

Experiment title:

Structural disorder in the quantum spin liquid candidate $Na_2BaCo(PO_4)_2$

number: HC-4369

Beamline:

Date of experiment:

ID22

from 22.09.2021 to 26.09.2021

Date of report:

Shifts:

Local contact(s):

Ola Grendal

13.08.2022

Experiment

Names and affiliations of the applicants:

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This experiment was focused on the structural study of the triangular quantum spin-liquid candidate $Na_2BaCo(PO_4)_2$ and its chemical analogs. In the case of $Na_2BaCo(PO_4)_2$, we confirmed trigonal symmetry but revised the space group as $P\bar{3}$ contrary to $P\bar{3}m1$ reported previously [PNAS 116, 14505] (2019)]. We have also observed a subtle disorder effect reflected by the unusually high displacement parameter of Na atoms. We are currently investigating this effect using NMR as the local probe.

In the second part of the experiment, we studied temperature-dependent crystal structure of the new compound Na₂SrCo(PO₄)₂ that proved to be even more interesting for the high-resolution setup of ID22. Here, reflection splitting was clearly observed at room temperature, indicative of the monoclinic symmetry. We then found two phase transitions upon heating, from $P2_1/a$ to C2/m around $650 \,\mathrm{K}$ and from C2/m to $P\bar{3}m1$ around $1025 \,\mathrm{K}$. The results on Na₂SrCo(PO₄)₂ have been **published** in [Phys. Rev. B **106**, 054415 (2022)].

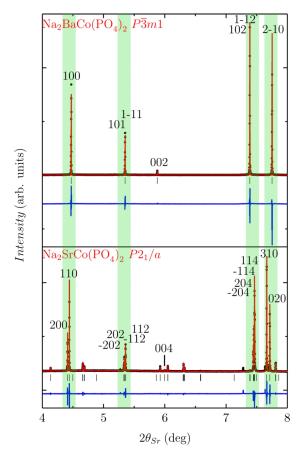


Figure 1: Comparison of room-temperature XRD data for $Na_2BaCo(PO_4)_2$ (trigonal, $P\bar{3}$) and $Na_2SrCo(PO_4)_2$ (monoclinic, $P2_1/a$). The 2θ values for the Ba compound were adjusted in order to match peak positions of the Sr phase.