REPORT FROM THE WORKSHOP ON LABORATORY SPECTROSCOPY IN SUPPORT OF HERSCHEL, SOFIA, AND ALMA

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EXECUTIVE SUMMARY

The goal of this Submillimeter and Far-Infrared Laboratory Spectroscopy Workshop was to develop a plan to deal with the harmful effect of spectral line confusion on the scientific return from the Herschel Space Observatory, the Stratospheric Observatory for Infrared Astronomy (SOFIA), and the Atacama Large Millimeter Array (ALMA). These major new facilities will open up the submillimeter region of the electromagnetic spectrum by making investigations of unprecedented high sensitivity and angular resolution possible. Much of the scientific interest will be in observations of spectral lines. For observations of the dense regions in which star formation occurs, the youngest stars and the proto-planetary disk material surrounding them possess spectra containing a few molecular species with extremely numerous, relatively strong transitions throughout the submillimeter. These species are likely to present a serious challenge, in as much as their emission will occupy a substantial part of the spectral range available, thus impeding the study of other important species. Thus, the discovery of new species of astrophysical and astrobiological interest will be severely hampered unless the spectral lines from these "weeds" can be removed from the data.

We have identified the most offensive weeds, which include six species plus their isotopically substituted variants. We propose that one (or ideally several) spectroscopic laboratories in the US be equipped with sources and detectors to cover the frequency range up to 2 THz, and that they each be funded to hire personnel to actively engage in a program of measuring the spectra of these weed species over a 2 to 3 year period from the present until the first Herschel data are available. Using a combination of traditional quantum state assignment and novel techniques involving measurement and classification of spectral lines measured at different temperatures, the data necessary to remove the weeds from astronomical spectra can be made available. Ongoing measurement and analysis efforts will be required to complete the process for ALMA, SOFIA and other submillimeter facilities.

1. THE NEW SUBMILLIMETER FACILITIES

Laboratory data form the basis for almost all astronomical investigations, but particularly for the study of star formation. The regions in which this important process occurs are studied in the spectral lines of a variety of molecular species. Many of these, at the temperature and densities of star-forming regions, have their most important transitions in the submillimeter range, which includes wavelengths between 1 mm and 0.1 mm. Given the great interest in studying star formation and the vast areas of spectral coverage, angular resolution, and sensitivity discovery space that will be opened up by Herschel, SOFIA, and ALMA, it is expected that these facilities will be used by astronomers with a wide range of expertise outside submillimeter spectroscopy. For these scientists, unidentified interfering spectral lines will be an especially vexing problem. Maximizing the overall return from submillimeter observations thus requires a community-based solution to this problem.

The three new facilities indicated above will all observe in the far-infrared and submillimeter spectral range. Herschel will observe from space, ALMA will operate from an extremely dry mountain location, and SOFIA will take data from the stratosphere – all in order to minimize absorption by species in the earth's atmosphere. SOFIA is expected to begin scientific operation in 2010 with a 20 year lifetime, ALMA will start full science operation in 2011 with a lifetime of many decades, but Herschel, scheduled for launch in 2008, will have a lifetime of only 3 to 4 years. Thus, dealing with submillimeter weeds is of greatest urgency for Herschel, both because it will be the first to be in operation, and because of the very limited opportunities to adjust observing strategies to deal with spectral confusion. It is of the utmost importance to deal with the most deleterious weeds affecting Herschel within the next 2-3 years, while establishing a longer term plan to improve general submillimeter spectroscopic knowledge.

2. DEFINITION AND IDENTIFICATION OF SUBMILLIMETER SPECTRAL WEEDS

The participants at the workshop agreed on the following characteristics of a "weed" for working purposes as a species with:

1. a relatively high abundance compared to that of H_2, on the order of $\sim 10^{-7}$
2. a dense rotational emission spectrum
3. an association with regions between 100 and 300 K
4. saturated bonds
5. a large moment of inertia and/or associated with internal degrees of freedom such as torsion
6. low-lying vibrational states
7. a spectrum that is particularly difficult to predict.

These characteristics collectively indicate that the species in question will have numerous, relatively strong transitions throughout the submillimeter frequency range in regions associated with star formation. Characteristics 5 and 6, in particular, explain why it is difficult to predict theoretically the frequencies of transitions of weeds with the accuracy of better than 1 MHz required for high-resolution submillimeter spectroscopy. The accuracy of extrapolations based on transitions measured at longer wavelengths rapidly deteriorates as one moves into the submillimeter, and there is thus no substitute for laboratory measurement of the species in question in the wavelength range of interest.

Given these characteristics, the panel identified the three most prominent (Class 1) weeds. They are CH_3OH (methanol), $HCOOCH_3$ (methyl formate), CH_3OCH_3 (dimethyl ether),CH_3CH_2CN (ethyl cyanide), and their isotopologues. Five somewhat less prominent (Class 2) weeds are C_2H_3CN (vinyl cyanide), SO_2 (sulfur dioxide), CH_3CN (methyl cyanide), HC_3N (cyanoacetylene), and CH_3CHO (acetaldehyde). According to the URL of Lovas, these species possess approximately half of the identified interstellar lines emanating from cold and hot portions of interstellar clouds through 700 GHz. Since many of the lines of the non-weeds arise from cooler portions of the interstellar medium, the effect of weeds on warmer regions is likely to be even greater.

Together, the spectra of these species have a major impact on ground-based submillimeter spectra obtained to date with single dish telescopes in surveys of modest sensitivity. These prominent weeds will certainly have a much greater impact on higher sensitivity and higher angular resolution studies that will be made with the next generation of submillimeter facilities. However, we should emphasize that the list above is certainly not a complete catalog of weeds, and that if additional resources and effort are available, there are undoubtedly others for which additional laboratory spectral studies would be very valuable. The above list of weeds, which itself comprises many more species due to the need to study the ^{13}C, ^{18}O, and D – substituted variants, includes just what we judge to be the most offensive species on which additional work is most urgently required. At least as significantly, most of the many U lines currently observed (more than 40% of the total in a recent IRAM survey near 1 mm) presumably are due to low lying vibrational and torsional states. Each species and each isotopic variation has a number of these states and each has its own rotational spectrum, thus *multiplying* the above assignment and analysis work by a significant factor. In addition, there are species that are of particularly great astronomical interest (which we might call "flowers") for which additional spectroscopic studies should be carried out so that their submillimeter transitions can be identified with confidence. This work is also critically deserving of support to maximize the scientific return of the new submillimeter facilities.

3. DEALING WITH THE WEEDS: THE CHALLENGE AND PROPOSED SOLUTION

The challenge posed by even this relatively restricted set of species is great. This is because the frequency range of interest is very wide (0.4 to 2 x 10^{12} Hz or λ = 0.75 to 0.15 mm) and the spectrum of each species must be measured with a spectral resolution of better than 1 MHz over this entire frequency range. We propose a technical solution having two major components.

The first is to obtain the entire laboratory spectrum of each weed. The major obstacle here is that there is at most one laboratory in the world equipped to cover this entire frequency range, and even then collecting the entire spectrum would be prohibitively expensive in terms of time and effort. There are, however, a number of spectroscopic laboratories in the United States that, if equipped with new source technology and detectors covering the submillimeter range of interest, could participate very effectively in obtaining the data needed. We thus feel that the initial step should be for these several laboratories to commit to this program, and then to be funded to acquire the required equipment. This must be followed by support for personnel to operate the spectrometers and collect and analyze the data. There are laboratories in Europe, Canada, and Japan that can potentially make significant contributions to this effort. We will support their efforts to obtain funding for equipment and personnel to join in this task. There is sufficient work to be done that if they are able to join the effort, a larger number of weeds can be characterized, more isotopologues can be studied, and the overall goal can be achieved sooner.

The second component of the solution is to analyze the spectroscopic information obtained through the efforts described above. We feel this can be accomplished with a two-pronged approach. The first prong is the assignment of quantum numbers to the levels of a given transition observed. This is an exceedingly time-consuming task since the weeds have thousands to tens of thousands of transitions within the submillimeter range of interest. Dealing with the entire spectrum will allow infrared techniques to be exploited in the submillimeter potentially greatly improving efficiency, but this will require a learning curve and development of software tools. As a result, this task most likely will not be completed before the Herschel launch, but is of great value. Furthermore, it must be carried out to some extent for the second prong of the approach which is to utilize intensity calibrated spectroscopy as a function of temperature. In this approach the entire spectrum is collected at multiple temperatures and compared with known calibration lines allowing the line strengths and energy levels to be determined. This technical solution requires relatively rapid data collection since the entire spectrum must be collected multiple times over temperature. It must be stressed that there are a number of technical innovations that are still being developed for the millimeter range which must be made to work well in the submillimeter to achieve the desired result.

An example of this type of spectroscopy is FASSST, an acronym for FAst Scan Submillimeter-wave Spectroscopic Technique, developed by Dr. F. De Lucia. FASSST or equivalent techniques such as FMSS (Frequency Multiplication Submillimeter Spectrometer) developed by Drouin and Pearson, yield the line strengths and upper and lower state energies of unassigned lines; i.e., those without assignment of quantum states. This will suffice to predict the weed spectrum for a specific model of an interstellar star-forming cloud, but this approach requires cross checking with assigned transitions, which is why the first prong of the solution must proceed in parallel with the second. Completion of the assignment of all quantum states, which is important for full understanding of the molecule's spectroscopy and structure, will plausibly follow.

It is critical to the success of this endeavor that the different laboratories maintain good communication with each other, in order to avoid duplication of effort, and to benefit from lessons learned in the limited time available. The different groups should also ensure rapid and wide dissemination of intermediate products, such as spectral atlases, as well as final products that will go into spectral line catalogs. While we do not propose a specific organizational structure for this effort, it does appear that the relevant groups are ready and willing to cooperate in pursuit of this important goal.

At present, it is not possible to make a precise determination of the funds required, but we have endeavored to make a reasonable estimate. At minimum, it is essential that at least one laboratory be equipped to carry out measurements throughout the Herschel spectral range. We estimate this cost to be $250,000 to $400,000 for a single lab. Obviously, having a full frequency capability in additional labs would both accelerate the generation of the needed data, and perhaps allow time for cross-checking the results. This would cost between $400,000 and $800,000. The cost of the personnel to fully utilize this new equipment is estimated to be between $200,000 and $300,000 per laboratory per year. This number includes funding for a graduate student, a postdoc, and minimal funding for the P.I., together with standard additional costs, fringe benefits, and indirect costs. Assuming that three laboratories are involved, the personnel cost would be between $600,000 and $900,000 per year for a minimum of three years. It is very important that a commitment to multiyear funding be obtained, since otherwise it will be extremely difficult to attract the skilled individuals required.

There are a number of possible funding mechanisms that must be explored to find the funding to solve the submillimeter spectral weed problem. We must investigate cross-agency funding, given that the new facilities are supported by the National Science Foundation (NSF) as well as by NASA. There may be some funds available in instrumentation programs that could be of relevance here. We will also work to encourage support for solving this problem on an international basis given that the three new facilities have involvement from Europe and Japan, as well as from North America. It is possible that a fraction of the Guest Observer funds for the Herschel Project can be made available to scientists proposing to attack this problem. This is similar to previous NASA funding of theory and laboratory astrophysics of importance for the Spitzer mission, but has the difficulty that these funds become available only after launch, which is too late to be starting to solve the problem. An initial attack on the weed problem in the very near future is required, although it could make a transition to support from the Herschel project at a later date. It is also possible that the NSF, either directly through the grants program, or through NRAO and the ALMA project, could contribute to support this vital laboratory spectroscopic effort.

A more complete understanding of the line confusion problem afflicting Herschel, SOFIA, and ALMA will permit users to extract the maximum exciting science from these new facilities. It will also produce spectroscopic results of importance in their own right for understanding the structure of complex, important molecular species. Finally, it will be making an important step towards training the next generation of spectroscopists with state-of-the-art equipment covering a relatively unexplored range of the spectrum.

4. RECOMMENDATIONS

1. The issue of spectral line confusion in the submillimeter spectral range from lines of "weed" species is an issue of immediate concern for Herschel, SOFIA, and ALMA, and should be recognized as such. A program to accurately measure the frequency of the weed transitions to enable their proper identification and removal from astronomical spectra is essential for obtaining the maximum scientific output from these new observatories.

2. We have identified a relatively small number of molecular species that are the worst offenders, but include their isotopic variants and many vibrational states. Measuring the transitions of the three Class 1 weeds and the five Class 2 weeds throughout the submillimeter to the required accuracy of better than 1 MHz is a significant task.

3. By using a combination of novel measurement techniques and traditional level assignments, it is possible to make significant progress in attacking the weed problem before the first Herschel data are available, but only if a start is made in the immediate future.

4. We have estimated the cost ($250,000 to $800,000) to equip spectroscopy laboratories for this task, and for the labor ($600,000 to $900,000 per year for a minimum of 3 years) to take and analyze the relevant data, and provide it to molecular line databases.

5. A variety of funding approaches must be investigated given the broad impact of the weed problem. The community must work with US funding agencies as well as with international collaborators to ensure a successful solution of this important problem, as well as measurement of transitions of astronomically important flower species.

Panel Members of the Laboratory Workshop on Submillimeter Spectroscopy in Support of Herschel, SOFIA, and ALMA on behalf of the workshop participants

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