A GBT Legacy Survey of Prebiotic Molecules Toward SgrB2(N-LMH) and TMC-1

Jan M. Hollis

NASA's Goddard Space Flight Center, Computational and Information Sciences and Technology Office, Greenbelt, MD, 20771 email: mhollis@milkyway.gsfc.nasa.gov

Anthony J. Remijan

National Radio Astronomy Observatory, 520 Edgemont Road, Charlottesville, VA 22903

email: aremijan@nrao.edu

Philip R. Jewell
National Radio Astronomy Observatory, 520 Edgemont Road, Charlottesville, VA 22903
email: pjewell@nrao.edu

Frank J. Lovas

NIST, Optical Technology Division, 100 Bureau Drive, Gaithersburg, MD 20899

email: lovas@nist.gov

Abstract

Astrobiology undoubtedly begins with the formation of prebiotic molecules in interstellar clouds. The inventory of interstellar molecules presently stands at ~140 different species. In the last two years, our team has used the GBT to detect 8 new interstellar molecules -- all are large (6 to 11 atoms), organic, and prebiotic in some measure. The reason for this unprecedented success is three-fold: The GBT is very sensitive with substantial beam efficiency in the range of 300 MHz to 50 GHz; the rotational transitions between low-energy levels of most prebiotic molecules fall in the range of 300 MHz to 50 GHz; and the GBT beam couples well to prototypical prebiotic molecule sources (e.g., SgrB2[N-LMH] and TMC-1) which are found to be very cold (~10 K) and spatially extended. Thus, we propose to conduct a GBT legacy spectroscopic survey of SgrB2(N-LMH) and TMC-1 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 these sources 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.

1.0 Scientific Justification

1.1. Background

A primary focus of current astrobiology research is to investigate our prebiotic molecular origins. As such, over the last several years there have been significant advances in this field primarily due to dedicated searches for large molecules that are possible precursors to molecules of biological importance (biomolecules) in the interstellar medium and in the atmospheres of comets. Successful dedicated searches with the Green Bank Telescope (GBT) in the last two years have led to the detections of interstellar aldehydes namely propenal (CH₂CHCHO) and propanal (CH₃CH₂CHO) (Hollis et al. 2004a), simple aldehyde sugars like glycolaldehyde (CH₂OHCHO) (Hollis et al. 2004b), the first keto ring molecule to be found in an interstellar cloud, cyclopropenone (c-H₂C₃O) (Hollis et al. 2006a), the third organic imine to be detected in an interstellar cloud, ketenimine (CH₂CNH) (Lovas et al. 2006b), and acetamide (CH₃CONH₂) (Hollis et al. 2006b), the largest interstellar molecule detected with a peptide bond. These searches and detections all took place in the direction of the Galactic center towards Sgr B2(N) in a region that has been named the ``Large Molecule Heimat" and have greatly enhanced our understanding of the distribution and abundance of these large organic molecules in interstellar clouds. However, dedicated searches are very limited in the identification for new interstellar species and transitions because they often cover only a restricted range of frequencies and bandwidth. What is needed is a complete survey over a large frequency range and bandwidth to obtain as much information as possible.

There are many specific reasons why a deep spectral line survey is important and timely and could significantly advance the field of astrobiology. First, although we have made significant progress in understanding the chemical content and formation mechanisms in interstellar clouds, we still cannot predict with certainty which species will be present. A number of species such as the 3-carbon sugar glyceraldehyde and the simplest amino acid, glycine, have eluded detection so far although models and the presence of precursor species suggest that these molecules should be present. A survey offers the possibility of ensemble averages of transitions, which may be the only way to make detections of the largest, most complex species for which the population is distributed over many energy states (large partition function). This technique was not feasible in the past since weak signatures of complex molecular species emitting or absorbing in the 300 MHz to 50 GHz region were not amenable to detection until the advent of the GBT.

Second, in practical terms, a sensitive and methodical survey is one of the most efficient ways to detect new species. Very often, targeted lines prove unobservable because of unexpected radio frequency interference (RFI) or confusion from interloping spectral lines. To achieve the detection, one must then observe another spectral line in the ensemble, but this often requires another observing proposal and thus delays the scientific result.

Third, large databases of laboratory spectroscopic transition frequencies exist already. A thorough, sensitive survey would allow astrochemists to utilize these databases to make firm, multi-transition identifications of species. This would greatly advance the field of astrochemistry by creating a comprehensive inventory of species. Furthermore, this legacy survey will contain unidentified spectral features that can be assigned to new interstellar species in a spectral region that contains low-energy transitions of complex prebiotic molecules and as such, would spur laboratory spectroscopists to make additional measurements of likely species.

Fourth, this survey will produce a complete inventory of known interstellar molecules and their transitions that can be evaluated and synergistically used as multiple probes of physical conditions. This is potentially one of the most important outcomes of this survey. To fully understand the role of interstellar clouds in our molecular origins, an inventory of molecular species is necessary in prototypical sources. For example, the trends in molecular abundances and distributions provide the keys to how they are formed.

Finally, this is an important and advantageous time to make this survey. The results will guide further instrumentation development on the GBT (specifically including the specifications for focal plane arrays at key frequencies), and can guide the scientific development of ALMA and the EVLA, both of which expect astrochemistry to be an important component of their scientific programs. The results may also be valuable to other projects such as the space-based Hershel/HIFI mission, which will be coming on line in just a few years.

Overall, inventories of molecules are important to understand astrochemistry and chemical evolution. This legacy survey will produce a complete inventory of known interstellar species that can be used as probes of physical conditions. The survey will also discover new interstellar species that will provide constraints that aid in our understanding of astrochemistry and chemical evolution.

1.2. Sources of Interest: SgrB2(N) and TMC-1

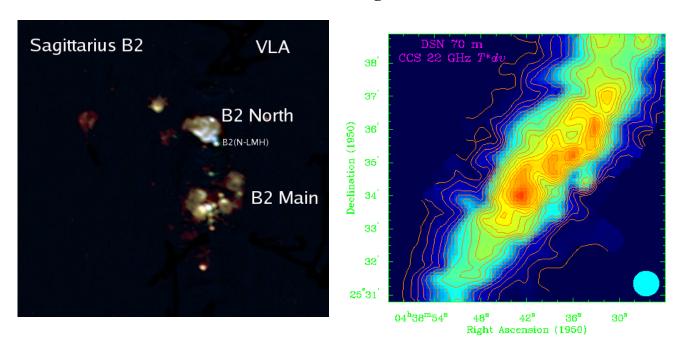


Figure 1. VLA 15.2 GHz data are red, the 22.1 GHz data are green, and the 43.7 GHz data are blue. All images were made with a beam 2".5x2".0 and a PA of 67°. Courtesy of Dave Boboltz – USNO.

Figure 2. Radio Map of CCS toward TMC-1 - Courtesy of Tom Kuiper (http://dsnra.jpl.nasa.gov/origins/).

The giant molecular cloud complex, Sagittarius B2(N) near the center of our Galaxy, is undoubtedly the preeminent source for the study of large complex interstellar molecules. Of the 141 interstellar molecules detected, more than half have been detected first in the Sagittarius B2 star-forming region. The Sgr B2 complex

is a star-forming region containing compact hot molecular cores of arcsecond dimensions, molecular maser emitting regions, and ultracompact continuum sources surrounded by larger-scale continuum features as well as molecular material extended on the order of arcminutes. In addition, small-scale and large-scale shock phenomenon characterize the complex. In particular, the hot molecular core known as the Large Molecule Heimat (LMH) has for the last ten years been the first source searched to detect and identify new large interstellar molecules since many of the large organic species have previously been confined to its ~5" diameter. However, the recent GBT detections of large organic molecules have suggested that prebiotic molecules found toward the SgrB2(N) complex are are extended, perhaps even on the order of the 2'x2' field shown in Figure 1.

The cold dark dust cloud Taurus Molecular Cloud 1 (TMC-1) is an elongated condensation that extends in a ridge more than 5'x15' in the southeast-northwest direction. It is located in the Heiles Cloud 2 group of dark clouds at a distance of about 140 pc. TMC-1 is the prototypical dark cloud and has been a primary target of several molecular line surveys because the chemistry and abundances of molecular species is completely different than what is seen in high mass star-forming regions like Sgr B2(N). For example, TMC-1 is an excellent place to search for members of the cyanopolyyne $H(C=C)_nCN$, methylcyanopolyyne $CH_3(C=C)_nCN$, and methylacetylene $CH_3(C=C)_nH$ (n=1,2,3, etc...) families, because it has been shown to be an abundant source of carbon chain molecules and other species. Using the GBT, we have detected the largest symmetric top species, methyltriacetylene (CH₃C₆H) (Remijan et al. 2006) as well as methylcyanodiacetylene (CH₃C₅N) (Snyder et al. 2006) and cyanoallene (CH₂CCHCN) (Lovas et al. 2006a) in dedicated searches. Previous cursory surveys document that TMC-1 contains a number of different carbon chain sequences and thus, TMC-1 is the optimal source for investigating the formation of carbon chain species. In addition, it has been suggested by Turner et al. (2000) that TMC-1 may be a region in which the transition from gas-phase chemistry to grain chemistry may need to be invoked to explain the abundances of certain partly hydrogen-saturated species. Thus, the study of this region is essential to understanding the formation of large carbon-bearing species and while this region is too cold to show continuum emission, molecular emission is easily detected and what is seen in Figure 2, is a DSN 22 GHz map of emission from the 2,1-1,0 transition of CCS.

1.3. Frequency coverage (300 MHz to 50 GHz) with the GBT

In Figures 3 and 4, we compare 1 GHz of passband at 230 GHz and 23 GHz toward SgrB2(N), respectively. While these two passbands are NOT on the same velocity scale, it can be seen that in Figure 3, the high-frequency bands are so full of lines by comparison that it is difficult, if not impossible, to reliably identify species simply due to all the line confusion. On the other hand, in Figure 4, the low frequency bands are relatively uncluttered. The prominent lines in this band are mainly recombination lines of hydrogen and helium and ammonia complexes.

Figure 5 presents a graph that represents the number of interstellar molecules as a function of constituent atoms. There are 141 total molecules. Notice that there is a high degree of isomerism (isomer pairs are illustrated in orange and yellow, triads in blue), suggesting that the formation of molecules is a quasi-random process that gets modified by ensuing gas or grain chemistry. Low energy transitions of large molecules fall in the range of 300 MHz to 50 GHz. Such molecules are organic and are spatially widespread. Low energy transitions of light molecules (e.g., H_2D^+) fall at much higher frequencies.

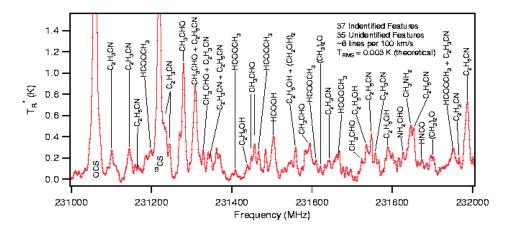


Figure 3. 1 GHz of bandwidth at 231.5 GHz taken with the SMT using the NRAO ALMA Band 6 receiver

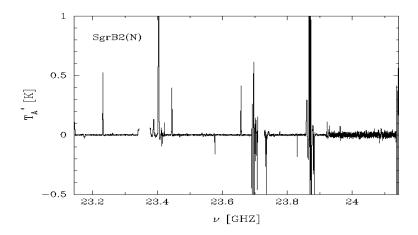


Figure 4. \sim 1 GHz of bandwidth near 23.6 GHz taken with the GBT from our dedicated surveys. Most of the strong emission and absorption features seen in this passband are due to simple species like ammonia (NH₃) or H and and He recombination lines.

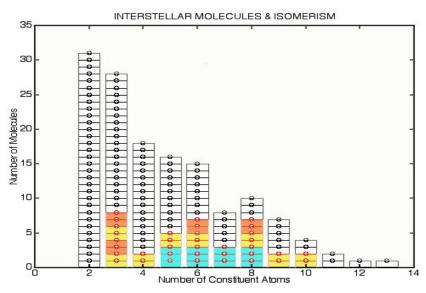


Figure 5. Graphical representation of the number of interstellar molecules as a function of constituent atoms.

1.4. Example: Understanding the Formation of Large Organic Molecules

Finally, why it is so important and advantageous to use the GBT? Over the last 2 years our team using the GBT has already detected 8 new interstellar molecules, a feat that is unequaled in such a short time by any other telescope or observing team in the history of molecular spectral line astronomy. Figure 6 shows those species we have detected toward SgrB2(N) with the GBT. From this graphical representation, it is possible to illustrate some of the chemical processes we believe are occurring in interstellar clouds that leads to the production of larger and larger interstellar species. First, successive hydrogen addition reactions account in the formation of ethylene glycol from glycolaldehyde which is the simplest possible aldehyde sugar. Successive hydrogen addition reactions also may account for the formation sequence of prop Ynal, prop Enal, and prop Anal and these species are important in the formation of amino acids. Oxygen addition accounts for the formation of cyclopropenone from cyclopropenylidene. Acetamide is one of two interstellar molecules with a peptide bond which is the way amino acids are polymerized into proteins. Acetamide can be formed in neutral radical reactions of the radicals CH₂ or CH₃ with formamide. Finally ketenimine can be isomerized from methyl formate by a process called tautomerization where the H atom migrates from the methyl group and finally attaches itself to the N. Because of the high activation barrier of some of these reactions, most of these reactions are probably powered by shocks in and surrounding the SgrB2(N) star-forming region.

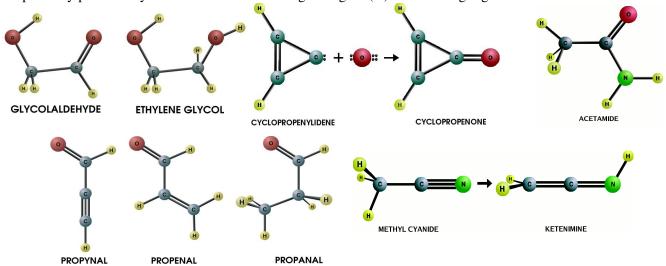


Figure 6. Molecular Species that our team has detected using the GBT toward Sgr B2(N) **METHYLCYANOACETYLENE METHYLCYANODIACETYLENE** CYANOALLENE **METHYLTRIACETYLENE**

Figure 7. Molecular Species that our team has detected using the GBT toward TMC-1

METHYLDIACETYLENE

Figure 7 shows the species we have detected toward TMC-1 with the GBT. In this case, carbon addition reactions account for methylcyanodiacetalene and methyltriacetylene from the simpler species on the left. Cyanoallene can be explained by neutral-radical reactions of the radical CN with allene. *However, only through a systematic and complete spectral line survey, will it be possible to accurately constrain the formation mechanisms of these and even more complex molecular species.*

Astrochemistry projects have been among the most productive research areas on the GBT, which has clearly demonstrated its unique power as a spectral line search instrument. The GBT beams are ideal for spatially widespread prebiotic species like we are finding now. Below 50 GHz, the GBT beams couple well to the extended molecular emission seen interstellar clouds. Because of the tremendous sensitivity, the GBT can reach an rms noise level of \sim 2 mK in two tracks on Sgr and in one track on TMC-1. Finally, the spectrometer is versatile and we have large spectral bandpasses with the existing equipment (e.g., 4x200 MHz = 24.4 kHz resolution; 4x50 MHz = 6.1 kHz resolution). For all these reasons, the GBT is the only telescope currently in operation in the world that can be used for such a deep spectral line survey.

2. Observing Strategy

We intend to use the position-switching mode of observation for both SgrB2(N-LMH) and TMC-1 and switch in azimuth 60 arcminutes off source every two minutes. Both sources are extended on the scale of several arcminutes and we have found that this procedure permits the detection of weak signals. For example, we know of other observers who have wasted valuable GBT time trying to nod just a few arcminutes between receiver beams, only to find later that this "more efficient" observing method actually switched into signal in the off position, thus precluding the detection of weak species like prebiotic molecules.

In the 300 MHz to 50 GHz frequency range of the GBT there is 40.4 GHz of useable bandwidth spread across 16 different receivers. What is described below is an approximation based on an average of how much time is needed to complete this survey. Having observed at almost every band on the GBT, we are aware of observational difficulties including RFI, the variation of system temperature across the bands and the loss of sensitivity due to weather and what occurs at the band extremes. Thus, some bands will require more observing time than what is described below, and some will require less. With this in mind, we assume an average value of the noise level expected in a particular amount of time on source.

For SgrB2 observations, we intend to use four 200 MHz bandpasses, but each successive bandpass will overlap the next one by 5 MHz so that no molecular lines will be lost due to ambiguities at the bandpass edges; this will result in 775 MHz of contiguous coverage for each observation (i.e., one 6 hr track on SgrB2). On average, we assume there will be 40.4/0.775 = 52 different tracks on SgrB2; to achieve a noise level of ~2 mK, will require that approximately 2 tracks be devoted to each tuning which results in a total of ~104 tracks for SgrB2. Similarly, for TMC-1 observations, we intend to use four 50 MHz bandpasses, which results in 175 MHz of contiguous coverage for each observation (i.e., one 13 hr track on TMC-1), On average, there will be 40.4/0.175 = 231 tracks on TMC-1; each track should result in a noise level of ~ 2 mK. Thus, the total time requested for this legacy proposal is 3627 hours; we could accomplish all SgrB2 observations in 2.5 yrs by observing an average of 4 tracks per month; we could accomplish all TMC-1 observations in 5 yrs by observing an average of 4 tracks per month. The foregoing time estimates are reasonable, given that some bandpasses will be plagued by

RFI, and, hence, will not be entirely observable (e.g., RFI due to communications satellites operating at 4 and 12 GHz). Moreover, we acknowledge that for very low frequencies, we may have to observe SgrB2 at 6.1 kHz channel spacing in order that good velocity resolution is achieved on spectral lines. These decisions will have to be made at the telescope since many of the receiver systems have not been used for spectroscopy of the expected weak lines that characterize prebiotic molecules.

3. Data Release Strategy and the Spectral Line Search Engine [SLiSE])

We are committed to a quarterly release of data to the astronomical community (assuming that we acquired data in that quarter). Furthermore, we will provide a web-based data-mining tool – SliSE (Spectral Line Search Engine) -- which we have already developed and demonstrated.

SLiSE is a data display tool that will contain all the fully reduced and calibrated archived data taken as part of this Legacy survey. SLiSE is fast, easy to use and contains the necessary functionality to display the data taken from spectral line searches. For example, SLiSE contains functions to overlay possible molecule identifications based on a current line catalog as well as overlaying H and He recombination lines. It is a java based applet, so it is platform independent and is easily accessed online. SLiSE will also be made available as a standalone data product where observers can have access to the legacy survey data but do not have to be online as well as having the opportunity to upload their own datasets of interest to search for possible identifications of molecular transitions. Currently the online version does not have the capability to upload your own dataset but we are working on that functionality in anticipation of this legacy survey.

In summary, SLiSE will be updated quarterly as long as data are taken during that quarter. Furthermore, both the online and standalone versions will be updated at the same time. This is to assure the community that they will have the most up-to-date data available. A screenshot of the basic SLiSE interface is seen in Figure 8.

SLiSE and this Legacy survey will be a valuable tool for the NRAO proposal system on the GBT and possibly other instruments. SLiSE will help in avoiding overlap with other proposals or previously archived data in passbands already observed. Furthermore, it will identify any contamination from known interstellar molecules or RFI that may conflict with a new proposed observation.

To conclude, this legacy survey will produce a complete inventory of known interstellar species accessible from the centimeter wavelength range that can be used as probes of physical conditions and to understand astrochemistry and chemical evolution. We anticipate that the survey will discover new interstellar species that will constrain chemical formation mechanisms. We will make the data available to the astronomical community in a timely, efficient, and most importantly, in an easy to use manner. We anticipate that these data will help guide the scientific development of ALMA, the EVLA, and Herschel, all of which expect astrochemistry to be an important component of their scientific programs.

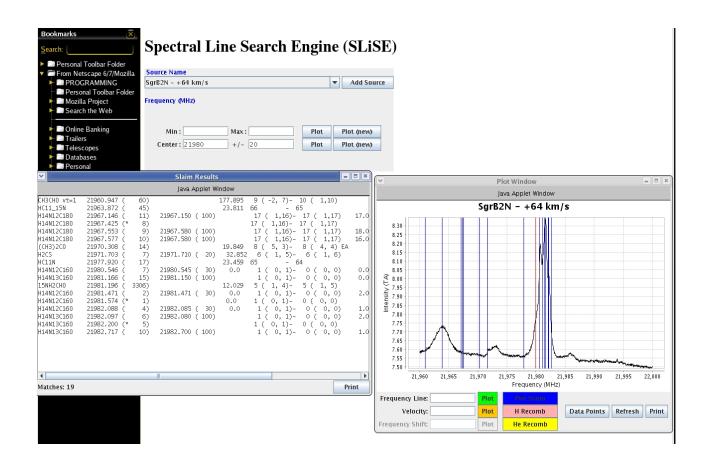


Figure 8. We have developed a slick and easy way to disseminate and display the survey data. The Spectral Line Search Engine (SLiSE) is computer-independent and easy to use via the web or standalone. The illustration above shows the basic online interface of SLiSE.

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