Experimental report

24/03/2022

Proposal: 5-31-2812 **Council:** 10/2020

Title: Crystal and magnetic structure of TbMgCo4D3.3

Research area: Chemistry

This proposal is a new proposal

Main proposer: Vitalii SHTENDER

Experimental team: Clemens RITTER

Local contacts: Clemens RITTER
Claire COLIN

Samples: TbMgCo4D3.3

Instrument	Requested days	Allocated days	From	To
D2B	2	2	21/06/2021	23/06/2021
D1B	1	0		

Abstract:

The aim of this proposal is to solve both the crystal and magnetic structures of TbMgCo4D3.3. This compound is interesting as for hydrogen storage and magnetocaloric application. Neutron diffraction experiments will be necessary to identify the positions of the D atoms in this deuteride. As the monoclinic distortion should be induced by the H(D) atom insertion, that will help us to understand why it is different from orthorhombic TbMgNi4D4 and cubic TbMgCo4D6 and the role played by Co for Ni substitution on the hydrogenation properties of TbMgNi4-xCox hydrides. In addition, the evolution of the NPD patterns versus temperature is required to solve the magnetic structure of TbMgCo4D3.3 and its evolution versus D content. These results will allow to complete the structural and magnetic phase diagram of TbMgCo4Hy hydrides and deuterides.

Progress report of proposal 5-31-2812

Proposal title: Crystal and magnetic structure of $TbMgCo_4D_{3.3}$

Dates of experiment: From 21/06/2021 To 23/06/2021

Main proposer: Vitalii Shtender and co-proposers: Martin Sahlberg and Valerie Paul-Boncour

Instrument responsible Clemens Ritter

The aim of this proposal was to study magnetic structure of the $TbMgCo_4D_{3.3}$ compound. Neutron powder diffractions have been measured at several temperatures for the corresponding sample according to magnetic curves M(T) (see proposal).

From the obtained results, it was preliminary found/refined structure of the deuteride. As for the magnetic structure we have tested the ferrimagnetic structure which gives satisfied result. The only issue now to ensure that nuclear structure does not changes at lower temperatures. For this reason, further experiment with the synchrotron source is planned. In the Figure 1 it is presented refined neutron diffractogram in the paramagnetic state.

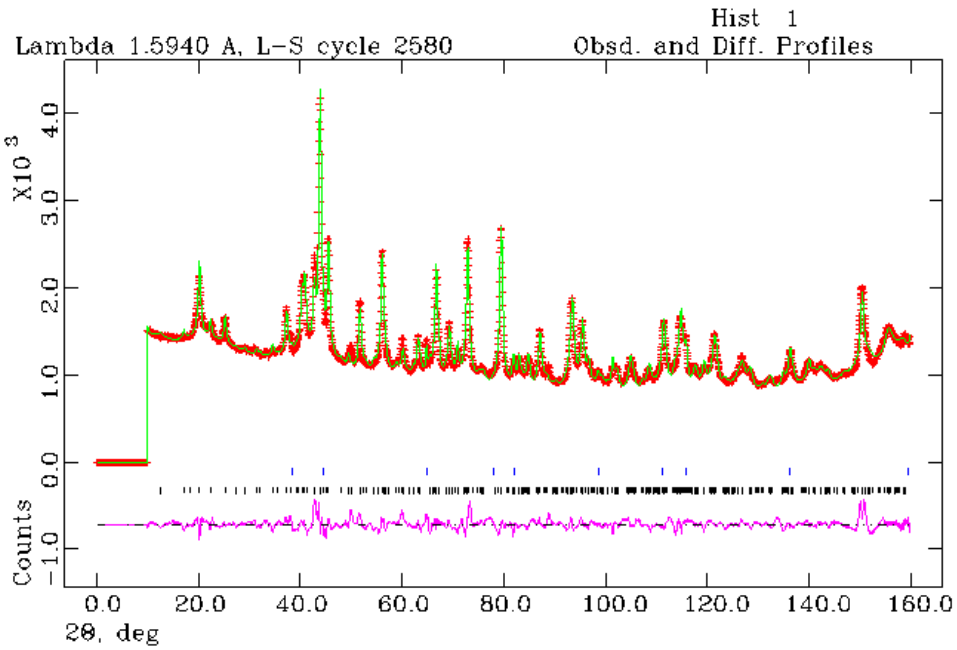

Fig. 1. Refined NPD pattern of $TbMgCo_4D_{3.3}$ compound at 175 K and its crystal structure.