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Neutron Scattering Structure and Dynamics in Hydrazine AL-ICE ACATRINEI, MONIKA HARTL, LUKE DAEMEN, Los Alamos National Laboratory, DIANA FORSTER, RAINER KICKBUSCH, PETER LUGER, DI-ETER LENTZ, Freie Universitat Berlin, LOS ALAMOS NATIONAL LABORA-TORY TEAM, FREIE UNIVERSITAT BERLIN COLLABORATION — The Lewis Acid Base theory is a fundamental concept in chemistry. One way of describing a chemical bond is to look at the charge distribution within a molecule. By studying the charge densities in electron-deficient compounds such as hydrazine borane, a more detailed view of the bonding situations is achieved. Our interest in hydrazine borane comes from many reasons. First of all it allows examining the experimental charge density of a so called donor acceptor bond on one of the simplest molecules. N2H4BH3 is a potential hydrogen storage material which has not been studied in detail so far. Finally, it contains N-N bonds that are of interest due to their torsional vibrations. We performed neutron powder diffraction on the powder diffractometer NPDF at 15K and 95K and determined the hydrogen positions in N2H4BH3. We synthesized the completely labelled compound N2D4(11BD3)2. We investigated the hydrogen bonding and the N-N torsional dynamics by using incoherent inelastic neutron scattering on the Filter Difference Spectrometer FDS. While IR and RAMAN spectroscopy only show weak signal for torsional and librational modes, these modes are quite strong in neutron vibrational spectroscopy. We present neutron diffraction data and vibrational spectra and their interpretation using molecular modelling calculations.

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