

TIA
0017
083593
P3

Final Report: NASA Grant NAG 5-3020
Astrophysical Data Program
Spectroscopic Data for an Astronomy Data Base

W. H. Parkinson & Peter L. Smith
October 31, 1997

1 Project Goals

When we began this work, very few of the atomic and molecular data used by astronomers in the analysis of astronomical spectra were available in on-line searchable databases. Our principal goal was to:

- make the most useful of the atomic data files of R. L. Kurucz (1995a,b) available on the WWW; and also to
- make the atomic data of R. L. Kelly for ultraviolet and vacuum ultraviolet lines [*i.e.*, essentially the same as the data in Kelly (1979) and Kelly (1987)] similarly available.

In addition, we proposed to improve access to parameters for simple molecules of interest to astronomers

2 Tasks Completed

2.1 Kurucz and Kelly data sets

The Kurucz and Kelly data sets were added to the WWW and the search engines were incrementally improved. The links are <<http://cfa-www.harvard.edu/amp/data/kur23/sekur.html>> and <<http://cfa-www.harvard.edu/amp/data/stats/kelly.html>>.

The average number of "hits" per week during the four month period July → October of this year was 210 ± 100 for the data from Kurucz CD 23, 76 ± 37 for the database containing the data on Kurucz CD 18, and 169 ± 72 for the Kelly database. [The contents of CD 18 are described in Kurucz (1995a,b); CD 23 is the merged and updated compilation of these files.]

Note that these may be serious underestimates of the actual usage: We collaborated with colleagues at the Plasma Physics Institute at the University of Hanover in Germany to create a mirror site and thereby improve access to the Kurucz and Kelly databases for people in Europe. We have no information about use rates at that site.

Our database work complements that of the NIST Atomic Data Centers, which have put some of their critically compiled "benchmark" atomic reference data onto the WWW at <http://aeldata.phy.nist.gov/nist_beta.html>.

2.2 Molecular data

Our molecular data projects were somewhat less successful. We did add links to compilations of molecular data measured at the Cfa (<<http://cfa-www.harvard.edu/amp/data/cfamols.html>>). However, the people in charge of the HITRAN database elected to have an independent WebSite <<http://www.HITRAN.com/>> and the publishers of the Berkeley Newsletter on Molecular

Spectroscopy backed out of a joint WWW project after we had spent considerable effort on a beta version.

Nevertheless, our efforts have encouraged other producers and compilers of molecular data used by astronomers to consider the WWW as a way to improve access. (One example is those at NIST who are converting the data of Huber & Herzberg (1979) to electronic form). The resulting improved access to these important atomic and molecular data sets are enhancing the analysis and interpretation of data from many spectroscopic space astrophysics missions, thus optimizing science return.

3 Other activities

3.1 Workshop

Smith helped to plan and organize a workshop on *Atomic and Molecular Data for Science and Technology* held at Harvard University in June 1996 and chaired the first Panel Discussion on *Data Needs*. Speakers at the workshop noted the increasing amount of useful atomic and molecular data that were available on the WWW. Our early version of the Kurucz database was cited as a pioneer example of such WWW databases.

This workshop concluded that a regular international meeting to discuss such issues was necessary. As a result, the *International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA)* was planned.

3.2 ICAMDATA

Smith was a member of the committee that developed the structure for the planned ICAMDATA series of meeting, selected the first International Advisory Board and the International Program Committee, and wrote the ICAMDATA charter. He also served on the Local Conference Committee for the first ICAMDATA meeting, which was held at NIST from Sept. 29 through Oct. 02, 1997.

4 Publications and Presentations

The Place for Atomic & Molecular Databases for Astronomy is the World Wide Web, P. L. Smith, J. R. Esmond, C. Heise & R. Kurucz, in *ATOMIC SPECTRA AND OSCILLATOR STRENGTHS FOR ASTROPHYSICAL AND LABORATORY PLASMAS - POSTER PAPERS*, ed. W.-U. L. Tchang-Brillet, J.-F. Wyart & C. J. Zeippen, [Paris: Observatoire de Paris], (1996).

On-Line Atomic & Molecular Data for Astronomy, P. L. Smith, J. R. Esmond, C. Heise & R. Kurucz, in *UV AND X-RAY SPECTROSCOPY OF ASTROPHYSICAL AND LABORATORY PLASMA*, ed. K. Yamashita & T. Watanabe, [Tokyo: Universal Academy Press], p.513 (1996).

5 References

- Huber, K. P., & Hergberg, G. H. 1979, *Constants of Diatomic Molecules*, [New York: Van Nostrand Reinhold].
- Kelly, R L 1979 *Atomic Emission Lines in the Near Ultraviolet; Hydrogen through Krypton*, NASA Tech. Mem. 80268.
- 1987 *Atomic and Ionic Spectrum Lines Below 2000 Å; Hydrogen through Krypton*, J. Phys. Chem. Ref. Data **16**, Suppl. 1.
- Kurucz, R. L. 1995a *The Kurucz Atomic and Molecular Database, Astrophysical Applications of Powerful New Databases*, eds. S. J. Adelman & W. L. Wiese, A.S.P. Conf. Ser. 78, p.205.
- 1995b *An Atomic and Molecular Data Bank for Stellar Spectroscopy*. eds. A. J. Sauval, B. Blomme, & N. Grevesse, A.S.P. Conf. Ser. 81, p.583.