Experimental report

01/05/2026

Proposal: EASY-1451 **Council:** 10/2024

Title: Structure of metal/ammonia intercalated NbSe2

Research area: Chemistry

This proposal is a new proposal

Main proposer: Simon James CLARKE

Experimental team:

Local contacts: Emmanuelle SUARD

Samples: ammonia-intercalated lithium rubidium niobium selenide (NH3)xLi0.2Rb0.2NbSe2

Instrument	Requested days	Allocated days	From	To
D2B	6	6	03/07/2025	04/07/2025

Abstract:

Niobium selenide can be intercalated with alkali metals and this controls the superconductivity. These compounds can also absorb small molecules. Here we propose to investigate the composition (NH3)xLi0.2Rb0.2NbSe2 in which ammonia is co-intercalated with Li and low temperature (~3K) superconductivity emerges.

EXPERIMENTAL REPORT

EXPERIMENT N° EASY-1451 INSTRUMENT D2B

DATES OF EXPERIMENT 03/07/2025 - 04/07/2025

TITLE Structure of lithium ammonia intercalate of ZrNCl

EXPERIMENTAL TEAM (names and affiliation)

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LOCAL CONTACT SUARD, Emmanuelle

Date of report 1/05/26

Multiple alkali metals may be intercalated into the layered superconductor $NbSe_2$. In this experiment we intercalated Rb at high temperatures and subsequently intercalated Li at low temperature using a solution of Li in liquid ammonia. Rietveld refinement against the 1.59 Å data is shown below in Figure 1. These systems are structurally challenging because of partial occupancies, the difficulty of locating disordered H (or even D) and the model shown below is approximate. Further investigations are in progress.

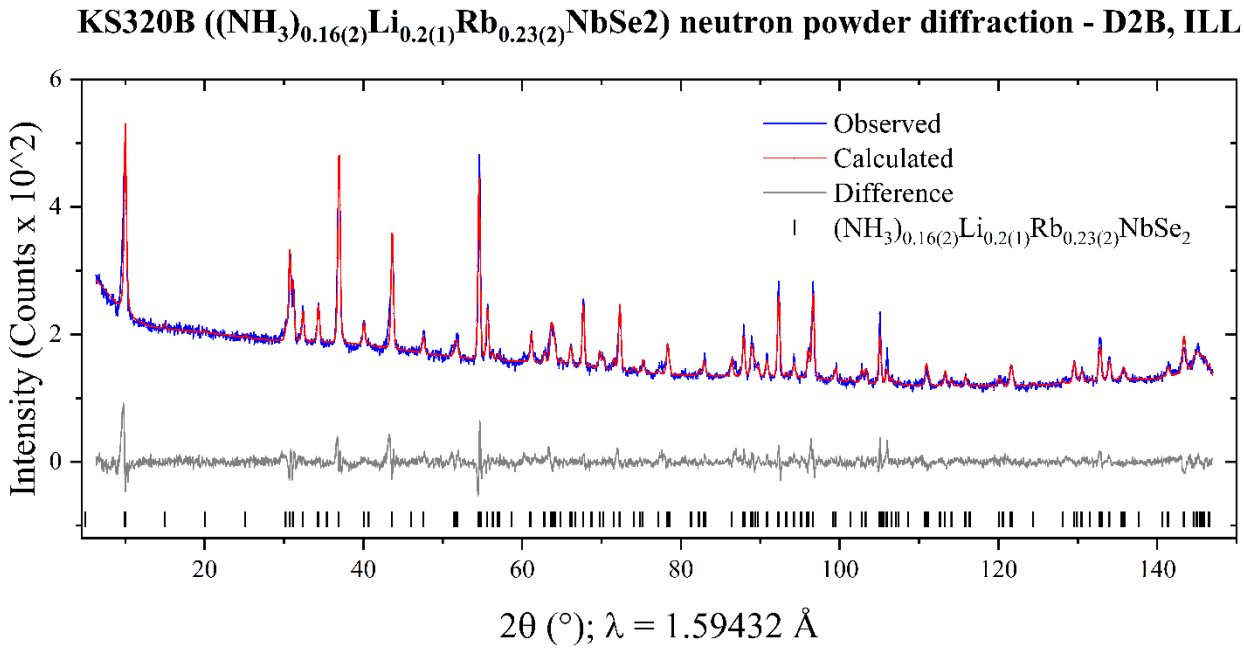


Figure 1: Rietveld refinement of Li,Rb,ammonia intercalated $NbSe_2$ measured at RT on the D2B diffractometer at ILL, showing the observed (black), calculated (red) and difference (gray) curves.

The tentative model for this is as shown in Figure 2. The current data have not yet enabled a definitive model to be deduced and further investigation is in progress. It is possible that a time-of-flight source may be more appropriate here because of the longer *d* spacing range available at the long and short ends. PDF measurements

may also be appropriate. But this was a useful experiment which will contribute to Katie Steele's D.Phil. thesis.

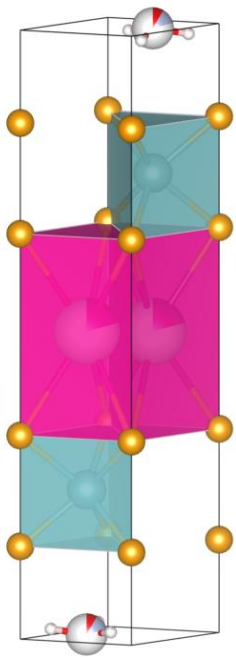


Figure 2: Tentative structural model used in Rietveld refinement. The data collected at 2.4 Å are shown also, but these did not enable the lowest d-spacing reflection to be measured. Blue polyhedra are Nb-centred. Purple polyhedra are Rb-centred. The lightly-occupied NH_3 and Li are likely ordered within each of the uncoloured layers, but the arrangement is likely not ordered along the stacking direction. But further examination is needed.