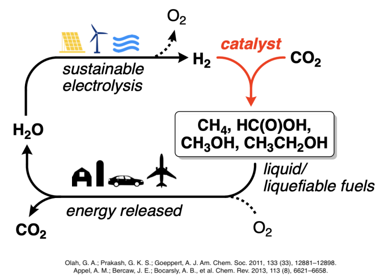
Hard-Soft-Acid-Base Mismatch for Renewable Fuel Production

Timmy Gee, Class of 2025

Due to the serious risk that climate change poses to society and the environment, a global transition to renewable energy is required. Hydrogen is an abundant resource with the potential to be utilized as an effective means of storing renewable energy. The benefits of a hydrogen-based liquid fuel include storage longevity, high energy density, and the potential to be employed in existing transportation infrastructure where fossil fuels currently dominate. While it has many beneficial properties, a hydrogen-based fuel is challenging to synthesize due to the chemical properties of elemental hydrogen. Hydrogen alone is not an effective fuel, nor does it readily react with other molecules required for its conversion to a liquid form with superior fuel properties. Therefore, a catalyst is required to facilitate the chemical reactions required for producing a practical hydrogen-based fuel. The complete process, from the production of our proposed hydrogen-based fuel to its combustion in transportation vehicles, is a fully renewable and carbon-neutral process.

Molecular hydrogen (H_2) can be obtained from the electrolysis of water (H_2O) using renewable energy such as wind or solar power. To be converted to a practical fuel, hydrogen must be chemically combined with a carbon source such as carbon dioxide (CO_2). My research focused on a novel method of catalyzing these reactions, which leverages the principles of Hard-Soft Acid-Base (HSAB) theory. According to HSAB theory, hard acids tend to form strong bonds to hard bases, while soft acids prefer to bond to soft bases. We hypothesized that a proposed chemical catalyst such as Silver Fluoride(AgF), which contains a mismatched soft acid and hard base, could split molecular hydrogen into two separate hydrogen ions capable of bonding to CO_2. For AgF to effectively catalyze the reaction, we needed to attach a N-Heterocyclic Carbene ligand (NHC ligand) to AgF. NHC ligands are large molecules that improve the bonding and reactivity properties of metal molecules such as AgF.



Hydrogen-based Liquid Renewable Fuel Cycle

Most of my time this summer was spent synthesizing a specific NHC ligand called IPr**. This ligand was previously proven to improve the reactivity of AgF. The process of developing IPr** spanned the entire duration of my research experience due to many experimental setbacks that resulted in impurities in our IPr** product. Much of my time was spent adapting previous research to improve the synthesis process. Additionally, each time I developed a precursor to our product, I analyzed it using Nuclear Magnetic Resonance (NMR) spectroscopy, a technique that relies on the absorption of radio waves by molecules in an extremely strong magnetic field. This data allowed for the identification of the chemical composition of my product.

I would like to thank the Kufe Family Research Fellowship for funding my summer research experience. I'm very grateful for the opportunity to engage in Professor Tate's Synthetic Chemistry laboratory and expand my chemistry knowledge.

Faculty Mentor: Dr. Brandon Tate
Funded by the Kufe Family Research Fellowship

References:

1. Olah, G. A.; Prakash, G. K. S.; Goeppert, A. J. Am. Chem. Soc. 2011, 133 (33), 12881–12898.
2. Appel, A. M.; Bercaw, J. E.; Bocarsly, A. B., et al. Chem. Rev. 2013, 113 (8), 6621–6658.
3. R. G. Pearson, J. Am. Chem. Soc. 1963, 85 (22), 3533–3539.
4. B. K. Tate, J. T. Nguyen, J. Bacsa, J. P. Sadighi, Chem. Eur. J. 2015, 21, 10160–10169.
5. E. A. Romero, P. M. Olsen, R. Jazzar, M. Soleilhavoup, M. Gembicky, G. Bertrand. Angew. Chem. 2017, 56, 4024–4027.
6. Leibowitz, Zach. 2024. Honors Thesis, Biochemistry Department, Bowdoin College
7. Weber, Simone & Loos, Christian & Rominger, Frank & Straub, Bernd. (2012). Synthesis of an extremely sterically shielding N-heterocyclic carbene ligand. Archive for organic chemistry. 2012. 226-242.