Information-calculating system Spectroscopy of Atmospheric Gases. The structure and main functions

C.N. Mikhailenko, Yu.L. Babikov, and V.F. Golovko

Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk

Received June 30, 2005

This paper describes the structure and main functional capabilities of the information-calculating system Spectroscopy of Atmospheric Gases. The system is a convenient tool for the Internet access to the results of investigation in spectroscopy of atmospheric gases and for the interactive solution of some spectroscopic problems. The system can be used both for research purposes and for teaching the courses of optics and molecular spectroscopy in the higher school.

Introduction

Today, spectroscopic data available on the Internet are, as a rule, presented either in the form of archives arranged as file sets or in the form of resources containing the tools for searching the data, a user may have a need in as well as for extracting these data from the databases and mapping those on the site. Examples are the sites of the banks like HITRAN (Ref. 1), JPL (Ref. 2), CDMS (Ref. 3), etc. Among the resources of the second type the database sites of the Physics Laboratory of the US National Institute of Standards and Technology (Ref. 4) can be mentioned, for example, the database of heterodyne frequency measurements (Ref. 5). At the Institute of Atmospheric Optics, since 1999, we have been developing the information-calculating system *Spectroscopy of Atmospheric Gases*, http://spectra.iao.ru (ICS SPECTRA). Its main distinction from all known information resources on molecular spectroscopy is that it allows the users to solve applied spectroscopic problems interactively.

The main functions of the system are to provide access, via Internet, to the information on absorption spectra of atmospheric gases and solution of some problems in molecular spectroscopy in the interactive mode. Among the problems that can be solved with the system there are: 1) search, retrieval, and visualization of data on spectral line parameters; 2) preparation by users of their own gas mixtures; 3) simulation of high and low resolution laboratory spectra; 4) solution of the direct spectroscopic problem by the effective-operators method; 5) download the search results to a user's computer for their subsequent processing, or saving those in the system for use in the next sessions, later. Registration in the system is not obligatory. Both registered and non-registered users can work with the system, though registration allows access to a wider choice of the system's functional capabilities.

The construction principles, the structure, and technological aspects of implementation of the system's first version (http://spectra1.iao.ru) are briefly described in Ref. 6. Reference 7, thoroughly discussed one of the system's parts, namely, "direct spectroscopic problem" which allows a user to perform his/her own calculations of the vibrational-rotational spectra of water and ozone molecules by use of preset parameters of the effective Hamiltonian operators and dipole moment of the transition. In this paper, we do not consider this task in detail.

Our database of spectral line parameters is based on the HITRAN-2004 databanks (Ref. 8) and its updates for the year 2005, and GEISA-97 (Ref. 9). Besides, the database of spectral line parameters contains the data on the molecules of water, carbon dioxide (Ref. 10), and hydrogen sulphide, unavailable in other banks of spectroscopic information (Ref. 11). The data on six isotopic modifications of the water molecule were obtained from the results published in Refs. 12 and 13. The information on high-temperature spectra is provided by HITEMP (Ref. 14) and CDSD-1000 (Ref. 15) banks, and calculations based on data from Refs. 12 and 13. The original data included in the system was obtained at the IAO SB RAS in cooperation with the leading specialists in molecular spectroscopy from France, the USA, and China.

Earlier, the IAO laboratory of theoretical spectroscopy developed local information systems for personal computers, AIRSENTRY (Ref. 16), TDS (Ref. 17), and GEISA-PC (Ref. 18), which often have a larger number of functional capabilities. Our system is based on these information systems. We would like to mention one important circumstance. The toolkits of the ICS SPECTRA do not allow modeling the absorption/emission spectra of optically inhomogeneous media. So, the title of the ICS SPECTRA *Spectroscopy of Atmospheric Gases* is not related only to the atmospheric spectroscopy. Similar calculations dealing with, for example, the propagation of radiation through the atmosphere, can be performed with the AIRSENTRY system as well.

0235-6880/05/09 685-11 $02.00

We would like also to mention the information resource on molecular spectroscopy (Atmospheric spectroscopy, http://saga.atmos.iao.ru), a part of the web-portal http://atmos.iao.ru, which has also been developed at the IAO SB RAS. The purpose of this resource is somewhat different to that of the system we present in this paper. The main concern of the authors was the development of the information model of a subject area, which is in this case the molecular spectroscopy, and a structured data model of this subject, i.e., the development of operations with these data, study of ontologies, etc.

System structure

The ICS SPECTRA is a program complex designed to retrieve information from databases, process it, and display the results in a text or graphical format. It is a special feature of this complex that the user interface is built-up on basis of Internet technologies. The architecture of this complex is traditional for the program systems of this kind and consists of the main program aimed at processing the user's queries and mapping the information and it is arranged according to the module principle comprising the class and subprogram library, and a database.

The database is an essential part of the system. It consists of three parts, a subject oriented database, a reference database, and the database of administrative information and metadata. The content of all these three parts is described in Ref. 6. The database operates under the DBMS MySQL (Ref. 19). The part of the data that does not require search by different criteria is stored in the file system. Metadata involves menu description and references to the data stored in the database.

The library of subprogram classes consists of three parts: the library of computational modules, PHP class library (Ref. 20) and a service library. Computational modules are written in C^{++} or Fortran language. The system's main computational modules are the programs of calculating different spectral functions (written in C^{++}) and the GIP program (Refs. 7 and 21) for solution of the direct spectroscopic problems (is written in Fortran). The PHP class library is a set of classes, which are abstractions of the entities both of the subject domain (molecules and their isotopic forms, spectral bands, gas mixtures, mixtures of isotopomers, spectra, etc.) and of those, essential for system's functioning (users and groups, user sessions, menu, graphics). The service library is written in PHP (Ref. 22) and includes a set of auxiliary functions used both in classes and in the main program.

The main program is written in the PHP language and performs the following functions:

– user authorization;

– management of user interaction with the system;

– processing of user's query (URL) to the system generated by the *menu* module;

– execution of a query by accessing the database and performing necessary computations;

– generation of an HTML-page with the results of query on the basis of the available template.

To build page templates, we used the template processor SMARTY (Ref. 22). We have added a new frame to it, namely, a template that can be activated. As a rule, the frame consists of two parts: a PHP code which accesses the corresponding functions of the class library to acquire data and the very template to generate an HTML-code. We believe that this approach makes the system's architecture solution ordered and complete.

The main capabilities of the system

The system is aimed at giving the access to spectroscopic data so that on this basis users can solve a set of applied problems. Figure 1 shows a title page of the system as it is seen by a registered user.

As is seen from Fig. 1, along with the title page the user has an access to six system's sections: *Molecules*, *Gas mixture spectra*, *Cross-sections*, *Direct problem*, *Auxiliary data*, and *Saved spectra*.

The system's sections can be accessed by pressing a corresponding button in the system's menu. To press the desired button, a user must click it with the mouse.

The section *Molecules* is meant for giving information on spectral line parameters and modeling the spectra in the profile *Molecule/Isotopic species/Band*. By pressing the button corresponding to this section, a user goes to the page *Molecules/Survey*. This page is shown in Fig. 2. The section contains a list of 45 molecules, for which the system has information on their spectral line parameters (a table in the left part of the window). Figure 2 shows a fragment of this table. To select a desired molecule, a user must click at its chemical formula in the second column of the list. In the right-hand part of the window, there appears general information on the molecule chosen, namely, its number, code, formula, weight, composition, partition function of each of the molecule's isotopic species, and the range of temperatures, for which it is possible to calculate the spectrum. In this block, there is a citation list where the data on spectral line parameters for the selected molecule can be found. To obtain information on the vibrational-rotational bands of the molecule, the user must select one isotopic species in the list if references selected. To select an isotopic species, the user must press the button Code for the selected source of data. Figure 3 shows the result of such a selection for the molecule $H_2{}^{33}S$ from the IAO database (the page *Molecules/Bands*).

The section *Gas mixture spectra* is designed to provide information on spectral line parameters and simulate the spectra in the profile *Gas Mixture/Range*. Having pressed the button that corresponds to this section, the user goes to the page *Gas mixture spectra /Parameters* (Fig. 4).

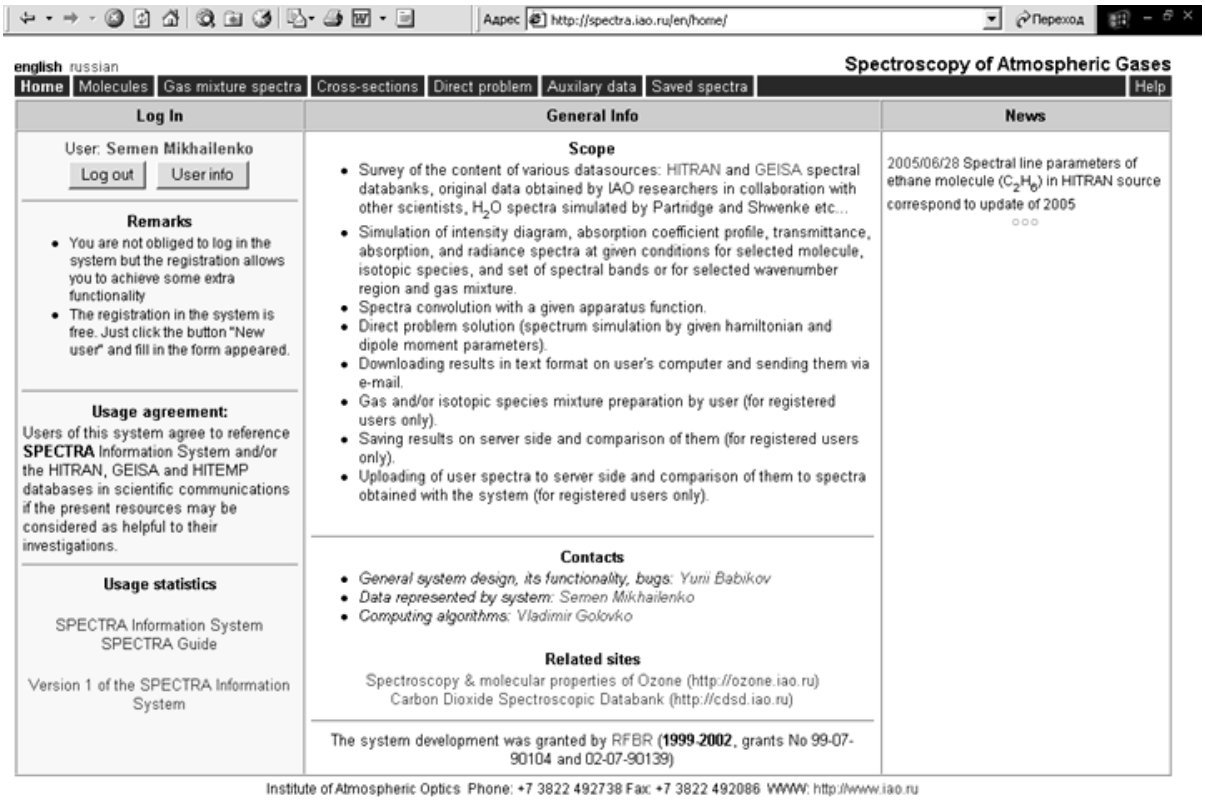

Fig. 1. Title page of the SPECTRA system.

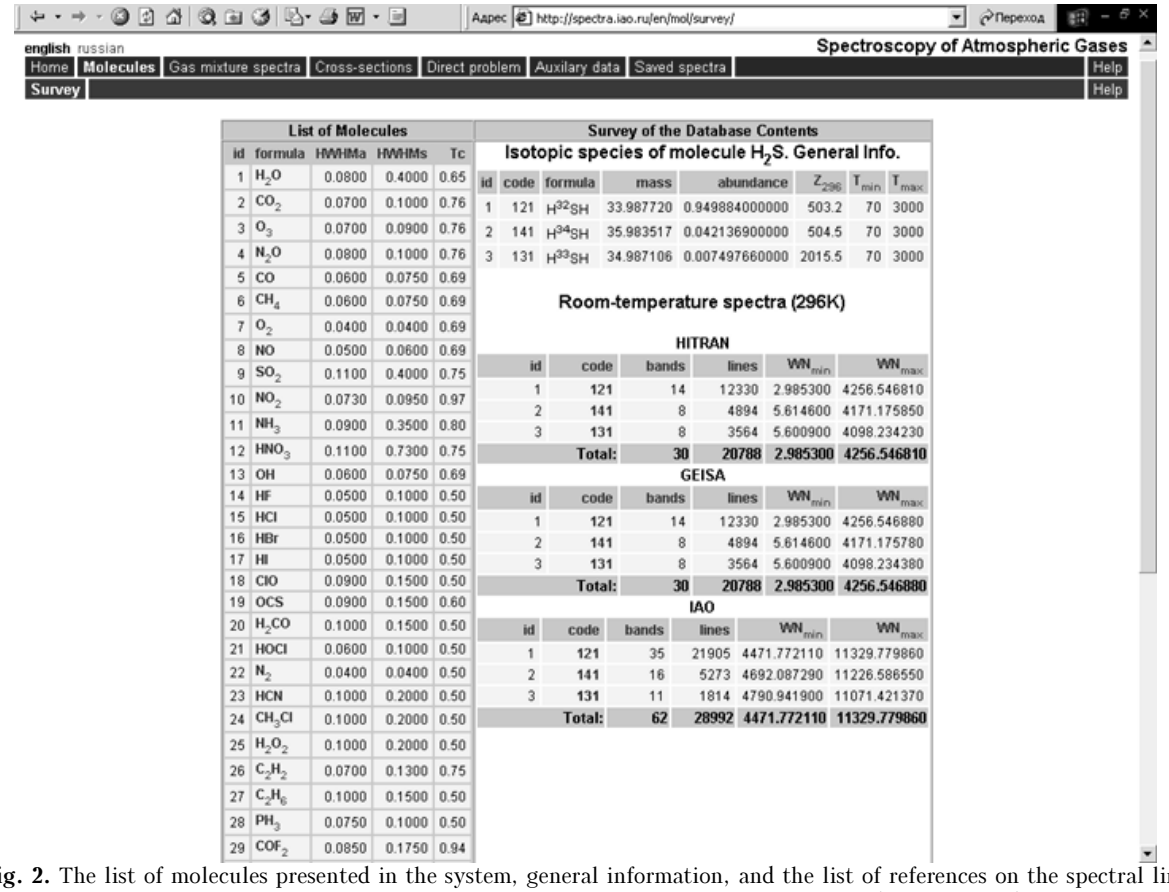

Fig. 2. The list of molecules presented in the system, general information, and the list of references on the spectral line parameters for a chosen molecule with the example of the molecule of hydrogen sulphide.

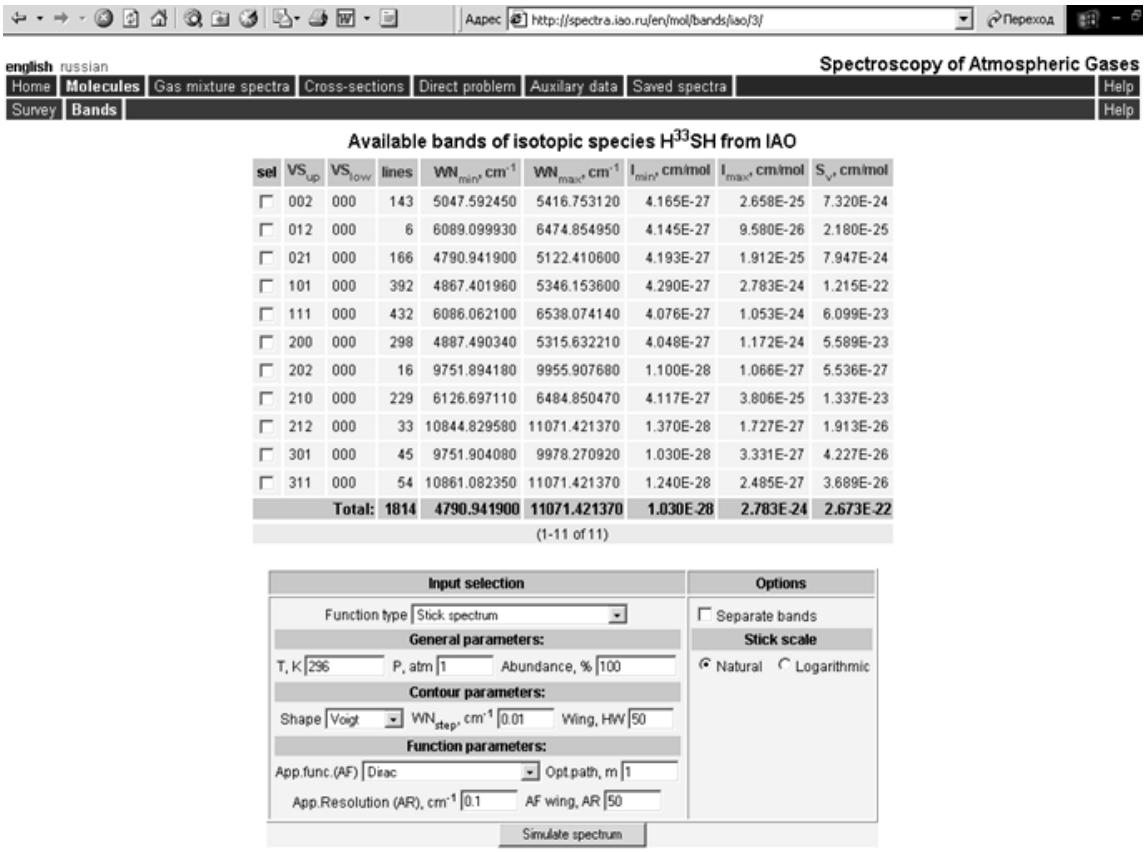

Fig. 3. The list of vibrational-rotational bands with the example of the $H_2{}^{33}S$ molecule from the IAO databank.

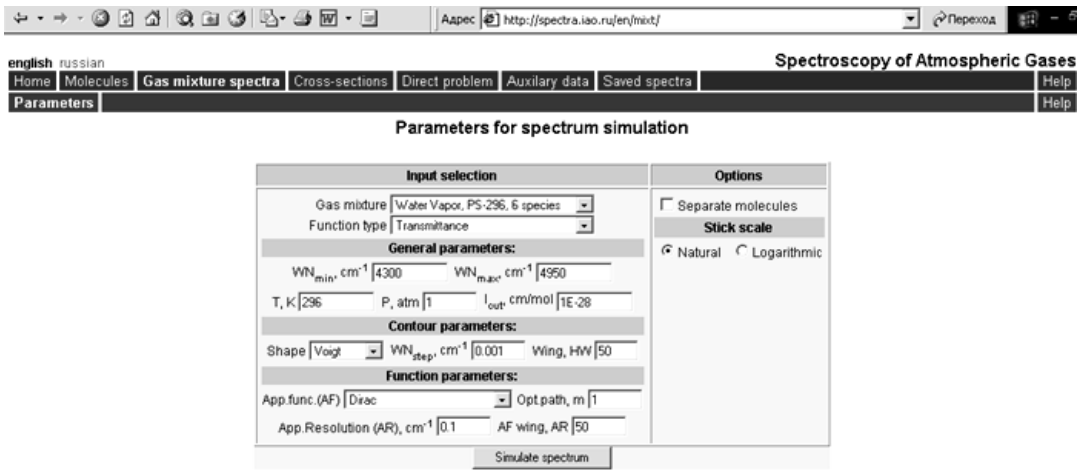

Fig. 4. Parameter selector for calculating the spectrum of a chosen gas mixture in a specified wave number region.

The user specifies the parameters in the spectral parameter selector by selecting a gas mixture and the type of a spectral function, setting a spectral range, pressure, temperature, path, etc., and thus he/she can calculate the spectrum of the desired gas mixture under the desired conditions and in the desired spectral interval.

The section *Cross-sections* allows a user to look through the experimental information on the absorption cross sections of seven molecules, namely N_2O, SO_2, NO_2, SF_6, $ClONO_2$, HNO_4, and N_2O_5. The system contains information on the absorption cross sections of the molecules listed, which corresponds to the HITRAN data. Note that the information on spectral line parameters taken from this source corresponds to HITRAN 2004 (including the 2005 updates), while the information on absorption cross sections corresponds to HITRAN-2000. Figure 5 shows the page *Cross-sections/ Survey*.

On the left, in Fig. 5, there is a list of molecules for which the system presents the data on their absorption cross sections. On the right, there is a list of experimental spectra of a selected molecule.

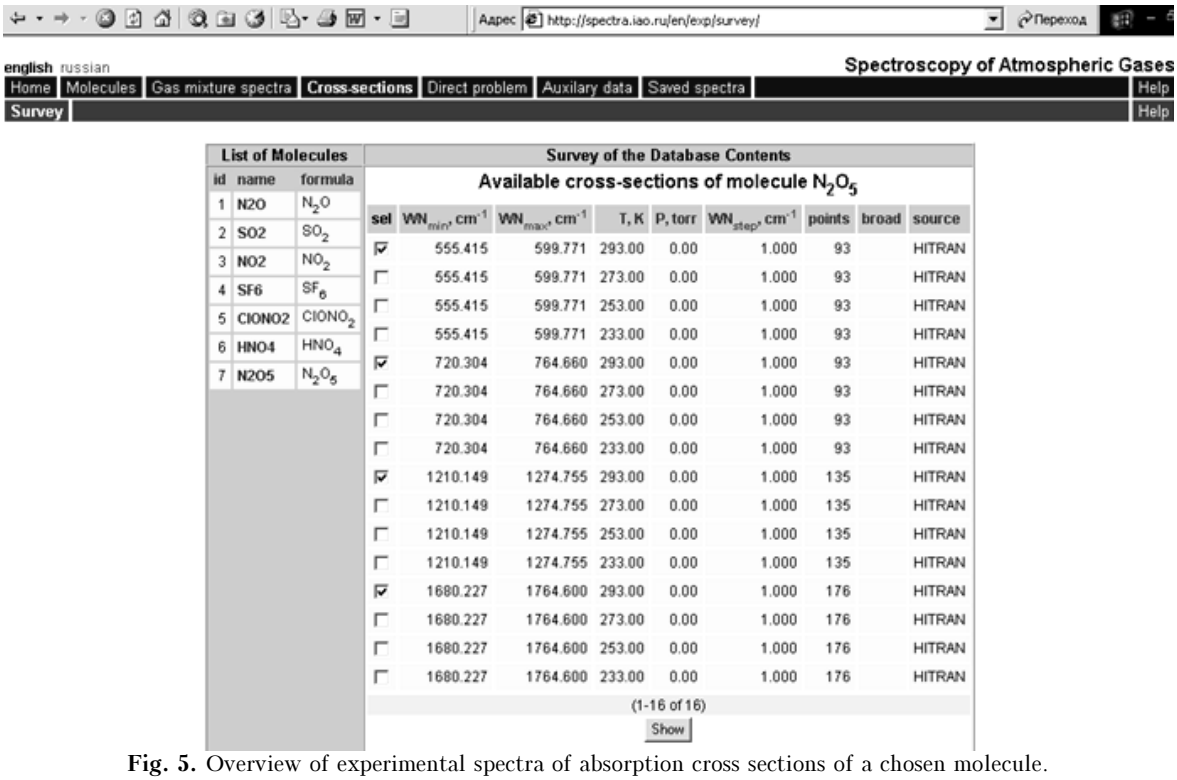

Fig. 5. Overview of experimental spectra of absorption cross sections of a chosen molecule.

The section *Direct Problem* allows a user to calculate vibrational-rotational spectra of water and ozone molecules by use of preset parameters of Hamiltonian and transition dipole moment. Description of this section and of user's calculation of the spectra is given in Ref. 7. Note that to successfully exploit this section, a user must have knowledge of the basics of effective operators theory and its applications to the problems of molecular spectroscopy.

The section *Auxiliary data* consists of two subsections: 1) *Auxiliary data/Gas mixtures* and 2) *Auxiliary data/Mixtures of isotopic species*. This section is designed for users needed in the formation of gas mixtures containing different molecular components (Subsection 1), and mixtures of isotopic modifications of a chosen molecule (Subsection 2). Subsection 1 contains a list of standard mixtures and user formed mixtures. Subsection 2 (Fig. 6) contains a list of molecules, for which it is possible to form mixtures of isotopic modifications (left part of the page).

This list is the same as that in the section *Molecules/Survey*. In the right-hand part of the page there is a list of isotopic species of a selected molecule. Mixtures of isotopic modifications of molecules and gas mixtures in Subsection 1 can be of three types:

1) standard mixtures within the system (Mixture Nos.1 and 9, Fig. 6);

2) user defined mixtures accessible to other users (Mixtures Nos. 4, 6, 13, 15, 22, 27, 28, Fig. 6);

3) personal user mixtures inaccessible to other users (Mixtures Nos. 5, 7, 10, 16, 18, 23, 24, Fig. 6).

When preparing a mixture, a user can make it publicly accessible or personal. A user has the right to modify and delete the mixtures of the second and third types. Only registered users can prepare mixtures. Non-registered users can only look through the publicly accessible mixtures.

Note that in the list of gas mixtures, there are standard mixtures corresponding to ten atmospheric models (Mixtures 1–10 of the section *Auxiliary data/Gas mixtures*). Again, we emphasize that this does not mean the possibility of modeling atmospheric spectra. By using these mixtures a user can simulate laboratory spectra for the mixtures that correspond to the atmospheric gas content.

The section *Saved spectra* is accessible to authorized users only and it is designated for manipulations with the spectra earlier simulated or uploaded by the user. The spectra of this type can be obtained by using the system's tools or they can be loaded to the system from the user's computer. The section is intended for loading and storage of spectra, their comparison, and deleting of unnecessary spectra.

Reference or help system

In addition to the above listed sections there is also a help system, in the ICS. It can be accessed by pressing "Help" box on the right edge of the menu. The information is mapped in a separate browser window (Fig. 7). The window is divided in two parts. On the left, there are *Contents*. On the right, there is information about a selected system's section.

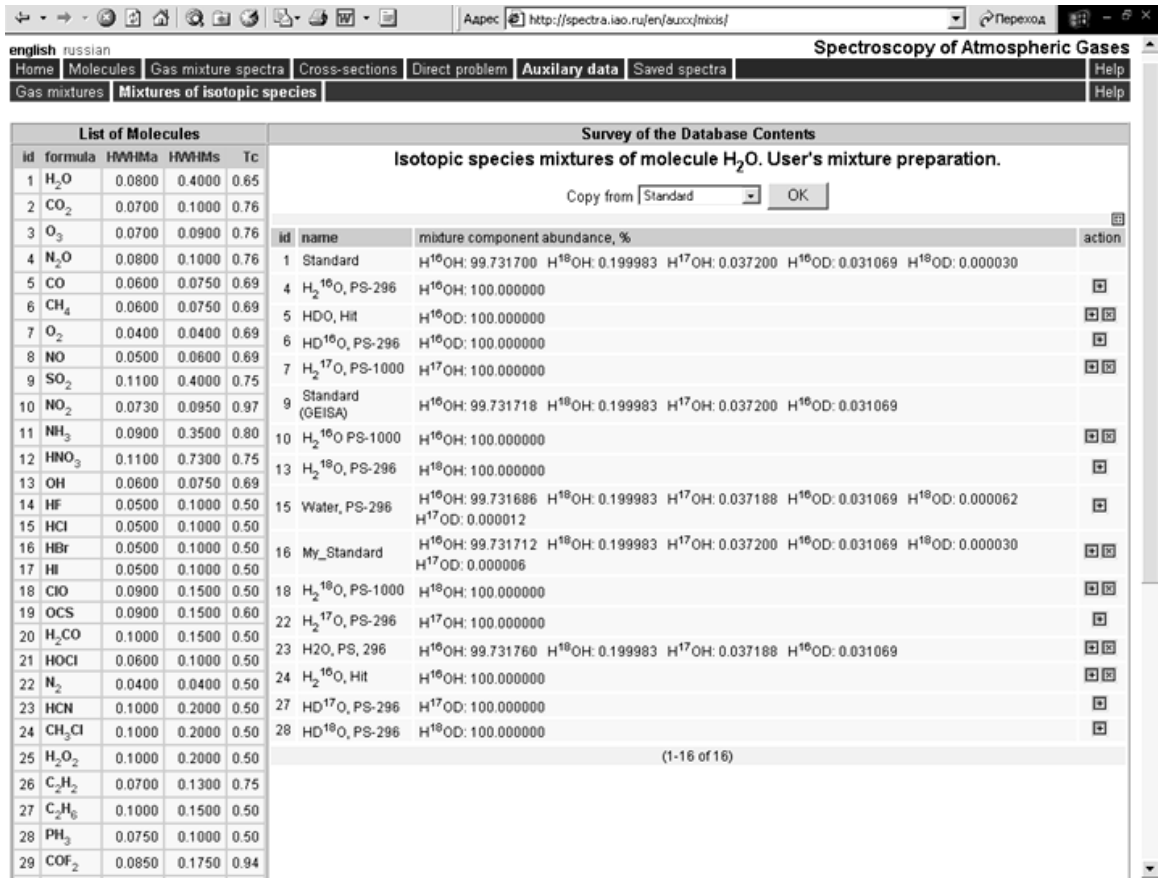

Fig. 6. A list of mixtures of isotopic modifications with the example of the water molecule.

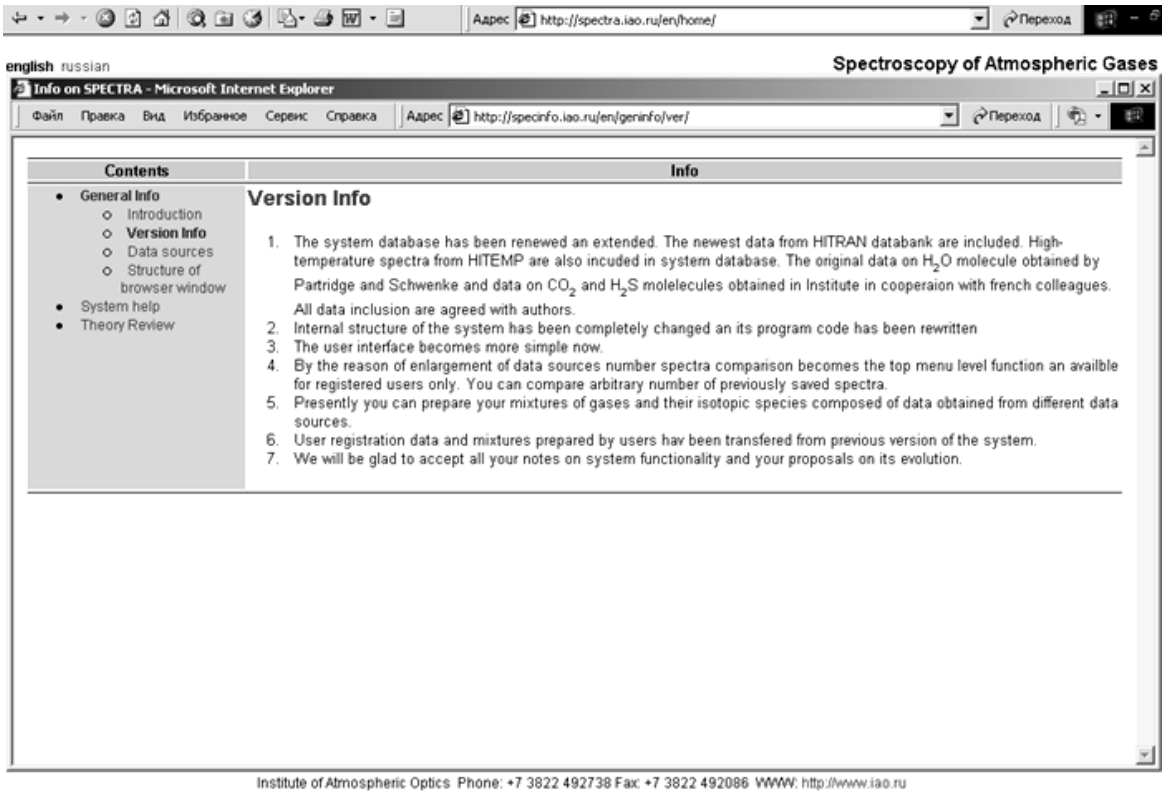

Fig. 7. A typical view of the help window.

The ICS help system consists of three parts (Fig. 7): *General Info*; *System help*; *Theory Review*.

The part *General Information* gives a brief annotation on the ICS (*Introduction*), the information on the current system's version (*Version Info*), and six sources of data on spectral line parameters: HITRAN, GEISA, HITEMP, CDSD, PS, and IAO (*Data sources*). It also describes browser window structure (*Structure of browser window*).

The part *System help* gives a thorough description of all the six system's sections. In this part of the help system, section titles fully agree with the ICS section titles.

In the part *Theory Review*, there are definitions and main formulas for calculation of spectral functions (the sections *Spectrum functions* and *Absorption Coefficient*), spectral line contours (*Line shapes*), temperature and pressure dependences of the characteristics to be calculated (*Pressure and Temperature Dependences*), convolution of high-resolution spectrum with the instrumental function (*Convolution of spectra*).

Frequently Asked Questions (FAQs)

As noted above in this paper, the system's main objectives are the access to spectroscopic information and interactive solution of some spectroscopic problems. We decided to give explanations to the main questions regarding implementation of the system's functions in the form of answers to the questions that often arise when working with the systems of this kind.

First, in the Sections **Introduction** and **System Structure**, it has already been said that this version of the system allows calculations of spectra to be made only for optically homogeneous media. Thus, this system does not allow modeling the atmospheric spectra or spectra of gas media with an inhomogeneous distribution of temperature, pressure, concentrations, etc.

What spectroscopic information and for which molecules can be found in the system?

The system provides two types of spectroscopic information: spectral line parameters (both experimental and calculated) and experimental spectra of low resolution (absorption cross sections). The list of molecules, for which the system has data on spectral line parameters can be found in the section *Molecules/Survey* (see Fig. 2). For each molecule, there is a set of isotopic species and a list of literature on the spectral line parameters. The banks HITEMP, CDSD, and PS contain only calculated data. The banks HITRAN, GEISA, and IAO are compilations containing both calculated and experimental data.

The molecules for which there is information on experimental absorption cross sections are listed in the section *Cross-sections/Survey* (see Fig. 5). Data from this section can be downloaded to a user's computer only in a graphical form.

How can I get information on the spectral line parameters for a separate band of the molecule I have selected?

To obtain the data on spectral line parameters for a separate band (or a group of bands) of a molecule selected, you will need to go to the section *Molecules*. For example, a mouse click of the hydrogen sulphide formula (molecule No. 31 in the list of molecules on the page *Molecules/Survey*) will call information saying that the data on spectral line parameters for this molecule are stored in three databanks, namely, HITRAN, GEISA, and IAO (see Fig. 2). Then, by clicking code *131* of the isotopic species $H_2{}^{33}S$ from the IAO bank you obtain information on eleven spectral bands of selected molecule (see. Fig. 3). Click the desired bands with the mouse in the left column to select them from the list. Under the band list, there is a selector of spectral parameters. To obtain information about a spectral line parameter, the box *Function type* on the left side of the selector (*Input selection*) must be set to *Stick spectrum*. If you have chosen more than one band from the list, then on the right side of the selector, for your convenience, you may check the field *Separate bands*. After this, press the button *Simulate spectrum* at the bottom of the spectral parameter selector. The result of the query is shown on the page *Molecules/Simulation* (Fig. 8).

As is seen from Fig. 8, separation of the bands consists in displaying of the corresponding lines in different colors.

How can I obtain information on spectral line parameters for a gas mixture for some particular wave numbers?

To obtain spectral line parameters of a gas mixture in some spectral range, you will need to go to the section *Gas mixture spectra* and formulate your query using the selector for the parameters of the spectrum to be modeled (see Fig. 4). To formulate the task for the system, you need to specify your target gas mixture. The mixture can be selected from the pop-up list of mixtures (selector parameter *Gas mixture*). Figure 4 shows an example of obtaining information on six isotopic modifications of the water molecule (the mixture *Water Vapor, PS-296, 6 species*) from the PS databank in the wave number range from 4300 to 4950 cm^{-1}. The answer to the query is displayed on the page *Gas mixture spectra/Simulation*. This page looks similar to that of *Molecules/Simulation* in Fig. 8. If a gas mixture contains different molecular components, then their lines can be shown in different colors like the lines of different bands in Fig. 8.

How can I get the information on spectral line parameters in the text format?

It is possible to obtain information on spectral line parameters as a text file from the pages *Molecules/Simulation* (Fig. 8) or *Gas mixture spectra/Simulation* by pressing the button *Show*, which is placed between the graphical representation of the spectrum and the spectral parameter selector. The text file is loaded as a separate browser window. If the file is large enough, its load can take time. A *.zip text file can also be downloaded to a user's computer. To do this, make use of the button *Download*. Another way of obtaining the desired information is to send a *.zip file via e-mail using the button *E-mail*.

How can I calculate transmission (absorption, emission) spectrum or absorption coefficient?

One can calculate all the four spectral functions using the parameter selector to calculate the spectrum either in the section *Molecules* (see Figs. 3 and 8) or in *Gas mixture spectra* section (see Fig. 4).

To calculate the spectrum in a specified wave number range, use the selector and select a gas mixture in the field *Gas mixture*, specify the type of the function to be modeled by selecting it from the pop-up list in the *Function type* window, and specify the wave number range (parameters WN_{min}, and WN_{max}, cm^{-1}). Temperature, pressure, path length, and intensity cutoff for the lines that you wish to be taken into account in modeling are found in the corresponding selector fields. In calculations of absorption, transmission, and emission coefficients you need to pay attention to the *Contour parameters*, namely, contour shape, line wing width (in half-widths) and the modeling step. If you have chosen a wide spectral range, which involves a large number of lines of a gas mixture, and a very small modeling step, it can be time consuming to calculate the spectrum. The system allows for the influence of the instrumental function. Function type is selected from the pop-up list of the field *App. func.* (AF). In this case, instrumental resolution must be specified in the field *App. Resolution* (AR), cm^{-1}. Figure 9 shows the calculated result of the transmission spectrum for the mixture *Water Vapor, PS-296, 6 species* in a range of 4600–4650 cm^{-1}. The calculation was performed for normal temperature

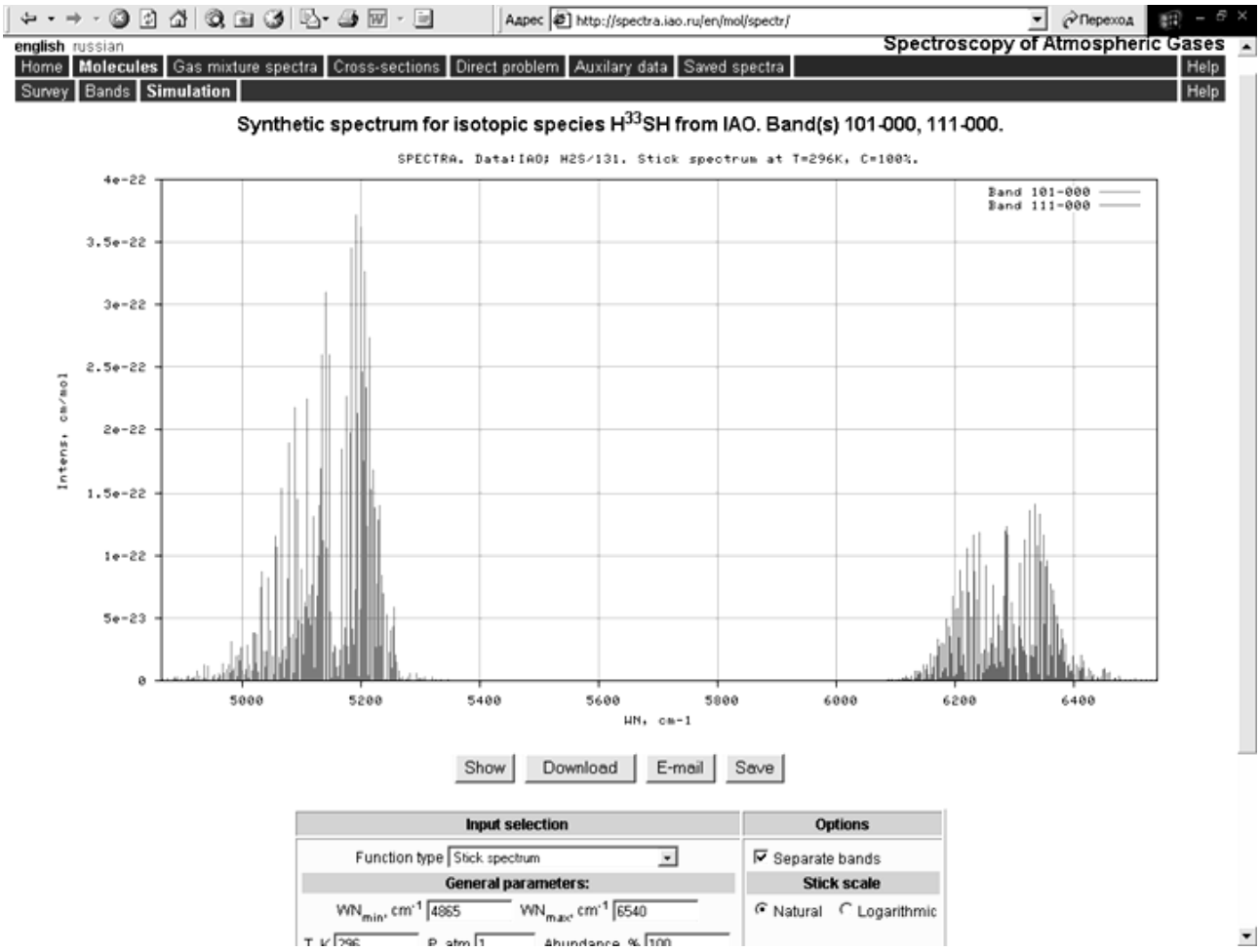

Fig. 8. The calculated results on the spectrum (intensity diagram) for the chosen bands of the $H_2{}^{33}S$ molecule.

(296 K), pressure of 0.2 atm, and path length of 100 m. In the calculation, we used a Voigt contour with the wing as wide as 50 half-widths. We also took into account all the lines with the intensity higher than 1×10^{-28} cm/mol, frequency step was 0.001 cm^{-1}. The influence of the instrumental function was neglected (Dirac instrumental function). The calculation time did not exceed 3–4 s. The calculated result is shown in Fig. 9. Between the spectrum plot and the selector, there is a vertically reduced diagram of intensities.

Spectral functions in the section *Molecules* for a group of selected bands are calculated in a similar way. As is seen from Figs. 3 and 4, the parameter selectors for modeling the spectrum in these sections are the same.

How can I save obtained information on the server side?

As mentioned above, this option is available for authorized users only, since one of the attributes of the information to be saved is the user's name. The obtained information can be saved on the server's side from the pages *Molecules/Simulation* (see Fig. 8) and *Gas mixture spectra/Simulation* (see Fig. 9) by pressing the button *Save* placed between the spectrum plotted and the spectrum parameter selector. The information saved can be accessed through the section *Saved spectra* shown in Fig. 10. Saved spectra are classified into six types (the field *Spectrum type* in Fig. 10) and correspond to six types of spectral functions in the parameter selector (see Figs. 3 and 4). For example, the spectrum from Fig. 8 is saved in the considered section as *Stick spectrum*, which was the last note in the list in Fig. 10. The spectrum shown in Fig. 9 can be saved as *Transmission spectrum* in the section *Saved spectra*. In Fig. 10, the spectra derived by means of the system's tools are marked with "S". Those spectra which were loaded to the system from the user's computer are marked by the indicator "U".

How can I prepare a mixture of isotopic species of the molecule selected?

This service is accessible to the registered users only. To prepare a mixture of the isotopomers, you must go to the section *Auxiliary data/Mixtures of isotopic species* shown in Fig. 6.

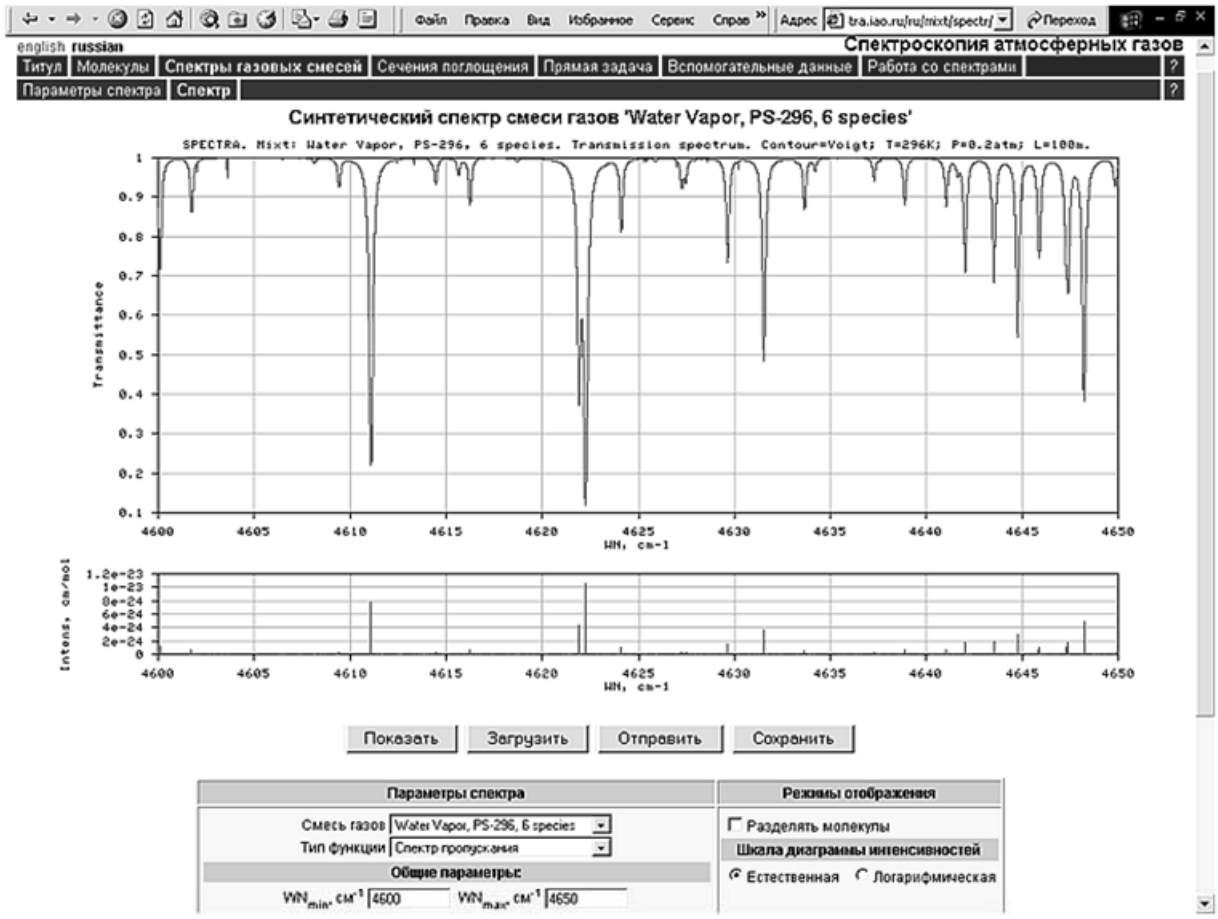

Fig. 9. The calculated results on the transmission spectrum of the chosen gas mixture in a specified wave number range.

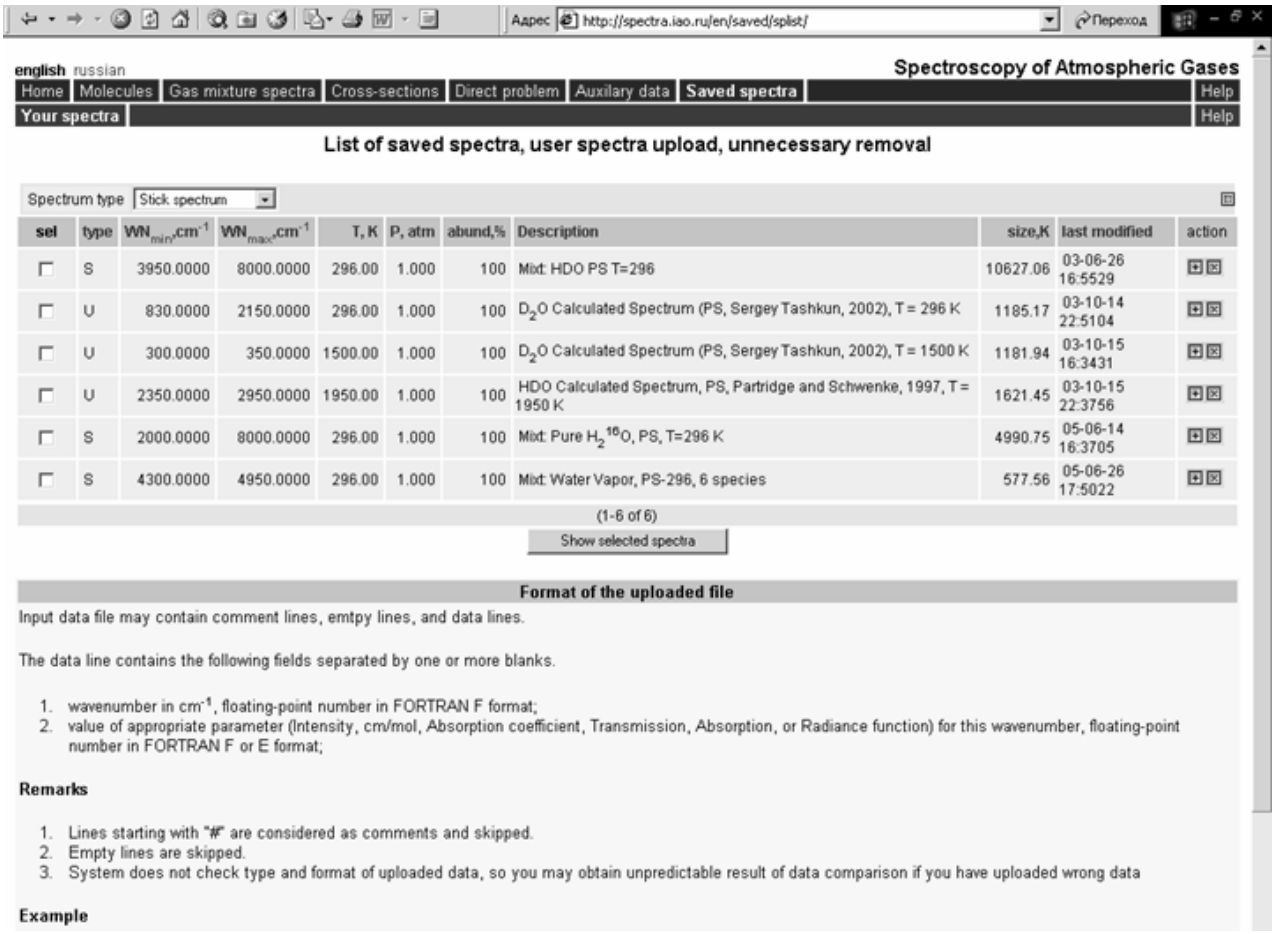

Fig. 10. An example of user's saved spectra (intensity diagrams).

To select a desired molecule, press the button corresponding to the formula of this molecule in the list of molecules. A new mixture can be prepared either by copying an already existing mixture (selected from a pop-up list in the field *Copy from*) or by forming a new one. When you have chosen the method, press the button *Add* in the upper right corner of the mixtures list. As soon as you have pressed *Add*, in the screen there appears the form *Add user's mixture*. The form lists all the isotopic species of the selected molecule and the relevant bibliography on the spectral line parameters. The user must fill in the field *name*, enter the values of relative concentrations of the desired isotopic modifications of the molecule, and to cite the references from which the spectral line parameters have been taken.

When you have filled in the form and pressed the button *OK*, a new record will appear in the list of mixtures. In front of the name of the user mixture, there are buttons for modifying and deleting this mixture (the field *Action*). When you press the button *Modify*, there appears the form *Modify user's mixture* similar to the form *Add user's mixture*. To save the modifications, you have typed in the form, press *OK*.

When isotopic mixtures of important molecules have been prepared, you can proceed to preparing a gas mixture.

How can I prepare a gas mixture?

This service is accessible to the authorized users only. To prepare a gas mixture, you will need to go to the section *Auxiliary data/Gas mixtures*. This page shows a list of all the gas mixtures accessible to the users of this system. The procedure of preparing a new gas mixture is similar to the above procedure of preparing the isotopic mixtures of molecules. If you press the button *Add*, there will appear the form *Add user's mixture*. The form contains all the 45 molecular components contained in the lists of molecules (see Figs. 2 and 6).

The form can be filled in and saved in the way, similar to that in creating a mixture of isotopic species of a molecule. For each molecule, a mixture of isotopic species is selected from a pop-up list *Isotopic species mixture*, which is found in front of each molecular formula. Once you have filled in the form and pressed *OK*, there will appear a new record in the list of gas mixtures. The new record will also appear in the pop-up list of the *Gas mixture* box in

the parameter selector for the spectrum modeling (see Figs. 4 and 9).

Concluding remarks

The SPECTRA information-calculating system provides, via Internet, the access not only to the known spectroscopic databanks (Refs. 8, 9, and 14), but also to the data not provided in other banks (Refs. 10, 11, and 15). It is a specific feature of this system the possibility of interactively solving some spectroscopic problems on modeling the high- and low-resolution spectra for the molecules of many atmospheric gases.

The toolkit of this system allows a user to solve direct spectroscopic problems and calculate molecular spectra for those spectral ranges and conditions that are not presented in the system's database of spectral line parameters.

This system will be useful for the specialists in molecular spectroscopy, atmospheric optics, and other branches connected with the use of data on spectral properties of gaseous media. Besides, the system can be used as a training aid in delivering lectures and conducting practical lessons in optics and molecular spectroscopy at higher education facilities (faculties, departments) of physics and/or chemistry.

Acknowledgments

The authors of this paper would like to acknowledge S.A. Tashkun, V.I. Perevalov, and Vl.G. Tyuterev for collaboration and contribution to the development of this system, and Yu.A. Poplavsky and V.A. Kapitanov for useful remarks and discussions that yielded some corrections to the spectrum simulation.

The work was partly supported by the program No. 2.10 of the Russian Academy of Sciences *Optical Spectroscopy and Frequency Standards*.

References

1. http://www.hitran.com
2. http://spec.jpl.nasa.gov
3. http://www.cdms.de
4. http://physics.nist.gov
5. http://physics.nist.gov/PhysRefData/wavenum/html/spect.html
6. Yu.L. Babikov, A. Barbe, V.F. Golovko, S.N. Mikhailenko, and Vl.G. Tyuterev, in: *Proc. Third All-Russian Conf. on Electronic Libraries: Perspective Methods and Technologies, Electronic Collections* (Petrozavodsk, 2001), pp. 183–187.
7. S.N. Mikhailenko, S.A. Tashkun, Yu.L. Babikov, V.F. Golovko, and Vl.G. Tyuterev, Atmos. Oceanic Opt. **17**, No. 11, 821–831 (2004).
8. L.S. Rothman, D. Jacquemart, A. Barbe, D.C. Benner, M. Birk, L.R. Brown, M.R. Carleer, C. Chackerian, Jr., K. Chance, V. Dana, Devi V. Malathy, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S.T. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, Auwera J. Vander, P. Varanasi, and G. Wagner, J. Quant. Spectrosc. Radiat. Transfer (in print).
9. N. Jacquinet-Husson, E. Arie, J. Ballard, A. Barbe, G. Bjoraker, B. Bonnet, L.R. Brown, C. Camy-Peyret, J.-P. Champion, A. Chedin, A. Chursin, C. Clerbaux, G. Duxbury, J.-M. Flaud, N. Fourrie, A. Fayt, G. Graner, R.R. Gamache, A. Goldman, V. Golovko, G. Guelachvili, J.-M. Hartmann, J.-C. Hilico, J. Hillman, G. Lefevre, E. Lellouch, S.N. Mikhailenko, O.V. Naumenko, V. Nemtchinov, D.A. Newnham, A. Nikitin, J. Orphal, A. Perrin, D.C. Reuter, C.P. Rinsland, L. Rosenmann, L.S. Rothman, N.A. Scott, J. Selby, L.N. Sinitsa, J.M. Sirota, M.A.H. Smith, K.M. Smith, Vl.G. Tyuterev, R.H. Tipping, S. Urban, P. Varanasi, and M. Weber, J. Quant. Spectrosc. Radiat. Transfer **62** No. 2, 205–254 (1999).
10. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, J. Quant. Spectrosc. Radiat. Transfer (in print).
11. O.V. Naumenko and E.R. Polovtseva, Atmos. Oceanic Opt. **16**, No. 11, 900–906 (2003).
12. H. Partridge and D.W. Schwenke, J. Chem. Phys. **106**, No. 11, 4618–4639 (1997).
13. D.W. Schwenke and H. Partridge, J. Chem. Phys. **113**, No. 16, 6592–6597, (2000).
14. L.S. Rothman, C. Camy-Peyret, J.-M. Flaud, R.R. Gamache, D. Goorvitch, A. Goldman, R.L. Hawkins, J. Schroeder, J.E.A. Selby, and E.B. Watson, J. Quant. Spectrosc. Radiat. Transfer (in preparation).
15. S.A. Tashkun, V.I. Perevalov, J.L. Teffo, A.D. Bykov, and N.N. Lavrentieva, J. Quant. Spectrosc. Radiat. Transfer **82**, Nos. 1–4, 165–197 (2003).
16. V.F. Golovko, A.V. Nikitin, A.A. Chursin, and Vl.G. Tyuterev, in: *Proc. of the 2nd Intern. Workshop ADBIS95* (Moscow, 1995), Vol. 2, pp. 12–14.
17. Vl.G. Tyuterev, Yu.L. Babikov, S.A. Tashkun, V.I. Perevalov, A.V. Nikitin, J.-P. Champion, Ch. Wenger, C. Pierre, G. Pierre, J.-C. Hilico, and M. Loete, J. Quant. Spectrosc. Radiat. Transfer **52**, Nos. 3/4, 459–479 (1994).
18. N. Husson, B. Bonnet, A. Chedin, N.A. Scott, A.A. Chursin, V.F. Golovko, and Vl.G. Tyuterev, J. Quant. Spectrosc. Radiat. Transfer **52**, Nos. 3/4, 425–438 (1994).
19. http://www.mysql.org
20. http://www.php.net
21. S.A. Tashkun and Vl.G. Tyuterev, Proc. SPIE **2205**, 188–191 (1994).
22. http://smarty.php.net