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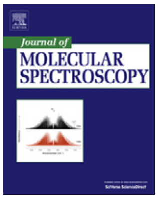

An analysis of a preliminary ALMA Orion KL spectrum via the use of complete experimental spectra from the laboratory

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ABSTRACT

Preliminary Atacama Large Millimeter/Submillimeter Array (ALMA) science verification data for a single pixel centered on the hot core of Orion KL (R. A. = 05 h 35 m 14.35 s, Dec = –05°22′35″ (J2000)) are available as this special issue on broadband spectroscopy is coming to press. As part of this verification process it is useful to compare simulations based on laboratory spectroscopy with ALMA results. This provides not only a test of instrumentation and analysis, but also a test of astrophysical assumptions such as local thermodynamic equilibrium (LTE) and the temperature variations within telescope beams. However, these tests are spectroscopically limited because it is well known that astrophysical spectra contain large numbers of unknown lines, many of which are presumably due to unanalyzed rotational spectra in excited vibrational states of a relatively few molecules. To address this issue we have previously discussed the use of broadband complete experimental spectra (CES) that is obtained from the analysis of several hundred intensity calibrated spectra taken over a range of temperatures. In this paper we will compare these CES with the similarly complete astrophysical spectra.

1. Introduction

The preliminary Science Verification data from ALMA provide an opportunity to compare the astrophysical data from a large broadband interferometer with the underlying laboratory database. In the millimeter and submillimeter spectral region (mm/submm) both laboratory [1–3] and astrophysical spectroscopy [4–10] began as narrow band experimental subjects, limited by the availability of technology. In the laboratory, quantum mechanical (QM) models were developed to select observation frequencies for the narrow band bootstrap observation, analysis, and prediction cycles. The resultant QM models were then used to calculate synthetic spectra for astrophysical use over broad spectral regions [11,12].

This approach has been enormously successful, as testified to by the development of ALMA, Herschel, SOFIA [13–15], their host of antecedent telescopes, and the growth of ever larger user communities. This success has led to telescopes of not only greater sensitivity and angular resolution, but also considerably greater bandwidth. One example is the WIDAR digital cross correlator, which was produced by Canada for use on the Karl G. Jansky Very Large Array (VLA). WIDAR cross-correlates the data from the 27 individual antennas to produce 351 independent correlations for spectral bands covering up to 8 GHz of bandwidth in each polarization. The 8 GHz band can be divided into 128 independent subbands, at a spectral (channel) resolution ranging from 1 MHz to less than 0.1 Hz. The ALMA instrument has two correlators with similar design specifications. At 275 GHz, 1 km s^{-1} is equivalent to 922 kHz for low redshifts, so the ALMA device can be used to analyze 8000 km s^{-1} of velocity or nearly 3% of the rest frequency. Such a large instantaneous coverage is conducive for line searches.

A byproduct of the enormous advances in sensitivity and spectral coverage of these telescopes is the rapidly growing number of astrophysically observable lines that are not included in the QM based astrophysical catalogs. It is generally assumed that many of these unassigned lines, typically referred to as the astrophysical weeds, are due to unanalyzed low lying excited vibrational states of a relatively few molecules [16]. While in some sense these unassigned lines are due to the small cumulative amount of mm/submm spectroscopy, there is a more fundamental reason. Briefly, the excited vibrational states are typically perturbed, often in very complex ways, and their analyses can be orders of magnitude more challenging than for the states included in the QM catalogs.

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We have previously described and demonstrated a laboratory approach to this problem that eliminates the need for the complicated and time consuming assignment and analysis process [17,18]. It depends upon the collection of intensity calibrated, complete laboratory data at many (in principle two, but typically 100–1000) temperatures. From these data it is possible to calculate the astrophysically significant line strengths and lower state energies of spectral lines without the need for quantum assignment. More recently we have shown an additional frequency point-by-point analysis procedure that is especially useful for regions of overlapping spectral features [18]. It is this latter procedure we will use in this paper to calculate the spectral simulations at astrophysical temperatures.

It was anticipated that the impact of unknown lines would be greater in ALMA than for earlier telescopes because its high angular resolution would (1) make possible the study of smaller, hotter regions and (2) the linewidths (and thus the ability to resolve more and weaker lines) could be narrower because the beam would average turbulence and other relative motion over smaller regions. Additionally, the larger S/N would often drive the astronomical spectra to the noise free, spectroscopic confusion limit.

In this paper we will (1) very briefly review our general strategy and laboratory procedures, (2) consider the ALMA spectrum from a single pixel of the Science Verification data, (3) show a comparison between the ALMA data and simulations based on very simple models, and (4) consider straightforward extensions to these simple models.

2. Background

We have previously described the spectroscopic methods and procedures used to generate CES across broad spectral regions in the mm/submm as a function of temperature [17–19].

2.1. Analysis

For each species and spectral region, we first selected 50–200 assigned lines that are included in the QM catalogs [11,12] to use as intensity references. With the strengths $S_{ij}\mu^2$ and lower state energy levels E_l (from the QM analyses) and Doppler widths $\delta\nu_D$ and line frequencies ν_0 (from the temperatures and measured frequencies from the experiment), we fit the measured peak absorbance of these reference lines to

$$A_{\text{peak}} = L\alpha_{\text{peak}}(T) = \frac{nL}{Q}\frac{8\pi^3}{3ch}(1-e^{-h\nu_0/kT})S_{ij}\mu^2 e^{-E_l/kT}\sqrt{\frac{\ln(2)}{\pi}}\frac{\nu_0}{\delta\nu_D} \quad (1)$$

to obtain the spectroscopic temperature T and nL/Q for each of the 100–1000 spectra of varying temperature. Here n is the number density, L the effective path length, and Q the partition function. Because we use this equation not only for the determination of T and nL/Q but also inversely for the calculation of the simulated spectrum, errors associated with linewidths and other systematic experimental errors cancel.

Although we originally used an inversion of Eq. (1) to calculate the line strengths $S_{ij}\mu^2$ and lower state energy levels E_l for the many experimental lines not in the QM catalog, we have more recently first processed the data without the identification of individual lines in the spectra. This analysis predicts the spectra as a function of temperature on a frequency point-by-point basis.

The Doppler width (HWHM) is given by

$$\delta\nu_D = \sqrt{\frac{2N_a k\ln(2)}{Mc^2}}\sqrt{T}\nu_0 = W\sqrt{T}\nu_0 \quad (2)$$

and the absorbance *as a function of frequency* can be rewritten as

$$A(\nu) = \frac{8\pi^3}{3ch}\sqrt{\frac{\ln(2)}{\pi}}\frac{nL}{Q}\frac{\nu_0(1-e^{-\frac{h\nu_0}{kT}})}{\delta\nu_D}S_{ij}\mu^2 e^{-\frac{E_l}{kT}}e^{-\ln(2)(\frac{\nu-\nu_0}{\delta\nu_D})^2} \quad (3)$$

where N_a is Avogadro's number, and M is the molecular mass. The absorbance normalized by the nL/Q factor becomes

$$\begin{aligned}\frac{A(\nu)}{nL/Q} &= \frac{8\pi^3}{3ch}\sqrt{\frac{\ln(2)}{\pi}}\frac{1}{W}\frac{(1-e^{-\frac{h\nu_0}{kT}})}{\sqrt{T}}S_{ij}\mu^2 e^{-\frac{E_l}{kT}}e^{-\frac{\ln(2)}{W^2T}(1-\frac{\nu}{\nu_0})^2}\\ &= K\frac{(1-e^{-\frac{h\nu_0}{kT}})}{\sqrt{T}}\tilde{S}_{ij}\mu^2 e^{-\frac{\tilde{E}(\nu)}{kT}} \quad (4)\end{aligned}$$

with

$$\tilde{E}(\nu) = E_L + k\frac{\ln(2)}{W^2}\left(1-\frac{\nu}{\nu_0}\right)^2 \quad (5)$$

In Eq. (4) every frequency slice of the data ($\sim 2\times10^6$ frequency points at each temperature) is represented by two parameters $\tilde{S}_{ij}\mu^2$ and $\tilde{E}$. On line center $\tilde{E}$ is the lower state energy and $\tilde{S}_{ij}\mu^2$ corresponds to the line strength. Off of line center, the meanings of $\tilde{S}_{ij}\mu^2$ and $\tilde{E}$ are less physical, but Eq. (4) is still a valid fitting function for describing the spectral intensity. To present these data in the usual astrophysical catalog format, we simply use a peak finder to identify the lines and catalog the on-line-center values of $\tilde{S}_{ij}\mu^2$ and $\tilde{E}$.

3. Comparison of laboratory and ALMA spectra

The hot core of Orion KL (R. A. = 05 h 35 m 14.35 s, Dec = −05°22′35″ (J2000)) [20] was chosen as one of the targets of ALMA's Science Verification program for Band 6 (211–275 GHz) [21] because it is one of the most studied molecular sources and one for which a number of spectral surveys exist for comparison [22–25]. Preliminary data for a single pixel (of a 1024 × 1024 array of pixels) centered on the hot core of Orion KL have become available and it is these data that we use in this work.

In this section we will consider how well simple models based on CES can simulate this ALMA spectrum for a number of the astrophysical 'weed' molecules. Issues that are addressed include the completeness of the laboratory spectroscopic basis in the context of this real astrophysical example and how well the simplest LTE models of the interstellar medium can account for the astrophysical spectrum.

While it is possible to do numerical fits of the CES simulations to the ALMA spectrum (in a similar fashion as in our laboratory fits to determine nL/Q and T, but with additional consideration of lineshapes and optical depth) to determine astronomical column density and temperature, we have chosen not to do so in these preliminary results. It will be especially interesting to see the statistical results of such analyses, especially in regards to the detection of species with many weak lines.

3.1. How complete are astrophysical catalogs?

We have previously asked the question, "How complete are astrophysical catalogs?" and have answered this question experimentally by sorting both synthetic spectra based on the QM catalogs and experimental spectra according to intensity [26]. Fig. 1 reproduces two of these comparisons at 300 K. The location of the divergence between the QM and experimental results in these plots can be quantitatively calculated and is related to the first unassigned vibrational state for each molecule. We have calculated the location of this point as a function of temperature for a number of species. These results are shown in Fig. 2. At the 190 K used in this paper for the simulations of ethyl cyanide, vinyl cyanide, and