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Introduction to submillimeter, millimeter and microwave spectral line catalog

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ABSTRACT

This note is an introduction to the reprint of the 1998 *JQSRT* paper "Submillimeter, millimeter, and microwave spectral line catalog" by H.M. Pickett et al. We describe the timeliness and significance of the article and the extensive use of our spectral line catalog as well as discuss more recent profound developments.

Our 1998 *JQSRT* paper [1] was written to document a number of substantial improvements in what has become commonly known as the JPL spectral line catalog. Historically, the paper represented a change from the Robert L. Poynter founded catalog captured in a 1985 *Applied Optics* paper with the same title [2] and the Herbert M. Pickett and Edward A. Cohen lead catalog era. The timing of the paper closely coincided with the development of major projects in Atmospheric Chemistry and the Astrophysics that utilized and funded catalog development. In Atmospheric Chemistry, the Earth Observing System Microwave Limb Sounder was in full development and was launched in July 2004. In Astrophysics, the call for instruments for what is now the Herschel Space Observatory had been issued, the Stratospheric Observatory for Infrared Astronomy (SOFIA) had started development and so had the Atacama Large Millimeter Array (ALMA). The scope of these projects was a harbinger of significant changes between the users of spectroscopic data and the producers of spectroscopic data underscored by the large project requirement to make spectroscopic data easily available to software engineers and others with no spectroscopic training. The large number of citations from the astronomic and atmospheric science communities is a testament to the enduring relevance and need for this work.

The JPL spectral line catalog was founded to address the fundamental difficulty in converting laboratory measurements, which in the rotational band historically consisted of a few carefully measured rotational transitions painstakingly fit to a molecular Hamiltonian model, into a global set of transition predictions that could be used to identify absorption or emission features from astronomical or atmospheric sources corresponding to transitions that were not observed in the laboratory. The philosophy set forth in the catalog paper continues in practice today as these project based needs have only intensified. This philosophy, in a nutshell, remains to critically analyze the literature transitions with the SPFIT/SPCAT suit of programs [3] and to generate a set of predictions utilizing the best available information for the electric dipole moment. This results in a common output format, consistent error propagation as well as a consistent critical review of the published literature facilitating a professional judgment on the accuracy of the calculation and the quality of the literature data. We note that this approach does require the cataloger to be an experienced molecular spectroscopist who could

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otherwise be capable of performing the original spectroscopic research.

The paper draws attention to the changing reality of the interface between spectral data generators and spectral data users. In the early years of atmospheric chemistry and astrophysics, the data generators and users were often the same person looking to understand one or two molecular species based on a few transitions. However, atmospheric chemistry and long wavelength astrophysics have subsequently evolved into sophisticated sciences in their own right so that those now trained in those areas are unlikely to have much knowledge of molecular spectroscopy. Additionally, measurement technology has improved enormously, facilitating the collection of enormous quantities of data in both the laboratory and through remote sensing. More importantly, the teams of specialists that develop large projects and their data pipelines are less likely to have extensive knowledge about molecular spectroscopy than the scientists interpreting the data. As a result, it is critical to large projects that the required molecular data be traceable, as trustworthy as possible, and available in a form that can be ingested by a computer without the intervention of someone who knows the details of molecular physics. The critical element in this interface between data users and data generators is a spectral line catalog. In 1998, the JPL submillimeter, millimeter, and microwave spectral line catalog was the first attempt to fulfill the interface role in the rotational band.

The paper is still particularly significant due to it capturing the initial wave of modern computing and documenting, though primitive by modern standards, the transition to a machine readable format on the World Wide Web compared to a magnetic tape distributed by request format of the previous decade represented a major revolution in data distribution. It also documented a significant increase in knowledge of trace atmospheric species and the explosion of known astrophysical species while providing a literature reference for the users and funding agencies of the catalog. The major projects that were under development at the time of the paper continue to dominate the need for spectral line catalogs. Regardless of need, funding for catalogs remains a significant challenge. The intervening years have seen a steady but low level of support for the Atmospheric Chemistry portion of the JPL spectral line catalog. However, the astrophysics side of the JPL catalog was not funded between 1999 and 2009. As a result, a second line catalog, The Cologne Database for Molecular Spectroscopy (CDMS) [4,5], was started in Europe with one of the co-authors, H.S.P. Müller, being a primary proponent to cope with the enormous need for additions and improvements in calculations of astrophysically relevant molecular species. The CDMS catalog continues the philosophy of the 1998 paper and utilizes the same programs and the same general analysis approach.

The interface role the JPL and CDMS catalogs play between the users of molecular data and those producing molecular data can easily be seen in a number of laboratory projects that have been undertaken to address particularly glaring needs for molecular data pointed out by multiple catalog users. These include detection of larger molecules [6–8], careful analysis of hyperfine effects [9], identification of excited vibrational states [10] and fundamental detection of new species [11]. Additionally, molecular species for which data is unavailable in catalogs, but is needed by the observing community in both atmospheric chemistry and astrophysics quickly obtains a high degree of visibility. This visibility enormously improves the possibility of a spectroscopy group obtaining funding to study the identified species.

In spite of the paper's continued relevance in explaining how molecular calculations are performed and how errors propagate, it also points out how much the field of spectroscopy has changed in the intervening 12 years. First, though modern in 1998, ascii text on the World Wide Web is by comparison with a modern relational or object oriented database a primitive format. Data analysis and observation planning tools for Herschel, ALMA and SOFIA would like to utilize virtual observatory constructs that utilize server query language, facilitating simultaneous multi-wavelength analysis of astronomical objects. The planetary community now desires to simulate planetary atmospheres including many hot extra solar planets to determine optimal wavelengths to study chemistry and dynamics, and finally the atmospheric community is shifting to whole Earth monitoring and measurement of the global energy balance. All of these applications require the spectral line data in conjunction with chemical, dynamical, excitation and radiative transfer models. Data for these complex analyses require (data is plural) not only the line frequencies, energy levels and strengths provided in line catalogs but also line widths, excitation rates and other sorts of inputs. This leads directly to the need to have catalogs be far more complete, consistent and in modern database formats that can easily be combined by analysis or planning programs.

The need for catalogs is growing ever more critical to the science investigations they support, however, the divergence between spectroscopic and atmospheric chemistry, astrophysics or planetary science continues to widen as the respective fields mature. As a result, the need to support an interface between the data users and generators becomes progressively less obvious to each side. Additionally, catalogers generally do not generate the numbers of citable papers that pure scientists would so in the academic setting database management is not a viable tenure track occupation. These difficulties make it a requirement for the agencies funding the overall scientific investigations to realize what is required to extract the desired atmospheric chemistry, planetary science or astrophysics and make sure that a fully integrated program is in place. Should this come to pass, the long term relevance of the 1998 submillimeter, millimeter and microwave spectral line catalog paper in the fields of atmospheric chemistry, planetary science, astrophysics and spectroscopy will be to usher in the maturation of fields and the importance of simple interfaces that allow each to maximize scientific productivity.

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