Astro2020 Science White Paper

OBSERVATIONAL ASTROCHEMISTRY IN THE NEXT DECADE

Thematic Areas: ☒ Planetary Systems ☒ Star and Planet Formation - *with an emphasis on Astrochemistry*

☐Formation and Evolution of Compact Objects ☐ Cosmology and Fundamental Physics

☐Stars and Stellar Evolution ☐Resolved Stellar Populations and their Environments

☐Galaxy Evolution ☐Multi-Messenger Astronomy and Astrophysics

Principal Author:
Name: Anthony Remijan
Institution: National Radio Astronomy Observatory
Email: aremijan@nrao.edu
Phone: 434-244-6848

Co-authors: (names and institutions)
Crystal Brogan - National Radio Astronomy Observatory
L. Ilsedore Cleeves - University of Virginia
Martin Cordiner - NASA Goddard Space Flight Center
David Frayer – Green Bank Observatory
Rachel Friesen - National Radio Astronomy Observatory
Robin T. Garrod - University of Virginia
Ryan Loomis - National Radio Astronomy Observatory
Felix J. Lockman– Green Bank Observatory
Michael C McCarthy - Harvard-Smithsonian Center for Astrophysics
Brett A. McGuire - National Radio Astronomy Observatory
Stefanie Milam - NASA Goddard Space Flight Center
Al Wootten - National Radio Astronomy Observatory
Ci Xue - University of Virginia

Abstract (optional):

Observational Astrochemistry in the Next Decade

Background:
2020 marks 50 years since the astronomical discovery of interstellar carbon monoxide (CO) (Wilson, Jefferts & Penzias 1970) and 51 years since the detection of the first polyatomic molecules ammonia (NH_3) (Cheung et al. 1969a), water (H_2O) (Cheung et al. 1969b) and formaldehyde (H_2CO) (Snyder et al. 1969) at radio frequencies. **The discoveries of these species changed the landscape of astronomical observations and astronomical discovery has now become chemical discovery.** For example, the CO/H_2 relationship was instrumental in our understanding the gas content of the universe (see for example recent investigations such as Cormier et al. 2018, Gaches & Offner 2018 and Carleton et al. 2017 and references therein and Frerking, Langer & Wilson 1982 for a historical perspective). For the first time, there were diagnostics that could be used to measure the invisible molecular gas that was present in nearly all astronomical objects - from the most distant galaxies to nearby star forming regions (Castignani et al. 2019 & Law et al. 2018). In addition, interstellar molecules were found to be good proxies for various physical conditions. Ammonia was found to be an excellent thermometer to measure gas temperature (e.g., Friesen et al. 2009 & Billington et al. 2019); heavier species such as CS (Penzias et al. 1971) were found to trace regions of high gas density (e.g., Saito et al. 2018 & Patoka et al. 2018); ionic species such as HCO+ (first detected as "X-ogen" in 1970 – Buhl & Snyder 1970) became instrumental in our understanding of the partially ionized and diffuse ISM (e.g., Gerin et al. 2019 & Zhou et al. 2018); and finally massive refractory elements such as SiO (Wilson et al. 1971) proved to be excellent tracers of astronomical shocks (e.g., Burkhardt et al. 2016 & Csengeri et al. 2018). Since these seminal detections, a total of 204 distinct molecules (and numerous isotopologues) have been detected in a variety of astronomical environments (e.g. Hashimoto et al. 2018 & Cordiner et al. 2018 and references therein). In this paper, we will propose the next suite of observations and instrumentation ***necessary*** to take that leap of astrochemical discovery in the next decade.

Proposed Statement of Need for Astrochemical Observations: 2020 - 2030:
Quite simply, in order to continue to make progress in our understanding of the nature of star formation and galaxy evolution, and specifically how the chemical and physical nature of molecular material changes as we move from the diffuse interstellar medium to compact cores and eventually disks with planetary systems, **as a community, we need astronomical & astrochemical observations made with:**

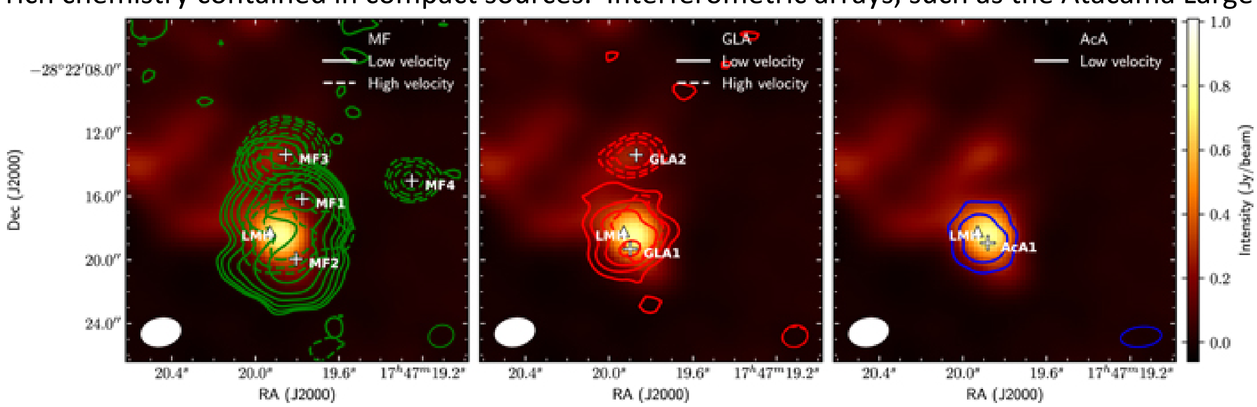
1. A large (100-m class) single dish radio telescope with excellent surface brightness sensitivity **(< 1mK RMS), that cover a wide field-of-view (30' x 30' FOV) sensitive** to extended emission. Observations of large astronomical molecules (LAMs) have shown distributions that extend over arcminutes. The observations of the molecules are absolutely dependent on a facility with high sensitivity and relatively large field of view.
2. Broadband frequency coverage in the 1 - 50 GHz frequency range with **instantaneous spectral coverage (20 GHz of instantaneous bandwidth) at high resolution (0.05 km/s spectral resolution).** Observations over the last decade have shown that the detection of LAMs is optimized at frequencies below 50 GHz where a) the Boltzmann distribution for these molecules peaks and b) non-thermal excitation processes (e.g. maser action)

pumps low line strength transitions. The full frequency range is essential to properly characterize the excitation condition of the molecular species.

3. The ability to map the spatial extent of low surface brightness emission (**< 1mK RMS in less than 10 hours @ 18GHz)** of these large astronomical molecules in a reasonable amount of time. Ideally, the mapping would take place using focal plane arrays or phased array feeds over the frequency range specified in 2). Interferometric observations have shown to be ineffective in mapping the extended distribution of large molecular emission at low frequencies - the emission is completely resolved out by the array.

Untapped Discovery Space:

The past 50 years of astrochemical discovery has provided a remarkable chemical inventory that has been effectively used for astrophysical diagnostics across a wide range of environments (McGuire 2018). *However, the full utility of these molecules to understand the physical and chemical nature of the universe will not be fully realized until a systematic and testable chemical theory is produced that will explain the formation chemistry of these molecular species - or molecular families.* Currently, astrochemical models are restricted. While current astronomical observations have provided the molecular inventory, observations have not effectively generated the relative spatial concentrations of these molecules towards astronomical sources. These "chemical maps" (Figure 1.) are essential to providing the appropriate calibration to astrochemical models. The past decade of astrochemical observations have started to show a rich chemistry contained in compact sources. Interferometric arrays, such as the Atacama Large



> **Figure 1:** Emission contours from the chemical maps of Methyl Formate (MF) (left), Glycolaldehyde (GLA) (middle), and Acetic Acid (AcA) (right) overlaid on the continuum emission at 85.9 GHz (background color image) towards Sagittarius B2(N) high mass star forming region. (Reproduced from Xue et al. 2019).

Millimeter/submillimeter Array (ALMA), have been able to look at the hot, compact emission regions of star forming regions (e.g. Xue et al. 2019, Jorgensen et al. 2018 & Belloche et al. 2016), evolved stars (e.g., Cernicharo et al. 2018) and external galaxies (e.g. Meier et al. 2015). These observations are starting to show distinct physical and chemical differentiation on size scales close to the proposed conditions of the pre-solar nebula. These data will be essential to further chemical theory to explain the formation of these (and other) large astronomical molecules. The component that is missing from these observations is found in the new molecule detections.

ALMA has NOT provided the anticipated avalanche of new molecule detections. In fact, only 3 new molecules have been detected with ALMA (Zeng et al. 2019, McGuire et al. 2017 & Belloche et al. 2017) while the bulk of the new detections have taken place with the IRAM 30-m telescope and the Green Bank Observatory 100-m Green Bank Telescope (GBT) (McGuire 2018). The signal coming over the last decade of molecular discovery clearly indicates that ***there is an extended, diffuse molecular emission component of the interstellar medium that is rich in LAMs.***

As further justification of this extended cool component, Figure 2 shows the detection of the absorption profiles of the LAMs, cyanoacetylene (HC_3N), methyl cyanide (CH_3CN), acetaldehyde (CH_3CHO), and formamide (NH_2CHO) shown in blue (Corby PhD Thesis, 2016). Vertical lines indicate the local standard of rest (LSR) velocities of absorption in and along the line-of-site towards the Sagittarius B2(N) - SgrB2(N) high mass star forming region. **This data provide clear evidence for an extended, cold region of emission that contains a chemistry conducive to the formation of LAMs.** These observations were taken as part of the GBT PRIMOS Key Science program toward SgrB2(N) between 1-50 GHz. This region alone accounts for more than 67 of the 204 astronomical molecule detections (McGuire 2018). The first detection of H_2CO taken in 1969 was in absorption, in the cool envelope surrounding this region of the Galaxy.

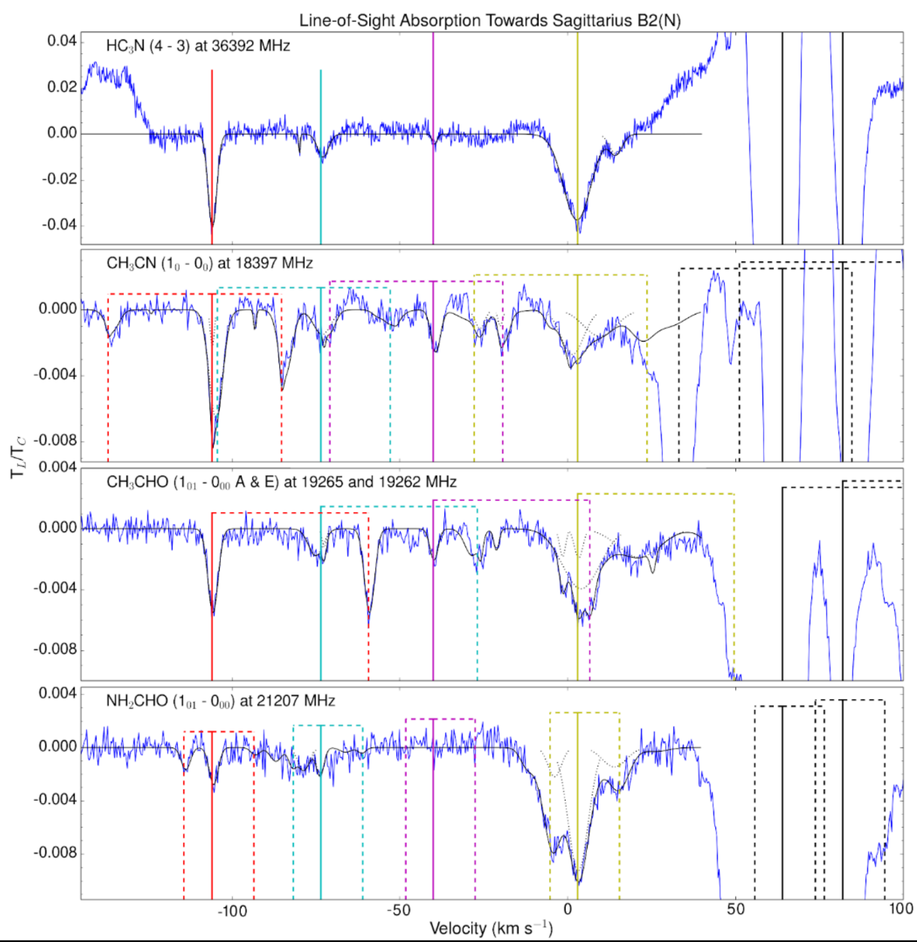


Figure 2: Line of sight absorption of select large astronomical molecules (LAMs) toward the high mas star forming region SgrB2(N). (Reproduced from Corby et al. 2016).

Objectives:

Observations in Figure 2 lead to the following unanswered questions to address in the next decade:

1. What is the extent of molecular complexity in the interstellar medium?
2. What is the distribution and excitation of this material in these conditions?
3. Can chemical theory explain the formation of these large astronomical molecules under these conditions?
4. Can we trace the chemical evolution from these diffuse structures down to compact cores that eventually lead to star and planet formation?
5. Is the chemistry found in these regions more/less conducive to the formation of larger complex molecules that could be of biological interest?
6. Can we use molecular tracers in these environments to help identify the carriers of the mysterious diffuse interstellar bands (DIBs) and the unidentified infrared bands (UIBs)?

The Star Formation Connection:

The process of star formation is highly connected to interstellar chemistry and molecular distributions. Surveys of continuum emission from cold dust with the Herschel Space Observatory and ground-based single dishes like the James Clerk Maxwell Telescope have revealed the filamentary nature of star-forming clouds (e.g., Bresnahan et al. 2018 & Broekhoven-Fiene et al. 2018), but without kinematic information cannot fully characterize their role in the star formation process. The changing physical conditions as regions within molecular clouds evolve from warmer, lower density conditions to the extremely cold and dense filaments and cores within which stars are born require observations across a broad range of molecular tracers. In particular, several large surveys have taken advantage of focal plane arrays to map emission from the 24 GHz NH_3 inversion transitions (and other molecular tracers), toward nearby star-forming regions within the Gould Belt (GAS, Friesen et al. 2017), more distant, high-mass clouds (KEYSTONE, Keown et al., in prep), and across the galactic plane (RAMPS, Hogge et al. 2018). Early results from these surveys have revealed, however, that with sufficient sensitivity NH_3 also traces the transition between turbulent cloud and quiescent cores and filaments, allowing direct measurements of where and how the supersonic cloud turbulence is dissipated at the boundaries of filaments and cores (Chen et al., in prep).

This new and exciting development shows the need for sensitivity over wide scales to detect faint emission lines, and for increased spectrometer flexibility to simultaneously target additional lines.

The Comet Connection:

Cometary ices represent an end-point in the chemical evolution of the ISM. Comparison of cometary and interstellar abundances therefore provides unique insights into the thermal and chemical evolution of matter during solar system formation. Every substantial improvement in radio spectral line sensitivity leads to detections of new cometary gases, of ever-increasing complexity (Biver 2005). Large aperture facilities or the more-than an order-of-magnitude sensitivity improvement afforded by interferometric arrays like ALMA used in auto-correlation (i.e. single-dish mode) is likely to result in a plethora of new molecular detections that will dramatically improve our understanding of the complex chemistry occurring during comet (and protosolar disk) formation.

Searching for molecules in warmer environments - the need for more collecting area at mm/sub-mm wavelengths:

Finally, at temperatures above the ~10 K found in the cold interstellar medium, molecular excitation conditions favor the detection of molecules at higher frequencies (above ~70 GHz). However, as previously stated, the spectroscopic sensitivity of arrays is severely limited for extended sources, which are filtered out by the interferometer on spatial scales >~5-10''. To open up the molecular discovery space in warm, extended sources, single-dish (non-interferometric) observations are required. These observations again support a large, single dish antenna with excellent surface brightness sensitivity with a large FOV and mapping speed (or interferometric arrays used in auto-correlation mode). This would lead to a significant expansion of our knowledge of the molecular inventories in hot cores, cometary comae, evolved stellar envelopes, and other sources larger than a few arcseconds in size.

Commitment to New Discovery:

The need to continue the discovery of new astronomical molecules, especially in the cold and warm regions of the interstellar medium must continue into the next decade as the discovery relates to star and planet formation through galaxy evolution. In addition, an understanding of the chemistry of these regions is starting to uncover discovery space that can lead to answering the questions on the nature, formation and direct observations of PAHs (or related molecules) in astronomical environments. The circumstantial evidence for the PAHs has been around for decades but a single, unique PAH has not, as of yet, been detected in the gas phase of the ISM. Figure 3 shows the first detection of an astronomical molecule with a formation chemistry related to PAHs - benzonitrile (c-C_6H_5CN). The need to continue on the successful searches for large astronomical molecules like benzonitrile is therefore critical.

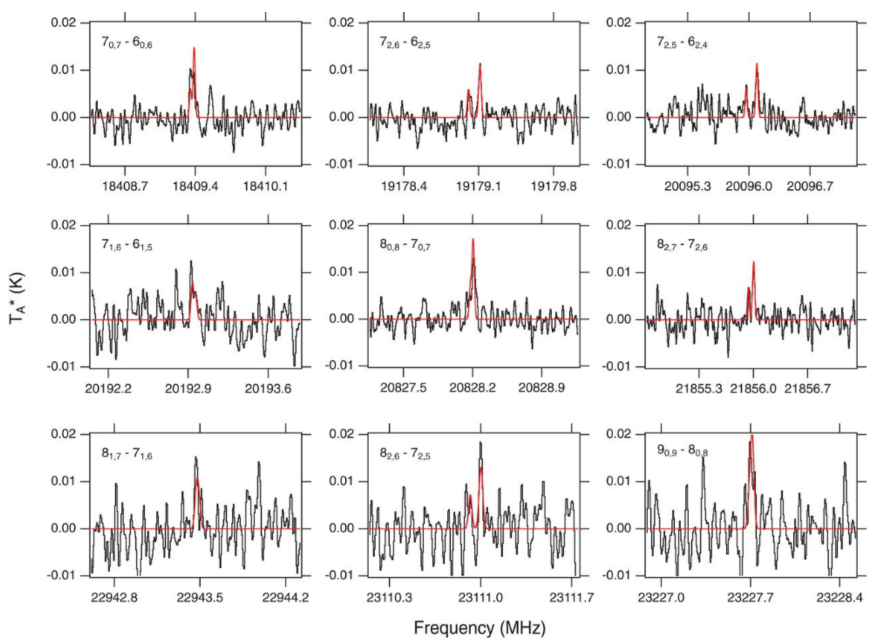


Figure 3: Initial detection of benzonitrile toward the cold, dark cloud TMC-1 (Reproduced from McGuire et al. 2018). This molecule has now been detected toward several more dark clouds – a link to carbon ring chemistry

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