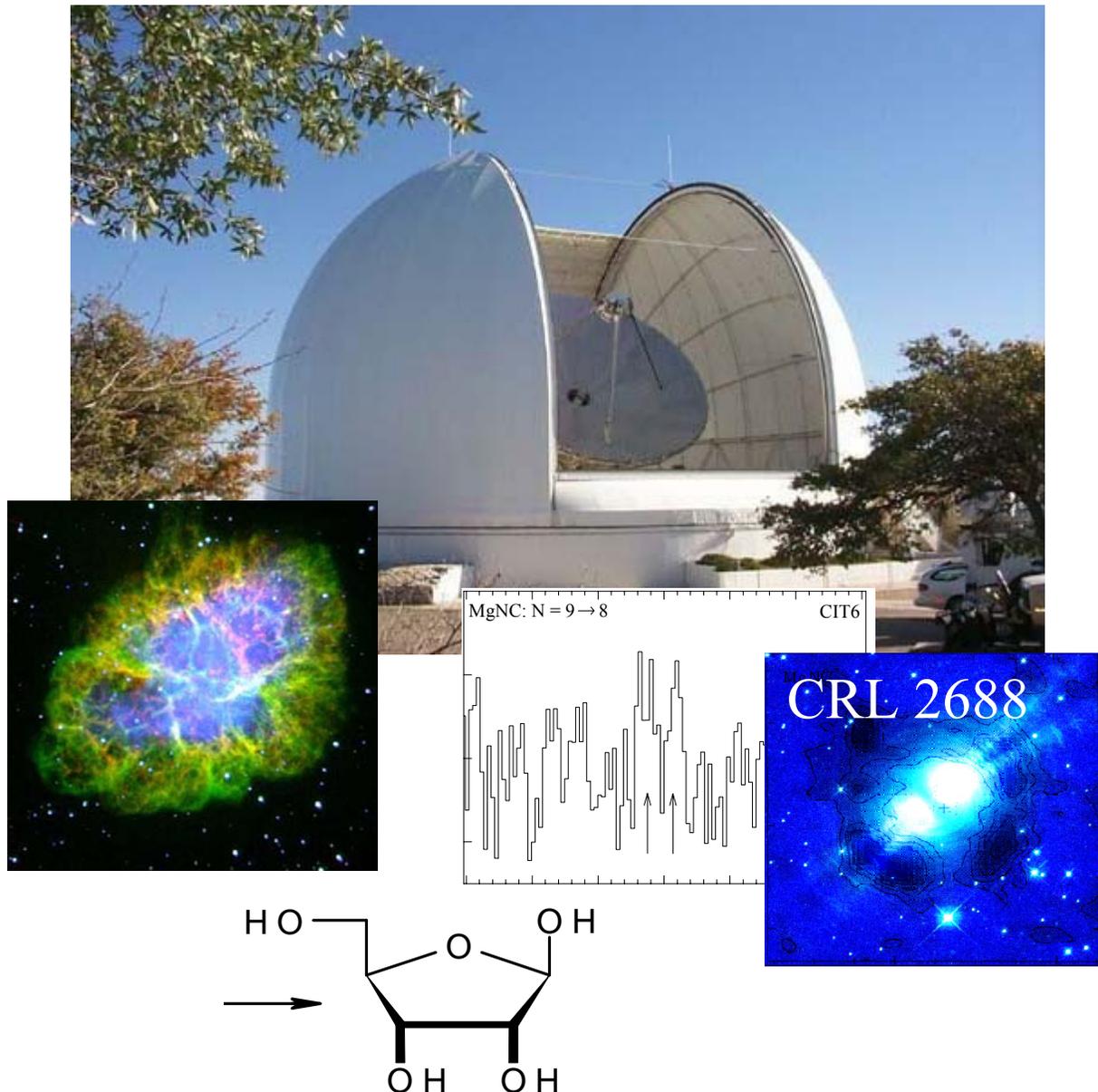


# Interstellar Molecules as Probes of Star Formation and Prebiotic Chemistry:

## A Laboratory in Radio Astronomy

L. M. Ziurys and A.J. Apponi



## I. Goals and Relevance to Astrobiology

Before even the simplest of living cells can form, the chemical compounds that compose the organism must exist. Astrochemistry therefore contributes to Astrobiology by studying (mostly organic) molecules in the interstellar medium, i.e. the vast regions of space between the stars. Such molecules likely contribute to the building blocks of life in the Universe. Astronomy conducted at millimeter wavelengths (0.3-3 mm) has been a primary tool of this research, not only for the discovery of new molecular species, but also in examining their abundances and distributions in the Galaxy. During this laboratory at the Arizona Radio Observatory (ARO) you will measure the spectra of three different interstellar molecules towards the Orion molecular cloud to investigate chemical abundances and trace evidence of star formation.

As the field of astrochemistry evolves, interstellar molecules are being found with ever greater complexity. The recent detection of such compounds as glycolaldehyde in interstellar space, a two-carbon sugar, suggests that three, four, and maybe even five-carbon sugars are also present. What other biogenic compounds might exist? Amino acids? Phosphate esters? How would such molecules be transported to planets? Would they survive the collapse of molecular clouds into solar systems? These are some of the questions astrochemistry is trying to answer.

It is clear that the 5-carbon sugar ribose is of tremendous biological importance, given the structure of DNA and RNA. Yet, ribose itself is not a stable compound in aqueous solution, casting some doubt on the viability of the proposed “RNA world” on early Earth. But what if ribose came from a different environment, where water was not an issue? What if ribose came from interstellar space? Although simpler chemical species than ribose will be studied, this laboratory will illustrate the basic principles and techniques surrounding the investigation of all interstellar molecules, and give some insight into the amazing chemistry occurring between the stars.

## II. Introduction

### i) *Interstellar Molecules: An Overview*

The discovery of interstellar molecules and the establishment of the field of astrochemistry began in the late 1960s with the discovery of H<sub>2</sub>O, NH<sub>3</sub> and CO (Cheung et al. 1968, Wilson et al. 1970). At the time it was thought that the interstellar medium, i.e. the gas and material between the stars, was primarily atomic in nature, and that this environment was too harsh and rarefied for anything more complicated than a few simple diatomic (two-atom) molecules to exist. But now we estimate that 50% of the material in the inner part of the Milky Way Galaxy is molecular in nature, and the current list of known, gas-phase, interstellar molecules is over 120 (see Table 1), not including isotopic variants. Much molecular material also exists in external galaxies, as well (Mauersberger et al 1989). We can now truly talk about a “molecular universe.”

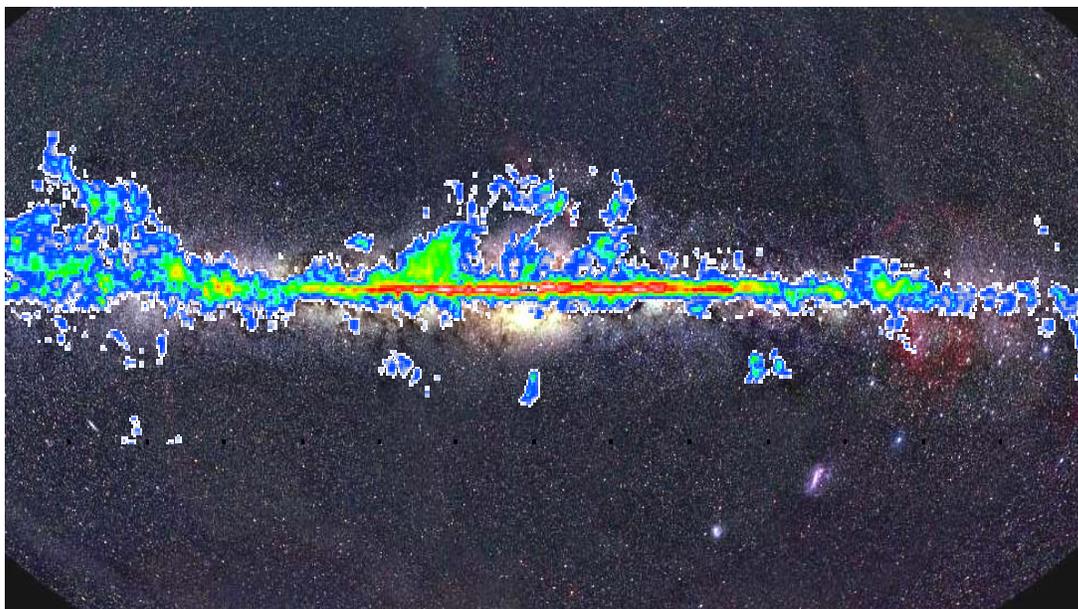
**Table 1.** Known Interstellar Molecules

2		3		4		5		6		7		8		9		10	
H <sub>2</sub>	CH <sup>+</sup>	H <sub>2</sub> O	C <sub>3</sub>	NH <sub>3</sub>	SiH <sub>4</sub>	CH <sub>3</sub> OH	CH <sub>3</sub> CHO	CH <sub>3</sub> CO <sub>2</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> COCH <sub>3</sub>							
OH	CN	H <sub>2</sub> S	MgNC	H <sub>3</sub> O <sup>+</sup>	CH <sub>4</sub>	NH <sub>2</sub> CHO	CH <sub>3</sub> NH <sub>2</sub>	HCO <sub>2</sub> CH <sub>3</sub>	(CH <sub>3</sub> ) <sub>2</sub> O	CH <sub>3</sub> (C≡C) <sub>2</sub> CN							
SO	CO	SO <sub>2</sub>	NaCN	H <sub>2</sub> CO	CHOOH	CH <sub>3</sub> CN	CH <sub>3</sub> CCH	CH <sub>3</sub> C <sub>2</sub> CN	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>2</sub> OH) <sub>2</sub>							
SO <sup>+</sup>	CS	NNH <sup>+</sup>	CH <sub>2</sub>	H <sub>2</sub> CS	HC≡CCN	CH <sub>3</sub> NC	CH <sub>2</sub> CHCN	C <sub>7</sub> H	H(C≡C) <sub>3</sub> CN								
SiO	C <sub>2</sub>	HNO	MgCN	HNCO	CH <sub>2</sub> NH	CH <sub>3</sub> SH	H(C≡C) <sub>2</sub> CN	H <sub>2</sub> C <sub>6</sub>	H(C≡C) <sub>2</sub> CH <sub>3</sub>								
SiS	SiC	SiH <sub>2</sub>	HOC <sup>+</sup>	HNCS	NH <sub>2</sub> CN	C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>2</sub> OHCHO	C <sub>8</sub> H								<b>11</b>
NO	CP	NH <sub>2</sub>	HCN	CCCN	H <sub>2</sub> CCO	HC <sub>2</sub> CHO	c-CH <sub>2</sub> OCH <sub>2</sub>	HC <sub>6</sub> H									H(C≡C) <sub>4</sub> CN
NS	CO <sup>+</sup>	H <sub>3</sub> <sup>+</sup>	HNC	HCO <sub>2</sub> <sup>+</sup>	C <sub>4</sub> H	CH <sub>2</sub> =CH <sub>2</sub>	H <sub>2</sub> CC(OH)H										
HCl	HF	NNO	AINC	CCCH	c-C <sub>3</sub> H <sub>2</sub>	H <sub>2</sub> C <sub>4</sub>											<b>12</b>
NaCl	SH	HCO	SiCN	c-C <sub>3</sub> H	CH <sub>2</sub> CN	HC <sub>3</sub> NH <sup>+</sup>											C <sub>6</sub> H <sub>6</sub>
KCl	HD	HCO <sup>+</sup>	SiNC	CCCO	C <sub>5</sub>	C <sub>5</sub> N											
AlCl		OCS	H <sub>2</sub> D <sup>+</sup>	C <sub>3</sub> S	SiC <sub>4</sub>	C <sub>5</sub> S?											<b>13</b>
AlF		CCH	NH <sub>2</sub>	HCCH	H <sub>2</sub> C <sub>3</sub>												H(C≡C) <sub>5</sub> CN
PN		HCS <sup>+</sup>	KCN	HCNH <sup>+</sup>	HCCNC												
SiN		c-SiCC		HCCN	HNCCC												
NH		CCO		H <sub>2</sub> CN	H <sub>2</sub> COH <sup>+</sup>												
CH		CCS		c-SiC <sub>3</sub>													
				CH <sub>2</sub> D <sup>+</sup> ?													

The chemical species in Table 1 (listed by number of atoms) illustrate the complexity and “non-terrestrial” nature of interstellar chemistry. About 50% of the compounds found in the interstellar medium (ISM) are not stable under normal lab conditions, namely free radicals and molecular ions. These species would be more common as reaction intermediates in terrestrial chemistry. On the other hand, many of these molecules are found in abundance on earth: H<sub>2</sub>O, CH<sub>3</sub>OH, CH<sub>3</sub>CH<sub>2</sub>OH, (CH<sub>3</sub>)<sub>2</sub>O, etc. Even acetone has been found, and after some debate, a simple sugar, glycolaldehyde. The presence of several “natural products” in interstellar space with common organic functional groups naturally leads one to speculate on the complexity of interstellar chemistry.

## ii) *Molecular Clouds and Gas Envelopes Around Old Stars: Interstellar Flasks*

These questions can first be addressed by considering where these gas-phase molecules exist in space and under what physical conditions. In our galaxy, as well as external galaxies, molecules are present in two types of objects: 1) so called “molecular” or dense clouds, and 2) gaseous envelopes around old stars, known as asymptotic giant branch (AGB) stars, as a result of mass loss from the star in the later phases of helium-burning (e.g. Bloeker 1999). As one might expect, these objects have similar physical conditions. Molecular clouds usually have gas kinetic temperatures in the range  $T_k \sim 10$ -50 K, but in rare, small, confined regions towards young stars,  $T_k$  can be greater than 1000 K. Circumstellar envelopes (CSE’s) are cold in the outer part, but heat up to as high as  $\sim 1000$  K at the inner shell near the star. These regions are also important sources of interstellar dust, which condenses out of hot gas being blown off the stellar surface.



**Figure 1:** The distribution of molecular clouds in our galaxy, as traced in emission of carbon monoxide at 115 GHz (CO:  $J = 1 \rightarrow 0$  transition).

Densities of molecular clouds fall in the range  $10^3 - 10^6$  molecules  $\text{cm}^{-3}$ , corresponding to pressures of  $10^{-15} - 10^{-12}$  torr at 10 K. Hence, while these objects are “dense” by interstellar standards, they are ultra-high vacuum in comparison with the terrestrial environment. For CSE’s there is a density gradient, with  $n \sim 10^{10}$   $\text{cm}^{-3}$  close to the star in the inner shell, falling to  $\sim 10^5$   $\text{cm}^{-3}$  at the outer edge.

Both molecular clouds and CSE’s play important roles in astrochemistry and astrobiology. Many of these clouds eventually collapse into stars and accompanying planetary systems. Our own solar system began, for example, as a molecular cloud. Many of these clouds are also very massive – up to  $10^6$  solar masses, and hence contain a tremendous amount of material, mostly in molecular form (as opposed to single atoms or dust particles). CSE’s are important because they are a source of heavy elements to the interstellar medium: carbon, oxygen, magnesium, phosphorus, and so forth.

### iii) *Radio Spectroscopy of Interstellar Molecules*

Astrochemistry involves detecting a wide variety of chemical species and evaluating their abundances. Despite the fact that signals from molecules may be coming from thousands of light years away, a quantitative analysis can be performed on interstellar gas mixtures through the use of radio telescopes and remote sensing. Radio telescopes at first glance may seem an odd tool for a chemist, but these instruments basically exploit fundamental principles of molecular spectroscopy in a similar manner to a laboratory spectrometer.

Molecules have rotational, vibrational, and electronic energy levels, as illustrated in Figure 2. The electronic energy levels, shown here for a diatomic (two-atom) molecule, depend on the internuclear distance and are represented by potential “wells.” Within

each well are the vibrational energy levels, which arise from the spring motion of chemical bonds, as well as rotational energy levels, produced by end-over-end physical rotation of the molecule about its center of mass. A change in *electronic* energy levels require an electron to change molecular orbitals and these changes correspond to the largest energy differences and relatively high energy photons, in the optical and ultraviolet regions of the electromagnetic spectrum. Changes in *vibrational* energy levels correspond to photon energies in the infrared region, while differences in *rotational* energy levels yield photons in the millimeter and sub-millimeter radio regimes at frequencies of  $\sim 30\text{-}300$  GHz.

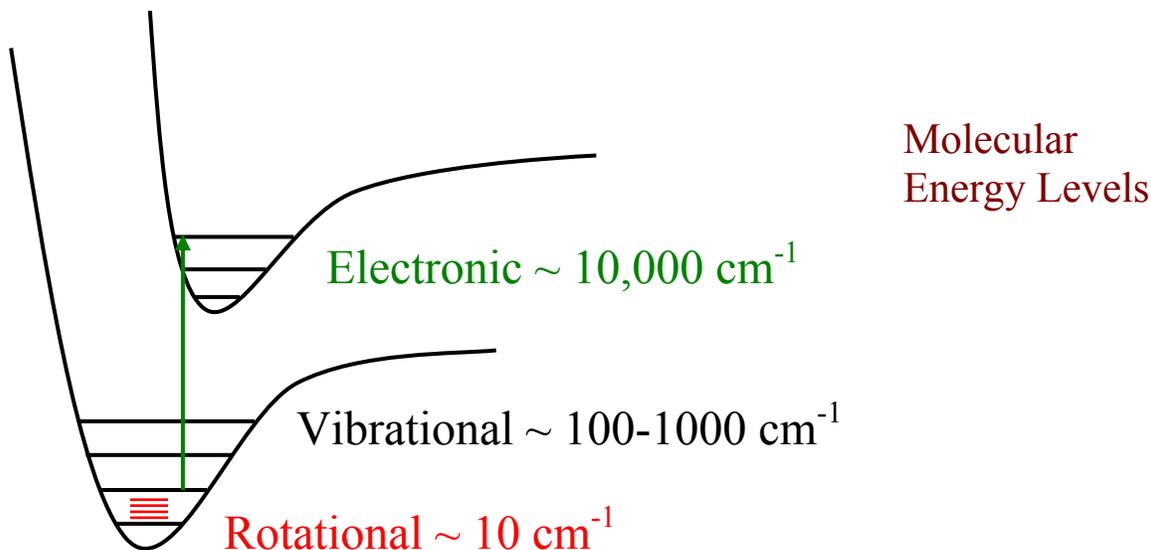


Figure 2: Energy levels of a diatomic molecule. The potential wells are individual electronic states. Within each of these “wells” lie vibrational and rotational levels.

The kinetic energy of other molecules’ collisions with a given molecule can be converted to the molecule’s own internal energy, causing the molecule to be at higher energy levels. From a higher level a molecule can then spontaneously decay to lower levels, resulting in the emission of photons at an energy (and therefore a characteristic frequency or wavelength) corresponding to the energy difference between the two levels. Given typical interstellar temperatures of 10-50 K, it turns out that usually only rotational energy levels of a given molecule are populated. The energies of the rotational levels, and hence energy differences, depend exclusively on the masses of the atoms forming the molecule, the bond lengths, and the molecular geometries, i.e., the “moments of inertia” of a given molecule. A diatomic molecule has two axes it can physically rotate around, as shown in Figure 3. These axes correspond to moments of inertia,  $I = \mu r^2$ , where  $r$  is the distance between the nuclei (or bond length) and the reduced mass  $\mu = m_a m_b / (m_a + m_b)$ , where  $m_a$  and  $m_b$  are the masses of the two atoms. These moments of inertia, called  $I_b$  and  $I_c$ , are equivalent, i.e.  $I_b = I_c = I$ .  $I$  determines the spacing of rotational energy levels of the molecule, and is used to define the “rotational constant”  $B$ , where  $B = h / (8\pi^2 I)$  and  $h$  is the Planck constant.



Diatomic molecules are the simplest cases, and polyatomic species naturally produce more complicated patterns defined by two or three differing moments of inertia. These molecules, in spectroscopic jargon, are labeled “symmetric” and “asymmetric” tops. The principle, however, is the same. Another detail is that rotating molecules are subject to centrifugal force, causing bonds to lengthen as the speed of rotation increases. This effect necessitates a small correction which depends on the quantum number  $J$ . A more correct energy level formula is thus:

$$E_{\text{rot}} = BJ(J+1) - DJ^2(J+1)^2, \quad (3)$$

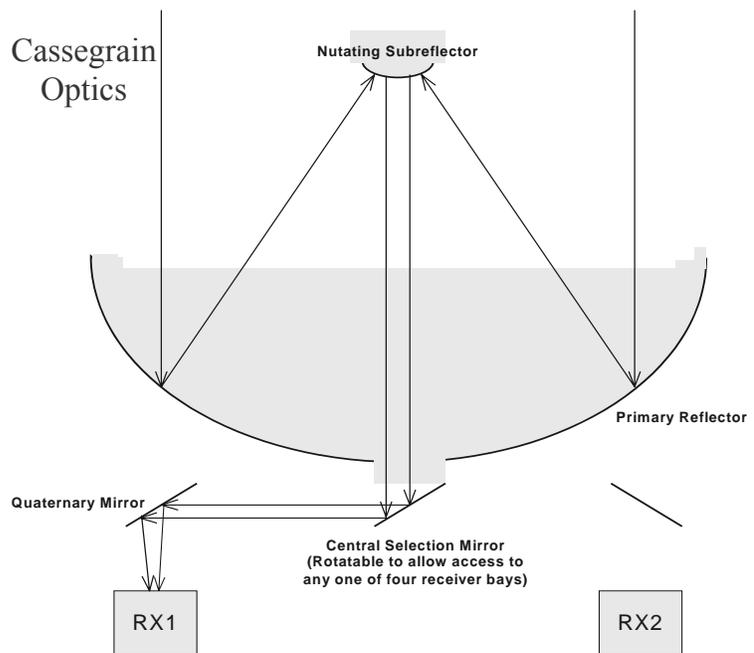
which yields

$$\nu = 2B(J+1) - 4D(J+1)^3, \quad (4)$$

where  $D$  is the “centrifugal distortion” constant. Since we can measure the frequencies of spectral lines to one part in  $10^7$ , small corrections such as centrifugal distortion are absolutely necessary to identify any interstellar species.

#### iv) Radio Telescopes and Receivers: A Hitchhiker’s Guide

A radio telescope is basically a large satellite dish with an extremely smooth surface. The Arizona Radio Observatory (ARO) dish is 12 meters in diameter with a surface accurate to better than 0.1 mm. As shown in Figure 5, the signal from the sky is focused from the “primary reflector” to the “secondary” mirror or “sub-reflector,” which in turn directs the signal through an opening in the primary. The signal is then directed by mirrors into the appropriate detectors, or *receivers*. Any dish has a limited *angular resolution* or *diffraction limit*, meaning that it cannot distinguish two sources of radiation separated on the sky by less than a certain angle  $\theta$ . A patch of sky whose diameter



**Figure 5:** Basic optics of the 12 m radio telescope leading to the heterodyne detector systems.

is  $\sim\theta$  is called the *beam* of a radio telescope, which determines how detailed a mapping it can do. For a telescope diameter  $D$  and observing wavelength  $\lambda$ , the beam diameter is  $\theta \cong 1.2\lambda/D$ . For your observations,  $D = 12$  m and  $\lambda = 3$  mm, so  $\theta \cong 0.0003$  radians = 62

arcseconds = about 1/30 of the diameter of the Moon = a US quarter seen at a distance of 80 meters = ~angular resolution of the human eye. [With regard to the last, plug in for yourself: pupil size = 2.5 mm (brightly lit situation) and  $\lambda = 5 \times 10^{-7}$  m (middle of visual spectrum). Also, do the experiment with the quarter!]

The signals from interstellar space are very weak and must be amplified while at the same time minimizing the inevitable addition of instrumental random noise to the signal. The “superheterodyne” technique is used where the signal from the sky is “mixed” (combined) with a “local oscillator” in a device called the “mixer.” In this way the sky signal (at a frequency  $\nu_{\text{sky}}$ , say, of 115 GHz) is converted to a much lower frequency, called the “intermediate frequency”  $\nu_{\text{I.F.}}$ , where it can be more conveniently and accurately handled. The mixer generates the intermediate frequency  $\nu_{\text{I.F.}}$  by multiplying the sky signal with the local oscillator signal (at frequency  $\nu_{\text{L.O.}}$ ), which is mathematically equivalent to producing sums and differences of all incoming frequencies. This intermediate frequency is then immediately sent to a low-noise amplifier constructed such that only a certain range of frequencies (a certain bandwidth) is amplified. For the ARO receivers,  $\nu_{\text{I.F.}} = 1.5$  GHz with a bandwidth of 1.0 GHz centered on that frequency.

The use of the mixer and amplifier combination thus determines which sky frequency is observed. In practice at ARO one chooses a value of  $\nu_{\text{L.O.}}$  (“sets the L.O.”) to get the desired sky frequency according to:

$$\nu_{\text{L.O.}} = \nu_{\text{sky}} - 1.5 \text{ GHz} \quad (5)$$

The local oscillator must maintain a very stable frequency because any drifting with time would cause the sky frequency also to change. Thus before observing begins, the telescope operator will stabilize the L.O. frequency (to about 1 part in  $10^9$ ) using a “phase-lock loop,” as well as set the L.O. to the desired frequency.

The I.F. signal is next sent to a spectrometer, which divides the signal of bandwidth 1.0 GHz into a large number (say, 256) of spectral frequency channels (a “filter bank”), each at a different frequency. Numerous spectral resolutions are available. Note that a complete spectrum is obtained at once, without having to take the time to consecutively scan to different frequencies.

The signals from the spectrometer are subsequently sent to a computer disk. In order to reduce the noise in a measurement (i.e., increase the *signal-to-noise ratio*) data is collected, or “signal-averaged,” usually over a 6 minute integration period. These 6 minute “scans” are recorded to the disk under a unique scan number, which is used as an identifier for the subsequent data reduction that you will be doing. Because the stability of the electronics is excellent, one can in turn average a large number of scans to obtain one spectrum with much improved signal-to-noise ratio. You will also be able to average (for each scan) the recorded signals from two completely independent sets of receiver electronics. This duplication allows, for other types of observations, the polarization of signals to be measured, but for us it gives a 2-for-1 deal and nicely improves our signal-to-noise ratio.

The noise level ( $T_{\text{rms}}$ ) of any measurement, which we want to minimize, follows the radiometer equation:

$$T_{\text{rms}}(1\sigma) = \frac{2T_{\text{sys}}}{\sqrt{B_W \tau}}, \quad (6)$$

where  $B_W$  is the bandwidth (or spectral resolution) of the individual channels of the spectrometer,  $\tau$  is the total integration time, and  $T_{\text{sys}}$  is the “system temperature,” a measure of the power from the electronics and the sky that competes with the desired signal power. The intensity scale in radio astronomy is often expressed in temperature units (Kelvins), a so-called *antenna temperature*, but beware: this temperature often has little to do with any physical temperature being measured. It is rather a measure (through a thermodynamic relation) of the incident energy flux (joules/sec/Hz-of-bandwidth) falling on the antenna in the direction in which it is pointed.

The system temperature can vary with time because sky conditions change with source elevation above the horizon and with weather. Typically,  $T_{\text{sys}}$  is therefore measured every scan or every other scan with a “cal scan.” Recorded signals are actually voltages, and the cal scan determines the voltage-to-temperature conversion scale by recording the voltage of the system while looking at two known signals: a “load” at ambient temperature and a blank sky position, which exhibits a colder temperature.

Another basic observing technique to correct for instrumental errors, especially those affecting the baseline (or zero level) of the spectra, is “position-switching.” To remove electronic and sky instabilities, scans are actually composed of the average *difference* between signals taken with the dish pointed “on-source” and then pointed “off-source,” going back and forth at ~30-second intervals.

Two other techniques are important at the telescope: “pointing” and “focusing.” The surface of the dish is precise, but nevertheless suffers from gravitational deformations, especially as it tilts far over from the straight-up, “bird-bath” position. These deformations both de-focus the telescope, as well as cause it to aim (point) incorrectly. The pointing calibration is accomplished by observing a strong source of known position (such as a planet), which then generates small, real-time corrections so that the telescope physically points at the desired coordinates in the sky. “Focusing” simply consists of moving the sub-reflector slightly in and out to optimize its position for maximum signal strength. Both pointing and focusing will be done during this activity.

### III. Lab Exercise

This lab will focus on measuring spectra of three different interstellar molecules towards the Orion molecular cloud. This cloud is located behind the famous Orion Nebula (Messier 42), part of the “sword” in Orion (be sure to see it with your naked eye some evening). The molecules to be observed are  $\text{HC}_3\text{N}$ ,  $\text{CO}$ , and  $\text{CH}_3\text{CN}$ .

HC<sub>3</sub>N: Here multiple rotational transitions will be observed over the 2 and 3 mm wavelength range. You will calculate the frequencies of observation before you start. These observations will illustrate the precision of interstellar molecular spectroscopy, and then be used to construct a “rotational diagram” from which a molecule “column density” can be extracted, as well as the temperature of the gas-phase HC<sub>3</sub>N.

CO: Here the  $J = 1 \rightarrow 0$  transition at 115 GHz will be observed at two positions towards Orion-KL, a region of young star formation. These spectra will show the presence of a “bipolar outflow” originating from a young star. The outflow contains molecules that are red-shifted (moving away from Earth) and blue-shifted (moving towards Earth). The measured spectra will thus show “red-shifted” and “blue-shifted” wings, which the observer will use to interpret the geometry of the outflow.

CH<sub>3</sub>CN: In this case the  $J = 8 \rightarrow 7$  transition will be observed. This molecule is more complicated than CO, a diatomic, and HC<sub>3</sub>N, a linear molecule. CH<sub>3</sub>CN is a symmetric top, and hence has two different moments of inertia, requiring the energy level pattern to be characterized by two quantum numbers, J and K. As a result, the  $J = 8 \rightarrow 7$  transition actually consists of many lines, labeled by quantum number K, so-called “K-ladder” structure. You will measure the relative intensities of these K-ladder lines to estimate the kinetic temperature of the CH<sub>3</sub>CN.

**First:** Calculate the rotational transitions of HC<sub>3</sub>N in the range 65 – 170 GHz. This range is that covered by the ARO receivers (although there are atmospheric lines of O<sub>2</sub> that prevent observations near 118 GHz). Pick at least four transitions to observe at the telescope. The rotational constants are:

$$B = 4549.058 \text{ MHz}$$
$$D = 0.5439 \text{ kHz}$$

### **Observing Procedure**

You will begin your observing session by logging onto the observer’s computer. The operator will help you do this.

### **HC<sub>3</sub>N Observations**

The session will begin with observations of HC<sub>3</sub>N. When you arrive at the telescope, give the operator the frequencies of the HC<sub>3</sub>N lines that you wish to observe. You will start with one line, and the operator will tune the local oscillator and radio receiver to its frequency. You can actually watch the operator do this tuning. The operator may ask what source you are observing. The source and 1950.0 coordinates are:

$$\text{Orion-KL } (V_{\text{LSR}} = 9.0 \text{ km/s}) \quad \alpha = 5^{\text{h}} 32^{\text{m}} 47.5^{\text{s}}$$
$$\delta = 5^{\circ} 24'23''$$

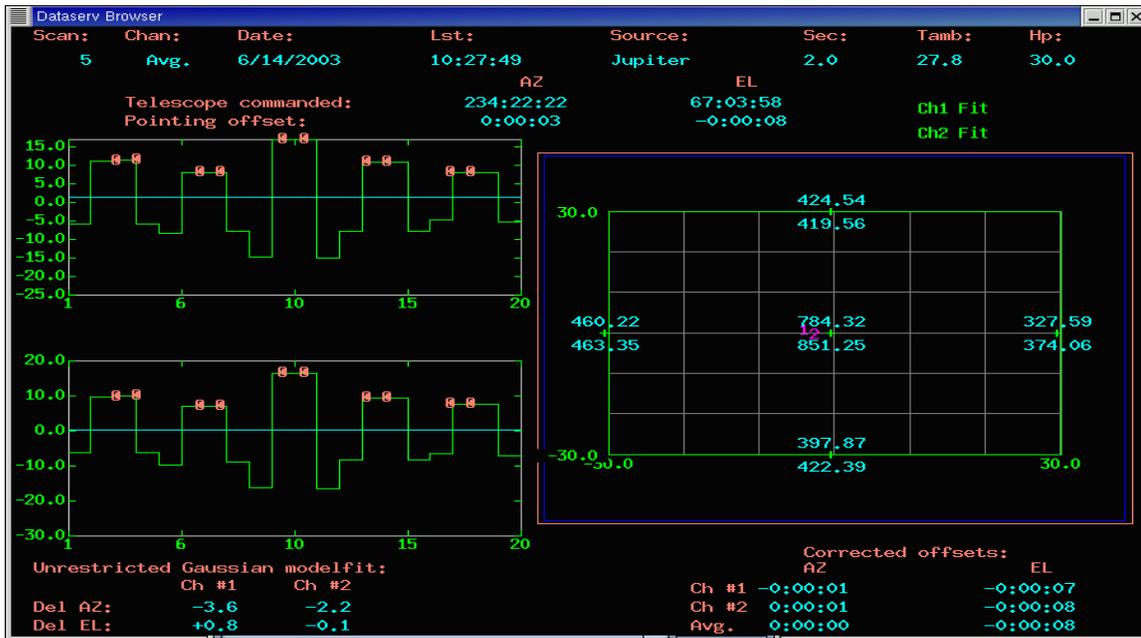


Figure 6: A pointing “5-point” scan displayed in “Dataserve.”

This source can be found in the LMZ.CAT catalog at the telescope.  $V_{LSR}$  is the Doppler correction for this source relative to our “solar neighborhood” velocity. It is called “velocity with respect to the Local Standard of Rest,” hence  $V_{LSR}$ .

Once the receiver is tuned, you will have to choose a planet for pointing and focusing. Ask the operator to set up “CATALOG TOOL” so you can find a handy planet. It is best to pick one close in the sky to your source. First, a “five-point” pointing needs to be done on the planet. The operator will move the telescope and measure five positions across the planet: nominal center position and  $\sim 0.5$  beamwidth north, south, east and west of the planet. These data will appear on the “Dataserve” computer terminal. The intensity of the planet, in janskys, will be displayed at the five positions measured, as well as pointing corrections in azimuth and elevation, as shown in Figure 6. These are the corrections you will need to “fine tune” the pointing of the telescope when you make your measurements in Orion. A few such pointing scans may have to be done to achieve a consistent set of pointing corrections. The operator will put the new corrections into the telescope drive computer.

The next task is to focus the telescope. The operator will move the focus to a series of positions and measure the temperature of the planet at each position. The computer will produce a plot of focus versus intensity (see Figure 7), and then do a fit to the peak of this curve, which is the optimal focus position. You may have to iterate a few times with the focus.

Next are the spectral line measurements. Give the operator your source name and position from the catalog and he will put in the Doppler correction and steer the telescope to the source. You will have to tell the operator:

- 1) Observing procedure: position-switching with off position = 30' west in azimuth
- 2) Scan time: 6 minutes
- 3) Spectrometer Backend Set-up: Use filter banks: 1000/1000; series/series: MAC:  
600\_2k\_2

The telescope will measure an off-position set. The spectrometer set-up places each receiver channel into its own filter bank of 256 1-MHz channels, and splits the Millimeter AutoCorrelator (MAC) in half for each channel. The MAC is a 1.5 bit autocorrelating digitizer that can sample the telescope IF at a rate up to 2 GHz. A digital waveform is generated by comparing adjacent samples of data and representing those that are increasing with time a 1, those that are decreasing with time a -1 and those that remain the same a 0. Bit resolution is dramatically improved by averaging in the time domain, e. g. Average (1+0) = 0.5, Average (1+1+0) = 0.7, etc. The frequency information is obtained by fast Fourier transform of the generated wave. For more detail, see the ARO website: <http://aro.as.arizona.edu>.

Once the spectrometers (also called “backends”) are connected, the operator will start with a calibration scan to establish the  $T_{\text{sys}}$  and hence the temperature scale, then take the first spectral line scan. When finished, it will be recorded under a scan number that the operator will log. Pull the scan up on the computer screen. You will have to “reduce” the data by averaging the two receiver channels (see Appendix for commands). It is best that you first look at each channel and see if they agree, and then take the average. You will want to do this separately for the filter bank and MAC data (see Appendix).

Compare your data. Do you have sufficient signal-to-noise to see the HC<sub>3</sub>N line, and then measure its intensity accurately? If not, take a few more scans and average them. It is recommended to take ~2 scans for each HC<sub>3</sub>N line.

When one transition has been successfully measured, continue with the next one. The operator will have to retune for each frequency. Measure at least four transitions. Make a hardcopy of each spectrum for analysis. Removing a baseline from your final spectrum will be useful. You may also fit a Gaussian profile to each spectrum to determine the intensity and line width.

## CO

Ask the operator to tune to the CO:  $J = 1 \rightarrow 0$  frequency at 115,271.202 MHz. Because pointing is critical for this observation, you must repeat the pointing and focusing procedure as previously described. Then go back to Orion and take a scan. The line will be very strong, but if you enlarge the spectrum on the computer screen you will see that broad “wings” exist on either side of the main feature. Make sure you take enough scans to have sufficient signal-to-noise to discern the wings, then take data at two other positions: 1) 30” north of center, and 2) 30” east of center. Again, take enough scans to see the wings. You should see the shape of the line wings change at each position. Make hard copies of all final averaged spectra.

## CH<sub>3</sub>CN

Now tune to the  $J = 8 \rightarrow 7$  transition of CH<sub>3</sub>CN at 147,124.0 MHz. You do not need to point or focus. Observe a spectrum at the center position. You should see multiple lines called “K-components” with spacings roughly 1:3:5:7:9... This pattern is characteristic of a symmetric top. Take a sufficient number of scans such that you can readily measure the intensities of at least six K-components.

## IV. Analysis

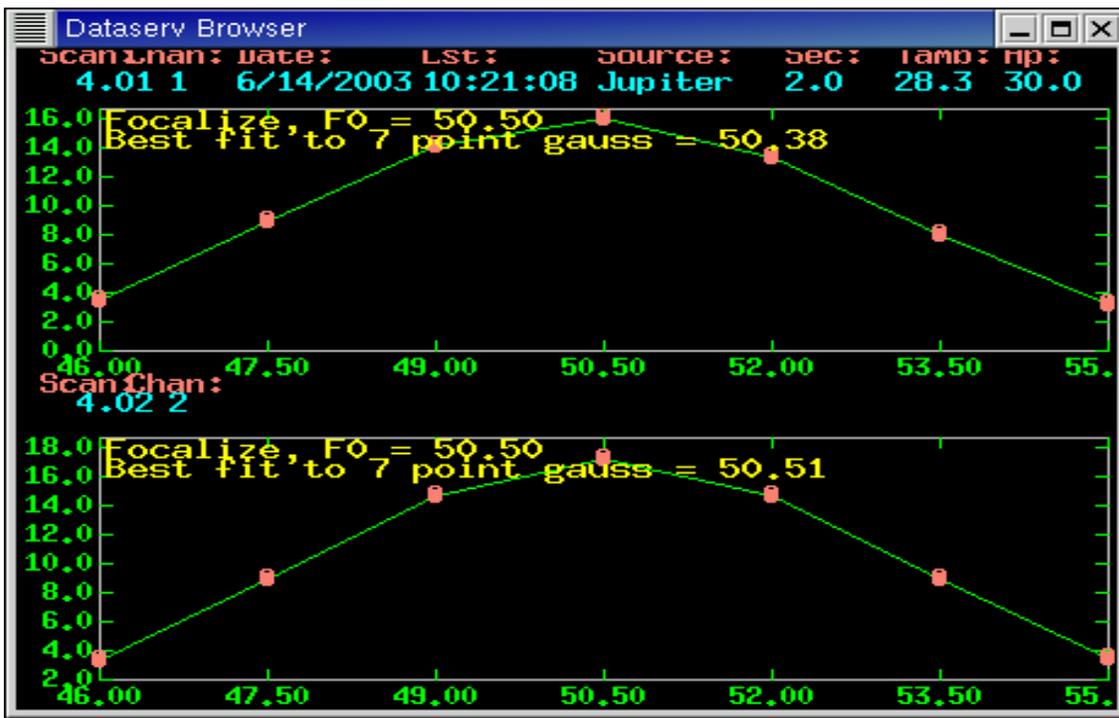


Figure 6: A “focus” scan which shows planet intensity as a function of focus positions.

## HC<sub>3</sub>N

Now use your HC<sub>3</sub>N data to construct a “rotational diagram” from which you can determine a “column density” ( $N_{\text{tot}}$ ) of HC<sub>3</sub>N, and a temperature characteristic of the molecule, called a “rotational temperature”  $T_{\text{rot}}$ . The column density is the total number of HC<sub>3</sub>N molecules along a 1 cm<sup>2</sup> cross-section column running from Kitt Peak out towards Orion and beyond! Unfortunately we can only measure this projected density; to estimate the usual volume density (molecules cm<sup>-3</sup>) we must somehow have an estimate of the depth of the molecular cloud along the line of sight. Do you have any ideas as to how we could estimate this?

The basis for determining the rotational temperature (as well as the kinetic temperature you will determine for CH<sub>3</sub>CN below) is the so-called Maxwell-Boltzmann distribution. A collection of molecules, each having many possible energy states, will occupy the energy states according to the effective temperature of whatever process (e.g., collisions with other molecules, absorption of photons) is providing the energy. For a given temperature, the Maxwell-Boltzmann formula predicts what fraction of the molecules will be in any energy state, and therefore also how strong various energy changes (producing spectral lines) will be. By observing the strengths of the spectral lines, we can thus measure the temperature of the gas.

For each transition observed, measure the peak intensity  $T_L$  in K, and the full-width-half-maximum (FWHM) line width  $V_{1/2}$ . These quantities are a measure of the amount of HC<sub>3</sub>N present per rotational level. You will use these data in a fit to the following formula:

$$\log\left(\frac{3kT_L V_{1/2}}{8\pi^3 \nu S_{ij} \mu_0^2}\right) = \log\left(\frac{N_{\text{tot}}}{\zeta_{\text{rot}}}\right) - E_u \log\left(\frac{e}{T_{\text{rot}}}\right). \quad (7)$$

Here  $\nu$  is the frequency of the transition,  $S_{ij}$  is the intrinsic quantum mechanical line strength,  $\mu_0$  the permanent electric dipole moment of the molecule,  $\zeta_{\text{rot}}$  the rotational partition function,  $e$  is the natural base number 2.718, and  $E_u$  the energy of the upper level for a transition  $J + 1 \rightarrow J$ . For a linear molecule,  $S_{ij} = J + 1$ , and  $\mu_0 = 3.724$  debyes for HC<sub>3</sub>N. The partition function can be approximated as  $\zeta_{\text{rot}} \cong B/T_{\text{rot}}$ , and  $E_u$  must be calculated for each K value.

Now plot (one point for each of your measured lines) the left side of equation (7) (which is a number based on your observations once you plug everything in!) versus  $E_u$ (K). You should get approximately a straight line with a negative slope; make an “eyeball” linear fit to the data points and determine its slope. This slope equals  $-\log e/T_{\text{rot}}$ , finally yielding the rotational temperature  $T_{\text{rot}}$ . Then from the Y-intercept, find  $\log(N_{\text{tot}}/\zeta_{\text{rot}})$  and thus  $N_{\text{tot}}$ .

## CO

Use your spectrum to construct a rough picture of the orientation of the bipolar outflow as we observe it on the sky.

## CH<sub>3</sub>CN

These data will be used to estimate the gas kinetic temperature. The different K-component lines lie at different energies, and hence, as explained above, comparing their relative intensities (called  $T_L(K)$ ) yields the kinetic temperature  $T_K$  of the gas. The following formula will be used to solve for  $T_K$ :

$$\frac{T_L(K)}{T_L(K')} = \frac{g(K)}{g(K')} \cdot \frac{J^2 - K^2}{J^2 - K'^2} \cdot \exp\left(\frac{-E(K) - E(K')}{kT_K}\right) \quad (8)$$

$T_L(K)$  and  $T_L(K')$  are the intensities of two K components and  $g(K)$  and  $g(K')$  are the respective “statistical degeneracies,” which has a value of 2 for  $K = 3, 6, 9, \dots$  and 1 for all other K’s.  $E(K)$  and  $E(K')$  are the energies of the K and  $K'$  levels, given by the formula:

$$E(K) = B J (J+1) - (A-B) K^2 \quad (9)$$

For methyl cyanide,  $A = 158,099.0$  MHz, and  $B = 9,198.83$  MHz. You will have many combinations of K components to compare, and they may give a range of values. Calculate several. Compare the temperatures obtained with that found for  $\text{HC}_3\text{N}$ .

## V. References

Bloecker, T. I.A.U. Symposium **191**, p. 21 (1999).

Mauersberger, R., Henkel, C., and Schilke, P. *Ap.J. S.* **156**, 263 (1989).

Wilson, R.W., Jefferts, K. and Penzias, A.A., *Ap.J.* **161**, L43 (1970).

Rohlfs, K. and Wilson, T.L. (2003) *Tools of Radio Astronomy*, Springer-Verlag.

Chapter 8 (sections 1-4 ONLY): Observational Methods

Chapter 11: Spectral Line Fundamentals

Chapter 14: Molecules in Interstellar Space

Turner, B.E. and Ziurys, L. M. (1988) “Interstellar Molecules and Astrochemistry” in *Galactic and Extragalactic Radio Astronomy*, 2<sup>nd</sup> ed., Verschuur, G.L and Kellerman, K.I. (eds.), Springer-Verlag.

## APPENDIX I: Simple commands for data reduction

UNIPOPS is a data reduction program used for the KP12m telescope. Spectral line telescope data is generally reduced to a Cartesian plot of frequency offset (MHz) vs. intensity (K). The frequency offset is relative to the rest frame of the molecule where all Doppler shifts have been accounted for in the operating software. In general, the data acquisition and reduction occurs as an interactive process of: (i) a calibration scan is taken, (ii) a short (about 6 minute) data scan is taken and written to the hard drive, (iii) the data is accumulated and averaged using a weighting function, (iv) a baseline is removed if necessary, and (v) steps (i) – (iv) are repeated until the desired signal to noise is achieved.

UNIPOPS is used to retrieve raw KP12m data from the disk and reduce each series of spectral line observations to a single Cartesian plot using a weighted average for each scan. UNIPOPS is able to do this in a number of ways, but we will stick to the absolute basics here. The data are written to the disk, each with its own unique scan number. There is a base scan number and a subscan number. The base scan number is listed sequentially for each observation made. The subscan number is listed as a decimal to the base number and corresponds to the different backends used for the observation. There will be 4 subscan numbers for this exercise, e.g. 2.01, 2.03, 2.11 and 2.12 where the 01 and 02 subscans are the filterbanks and the 11 and 12 are the MAC.

### *A Quick Look at Each Scan*

The first thing we will probably want to do is look at the raw data for each individual scan. This is done using the *get* command or the *f* and *s* macros in the following syntax:

```
LineF> get <scan>.<subscan> page show
LineF> <scan> f
LineF> <scan> s
```

To switch between the filterbanks and MAC use the following commands:

```
LineF> hcdata // changes the prompt to LineH> for MAC data
LineH> fbdata // changes the prompt to LineF> for filterbank data
```

The *get* command takes the scan denoted by *<scan>.<subscan>* and places it into the plotting array—NOTE when using *get hcdata* and *fbdata* are not needed. The commands *page* and *show* are added to actually plot the data to the screen. The macros *f* and *s* show the first and second filterbank or MAC channels on the screen with only a single command depending on the current prompt.

### *Averaging Two or More Scans Together*

If you have two or more scans towards the same position on the sky, at the same frequency and same resolution, that data can be averaged together to improve the signal to noise. To do this is relatively easy as long as the scans are taken sequentially.

```
LineF> empty // make sure the accumulation array is empty
LineF> add(<scanlow>, <scanhigh>)
LineF> c1 // macro to average all of the first filterbank data together
LineF> c2 // macro to average all of the second filterbank data
LineF> cb // macro to average both the first and second filterbanks together
```

### *Removing a Baseline and Determining Line Parameters*

Usually a polynomial baseline of order a few is needed to determine line parameter information. There are built in macros for each of these in the program:

```
LineF> nfit = <baseline order> // nfit is the order of the polynomial used in the fit
LineF> bset // will prompt you for mouse clicks in up to 16 regions
LineF> bshape bshow // optional commands to preview how the fit will look
LineF> baseline page show // removes the baseline and replots the spectrum
```

After a baseline is removed, Gaussian profiles are fit to each feature.

```
LineF> gset // will prompt you to select the left, center and right of the peaks
LineF> gshow // calculates the results and plots them on the screen.
```

If the fit does not converge, try setting the adverb *niter* = 1000 and run *gshow* again.

### *Enlarging a Spectrum*

There are two important commands for enlarging regions of the displayed spectrum

```
LineF> yrange(<min>, <max>) page show
LineF> xrange(<min>, <max>) page show
```

The command *yrange* expands the y-scale and *xrange* expands the x-scale. The arguments *<min>* and *<max>* have the same units as the current axis assignments.

Expansion of either scale can be done using the mouse in the following way:

```
LineF> yrange(tcur, tcur) // NOTE: tcur is the actual argument
LineF> xrange(xcur, xcur) // NOTE: xcur is the actual argument.
```

The arguments *tcur* and *xcur* prompt the user for a left mouse click over the graphics window corresponding to either the temperature (y-scale) or current x-scale position.

### *Printing and Exporting Data*

To print any graphic shown on the screen use the command *gcopy* and to print the scan information, use the commands *header* *tcopy*.

### *Other Data Reduction*

More sophisticated reduction may be necessary to show outflow characteristics and to reduce pointing and focus data. These will be shown to you as needed at the telescope.