ESRF	**Experiment title:** **Dynamic and electronic coupling of encaged atoms in the Ba_8Si_{46} clathrate**	**Experiment number:** **HS-3310**
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Shifts:	**Local contact(s):** Alexei BOSSAK	*Received at ESRF:*

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Report:

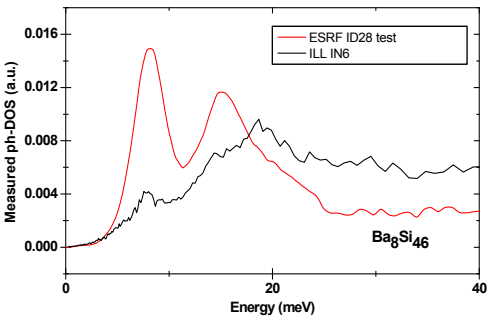

Fig1. *Generalized total inelastic scattering signal of Ba8Si46 as obtained by IXS and by INS. The rattling modes are better evidenced by IXS.*

Silicon clathrates are intercalated forms of sp^3 silicon that allow to multiply the pressure stability of the tetrahedral Si arrangement by a factor of four. This extraordinary stability is nevertheless affected by the presence of two "isostructural" transitions whose exact nature remains unclear. The aim of the proposal was to study the pressure evolution of the total phonon density of states to explore the nature of the observed instabilities. We were in particular interested in the characteristic rattling Einstein-type modes of the guest species (Ba in this case) which allow to monitor hybridization changes or even the integrity of the cage-structure**.**

The IXS signal of Ba_8Si_{46} taken outside the diamond anvil cell and after data treatment is shown in Fig 1. It is clearly appreciable that the contrast offered by the x-ray scattering cross sections allows for a better observation of the low energy rattling modes.

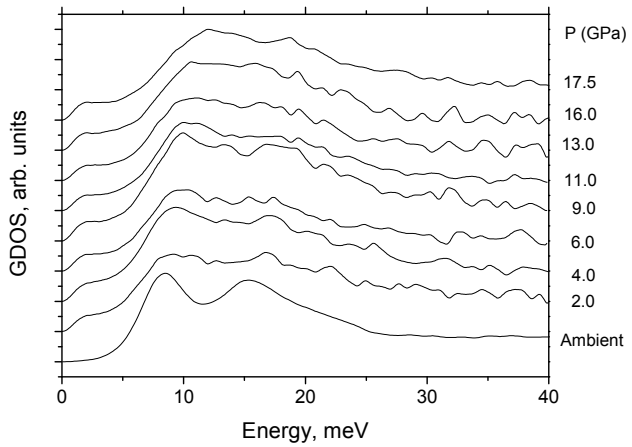

Fig2. *Pressure evolution of the GDOS of Ba8Si46 as obtained by IXS.*

The obtained evolution of the same signal under pressure is shown in Fig. 2 and compared with the signal at ambient conditions. The important reduction of S/N is due to the x-ray attenuation by the sample environment. In spite of these losses, the analysis of the obtained signal is providing quantitative information in relation with the isostructural transition that will be soon submitted for publication.