

# Project Report



**Application No.** 2009  
**Short title** Li-disorder in the hydrogen storage material  $\text{LiCe}(\text{BH}_4)_3\text{Cl}$  and detailed investigation of hydrogen positions

## Objectives: short, medium and long term (<250 words)

1. Short term: Perform powder diffraction measurement of the tripple-isotope-substituted material  $7\text{-LiCe}(11\text{-BD}_4)_3\text{Cl}$ .
2. Medium term: Analyse data to obtained detail structural information about the  $7\text{-LiCe}(11\text{-BD}_4)_3\text{Cl}$  phase; especially regarding Li disorder.
3. Long term: Publish results.

## Brief summary of work carried out:

The measurements where carried out as planned at ambient temperature and 8K. The two measurements were separated by about 1.5 month due to a scheduled maintenance period for the JEEP II reactor which was unproblematic since the sample is stable.

The data where analysed with the Rietveld method and the results are already submitted for publication to the journal RSC Advances in a joint manuscript with the experts from the host partner (authors: Jørn Eirik Olsen, Christoph Frommen, Torben R. Jensen, Magnus H. Sørby and Bjørn C. Hauback) with due acknowledgment to H2FC.

## Main achievements intended for publication <250 words

The aim of the measurements was to obtained detailed crystal structure information about the investigated phase. In particular, it was a goal to establish whether the Li ions were disordered or ordered in the structure, since conflicting reports on this topic is found in the literature

The model with disordered Li distribution gave a small but significant improvement in the Rietveld fits to the experimental data, compared to the ordered model, both at ambient temperature and 8 K. It was therefore concluded that the Li-ion distribution is indeed disordered and the disorder persist at very low temperatures.

The findings will aid in the understanding of the fast Li-ion conductivity reported in  $\text{LiCe}(\text{BH}_4)_3\text{Cl}$  and similar compounds and also in the understanding of the dynamics of hydrogen sorption processes since they involve ion diffusion in the solid state.

## Difficulties encountered <250 words

The sample was characterized by powder X-ray diffraction prior to the PND measurements and only some very minor peaks from impurity phases were observed. However, the Bragg peaks from the impurity phase(s) appeared much stronger in the PND data. This indicates that the impurity phase(s) contain mostly light elements, such as boron, hydrogen and/or lithium, but phase identification was not successful. The impurity peaks overlapped partly with peaks from main phase and the data were therefore not useful for obtaining more accurate hydrogen (deuterium) positions than those reported earlier. Fortunately, the data were still of sufficient quality to test models of ordered and disordered Li-ion distribution, which was the main objective of the investigation.

**Further comments:**