Experimental report

01/09/2022

Proposal: 6-02-622 **Council:** 10/2020

Title: Dihydrogen Bonding in Aqueous NaBH4 Solutions by Polarized Neutron Diffraction

Research area: Chemistry

This proposal is a resubmission of 6-02-609

Main proposer: Marie Claire BELLISSENT FUNEL

Experimental team: Marie Claire BELLISSENT FUNEL

Local contacts: Anne STUNAULT

Samples: BH2O/NaBH4+H2O
BH1O/NaBH4+H2O
BH55/NaBH4+H2O
NaOH+H2O

Instrument	Requested days	Allocated days	From	To
D3	7	11	25/08/2021	02/09/2021

Abstract:

As an electron-rich ligand, borohydride (BH4) forms various dihydrogen-bonded complexes with protic donors that possess diverse chemical properties. It influences the structure, reactivity, and selectivity both in solution and in the solid state, and has great potential utility in catalysis, crystal engineering, and materials chemistry. In conventional neutron diffraction measurement for liquids containing many hydrogen atoms, the sample is substituted with deuterons neglecting the isotope effect. However, since the hydrogen bond is sensitive to deuterated substitution, polarized neutron diffraction for the solution without substitution should be performed to reveal more precise information of hydrogen bond in BH4 solution. The obtained structure data will be applied to empirical potential structure refinement (EPSR) modeling with X-ray diffraction data conducted previously. BH4- hydration forms, dihydrogen bonding number, and water molecular orientation, especially the dihydrogen bonding in aqueous NaBH4 solutions will be revealed. The concentration and temperature effects on dihydrogen bonding will be discussed.

We intended to use Polarized neutron diffraction for aqueous $NaBH_4$ solution without hydrogen to deuterium substitution to reveal some more precise information of hydrogen bond between BH_4^- ion and water.

The experiment carried out on D3 instrument fully failed, all for technical reasons: The polarized 3He filling station died during our experiment. There was no hope of having it working before the end of the cycle. Moreover, added to the lack of polarized 3He, the RF coils have been out of work.