Microwave, Millimeter, Submillimeter, and Far Infrared Spectral Databases

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Abstract

The spectrum of most known astrophysical molecules is derived from transitions between a few hundred to a few hundred thousand energy levels populated at room temperature. In the microwave and millimeter wave regions, spectroscopy is almost always performed with traditional microwave techniques. In the submillimeter and far infrared microwave technique becomes progressively more technologically challenging and infrared techniques become more widely employed as the wavelength gets shorter. Infrared techniques are typically one to two orders of magnitude less precise but they do generate all the strong features in the spectrum. With microwave technique, it is generally impossible and rarely necessary to measure every single transition of a molecular species, so careful fitting of quantum mechanical Hamiltonians to the transitions measured are required to produce the complete spectral picture of the molecule required by astronomers. The fitting process produces the most precise data possible and is required in the interpret heterodyne observations.

The drawback of traditional microwave technique is that precise knowledge of the band origins of low lying excited states is rarely gained. The fitting of data interpolates well for the range of quantum numbers where there is laboratory data, but extrapolation is almost never precise. The majority of high- resolution spectroscopic data is millimeter or longer in wavelength and a very limited number of molecules have ever been studied with microwave techniques at wavelengths shorter than 0.3 mm. The situation with infrared technique is similarly dire in the submillimeter and far infrared because the black body sources used are competing with a very significant thermal background making the signal to noise poor. Regardless of the technique used the data must be archived in a way useful for the interpretation of observations.

The consequence to any archiving spectral database is that there is very limited high-resolution data available in the submillimeter and far infrared and the traditional infrared catalogs generally do not extend into the region. Additionally most astrophysical molecules are not very rigid further complicating the analysis and prediction of transitions. The JPL Submillimeter, Millimeter and Microwave Spectral line Catalog is an attempt to compile a complete and consistent set of spectroscopic data to support observations and observation planning.

1. Introduction

Atomic and molecular spectral line catalogs and databases facilitate the first step in reduction of astronomical spectra through the assignment of the observed spectral feature. The line strengths provided in many of the databases allows for determination of column density, effective temperature and when multiple transitions are observed the details on excitation conditions can be derived. The line shape allows for study of the local dynamics and provides some information on the line of sight. Since the molecular physics literature is well scattered in many journals and has many high quality publications prior to the electronic abstract data base searches of today. As a result, it is critical to collect, compile and catalog the existing data in a form convenient for interpreting astrophysical observations.

There are four basic types of databases available. The microwave catalog database is where a set of rotational measurements is combined with a molecular Hamiltonian in least squares fitting procedure to predict all the unmeasured transitions. The second type is an infrared catalog where complete sets of high-resolution, rotationally resolved, infrared measurements are cataloged. The third type is an infrared database where low-resolution infrared measurements give the band structure and intensity, but provide no line resolution. The final type of database is the atomic line catalog where the transitions and transition moments of atoms and highly ionized atoms are recorded.

2. Microwave Catalogs

Microwave, Millimeter and Submillimter spectral line catalogs have greatly aided astronomy in the radio through submillimeter spectral region. Four different catalogs have been assembled and two, which use the same format, are active. The two inactive catalogs are the NIST Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions (Lovas 1992) and the Smithsonian Astrophysical Observatory Database SAO92 (Chance *et al.*, 1994). The two active catalogs JPL Submillimeter, Millimeter and Microwave Spectral Line Catalog (Pickett *et al.*, 1998) and the Cologne Database for Molecular Spectroscopy (Muller *et al.*, 2001) both employ an analysis program written by Herbert Pickett (1991). The use of one program to analyze the molecular data provides a consistent data format in a machine-readable form. It also assures the spin statistics, partition functions and line strengths are calculated in a consistent way. Combined there are over 150 molecules cataloged, however, this is only a subset of approximately 130 known interstellar molecules and both catalogs are very short on isotopic species and rotational states of vibrationally excited states. Additionally there are very few potentially detectable molecules and no attempt has been made to catalog the ro-vibrational or ro-torsional transitions sure to be observed in the far infrared.

3. Infrared Catalogs

Several infrared catalogs have been assembled, mostly to support atmospheric chemistry studies. These catalogs include HITRAN and HITEMP (Rothman *et al.*, 1998) and GEISA (Jacquinet-Husson *et al.*, 1999). Additionally a calibration catalog with heterodyne measurements in the infrared is maintained by NIST (Chu *et al.*, 1999). In these cases the number of species is rather limited with 37 molecules in HITRAN and HITEMP, slightly more than 40 molecules in GEISA and 5 molecules in NIST Wavenumber Calibration Tables from Heterodyne measurements. These catalogs are limited below 500 wavenumbers, generally only including microwave data. They are rotationally resolved, have measured line and band strengths and are generally accurate to 0.001 wavenumbers, especially below 3 microns. Unfortunately very few of the known astrophysical molecules are contained in either catalog and there is only a very limited effort to address this relative to molecules in the outer planets.

3.1. Infrared Database

A wide selection of Infrared Databases is available of analytical chemistry applications. These generally focus on gas or liquid phase low-resolution spectroscopy in the 400-4000 wavenumber spectral window. The free and easy to access databases include the NIST/EPA gas phase Infrared Database, the NIST Quantitative Infrared Database and the NIST Chemistry WebBook (all can be found from http://www.nist.gov). Another very complete system is the Integrated Spectral Database System for Organic Compunds, which has over 47,000 spectra available. Virtually every chemical company line Sigma-Aldrich or Sadtler has a available data base as do all the spectrometer makers Bio-rad, Bruker, Nicolet. The analytical chemistry Coblentz Society also has an Infrared database. These databases and spectra will provide band location, but they do not provide line resolved data and generally do not provide intensity data. As a result, they are only useful in potentially (not unambiguously) identifying spectral features like the 3 micron PAH feature.

3.2. Atomic Line Catalogs

The atomic physics community has several databases, mostly supporting plasma physics and observations in the UV and X-ray spectral regions. These catalog the observed and calculated atomic transitions for charged and uncharged atoms. The Harvard Center for Astrophysics web site http://cfa-www.harvard.edu/amdata provides links to a number of sites. The NIST Atomic Spectra Database has an easy to use access form. Collectively these databases are relatively complete, but are known to have some problems with intensities, transition frequencies. A major challenge remains the development of a complete catalog and keeping up with the rapid instrumental progress towards progressively wider wavelength coverage and higher resolution.

4. Conclusions

A great deal of atomic an molecular data has been collected and compiled in catalogs. Unfortunately only the Microwave Catalogs and some of the Atomic Line Catalogs were developed to support Astronomy. The catalogs supporting astronomy are generally not as complete as desirable or as easy to use as desirable. In the case of the microwave catalogs, may of the species missing pose significant theoretical challenges to calculating energy levels and transition strengths or significant challenges to collecting the fundamental data needed as an input to the database. As result, an enormous amount of work is required to upgrade the exiting databases to address the needs of missions like FUZE, Herschel or SOFIA. Ideally this should be done prior to launch, however it is all to often an afterthought once data arrives.

There are also some glairing holes in the available catalogs. These include little or no rotationally resolved data in the entire infrared region and no catalog of electronic transition of molecules in near infrared to UV. The infrared space observatory, ISO, has provided many wonderful spectra of the CH stretch band in the interstellar medium. Unfortunately, very few of the approximately 100 known molecules with a CH bond have line resolved infrared spectra available or cataloged. As a result, not much can be concluded about the ISO CH stretch bands. Similar statements can be made about the diffuse interstellar bands. Ultimately the resolution of all these quandaries will require catalogs of line resolved atomic and molecular data.

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