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NSF and NASA Support for Laboratory Measurements Associated with Spectroscopic Observations using ALMA, Herschel, and the Great Observatories

Summary

Spectroscopy is an extremely powerful and fundamental tool for astronomy. It provides unique information on the composition of, and physical conditions in objects ranging from planetary atmospheres to distant galaxies. The most fundamental aspect of astronomical spectroscopy is the ability to identify spectral lines of gas phase molecules and features produced by small particles (dust grains). Having pushed into the infrared with unprecedented sensitivity and good spectral resolution, the Spitzer Space Observatory has been dealing with lack of laboratory data with which to identify observed spectral features in the Milky Way and external galaxies. The James Webb Space Telescope (JWST) will face this same problem. The ground-based Atacama Large Millimeter Array (ALMA) and the Herschel Space Observatory, two new facilities coming on line by the end of this decade, will operate in the submillimeter range of the electromagnetic spectrum, where a host of molecular emission lines are potentially powerful probes. Existing laboratory data are extremely sparse and will surely be inadequate to deal with the thousands of spectral lines that will be observed in star-forming molecular clouds as well as protostellar disks.

It is thus of great urgency that the NSF and NASA work together to develop a program to support critical laboratory astrophysical measurements that will be required for these new observatories, as well as for Spitzer and JWST. Given that ALMA is the largest project ever funded by NSF, and that Spitzer, Herschel, and JWST represent a major fraction of NASA's investment in astrophysics, it is evident that the issue of lack of laboratory data cuts across agency lines. We thus feel it is appropriate and timely that an interagency program be set up to fund laboratory spectroscopy and other studies including collision and reaction rate measurements necessary to maximize the scientific return from these ground and space-based astronomical facilities. This should be a competitive program, which can draw on the talents and use the facilities already in place, as well as train students and develop new facilities to carry out an ongoing program of laboratory research which will be of enormous value to a very broad scientific community.

Spectroscopic Focus and Data Requirements

Like any astronomical measurement, spectroscopy is dependent on telescopes to collect signals, and detectors to measure them. The additional feature is the spectral resolution, Δf, which expressed as a fraction of the observing frequency f, can range from $f/\Delta f$ equal to a few hundred for IR grating spectrometers on Spitzer, to 10^7 for the HIFI heterodyne instrument on Herschel. The different spectral resolution is connected with the type of spectral features being emphasized for study: solid state features are well adapted to low resolution, broadband spectroscopy, while the highest spectral resolution available is used to study the motions of gas phase molecules in quiescent pre-stellar cores. The type of observation and resolution are connected to the type of laboratory data required for exploitation of the different types of spectroscopy.

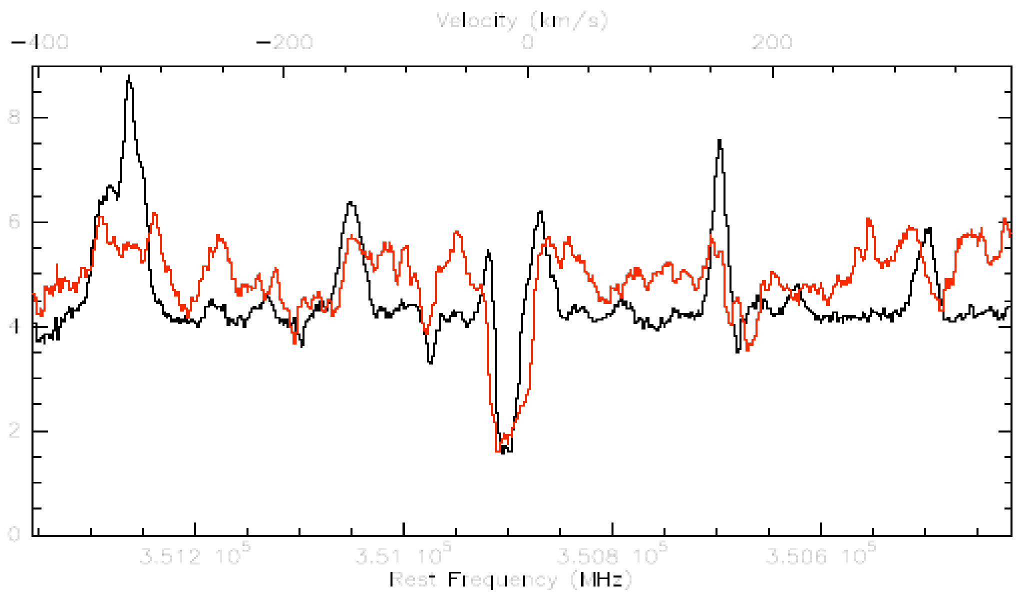
To exploit the spectral features produced by interstellar dust grains, laboratory data is needed for a large variety of candidate materials, which can exist in various mixtures, three dimensional structures, and for very small grains, ionization states. For gas phase molecular spectroscopy, the number of species detected in interstellar clouds exceeds 120 (not including isotopically substituted variants). Each of these needs very high precision spectra from cm wavelengths to the infrared. A frequency error of 1 MHz corresponds to a velocity error of 0.3 kms^{-1} at a frequency of 1 THz (where ALMA and HERSCHEL will be observing), which is significant for searching for infall motions associated with the early phases of star formation. These considerations have a major impact on the laboratory data needed and on the laboratory equipment required to obtain it.

Existing Databases

A variety of databases exist covering different spectral regions, having different degrees of completeness, and with differing frequency precision. Atomic databases (e.g. NIST and Kurucz), which are relatively comprehensive for astronomical purposes, cover transitions in the UV, visible, and infrared regions. Organic compounds are included in a number of databases which include gases, solids, and liquids, but mostly at relatively low spectral resolution. The infrared region is covered by databases including HITRAN, GEISA, HITEMP, ATMOS, and others. However, these focus on molecules of interest for atmospheric modeling and have moderate spectral resolution. When we get to the submillimeter region and demand high spectral resolution, there are really only two substantial catalogs, the JPL Submillimeter, Millimeter and Microwave Spectral Line Catalog and the Cologne Database for Molecular Spectroscopy. Even these, which include several hundred molecular species, have major deficiencies, particularly in the areas of ro-vibrational transitions, isotopically substituted species, and rotational transitions in excited vibrational states. In addition, the data available for many molecules which have already been observed to be abundant in warm, dense interstellar clouds are inadequate for much of the submillimeter region. The accuracy of line frequencies extrapolated from existing lower frequency measurements is simply not good enough for Herschel HIFI and ALMA, in particular. The shorter wavelength data available have proven incomplete for identification of spectral features observed by Spitzer, so that it is clear that a major effort is necessary to obtain laboratory data for these facilities, and for JWST as well.

The Challenge of ALMA and Herschel

In part because they have the highest spectral resolution, and because they operate in the relatively unexplored submillimeter spectral region, ALMA and HERSCHEL face particularly severe challenges in terms of laboratory data required to exploit the spectra they will obtain. The spectroscopy of many of the already-detected species in the submillimeter region is not understood. Consequently, the observer will be faced with a plethora of unidentified lines, which can be considered to be "contaminants" if one is trying to study a particular species which is being used to trace temperature, density, ionization, and other physical parameters. An example is shown in Figure 1, which plots spectra taken at the Caltech Submillimeter Observatory at two positions in the SgrB2 molecular cloud (indicated by two different curves) at a frequency near 350 GHz (spectra provided by Dr. D. Lis, Caltech). It is immediately evident that this range, which is less than 100 MHz wide, has tens of spectral lines which certainly can be identified, and that as one goes to weaker and weaker lines, it becomes almost impossible to distinguish between "real" spectral features and noise. It is clear that to fully utilize this type of data, the strong lines must all be known so that they can be 'removed', in order that the weaker features can be unambiguously identified and studied.



Thus, we can enumerate several steps that need to be taken regarding these species, considering for the moment only the issue of spectral line calculations.

- Identify common "contaminant" molecules, such as methanol and ethyl cyanide.
- Obtain laboratory data for these species which must be good to very high rotational quantum numbers and include vibrationally and torsionally excited states of abundant species such as CH_3CN and CH_3CH_3CN.
- Very high frequency accuracy must be maintained on lines used to study kinematics of cold objects.

- Make predictions covering the submm range for all known species having transitions of reasonable strength. This should include excited torsional states of internal rotors and some electronic transitions (C_3H).
- Measure “hot bands” of simple species likely to be observed in extreme environments around young stars, e.g. H_2O, HCN, HC_3N,…
- Measure submillimeter spectra of diatomic molecules known in stellar atmospheres.

This is obviously a major challenge. But in fact this addresses only the measurement aspect of the problem. To really “solve” a single species requires a number of steps

1. Ab initio calculation of dipole moments and moments of inertia
2. Laboratory measurements from microwave through submillimeter range
3. Fitting theoretical model for molecular structure to observed spectra to obtain as complete a set of accurate predicted line frequencies and intensities as possible
4. Catalog results and integrate into existing data base.

Each of the above four steps is an important and legitimate activity in support of these major new ground- and space-based facilities. Consequently, a funding program should allow people to propose for the most critical aspects of any of these four steps.

Program Concept

As indicated above, NASA is making major investments in new space observatories, especially covering submillimeter and infrared regions of the spectrum. NSF, together with international partners, is developing the ALMA array which will observe at millimeter and submillimeter wavelengths. Compared with the situation at optical and shorter wavelengths, the lack of laboratory data is more dramatic, in part because both ALMA and Herschel HIFI have exceptional spectral resolution in a relatively unexplored spectral regime. However, ongoing observations with the Spitzer Space Observatory Infrared Spectrometer (IRS) also indicate significant gaps in laboratory data. The NIRSpec instrument on JWST will likely also reveal new spectral features that demand laboratory work for identification.

Spitzer is currently operating extremely well. The Herschel Space Observatory is expected to be launched in 2008, and ALMA will gradually ramp up towards the end of the decade. The launch date for JWST is currently 2013. Thus, while there is clearly work to be done in support of JWST spectroscopy, the schedule is considerably less pressing than for Spitzer, Herschel, and ALMA. We thus envision a program that will initially be focused on solid state spectroscopy relevant to Spitzer and Herschel (low resolution instruments), and primarily gas phase molecular spectroscopy in support of Herschel HIFI and ALMA.

There are facilities for millimeter and submillimeter spectroscopy at several institutions in the United States, covering different frequency ranges with different capability. There are also groups capable of carrying out various quantum mechanical calculations necessary to model molecular structure and interactions. There are also individuals with expertise in analysis of molecular data, and capability of working on database issues associated with spectroscopy of gas phase and solid state features. All of these individuals, groups, and institutions can contribute to gathering, analyzing, and cataloguing molecular data in support of the new astronomical facilities. We thus feel that the best method to get the job done is for NSF and NASA to support a joint funding effort. A small number of individuals from within the agencies and in the community could structure the program to make sure that the research topics are consistent with the most urgent needs. As time goes on, this group could also monitor new proposals and awards to ensure that there is no duplication of effort, and that the most important issues are being addressed. We estimate that with a funding level of $500,000 per year, an appreciable fraction of the most important molecules and solid state features can be addressed over a five year period. It may be possible that some of the most critical problems in collisional and chemical reaction rates can also be addressed, but making a major inroad on these would require approximately twice this funding level.

Most of the laboratory measurements that will be carried out as part of this effort would not, on their own, qualify as being of major interest purely from the point of view of quantum chemistry or molecular dynamics. However, they are of the utmost importance for being able to exploit new astronomical facilities in which billions of dollars will have been invested. Thus, the critical issue is to define the criteria for successful proposals to this program as how they will enhance the scientific return of major ongoing and upcoming space- and ground-based missions. There does not appear to be a need to have a new program set up to address this need; there exist programs within both NSF and NASA which can support this laboratory research. What is really essential is the recognition of the importance of this type of work, and the evident scientific return that it will provide for a miniscule fraction of the facility cost.