

Chapter 3

Observational Astronomy

3.1 Observational Requirements for Interstellar Detections

Many members of the astrochemistry community dedicate a significant portion of their allocated observing time to the search for complex organic molecules in hot cores. While many hot cores have been identified, systematic spectral line surveys have only been conducted toward a handful of sources (see [4, 24, 25]). Perhaps the best known hot core is Sgr B2(N-LMH), which is found to have among the highest column densities of large organics ever detected [14]. Line confusion is very high in this source, however, due to the large number of species present therein. The observed abundances of complex species in the Orion Hot Core and Compact Ridge have therefore been widely used as the basis for existing hot core models [3] since the line confusion is greatly decreased due to the lower temperatures and narrower line profiles of these hot cores relative to Sgr B2(N-LMH). This increased possibility of a definitive detection of complex molecules in Orion combined with the observed molecular richness of Sgr B2(N-LMH) make these sources the primary targets for complex molecule searches in hot cores. Other less widely studied sources that display similar chemical complexity include the W51 e1/e2 hot cores and the low mass hot corino recently discovered toward IRAS 16293-2422.

The search for molecules in hot cores is most often limited by the availability of laboratory spectral information. For example, $\sim 55\%$ of the lines observed in the recent 3 mm survey of the Sgr B2(N-LMH) source remain unidentified [4]. Yet searches for many of even the simplest species found in primitive solar system materials have not been undertaken, and quite often the observed lines for these molecules are below the RMS limit for existing surveys. In addition, hot core sources are plagued with line confusion. Indeed, the confusion limit is often reached before the desired RMS level. Added to these factors is the ongoing debate within the field as to how many lines are required before one can claim a complex molecule detection, and this number seems to only be increasing. Complex molecule searches are only feasible if there are spectral windows within which the molecule has several strong lines and that are clear of line confusion.

The recent debate over the reported detection of glycine in the Sgr B2(N-LMH) source [26] has led to the development of a set of “essential criteria for establishing the identification of a new interstellar molecule [27].” These criteria are:

1. Rest frequencies for the molecule should be known to high accuracy.
2. Detected transitions should be consistently observed at the same source velocity.
3. Correction for beam dilution should be handled systematically.
4. The relative line intensities should be consistent with a given rotational temperature or quantitative physical source model.
5. Confirming transitions between connected states should be detected.

The high resolution laboratory studies discussed in Chapter 2 ensure that the first criterion is met. The most effective way to ensure that the other criteria are met is to conduct observational searches in many different frequency ranges such that a large number of

transitions are observed and a wide range of energies are probed. Aperture synthesis observations are also required such that the spatial scale of the emission can be determined and appropriate beam dilution corrections can be applied.

3.2 Observatories

The criteria outlined above require the use of several observatories for complex molecule searches in hot cores. Typical rotational temperatures in these sources are on the order of 100–300 K [28], and the Boltzmann peak for 2C and 3C species is near 230 GHz at these temperatures. The 1 mm receivers of the CSO and OVRO are therefore ideally suited for hot core observations of prebiotic species such as those studied in this thesis. Observations at lower frequencies are often more straightforward, however, because of the high line density at millimeter wavelengths, and so complimentary microwave GBT studies are also conducted. For example, the Sgr B2(N-LMH) line density is greater than 6 lines per 100 MHz at millimeter wavelengths [4], yet the line density observed in this source with the GBT is less than 3 lines per 100 MHz. GBT observations also allow for a wider range of transition energies to be probed, leading to a more complete understanding of molecular excitation mechanisms. In addition, the larger beams of the CSO and GBT are more sensitive to extended molecular emission, as the OVRO beam often resolves out extended emission. Studies combining single-dish and interferometric observations are therefore required for a complete understanding of the molecular physics in and around a hot core.

The observations conducted for this thesis involved 1 mm spectral line searches with the CSO, 3 mm and 1 mm spectral line searches and imaging with OVRO, and microwave spectral line searches with the GBT. The operating parameters of the observatories used in these studies are summarized in Table 3.1. This summary is not intended to be a complete

overview of the capabilities of these observatories, but rather a synopsis of the observing setups relevant to hot core complex molecule searches.

Table 3.1: A summary of the observatories used in these studies.

Receiver	Frequency (GHz)	T_{sys} (K)	FWHM (arcsec)	Bandwidth (MHz)	Aperture Efficiency
GBT					
K	18.0 - 26.5	30 - 40	37	50, 200	55%
K_a	26.0 - 40.0	30 - 40	30	50, 200	55%
Q	40.0 - 52.0	60 - 130	16	50, 200	40%
OVRO (combined L + E configurations)					
3 mm	86 - 116	350	7×5	1.8 - 480	65%
1 mm	210 - 270	400	5×2	1.8 - 480	40%
CSO					
1 mm	180 - 280	300	30	50, 500, 1500	70%
0.87 mm	280 - 400	300	25	50, 500, 1500	75%

3.3 Column Density Calculations

3.3.1 Rotation Diagrams

The rotation diagram approach can be used to determine the rotational temperature and column density of a species in the limit of local thermal equilibrium (LTE), optically thin emission, and negligible background radiation brightness. Under these simplest of possible conditions the integrated intensity of a transition, $\int_{-\infty}^{\infty} T_b dv$, is:

$$\int_{-\infty}^{\infty} T_b dv = \frac{hc^3}{8\pi k\nu^2} A g_u \frac{N_T}{Q(T_{rot})} e^{-E_u/kT_{rot}} \quad (3.1)$$

where ν is the transition frequency, N_T is the beam averaged total column density, A is the transition Einstein A -coefficient, g_u is the upper state degeneracy, $Q(T_{rot})$ is the partition

function, T_{rot} is the molecular rotational temperature, and E_u is the transition upper state energy [29]. A rotation diagram is then the plot of $\ln\left[(8\pi k\nu^2)/(hc^3 Ag_u)\int_{-\infty}^{\infty} T_b dv\right]$ versus E_u , which gives a line with slope inversely proportional to T_{rot} and with intercept equal to $\ln(N_T/Q(T_{rot}))$.

The mechanisms for determining the integrated intensity ($\int_{-\infty}^{\infty} T_b dv$), the Einstein A-coefficients times the upper state degeneracy (Ag_u), and the molecular partition function ($Q(T_{rot})$) are outlined below.

3.3.2 Integrated Intensities

The integrated intensity of a transition can be calculated by:

$$\int_{-\infty}^{\infty} T_b dv = 1.064 T_b \Delta v \quad (3.2)$$

where T_b is the peak brightness temperature of the line and Δv is its full width half maximum (FWHM). T_b can be approximated as T_{MB} , the peak line intensity (T_A^*) corrected to the main beam temperature scale by the relationship $T_{MB} = T_A^*/\eta$, where η is the aperture efficiency.

Beam dilution effects must be considered when the beam and source sizes are unequal. In this case, $T_b = BT_{MB}$, where the beam filling factor, B , can be calculated from the relationship between the source size, θ_s , and the beam size, θ_b , by:

$$B = \frac{\theta_s^2}{\theta_s^2 + \theta_b^2} \quad (3.3)$$

For interferometric observations, T_A^* (in K) can be determined by:

$$T_A^* = \frac{1.22 \times 10^6 Int}{\theta_A \theta_B \nu^2} \quad (3.4)$$

where θ_A and θ_B are the beam FWHMs, Int is the peak intensity in Jy/Beam, and ν is in GHz.

3.3.3 Line Strengths

The line strengths in terms of the Einstein A-coefficients times the upper state degeneracy (Ag_u) for a given transition can be calculated from the information given in the .cat files associated with the JPL CALPGM program. These files are generated by SPCAT (see Appendix C), and such files are available for a wide variety of species in the submillimeter and microwave spectral line catalog available at <http://spec.jpl.nasa.gov>. The line strengths are given here as the *log* of the intensity, I. For a given transition, then:

$$I = \sum_1^j 10^{\log I_j} \quad (3.5)$$

which accounts for multiple transitions contributing to the integrated intensity of the line, and the resultant intensity is in units of nm^2MHz . The line strength, Ag_u , can then be calculated by the relationship:

$$Ag_u = \frac{2.7964 \times 10^{-16} I \nu^2 Q(T)}{e^{-E_l/kT} - e^{-E_u/kT}} \quad (3.6)$$

when ν is in MHz and I is in nm^2MHz [30].

3.3.4 Molecular Partition Functions

Neglecting centrifugal distortion, the partition function for an asymmetric rotor is given by:

$$Q(T) = \left[\prod_{i=0}^{3N-6} \left(\frac{e^{-E_i/2kT}}{1 - e^{-E_i/kT}} \right) \right] \sqrt{\frac{\pi}{ABC} \left(\frac{kT}{h} \right)^3} \quad (3.7)$$

where $\prod \left(\frac{e^{-E_i/2kT}}{1 - e^{-E_i/kT}} \right)$ is the total vibrational state partition function, the E_i 's are the energies of the normal modes of vibration, $\sqrt{\frac{\pi}{ABC} \left(\frac{kT}{h} \right)^3}$ is the rotational partition function, and A , B , and C are the rotational constants. The rotational constants determined for the ground state and the n vibrational states populated at T are used such that the molecular partition function is approximated as:

$$Q(T) \approx \sum_{i=0}^n e^{-E_i/kT} \sqrt{\frac{\pi}{A_i B_i C_i} \left(\frac{kT}{h} \right)^3} \quad (3.8)$$