Ningyi Lyu

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Education

Yale University **Aug 2019-Present**
Graduate Student in Chemistry Department

Grinnell College (B.A.) **Aug 2015-May 2019**
Major: Chemistry, Concentration: East Asian Studies

Research Experience

DFT and NBO Studies of Aldehyde Vicinal Proton-Proton Coupling Constant
Advisor: Dr. T. Andrew Mobley (Grinnell) *Jan 2017-May 2019*
Employed electronic structure theory to discuss reasons behind the observed small proton-proton vicinal coupling constant ($^3J_{HH}$) of aliphatic aldehydes. We proposed that the aldehyde geometry is unfavorable for a large $^3J_{HH}$, and the electron withdrawing effect of the aldehyde oxygen atom to the coupling pathway decreases $^3J_{HH}$ by lowering the contribution of Fermi-contact (FC) term.

- Applied Gaussian 09 program to perform energetic calculations and NMR parameter calculations, including Single Point Energy Calculation, Geometry Optimization, Spin-Spin Coupling Constant (SSCC) Calculation and Coordinate Scan.
- Applied NBO 6.0 package (installed in G09) to perform NBO analyses, including Natural Bond Orbital Analysis, Natural Population Analysis, Second-Order Perturbative Analysis of Donor-Acceptor Interactions, Energetic Analysis with NBO Deletion, Geometry Optimization with NBO Deletion, Pairwise Steric Interaction Energetic Analysis, Natural J-Coupling Analysis and NBOPLOT Orbital Visualization.
- Developed a “hybrid molecule” model to investigate how the electron withdrawing effect on the coupling pathway could alter the Fermi-Contact term of coupling constant.
- Evaluated the performance of different approximate functionals in Density Functional Theory (DFT) in predicting spin-spin coupling constants.

Computational Investigations of Radical Anion Cyclization Reactions of Unsaturated Ketones
Advisor: Dr. James E. Swartz (Grinnell) *Jan 2018-May 2019*
Mechanism of unsaturated ketone radical anion cyclization reaction was studied with computational approaches. We proposed that during the cyclization process, the bond formation process might be barrierless while possible transition states come from prior dihedral adjustments.

- Applied Gaussian 09 program to perform energetic calculations, including Single Point Energy Calculation, Geometry Optimization, Transition State Optimization with Berny Algorithm and Synchronous Transit-Guided Quasi-Newton Method, Vibrational Analysis, Intrinsic Reaction Coordinate Search and Minimal Energy Pathway Scan.
- Applied PyMOL 2.2 package to perform conformational search using force field methods.
- Applied MOPAC 2016 program to perform semiempirical energetic calculations with

explicitly expressed solvation environment constructed in Packmol-16.
- Evaluated the performance of different approximate functionals in DFT by comparing single point energy calculation results between DFT, high-order electron-correlation methods and composite extrapolation approaches.

Towards an Anthropological Understanding of Ancient Chinese Wine
Advisor: Dr. Qiaomei Tang (Grinnell) *Jan 2018-May 2019*
Developed a biological chemical model to study the alcohol concentration of ancient Chinese wine.

Teaching Experience

Yale:
General Chemistry Lecture Teaching Assistant Jan 2020-May 2020
Lab Teaching Assistant Sep 2019-Dec 2019
Grinnell:
General Chemistry Lecture Teaching Assistant Aug 2018-Present
Lab Teaching Assistant Aug 2018-Present
Grader Aug 2017-Dec 2017
Inorganic and Analytical Chemistry Grader Jan 2018-May 2018

Publication and Presentation

"Computational Investigations of the Radical Anion Cyclization Reaction of 6-hepten-2-one." **Ningyi Lyu** and James E. Swartz. Presented by Ningyi Lyu at the 2018 ACS Midwest Regional Meeting, Ames, IA, USA, Oct 21st-23rd, 2018.

"Theoretical Exploration of (Un)expectedly Small Aldehyde $^{3}J_{HH}$ Values: an NBO Perspective." **Ningyi Lyu** and T. Andrew Mobley. Presented by Ningyi Lyu at the 2018 SMASH Small Molecule NMR Conference, Philadelphia, PA, USA, Sep 16th-19th, 2018.

Yang, Y., Li, H., Zhu, H., Shang, S., **Lyu, N.**, Song, W. "Intersection scan model and probability inference for vision based small-scale urban intersection detection." Conference Paper. 2017 IEEE Intelligent Vehicles Symposium, Los Angles, CA, USA. DOI: 10.1109/IVS.2017.7995905.

Yang, Y., Li, H., Zhu, H. **Lyu, N.** Song, W. "Small-scale intersection scan model for UGV in urban environment." Conference Paper. 2017 American Control Conference, Seattle, WA, USA. DOI: 10.23919/ACC.2017.7963605.

Manuscript in Preparation

Lyu, N. Mobley, T. A. "Theoretical Exploration of Small Aldehyde $^{3}J_{HH}$ Values: an NBO Perspective." In Preparation. Planning to submit to *Magnetic Resonance in Chemistry*.

Honors and Awards

Honors in Chemistry, Grinnell College
Phi Beta Kappa, Beta Chapter of Iowa