Transmission IR Studies of Hydrogen Storage Materials

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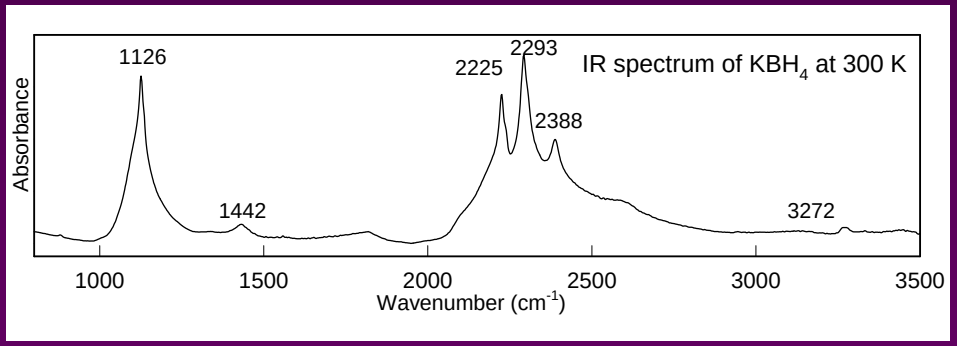
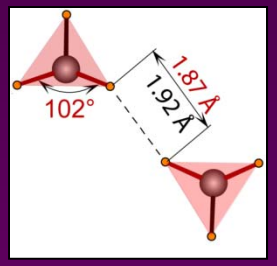
Borohydrides such as $NaBH_4$ and $LiBH_4$ are attractive as hydrogen storage materials because of their high weight percentages of hydrogen. However, it has been observed that the amount of hydrogen released from the thermal decomposition of borohydrides is less than expected and it has been hypothesized that this is because stable intermediates form. The following reaction sequence has been proposed involving formation of a stable $B_{12}H_{12}^{2-}$ anion.

$$NaBH_4 \rightarrow 1/12 Na_2B_{12}H_{12} + 5/6 NaH + 13/12 H_2$$
$$1/12 Na_2B_{12}H_{12} \rightarrow NaH + B + 3/2 H_2$$

To determine if this reaction occurs, IR spectra were obtained for salts containing the BH_4- and $B_{12}H_{12}^{2-}$ anions as a function of temperature. Spectra obtained at room temperature are shown below.





BH_4^-

$B_{12}H_{12}^{-2}$