Project Report 2026

Hydrogen positions in magnesium borohydride ammoniates

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Objectives: short, medium and long term

Investigate the novel Sr(11BD4)2·2ND3 in order to solve the crystal structure and obtain precise H positions by combined powder neutron diffraction and powder X-ray diffraction.

Brief summary of work carried out

Sr(BD4)2(ND3)2 was characterized for X hours using X detector and λ = 1.5539 Å

Main achievements intended for publication

From PXD data we recently indexed and solved the crystal structure of the new compound Sr(BH4)2(NH3)2. As a consequence of the high D-sensitivity using neutron diffraction, precise D-positions have been obtained for Sr(BD4)2(ND3)2. The PND data obtained reveals that the unit cell obtained by PXD is in fact a sub-cell of the true unit cell for Sr(BH4)2(NH3)2. One publication concerning structure and properties of Sr(BH4)2(NH3)2 is in progress.

Difficulties encountered

None.

Further comments

None.