CALIFORNIA INSTITUTE OF TECHNOLOGY

Division of Chemistry and Chemical Engineering
Mail Code 150-21
Pasadena, California 91125

Brett A. McGuire
Graduate Student

Phone: (626) 395-6791
e-mail: bmcguire@caltech.edu

To Whom It May Concern,

It is with great excitement that I am submitting the proposal entitled *The Cosmic Origins of Complex Prebiotic Molecular Material: A Combined Observational and Laboratory Investigation* for consideration for a 2014 National Radio Astronomy Observatory Jansky Fellowship. This work will utilize a one-of-a-kind, state-of-the-art laboratory instrument to probe, for the first time, the far-infrared spectra of complex interstellar ice analogs. Utilizing these results, I will directly determine, for the first time, the abundance and distribution of water and methanol ices, fundamental prebiotic precursors, in complex molecular clouds and protoplanetary disks using Herschel and SOFIA observations. These first-of-their-kind observations will provide unparalled insight into the physical and chemical evolution of molecular complexity in these regions. Finally, an expansive education and outreach program, through a partnership with the *Ph.Detours* program, will bring the results of this research to a public audience of more than 7 million annual viewers.

The primary host institution for this fellowship will be the NRAO Headquarters in Charlottesville, VA. Dr. Anthony J. Remijan, a world-renowned expert in the field, will serve as the primary advisor for this project. To facilitate the acquisition of the foundational laboratory measurements for this project, an extended working visit at the California Institute of Technology will occurr during the first year in cooperation with Professor Geoffrey A. Blake.

In the case of an institutional conflict with the NRAO Headquarters, the first backup institution will be the University of Virginia, again under the supervision of Dr. Remijan, who holds an adjunct faculty position at UVa. The second backup institution will be Harvard University and the Harvard-Smithsonian Center for Astrophysics, under the supervision of Dr. Michael McCarthy.

Thank you very much for your consideration, and I look forwarding to hearing from you.

Sincerely,

Brett A. McGuire

Brett A. McGuire

Blake Group
160 South Mudd
California Institute of Technology
1200 E California Blvd
Mail Code 150-21
Pasadena, CA 91125

Phone: (217) 549-5729
Office: (626) 395-6791
`bmcguire@caltech.edu`

Education

Ph.D. Physical Chemistry, California Institute of Technology, 2014 (Expected)
4.00 Cumulative GPA

M.S. Physical Chemistry, Emory University, 2011
3.63 Cumulative GPA

B.S. Chemistry, University of Illinois at Urbana-Champaign, 2009
3.75 Chemistry GPA, 3.68 Cumulative GPA
Graduated with Highest Distinction

Charleston High School; Charleston, IL, 2005
Valedictorian

Research Experience

Graduate Research Assistant — September 2011 - Present
California Institute of Technology — Advisor: Geoffrey A. Blake

Graduate Research Assistant — July 2009 - September 2011
Emory University — Advisor: Susanna L. Widicus Weaver

Undergraduate Research Assistant — October 2006 - June 2009
University of Illinois at Urbana-Champaign — Advisor: Benjamin J. McCall

Research Expertise

- *Laboratory Astrophysics:* High-resolution, gas phase spectroscopy of transient, reactive molecules. Design, construction, and use of supersonic expansion discharge sources. Microwave, millimeter, and sub-millimeter spectroscopy of astrochemically-relevant species. Fourier-transform Microwave Spectroscopy. Chirped-Pulse Microwave Spectroscopy. Cavity ring-down spectroscopy. Time-domain THz spectroscopy of solid-phase species. High vacuum systems. Structure optimization and potential energy surfaces of molecules using Gaussian 09. Assignment of pure rotational and rovibronic transitions of gas phase molecules.
- *Observational Astronomy:* Have been trained on, and conducted observations with, the Caltech Submillimeter Observatory (CSO), the W. M. Keck Observatory, the 100 m Green Bank Telescope (GBT), and the Combined Array for Research in Millimeter-wave Astronomy (CARMA). Additionally have experience in processing and analyzing data collected with the Herschel Space Telescope, the NRAO 12 m Kitt Peak Telescope, and the Berkeley-Illinois-Maryland Array (BIMA).

Honors and Awards

6/13 2013 Rao Prize at the 68th International Symposium on Molecular Spectroscopy

9/11 National Science Foundation Graduate Research Program Fellow

9/09-12/11 Robert W. Woodruff Fellow, Emory University

5/11-12/11 Curriculum Development Fellow, Emory University

5/11 Young Researcher Travel Grant, IAU Symposium 280

5/10 National Science Foundation Graduate Research Fellowship Honorable Mention

12/07-05/09 List of Teachers Ranked as Excellent by Their Students, University of Illinois (4 Semesters)

8/05-5/09 University of Illinois James Scholar

Teaching Experience

- Completed Caltech Project for Effective Teaching Pedagogy Workshop Series
  California Institute of Technology, Fall 2011 - Spring 2013
- Curriculum Development Fellow, Physical Chemistry Lab
  Emory University, Summer 2011 - Fall 2011
- Teaching Assistant, General Chemistry Labs I & II
  Emory University, Fall 2009 - Spring 2010
- Head Teaching Assistant, Accelerated General Chemistry Labs I & II
  University of Illinois, Summer 2008 - Spring 2009
  - Redesigned and modernized assignments for the course, including lab reports and pre-labs, to increase student comprehension and preparedness as well as scientific writing ability. Designed a new grading system to better reflect student performance in the course.
  - In addition to teaching an individual lab section, responsible for the day-to-day running of a laboratory course for over 220 advanced chemistry students. Led a team of 9 teaching assistants in running 11 separate laboratory sections of students. Achieved one of the highest retention rates for students continuing in the program from first semester in recent years. Designed formatting guides, course manual supplements, and gave substitute lectures for the professor when necessary. Additionally, gave a number of original lectures on course structure, scientific writing, and the data analysis and calculations behind the experiments.
- Teaching Assistant, Accelerated General Chemistry Labs I & II
  University of Illinois, Fall 2007 - Spring 2008

Mentoring Experience

- Undergraduate Students Mentored
  - Mr. Daniel Guth, Mr. Jerry Feng, Ms. Mary Radhuber, Mr. Jay Kroll, Ms. Sophie Lang, Mr. Patrick Lanter, Mr. Daniel Sudryznsky
- Lead Mentor, Chemistry Enrichment Project
  University if Illinois, Fall 2008

Service & Outreach

- Organizing Committee, 2014 Astrobiology Graduate Conference
- Student Representative, Chemistry Graduate Studies Committee
  California Institute of Technology, Spring 2013 - Present
- Organizing Committee, Chemistry & Chemical Engineering 2013 Seminar Day
  California Institute of Technology
- Organizing Committee, Chemistry & Chemical Engineering 2012 Seminar Day
  California Institute of Technology
- Group Leader, Kids and Chemistry Outreach Program
  University of Illinois, Fall 2006 - Spring 2007
- Kids and Chemistry Outreach Program
  University of Illinois, Fall 2005 - Spring 2006

Refereed Publications

[12] Neill, J. L., Bergin, E. A., Lis, D.C., Schilke, P., Crockett, N. R., Favre, C., Emprechtinger, M., Comito, C., Qin, S.-L., Anderson, D., Burkhardt, A. M., Chen, J.-H., Harris, B. J., Lord, S. D., McGuire, B. A., McNeill, T. D., Monje, R. R., Phillips, T. G., Steber, A. L., Vasyunina, T., & Yu, S., "*Herschel* observations of EXtraordinary Sources: Analysis of the full Herschel/HIFI molecular line survey of Sagittarius B2(N)," **2013**, submitted to the *Astrophysical Journal*.

[11] Crockett, N. R., Bergin, E. A., Neill, J. L., Favre, C., Schilke, P., Lis, D. C., Bell, T. A., Blake, G. A., Cernicharo, J., Emrpechtinger, M., Esplugues, G. B., Gupta, H., Kleshcheva, M., Lord, S., Marcelino, N., McGuire, B. A., Pearson, J., Phillips, T. G., Plume, R., van der Tak, F., Tercero, B., & Yu, S., "*Herschel* observations of EXtraordinary Sources: Analysis of the HIFI 1.2 THz wide spectral survey toward Orion KL I. methods," **2013**, submitted to the *Astrophysical Journal*.

[10] McGuire, B. A., Carroll, P. B., Gratier, P. Guzmán, V, Pety, J., Roueff, E., Gerin, M., Blake, G. A., and Remijan, A. J., "An observational investigation of the identity of B11244 (l-C_3H^+/C_3H^-)," **2013**, *Astrophysical Journal*, in revision.

[9] Allodi, M. A., Ioppolo, S., Kelley, M. J., McGuire, B. A., & Blake, G. A., "The structure and dynamics of carbon dioxide and water containing ices investigated via THz and mid-IR spectroscopy," **2013**, *Physical Chemistry Chemical Physics*, in revision.

[8] Remijan, A. J., Snyder, L. E., McGuire, B. A., Kuo, H., Looney, L. W., Friedel, D. N., Golubiatnikov, G. Y., Lovas, F. J., Iluyshin, V. V., Alekseev, E. A., Dyubko, S. F., McCall, B. J., & Hollis, J. M., "Observational results of a multi-telescope campaign in search of interstellar urea [$(NH_2)_2CO$]," **2013**, *Astrophysical Journal*, in revision.

[7] McGuire, B. A., Carroll, P. B., Blake, G. A., Hollis, J. M., Lovas, F., Jewell, P. R. & Remijan, A. J., "A search for l-C_3H^+ in Sgr B2(N), Sgr B2(OH) and the Dark Cloud TMC-1," **2013** *Astrophys. J.*, 774, 56.

[6] Carroll, P. B., McGuire, B. A., Zaleski, D. P., Neill, J. L., Pate, B. H., and Widicus Weaver, S. L., "The rotational spectra of glycolaldehyde isotopologues measured in natural abundance by chirped-pulse Fourier transform microwave spectroscopy," **2013** *J. Mol. Spec.*, 284-285, 21.

[5] McGuire, B. A., Loomis, R. A., Charness, C. M., Corby J. F., Blake, G. A., Hollis, J. M., Lovas, F. J., Jewell, P. R., & Remijan, A. J., "Interstellar Carbodiimide (HNCNH) - A New Astronomical Detection from the GBT PRIMOS Survey via Maser Emission Features," **2012** *Astrophys. J. Lett.*, 758, L33.

[4] Pulliam, R., McGuire, B. A., and Remijan, A. J., "A Search for Interstellar Hydroxylamine (NH_2OH) toward Select Astronomical Sources," **2012** *Astrophys. J.*, 751, 1.

[3] McGuire, B. A., Wang, Y., Bowman, J. M., and Widicus Weaver, S. L., "Do H_5^+ and Its Isotopologues Have Rotational Spectra?" **2011** *J. Phys. Chem. Lett.*, 2, 1405-1407.

[2] Crabtree, K. N., Kauffman, C. A., Tom, B. A., Beçka, E., McGuire, B. A., and McCall, B. J., "Nuclear Spin Dependence of the Reaction of H_3^+ with H_2 II. Experimental Measurements." **2011** *J. Chem. Phys.*, 134, 194311.

[1] Lovas, F. J., Plusquellic, D. F., Widicus Weaver, S. L., McGuire, B. A., and Blake, G. A., "Organic compounds in the $C_3H_6O_3$ family: Microwave spectrum of cis-cis dimethyl carbonate." **2010** *J. Mol. Spec.*, 264, 10-18.

Book Chapters, Conference Proceedings, and Other Publications

[4] McGuire, B. A. & Remijan, A. J., "Molecular Line Surveys."
Encyclopedia of Astrobiology, Gargaud, M., Ed.; Springer Reference (**2013**).

[3] McGuire, B. A., Carroll, P. B., & Remijan, A. J., "A CSO Broadband Spectral Line Survey of Sgr B2(N)-LMH from 260 - 286 GHz."
2013, *arXiv/astro-ph: 1306.0927*

[2] Lovas, F. J., Plusquellic, D. F., Widicus Weaver, S. L., McGuire, B. A., & Blake, G. A., "Organic compounds in the $C_3H_6O_3$ family: Microwave spectrum of cis-cis dimethyl carbonate."
Proc. Of: The 2010 NASA Laboratory Astrophysics Workshop, **2011**.

[1] Carroll, P. B., McGuire, B. A., & Widicus Weaver, S. L., "Construction of a High-Resolution Terahertz Cavity Ringdown Spectrometer."
Proc. of: The 2010 NASA Laboratory Astrophysics Workshop, **2011**.

Lectures and Invited Talks

[5] McGuire, B. A., "Beer's Law with a pathlength of 10^{16} m."
Kliegel Lectures in Planetary Science, California Institute of Technology, October 1, 2013.

[4] McGuire, B. A., "Beer's Law with a pathlength of 10^{16} m."
Summer Chemical Physics Seminar, California Institute of Technology, September 20, 2013.

[3] McGuire, B. A., "Unraveling the complexities of prebiotic interstellar chemistry through laboratory astrophysics and observational astronomy."
Gray-Hill Seminar Series, Occidental College, July 19, 2013.

[2] McGuire, B. A., "Exploring interstellar chemical inventories using astronomical observations and laboratory astrophysics."
California Institute of Technology, November 8, 2012.

[1] McGuire, B. A., "Exploring interstellar chemical inventories using cm-wave observations at the Green Bank Telescope."
Kliegel Lectures in Planetary Science, California Institute of Technology, October 23, 2012.

Selected Recent Conference Talks (12 Total From 2008 - Present)

- McGuire, B. A., Carroll, P. B., Corby, J. F., Loomis, R. L., Blake, G. A., Hollis, J. M., Lovas, F. J., Jewell, P. R., & Remijan, A. J., "The publicly available Prebiotic Interstellar Molecular Survey (PRIMOS): Expanding spectroscopic characterizations, extending to new sources, and adding to the known molecular inventory."
68th International Symposium on Molecular Spectroscopy, June 21, 2013.
- McGuire, B. A., Loomis, R. A., Charness., C. M., Corby, J. F., Blake, G. A., Hollis, J. M., Lovas, F. J., Jewell, P. R., & Remijan, A. J., "A new methodology for the detection of low-abundance species in the ISM: detection of interstellar carbodiimide (HNCNH)."
68th International Symposium on Molecular Spectroscopy, June 19, 2013.

- McGuire, B. A., Ioppolo, S., Allodi, M. A., Kelley, M. J., & Blake, G. A., "Terahertz time domain spectroscopy of interstellar ice analogs."
  2013 Astrobiology Graduate Student Conference, June 12, 2013.
- McGuire, B. A., Pulliam, R. L., & Remijan, A. J., "A search for interstellar hydroxylamine (NH_2OH)."
  Astrobiology Science Conference, April 18, 2012.
- McGuire, B. A., "Investigating the chemical complexity of the interstellar medium with ALMA."
  The Molecular Universe: IAU Symposium 280, 2011.

Selected Conference Poster Presentations (9 Total From 2009 - Present)

- McGuire, B. A., Ioppolo, S., Allodi, M. A., Kelley, M. J., & Blake, G. A., "Terahertz time-domain spectroscopy of complex organic molecules in astrophysically-relevant ices."
  246th Meeting of the American Chemical Society, September 11, 2013.
- McGuire, B. A., Loomis, R. A., Charness., C. M., Corby, J. F., Blake, G. A., Hollis, J. M., Lovas, F. J., Jewell, P. R., & Remijan, A. J., "Interstellar carbodiimide (HNCNH): A new astronomical detection from the GBT PRIMOS survey via maser emission features. "
  221st Meeting of the American Astronomical Society, January 9, 2013.
- McGuire, B. A., Wang, Y., Bowman, J. M, & Widicus Weaver, S. L., "Progress towards the rotational spectrum of H_5^+ and its isotopologues."
  The Molecular Universe: IAU Symposium 280, 2011.
- McGuire, B. A., Carroll, P. B., & Widicus Weaver, S. L., "Design and Construction of a High-Resolution Terahertz Cavity Ringdown Spectrometer."
  Spectroscopy 2011, ALMA: Extending the Limits of Astrophysical Spectroscopy, January 15-17, 2011.
- Carroll, P. B., McGuire, B. A., & Widicus Weaver, S. L., "Construction of a High-Resolution Terahertz Cavity Ringdown Spectrometer."
  2010 NASA Laboratory Astrophysics Workshop, October 25-28, 2010.

Unraveling the Complexities of Prebiotic Interstellar Chemistry through Laboratory Astrophysics and Observational Astronomy

Introduction. A unifying goal of my research is to use my skills as a laboratory chemist to aid in the interpretation of astronomical observations of our molecular universe. While the specific techniques and targeted science have evolved as my career has progressed, my focus has always been astrochemistry. Recently, I have made an effort to move beyond my training as a laboratory chemist to gain experience as an observational astronomer through both the collection and analysis of observational spectra relevant to my interests. Here, I have chosen to present a selection of my work which demonstrates my range of expertise, highlights my interests in the field of astrochemistry, and narrates my growth as a scientist.

The Simplest Polyatomic Ion - H_3^+. My undergraduate work with Ben McCall awoke in me a fascination for exploring problems which were experimentally challenging and whose answers offered substantial insight into the chemical evolution of the Universe. A key constraint in the study of these processes is temperature, for which an accurate observational probe is highly desirable. Because of its ubiquity in the universe, the ability to use hydrogen as this probe would be invaluable. Indeed, using simple Boltzmann statistics, the ortho-to-para ratio of the hydrogenic cation H_3^+ can yield an accurate temperature if one assumes the ratio is dominantly determined by the kinetic temperature of the gas [1]. However, the reaction of H_3^+ with H_2 (see Equation 1), which has not been extensively studied, can directly alter this ratio. Thus, the usefulness of this ratio as a probe of temperature is dependent on a rigorous understanding of this reaction.

$$H_3^+ + H_2 \rightarrow (H_5^+) \rightarrow H_3^+ + H_2 \tag{1}$$

H_3^+ is a transient, highly reactive species and as such is difficult to produce and study experimentally. To address this, I designed and constructed a liquid nitrogen-cooled hollow cathode plasma discharge cell to efficiently produce H_3^+ at low temperatures. I then coupled this source with a difference frequency generation laser system, in a White-type multi-pass arrangement, for direct absorption spectroscopy. Experimental results from this system have solidified our understanding of the effects the reaction of H_3^+ with H_2 have on the observed ortho-to-para ratio of H_3^+ [2]. These studies show that yet more complex processes than those examined are likely at play, and follow-up experimental work is planned.

Increasing Complexity: The Case of H_5^+. As I moved on from Ben's group, I continued to be intrigued by these simple, yet highly important species. H_3^+, and by association H_5^+, is thought to be a key reaction intermediate in interstellar processes and a foundational species in ion-neutral chemistry leading to the more complex species observed in the interstellar medium (ISM) [3]. I had moved from laboratory studies in the infrared, to those in the microwave and sub-millimeter regions of the spectrum, focusing on pure-rotational transitions of molecules. I was also beginning to take an interest in single-dish millimeter and sub-millimeter radio astronomy observations, with a particular interest in the detection of new molecular species. It struck me that while both H_3^+ and H_2 are well-known interstellar molecules, the intermediate species in the reaction of these two molecules, H_5^+, is not. I therefore endeavored to explore the possibility of measuring the laboratory spectra of H_5^+ in the millimeter and sub-millimeter, to enable searches for this molecule in observational spectra.

Rigorous Diffusion Monte Carlo simulations allowed for the calculation of highly-accurate structures for H_5^+ and all of its deuterated isotopologues. Molecules with completely symmetric structures possess no permanent dipole moment, and will thus display no pure-rotational spectra. The results of these simulations indicated that while H_4D^+, $H_3D_2^+$, and $H_2D_3^+$ all displayed permanent dipole moments, H_5^+, HD_4^+, and D_5^+ did not [4]. While the sensitivity of laboratory spectroscopic techniques is likely not yet sufficiently high to detect any of these species [5], we provided simulated pure-rotational spectra for all three species with permanent dipole moments, to be used a guide for future laboratory efforts. The identification of H_5^+ or its deuterated isotoplogues in the ISM based on such studies will be an important step forward in our understanding of the very roots of molecular complexity.

Exploring Prebiotic Chemical Pathways - $\mathbf{NH_2OH}$. H_3^+ serves as an important reaction intermediate in the formation of complex species through ion-molecule reactions. Perhaps the most enigmatic of these species is glycine (NH_2CH_2COOH), the simplest of the amino acids which are the building blocks of the biopolymers comprising life as we know it. Glycine has been found in meteorites and comets, most recently and notably in pristine samples from comet Wild 2 returned by the NASA STARDUST mission [6]. However, a detection of glycine in the gas-phase molecular environments these comets and meteorites form from, is so far lacking. This is likely due to its low abundance and complex spectra. Indeed, recent state-of-the-art models by R. Garrod predict that under ideal circumstances, it will take the full capabilities of our most powerful observatory, ALMA, to detect glycine [7]. It is therefore essential that we have a foreknowledge of the best environments in which to search for glycine and by extension, the most favorable environments in which glycine may form.

The reaction of hydroxylamine (NH_2OH), and even more favorably protonated hydroxylamine (NH_3OH^+) which is formed by reaction of NH_2OH with H_3^+, with acetic acid (CH_3COOH), has been proposed as an efficient route to the formation of interstellar glycine in the gas-phase [8] (see Equation 2).

$$NH_3OH^+ + CH_3COOH \rightarrow NH_3CH_2COOH^+ + H_2O \tag{2}$$

Neutral NH_2OH had been predicted by gas-grain chemical models to be highly abundant in warm star-forming regions [9]. As my first true foray into the field of observational astronomy, my colleagues and I undertook an observational campaign to detect and quantify this abundance in seven distinct interstellar environments [10]. In each case, the observations resulted in a clear non-detection of NH_2OH, with upper limits to the abundance as much as 10^6 times lower than those predicted by the models. As a result of these studies, these models were revised, and now predict that there is **no** viable gas-phase route to the formation of glycine in the ISM. Instead, it is most likely formed through reactions within the icy surfaces of interstellar dust grains [7].

Complex Chemistry in Interstellar Ices. Indeed, much observational evidence is now pointing to the importance of the interplay between reactions occurring in the gas phase and those occurring in the solid phase in ices. I recently published the first detection of carbodiimide (HNCNH), the tautomer of the long-known interstellar species cyanamide (NH_2CN) in the Sgr B2(N) molecular cloud [11]. The possibility of detecting HNCNH had long been dismissed as its abundance is only ∼1% of NH_2CN at room temperature; much less at lower temperatures. However, recent experimental work has shown that when NH_2CN is embedded in water ice, such as in the icy surfaces of dust grains, tautomerization to HNCNH is somewhat stabilized. As a result, abundances of HNCNH as high as 13% of those of NH_2CN are possible [12]. Additionally, the energy level structure of HNCNH is such that transitions occurring around 5, 25, and 45 GHz were observed to be masing, greatly enhancing their observed brightness to detectable levels. It was only through the combination of these two factors that we were able to detect this species in the ISM. This work highlights the importance of reactions occurring within interstellar ices, as well as the stabilizing influence of the ices themselves, to the formation of complex molecules in the interstellar medium.

My most recent laboratory work has been the construction of a novel time-domain THz spectrometer to study these important interstellar ices in a region of the spectrum which has been largely unexplored. While only in its infancy, this ground-breaking work is already displaying the promise of these observations in the study of these systems. The details of this spectrometer, as well as my plans for its applications going forward, lay the foundation of the first year of my proposed research, and are detailed further in that document.

References

[1] McCall et al. 1999, ApJ, 522, 338.

[2] Crabtree et al. 2011, JCP, 134, 194311.

[3] B.J. McCall, PhD Thesis, University of Chicago, June 2001.

[4] McGuire et al. 2011, JPCL, 2, 1405.

[5] Alligood DePrince et al. 2013, Rev. Sci. Inst., 84, 075107.

[6] Elsila et al. 2009, Meteor. & Planet. Sci., 44, 1323.

[7] Garrod 2013, ApJ, 765, 60.

[8] Snow et al. 2007, JACS, 129, 9910.

[9] Garrod et al. 2008, ApJ, 682, 283.

[10] Pulliam et al. 2012, ApJ, 751, 1.

[11] McGuire et al. 2012, ApJL, 758, L33.

[12] Duverney et al., JPC, 109, 603.

The Cosmic Origins of Complex Prebiotic Molecular Material: A Combined Observational and Laboratory Investigation

One of the most fundamental scientific questions that remains largely unexplored is the investigation of our prebiotic molecular origins in the universe. What were the properties that led to the evolution of complex organics in stellar systems? Where are the building blocks of organic molecules located in astronomical environments? And finally, how does this organic material make its way into early planetary systems? This proposal outlines an integrated laboratory and observational program that seeks to directly address these questions, during which time my primary host institution will be the NRAO Headquarters. Initially, I will use a time-domain THz spectrometer constructed at Caltech, the only facility worldwide equipped to conduct this research, to study astrophysical ices in this largely unexplored region of the electromagentic spectrum. I will then use the laboratory measurements to probe directly, for the first time, the abundance and distribution of water and methanol ices in protoplanetary disks and molecular clouds. These results will then inform observational campaigns with the GBT, VLA, and ALMA to correlate these ice abundances with gas-phase molecular complexity. The initial steps of this program will take advantage of my expertise with laboratory spectroscopy and single-dish observational astronomy of molecular clouds. The latter two thirds will allow me to expand my skill set to become an expert in the study of solid-phase species and protoplanetary disks. This unique combination of skills will allow me to address fundamental questions of our origins from a unique vantage point. Given my knowledge, experience, and access, I am currently the best qualified researcher worldwide to perform these groundbreaking studies.

Introduction. Understanding the origin of life on Earth has long fascinated the minds of the global community and has been a driving factor in interdisciplinary research for centuries. The most recent major discovery in this area has been the detection of glycine (NH_2CH_2COOH), the simplest amino acid, in cometary samples returned by the NASA STARDUST mission [1]. Indeed, the open questions left by these discoveries, both in the public and scientific communities, hold such fascination that NASA has designated the understanding of our "Cosmic Origins" as a key mission priority. Until quite recently, our ability to explore the possibilities of the more widespread formation of life in the Universe has been limited to an environmental sample set of one: our own Solar System. With the advent of the Atacama Large Millimeter Array (ALMA), we now possess the tools to study star-forming regions and protoplanetary disks, the evolutionary precursors to solar systems, at spectral and spatial resolutions never before obtainable. These studies are essential for understanding the conditions under which solar systems and planets form. Despite these advances, we have yet to detect even glycine outside of our own solar system. In fact, my previous observational work has shown the only efficient route to glycine formation is through solid-phase reactions within the icy mantles of interstellar dust grains [2]. Unfortunately, our current understanding of the composition of these astrophysical ices is limited to only a few major constituents, and is hampered by the need to conduct these observations in the infrared, where laboratory databases exist.

To address these concerns, I will conduct an integrated laboratory spectroscopy and observational astronomy project. First, I will characterize astrophysical ice analogs of the major known ice constituents, specifically water and methanol, using time-domain THz spectroscopy, opening a new region of the electromagnetic spectrum for observation of these species. I will then use SOFIA and Herschel PACS/SPIRE archive data with these laboratory measurements to constrain the composition and thermal history of the ices in protoplanetary disks and the pre-eminent complex molecular source, Sgr B2(N).

Exploring Molecular Evolution in the ISM. While the number of known molecules identified in the gas phase continues to increase (8 new molecules have been identified so far in 2013 [3–9]), identification of solid-phase molecules has been remarkably slower. Indeed, the identification of complex species, such as methyl formate (CH_3OCHO), which are widely observed in high abundance in the gas-phase but must be formed primarily in the solid-phase [2,10], is so far lacking. Additionally, the number of sources in which *any* measurements of ices have been made is limited. This is likely due to several factors.

First, the features arising from these solid-phase species in the infrared are often relatively broad, resulting in overlapping and confused signals in observations. Second, the sample set of sources from which we may observe these species in ices is limited, relative to gas-phase species, as we can observe these species only in absorption, rather than emission. Observations in the THz region of the spectrum will resolve both of these issues. Here, $h\nu$ is sufficiently small that temperatures less than ~150 K can provide detectable emission, and absorption can occur against background continuum. The combination of these factors vastly increases the number of target sources available for observation. Preliminary indications are that the spectra of solid-phase molecules in the THz are more distinctive than those in the infrared and provide information on the structure, temperature, and thermal history of the ice. Preliminary indications are that the spectra of solid-phase molecules in the THz are more distinctive than those in the infrared and provide information on the structure, temperature, and thermal history of the ice (see, e.g. [11–15]). The vast majority of molecules of interest, however, remain unexplored.

THz Spectroscopy of Astrophysical Ices. The Blake Group has constructed a one-of-a-kind THz time-domain spectrometer capable of collecting broadband spectra of astrophysically-relevant ices over the range of 0.3 - 7.5 THz. The details of this spectrometer and the techniques used are given in [16]. Briefly, ices are deposited via a vapor deposition line onto a silicon substrate cooled to 8 - 300 K in a closed-cycle helium cryostat evacuated to high vacuum pressures. The sample is then simultaneously interrogated in the THz (0.3 - 7.5 THz) and in the infrared (400 - 4000 cm^{-1}). As the THz detection is a natively time-domain technique, it has the added benefit of sampling not only the magnitude of the THz pulse, but also the phase. As such, the fully complex optical constants (n and k) are directly sampled, increasing the accuracy with which these constants can be measured.

Initial work with this spectrometer has been crude and exploratory, focused primarily on the spectra of water ices [16] and methanol. Despite having a relatively low resolution ($\Delta\nu$ ~100 GHz), these studies reveal the expected richness of ice signatures in the THz.

These spectra demonstrate the need for higher-resolution data. The spectrometer has in fact recently been upgraded to a resolution of $\sim$10 GHz. Interstellar ices will certainly be more complex than these simple, pure samples, and studies of astrophysically-relevant mixtures are necessary to conduct meaningful searches for these molecules in the ISM. My work will therefore focus primarily on the establishment of this database and some initial astrophysically-relevant mixtures of the major ice constituents. Specifically, during an extended visit to Caltech during my first year, I will obtain high-resolution spectra of pure water, pure methanol, and mixtures of the two with each other, as these speak directly to my goal of understanding the role of methanol ice in molecular complexity.

Herschel and SOFIA Observations of Astrophysical Ices. Understanding the interplay between the gas- and solid-phase chemistry occurring in molecular clouds and protoplanetary disks is essential to grasping the larger picture of the physical and chemical evolution of these regions. Much work to understand the gas phase side of this broader view has been conducted using single-dish measurements in complex clouds (see, e.g. the PRIMOS project [4, 5, 17]). Some targeted interferometric work has been conducted as well [18, 19]. Existing observatories can provide a much-needed intermediate product in the near future. High-resolution, broadband interferometric surveys of molecular clouds and protoplanetary disks, however, will require the full capabilities of ALMA which will not be available in these modes for many years.

Studies of solid-phase species in these regions are historically more limited. In fact, two of the most recent state-of-the-art observational studies of the famous TW Hydrae protoplanetary disk merely infer the abundance of solid-phase species from gas-phase observations [20, 21]. Direct measurements of solid-phase abundances in these regions will provide the next leap in our understanding. Here, I will apply the insight gained from the laboratory investigations outlined above to observations of interstellar ices from the Herschel Archive and new observations using the FIFI spectrometer onboard the Stratospheric Observatory for Infrared Astronomy (SOFIA). These studies will allow for the first time the direct determination of solid-phase abundances, as well as the physical state (crystalline versus amorphous), of molecular species which are keystones in the physical and chemical evolution of these sources.

My first goal will be to mine this archive and analyze the data with the dual objectives of quantifying the abundance fraction of crystalline versus amorphous water ice, as well as the abundance of methanol ice, in these disks. In fact, the well-ordered temperature structure of disks means that such studies can for the first time determine the radial location of the ice within the disk. By observing these distributions across a number of disks at different evolutionary time scales, we can begin to piece together the larger picture of both water and complex chemical evolution in these regions. This picture can then in turn be used to understand the evolutionary origin of: (i) Earth's own water supply and (ii) complex organic molecules in our solar system. I aim to determine whether increased molecular complexity in ices, as indicated by the methanol fraction, leads to an increased complexity observed in the gas-phase as well.

This study will provide an inventory of environments in which the Herschel and SOFIA results are sensitive to the cooler dust components, thus providing excellent constraints on the initial composition of ices in the regions. These will then inform observational proposals in the latter part of my tenure using the GBT, VLA, and ALMA to correlate the ice abundances with grain mantle heating and high temperature gas phase chemistry in hot cores and disks.

Education & Outreach. Finally, I will engage in a unique outreach and education program during my tenure as a fellow. My primary focus will be a collaboration with the Ph.Detours outreach initiative. Ph.Detours is an online video outreach program started by Jorge Cham, the author of the widely acclaimed PhD Comics, and Alex Lockwood, the star of the 2012 PhD Comics Movie. Each episode (∼5 minutes) focuses on a current topic in cutting-edge research. Alex interviews researchers, faculty, and PhD students involved and helps to present their research in language approachable to a general viewing audience. So far, they have covered topics ranging from the Mars Curiosity rover to the scientific study of the impact of comic books on society.[1] These episodes reach an audience of over 7 million annual viewers, with each episode typically receiving between 25,000 and 120,000 views. Each year, I will work with Alex and Jorge to select several new topics to explore, travel with the team to the site, and participate on-screen in the videos. Our first collaboration will focus on the SOFIA aircraft and telescope, highlighting my own research and observations discussed previously, as well as the big picture of SOFIA's scientific reach.

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[1] The most successful video, featuring the Mars Curiosity team, can be seen at http://youtu.be/sSpfJeVpZSg.