Adsorption and Reaction of *ortho*-Carborane on Pt(111)

Final Report

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REU Program

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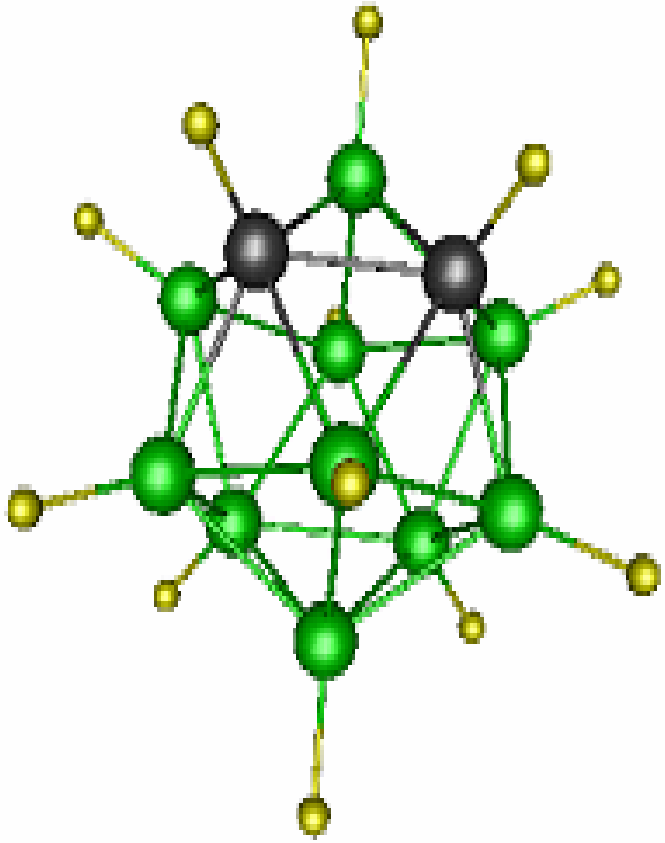
ortho-Carborane adsorbed on Pt(111)

- *ortho*-Carborane, more commonly o-Carborane $C_2H_{12}B_{10}$
- Present on surface of platinum, Miller Index 111
- Boron Cage Structure
- 8.3% Hydrogen by mass

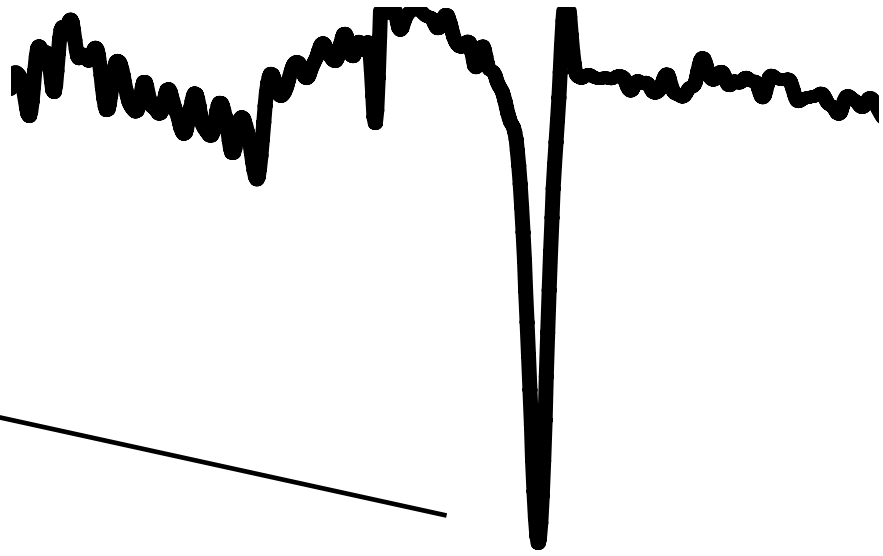


Motivations

- Hydrogen Storage is a key challenge to realizing a hydrogen economy
  - DOE goal is a viable storage mechanism 9% H_2 by mass by 2015
  - Metal catalyzed release and uptake of hydrogen in complex hydrides is a promising approach
  - Because boron is one of the lightest elements, boron hydrides are good candidates for hydrogen storage
- Catalytic surface chemistry of BH bonds has never been studied before
  - Characterize nature of bonding of carborane with Pt(111)
  - Explore thermal evolution of molecule
  - Study various other properties of molecule
  - May lead to optimization of well known techniques using carborane, such as thin film vapor deposition

Surface Science Methods

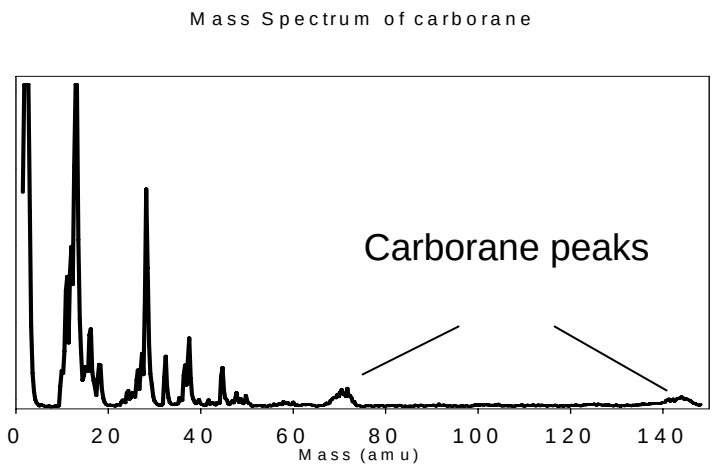
- Reflection Absorption Infrared Spectroscopy (RAIRS)
  - If a bond is present it will produce a “peak”



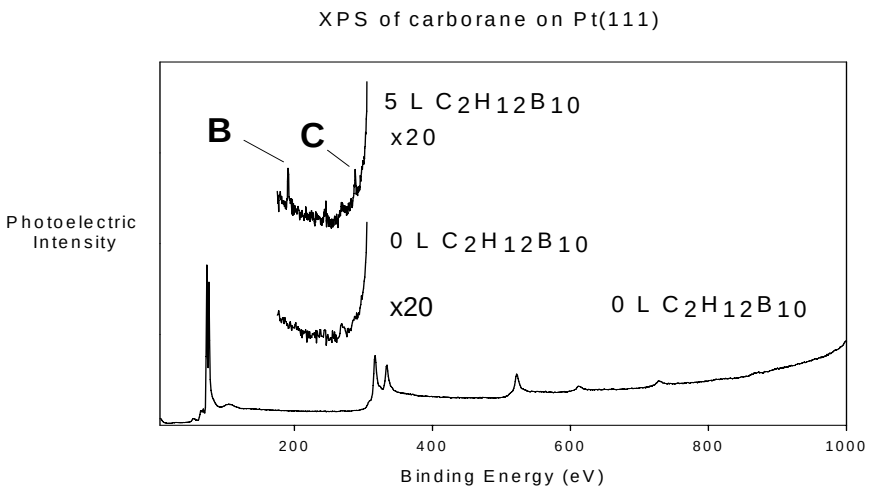
- Mass Spectrometry
- Temperature Programmed Desorption (TPD)
- X-Ray Photoelectron Spectroscopy

Apparatus

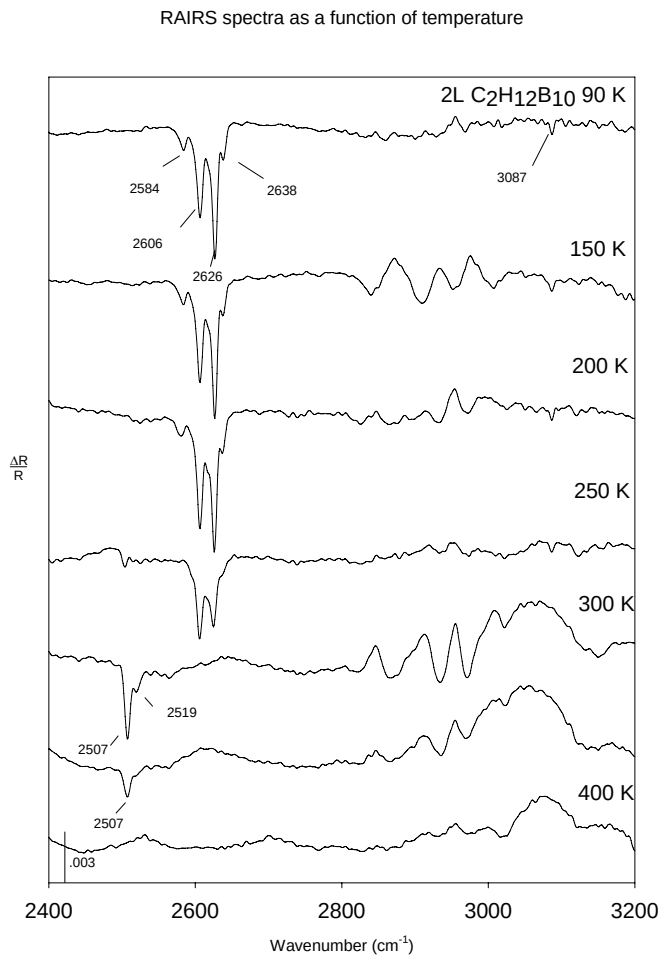
- Ultra High Vacuum (UHV)
  - Pressure = 10^{-11} torr
  - Needed for well-defined surface conditions
- Mass Spectrum of carborane sample at 10^{-7} torr



- XPS of 5 L carborane on Pt(111) surface
  - 1 L =1 x 10^{-6} torr sec ~1 molecular layer



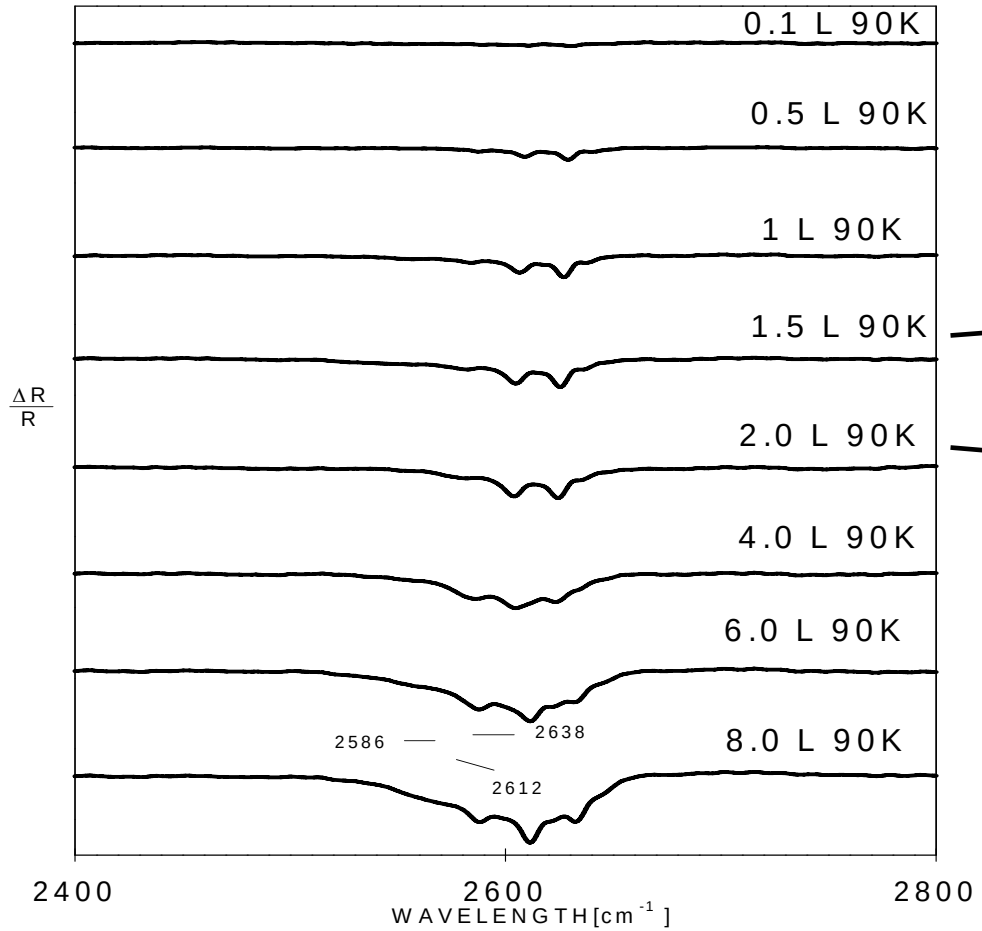
RAIRS Thermal Evolution of *ortho*-Carborane on Pt(111)



InSb Detector
Wavenumbers 1880-4000

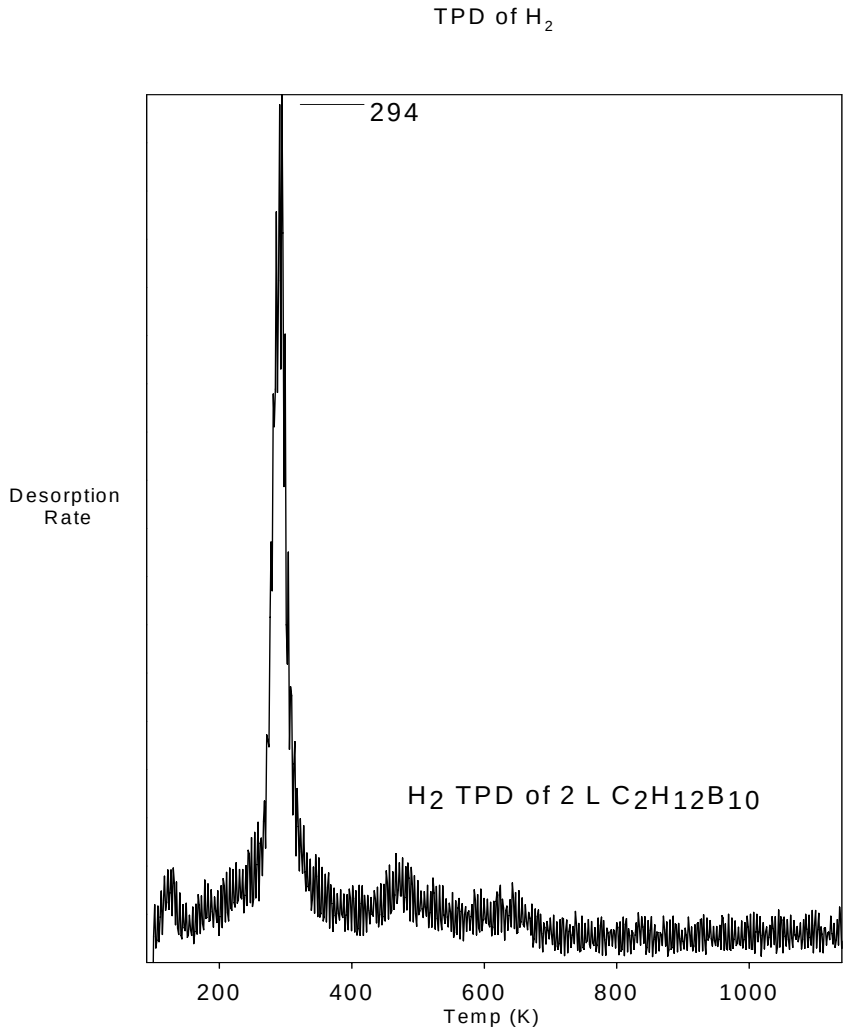
- 90 K molecular adsorption
- No reaction 90-250 K
- New surface species with BH bonds at 300 K
- Loss of all BH bonds by 400 K

RAIR SPECTRA OF *ortho*-CARBORANE AS FUNCTION OF EXPOSURE



Similar Intensity of BH bonds indicate formation of monolayer at 1.5 L

TPD (Temperature Programmed Desorption)



Supports IR data, consistent with shift observed at 300 K, as well as thermal stability to 250 K

Conclusions

- *ortho*-Carborane is thermally stable on Pt(111) through 250 K
- Chemical reaction at 300 K is indicated by a red shift, as well as a decrease in intensity at 300 K. This is supported by TPD results
- *ortho*-Carborane forms a monolayer on Pt(111) at about a 1.5 L exposure
- BH bonds broken at 400 K
- CH bonds broken at 300 K
- Pt(111) catalyzes thermal decomposition of carborane

Future Directions

- Fully Analyze Results
  - Analyze MCT results for information on BB bonds
  - Explain Lack of BH bonds after introduction of H_2 after annealing to 300 K
  - Determine if D_2 exchange is really what is occuring at 250 K
- Repeat Experiments Under Optimized Conditions
- Explore Avenues Not Possible with Current Apparatus, more TPD and XPS

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