Atomic Data and Databases on the Internet: Entering 1996*

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Abstract

In this report the current situation with availability and management of atomic data on the Internet is reviewed.

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*Electronic version can be found at http://plasma-gate.weizmann.ac.il/~fnralch/app.dvi.

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1   Introduction

Only 3-4 years ago the Internet was used practically only for e-mail correspondence. Since then the exploding development of Internet systems, mainly of the World-Wide Web[1], has utterly changed the methods of scientific information exchange. Though unlike astro- or high-energy physicists, the atomic and plasma community have not paid enough attention to utilizing those new opportunities in practical work, the situation with proliferation of atomic data on the Internet rapidly changes to better.

We review here the availability of and access to the 'wired' atomic data. This report may be thought of as the next in the chain of analogous papers [1, 2, 3]. Although because of incredibly rapid changes in on-line atomic data distribution such a review is condemned to be out of date almost straight after completing, nevertheless, we hope that at least those researchers, who are not too familiar with existing on-line atomic databases, will find new information. In what follows, we will not stress a distinction between *databases* that give search and selection options and *datasets* that are mostly ASCII or PostScript files though this should be kept in mind. Note also that availability of mostly *atomic*, not molecular, data will be discussed. In addition, no evaluation of the accuracy of concrete datasets will be provided.

In Section 2 we present the main advantages the World-Wide Web gives to atomic data users. An effort at a comprehensive list of existing databases is given in Section 3. Two proposals aiming more easy and convenient access to already available and new atomic data are formulated in Section 4. Section 5 contains the concluding remarks.

2   World-Wide Web and Database Management

Currently, an access to the on-line atomic data is implemented via four protocols, viz., Telnet, e-mail, FTP, and HTTP. The HTTP-based World-Wide Web software not only supports the other protocols but also offers many additional options. As was correctly noted in Ref. [3], the World-Wide Web has become a *de facto* standard in modern scientific information exchange.

The most attractive feature of the WWW is its user-friendly, extremely clear interface. While in order to work with databases using other protocols one has firstly to look through many-page manuals, the formation of an input on the Web can easily be accomplished already at the very first connection to database. Besides, some non-WWW databases run under special operating systems and/or environment that has firstly to be learned — this circumstance is totally avoided in the WWW since the same client (user) software is used for all Web databases. Another very important advantage of the Web is that its language, HTML, was initially made to support various text formats, images, etc., which makes the output far richer than in other systems. Though the principles of the WWW are based on free access ideology, nevertheless, the access can be restricted by using authentication mechanisms. Most

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[1]The glossary of some Internet terms is given in Appendix I.

of client (browsers) and server (HTTP daemons) software is free for educational, academic and governmental organizations. Finally, the progress of the World-Wide Web and related software is so fast that we can undoubtedly expect many new impressive features and options to appear in the very nearest future.

3   Atomic Databases

In this Section we alphabetically list the on-line atomic databases and datasets with we are familiar as of January 1996. No restricted access databases (e.g., ADAS database) are reviewed here. The related URLs are given in parentheses after the database names, and the collections of data with no search options have the star superscript. The summary table is given in Appendix II where the names of persons responsible for database operation and/or maintainance can be found. Probably, it is hardly possible to list *all* existing on-line atomic databases so we sincerely apologize to the authors of the missed links.

The permanently updated hypertext list of atomic data and databases on the Internet can be found at the URL *http://plasma-gate.weizmann.ac.il/DBfAPP.html*.

3.1   Atomic Data for Astrophysics* (*http://www.pa.uky.edu/~verner/atom.html*)

This collection which is located at the University of Kentucky includes both local data sets and many links to other hosts (mainly to the CDS catalogues) storing atomic data. The various datasets and links are conveniently sorted by processes or characteristics, e.g., recombination, photoionization, charge transfer, energy levels, Stark broadening, etc. The local data are given as ASCII and/or PostScript tables with additional description text files.

3.2   Atomic Data for Resonance Absorption Lines* (*http://www.dao.nrc.ca/~dcm/atomic_data.html*)

On the WWW server of Herzberg Institute of Astrophysics, Canada, one can find an updated version of tables published in [4]. The available data are wavelengths, transition probabilities, oscillator strengths, damping constants. For some of A- and f-values the estimated accuracy is presented. The data are given as ASCII files for different elements, the finding wavelength list being available as well.

3.3   BIBL Spectral Bibliography Database (*http://plasma-gate.weizmann.ac.il/bibl.html*)

The BIBL database which was created and is maintained by efforts of Department of Atomic Spectroscopy at the Institute of Spectroscopy, Troitsk, Russia, is not a true *on-line* database. The BIBL was made for use on IBM-PC compatibles and is added to this list so long as it can be freely downloaded from the Weizmann Plasma-Gate site. This database contains

very detailed information on more than 4000 papers in various fields of atomic and plasma spectroscopy and has multiple options as for searching, editing and adding the data.

3.4 CCP7 Data Library* (*ftp://ccp7.st-and.ac.uk/ccp7/*)

One of the Collaborative Computational Projects (United Kingdom), CCP7, is devoted to the analysis of astronomical spectra. CCP7 maintains an unrivalled software library with atomic and molecular data at the anonymous FTP-site of the University of St. Andrews, UK. Some of data are presented as files which can only be read with specific software while the others can be utilized independently. This data depository contains R. L. Kurucz CD-ROM data, line list for LTE spectrum modeling and other data.

3.5 Centre de Données astronomiques de Strasbourg (*http://cdsweb.u-strasbg.fr/cats/VI.html*)

Although the main aim of CDS is to collect astronomical data, it contains also about 20 catalogues (datasets) of spectroscopic and collisional atomic data published during last 40 years. Available are such data as energy levels and transition probabilities from NIST compilations, atomic spectra line list, some of Kurucz data, to name a few. Most of catalogues can be retrieved via FTP though some should be requested only by sending an e-mail to *question@simbad.u-strasbg.fr*. The atomic data tables from major astronomical journals are available at CDS as well (*http://cdsweb.u-strasbg.fr/cats/J.html*). Note that links to CDS atomic data (both catalogues and tables) sorted by processes or characteristics can be found at the Atomic Data for Astrophysics site (see above).

3.6 DASGAL Bibliography Database on Atomic Line Shapes and Shifts (*http://www.obspm.fr/departement/dasgal/lesage/*)

This bibliographic database which was created at the Department of "Astrophysique Stellaire et Galactique" of the Observatory of Paris-Meudon covers period from 1977 till 1992. The available references on line shapes and shifts are the result of joint work of Observatory of Paris-Meudon and NIST[5]. The database has search options by author, year, effect (Stark, Zeeman,...), element and title. There exist both English and French versions of this database.

3.7 GAPHYOR Data Center (*http://gaphyor.lpgp.u-psud.fr/*)

The GAPHYOR (GAz-PHYsics-ORsay) database at Centre de Données, Orsay, France covers very broad range of bibliographic data on properties of isolated atoms and molecules, collisions with photons, electrons and heavy particles (atoms and molecules), and macroscopic properties of gases. By the middle of 1995, the total number of entries had approached half

a million. The WWW GAPHYOR database is now of version 1.1 and is rapidly advancing. New search options are being developed in addition to already available selection of chemical element(s) and physical process or characteristics. The quests for expert's reports can also be sent by e-mail to *gaphyor@lpgp.u-psud.fr* but this service is not free of charge.

3.8   Harvard-Smithsonian Center for Astrophysics Databases (*http://cfa-www.harvard.edu/amp/data/amdata.html*)

These are three databases which cover the atomic linelists from R. L. Kurucz's CD-ROMs No. 18 and No. 23[6] and R. L. Kelly's compilation of spectral lines below 2000 Å [7]. The newest of these databases (Kurucz CD-ROM No. 23, European mirror is located at *http://leanda.pmp.uni-hannover.de:9000/projekte/kurucz/sekur.html*) has many options in configuring both input and output while for two others the search procedures currently include only wavelength range and/or ion range selection. Note also that some molecular data as well as the list of other atomic and molecular databases are presented on this server.

3.9   IAEA Atomic and Molecular Data Information System (*telnet://aladdin@ripcrs01.iaea.or.at*)

This database (AMDIS) which contains mainly collisional data is located at the International Atomic Energy Agency, Vienna, Austria. The IAEA AMDIS (don't mix with the NIFS AMDIS!) consists of three databases:

- ALADDIN – recommended and evaluated data for atomic and molecular collisions and particle-surface interactions;

- AMBDS – Atomic+Molecular Bibliographic Data Retrieval System;

- AMBB – Electronic Bulletin Board with Atomic+Molecular related news.

The ALADDIN, which goes from **A L**abelled **A**tomic **D**ata **In**terface, is the system adopted by the IAEA and the Atomic Data Centre Network for the exchange of data since 1988[8]. The non-registered users may work with userid *guest* but may not save the search results into a file. In order to become a registered user, send an e-mail to *psm@ripcrs01.iaea.or.at*. In addition to the IAEA interactive system, ALADDIN is also available as a set of FORTRAN-77 codes and data files which can be downloaded, e.g., from anonymous FTP-site at *ftp://ripcrs01.iaea.or.at/pu*

3.10   LLNL Elastic Photon-Atom Scattering Database (*http://www-phys.llnl.gov/V_Div/scattering/elastic.html*)

The programs and data presented in this database (Lawrence Livermore National Laboratory) are useful for evaluating Rayleigh scattering, the contribution to elastic scattering made by the bound electrons of an atom, which dominates elastic scattering for most of the x-ray and low-energy gamma-ray regimes. These data are based on the anomalous-scattering-factor

(ASF) approximation. The existing interface provides access to ASFs for any choice of atom and photon energy, the differential/total cross sections and angular dependence of ASFs can be generated as well.

3.11 Masaryk University Collection of Data[*] (*http://www.sci.muni.cz/physics/archives.htm*)

On the anonymous FTP server of Masaryk University, Czech Republic, one can find a small set of atomic data for some of noble gas and alkaline *atoms*. This host contains collisional cross sections as well as spectroscopic data like energies and transition probabilities.

3.12 NIFS Database (*telnet://msp.nifs.ac.jp*)

This is a large databank of collisional processes characteristics which is located at the National Institute for Fusion Science (NIFS), Nagoya, Japan. Actually, it consists of a few databases under common envelope of the Fujitsu Advanced Information Retrieval System (FAIRS), among them:

- AMDIS – Atomic and Molecular Data Interactive System;

- BACKS – Backscattering of Ions from Solids in Normal Incidence;

- CHART – Charge Transfer between Atoms and Ions;

- SPUTY – Sputtering Yields of Monoatomic Solids.

Four additional databases located at NIFS are the plasma-fusion-atomic excerpts from the well-known commercial INSPEC$^{\circledR}$ database and the ORNL bibliographic database (see below). The original NIFS databases contain very detailed and extensive information on such collisional processes as, e.g., electron impact excitation and ionization, charge transfer, etc. As of the end of 1995, the AMDIS contains 4303 sets of electron-ion excitation cross sections and 1302 sets of electron-ion ionization cross sections. The selected data sets can be downloaded with FTP or plotted on a screen. There is no anonymous access to the NIFS database so in order to get a userid with a password one has to send a request to Research Information Center, NIFS, Nagoya 464-01, Japan.

3.13 NIST Atomic Spectroscopy Database (*http://aeldata.phy.nist.gov/nist_atomic_spectra.html*)

This database (currently version 1.0) is a part of the NASA Astrophysics Data System which is based purely on the World Wide Web. ASD contains critically evaluated data on energy levels, wavelengths and transition probabilities and reflects the most up-to-date state for these spectroscopic data. Currently, included are data of various degree of completeness for 36

elements. The search options are very basic, though full-size help is available on-line. There also exists a telnet version of ASD (*telnet://asd@atm.phy.nist.gov*) which contains data only for four elements.

3.14   NIST Atomic Transition Probability Bibliographic Database (*http://physics.nist.gov/PhysRefData/fvalbib/reffrm0.html*)

The NIST A-value bibliographic database is one of the first WWW atomic databases. This databank (current version is already 3.0) contains about 3000 references up to 1994 which are part of the collection of the Data Center on Atomic Transition Probabilities at NIST. The multiple selection criteria include element, isoelectronic sequence, author, journal, year of publication, method of calculation/measurement, etc.

3.15   Opacity Project TOPbase (*http://cdsarc.u-strasbg.fr/OP.html*)

The TOPbase[9] is a data management system (DMS) which was designed specially for presentation of the results from the widely-known Opacity Project[10]. This database which is located at the Centre de Données astronomiques at Strasbourg, France, contains energy levels, wavelengths, oscillator strengths and photoionization cross sections for ions of many astrophysically abundant elements. Like other DMSs, the TOPbase offers multiple options as for selection and presentation of available data including possibilities for graphical output. The TOPbase site can be directly reached at the host *cdsarc.u-strasbg.fr* with *topbase* as userid and *Seaton+* as password.

3.16   ORNL Controlled Fusion Atomic Data Center Databases (*http://www-cfadc.phy.ornl.gov/*)

In addition to collection of ALADDIN codes/data and a list of atomic and plasma databases, on the CFADC home page one can find a link to categorized bibliographic database of about 30,000 references dating from 1978 to present (work on adding 30,000 references till 1978 is in progress). All data are divided into 9 categories and tens of subcategories which embrace practically all atomic processes and characteristics related to nuclear fusion. User can select input parameters from the list of (sub)categories or make a search by author name. The other refined database at the CFADC presents experimental ionization cross sections measured in the Physics Division at ORNL. The CFADC host serves also as a temporary location of *Atomic Data and Nuclear Data Tables* journal and *Theoretical Atomic, Molecular, and Optical Community* WWW home pages.

3.17 SAM Project Data*
(*http://aniara.gsfc.nasa.gov/sam/sam.html*)

The aim of the "Systematic, Accurate, Multiconfiguration calculations" project which has recently been initiated by international collaboration of atomic theory groups is to produce, collect and distribute accurate atomic data with special attention paid to uncertainty evaluation. The SAM results – oscillator strengths, energy levels, wavelengths, hyperfine structure parameters – are stored mainly as PostScript (PS) or DVI sources of SAM collaborators papers or, in few cases, as PS, DVI or ASCII files of data tables. It should be added that one can find there a lot of data on intercombination and forbidden lines which are not well presented yet in other databases.

3.18 Uppsala University Databases
(*http://xray.uu.se/*)

The X-Ray WWW server at the Department of Physics at Uppsala University, Sweden, stores various information related to X-ray physics. One can find there the COREX database of core edge (inner shell) excitation spectra of gas phase atoms and molecules with bibliographies, the database of Henke scattering factors[11], a list of electron binding energies in eV for the elements in their natural forms, and a list of X-ray emission lines. The first two databases feature search by keywords with graphical output while the lists are the ASCII files. Note that Henke scattering factors can also be found at the URLs *ftp://grace.lbl.gov/pub/sf/* and *ftp://xray1.physics.sunysb.edu/pub/henke.*

3.19 Vienna Atomic Line Database
(*mailto:vald@galileo.ast.univie.ac.at*)

The only atomic database which is based solely on the e-mail interface is the Vienna Atomic Line Database (VALD) at the Institut für Astronomie, Vienna, Austria. The VALD includes data on atomic line parameters and provide tools for selecting subsets of lines for typical astrophysical applications. The data sets are extracted from different sources and are then critically evaluated. To become a VALD client, send an e-mail with your full name and **all** e-mail addresses you may use to the VALD administrator at *valdadm@galileo.ast.univie.ac.at.* With registration confirmation, user receives the VALD manual.

4 Proposals

Concerning the nearest improvement of an access to the on-line atomic data, we would like to pay attention of the Discussion Group to the following two proposals:

1. *Organization of two hosts — in the U.S.A. and in Europe — that would serve as mirrors of existing databases.*

Firstly, such mirrors should greatly facilitate an access to already available data. Practically all database host computers are not dedicated to atomic database management alone, and scheduled and unforeseen shut-downs due to activity not related to database management are not very uncommon. For instance, the NIFS databases are down almost every Saturday and Sunday. Secondly, the mirror service team might supplement the copies of non-Web databases with WWW interface. This task seems to be neither enormous nor unreal because the modern management tools like, e.g., PERL computing language, proved to be very successful in such applications. Thirdly, the mirrors may also serve as a repository of a free atomic software and even may run simple atomic codes under WWW envelope. In addition, the data on the mirrors might be filtered to avoid unnecessary duplication.

The operation of large WWW databases shows that middle-class workstations with sufficient disk space would be quite suitable for storing huge amounts of data and processing multiple simultaneous user requests.

2.   *Use of the e-Prints archive (URL http://xxx.lanl.gov).*

When visiting the WWW home pages of various atomic laboratories, one can easily notice that almost all hosts contain the copies of local group publications in different formats. Now the natural question arises why not to put them onto entirely automated system with different access modes, well developed search and selection options, immediate notification of new submissions, and possibility of free retrieval of papers? Fortunately, such a system does exist already for about 5 years and has *really* become the primary means in distribution of ongoing scientific information in high-energy physics, astrophysics, quantum physics, etc. Probably, the main widespread prejudice against e-prints is the lack of refereeing which is believed to lead to dissemination of low-quality results. No matter how solid this argument would be – have you never seen questionable papers in refereed journals? – it must be admitted that for some fields of physics such an open distribution of research works well and has real advantages for researchers in developed and especially undeveloped countries. It is a pity that the Plasma Physics (started from February 1995) and Atomic, Molecular, and Optical Physics (started from September 1995) e-prints archives still stand out for their very low load comparing to most other archives.

5   Conclusion

Although the 'wired' atomic data are becoming more easy accessible, the existing opportunities provided by the World-Wide Web are not fully utilized yet. We believe that the activity of this Discussion Group in coordination of joint efforts in further development of electronic atomic databases as well as the regular, biennial 'International Conference on Atomic and

Molecular Data for Science and Technology' recently proposed by A. Dalgarno and R. K. Janev can be extremely effective.

6   Acknowledgments

<div align="center">**REFERENCES**</div>

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Appendix I

Glossary of Internet terms

FTP:

File Transfer Protocol – a client-server protocol which allows a user on one computer to transfer files to and from another computer over the Internet. Also the client program the user executes to transfer files.

HTML:

HyperText Markup Language – hypertext document format used by the World-Wide Web.

HTTP:

HyperText Transfer Protocol – the client-server protocol used on the World-Wide Web for the exchange of HTML documents.

Telnet:

The Internet standard protocol for remote login.

URL:

Uniform Resource Locator – a draft standard for specifying an object on the Internet, such as a file or newsgroup. URLs are used extensively on the World-Wide Web. They are used in HTML documents to specify the target of a hyperlink. Examples:

> *http://plasma-gate.weizmann.ac.il/DBfAPP.html*
> *news:sci.physics.plasma*
> *telnet://aladdin@ripcrs01.iaea.or.at* — here *aladdin* is the userid.
> *ftp://topbase:Seaton+@cdsarc.u-strasbg.fr/users* — here *topbase* is the userid
and *Seaton+* is the password.

WWW:

World-Wide Web (also W3) – An Internet client-server hypertext distributed information retrieval system. On the WWW everything (documents, menus, indices) is represented to the user as a hypertext object in HTML format. Hypertext links refer to other documents by their URLs. These can refer to local or remote resources accessible via FTP, Gopher, Telnet or news, as well as those available via the HTTP protocol used to transfer hypertext documents.

Appendix II

Atomic Databases

NAME	COUNTRY	CONTACT	ACCESS	DATA
TOPbase	France	**C.Mendoza**	Telnet	EL,OS,TP,PH,WL
NIFS	Japan	**H.Tawara,T.Kato**	Telnet	EX,IN,CT,HP
NIST ASD	U.S.A.	**W.C.Martin**	WWW,Telnet	EL,OS,TP,WL
CfA Harvard	U.S.A.	**P.L.Smith**	WWW	EL,OS,TP,WL
CDS	France	—	FTP	VSC
CFADC	U.S.A.	**D.R.Schultz**	WWW	IN,Bibl: VSC
GAPHYOR	France	**J.L.Delcroix**	WWW,E-mail	Bibl: VSC
IAEA AMDIS	Austria	**R.K.Janev**	Telnet	EX,IN,CT,HP,Bibl
VALD	Austria	**F.Kupka**	E-mail	EL,OS,TP
CCP7	U.K.	**C.S.Jeffery**	FTP	EL,WL
SAM	U.S.A.	**T.Brage**	WWW	EL,OS,TP,HS
DASGAL	France	**A.Lesage**	WWW	Bibl: LS,SH
ADA	U.S.A.	**D.Verner**	WWW	VSC
NIST ATPBD	U.S.A.	**P.J.Mohr**	WWW	Bibl: OS,TP
ADRAL	Canada	**D.C.Morton**	WWW	EL,OS,TP
BIBL	Russia	**A.N.Ryabtsev**	FTP	Bibl: VSC
LANL EPAS	U.S.A.	**L.Kissel**	WWW	SF
Uppsala U.	Sweden	—	WWW	SF,WL,OS

Data keys:

Bibl: XXX - bibliography for XXX; CT - charge transfer cross sections; EL - energy levels; EX - electron impact excitation cross sections; HP - heavy-particles interaction cross sections; HS - hyperfine structure parameters; IN - electron impact ionization cross sections; LS - line shapes; OS - oscillator strengths; PH - photoionization cross sections; SH - line shifts; SF - scattering factors; TP - transition probabilities; VSC - various spectroscopic and collisional data; WL - wavelengths.