Spectr-W^3 online database on atomic properties of multicharged ions

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Abstract. The Spectr-W^3 information-reference system was developed in 2001–2013 and realized as an online Web resource based on the factual atomic database Spectr-W^3. The information accumulated in the Spectr-W^3 atomic database contains about 450,000 records and includes the experimental and theoretical data on ionization potentials, energy levels, wavelengths, radiation transition probabilities, and oscillator strengths, and the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. Those data were extracted from publications in physical journals, proceedings of the related conferences, special-purpose publications on atomic data, provided directly by authors. The information is supplied with references to the original sources and comments, elucidating the details of experimental measurements or calculations. To date, the Spectr-W^3 atomic database is still the largest factual database in the world, containing the information on spectral properties of multicharged ions. In 2014, the new stage in the development of the Spectr-W^3 atomic database started. The purpose of this stage is the creation of a new information section of the Spectr-W^3 database. This section would contain the information on the x-ray emission spectrograms registered from various plasma sources.

1. Introduction

Presently, the advances in the field of top technologies essentially depend on the availability of reliable and consistent data on the fundamental spectral properties of atoms and ions. The reason is that these properties are responsible for the interactions of matter with electromagnetic radiation and particle beams. Accordingly, the relevant data form the basis for upgrading high-precision diagnostic tools for the Inertial Confinement Fusion (ICF) studies and astrophysical research as well as for the development of tabletop x-ray radiation sources for semiconductor micromachining, microlithography, diffractometry, studies of ultra-fast chemical reactions, and many other technological and scientific applications. However, this kind of data, resulting from costly calculations and experiments, are dissipated over a great number of original papers and are often published in an incomplete form. Therefore, the needs for systematization and adequate interpretation of spectral properties of atoms and ions along with the availability to effectively employ large-scale data sets for the applied research unambiguously assume the development of appropriate atomic databases (ADBs).

A tremendous progress in the novel information technologies achieved in the last two decades on the basis of the World-Wide Web (WWW) has shown a very good potential for a worldwide exchange of scientific and technological information, including the atomic data. The most attractive features are friendly and understandable user interface, and powerful HTML language for creating and displaying hypertext documents able to support not only different alphanumeric formats but also graphics, including figures, formulas, tables, etc. Besides, WWW software is based on the standard operating systems of personal computers (PCs) and workstations and hence can readily be mastered by users.

A serious long-term effort made in 1988-95 at Multicharged-Ion Spectra Data Center (MISDC) of SRC VNIIFTRI resulted in the development of a factual atomic database SPECTR, which later served as a certified Database of Russian State Service of Standard Reference Data. Previously, the relevant atomic database (SPECTR ADB), implemented using the FoxPro DBMS (database-management software) for IBM-compatible PCs, was available to users locally at MISDC and was also distributed by the authors upon the agreement with the interested organizations. The SPECTR ADB was successfully used in a number of laboratories and universities worldwide, including RFNC-VNIITF. This database accumulated a considerable amount of factual information on the spectral properties of multicharged ions, low-ionized and neutral atoms, obtained at the leading research centers and university laboratories, which had been pursuing the studies in atomic physics, plasma spectroscopy and astrophysics over several decades.

The information accumulated in the SPECTR ADB included the experimental and theoretical data on ionization potentials, energy levels, wavelengths, radiation and autoionization transition probabilities, and parameters used in analytical expressions to approximate collisional cross-sections and electron transition rates in atoms and ions. The information was supplied with the references to the original sources and comments, elucidating the details of experimental measurements or calculations. The SPECTR ADB accumulated practically all the experimental data for the x-ray spectral range published up to 1994. Publications also served as a source to obtain the theoretical data. It should be noted that a significant portion of theoretical data was calculated specially for the SPECTR ADB by the highly-qualified experts of a number of universities and institutes of Russia and the Former Soviet Union: the Institute of Theoretical Physics and Astronomy of Lithuanian Academy of Sciences, the Institute for Spectroscopy of Russian Academy of Sciences, Voronezh State University, MISDC of SRC VNIIFTRI, Uzhgorod State University (Ukraine), and RFNC-VNIITF. The data were calculated using various theoretical methods and were published in detail mostly in paper collections, preprints and reports of the relevant institutions. Therefore, the SPECTR ADB was the only resource for the world scientific community presenting a full-scale access to these data.

In the middle of 1990-ties, RFNC-VNIITF specialists gained a wide experience in creating specialized Websites covering many directions of the research and spin-off activities. This resulted in a number of developments for the Web-versions of databases using the up-to-date commercial DBMS like ORACLE thus enabling to create the SPECTR-W^3 information-reference system in 2001-2014. The system is implemented as an online Web resource providing an access to the redeveloped and considerably extended Web-version of the SPECTR ADB, called SPECTR-W^3, and presenting the relevant additional information. The project to create the SPECTR-W^3 Web resource was carried out through the employment of the advanced technologies of the large-scale database development and Web-programming on the base of up-to-date software of leading world manufacturers. Using the tools of the Oracle-8 DBMS, a throughout revision and necessary correction of the previously accumulated data were performed from the viewpoint of their completeness, consistency, reliability, presence of doubled records, and compliance with the current state-of-the-art. With the follow-on data optimization, this enabled to significantly reduce the original amount of records. The SPECTR-W^3 ADB also incorporated new theoretical data and the results of high-resolution spectroscopic measurements obtained after 1995.

To date, the information accumulated in the SPECTR-W^3 ADB contains about 450,000 records and includes experimental, calculated, and compiled data on ionization potentials, energy levels, wavelengths, radiation transition probabilities and oscillator strengths, and the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. The SPECTR-W^3 site (http://spectr-w3.snz.ru) has been operating on the Web freely accessible round-the-clock since May 2002. Its homepage was integrated into the family of specialized databases for atomic and plasma physics on the Internet (http://plasma-gate.weizmann.ac.il/DBfAPP.html). Now the SPECTR-W^3 Web-resource serves about 50 visiting sessions per day from universities and research laboratories worldwide as well as from telecommunication companies and individuals. A number of experts also use the fully functional local version of the SPECTR-W^3 database, SPECTR-CD, created for the off-line operation on the Windows PCs. The SPECTR-CD setup package is available for a non-profit personal use on the SPECTR-W^3 homepage. It can be seen that to date the SPECTR-W^3 ADB is still the largest factual database in the world, containing the information on spectral properties of multicharged ions, as exemplified in part by active use of the SPECTR-W^3 ADB and SPECTR-CD.

2. The structure and interface of ADB SPECTR-W^3

The SPECTR-W^3 ADB contains data on 1) ionization potentials of atoms and ions, 2) excited energy levels, 3) wavelengths, radiation and autoionization probabilities for transitions in atoms and ions, 4) cross sections and rates of different collisional processes and 5) bibliographic information, thus consisting of five informational sections. To organize access to the Windows-based database, five query pages were designed using the well-proven Active Server Pages (ASP) technology. The example of Energy levels query page is presented in figure 1.

User specifies the data of interest, presses the Search button, and receives the query result in the form, presented in Figure 2. The query result may be sorted by any field of record. Note, when the user clicks on an appropriate reference in Reference field, the information on a data source is displayed (see figure 3).

As the ionization potentials, of atomic-level energies, radiative-transition wavelengths, probabilities, and oscillator strengths of are the digital data, their values are directly displayed after the query processes, as it is shown in figure 2. In the case of the collisional database section, the query result is represented by an analytic function of the particle energy (or temperature). For this kind of information, we used a set of parameters enabling to approximate cross sections or rates by using simple formulas. The example of the query result on the collisional data is shown in figure 4 with the related function FNRC1 presented in figure 5.

In parallel with the development of the Web-site pages, the activities are being carried out to put the pages on Apache Web-server. Using the Web-programming technologies, an algorithm to temporarily dump previous information inquires sent by user to the SPECTR-W^3 ADB is selected, which would be compatible both with Unix/Linux and Windows platforms. The algorithm uses portions of information recorded automatically on the users computer hard disk (the so called cookies). A version of data display at the users request in the form of HTML-marked Web-table was implemented with maximum number of the records displayed being specified by the user. Other version of data display in the plain text format and in the form of a Web-table to be emailed to the user is also being developed.

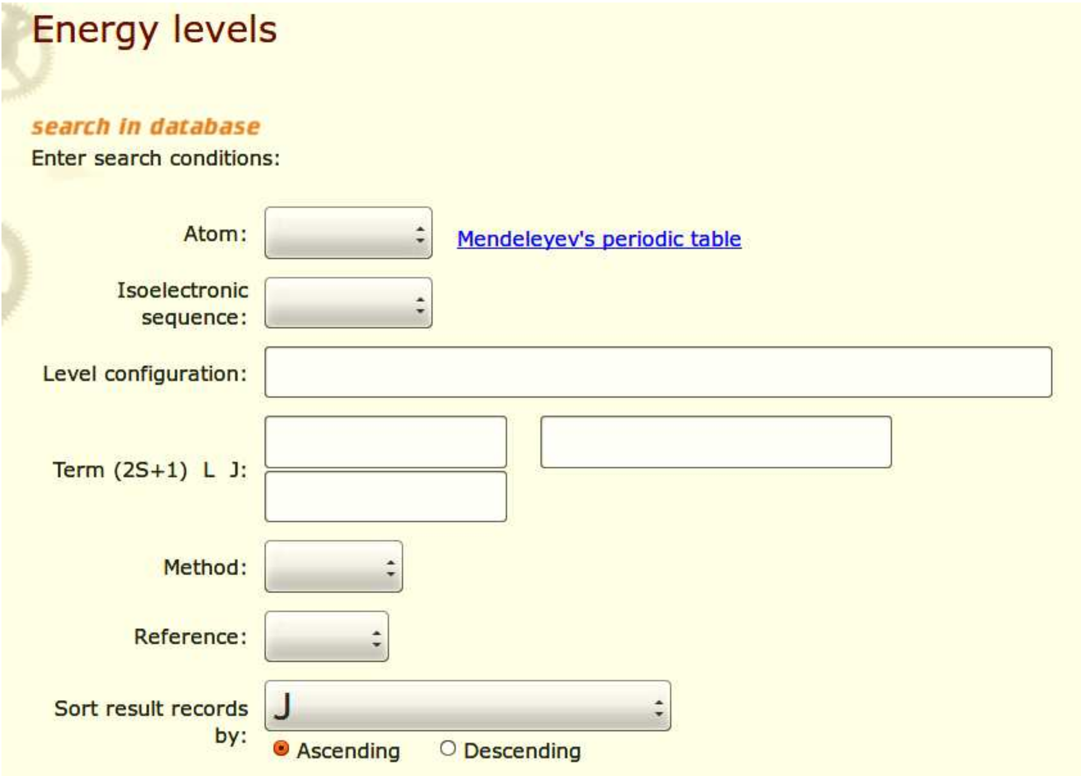
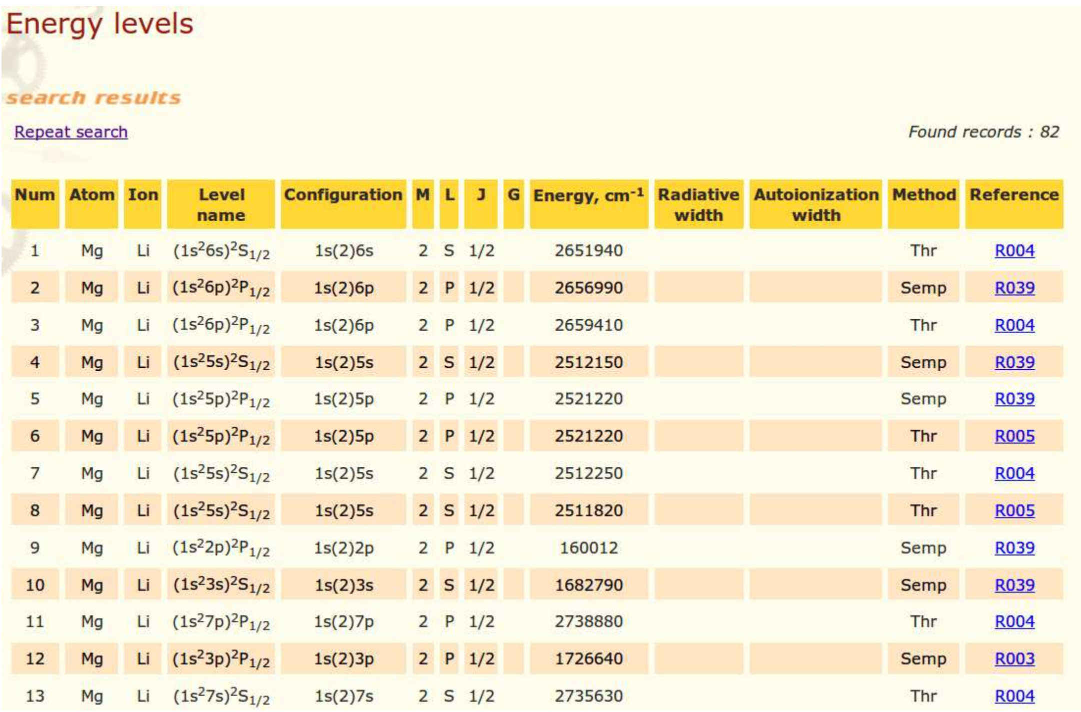


Figure 1. Energy level query page.



Energy levels

search results

Repeat search

Found records : 82

Num	Atom	Ion	Level name	Configuration	M	L	J	G	Energy, cm^{-1}	Radiative width	Autoionization width	Method	Reference
1	Mg	Li	$(1s^26s)^2S_{1/2}$	1s(2)6s	2	S	1/2		2651940			Thr	R004
2	Mg	Li	$(1s^26p)^2P_{1/2}$	1s(2)6p	2	P	1/2		2656990			Semp	R039
3	Mg	Li	$(1s^26p)^2P_{1/2}$	1s(2)6p	2	P	1/2		2659410			Thr	R004
4	Mg	Li	$(1s^25s)^2S_{1/2}$	1s(2)5s	2	S	1/2		2512150			Semp	R039
5	Mg	Li	$(1s^25p)^2P_{1/2}$	1s(2)5p	2	P	1/2		2521220			Semp	R039
6	Mg	Li	$(1s^25p)^2P_{1/2}$	1s(2)5p	2	P	1/2		2521220			Thr	R005
7	Mg	Li	$(1s^25s)^2S_{1/2}$	1s(2)5s	2	S	1/2		2512250			Thr	R004
8	Mg	Li	$(1s^25s)^2S_{1/2}$	1s(2)5s	2	S	1/2		2511820			Thr	R005
9	Mg	Li	$(1s^22p)^2P_{1/2}$	1s(2)2p	2	P	1/2		160012			Semp	R039
10	Mg	Li	$(1s^23s)^2S_{1/2}$	1s(2)3s	2	S	1/2		1682790			Semp	R039
11	Mg	Li	$(1s^27p)^2P_{1/2}$	1s(2)7p	2	P	1/2		2738880			Thr	R004
12	Mg	Li	$(1s^23p)^2P_{1/2}$	1s(2)3p	2	P	1/2		1726640			Semp	R003
13	Mg	Li	$(1s^27s)^2S_{1/2}$	1s(2)7s	2	S	1/2		2735630			Thr	R004

Figure 2. The example of the energy levels query result.

reference

Reference code:
R004
Author:
Knight P.E., Sanders F.C.
Journal:
Physical Review, 1981, v.22A, No.4, pp.1361-1369
Title:
S, p and d states of three-electron ions via z-dependent perturbation theory

Figure 3. The information on a data source R004.

Collision data

search results

Repeat search

Found records : 2247

Num	Atom	Initial Ion	Initial level	Final level	Approximation function name	a_0	a_1	a_2	a_3	a_4	a_5
1	Al	HE	$(1s^2)^1S_0$	$(1s3p)^1P_1$	FNRC1	1	12	137.3	.407	-.186	.756
2	Al	HE	$(1s2s)^3S_1$	$(1s3p)^3P$	FNRC1	1	12	21.39	-47.8	75.2	80.1
3	Al	HE	$(1s2s)^1S_0$	$(1s3p)^1P_1$	FNRC1	1	12	20.56	-50.4	74.4	88.2
4	Al	HE	$(1s2p)^3P$	$(1s3s)^3S_1$	FNRC1	1	12	20.13	-3.5	5.71	4.38
5	Al	HE	$(1s3s)^3S_1$	$(1s3p)^3P$	FNRC1	1	12	.272	2080	1.57	290
6	Al	HE	$(1s3p)^3P$	$(1s3d)^3D$	FNRC1	1	12	.155	1020	.556	134
7	Al	HE	$(1s^2)^1S_0$	$(1s3s)^1S_0$	FNRC2	2	12	137.1	.201	-.116	.0204
8	Al	HE	$(1s2s)^3S_1$	$(1s3s)^3S_1$	FNRC2	2	12	21.12	41.3	-14.2	3.34
9	Al	HE	$(1s2s)^1S_0$	$(1s3d)^1D_2$	FNRC2	2	12	20.52	120	-98.4	24.8
10	Al	HE	$(1s2s)^1S_0$	$(1s3s)^3S_1$	FNRC3	3	12	20.13	9.32	-12	5.72

Figure 4. The example of the collisional data query result.

approximation function

Electron impact excitation rate coefficient [cm^3s^{-1}] averaged over the Maxwellian energy distribution of electrons represented by the FNRC1 approximation function is defined as follows.

$$\langle v\sigma_{ij} \rangle = \frac{3.62\times10^{-15}}{a_1^4 g_i \sqrt{T_e}}\left[a_3 \exp(-y) + (a_4 + a_5)E_1(y)\right],$$

$$y = \frac{T_e}{a_2 \cdot 13.606},$$

where T_e[eV] is electron temperature, g_i is the statistical weight of the initial state, $g_i = (2S_i + 1)(2L_i + 1)$ or $(2J_i + 1)$ or $g(n_i)$ (n is the principal quantum number of the initial state).

The relevant script FNRC1.m for MatLab™ is placed here.

Figure 5. The function FNRC1 used for calculation of the rate of electron impact excitation.

In 2014, the new stage in the development of the Spectr-W^3 atomic database started. The purpose of this stage is the creation of a new information section of the Spectr-W^3 database.

This section would contain the information on X-ray emission spectrograms registered from various plasma sources. In the present time, the relevant software has been created and tested for the Spectr-CD local version of the database. The set of the spectrograms mostly obtained in the laser-produced-plasma experiments was also prepared. In 2015, the section Emission spectrograms will be available in the Web-version of the Spectr-W^3 database.

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