Project Report 2062

The Crystal Structure of NdGaDx

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Objectives: short, medium and long term

The objective if the project is to determine the structure of NdGaDx as an analogue to GdGaHx.

Brief summary of work carried out

Neutron Powder Diffraction of NdGaDx and NdGa samples. The atomic coordinates of the deuterium atoms were located using density maps. Refinement using the Rietveld method on combining X-ray and neutron data was done to solve the structure of the deuteride.

Main achievements intended for publication

The deuterium atoms have been located in the NdGaDx structure, to our knowlage the first ReGa (Re=rare earth metal) hydride (deuteride) structure which has been determined.

Difficulties encountered

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Further comments

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