ESRF	**Experiment title:** Search for the ideal antiferroelectric soft mode in the francisite $Cu_3Bi(SeO_3)_2O_2Cl$	**Experiment number**: HC-4041
Beamline: ID28	**Date of experiment**: from: 12/09/2018 to: 17/09/2018	**Date of report**: 29/02/2020
Shifts: 12	**Local contact(s)**: Luigi Paolasini, Alexei Bossak	*Received at ESRF:*

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Report:

The following experiments were performed:

- Inelastic scans at the Z point (5 0 -0.5) at 8 different temperatures between room temperature and the transition at 115 K
- Phonon dispersion along the 5 0 -0.5+L and (5+H 0 -05) direction at two temperatures
- Diffuse scattering in fine temperature steps between room temperature and ~100 K.

The experiment was successful and confirmed the presence of the expected soft mode as hypothesized in the proposal. The results were integrated in a paper that was accepted in Physical Review Letters (2020, in print). See also https://arxiv.org/abs/1907.12069.

Abstract of the accepted paper:

Model materials are precious test cases for elementary theories and provide building blocks for the understanding of more complex cases. Here, we describe the lattice dynamics of the structural phase transition in francisite $Cu_3Bi(SeO_3)_2O_2Cl$ at 115 K and show that it provides a rare archetype of a transition driven by a soft antipolar phonon mode. In the high-symmetry phase at hightemperatures, the soft mode is found at (0,0,0.5) at the Brillouin zone boundary and is measured by inelastic X-ray scattering and thermal diffuse scattering. In the low-symmetry phase, this softmode is folded back onto the center of the Brillouin zone as a result of the doubling of the unit cell, and appears as a fully symmetric mode that can be tracked by Raman spectroscopy. On both sides of the transition, the mode energy squared follows a linear behaviour over a large temperature range. First-principles calculations reveal that, surprisingly, the flat phonon band calculated for the high-symmetry phase seems incompatible with the displacive character found experimentally. We discuss this unusual behavior in the context of an ideal Kittel model of an antiferroelectric transition.