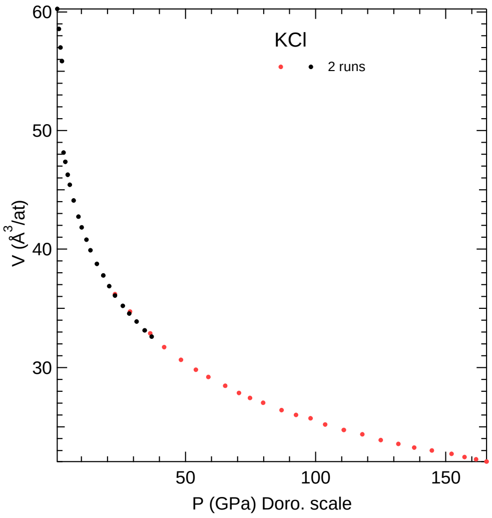

Figure 2: 300K-Equation of state of KCl, compressed in a quasi-hydrostatic pressure medium in a diamond anvil cell. The B2 phase P-V points can be fitted by a Vinet EoS with the following parameters: V_0 =55.859 A^3, K_0 =15.3 GPa, K'_0=5.98.

The volume of NaCl as a function of ruby pressure has been measured up to 155 GPa. Under moderate pressure, if the pressure is calculated from this NaCl volume using Decker scale [1], a slightly lower pressure (~1-2%) than ruby pressure is found (**Fig. 3**). It either suggests that Decker scale underestimates pressure, but not as much as suggested in Ref. [2], or that the Ruby scale [3] overestimates pressure. We favor the last hypothesis, because Al and Cu EoS derived from ultrasound measurements are also slightly lower than the ruby pressure.

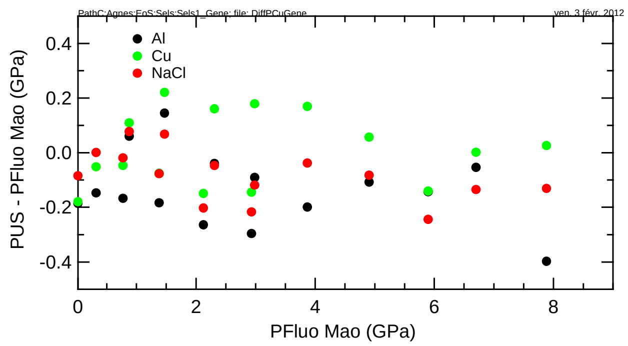

Figure 3: Difference between PUS(V) (pressure calculated using Ultra Sound EoS parameters [1]) and PFluo Mao (pressure from ruby fluoresence [3]), for NaCl, Cu and Al, as a function of PFluoMao. Data from last experimental run.

[1] D.L. Decker *et al.*, High-pressure calibration – a critical review, J. Phys Chem Ref. Data 1, 773, 1972
[2] B. Li *et al.*, P calibration to 20 GPa by simultaneous use of ultrasonic and x-ray techniques, J. Appl. Phys. 98, 13521, 2005
[3] Mao H.K., Xu J., and Bell P.M. (1986) J . Geophys. Res. 91, 4673.