Supplementary Electronic Information

Hydrogen mediated affinity of ions found in compressed potassium amidoborane, K[NH2BH3]

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Materials and Methods

1. Characterization of sample material

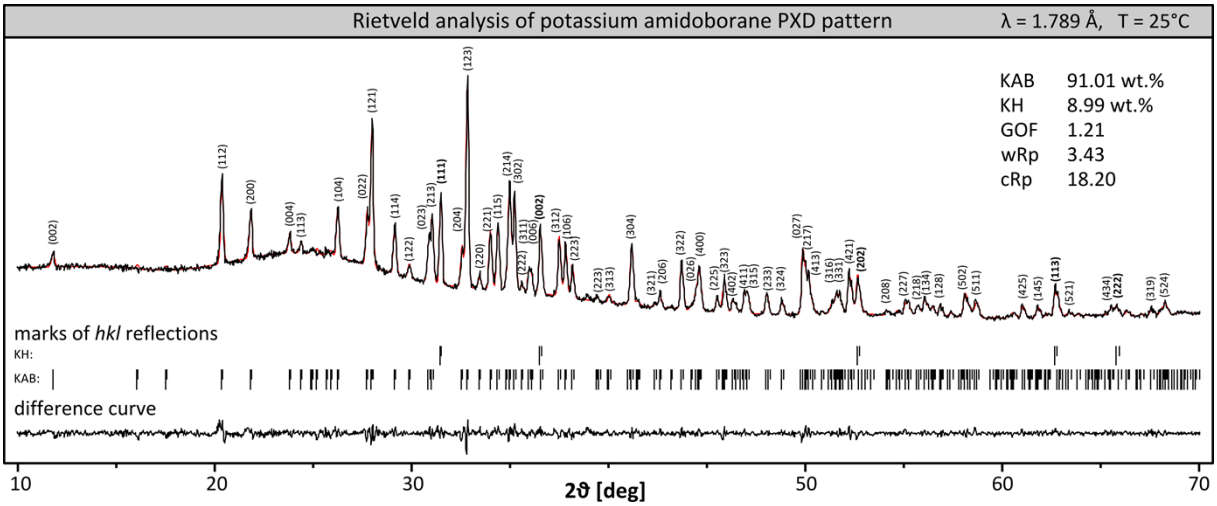

Figure S1. Powder X-ray diffraction (PXRD) pattern of potassium amidoborane (KAB) sample used for study.

2. High-pressure measurements

Diamond anvil cell with type-I diamonds of 500 μm culet size was used for the high-pressure experiments. A stainless steel gasket was preindented to ~35 μm thickness and then a hole of ~155 μm in diameter was drilled in the center as a sample chamber. Polycrystaline sample, powder of KAB, along with some ruby crystals (in form of sphere) for in situ pressure measurement, were loaded in the sample chamber inside the glovebox. Pressure was calibrated from the shift of Ruby fluorescence. No pressure medium was used in the sample chamber because sample material is fairly soft.

2.1. Raman measurements

Raman spectra were collected in backscattered geometry using custom disigned setup for micro-Raman measurements based on monochromator Jobin Yvon THR1000 (focal length 1000 mm) equipped with a single grating (with 1200 grooves mm^{-1}) giving a resolution of ~1 cm^{-1}, notch filters (Keiser Optical Systems) and thermoelectrically cooled (-75^{0}C) (Peltier effect) CCD (Horiba Synapse) detection.

He-Ne laser (Melles-Griot) line 632.8 nm was used for sample excitation.

2. 2.X-ray diffraction measurements

2.2.1. Ambient pressure sample characterisation
Powder X-ray diffraction patterns of solids (sealed under argon inside 0.6 mm thick quartz capillaries) were measured using Bruker D8 Discover diffractometer with 2D Vantec detector (parallel beam; CoKα λ ~ 1.789 Å), denoted here as.

2.2.2. High-pressure measurements

Angle dispersive powder X-ray diffraction patterns of solids were collected at ID 09 of European Synchrotron Radiation Facilities (ESRF) (λ=0.414552 Å). Pressure was estimated using „on-line“ setup for Raman measurements.

3. DFT calculations

The numerical calculations were performed using density-functional-theory (DFT) with the Perdew-Burke-Ernzerhof (PBE) parametrization of the generalized gradient approximation, as implemented in the VASP (ver. 4.6) and CASTEP codes. Lattice parameters and atomic ositions were optimized by seeking a total minimum energy based on density-functional theory and the plane-wave pseudopotential method. In order to perform the geometry optimization, the following thresholds were applied for a convergence window of two successive self-consistent steps: total energy change smaller than 1x 10 -6 eV/atom, maximum force per atom below 0.005 eV/Å, pressure smaller than 0.01 GPa, and maximum atomic displacement not exceeding 1x 10- 3Å. The BFGS minimizer was employed to carry out the unit cell optimization. The quality of this basis set was kept fixed as the unit cell volume varied during geometry optimization.

After optimization of the lattice parameters and atomic positions, the normal-mode vibrational analysis was performed with ab-initio lattice dynamics. Calculations were performed using again the PBE exchange-correlation functional. Brillouin-zone integration was performed according to the Monkhorst-Pack scheme with a sufficiently dense mesh of k-points to yield accurate convergence. The normal modes of the selected phases were derived from dynamical matrices calculated using small displacement method. Raman and IR intensities were calculated according to the scheme implemented in CASTEP program package.