ESRF	**Experiment title:** Crystal structure of Bechgaard salts under pressure	**Experiment number:** HS-3107
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Shifts: 9	**Local contact(s):** Dr. Michael HANFLAND (e-mail: hanfland@esrf.fr)	*Received at ESRF:*

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Report:

The high-pressure experiment has been performed on two isostructural organic Bechgaard-Fabre salts $(TMTTF)_2PF_6$ and $(TMTSF)_2PF_6$. These compounds are characterized by a very anisotropic crystal structure and represent model examples of quasi-one-dimensional conducting systems [1]. The main goal of the experiment was to obtain the pressure dependence of the lattice constants and the unit cell volume which is very important for the analysis of infrared spectroscopy data and dc transport measurements. In addition, the possibility of structural transformations under high pressure had to be verified.

The single crystal diffraction experiments on each compound loaded in the diamond anvil cell (DAC) filled with helium as pressure transmitting medium have been performed at room temperature. The DAC rotation angle varied from $-30°$ to $+30°$ for $(TMTTF)_2PF_6$ and from $-20°$ to $+20°$ for $(TMTSF)_2PF_6$ with $-2°$ step. In addition, a powder diffraction experiment has been done on $(TMTSF)_2PF_6$, in order to verify the pressure induced structural transition. Data collection has been performed from 0 to 10 GPa, some pressure points have been collected on pressure release. The pressure has been determined using a ruby luminescence system.

The 2D diffraction patterns have been processed with the Fit2D software [2] and the single crystal data have been analyzed using the XDS package [3]. The pressure dependence of the normalized cell parameters of $(TMTTF)_2PF_6$ and $(TMTSF)_2PF_6$ compounds is shown in Fig. 1.

Another important result of the experiment is the evidence for structural phase transitions in both compounds, which occur at around 8.5 and 5.5 GPa in $(TMTTF)_2PF_6$

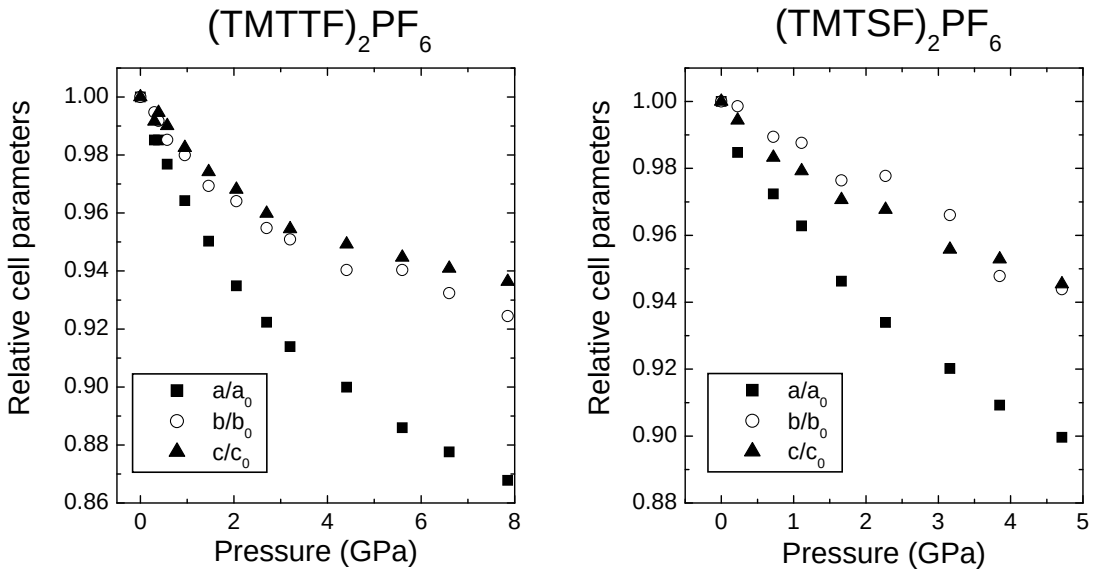

Fig. 1. Normalized cell parameters of $(TMTTF)_2PF_6$ and $(TMTSF)_2PF_6$ salts as a function of pressure.

and $(TMTSF)_2PF_6$, respectively. Preliminary analysis reveals the abrupt change of the γ angle and b lattice constant across the transition pressure as it is demonstrated in Fig. 2. The transition pressure offset of 3 GPa between the two compounds is in good agreement with the generic phase diagram of the Bechgaard-Fabre salts [1]. However, more detailed analysis of the data is necessary in order to determine the structure and symmetry of the high pressure phase in both compounds.

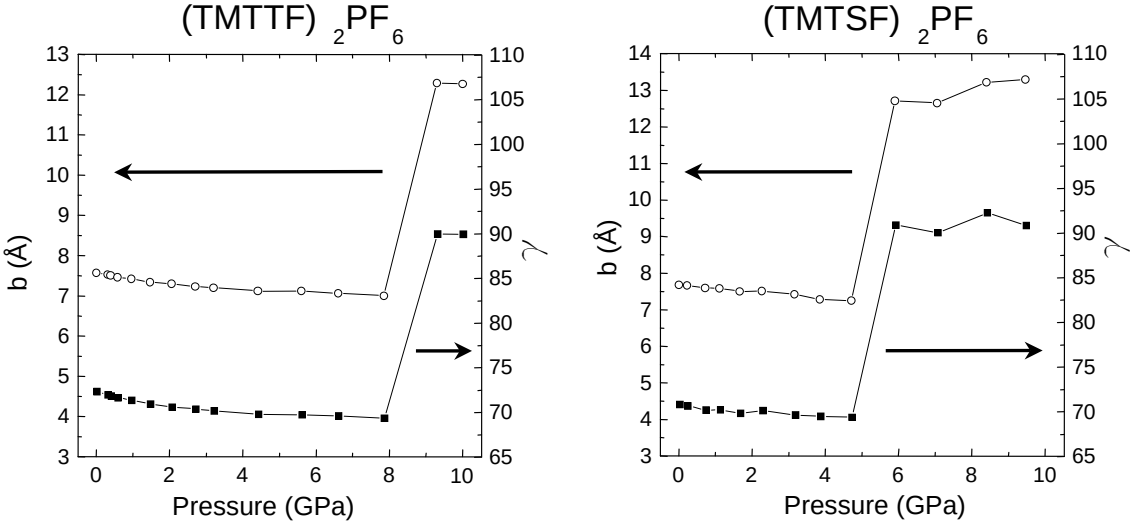

Fig. 2. Change of the lattice parameters b and γ across the structural phase transition.

References:
[1] D. Jerome, *Chem. Rev.* **104**, 5565 (2004).
[2] A. P. Hammersley, S. O. Svensson, M. Hanfland, A. N. Fitch, and D. Häusermann, *High Press. Res.* **14**, 235 (1996).
[3] W. Kabsch, *J. Appl. Cryst.* **26**, 795-800 (1993).