Experimental report

17/08/2021

Proposal: 5-21-1137 **Council:** 10/2019

Title: A Variable Temperature Investigation of Ba7Li3Ru4O20; a disordered, mixed geometry structure

Research area: Chemistry

This proposal is a new proposal

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Samples: Ba7Li3Ru4O20

Instrument	Requested days	Allocated days	From	To
D2B	2	2	24/08/2020	26/08/2020

Abstract:

We are asking for beam-time to investigate the hexagonal structure of Ba7Li3Ru4O20 using neutrons. We have recently reported exceptional transport properties in two hexagonal perovskite derivatives, Ba3MNbO8.5 and Ba7Nb4MoO20. These materials have great potential for many technological applications such as electrolyte materials in solid-state fuel cells and in multiple sensor devices. Intensive variable temperature diffraction studies have shown us that there are several key structural pre-requisites which work to aid ionic transport within these hexagonal unit cells. The transport properties of the 7-layered hexagonal material, Ba7Li3Ru4O20, are currently being investigated at the University of Aberdeen as the structure possesses several of these key features.

There was an amendment to the material described within the proposal. Instead of measuring the Li based material, another similar hexagonal perovskite ($Ba_6Nb_{1.5}W_{1.5}O_{14.25}$) was measured. We could not synthesise the Li-based material to a high enough purity, and it was incredibly air sensitive.

The sample was measured in August 2020 in a silica tube, backgrounds were run on D2B. Variable temperature measurements were taken between room temp and 800^{o}C.

RITTER emailed the data to WILDMAN upon completion.

Currently the Rietveld analysis of the data is going well. It is a new composition with a supercell structure similar to that of γ-$Ba_4Nb_2O_9$ (high temperature polymorph). The phase is stable across the entire temperature range, which is in contrast to γ-$Ba_4Nb_2O_9$. There are > 90 atoms in the unit cell. In $Ba_4NbWO_{9.5}$, there are 4 additional oxygen sites within the unit cell which are highly disordered and vacancies are distributed across them. This additional disorder, injected into these 2D layers is the reason for the increased proton conductivity of the tungsten analogue (compared to $Ba_4Nb_2O_9$).

The neutron diffraction analysis will be published alongside the physical property measurements of $Ba_4NbWO_{9.5}$ in due course. We will aim to publish in Chemistry of Materials.