

# Project Report 2040



## Structural characterization of $\text{Sr}(\text{11BD4})_2 \cdot 2\text{ND3}$ by powder neutron diffraction

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### Objectives: short, medium and long term

Our aim was to determine precise H-positions for  $\text{Mg}(\text{11BD4})_2 \cdot n\text{ND3}$  ( $n=3$  and  $6$ ) in order to determine dihydrogen bonds between  $\text{H}^+$  from  $\text{NH}_3$  and  $\text{H}^-$   $\text{BH}_4$ . We speculate that this has a strong influence on the hydrogen release from these compounds.

### Brief summary of work carried out

$\text{Mg}(\text{11BD4})_2(\text{ND}_3)_3$  and  $\text{Mg}(\text{11BD4})_2(\text{ND}_3)_6$  was characterized by PND for approximately 48 hours for each sample using wavelength,  $\lambda = 1.5539 \text{ \AA}$ .

### Main achievements intended for publication

The detailed analysis of the PND data for  $\text{Mg}(\text{11BD4})_2 \cdot n\text{ND}_3$  ( $n=3$  and  $6$ ) is in progress.

### Difficulties encountered

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### Further comments

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