Infrared Spectroscopy of a Copper-Hydride Molecule

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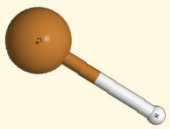
Objective

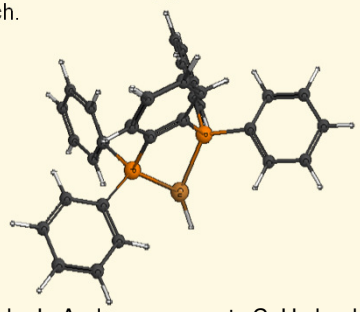
- The objective of this research was to locate the region where Copper-Hydride is found in both IR and NMR spectra.

Rationale

- It is essential to understand Metal-Hydrogen bonding to find a safer and lighter hydrogen storage material.
- The infrared spectra of (BDP)CuH and $(PPh_3)_3CuH$ have not been observed in previous research.

Molecules





Background

- Previous research conducted by L. Andrews suggests CuH should show up around 1800 cm^{-1}.
- Copper Hydride is unstable by itself.
- Stable only when attached to ligands with low concentrations of CuH making it difficult to see on IR spectra.
- The ligands change where CuH shows up on the spectra.

Experimental Design

- A solution Phase Infrared Spectroscopy (IR), using a Nicolett AVATAR (360 FT-IR), of (BDP)CuH was performed for this experiment.
- The solution used was (BDP)CuH (Sigma-Aldrich) which consists of 71% toluene, 28.6% polymethylhydrosiloxane, .38% triphenylphosphine, .07% copper-hydride.
- A background of proportionate amounts of toluene and polymethylhydrosiloxane was taken.
- An IR spectra of (BDP)CuH was then taken.
- WebMo was used to calculate where different vibrational frequencies (stretches) should be observed in the spectrum.
- The WebMo basis sets used were B3LYP and CC-pVTZ.

References

1. **Infrared Spectra and DFT Calculations for the Coinage Metal Hydrides MH, (H2)MH, MH2, M2H, M2H-, and (H2)CuHCu in Solid Argon, Neon, and HydrogenXuefeng Wang and, Lester Andrews*, Laurent Manceron, and Colin Marsden** ***The Journal of Physical Chemistry A 2003 107 (41), 8492-8505***
2. **(BDP)CuH: A "Hot" Stryker's Reagent for Use in Achiral Conjugate ReductionsBenjamin A. Baker,arko V. Bokovi, and, and Bruce H. Lipshutz*** ***Organic Letters 2008 10 (2), 289-292***

Acknowledgments

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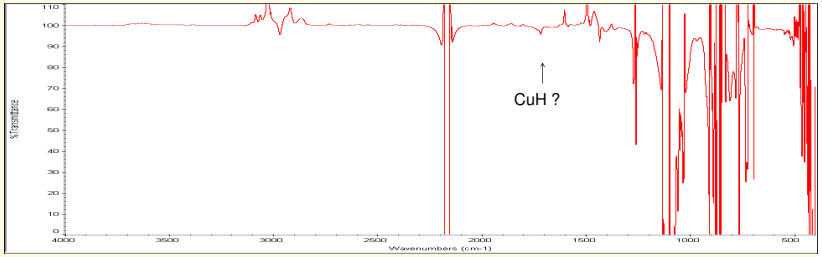
•Thanks to Dr. Warren Gallagher and Dr. Jim Phillips for their expertise and advice.

Expected Results

- L. Andrews et. al. conducted infrared spectroscopy of coinage metal hydrides and found that CuH shows up at 1879.8 cm^{-1} in an argon matrix.
- CuH strecth is calculated by WebMo at 1823 cm^{-1}.
- (BDP)CuH vibrational frequencies were calculated using WebMo.
- The CuH stretch in (BDP)CuH should show up at 1753 cm^{-1} according to calculations made by WebMo.
- B. Baker et. al. took an NMR of (BDP)CuH and found the hydride peak to show up at δ= 1.49 ppm.

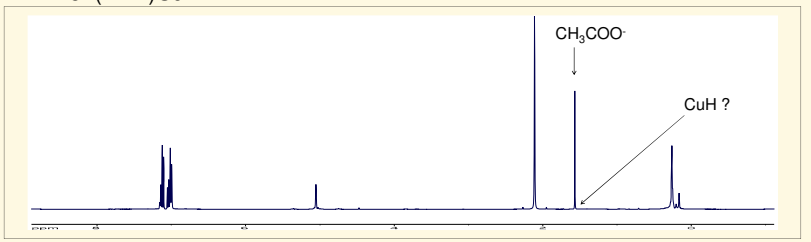
Results from Experiment

IR of (BDP)CuH



- CuH stretch is expected to be observed around 1700 cm^{-1}.

NMR of (BDP)CuH



- Hydride peak is expected to be observed at δ= 1.49 ppm.
- Acetate peak is observed at δ= 1.55 ppm, which would obscure the hydride peak at δ= 1.49 ppm.

Conclusion/Future work

- After successfully obtaining the IR spectra of BDP-CuH, we hope to positively identify the Cu-H stretch.
- Perform a successful solid phase IR of triphenylphosphine Cu-H (Stryker's Reagent).
- Compare to WebMo calculations.