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Nuclear Magnetic Resonance Studies of Sodiumaluminohexahydride (Na3AlH6)

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Many applications of modern physics require the investigator to understand the behavior of specific atoms in compounds. The behavior and structure of molecules such as sodiumaluminohexahydride (Na₃AlH₆) is relevant to the field of hydrogen storage. In this study, we used Nuclear Magnetic Resonance to examine the behavior of sodium, aluminum and hydrogen atoms in the compound sodiumaluminohexahydride. Sodiumaluminohexahydride consists of a covalently bonded AlH₆ anion that forms an ionic bond with a sodium cation. Particularly, we investigated the atomic motion at various temperatures by looking at the motional averaging of the atoms as a function of temperature from 23°C to 240°C. Atoms in motion will return results from the nuclear magnetic resonance experiments which are distinguishable from that atom when it is stationary. For example, the precise frequency of a ²³Na atom in Na₃AlH₆ depends on the orientation of the local hydrogen nuclear spins. From these results we can determine whether the atoms are in motion. Over this range of temperatures, our measurements are consistent with a model in which hydrogen atoms in the AlH₆ group rotate isotropically, while the sodium atoms diffuse through the solid. As the temperature increased, we saw evidence of increased sodium diffusion. We believe that the aluminum atoms are not moving and, though the hydrogen atoms are rotating, there is no translational component of diffusion.