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NRAO Facility

Green Bank, West Virginia

Posters: Titles & Abstracts

Gilles Adande, Lucy M. Ziurys, and DeWayne Halfen
University of Arizona

H-1

“Mapping of the distribution of HSCN and HNCS in Sgr B₂”

Sulfur is an abundant element in the galaxy, and main sulfur-bearing species (SO, CS, SO₂, H₂S) are sometimes used as moderate tracers for shock chemistry or as chemical clocks. Our understanding of sulfur chemistry is however still incomplete. In dense molecular clouds, the identity and abundance of the main sulfur reservoir is still discussed, as well as the chemical processes leading to the observed sulfur complexity.

One interesting way to investigate sulfur chemistry is by observing metastable isomers. A particular pair of interest is HNCS and its metastable isomer HSCN. We have been conducting mapping observations of the $8_{0,8} \rightarrow 7_{0,7}$ transition of these two species in the Sgr B₂ giant molecular cloud. Preliminary results show that emission from both species is extended over a 5' * 3' region around Sgr B₂(GC).

The study will shed light on the spatial extent of the chemical processes leading to these molecules, and provide new data useful for sulfur species in astrochemical models.

Thomas A. Anderson, Jay A. Kroll, and Susanna L. Widicus Weaver
Department of Chemistry, Emory University, Atlanta, GA 30322

H-2

“Spectroscopy of Prebiotic Molecules Formed from O(¹D) Insertion Reactions”

Many important molecules in astrochemistry are unstable or reactive species, and therefore difficult to study in the lab. Three such molecules are methoxymethanol (CH₃OCH₂OH), methanediol (HOCH₂OH), and aminomethanol (NH₂CH₂OH). These molecules are predicted to form on grain surfaces in the initial steps of interstellar prebiotic molecular evolution. Once in the gas phase, these molecules are thought to be precursors to complex molecules such as sugars and amino acids. To test these prebiotic interstellar chemical pathways, a pure rotational spectrum is required for comparison to interstellar line surveys. Given the reactivity and instability of these molecules under normal laboratory conditions, an efficient chemical formation mechanism is required before such laboratory studies can be conducted. O(¹D) insertion reactions are one possible production route. O(¹D) insertion reactions into C-H bonds are highly exothermic, and therefore highly efficient. We have constructed a supersonic expansion source which allows O(¹D) to react with organic molecules on-the-fly, in the gas phase. The products are stabilized and isolated in the expansion, allowing spectroscopic study. We will present our experimental design and our progress toward obtaining high-resolution gas-phase spectra of these molecules.

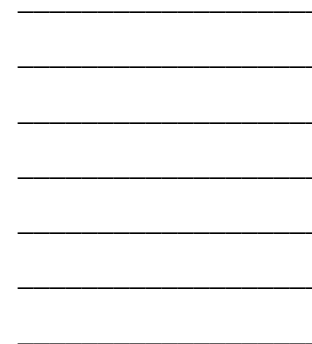
Brandon Carroll and Susanna L. Widicus Weaver

H-3

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“Laboratory Spectroscopy of ‘Interstellar Weeds’ and other Complex Organic Molecules”

With the eminent launch of the Herschel Space Observatory and completion of the Atacama Large Millimeter Array (ALMA), a number of high-resolution spectral line surveys of interstellar clouds will soon become available. These surveys will be difficult to interpret due to the presence of so-called “interstellar weeds,” or highly abundant molecules with strong and dense spectra across the millimeter and submillimeter windows. In order to effectively use these surveys to identify new interstellar molecules, it is necessary to obtain complete spectral assignments for the known molecules. Using a newly-constructed direct absorption spectrometer, we have begun collecting spectral catalogs of several interstellar weeds in the 140-220 GHz frequency range. In addition to studying interstellar weeds, we are using this spectrometer to investigate several complex organic molecules predicted to be present in interstellar clouds. We will report our initial results from these studies.



Martin Cordiner,[†] T. J. Millar[‡]

H-4

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“Carbon chains and anions in the density-enhanced shells of IRC+10216”

A new, more physically realistic chemical model is presented for the carbon-rich circumstellar envelope of the AGB star IRC+10216, which includes shells of matter with densities that are enhanced relative to the surrounding circumstellar medium. The chemical model uses an updated reaction network and a more detailed anion chemistry. In particular, new mechanisms are considered for the formation of CN⁻, C₃N⁻ and C₂H⁻. New reactions involving H⁻ are included which result in the production of significant amounts of C₂H⁻ and CN⁻ in the inner envelope such that these species may be detectable in IRC+10216 despite the very low theorized radiative electron attachment rates of their parent neutral species. The calculated radial molecular abundance profiles for the hydrocarbons C₂H, C₄H and C₆H and the cyanopolynes HC₃N and HC₅N show narrow peaks, which are in better agreement with observations than previous models. Thus, the narrow rings observed in molecular microwave emission [1,2] surrounding IRC+10216 are interpreted as arising in regions of the envelope where the gas and dust densities are greater than the surrounding circumstellar medium.



References:

[1] Guélin, M., Neining, N., Lucas, R. and Cernicharo, J. 1999, The Physics and Chemistry of the Interstellar Medium, Proceedings of the 3rd Cologne-Zermatt Symposium, 326, CGA-Verlag, Herdecke

[2] Dinh-V-Trung and Lim, J. 2008, ApJ, 678, 303

Jessica Dodd[†] and Lucy Ziurys[‡]

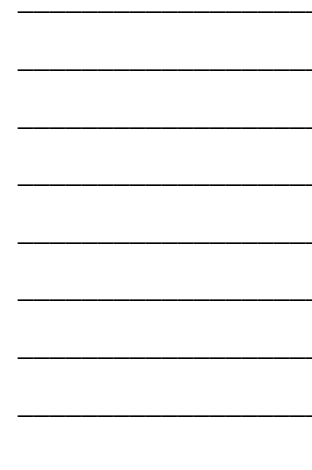
L-1

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“Chemistry in Protoplanetary and Planetary Nebulae”

Intermediate mass stars evolve off of the Asymptotic Giant Branch and continue through the Protoplanetary Nebulae (PPNe) and Planetary Nebulae (PNe) phases. Molecules that formed in the circumstellar envelope of the AGB star will be carried on into the Protoplanetary Nebula stage. In the following Planetary Nebula phase, the central star becomes a hot UV emitter. This UV radiation can ionize the surrounding material, and so it was previously thought that many if not all molecules would be destroyed in this environment. Radio observations have proven otherwise with a number of molecules persisting far into and even surviving through these late stages of stellar evolution. Radio observations and rotational spectroscopy can be used to identify molecules and measure their abundances. The $^{12}\text{CO}(2-1)$ and $^{13}\text{CO}(2-1)$ rotational transitions have been measured in a number of planetary nebulae using the Arizona Radio Observatory SMT on Mt. Graham. These observations will be used to calculate the $^{12}\text{C}/^{13}\text{C}$ isotope ratio which can provide information about processes occurring during stellar nucleosynthesis. Also, a search for the molecule CS in Planetary Nebulae is under way with two possible detections so far. It was previously thought that this molecule was destroyed during the transition from a PPN to a PN, but these new observations made with the ARO 12-m telescope on Kitt Peak suggest otherwise.



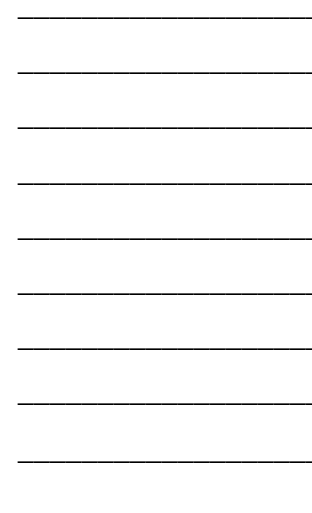
Brian J. Drouin and John C. Pearson

H-7

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“The JPL Millimeter and Submillimeter Spectral Line Catalog”

Recent concerns regarding interstellar line confusion has revived astrophysical support for the Jet Propulsion Laboratory’s Millimeter and Submillimeter Spectral Line Catalog. This catalog was originally designed as a tool for the planning and interpretation of atmospheric, planetary and astronomical observations at long wavelengths. The traditional format (ASCII files available via ftp or http) has been sufficient for atmospheric science missions and individual astronomers; however the complexity of astrophysical sources and the comprehensive spectra expected from future telescopes (e.g. Herschel and ALMA) require a more modern approach to the database and its tools. The current catalog interface is designed for (human) users who might browse and search the contents. Users with large data analysis problems have been required to develop their own assimilation tools. However, the large data analysis problem is likely to become the regular problem; therefore the development of astronomical data analysis tools that seamlessly utilize the comprehensive spectroscopic data will be a primary driver for the upgrades. Some of the planned upgrades include: the file infra-structure will be cast into a database structure compatible with modern client tools; the development of a systematic and user/machine-friendly citation tool. Synergistic upgrades for the atmospheric usage of the database will also be highlighted. We will also discuss new or planned changes to the catalog species.



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“Gas Phase Reactions of CH_3^+ with a Series of Homo- and Heterocyclic Molecules”

In gas phase ion chemistry the growth of larger molecules is known to occur through association of ions and neutrals. Where the ion attaches to the neutral is important because it can influence the possibility of additional associations, effectively enabling or terminating further molecular growth. The methyl cation, CH_3^+ , is an important species in the interstellar medium and in the ionosphere of Titan. Interest in Titan has increased recently due to the continuing success of the Cassini Mission. Experimental data involving this ion are important to correctly model the chemistry occurring in the Titan atmosphere. As a contribution to this, rate coefficients and product distributions have been determined for reactions of CH_3^+ with a series of cyclic molecules: benzene (C_6H_6), cyclohexane (C_6H_{12}), pyridine ($\text{C}_5\text{H}_5\text{N}$), pyrimidine ($\text{C}_4\text{H}_4\text{N}_2$), piperidine ($\text{C}_5\text{H}_{11}\text{N}$), 1,4-dioxane ($\text{C}_4\text{H}_8\text{O}_2$), furan ($\text{C}_4\text{H}_4\text{O}$), pyrrole ($\text{C}_4\text{H}_5\text{N}$), and pyrrolidine ($\text{C}_4\text{H}_9\text{N}$). Unexpectedly, association with the methyl cation was competitive with proton transfer, charge transfer and hydride abstraction product channels in reactions involving unsaturated species where there were π electrons in the ring. No association was observed for cases where there were no π electrons available. The significance of this to modeling the Titan atmosphere and the interstellar medium will be discussed.

Keywords: SIFT, ion-neutral reactions, association reactions

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H-9

[†]Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX[‡]Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, and the School of Engineering & Applied Sciences, Harvard University, Cambridge, MA“A Survey of C_4H , C_6H and C_6H^- with the Green Bank Telescope”¹

The carbon chain negative ion C_6H^- and the structurally similar radicals C_4H and C_6H were surveyed with the 100 m Green Bank Telescope toward 24 galactic molecular sources. The most readily observed molecular anion to date, C_6H^- was detected in two new sources: the dark clouds L1544 and L1521F, where it was found to be present at the level of $2.5\% \pm 0.8\%$ and $4\% \pm 1\%$, respectively relative to neutral C_6H . The C_4H radical was detected in nearly all dark clouds surveyed—in six for the first time; C_6H was detected in six new sources: five dark clouds and one translucent cloud. The observed $\text{C}_6\text{H}^-/\text{C}_6\text{H}$ (1%–4%) and $\text{C}_6\text{H}/\text{C}_4\text{H}$ (0.2%–1%) ratios in these sources suggest that C_6H^- may be close to detection in other dark clouds. The fractional ionization estimated from the $\text{C}_6\text{H}^-/\text{C}_6\text{H}$ ratio in L1544 and L1521F of 10^{-8} to 10^{-7} is comparable to earlier determinations from positive molecular ions. A close correlation is found between the column densities of C_6H and C_4H , similar to correlations previously observed between the cyanopolyynes HC_3N and HC_5N , and between C_4H and the cyanopolyynes², suggesting that long carbon chains are probably formed by similar processes in interstellar clouds.

¹ Gupta H., Gottlieb, C. A., McCarthy, M. C., & Thaddeus, P. 2009, *ApJ*, **691**, 1494.² Federman, S. R., Huntress, W. T., Jr., & Prasad, S. S. 1990, *ApJ*, **354**, 504.

Nanase Harada and Eric Herbst

L-2

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“A New Interstellar Model For High-Temperature Time-Dependent Kinetics”

We have developed a kinetic approach to investigate time-dependent, high-temperature interstellar chemistry that can occur up to 1000 K. The network used is an expanded OSU gas-phase network, which includes both exothermic processes with barriers and endothermic reactions. Some hydrogenation reactions with barriers, which do not happen at lower temperatures start having great impact on the chemistry at temperatures greater than 100 K or so. As a result, H₂O becomes a dominant form of oxygen instead of atomic oxygen, which is more dominant in cold clouds, and NH₃ becomes more dominant than atomic nitrogen. Because of the high abundance of H₂O and NH₃, H₃O⁺ and NH₄⁺ become the dominant forms of ions. Other species that became more abundant with increasing temperature are CH₄, HCN, and C₂H₂. Higher abundances of H₂O and CH₄ are also obtained by a thermodynamic model (Markwick et al) although it does not produce the variety of molecules that have been observed in high-temperature sources. When an appropriate cosmic-ray induced ionization or X-ray ionization is incorporated, this expanded network can be applied to dynamic models such as those needed for active galactic nuclei, which will be observed in some detail when ALMA becomes fully operational.

George Hassel,[†] Eric Herbst,[†] and Ted Bergin[‡]

L-6

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“Shocks as a Molecular Cloud Formation Mechanism: the Astrochemistry Context”

We investigate the initial synthesis of molecular ices and subsequent evolution of complex gas phase molecules during the formation of a cold molecular cloud after the passage of a shock. The Ohio State gas-grain reaction network is modified to simulate the evolution of physical conditions from those of the diffuse interstellar medium to the initial stages of a dark cloud. The inclusion of newly measured rates of photodesorption is required to more accurately model this transitional period. In contrast with a more common pseudo-time-dependent approach, water ice is produced on grains and CO is produced in the gas phase, then accretes to grains in intermediate stages of dark cloud formation. For the ices, this enhances the production of CO₂ and inhibits the formation of CH₄. In the gas phase, this can alter the C/O ratio from an O-rich state toward unity. Overall, the results show that dense cores will condense from molecular gas rather than atomic, ionized gas.

David Horne,[†] Erika Gibb,[†] T. Rettig,[‡] and S. Brittain[§]

H-10

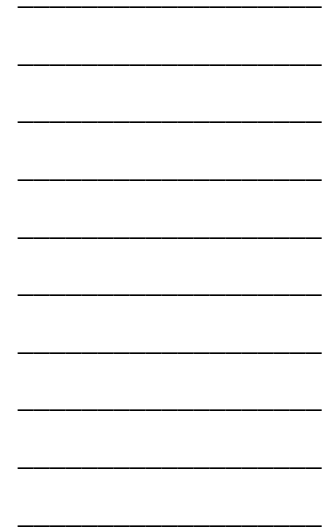
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“Investigating Dust/Gas Stratification in the Disks of Young Stellar Objects”

The distribution of gas compared to dust in the circumstellar disks of young stellar objects (YSO's) is crucial to our understanding of the early evolution of planetary bodies. Planetary formation models indicate that dust density in the mid-plane of a protoplanetary disk is critical to the formation timescale of planetary bodies, but turbulent mixing may act to distribute dust to higher scale heights. Observations of gas/dust stratification provide a good measure of internal disk dynamics and potential formation of planetesimals. Rettig et al. (2006) reported observational evidence of stratification in the disks of four class II T Tauri stars utilizing NIRSPEC observations of ^{12}CO , ^{13}CO and C^{18}O fundamental and ^{12}CO overtone absorption lines to measure the column density of gas along the line of sight. Here we study this effect for a larger sample of T Tauri stars. Since our sample consists of low mass stars that often exhibit photospheric CO absorption at K-band, our analysis has been adapted to incorporate NEXTGEN (Hauschildt, 1999) and MARCS synthetic photospheric spectra. Photospheric features may then be extracted from the target spectrum using custom written algorithms. These methods have allowed the gas/dust ratio as a function of inclination to be accurately derived for a greater range of sources. We present results for 6 additional sources and discuss the correlation of the gas/dust ratio with disk inclination for these observations with respect to the findings of Rettig et al. (2006).



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H-11

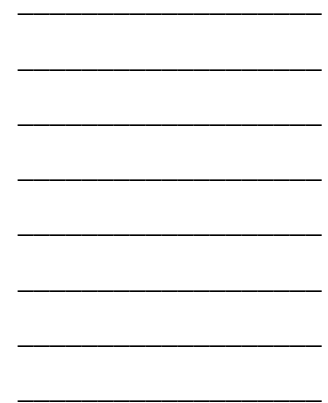
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“Variability of the Cosmic-Ray Ionization Rate in Diffuse Molecular Clouds”

The energy spectrum of cosmic-rays --- a product of particle acceleration and subsequent diffusion --- is generally assumed to be uniform throughout the Galaxy. As a result, the cosmic-ray ionization rate inferred in similar environments (e.g. in several diffuse clouds) should also be relatively constant. However, current estimates of the ionization rate in diffuse molecular clouds vary over the range $(1-8)\times 10^{-16} \text{ s}^{-1}$. In addition, there are a few sight lines with 3σ upper limits of $\zeta_2 < 10^{-16} \text{ s}^{-1}$, suggesting even lower ionization rates in some clouds. This roughly order of magnitude difference in the cosmic-ray ionization rate between sight lines contradicts the concept of a spatially uniform cosmic-ray flux.



We present cosmic-ray ionization rates derived from several published and unpublished spectroscopic observations of H_3^+ in diffuse cloud sight lines. These ionization rates are then compared with various other parameters (Galactic latitude, Galactic longitude, hydrogen column density) in a search for correlations. Also, sight lines in close proximity are compared to each other to determine the variability of the ionization rate on small spatial scales.

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Engineering & Applied Sciences, Harvard University, Cambridge, MA
“The Optical Spectrum of Thiozone”

The recent discovery and mapping of S₂ and SO₂ in the plume of Pele, one of the largest and most active volcanoes on Io, the innermost moon of Jupiter, suggests that other sulfur rich molecules may be abundant in this unusual planetary source.^{i ii} Optical images of Io in the range 3900Å – 5000Å conclude as much: the observed flux intensity cannot be attributed to transitions of these molecules alone.ⁱⁱⁱ

By means of 2-colour resonant-2-photon ionisation time of flight mass spectroscopy the optical spectrum of thiozone S₃ and other sulfur rich systems have now been detected. For thiozone a progression in the excited state bending mode is seen with a frequency of 350cm⁻¹ built onto the origin band at 433.82nm. In this talk our results are compared to prior experimental matrix and low-resolution gas-phase work. The prospects for finding these atomic clusters in the atmosphere of Io will be discussed.

ⁱ J. R. Spencer, K. L. Jessup, M. A. McGrath, G. E. Ballester and R. Yelle, *Science*, **288**, 1208-1210, 2008

ⁱⁱ A. Mollet, E. Lellouch, R. Moreno, M. A. Gurwell and C. Moore, *A&A*, **482**, 279-292, 2008

ⁱⁱⁱ P. Geissler, A. McEwen, C. Porco, D. Strobel, J. Saur, J. Ajello and R. West, *Icarus*, **172**, 127-140, 2004

Nadya Kunawicz, A. J. Markwick, and P. J. Woods
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“Potential metallicity tracers in extragalactic dark clouds”

A time-dependent model of a dark cloud was constructed, in an attempt to model these clouds in low metallicity environments such as external galaxies. The models were calculated with varying initial elemental abundances of carbon, oxygen, nitrogen, sulphur and the heavy metals Fe, Mg and Na (henceforth, M). These abundances were taken from observations of HII regions in the LMC and SMC. The results were used to identify potential metallicity tracer species in dark clouds. The most useful tracers were ratios of two species, notably CO/OH and HCO+/CO, which trace the underlying carbon abundance and the underlying M abundance respectively. In the future, these results can potentially be extrapolated, so that tracers observed in galaxies at high redshift will allow the calculation of the underlying metallicity of an extragalactic dark cloud.

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Weaver[†]

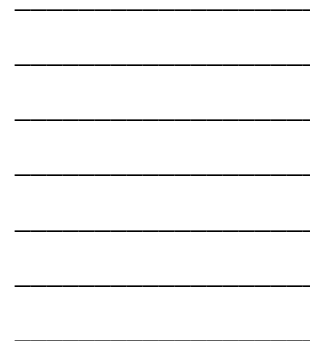
H-14

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*“Methanol Photodissociation and its Role in the Complex Chemistry of the
Interstellar Medium”*

Methanol has been observed to play a fundamental role in the complex organic chemistry of the interstellar medium. The primary dissociation products of methanol from cosmic ray-induced and external UV photons are all highly reactive radicals. These radicals are thought to be significant driving forces in the observed chemical complexity of interstellar clouds. However, quantitative branching ratios for methanol dissociation channels have not been determined experimentally. To address this problem, we are conducting quantitative, high-resolution THz spectroscopy experiments to monitor the products and branching ratios for gas-phase far-UV photodissociation of methanol. Here we will present the experimental design of the photolysis source and THz spectrometer. We will also present the initial results from a coupled gas/grain astrochemical model that explores the effects of the methanol dissociation branching ratios on complex organic interstellar chemistry.



Valerio Lattanzi,[†] Michael C. McCarthy,[‡] Patrick Thaddeus,[‡] and Sven
Thorwirth[§]

L-3

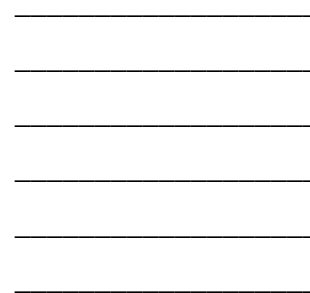
[†]Harvard-Smithsonian Center for Astrophysics, Cambridge, MA

[‡]Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, and the School
of Engineering & Applied Sciences, Harvard University, Cambridge, MA

[§]Max-Planck-Institut für Radioastronomie, Bonn, Germany

“Microwave Detection of Protonated SO₂ in Two Isomeric Forms”

By means of Fabry-Pérot FT microwave spectroscopy, the rotational spectrum of protonated sulfur dioxide in two distinct isomeric forms, a cis and a trans geometry, is reported. Searches for both isomers were based on theoretical structures obtained at the CCSD(T)/cc-pwCVQZ level of theory corrected for zero-point vibrational effects at the CCSD(T)/cc-pV(T+d)Z level. At a similarly high level of theory, the cis isomer is calculated to be the global minimum on the potential energy surface, but the trans isomer is predicted to lie only a few kcal/mol higher in energy. The identification of cis HOSO⁺ has been confirmed by detection of rotational lines of DOSO⁺ and HO³⁴SO⁺ at precisely the expected frequency shifts. Because sulfur dioxide is a well known interstellar and extragalactic species, and because it possesses a large proton affinity, HOSO⁺ is a excellent candidate for radioastronomical detection.



Avi M. Mandell,[†] Michael J. Mumma,[†] and Geoffrey Blake[‡]

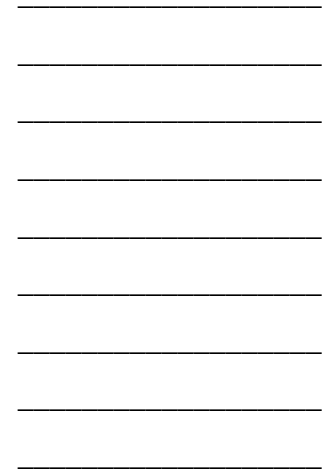
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[‡]California Institute of Technology

“Constraining the Characteristics of Warm Gas in the Planet-Forming Regions of Gas-Rich Circumstellar Disks”

H-15

Characterizing the gas chemistry in the planet-forming regions of young circumstellar disks is essential to understanding the origins of planetary systems. Near-infrared spectroscopy (1 – 5 microns) covers both low-energy and high-energy ro-vibrational transitions for a large variety of molecules, allowing accurate measurements of the excitation state and kinematics of the warm gas in the inner disk. Detection of new tracers of molecular chemistry can provide new insight into the thermodynamic and kinematic processes occurring in the inner disk. We have developed new reduction techniques to allow very accurate spectroscopic observations of Herbig Ae and T Tauri stars in the 3.0 – 3.7 micron wavelength range (L-band); our results reveal emission from multiple ro-vibrational transitions of OH, as well as lines of highly excited H₂O and possible evidence of other tracers. H₂O and OH (as a potential tracer of dissociated H₂O) provide an especially sensitive probe of the thermal environment in the planet-forming region. Of particular interest is the lack of H₂O features in spectra from higher-mass stars, while water is easily detected in TT stars; the reasons for this disparity are unclear. Detailed investigations of the excitation physics of molecular tracers in disks hold the potential to provide new constraints on the chemistry occurring in protoplanetary environments.



Oscar Martinez Jr., Brian R. Eichelberger, Zhibo Yang, Theodore P. Snow, and

Veronica M. Bierbaum

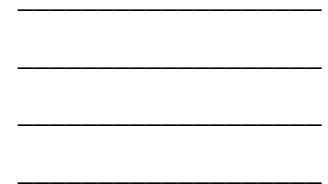
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Astronomy

“Gas Phase Anion Chemistry Relevant to the Interstellar Medium”

H-16

The apparent complexity of the chemistry in the interstellar medium (ISM) has been augmented by the recent discovery of anions. Of particular interest are those reactions contributing to physical processes governing the evolution of the structure and composition of the ISM. In particular, reactions occurring with predominant interstellar constituents dictate the majority of physical processes. This work represents a study of the reactivity of a variety of carbanions with the most prevalent interstellar neutral, hydrogen atom.



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H-17

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“Hydrogen Plasmas in a Cold Hollow Cathode”

H_3^+ is the key precursor to ion chemistry in the interstellar medium. It has been used as an astrophysical probe of conditions of temperature and density due to its ubiquity in a variety of environments. The distribution of ortho- and para- spin modifications of H_3^+ is particularly interesting in this regard. Consequently, it is important to understand the pathways through which changes to the H_3^+ spin distribution can occur. One possible pathway is the $H_3^+ + H_2 \rightarrow H_2 + H_3^+$ reaction, which proceeds by proton hop and proton exchange and is governed by the conservation of nuclear spin. Cordonnier et al.¹ studied this reaction at high temperature in a pulsed hollow cathode cell, but to facilitate the understanding of astronomical observations, we need lower temperature measurements. Recently, we have constructed a liquid nitrogen-cooled hollow cathode discharge source and coupled it with multipass absorption spectroscopy to measure the ortho:para ratio of H_3^+ in plasmas at a variety of para- H_2 enrichment levels at ~ 150 K. Previously, we have reported² experimental measurements of the branching ratio between proton hop and exchange in a hydrogenic plasma at ~ 80 K. Together, these experiments have allowed us to explore the temperature dependence of this branching ratio and provide valuable information for the interpretation of astronomical observations.

¹M. Cordonnier et al., J Chem Phys, **113**, 3181 (2000)

²B. A. Tom, M. B. Wiczer, A. A. Mills, K. N. Crabtree, and B. J. McCall, “Observation of nuclear spin selection rules in supersonically expanding plasmas containing H_3^+ ,” 63rd International Symposium on Molecular Spectroscopy (2008)

Justin L. Neill,[†] Matthew T. Muckle,[†] Daniel P. Zaleski,[†] Brooks H. Pate,[†] M. C. McCarthy,[‡] S. Spezzano,[‡] V. Lattanzi,[‡] A. J. Remijan[§]

L-4

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“Laboratory and Astronomical Detection of trans-Methyl Formate”

The rotational spectrum of the *trans* conformational isomer of methyl formate has been observed and assigned at the University of Virginia and the Harvard-Smithsonian Center for Astrophysics. A total of 22 transitions, 19 from the A-symmetry torsional state and 3 from the E-symmetry torsional state, have been detected in the laboratory so far, and quantum state connections between them have been confirmed by microwave-microwave double resonance experiments. In addition, a total of four transitions (three from the A-symmetry torsional state and one from the E) have been identified in GBT survey scans towards Sgr-B2(N), showing an abundance relative to the *cis* much greater than its calculated relative energy of 1800 cm^{-1} (Senent *et al.*, Ap.J. 627 (2005) 567-576) would predict. The spectral assignment is complicated by an extremely low barrier to internal rotation of the methyl group. Further measurements on the E-symmetry state are in progress. This detection could offer insight into the production mechanism of methyl formate in the interstellar medium.

Robin L. Pulliam and Lucy M. Ziurys

L-5

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“The Pure Rotational Spectra of CrS ($X^5\Pi_r$) and TiS ($X^3\Delta_r$)”

The pure rotational spectra of CrS ($X^5\Pi_r$) and TiS ($X^3\Delta_r$) have been measured using gas-phase direct absorption methods at submillimeter wavelengths. Both molecules were created by reacting H₂S gas with either chromium or titanium vapor, produced from a Broida oven. All spin components were observed in both molecules and lambda-doubling was resolved in the $\Omega=1,2$, and 3 ladders for CrS. The data were fit using a Hund’s case(a) Hamiltonian in both cases. The role of transition metal molecules in the chemistry of the interstellar medium is poorly understood. Using optical techniques, however, both chromium and titanium bearing species have been detected in space, primarily around stars [1-3]. Yet, there have been no confirmed detections of transition metal molecules in the gas phase using radio observations to date. The astrophysical implications of this research including future directions will be presented.

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Donghui Quan[†] and Eric Herbst[‡]

H-18

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“Modeling of CHNS Isomers in Hot and Cold Cores”

Recently we have applied gas-grain chemical reaction models for newly detected or confirmed CHNO isomers. Here we present an analogous study of the CHNS isomers. We applied two models: a warm-up envelope model to simulate the surroundings of hot cores and a constant low temperature model for the cold cores. Modeling results show reasonable agreement with reported HNCS observed abundances or upper limits in hot and cold cores. All CHNS isomers can be formed on the surface from smaller precursors and evaporate into the gas phase via thermal or non-thermal desorption according to the environment of dense cores. The two more stable isomers, HNCS and HSCN, showed higher peak abundances compared with the other two isomers studied, HCNS and HSCN, and may be easier to detect.

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 Matthew C. Sumner,[‡] Frank Rice,[‡] Jonas Zmuidzinas,[‡] Geoffrey A. Blake,[§] and
 Susanna L. Widicus Weaver[†]

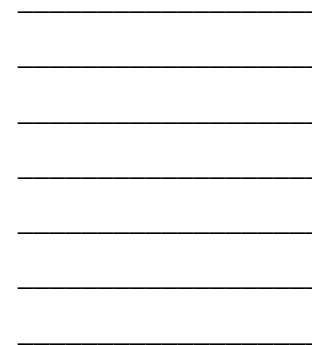
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“Submillimeter Spectral Line Survey of Orion”

Spectral line surveys of Orion have previously focused on determining the main molecular components of the cloud. Such surveys did not require the sensitivity often needed to identify new molecules with weak spectral signatures. We have recently completed a submillimeter survey of Orion with a new, highly-sensitive, broadband receiver at the Caltech Submillimeter Observatory (CSO). The primary objective of this work is to obtain the necessary information to identify new interstellar molecules, circumventing the need for dedicated searches for each individual molecular candidate. This survey surpasses the sensitivity of previously published surveys by an order of magnitude, with a noise level of ~30 mK. Preliminary analysis indicates that 80-90% of the observed lines have not been identified in previous surveys. We will report on the results of this survey, placing particular emphasis on the spectral analysis and line identification process.



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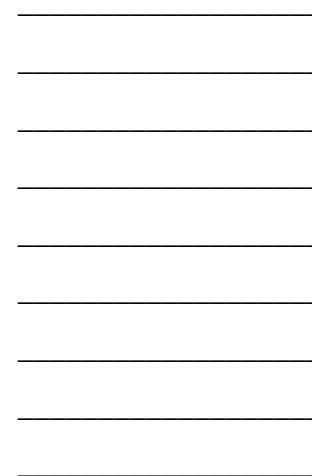
“Indirect Photochemical Excitation of Molecules Adsorbed on Grain Surfaces”

Modeling of stellar atmospheres where photochemistry plays a role is generally carried out by employing the known cross sections for DIRECT photochemistry of gas phase molecules. Yet, laboratory studies for the last 30 years have shown that INDIRECT photoexcitation is of major significance for adsorbed molecules. Here, electron-hole production within the solid leads to charge transfer to adsorbed molecules, followed by chemical bond breaking in the adsorbed molecule.

We are investigating the role of indirect photoexcitation on high area SiO₂ surfaces as models of silicate grains. Lyman- α radiation is used to cause photoexcitation of adsorbed molecules at monolayer coverage as well as molecules in ice layers on the SiO₂. Transmission FTIR spectroscopy sensitively detects surface chemical events at the 10⁻⁴ monolayer level of sensitivity.

The first stage of this research is almost completed- namely the calibration of the Lyman- α source. The photodecomposition of N₂O(g) is observed to produce NO(g) and this information is used to calibrate the Lyman- α lamp. Partial pressures of N₂O and NO are measured by transmission IR spectroscopy at 1 – 10 Torr during irradiation. A Lyman- α flux of ~2 x 10¹⁵ photons cm⁻²s⁻¹ is found. The rf-excited lamp operates at 1 Torr pressure with a flowing mixture of H₂ (10%) and Ar (90%), known to produce almost pure 10.2 eV radiation.

Work supported by NSF Center for Chemical Innovation (CCI) grant award 0847919- “Chemistry of the Universe”



Anthony J. Remijan,[†] J. M. Hollis,[‡] P. R. Jewell,[†] F. J. Lovas[§]

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“The GBT PRIMOS Project – Science, Status, and Suspicions”

In the Fall of 2007 we began observations to conduct a GBT legacy spectroscopic survey of SgrB2(N-LMH) in order to provide a complete inventory of known and unidentified species in the range of 300 MHz to 50 GHz. This survey will be the deepest spectral line survey to date toward this source at these frequencies and the data will be provided to the astronomical community on a quarterly basis (as available) as data accumulate in order to facilitate the identification of new interstellar species and deduce likely molecular formation chemistry. To date, we have completed 45 sessions toward Sgr B2N. This corresponds to ~245 hours completed out of 625 approved which is ~39% of the project. Over 720 individual spectral line features have been seen with ~240 of the 720 being unidentified. In this poster, I will summarize the science, current status of the observations and the suspicious transitions detected that may be from new molecular species. In addition, I will address the probability of the unambiguous identification of new molecules at these frequencies with exceeding low spectral line density. As always, researchers can obtain and analyze the raw or fully calibrated spectral line data available at: <http://www.cv.nrao.edu/~aremijan/PRIMOS/>.

- Detection of Interstellar Cyanoformaldehyde (CNCHO), Anthony J. Remijan, J. M. Hollis, F. J. Lovas, Wilmer D. Stork, P. R. Jewell, and D. S. Meier, 2008, ApJ, 675, L85
- Non-Thermal Continuum Toward SGRB2(N-LMH), J. M. Hollis, P. R. Jewell, Anthony J. Remijan, & F. J. Lovas, 2007, ApJ, 660, 125L
- Detection of Ketenimine (CH₂CNH) in SgrB2(N) Hot Cores, Lovas, F. J., Hollis, J. M., Remijan, Anthony J., & Jewell, P. R. 2006, ApJ, 645, L137
- Detection of Acetamide (CH₃CONH₂): The Largest Interstellar Molecule with a Peptide Bond,* Hollis, J. M., Lovas, F. J., Remijan, Anthony J., Jewell, P. R., Ilyushin, V. V., & Kleiner, I. 2006, ApJ, 643, L25

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*“Column Dependent Cosmic Ray Ionization Rate and its Implications for
Astrochemistry of Diffuse and Dense Clouds”*

In diffuse clouds, H₃⁺ and other molecules been observed in abundances that seem to indicate a cosmic ray ionization rate of $\zeta \sim 2.5 \times 10^{-16} \text{ s}^{-1}$, whereas abundances in dense clouds indicate a lower ζ of $\sim 10^{-17} \text{ s}^{-1}$. We consider energy losses of the cosmic rays due to ionization as well as magnetic field effects, and produce, using a Monte Carlo model, a column dependent ζ that ranges from $2 \times 10^{-15} \text{ s}^{-1}$ to $2 \times 10^{-17} \text{ s}^{-1}$. We apply this column-dependent rate to typical diffuse and dense conditions in a PDR model and discuss the results.

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“Discovery of a Carbon-Chain Rich Starless Core in Lupus”

Recently, Sakai et al. (2008) found that various carbon-chain molecules exist with high abundances in the vicinity of the class 0 protostars, IRAS04368+2557 (L1527) in Taurus, and IRAS15398-3359 in Lupus.^{1,2)} It has been thought that abundances of carbon-chain molecules rapidly decrease as evolution of starless cores, and becomes very low in star-forming cores. Such chemical evolution is well established observationally and theoretically, being used as a ‘chemical clock’.^{3,4)} In view of this conventional picture, detections of abundant carbon-chain molecules around the protostars are very surprising. In the above two sources, carbon-chain molecules are thought to be produced from CH₄ evaporated from grain mantles near the protostar (Warm Carbon Chain Chemistry : WCCC). A basic part of this mechanism is confirmed by chemical model simulations by Aikawa et al. (2008)⁵⁾ and Hassel et al. (2008)⁶⁾. WCCC is now attracting considerable attention as new chemistry in star-forming regions.

In order to understand an origin of WCCC, we conducted mapping observations of CCS ($J_N=4_3-3_2$; 45.379 GHz) and HC₃N ($J=5-4$; 45.490 GHz) in the 5'x4' area around IRAS 15398-3359 with Nobeyama 45 m telescope (NRO 45 m). The beam size is 37". As a result, we found a starless core with bright CCS and HC₃N emissions at 3' northwest from IRAS15398-3359. Then we further carried out observations of various carbon-chain molecules like C₄H, HC₃N, HC₅N, c-C₃H₂, CH₃CCH in the 45 GHz and 85 GHz bands with NRO 45 m, and detected all of them with high intensity. In particular, the peak brightness temperature of the C₄H ($N=10-9$) line is as high as 4 K. On the other hand, the HN₂⁺ ($J=1-0$) line is very weak toward the starless core position, while it is bright toward IRAS15398-3359. These results indicate that the starless core is in the early stage of chemical evolution.

It is well known that a famous starless core TMC-1 with rich carbon-chain molecules exists near the WCCC source, L1527. Existence of a similar starless core near another WCCC source, IRAS15398-3359, means that association of a carbon-chain-rich starless core with the WCCC source would not be accidental, considering that both sources are fairly rare. Sakai et al. (2009) proposed that WCCC would be caused by fast contraction of a parent core. In this case, carbon atoms will deplete onto dust grains before they are fixed to CO in the gas phase, and hence, CH₄ is efficiently produced on dust grains by hydrogenation of the carbon atoms. If such fast contraction is occurring in other cores near the WCCC source, existence of carbon-chain-rich starless cores is also expected. Therefore, the fast contraction scenario for the WCCC source naturally explains association of the young starless core near the WCCC source.

As discussed above, the fast contraction scenario for the WCCC sources is supported by the mapping observations of the surrounding clouds. For further confirmation, a search for the third and more WCCC sources is still important.

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 Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, and the School of
 Engineering & Applied Sciences, Harvard University, Cambridge, MA
 “An Exhaustive Isotopic Study of the Abundant Astronomical Molecule
 Cyclopropenylidene, $c\text{-C}_3\text{H}_2$ ”

Cyclopropenylidene, $c\text{-C}_3\text{H}_2$, is the most widely distributed ring in our galaxy; it has been detected in more than 50 astronomical sources, and its isotopic species $c\text{-C}_3\text{HD}$ has also been detected in a variety of cold clouds. Because of the high observed abundance and large deuterium fractionation for this small hydrocarbon ring, other isotopic species of $c\text{-C}_3\text{H}_2$ may be good candidates for astronomical detection.

For these reasons, an exhaustive isotopic study of $c\text{-C}_3\text{H}_2$ has now been undertaken in which rotational spectra of $c\text{-C}_3\text{D}_2$, $c\text{-C}_3\text{HD}$, and the carbon—13 isotopic species of $c\text{-C}_3\text{HD}$ and $c\text{-C}_3\text{H}_2$ have been detected in the centimeter-wave band by Fourier transform microwave (FTM) spectroscopy between 10 and 40~GHz. For $c\text{-C}_3\text{D}_2$, millimeter- and submillimeter-wave spectra were subsequently measured between 140 and 400~GHz. Rotational and centrifugal distortion constants derived either from previous measurements or those predicted from theory are compared with the precise constants determined here.

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“Formation of molecular hydrogen on amorphous silicates”

In this poster we describe the experimental methods – and present a selection of results – of our laboratory program on **the formation of hydrogen molecules on amorphous silicates**. The primary results consist of: 1. Efficiency of formation of H_2 on amorphous silicates of composition $(\text{Mg}_x \text{Fe}_{1-x})_2 \text{SiO}_4$ ($0 < x < 1$); 2. Energies of adsorption, diffusion and desorption of hydrogen atoms and molecules; 3. Connection between morphology and efficiency of H_2 formation; 4. Application of experimentally derived quantities of elementary steps of molecule formation to the determination of the efficiency of H_2 formation in actual ISM conditions.

I am grateful to NASA (APRA and Origins of Solar Systems) and NSF (Astronomy) for financial support of this research over the years.

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Research Web-page: <http://physics.syr.edu/astro>

David G. Whelan, Kelsey Johnson, and Rémy Indebetouw
University of Virginia

H-24

“Interpreting Three-Dimensional Radiative Transfer Models of Super Star Clusters”

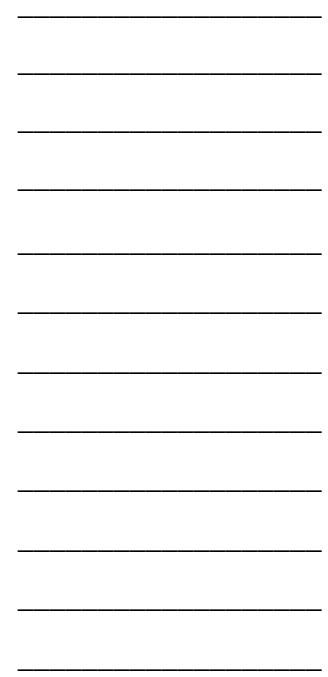
We present temperature and mass density profiles of three-dimensional radiative transfer models of natal super star clusters. Together with calculated spectral energy distributions (SEDs), these profiles allow us to analyse the transfer of radiation in a dusty cluster envelope across a variety of physical parameters, including size, total dust mass, and the ratio of clumpy to smooth dust. Degeneracies in the infrared flux (and therefore also color) due to viewing angle are a direct result of the clumpy nature of the envelope. These models therefore act to caution the observer about the limits of using infrared diagnostic tools to understand natal super star clusters.



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“Analysis of Ices Towards YSOs in Rho Ophiuchi”

H-25

Recent technological advances have sparked an exciting study of the chemistry in star forming regions. By combining Spitzer IRS and ground based observations, a more sensitive diagnostic of the composition of the material surrounding Young Stellar Objects (YSOs) can be performed. An important correlation to consider is the ice abundances with respect to the location of the YSO. For example, Pontoppidan (2006) found that CO₂ and CO abundances were enhanced toward the center of the cold Ophiuchus-F core, and recent results for the CO₂ ice feature at 15.2 μm also imply spatial variations within regions of star formation. However, Whittet et al. (2009) found similar CO₂ profiles for background objects consisting mainly of a polar component (85%) toward three distinct dark clouds, thus providing a benchmark of unprocessed ices to which processed ices can be compared. Here we present a combination of ground-based and space-based results for the stretching, bending, and libration modes of H₂O ice at 3μm, 6μm, and 13μm respectively, the stretching mode of CO ice at 4.67 μm, and the bending mode of CO₂ ice at 15.2μm of the Rho Ophiuchi star forming region. These data were taken with the Infrared Spectrometer (IRS) on the Spitzer Space Telescope and SpeX at the Infrared Telescope Facility (IRTF) located on Mauna Kea, HI. We measured abundances and used laboratory spectra to constrain the polar/apolar composition and the thermal history of the region. The abundances and profile shapes are compared while considering their location with respect to the Ophiuchus A, B, and F cores, and their evolutionary state. In the future, additional YSOs in the Taurus and Rho Ophiuchi regions will be similarly analyzed in order to correlate variations in the volatile composition of the material surrounding YSOs due to environmental factors and evolutionary state.



Paul M. Woods^{†‡} and Karen Willacy[‡]

H-26

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“Carbon isotopes in the Solar System”

The ratio of 12-carbon to 13-carbon throughout the Solar System shows homogeneity whether one looks at the centre, the Sun, or at the farthest components, comets. This homogeneity runs contrary to chemical models of carbon fractionation in the early Solar System, where distinct regions of similar $^{12}\text{C}/^{13}\text{C}$ ratio arise due to the chemical and physical processes which are ongoing in those regions. Here we present such a chemical model and discuss how heterogeneity can become homogeneity, and the implications this has for the formation of the Solar System.

Shanshan Yu, Brian J. Drouin, and John C. Pearson

H-27

Jet Propulsion Laboratory

“Terahertz spectroscopy of hydronium (H_3O^+) and acetylene ($\text{C}_2\text{H}_2/\text{C}_2\text{D}_2$)”

Herschel, SOFIA and ALMA will work in the terahertz region and will be able to detect weaker signals. Laboratory identifications of likely interstellar species such as CH_3OH_2^+ are desirable and laboratory spectroscopy of well-known species such as H_3O^+ needs to be extended to the terahertz region. This paper reports on laboratory results of H_3O^+ , C_2H_2 and C_2D_2 . Transitions in the 0.2–1.6 THz region have been measured for these molecules with the frequency multiplier submillimeter spectrometer (FMSS) at JPL [1]. The accuracy of these measurements is estimated to be 50–200 kHz. These observed lines were modeled together with prior data and significantly improved molecular parameters were obtained for these molecules with the combined data set. New frequency and intensity predictions were made to support astrophysics applications. At the same time, the development of a radio frequency (RF) discharge cell is underway with the hope to greatly improve ion production efficiency and to allow us to generate ions whose spectra have never been measured before.

[1] B. J. Drouin, F. W. Maiwald and J. C. Pearson, Rev. Sci. Instrum. 76, 093113 (2005).

Lindsay N. Zack, Robin L. Pulliam, and Lucy M. Ziurys

H-28

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“Rotational Spectroscopy of Zinc-Containing Molecules”

Molecules containing transition metals have been the focus of several low- and high-resolution spectroscopic studies. To date, however, molecules that contain zinc have been neglected by spectroscopists. Recently, millimeter/sub-millimeter direct-absorption techniques have been used to measure the gas-phase rotational spectra of three zinc-containing molecules: $\text{ZnS}(X^1\Sigma^+)$, $\text{ZnO}(X^1\Sigma^+$ and $a^3\Pi_1)$, and $\text{ZnOH}(X^2A')$. These molecules were produced in the gas phase by reacting zinc vapor, generated in a Broida-Type oven, with H_2S , N_2O , or H_2O for ZnS , ZnO , and ZnOH , respectively, under dc discharge conditions. The spectra of both ZnS and ZnO in the $X^1\Sigma^+$ ground state were recorded for up to five naturally-occurring zinc isotopologues, as well as several vibrationally excited states. In the low-lying $a^3\Pi_1$ excited state, the ZnO spectra was measured for three isotopologues and exhibits spin-orbit, spin-spin, and Λ -doubling interactions. The $\text{ZnOH}(X^2A')$ spectra features a K-ladder structure, indicative of a bent molecule, and spin-rotation doublets for each line. Several rotational transitions have been measured for each of these molecules, and rotational constants have been determined. Equilibrium parameters were also calculated for ZnS and ZnO . These techniques will be used to study other 3d metal-bearing species, in particular those of astrophysical interest, such as FeOH and CrOH .
