HARVARD COLLEGE OBSERVATORY
60 Garden Street, Cambridge, MA 02138
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Final Report: NASA Contract NAS5-32587

Spectroscopic Data for an Astronomy Database

W. H. Parkinson, Principal Investigator

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This project was motivated by the lack of online spectoscopic databases containing the atomic and molecular parameters -- wavelengths, energy levels and designations, oscillator strengths, cross sections, etc. -- used by those studying astronomical spectra, particularly spectra obtained using the Hubble Space Telescope and other NASA satellites.

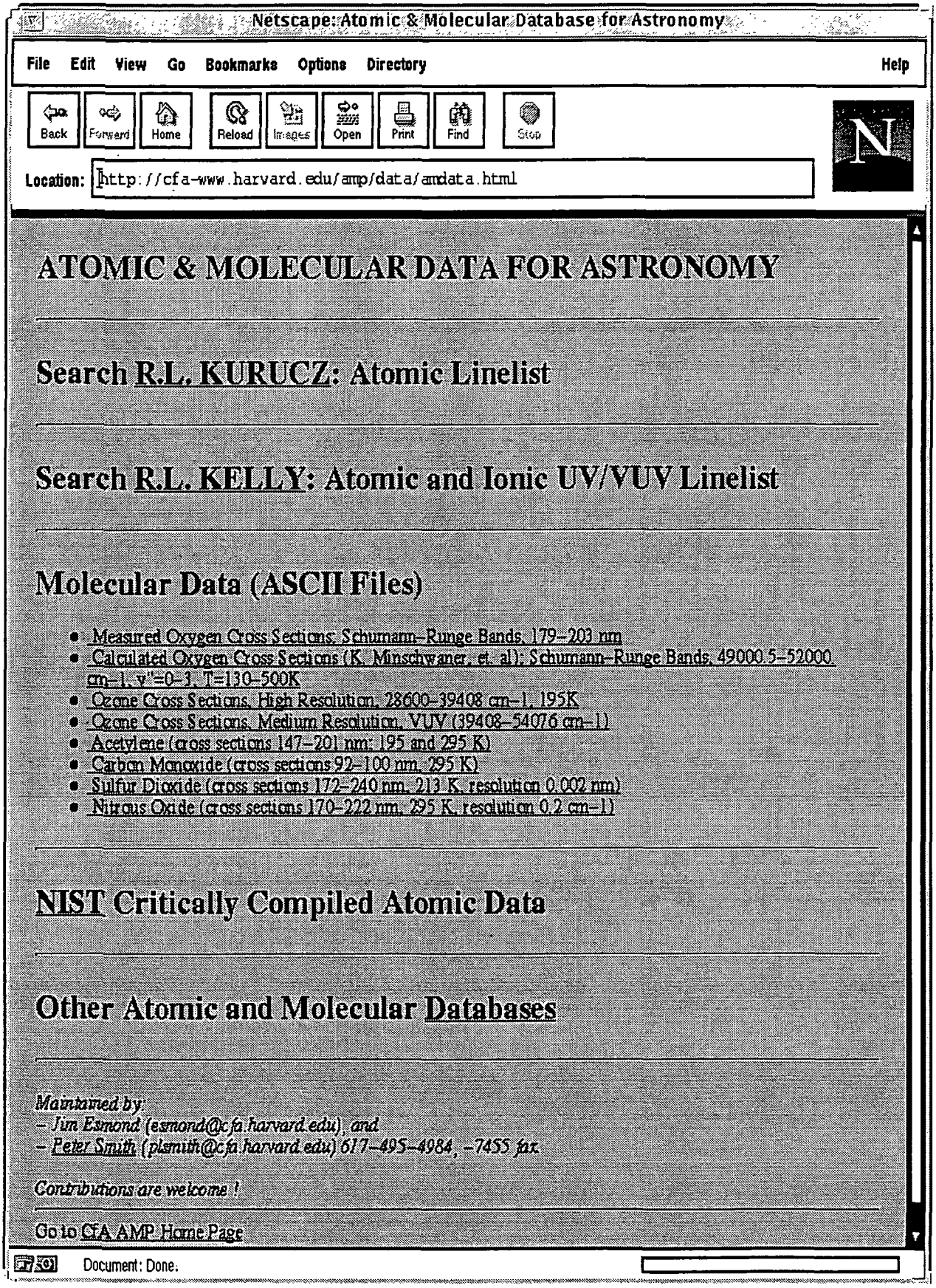
The database was implemented on the World Wide Web and can be accessed by using hypertext browsers, such as Mosaic and Netscape. The ULR is *http://cfa-www.harvard.edu/amp/data/amdata.html*.

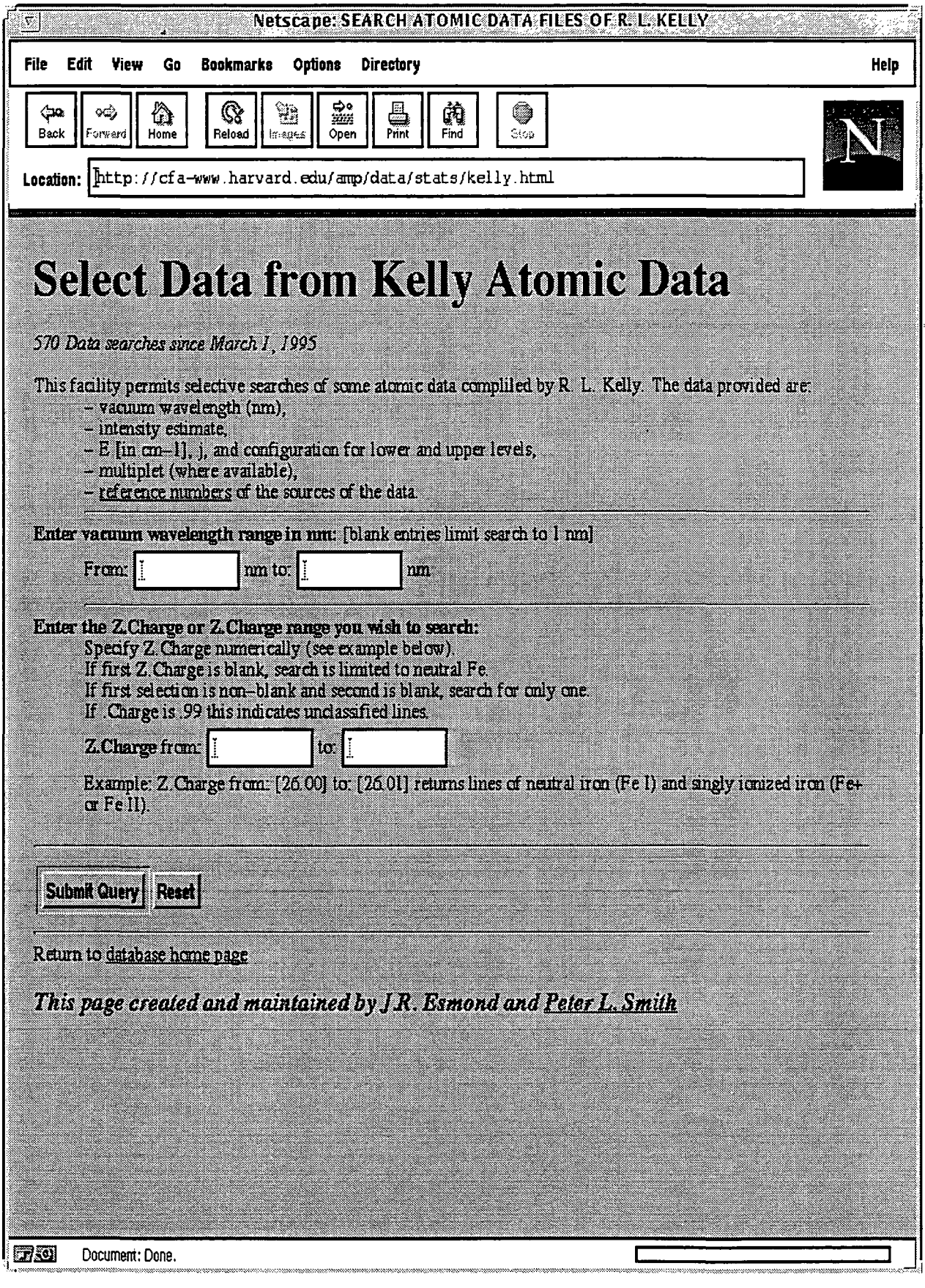
The principal data in the database are those of R. L. Kurucz, specifically 5 files from his CD-ROM 18 (see Kurucz, R. L., in *Laboratory and Astronomical High Resolution Spectra*, ed. A. J. Sauval et al., A.S.P. Conf. Ser. 81, 1995). A search routine using a Perl script has been implemented. About 10 searches per day have been logged.

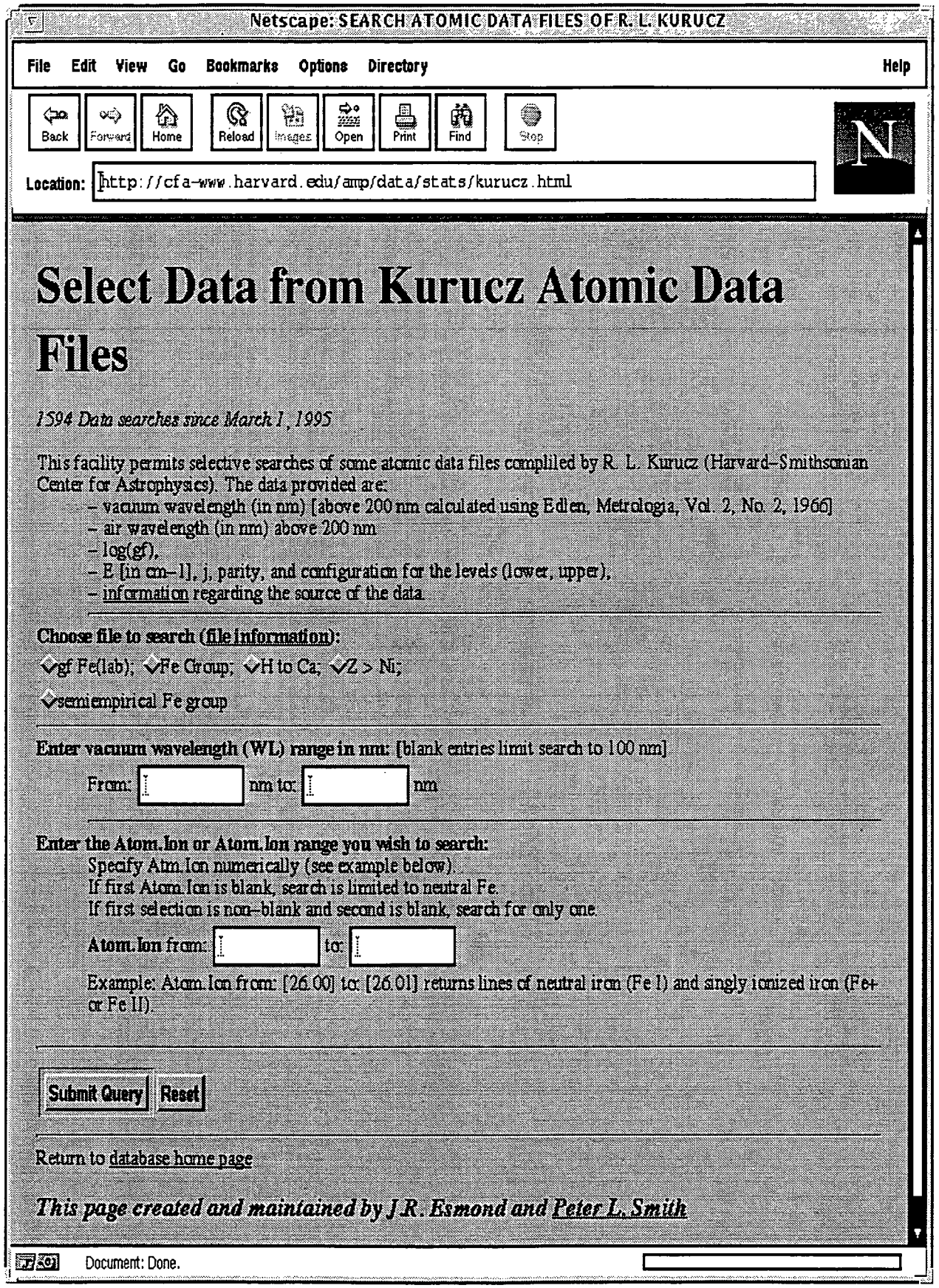
Other data in our online database include:
- the atomic data of R. L. Kelly;
- cross section data for O_2, O_3, NO, CO, C_2H_2, and SO_2; and
- links to other spectroscopy databases, such as that at NIST, that will of use to astronomers.

More details about these databases are given in the appended publications. Figures showing the database home page and the pages for searching the files are also appended.

Our online database was formally announced at two meetings: The *Eleventh International Colloquium on UV and X-Ray Spectroscopy of Laboratory and Astrophysical Plasmas* in Nagoya Japan (May 30 - June 2, 1995) and the *Fifth International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, in Paris (28 - 31 August, 1995). Papers that will be published in the proceeding of these meetings are appended.


Netscape: Atomic & Molecular Database for Astronomy
File Edit View Go Bookmarks Options Directory Help
Back Forward Home Reload Images Open Print Find Stop
Location: http://cfa-www.harvard.edu/amp/data/amdata.html
ATOMIC & MOLECULAR DATA FOR ASTRONOMY
Search R.L. KURUCZ: Atomic Linelist
Search R.L. KELLY: Atomic and Ionic UV/VUV Linelist
Molecular Data (ASCII Files)
Measured Oxygen Cross Sections: Schumann-Runge Bands, 179-203 nm
Calculated Oxygen Cross Sections (K. Minschwaner, et. al): Schumann-Runge Bands, 49000.5-52000 cm-1, v"=0-3, T=130-500K
Ozone Cross Sections, High Resolution, 28600-39408 cm-1, 195K
Ozone Cross Sections, Medium Resolution, VUV (39408-54076 cm-1)
Acetylene (cross sections 147-201 nm; 195 and 295 K)
Carbon Monoxide (cross sections 92-100 nm, 295 K)
Sulfur Dioxide (cross sections 172-240 nm, 213 K, resolution 0.002 nm)
Nitrous Oxide (cross sections 170-222 nm, 295 K, resolution 0.2 cm-1)
NIST Critically Compiled Atomic Data
Other Atomic and Molecular Databases
Maintained by:
- Jim Esmond (esmond@cfa.harvard.edu), and
- Peter Smith (plsmith@cfa.harvard.edu) 617-495-4984, -7455 fax
Contributions are welcome !
Go to CfA AMP Home Page
Document: Done.


Netscape: SEARCH ATOMIC DATA FILES OF R. L. KELLY
File Edit View Go Bookmarks Options Directory Help
Back Forward Home Reload Images Open Print Find Stop
Location: http://cfa-www.harvard.edu/amp/data/stats/kelly.html
Select Data from Kelly Atomic Data
570 Data searches since March 1, 1995
This facility permits selective searches of some atomic data compliled by R. L. Kelly. The data provided are:
– vacuum wavelength (nm),
– intensity estimate,
– E [in cm–1], j, and configuration for lower and upper levels,
– multiplet (where available),
– reference numbers of the sources of the data.
Enter vacuum wavelength range in nm: [blank entries limit search to 1 nm]
From: nm to: nm
Enter the Z.Charge or Z.Charge range you wish to search:
Specify Z.Charge numerically (see example below).
If first Z.Charge is blank, search is limited to neutral Fe.
If first selection is non–blank and second is blank, search for only one.
If .Charge is .99 this indicates unclassified lines.
Z.Charge from: to:
Example: Z.Charge from: [26.00] to: [26.01] returns lines of neutral iron (Fe I) and singly ionized iron (Fe+ or Fe II).
Submit Query Reset
Return to database home page
This page created and maintained by J.R. Esmond and Peter L. Smith
Document: Done.


Netscape: SEARCH ATOMIC DATA FILES OF R. L. KURUCZ
File Edit View Go Bookmarks Options Directory Help
Back Forward Home Reload Images Open Print Find Stop
Location: http://cfa-www.harvard.edu/amp/data/stats/kurucz.html
Select Data from Kurucz Atomic Data Files
1594 Data searches since March 1, 1995
This facility permits selective searches of some atomic data files compiled by R. L. Kurucz (Harvard-Smithsonian Center for Astrophysics). The data provided are:
– vacuum wavelength (in nm) [above 200 nm calculated using Edlen, Metrologia, Vol. 2, No. 2, 1966]
– air wavelength (in nm) above 200 nm
– log(gf),
– E [in cm–1], j, parity, and configuration for the levels (lower, upper),
– information regarding the source of the data
Choose file to search (file information):
gf Fe(lab); Fe Group; H to Ca; Z > Ni;
semiempirical Fe group
Enter vacuum wavelength (WL) range in nm: [blank entries limit search to 100 nm]
From: nm to: nm
Enter the Atom.Ion or Atom.Ion range you wish to search:
Specify Atm.Ion numerically (see example below).
If first Atom.Ion is blank, search is limited to neutral Fe.
If first selection is non-blank and second is blank, search for only one.
Atom.Ion from: to:
Example: Atom.Ion from: [26.00] to: [26.01] returns lines of neutral iron (Fe I) and singly ionized iron (Fe+ or Fe II).
Submit Query Reset
Return to database home page
This page created and maintained by J.R. Esmond and Peter L. Smith
Document: Done.

ON-LINE ATOMIC & MOLECULAR DATA FOR ASTRONOMY

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Abstract

Very few of the atomic and molecular data used in analyses of astronomical spectra are currently available in World Wide Web (WWW) databases that are searchable with hypertext browsers. We have begun to rectify this situation by making the extensive atomic data files of R. L. Kurucz and R. L. Kelly available with simple search procedures. We have also made a number of other useful atomic and molecular data files available on the WWW and have established links to other on-line atomic and molecular databases. All can be accessed from our database homepage with URL:
http://cfa-www.harvard.edu/amp/data/amdata.html.

1. Introduction

The "computer age" has influenced few areas of intellectual endeavor as much as it has astrophysics. Astronomers, astrophysicists, and space physicists have been at – and in some instances driven – the forefront of electronic information acquisition, storage, and manipulation. Rare is the practitioner in these fields who doesn't have a computer on his/her desk or very nearby, a computer used for planning and performing observations, data analyses, information searches, communication, and document preparation. Until recently, however, there has been an anomaly in the availability of data for modern astronomy: Few of the atomic and molecular data used in analyses of state-of-the-art astronomical spectra have been conveniently available in databases that are easily used.

There are a large number of relevant databases on the Internet; links to some for atomic and plasma physics can be reached with URL's:
http://plasma-gate.weizmann.ac.il/DBfAPP.html and
http://www-cfadc.phy.ornl.gov/databases.html.
However, many of these databases are simply FTP sites from which files can be obtained. Others, *e.g.*, (*i*), TOPBASE (Cunto *et al.* 1993), which provides access to the results of the Opacity Project; (*ii*), the International Atomic Energy Agency (IAEA) atomic and

molecular data compilation for support of fusion research, which uses the ALLADIN system (Hulse 1990) for management and exchange of data; (*iii*), the Research Information Center at the National Institute for Fusion Science (NIFS), which also has a specialized interface; and, (*iv*), the Vienna Atomic Line Data-Base (Piskunov *et al.* 1995), require registration and/or use of a dedicated database management system. The data in the Atomic Data and Analysis Structure database (http://patiala.phys.strath.ac.uk/adas/Mail.adas.html) are available only to members of the ADAS Consortium.

Other databases, such as that of (Kurucz 1995) and the HITRAN molecular database of Rothman *et al.* (1992), are not on the Internet, but are available through personal communication with their developers; another is available commercially (Lu).

The proliferation of specialized databases, with complicated access and specialized interfaces has – unexpectedly in this computer intensive age – made some fraction of atomic and molecular data harder to obtain than they were a decade ago, when printed paper was the only medium for distribution.

The lack of convenient access to the atomic and molecular data used by astronomers was noted at recent workshops. Group Recommendation *X.B.c* from the NASA Astrophysics UVGA Branch Laboratory Astrophysics Workshop held in Pasadena in February 1994 stated that, *"Electronic versions of [atomic and molecular databases] should be maintained, made available to outside users, and use standardized software"*. Similar recommendations were part of the discussion that concluded the recent Workshop on Laboratory & Astronomical High Resolution Spectra (Sauval *et al.* 1995).

2. Atomic & Molecular Data for Astronomy On the World Wide Web

In the last few years, the World Wide Web (WWW) has become the *de facto* standard for electronic exchange of information in many fields of human activity. WWW browsers such as *Mosiac* and *Netscape* are available to many astronomers and familiar to most. Their graphical interfaces are easy to learn and use. No passwords or registration are necessary. Real-time search capabilities are easy to implement, so downloading of large files containing unnecessary information – a frequent necessity when using FTP or TELNET – can be avoided.

Because of these advantages, we chose the WWW as a way to make atomic and molecular data available to astronomers. The URL of our database homepage is:

http://cfa-www.harvard.edu/amp/amdata.html.

2.1. Atomic Data of R. L. Kurucz and B. Bell

Our database now contains five files of atomic line parameters that are on Kurucz CD-ROM 18 (Kurucz 1995). These will soon be replaced by the data on Kurucz CD-ROM 23 (Kurucz & Bell 1995) that are, essentially, an update of the classic work of Kurucz & Peytremann (1975) supplemented by extensive data collected from published literature by Barbara Bell. The new data file will contain information for about 540,000 atomic lines for which there are measured energy levels.

We have provided a rudimentary search capability, so that users can search for lines of a given element and charge state in a given wavelength range. We plan to expand the search capability to include Boolean searches.

2.2. Atomic Data of R. L. Kelly

We have also made the atomic data of R. L. Kelly for about 90,000 ultraviolet and vacuum ultraviolet lines similarly available. These data are similar those in Kelly (1979) and Kelly (1987), but were obtained privately. The search capabilities are similar to those for the Kurucz data.

2.3. Molecular Data

Parkinson (1992) reviewed the status of molecular databases of interest to astronomy. None of the data discussed was readily available on-line.

As an example of what we hope others will do with molecular data of interest to astronomers, we have made cross section data for a number of molecules available. These include:

CO	from	92	to	100 nm	at	295 K	and	0.0006 nm	resolution
C_2H_2	"	147	"	201 "	"	195 and 295 K	"	0.0075 nm	"
SO_2	"	172	"	240 "	"	213 K	"	0.002 nm	"
NO	"	170	"	222 "	"	295 K	"	0.2 cm^{-1}	".

We intend to soon begin, as a demonstration project, an on-line "atlas" of ultraviolet spectroscopic data for N_2. Our cross section data (Stark *et al.* 1992) and unpublished line lists of Yoshino (1995) will be available.

We also intend to add selected portions of the HITRAN molecular database of Rothman *et al.* (1992). This has been developed over two decades with U. S. Air Force support to provide efficient access to many of the fundamental molecular parameters necessary for spectroscopic analyses of the Earth's atmosphere. We propose to extract molecular data of relevance to astronomy from the HITRAN data base, convert the parameters to those familiar and useful to astronomers, and place the data on the WWW.

2.4. Other On-line Atomic and Molecular Databases of Interest to Astronomers

Our work complements that of the Atomic Data Centers of the U. S. National Institute of Standards and Technology (NIST, formerly the National Bureau of Standards or NBS), which have begun to put some of their critically compiled atomic data onto the WWW. The URL for the "beta" version of this online database is:

http://aeldata.phy.nist.gov/nist_beta.html.

Searches for selected energy levels, wavelengths, or transition probabilities can be made. Bibliographic files are available with URL:

http://physics.nist.gov/PhysRefData/contents.html.

D. C. Morton has posted his list of atomic lines with $\lambda \geq 121$ nm that are likely to be seen in interstellar absorption (Morton 1991). The URL is:

http://www.dao.nrc.ca/~dcm/atomic_data.html.

There is no search mechanism.

3. Comments

We believe that the ready availability and ease of use of the World Wide Web and hypertext browsers make this medium the one of choice for access to the atomic and molecular parameters that are used by many astronomers. We encourage others to create WWW data sites and to support a migration away from databases with limited access and one-of-a-kind management systems.

4. Acknowledgements

This work was supported in part by NASA Contract NAS5-32587 to Harvard University and Grants NAGW 1486, 2528, and 3299 to the Smithsonian Astrophysical Observatory. CH was supported in part by a Feodor Lynen fellowship awarded by the Alexander von Humboldt-Stiftung. The authors thank W. H. Parkinson for his advice and support. PLS thanks the Colloquium organizers, who supported his attendance at the meeting and presentation of this paper.

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The Place for Atomic & Molecular Databases for Astronomy is the World Wide Web

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Abstract

Very few of the atomic and molecular data used in analyses of astronomical spectra are currently available in online databases that are searchable using the World Wide Web and with hypertext browsers. We believe that these new electronic tools provide a simple and readily available means of improving access to such data for astronomers. We have made the extensive atomic data files of R. L. Kurucz and R. L. Kelly available with simple search procedures, have provided access to number of other useful atomic and molecular data and bibliographic files, and have established links to other online atomic and molecular databases and information sources. All can be accessed from our database homepage with URL:

http://cfa-www.harvard.edu/amp/data/amdata.html.

Introduction

Until recently, the atomic and molecular data used by astronomers and astrophysicists in analyses of spectra and in photochemical models were distributed only in printed form. Searches were done "by hand"; required subsets of such data were created by transcription to paper or computer memory for further use.

This situation was in sharp contrast with the methods for acquiring the astronomical spectra, as astronomers, astrophysicists, and space physicists have long been at the forefront of electronic acquisition, storage, and manipulation of observational data. Rare is the practitioner in these fields who doesn't have, on his/her desk or very nearby, a computer used for planning and performing observations, data analyses, information searches, communication, and document preparation.

Recently, the atomic and molecular data used by astronomers has begun to become available electronically. The atomic line database of Kurucz (1995) and the HITRAN molecular database of Rothman *et al.* (1992) are available on CD-ROM from the authors. Three NIST (U.S. National Institute of Standards & Technology) atomic line and transition probability databases, *viz.*, Standard Reference Databases 24, 38, and 61, are available on floppy disk.

There are also a large number of relevant databases that can be obtained using FTP file transfer protocol. Ralchenko & Stambulchik (1995) lists many of these; others can be reached with with URL (uniform resource locator) http://www-cfadc.phy.ornl.gov/databases.html. However, many of these "online" databases are simply files that can be downloaded. Others, *e.g.*, (*i*), TOPBASE (Cunto *et al.* 1993), which provides access to the results of the Opacity Project; (*ii*), the International Atomic Energy Agency (IAEA) atomic and molecular data compilation for support of fusion research, which uses the ALLADIN system (Hulse 1990) for management and exchange of data; (*iii*), the data at the Research Information Center at the National Institute for Fusion Science (NIFS), which also has a specialized interface; and, (*iv*), the Vienna

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Atomic Line Data-Base (Piskunov *et al.* 1995), require registration and/or use of a dedicated database management system. The data in the Atomic Data and Analysis Structure database (Lang 1995) are presently available only to members of the ADAS Consortium.

The proliferation of specialized databases, with complicated access and specialized interfaces has – unexpectedly in this computer intensive age – made some fraction of atomic and molecular data harder to obtain than they were a decade ago, when printed paper was the only medium for distribution.

The lack of convenient access to the atomic and molecular data used by astronomers was noted at recent workshops. Group Recommendation *X.B.c* from the NASA Astrophysics UVGA Branch Laboratory Astrophysics Workshop held in Pasadena in February 1994 stated that, *"Electronic versions of [atomic and molecular databases] should be maintained, made available to outside users, and use standardized software"*. Similar recommendations were part of the discussion that concluded the recent Workshop on Laboratory & Astronomical High Resolution Spectra (Sauval *et al.* 1995).

We believe that the World Wide Web (or Internet – we use the terms synonymously), especially when used with hypertext browsers such as *Mosaic* or *Netscape*, has many features that merit consideration by data producers who want to facilitate use of their data and by those who want easy access to them. We discuss these advantages and introduce some WWW hypertext data sites in this paper.

Using the World Wide Web for Atomic & Molecular Databases for Astronomy

In the last few years, the World Wide Web (WWW) has become the *de facto* standard for electronic exchange of information in many fields of human activity. Hypertext browsers are available to many astronomers and familiar to most.

For data users, advantages of the WWW include graphical interfaces that are easy to learn and use. There are no requirements for passwords or registration and no special database management system instructions to learn and remember. When the WWW browsers include search capabilities, downloading of large files containing significant fractions of unnecessary information – a frequent necessity when using FTP or TELNET – can be avoided.

For data producers, real-time search capabilities are easy to implement. Plotting packages are available (one examples is discussed below). Subsets of a database can be made available when they are ready; there is no need, as there is in paper publication, to be complete before making data widely available. There are no publication costs. Typographical and other errors can be readily corrected.

Because of these advantages, we recommend the WWW as a way to make atomic and molecular data available to astronomers. Some examples of our use of the WWW in this way are discussed below. The URL of our database homepage is: http://cfa-www.harvard.edu/amp/data/amdata.html.

Atomic data of Kurucz and of Kelly

Our database now contains five files of atomic line parameters that are on Kurucz CD-ROM 18 (Kurucz 1995). These will soon be replaced by the data on Kurucz CD-ROM 23 (Kurucz & Bell 1995) that are essentially an update of the classic work of Kurucz & Peytremann (1975) supplemented by extensive data collected from published literature by Barbara Bell. The new data file will contain information for about 540,000 atomic lines for which there are measured energy levels. We have also made the atomic data of R. L. Kelly for about 90,000 ultraviolet and

vacuum ultraviolet lines similarly available. These data are similar to those in Kelly (1979) and Kelly (1987), but were obtained privately. We have provided a rudimentary search capability, so that users can search for lines of a given element and charge state in a given wavelength range. We plan to expand the search capability to include Boolean searches.

Molecular spectral and bibliographic data

As an preliminary example of what we hope others will do with molecular data of interest to astronomers, we have made ultraviolet wavelength cross section data for a number of molecules available (see the table below). The molecular bibliographic information available in the Berkeley Newsletter (Phillips, Davis & Eakin 1995) is also now online, as is the The Smithsonian Astrophysical Observatory atmospheric molecule database (Chance *et al.* 1994), which contains data for the 10 to 800 cm^{-1} range. There are no search mechanisms.

Molecular Cross Section Data Available in the CfA WWW Database									
CO	from	92	to	100 nm	at	295 K	and	0.0006 nm	resolution
C_2H_2	"	147	"	201 "	"	195 and 295 K	"	0.0075 nm	"
SO_2	"	172	"	240 "	"	213 K	"	0.002 nm	"
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We intend to soon begin, as a demonstration project, an online "atlas" of ultraviolet (~85 to 100 nm) spectroscopic data for N_2. Our cross section data (Stark *et al.* 1992) and unpublished line lists of Yoshino (1995) will be available. We also intend to add selected portions of the HITRAN molecular database of Rothman *et al.* (1992). We propose to extract molecular data of relevance to astronomy from the HITRAN data base, convert the parameters to those familiar and useful to astronomers, and place the data on the WWW with searching and graphical tools.

Other hypertext atomic and molecular databases of interest to astronomers

Our work complements that of the Atomic Data Centers of NIST, which have begun to put some of their critically compiled atomic data onto the WWW. The URL for the "beta" version of this online database is: http://aeldata.phy.nist.gov/nist_beta.html. Searches for selected energy levels, wavelengths, or transition probabilities can be made. Bibliographic files can be searched by starting with URL: http://physics.nist.gov/PhysRefData/contents.html. URL http://physics.nist.gov/PhysRefData/wavenum/html/spect.html provides a nice example of realtime plotting of data.

D. C. Morton has posted his list of atomic lines with $\lambda \geq 121$ nm that are likely to be seen in interstellar absorption (Morton 1991). The URL is: http://www.dao.nrc.ca/~dcm/atomic_data.html. There is no search mechanism.

Comments

We believe that the ready availability and ease of use of the World Wide Web and hypertext browsers make this medium the one of choice for access to the atomic and molecular parameters that are used by many astronomers. We encourage others to create WWW data sites and to support a migration away from databases with limited access and one-of-a-kind management systems.

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