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THz Spectroscopy and Spectroscopic Database for Astrophysics

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ABSTRACT

Molecule specific astronomical observations rely on precisely determined laboratory molecular data for interpretation. The Herschel Heterodyne Instrument for Far Infrared, a suite of SOFIA instruments, and ALMA are each well placed to expose the limitations of available molecular physics data and spectral line catalogs. Herschel and SOFIA will observe in high spectral resolution over the entire far infrared range. Accurate data to previously unimagined frequencies including infrared ro-vibrational and ro-torsional bands will be required for interpretation of the observations. Planned ALMA observations with a very small beam will reveal weaker emission features requiring accurate knowledge of higher quantum numbers and additional vibrational states. Historically, laboratory spectroscopy has been at the front of submillimeter technology development, but now astronomical receivers have an enormous capability advantage. Additionally, rotational spectroscopy is a relatively mature field attracting little interest from students and funding agencies. Molecular data base maintenance is tedious and difficult to justify as research. This severely limits funding opportunities even though data bases require the same level of expertise as research. We report the application of some relatively new receiver technology into a simple solid state THz spectrometer that has the performance required to collect the laboratory data required by astronomical observations. Further detail on the lack of preparation for upcoming missions by the JPL spectral line catalog is given.

1. Introduction

The first step in the interpretation of any spectroscopic astronomical observation is to identify the carriers of the emission or absorption features present. Identification has proven to be a challenge in all wavelengths. Atomic and Molecular Line catalogs provide the astronomical community with a tool to assist in the identification of spectral lines or bands. Any further interpretation of the identified lines for chemical, physical and energetic conditions requires more laboratory data including line strengths, energy levels and collision excitation cross sections. The energy levels, line strengths and cross sections are all input parameters for radiative transfer and collisional excitation models. The models and underlying molecular data enable the molecular abundances and physical conditions of the astrophysical object to be derived. Once this is done, the chemical evolution can be extracted by modeling the observed abundances. The existence of more than 130 different molecules and numerous isototopically substituted variants makes ready access to molecular data mandatory whenever there is astronomical spectroscopy.

The more than 130 different known astrophysical molecules have provided a unique picture of the current state-of-the-art in molecular physics. For diatomic molecules, there are neutrals, radicals and ions with fine structure, hyperfine structure and spin-orbit effects. Many of these molecules provide examples of interacting electronic bands. In addition to displaying all the effects seen in diatomics, the astrophysical triatomic molecules feature case studies in non-rigidity and interactions between vibrational states (e.g. H_2D^+, D_2H^+, H_2O^+, CH_2, NH_2, H_2O). The symmetric top molecules with three hydrogen atoms in the top (e.g. NH_3, H_3O^+, CH_3CCH, CH_3CN and CH_3NC) all eventually suffer from breakdown of separation of rotation and vibration higher K quantum numbers. Internal rotation theory, as it is known today, was developed to analyze the spectra of CH_3OH, CH_3CHO and CH_3COOH. What is known about two top internal rotors (e.g. CH_3OCH_3, CH_3COCH_3) was largely developed to support astronomy. Additionally, there are a number of known astrophysical molecules that are still at the cutting edge of molecular physics. These include extreme cases of non-rigidity (e.g. NH_2, CH_2, H_2O and H_2O^+), vibration-torsion interactions in three fold internal rotors (e.g CH_3OH and CH_3CH_2CN), Asymmetric-top asymmetric-frame internal rotation (e.g. CH_2DOH and CH_3CH_2OH) and coupling of multiple large amplitude motions (e.g. CH_3NH_2, CH_3CH_2OH, and CH_2DOCH_3).

Rotational spectroscopy, unlike infrared or optical spectroscopy, has historically only measured a few transitions with high accuracy due to technical limitations. The rest of the spectrum is determined by fitting a molecular model to the data. This process can have a number of serious limitations that depend strongly on the quality and range of quantum numbers and energy levels in the data set. As a result of the complexity of the molecular physics and the limitations of most molecular data sets, significant expertise is required to calculate and understand the spectra for most of the known astronomical species. Catalogs are necessary since accumulation of all the existing data represents a lifetime of work. The JPL Microwave, Millimeter and Submillimeter Spectral line Catalog (Pickett et al. (1998))

was created to be a repository of rotational molecular data for atmospheric chemistry and astrophysics. For the last 6 years only the atmospheric chemistry portion has been funded and regularly updated. The Cologne Database for Molecular Spectroscopy CDMS (Müller et al. (2005)) was created using the same approach and programs for molecular analysis. CDMS has filled in many missing species and updated a number of older entries with newer data, but even when combined, these database fall well short of what is ultimately need to support the astrophysical need of Herschel, SOFIA and ALMA.

2. Instrument Capability And Data Limitations

The Herschel Space Observatory, SOFIA and ALMA represent several billion dollars of investments by ESA, NASA and the NSF in far-infrared astronomy. A suite of extremely powerful spectroscopic instruments is planned for these missions primarily to study gas phase molecular emission and absorption in unprecedented detail. The bottom line is high resolution spectroscopy $R > 10^6$ will now be possible to 5 THz and $R = 5\text{x}10^5$ will be possible over the 5-28 μm region as well. ALMA will not suffer from the beam dilution that limits most single dish instruments, allowing it to observe and even image the most dense and highly excited astronomical regions to 950 GHz. Additionally, the instruments on Herschel, SOFIA and ALMA have wider instantaneous bandwidths allowing much more spectral coverage to be collected per observation. The improved technical capability of these instruments will result in spectra with thousands of molecular features. This results in an unprecedented need for larger quantum numbers, additional vibrational states and precise vibrational and torsional band spectra. Analyzing large line-confused observational data sets will require the underlying laboratory data to be accurate to 1/10 of observational resolution as well as available electronically for computer aided tools to assist in line identification.

The existing databases generally fill the needs for on line access, but a slightly closer examination of their contents relative to the rapidly approaching need results in some rather disturbing discoveries:

i Isotopic data is generally very limited if available at all.
ii There are few excited vibrational states (rotational hot bands).
iii Torsional or vibrational band data is nearly non-existent.
iv Many existing data sets end below 400 GHz and at small quantum numbers.

The implication of item $i - iii$ is there will be forest of U-lines with predictable intensity. Item *iv* emphasizes that the spectrum of many molecules with high abundance is unknown at the frequencies available to Herschel and SOFIA. The problem is already apparent at in 1-3mm spectral surveys where 1/3 of the lines are unassigned even though these are in the range of the existing data. The problem will be significantly worse for ALMA, Herschel and SOFIA where the consensus estimate above 800 GHz is that 80% of the lines will be initially unassigned at the line confusion limit.

A deeper investigation into the databases and available data results in a serious cause for alarm. The following has been noted:

i Many low J data sets are older and have systematic predictive errors.
ii There is little infrared data in the region below 400 cm^{-1} (12 THz).
iii Theoretical challenging species are in the worst shape.
iv There is no database of infrared or electronic transitions for astrophysical molecules.
v Very few of the potential discovery molecules are in catalogs (or have data).
vi Uncertainties generated in extrapolation are overly optimistic.

i) results in molecular data that is often too poor for careful velocity studies. This causes confusing and erroneous results on cloud collapse and dynamics studies. Item *ii* amplifies the fact that little is known about the long wavelength bands of large molecules. Current constraints of theory are recognized in item *iii*. A complete lack of a catalog for infrared and electronic transitions of known astrophysical molecules is pointed out in item *iv*. This is absolutely crazy since the electronic bands will be seen in absorption if the dust is not optically thick. The implication of item *v* is Herschel, SOFIA and ALMA all sold discovery science as a fundamental reason for their existence, but discoveries cannot be made without laboratory data to identify the carriers of lines. Lastly, item *vi* results in any extrapolated line position being much worse than expected. Additionally, many astronomical molecules have pathologies, like internal motions and non-rigidity, which make extrapolation a non-linear problem compounding the estimated errors in ways that are not obvious.

Figure 1 compares the best available calculation of CH_3OCH_3 (in the JPL catalog) to a laboratory spectrum at 845 GHz. The strong Q-branch origin is off by about 100 MHz and deviates from the predicted shape at higher J. As a result, it would be difficult to assign this in an astronomical spectrum and the band could easily be attributed to a PAH. The HCO^+ molecule, which has been called "the most stable molecule in the Universe", provides a second example. The ground state has been studied with microwave spectroscopy (Woods et al. (1975); Bogey et al. (1981); Sastry et al. (1981)) and laser sideband (van den Heuvel & Dymanus (1982)) to 1 THz and the three fundamental vibrational modes have been studied with infrared spectroscopy (Davies & Rothwell (1984); Kawaguchi et al. (1985); Davies et al. (1984,?); Foster et al. (1984); Gudeman et al. (1983); Amano (1983); Liu et al. (1988)). However, the available data failed to reproduce the observed transitions at 800 GHz within their error bars or 5 times the measurement uncertainty (Pearson & Drouin (2006)). Lastly there is no data on the electronic transitions. Given that HCO^+ is abundant in the diffuse ISM (Liszt & Lucas (1994)) and the only two recent diffuse interstellar band assignments were to a not very complex CH molecule (Watson (2001)), it is astonishing that the fundamental laboratory work remains to be done and that the lack of data is not glaringly apparent to those working in the field. Neither is the case primarily for lack of a comprehensive molecular database.

3. Current Status

The status of molecular databases for NASA astronomy is sad at best. In the optical there is no data base, in the infrared there is no database and in the far-infrared there has been no funding to support databases for the last 6 years. In Europe the situation is not much better with ESA recently retracting their commitment to support CDMS for the next three years, even though the Herschel observational planning tool uses the database. Virtual Observatories, Herschel, ALMA and SOFIA have all sought to address the problem, but so far there is no progress other than software to read what is already there into another data format. The recent Laboratory Astrophysics NRA calls explicitly solicit new research rather than data management efforts, so there has been no place to even apply for support. Unfortunately database preparation requires an enormous amount of experience and expertise that is generally easier to interested in doing research rather than community service. As a result, the only real solution is to pay for the database work to be done or to expect each astronomer to spend a significant amount of time maintaining their own data. From the point of molecular physics, it makes the most sense to collect all the available information together since vibrational and electronic spectra ultimately determine or use the rotational or obvious hot bands as a starting point. The combined approach requires more expertise and effort but it does allow for the known state of knowledge to be tracked.

It will require about 20-30 work years of effort catalog what is known about astrophysical molecules in the rotational, vibrational and optical. In just the rotational the known data could be completed in a 2-5 work years of effort. However, the existing data is not complete and a significant amount of new data will have to be generated to support observations additionally there are a wide range of molecules that are highly desirable to search for, which should be cataloged as well. Cataloging these results will require significantly more effort.

4. Conclusions

NASA, ESA and the NSF are spending billions of dollars building wonderfully powerful instruments with unprecedented exploration capability. Additionally similar sums of money are planned to support observations and data analysis, but there has been little thought or planning of the laboratory work and databases that will be required to support these missions. Currently database efforts are not funded and there is no mechanism to get funding within the current NASA NRA structure. NASA missions, Herschel and SOFIA, have explicitly been instructed not get into the laboratory astrophysics business and are not doing so. As a result, individual instrument users have one of three choices 1) propose only simple observations where the molecular physics is known e.g. CO, 2) Learn the molecular physics themselves and keep their own catalogs, or 3) not fully exploit the data and ignore the discovery potential of complex and potentially biogenic molecules.

The price of not funding a catalog effort is that NASA will have to provide larger grants for analysis of spectroscopic observations have fewer observers willing to perform spectroscopy and will ultimately be unable to optimally design the next generation of missions. Requesting individual missions to catalog 100 years of spectroscopy for their purposes is equally nearsighted, since molecules have spectral features at all wavelengths that do not dissociate them. Cataloging the rotational, vibrational and electronic bands simultaneously allows all wavelengths to benefit from investigations at other wavelengths and facilitates rapid updates when better laboratory data become available. Since this cuts across wavelengths and missions it only makes sense for this data to be provided as a service like catalogs of astronomical objects.

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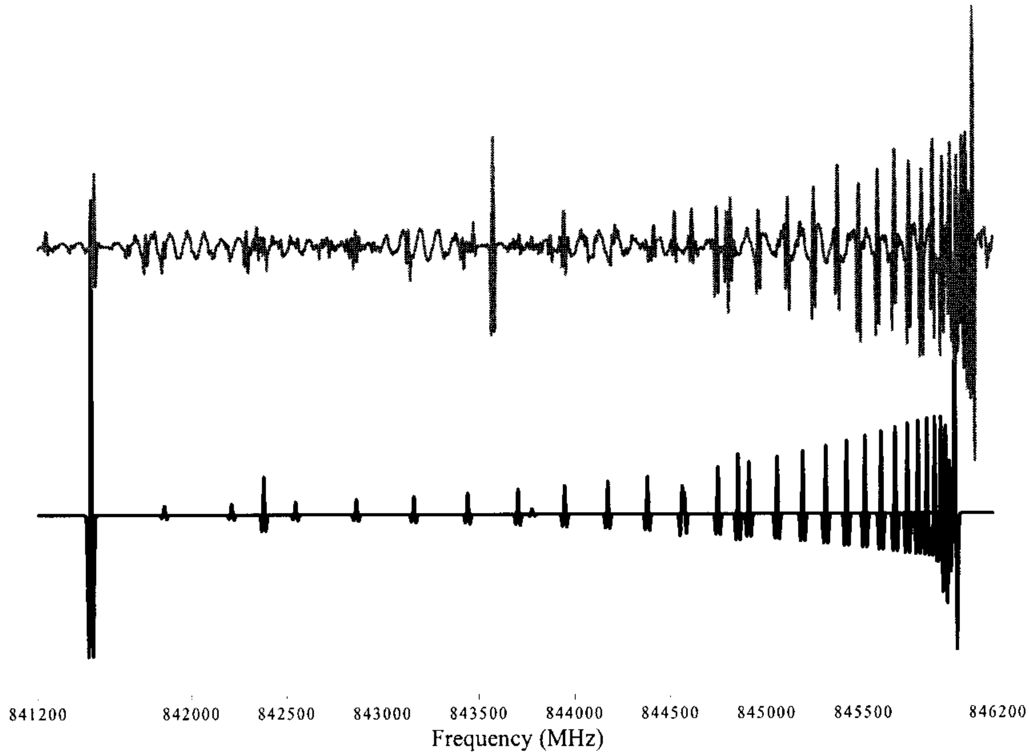

Fig. 1.— The second derivative laboratory absorption spectrum (grey) of dimethyl either (CH_3OCH_3) near 845 GHz compared to the JPL catalog prediction (black).

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