

# Adventures in Parahydrogen Matrix Isolation Infrared Spectroscopy

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The use of *para*-hydrogen (p-H<sub>2</sub>) as a host in matrix isolation studies began in 1998 when Momose and Shida started using solid p-H<sub>2</sub> to record the infrared spectrum of unstable molecules such as radicals and ions [1]. Sparked by the eloquent high-resolution laser studies of solid p-H<sub>2</sub> by Oka and co-workers [2], there was growing interest in developing so-called quantum hosts such as liquid helium and solid p-H<sub>2</sub> for matrix isolation studies. In principle quantum hosts offer several advantages - sharp guest species linewidths, weak cage effect for *in situ* photolysis studies, and tunneling mobility - over classical noble gas matrices such that new low temperature phenomena could be explored.

Research in the Anderson group started in 2000 at the University of Wyoming where we made several discoveries: guest species induce IR activity in the solid p-H<sub>2</sub> host [3], mobile *ortho*-hydrogen (o-H<sub>2</sub>) molecules present at controlled proportions can be used to form guest-(o-H<sub>2</sub>)<sub>N</sub> clusters [4], and we identified and developed a two-step UV/IR photolysis scheme to selectively produce hydrogen atoms (H-atoms) in order to study low temperature bimolecular chemical reactions [5]. We have focused our subsequent studies on the details of H-atom reactions with various guest species in solid p-H<sub>2</sub>.

In this talk I will highlight some new results that I think nicely illustrate how quantum hosts differ from classical matrix isolation hosts. From the beginning my work group has been interested in how *in situ* photochemistry inside solid p-H<sub>2</sub> can be utilized to create species that are difficult to generate any other way. In the current studies, we photolyze diborane (B<sub>2</sub>H<sub>6</sub>) at 193 nm to create two BH<sub>3</sub> fragments that easily escape the solvent cage and react with the p-H<sub>2</sub> host to generate BH<sub>5</sub>. The BH<sub>5</sub> chemical intermediate is a highly fluxional molecule and is thought to scramble the hydrogen atoms within the complex. Following the photolysis exposure, we observe recombination of the photofragments which indicate that BH<sub>5</sub> (or BH<sub>3</sub>) can diffuse through the p-H<sub>2</sub> matrix even at temperatures as low as 1.5 K. I will also show that the BH<sub>5</sub> species catalyzes p-H<sub>2</sub> → o-H<sub>2</sub> nuclear spin conversion in highly enriched p-H<sub>2</sub> solids at liquid helium temperatures via a mechanism that involves H<sub>2</sub>(v=1) vibrons. The fact that the BH<sub>5</sub> fragments are mobile and can recombine was unexpected and shows how quantum solids such as p-H<sub>2</sub> present unique environments for high resolution spectroscopy and reaction studies.

## References

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