
XX SYMPOSIUM ON HIGH-RESOLUTION
MOLECULAR SPECTROSCOPY (HighRus-2023)

“Electronic Structure of Atoms” Information System for Atomic Spectroscopy

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Received October 26, 2023; revised October 26, 2023; accepted November 5, 2023

Abstract—Russia’s “Electronic Structure of Atoms” information and reference system for atomic spectroscopy is described. Its main characteristics and capabilities for supporting scientific research and training of specialists are explained. The data array contains more than 234 000 levels, with great attention given to experimental data and uniform filling across Z , including classified levels and transitions of all rare earth and transuranium elements and their ions. Original means of visualizing scientific data in the form of spectrograms, quantograms, and Grotrian diagrams are proposed. Presenting spectral data in the form of color interactive diagrams promotes understanding and analysis of the properties of an atomic system. In combination with its functionality, the use of spectral data from the “Electronic Structure of Atoms” information system is an effective way of solving different scientific problems and training specialists.

Keywords: atomic spectroscopy, scientific visualization, Grotrian diagrams, spectrograms, quantograms

DOI: 10.1134/S0036024424050145

INTRODUCTION

Providing access for scientists and developers to information on the spectra of atomic systems is one of the most complex and pressing tasks of supporting research in a number of scientific and technical areas of fundamental physics and applied areas, from astrophysics and gas laser physics to elemental analysis and archaeology. Resources containing information on atomic spectroscopy have come a long way from reference tables to computer systems. They are represented today mainly by Internet resources organized as information retrieval systems with a Web interface [1].

A number of such systems are known. They have been developed and supported by leading scientific organizations in the world. In the United States, the ASD system is supported by the National Institute of Standards and Technology (NIST) [2]. Similar systems are NIFS (Japan) [3], AMODS (Korea) [4], and VALD (Austria) [5]. Each system has an extensive database of spectra of atoms and/or ions. A combination of existing databases for finding information on atomic spectroscopy across many resources simultaneously is also being developed. One such solution is the portal of the European consortium VAMDC [6].

A familiar information resource in Russia is the SPECTR-W3 data bank on the spectroscopic properties of atoms and ions, created and developed at the

Russian Federal Nuclear Center (Snezhinsk) [7]. Since 2002, the resource has been made publicly available on the Internet and is currently one of the most authoritative and frequently used domestic Internet information resources on atomic spectroscopy. In Russia, the “Electronic Structure of Atoms” (ESA) information system for atomic spectroscopy has been published on the Internet since 2005. It continues to be developed and is comparable in its main parameters to the leading world analogs [8, 9].

Information systems for atomic spectroscopy usually have much in common, due to the general task of providing the user with the most accurate and reliable data on the energy levels and radiative transitions of atomic systems. At the same time, creating an exhaustively complete information resource on atomic spectroscopy is a difficult task, due to the large volume and fragmentation of the source data. In reality, we observe the specialization of each information resources.

Atomic spectroscopy resources basically have the ability to provide data on levels and transitions in tabular form upon user requests, including filtering and sorting. However, they also include tools for scientific graphics, modeling, and data analysis, based on complex algorithms for processing them. If the functionality of tabular views is approximately equivalent for all

Table 1. Comparison of the main parameters of information system databases

Parameter	ASD NIST	MUNICIPALITY	SPECTR-W3	ESA
Number of records by level				
All levels	106 522	>550 000	30 000	83 823
For transuranic	3 300	0	51	4 969
For rare earth elements	18 516	333 000	1 834	17 887
Number of records according to transition				
All transitions	224 521	255 000 000	80 000	158 814
For transuranic elements	865	0	54	4 033
For rare earth	16 681	3 146 000	2 250	23 589

such resources, they differ substantially in the field of visualization and analysis.

The “Electronic Structure of Atoms” information system also contains and is actively developing a number of data visualization and analysis services that can be useful in solving a wide range of scientific and engineering problems. Features of the ESA system are largely determined by it being created and supported on the basis of a classical university (Novosibirsk State University) and institutes of the Siberian Branch of the Russian Academy of Sciences. It focuses largely on training of physicists. The ESA system is the only one of the world’s leading information systems on atomic spectroscopy that has interfaces in both Russian and English. This is of great importance for educational institutions that teach in Russian.

ESA INFORMATION SYSTEM DATABASE

The volume, completeness, and reliability of databases are some of the most important properties of information systems, and atomic spectroscopy systems in particular. Due to the large volumes of spectral data, the complexity of processing, and the need to keep them up to date, there is some specialization among existing systems with regard to individual groups of elements, parameters of levels, and transitions.

The priorities of the ESA system are determined by the tasks of general analytics and training specialists. They consist of supporting a database of experimentally obtained parameters of energy levels and radiative transitions of neutral atoms and atomic ions of all elements of the periodic table. Particular attention is given to uniformly filling the database for all values of atomic numbers Z , including how the spectra of rare earth and transuranium elements is presented. This distinguishes the ESA system from a number of other resources, including the NIST ASD. Priority is given to classified data when filling the database.

Table 1 compares the volume and completeness of the ESA database to information resources that are

authoritative and often used in practice around the world. Resources with extensive experimental data bases were selected: ASD NIST, VALD, and SPECTR-W3. The ESA database currently includes more than 234 000 records on energy levels and radiative transitions of atomic systems, which exceeds the database volumes of most other atomic spectroscopy resources. Although the total number of stored records about levels and transitions in the VALD database is much higher than in the ESA and other compared systems, this is the result of the VALD database including large volumes of calculated data that do not have the accuracy needed for many scientific tasks.

The ESA database presents elements of the periodic table with Z from 1 to 110. Among the parameters determined for different levels are the electronic configuration, the notation of the term and its energy value, the internal quantum number J , and the level’s lifetime. For transitions, they include configurations of the upper and lower levels; the values of wavelengths; the intensity of lines; the strength of oscillators; the probability of a transition; and the excitation cross section, which basically corresponds to the data structure of other information resources.

For a number of problems, it is essential to what extent the information resource is filled with information about electronic configurations and terms of levels, and whether the configurations and terms of the upper and lower levels are known for radiative transitions. The ESA system classifies a much greater number of levels and transitions than other compared systems, which is an important advantage of the resource.

PRESENTING SPECTRA IN THE FORM OF SPECTROGRAMS AND VIRTUAL SPECTROSCOPE IS ESA

An important characteristic of the effectiveness of a scientific information resource is the ability to present data using scientific graphics. The most common way of visually presenting spectra is through spectrograms. Table 2 compares some characteristics of spectro-

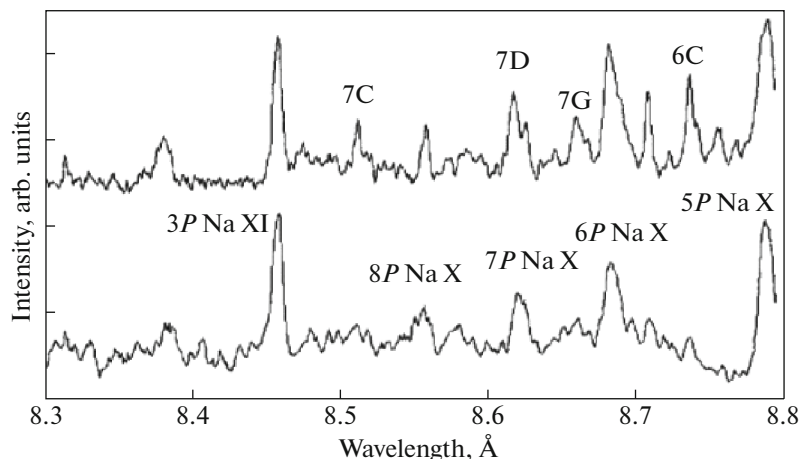
Table 2. Comparison of some properties of spectrograms generated by information resources on atomic spectroscopy

Parameters	SPECTR-W3	ASD NIST	VAMDC	IS ESA
What elements is it built for?	Only for items for which pictures are loaded	Does not work on elements with many lines	Is built for all elements	Is built for all elements
Relevance	Does not update automatically, databases do not match	Automatic creation from database	Automatic creation from database	Automatic creation from database
Permission	Bitmap image, max 800 pixels along axis	Raster image, 796 pixels along the axis	Vector drawing, scaled to fit the screen	Vector drawing, zoom tools
Chroma	Black and white (determined by the uploaded image)	Black and white	Black and white	Color in the optical range
Parameter Information	Matches the uploaded picture	Axis scale only	Only the value of the transition wavelengths	Axis scale displays wavelength when pointing at a line
Intensity information	Available	None	None	Weak transitions can be ignored using the sensitivity tool
Chart setup	Not provided	Range selection, line filtering during generation	Range selection, line filtering during generation	Range selection, interactive line filtering, scrolling

grams important for users that are generated by a number of information resources on atomic spectroscopy. The systems chosen for comparison were ESA, ASD NIST, SPECTR-W3, and VAMDC. Samples of spectrograms presented by these systems are shown in Figs. 1–3.

There are two fundamentally different approaches to displaying spectral data in graphical form. In SPECTR-W3, spectrograms are raster images not associated with data in the database. Such spectrograms are built manually by specialists and have a high quality of execution, but the building of such diagrams

is labor-intensive and in practice leads to shortages and the impossibility of automatic updating. There are very few such spectrograms in SPECTR-W3—only around 50 for almost 1500 atomic systems presented in the database. In the ASD NIST, VAMDC, and ESA systems, spectrograms are generated automatically from spectral information stored in the system database in any quantity, allowing for additional conditions imposed by the user. However, the quality of such spectrograms depends on the algorithms embedded in these programs. In many cases, today's are inferior to those performed manually by specialists.

**Fig. 1.** Densitogram in the SPECTR-W3 system.

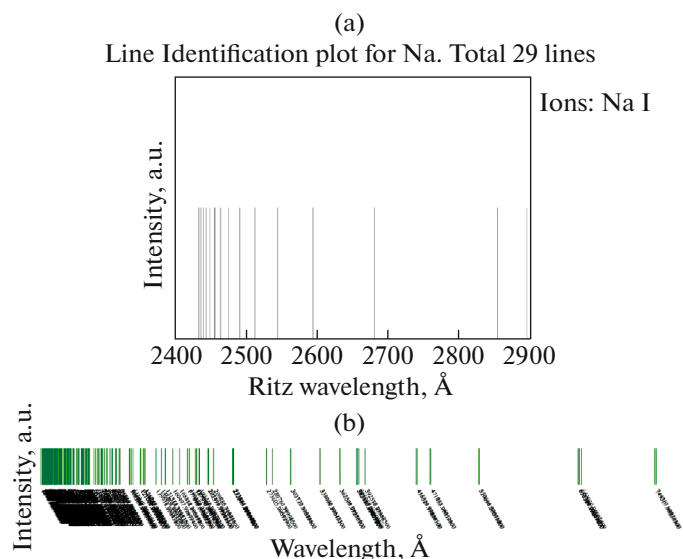


Fig. 2. Spectrogram of the sodium atom in the (a) NIST ASD and (b) VAMDC systems.

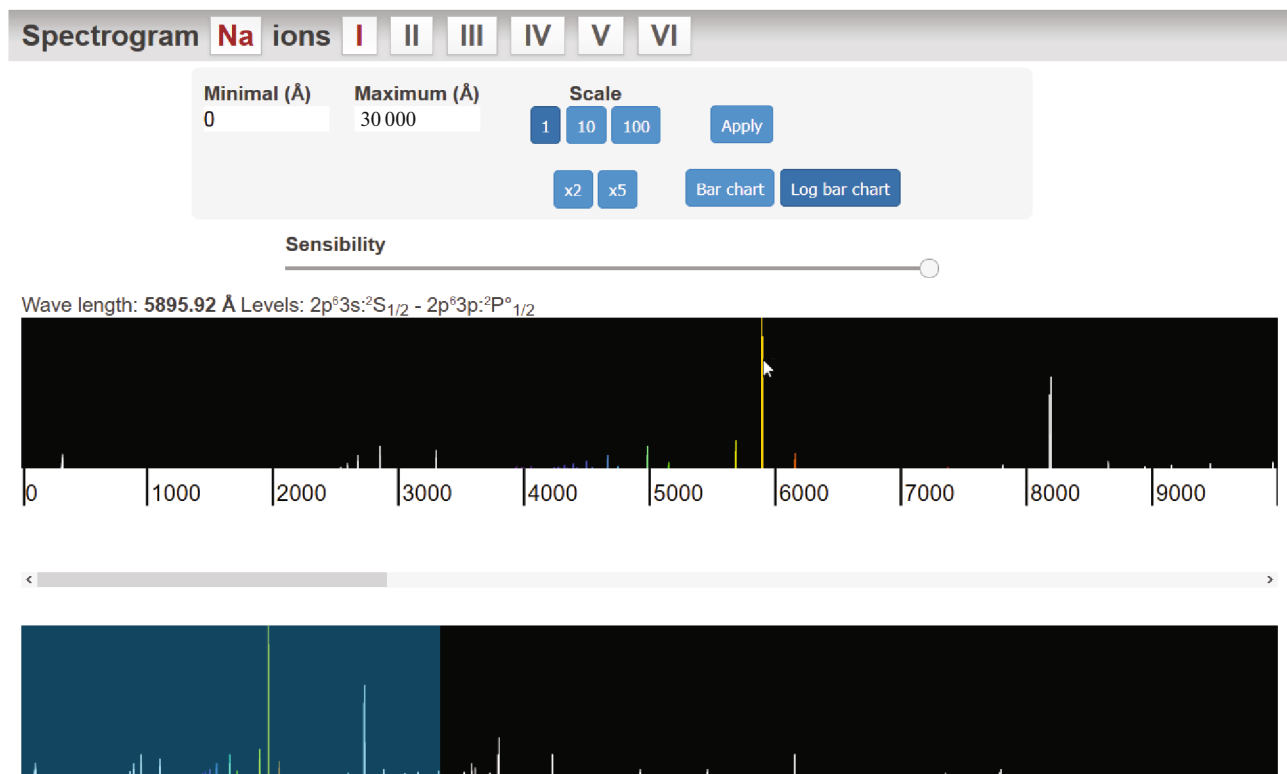


Fig. 3. Interface of the ESA virtual spectroscope when working with the spectrum of Na I. From top to bottom: (1) Virtual spectrometer control toolbar: windows for selecting the section of a spectrum, buttons for selecting scales of magnification, and a sensitivity tool for cutting off weak lines. (2) Fragment of a spectral range viewed with a magnification determined by the scaling factor. (3) Spectrogram of the full range of lines and scroller for adjusting the scaled spectrum window.

An essential parameter is the resolution of the spectrum diagrams, which is directly related to the amount of information that can be placed on a diagram. Unlike its analogs, vector graphics in the ESA

systems are supplemented with scrolling and scaling tools that allow us to enlarge a selected part of the spectrum in order to display fine and ultra-fine line structures even on small screens. Proper use of color

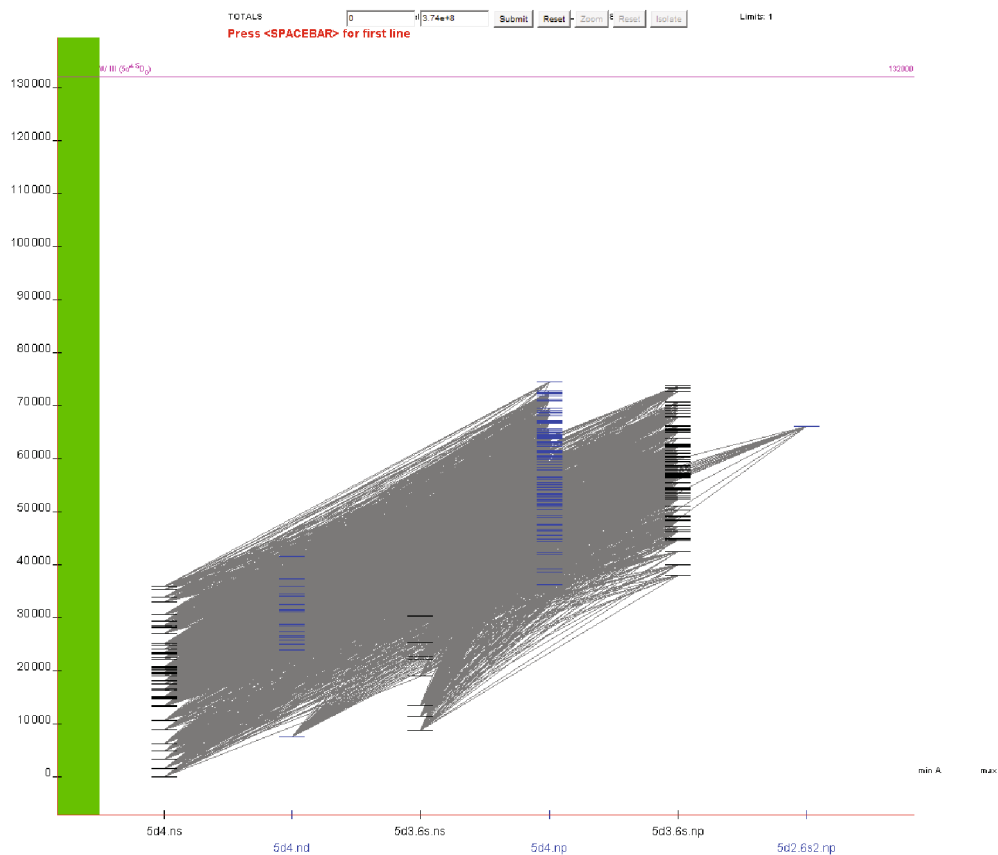


Fig. 4. Diagram of a W II atom in the ASD NIST system.

solutions can make the user’s work with scientific graphics much easier. In contrast to other information systems, the spectral lines of the optical range in the ESA system are shown in the appropriate color, like optical prismatic spectroscopes that are used everywhere in the educational process [10].

An important advantage of the ESA system is the availability of information about the parameters of transitions. In the ESA system, such information is presented on the spectrogram in the form of a wavelength scale, and the wavelength of a particular transition appears when the user points at the corresponding line (see Fig. 3).

The efficiency of working with a spectrogram is influenced by the possibility of customizing it for a specific task: choosing a range of the spectrum and filtering the displayed transitions according to certain parameters (e.g., intensity). This is most convenient in the ESA system, since it uses an interactive mode without reloading the page when changing the filtering and display parameters.

We can see the user properties of ESA spectrograms are in many respects superior to those generated automatically in other resources, and are not inferior to spectrograms created by specialists.

CONSTRUCTING GROTRIAN DIAGRAMS

Another way of visualizing the spectra of atomic systems is to present the electronic structure of an atom in the form of Grotrian diagrams, which are convenient in problems of generally analyzing the electronic structure of atoms and ions [8].

A Grotrian diagram is a complex graphic design that was created manually by specialists until recently. The process of creating diagrams is labor-intensive, so there is a constant shortage of them. There are also software versions of algorithms for constructing Grotrian diagrams. Today, this is possible in two Internet information resources on atomic spectroscopy: the NIST ASD and ESA systems.

Figure 4 shows an example of a Grotrian diagram automatically generated by the NIST ASD system for W II. We can see it is difficult to read the diagram, due to the lack of a line selection mechanism. In the ESA system, Grotrian diagrams are constructed dynamically on the basis of spectral information stored in the database of levels and transitions of atomic systems. Diagrams of 98 neutral atoms can be constructed in the ESA system (Pa, Fm, Md, No, and Lr transitions are not reflected in the diagrams, since there are still

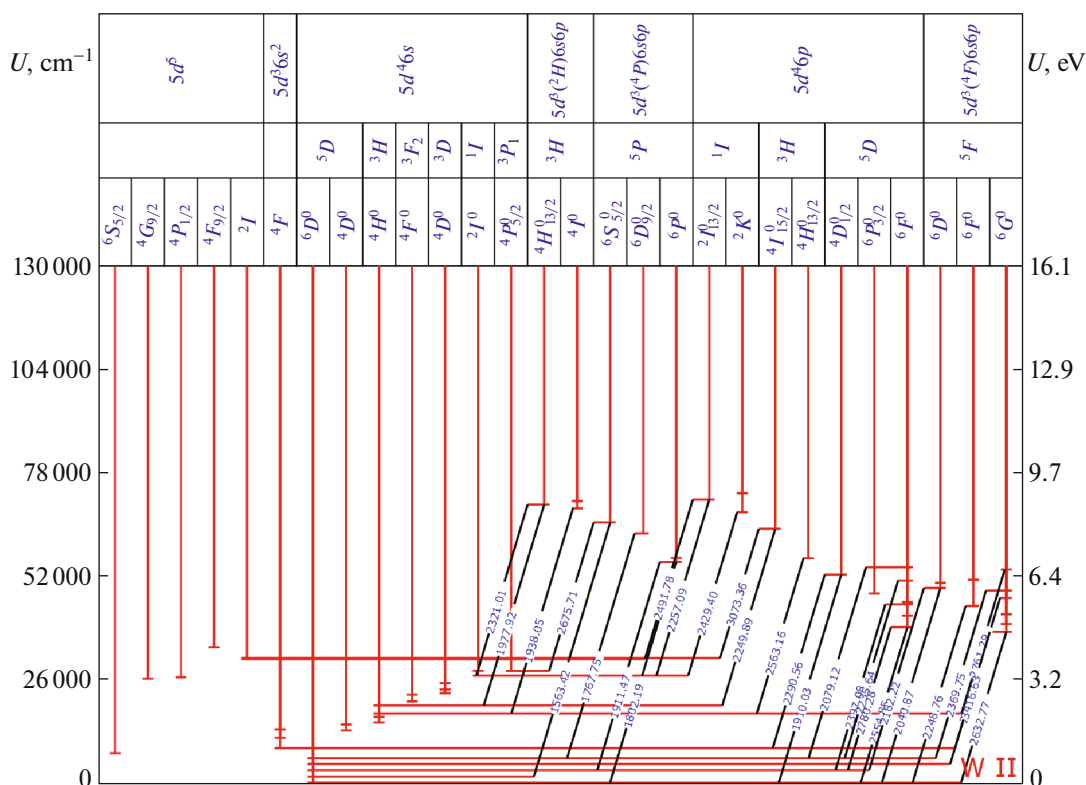


Fig. 5. Grotrian diagram for a W II atom in the “Electronic Structure of Atoms” information system. Levels and transitions are automatically selected when generating a diagram. The technique of spacing even and odd terms on opposite sides of the diagram from the central ground state was used. Energy levels are divided into groups according to the type of atomic residue and subgroups according to terms.

no data on classified transitions). Diagrams are also constructed for single and multiple transitions.

A number of solutions used in the ESA system ensure better quality of the resulting diagrams than

NIST ASD [11]. The main and most fundamental difference is the use of a special algorithm that allows the selection of information for placing on the diagram. The algorithm classifies levels and transitions accord-

Table 3. Comparison of the main characteristics of system for constructing Grotrian diagrams for various information resources on atomic spectroscopy

Parameters	ASD NIST	ESA system
Format and display area	Vector graphics, 1280 × 1024 pixels	Vector graphics scalable to fit window
Readability	Low: All spectrum lines overlap one another	High: Automatic selection of the number of lines needed to maintain readability
Technology and installation	Java applet; requires a Java installation with manual security configuration	JavaScript SVG; no installation required
Interactive capabilities	Displays information about levels and transitions	Displays information about levels and transitions, filtering according to transition wavelength and energy levels
Grouping levels by configuration and series	Configured by the user before plotting	Automatically adjusts, based on screen size and amount of data
Ability to open a diagram via a link	Filling out a form on the website	According to URL address. Just enter the link into the address bar of the browser. The link can be shared with other users

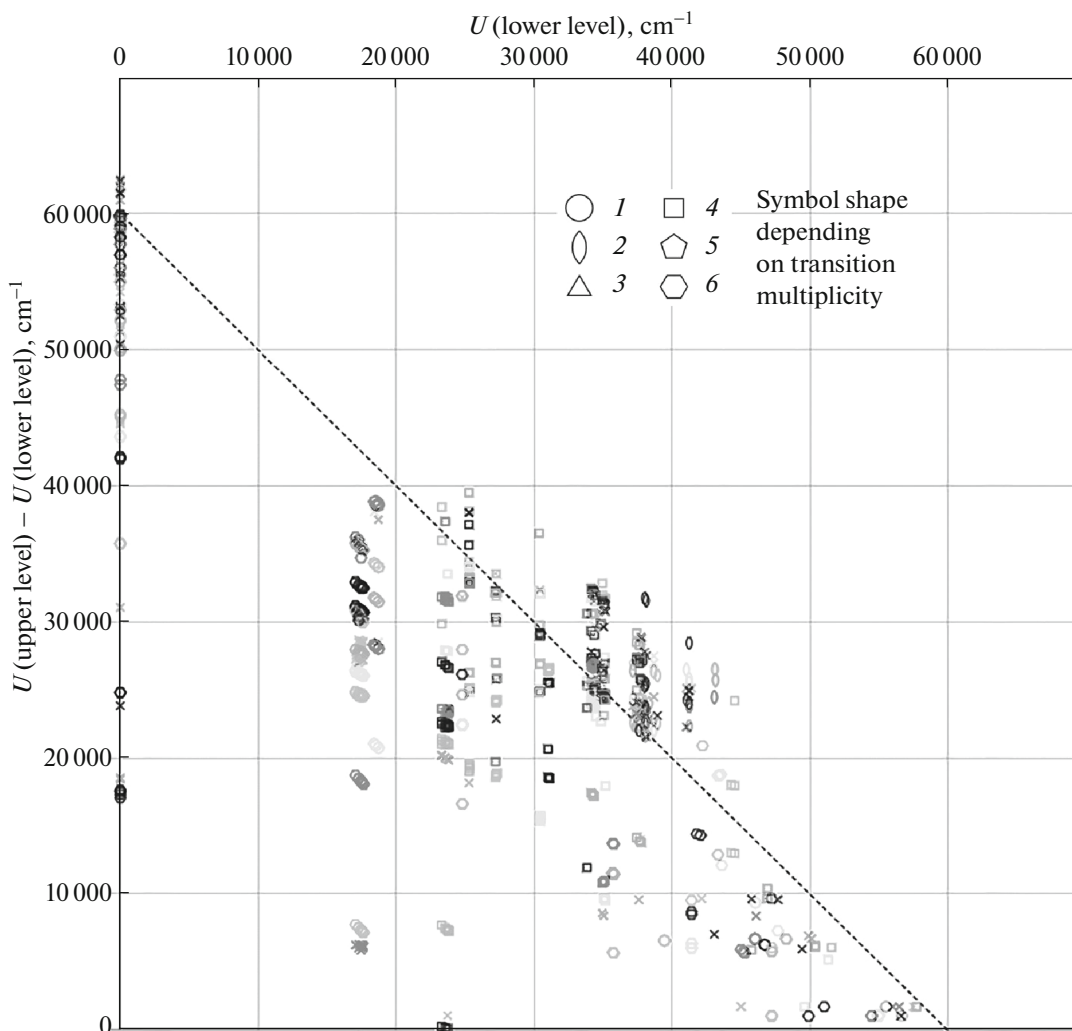


Fig. 6. Quantogram Mn I, plotted in axis coordinates X (lower level energy) and Y (differences in energy between the upper and lower levels of the transition). The dotted line is the boundary of ionization. Autoionization transitions lie above the limit of ionization. Denotations: \bigcirc singlet, \circ doublet, \triangle triplet, \square quartet, \pentagon pentet, \hexagon sextet, and \times prohibited transitions.

ing to a number of characteristics and then selects from each group such a number for placing on the diagram that, while maintaining general readability, it represents all the main features of the displayed spectrum.

The type of Grotrian diagram automatically constructed in the ESA system is shown in Fig. 5. The way it is constructed is based on separating even and odd levels to the right and left of the center line of the diagram. This way of constructing allows us to place a much larger number of lines than the traditional one, while maintaining the readability of the diagram by eliminating clusters of lines at one point and reducing their intersections.

Table 3 compares the ways of constructing Grotrian diagrams in the NIST ASD and ESA systems for a number of parameters. The ESA system's, which presents the electronic structure of atomic systems in

the form of Grotrian diagrams, allows us to construct diagrams for a greater number of such systems, while ensuring better readability.

QUANTOGRAMS

Changing the user properties of diagrams when switching to their computer execution allows the use of new, previously unused diagramming techniques, with the possibility of cognitively visualizing the electronic structure of atoms along with their interactivity and dynamics. The authors proposed one variant of such a diagramming technique in [12], which they call quantograms.

A coordinate system that differed slightly from Grotrian diagrams was chosen to construct quantograms: the energies of the levels of the atomic system are deposited along axes X and Y . The transition in

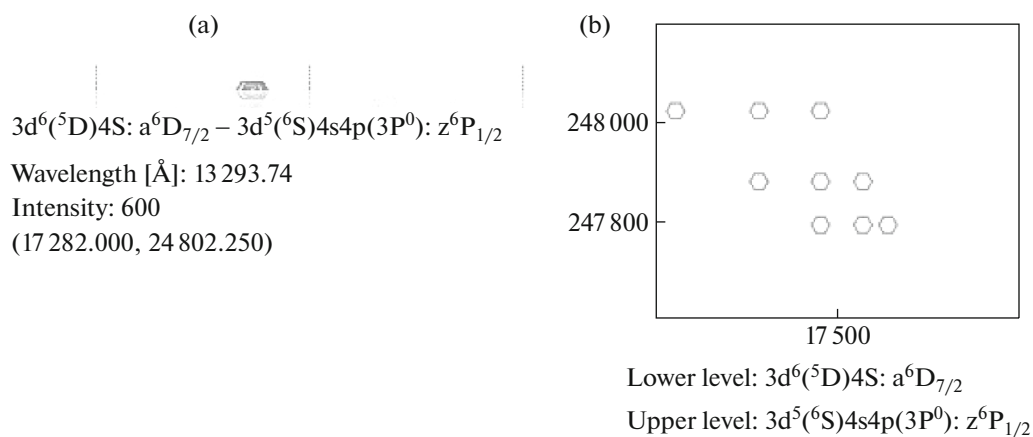


Fig. 7. Displaying multiplets on a quantogram. (a) Line in the spectrum of Mn I, selected on the quantogram by hovering the cursor and a tool that pops up. (b) Multiplet structure of the selected line, displayed in a separate window. Energy is indicated in cm^{-1} .

such a coordinate system is represented by a point whose X coordinate corresponds to the energy of the lower level, while the Y coordinate is energy of the upper level. All known transitions of the atomic structure can therefore be placed on a quantogram without loss of readability, in contrast to Grotrian diagrams. The quantogram field can be scaled to work with individual sections of the electronic structure (e.g., multiplets). Scaling is meaningless for a Grotrian diagram, due to the sizes of the segments representing transitions.

A series of transitions between energy levels on a quantogram are easily found as groups of points depicting transitions on the same vertical. Minor modification of the quantogram coordinates in $X = X$, $Y = Y - X$ allows us to visually compare energies of transitions. Those with similar energies are located near the same horizontal line (Fig. 6).

Representing the radiation transition on a quantogram by a dot opens up wide possibilities for associating pictograms with it by attaching inscriptions, color values, and other ways of enhancing information content. Dots are used to display singlet lines, diamonds are used for doublets, triangles are used for triplets, and so on.

When we hover over any transition, a tool appears showing the terms and configuration of its upper and lower levels, its wavelength, its intensity, and the coordinates of the transition. All transitions of fine term splitting are displayed when we click on a transition. The diagram is also easy to scale.

A separate window is used to display the selected multiplet. When we hover the cursor over the selected transition, all transitions that belong to this multiplet are selected (Fig. 7).

A sample program that generates quantograms has been created and integrated into the ESA system. The program is capable of generating quantograms for all

neutral atoms, along with ions of multiplicity 1–7 in the system database. All software is posted on the Internet in the public domain and can be used to solve scientific, technical, and educational problems. Experience with quantograms shows their advantage in clarity and readability over other types of visualizing the electronic structure of atoms in a number of cases and tasks. It is expected that the functionality of quantograms will be improved, distinguishing the new way of graphically representing atomic systems from traditional Grotrian diagrams.

CONCLUSIONS

The ESA database is one of the most complete Internet information resources on the spectra of atomic systems. At the same time, a number of features of the ESA database, including a large number of classified levels and transitions and better ways of studying spectra with high atomic numbers, allow us to recommend it for educational tasks and general analytical purposes that include working with the electronic structure of atomic systems throughout the range of atomic numbers Z .

The tools for visualizing atomic spectra in the form of spectrograms implemented in the ESA are much better than those in similar resources in terms of ease of use, due to their being created in the form of interactive applications and the use of vector graphics. Their use is especially effective for purposes of analytically working with spectra, and in training tasks in spectroscopy and related fields. Due to the simplicity and intuitiveness of the interface, working with spectrograms can be recommended even for high school students.

Presenting atomic spectra in the form of Grotrian diagrams automatically generated from the database system in the ESA system is a powerful tool for theo-

retically analyzing spectra and training specialists in the field of atomic physics and spectroscopy. Today, Grotrian diagrams are automatically created in both the NIST ASD and ESA systems. However, the construction algorithms used in the ESA system are more consistent with specialists constructing diagrams manually. They are more readable and better suited for both analyzing the electronic structure of an atomic system and training purposes.

The “Electronic Structure of Atoms” information system thus supports scientific research with spectral data on atomic systems, giving a researcher large amounts of up-to-date information on a wide range of parameters of energy levels and radiative transitions in tabular and graphical forms using spectrograms and Grotrian diagrams. At the same time, the general level of service is comparable to the best world analogs. It is therefore better to use the EAS system for some purposes, including general analytics of the electronic structure of atomic systems and training specialists in areas related to spectroscopy.

FUNDING

This work was supported by the Russian Foundation for Basic Research, project nos. 16-37-60094 and 16-07-00910.

CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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