

GRAPHICS SOFTWARE OF A SPECTROSCOPIC INFORMATION SYSTEM

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We advertise some functional capabilities of our computer large–database management system designed for simulation of gas–analysis procedure and for optimization of search for informative sections in the IR absorption spectra aiming at sounding of atmospheric gases and impurities. One of the computer versions was called GRASSP (Graphics System of Spectra). Its main application is the on–line display of spectroscopic data on the propagation of laser radiation through the atmosphere under various conditions or through model gas mixtures. Recommendations obtained on the basis of the graphs displayed by the system can be used for expert estimate of the efficiency of application of a spectrometric instrument under various atmospheric conditions or in technological cases.

Spectroscopic methods of gas analysis are the most promising ones for determining the concentrations of trace gaseous impurities in the atmosphere because of their selectivity, high sensitivity, and possibility of remote control¹ which makes them most suitable for solving the problems of ecological monitoring of air basin.

In recent years the problems of change in the gas composition of the atmosphere, in particular, the ozone problem,^{2,3} increase of CO₂ content (greenhouse effect), CO content (ignition of oil wells), etc. have occupied a special place in ecology. For example, one section of the international scientific program EUROTRAC³ called TOR (Tropospheric Ozone Researches) is devoted to the study of ozone formation in the atmosphere as well as of the chemical processes leading to its destruction. A number of papers^{4–6} demonstrate that the IR range is the most informative one for sounding of various atmospheric gases.

But the perfect experimental equipment must be supported by information about high–resolution spectra for successful application of spectroscopic methods. By now such spectroscopic databases on the IR spectra as GEISA,⁷ HITRAN,⁸ and ATLAS⁹ have been developed which have the software packages for management and optimal application of these bases along with the databases themselves. The application package LARA–1¹⁰ has also been developed, which uses the HITRAN–86 and GEISA–84 databases and is intended for simulation of laser radiation propagation through the atmosphere. More detailed list of papers is given in Ref. 9.

The tendency for development of a computer applied to spectroscopy becomes more pronounced¹¹ due to a huge amount of data. For example, GEISA–91 contains data on more than 700,000 molecular transitions. The authors of Ref. 12 have developed the program package for graphic display of spectroscopic information contained in databases on the absorption spectra of atmospheric gases. Initially the above–indicated program packages were intended for use on large computer complexes (see, for example Ref. 10), but recently there is a tendency for their adaptation to personal computers.^{12,13}

The objective of our paper, which as far as we know, has not yet been realized, is the development of the unique program based on the well–known simplest methods

designed for application on IBM PC AT/XT–compatible computers and characterized by highly–developed service and on–line access to the spectroscopic data. In addition, the computer information system¹³ presented here is distinguished by its functional capabilities listed below from the systems known in the literature^{10,12} and similarly tailored toward the study of atmospheric gases. Let us also note its principal difference from the TDS series computer systems¹⁴ tailored toward thorough investigation of molecules of a definite class.

Let us briefly note the principal distinctive features of the present version. First, the features peculiar to a mini–computer called for the solution of the following problems.

1. Database compression in internal format.
2. Fragmentation of the system to minimize the space occupied on a hard disk and to improve the system portability from one computer to another.
3. In connection with item 1, display of characteristics of all lines in any spectral region.

Second, the choice of concrete applied problems of gas analysis and atmospheric sounding has envisaged the following unique capabilities.

1. Graphic display of the transparency microwindows of the interfering atmospheric components to monitor the content of the examined gas components.
2. Display of the spectra with any prescribed resolution lower than it follows from the theory of line shapes.
3. Development of the interface between the databases on molecular and laser lines.

DESCRIPTION OF THE DATABASE MANAGEMENT SYSTEM

Figure 1 shows block diagram of the system. The system uses the databases (both spectroscopic database and that of the lines of lasing of CO₂ and CO lasers) and consists of a program package, which, in its turn, includes service programs and a graphical package. The spectroscopic database was stored on a hard disk in an internal format in the form of typed file that enables us to decrease the bank volume (e.g., the GEISA–84 base occupies 25 Mbyte memory in a text format, while in a packed format it

occupies only 18 Mbyte) and to organize it as a direct-access file for any spectral line. In our version the key access parameters are the transition wave numbers. Let us

note an important possibility of fragmentation of the database into separate working files by using special service programs that improves the system portability.

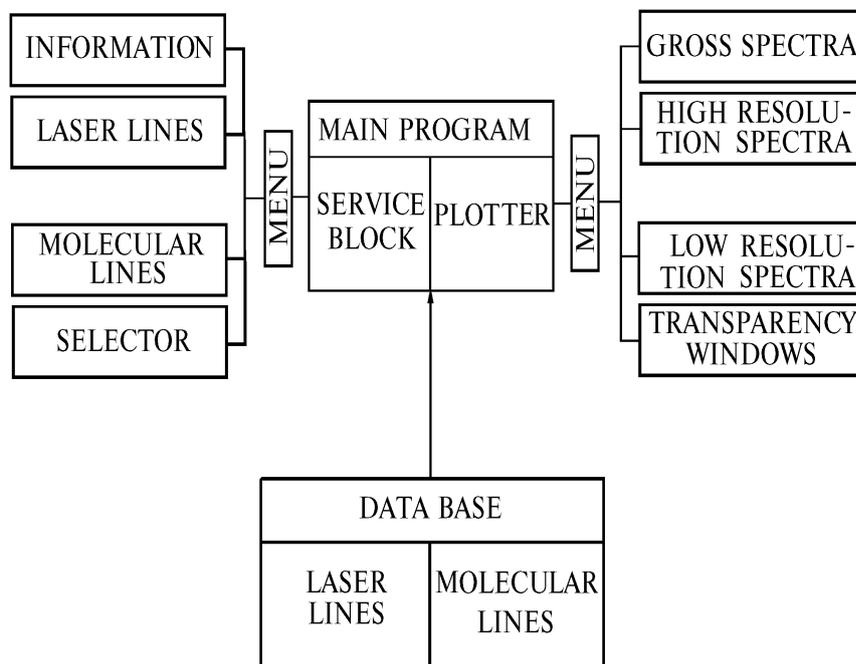


FIG. 1. Block diagram of the computer program for optimization of the search for informative sections in the IR absorption spectra and display of spectral data.

Any data array written in a standard international format can serve as a working file, while reformatting is executed by a special service program. The general management by the system is executed in an interactive mode and the system can operate with several working files selected in the mode of the main menu, which controls the block of service procedures and initiates the graphical package. Below we shortly describe the main options of menu operation.

The option HELP with its numerous suboptions enables us to retrieve data on the atmospheric models fed into the system, isotope natural distribution, lines of laser generation, etc. Moreover, it contains the system service manual.

The option SELECTOR is designed for selection of working files and cutoff the line intensities which are greater or less than the threshold ones. It contains a menu for selection of various molecules or separate isotopic modifications from a totality of 81.

The rest of the options LASER LINES, MOLECULAR LINES, and PLOTTER are designed for display of spectroscopic data. For example, calling the first two options in a special screen window, beginning from a certain prescribed wave number and moving step by step forward or backward we can browse the data from the databases on the laser lines or spectral transitions (line center, intensity, halfwidth, energy of the lower level, etc.). Additional data, such as the coefficient of temperature dependence of the halfwidth, adjacent laser line, references, and some others are displayed on the screen after pressing special keys. Moreover, the option MOLECULAR LINES is used for the above-indicated fragmentation of the database. The option PLOTTER loads the system graphical package which is described in detail in the next section.

GRAPHICAL SYSTEM

The graphical package is controlled by a special menu. Let us list its main operational modes; among them is the display of the transparency microwindows, which, as far as we know, has never been done in homemade or foreign systems of this kind.

1. Graphic display of the coefficient of absorption of any accessible gas or gas mixtures in the oxygen-nitrogen earth's atmosphere or of the atmosphere itself with a spectral resolution prescribed by the user.

2. Display of the function of the spectral absorption on 1-km path.

3. Display of the transparency microwindows of the atmosphere for sounding of its components or gaseous impurities.

4. Display of the gross spectra in the form of a set of vertical line segments whose lengths are proportional to the line intensities in logarithmic scale without display of a line shape. This mode is used for on-line retrieval of data on the absorption bands of an examined substance.

A set of additional parameters is specified with the help of special menu or is entered through the screen windows in the interactive mode. It includes the shape of absorption line (Lorentz or Gauss line), temperature, pressure of a mixture, and some other parameters. To calculate the coefficient of absorption of a gas mixture, we used the method of direct summation. For example, for the Lorentz line the coefficient of absorption $k(\omega)$ of the mixture of l gases was calculated from the well-known formula

$$k(\omega) = \frac{B}{\pi} \sum_{i=1}^l \frac{n_i}{(\omega_i - \omega_{0i})^2 + \gamma_i^2} S_i \gamma_i, \quad (1)$$

where S_i is the intensity of the line of absorption by the i th component of the mixture (cm/mol) under the normal conditions, γ_i is the line halfwidth (cm⁻¹/atm) under the normal conditions (broadening by air), ω_{0i} specifies the line center (cm⁻¹), and n_i is the relative volume concentration. The quantity B indicates the concentration of molecules at a pressure of 1 atm and a temperature of 296 K. The values of n_i are calculated as the product of the relative concentration of the component in the atmosphere and the natural occurrence of the isotopic modification or are specified by the user. For the main atmospheric components the statistical sums were calculated in the temperature interval 200–350 K with a step of 1 K. Therefore, using the coefficient of temperature dependence of the halfwidth and the simple formula for line broadening by pressure, one can calculate the coefficients of absorption under various external conditions that allows one to simulate the propagation of radiation at different altitudes.

SIMULATION OF MEASUREMENTS BY SPECTRAL INSTRUMENTS

Though this system is designed first of all for graphic display of the theoretical spectra, it opens a number of possibilities for simulating the spectra recorded by real instruments with an *a priori* known instrumental function and for solving some applied problems of laser atmospheric sounding. Equation (1) was used to retrieve the theoretical coefficient of absorption. Calculations were performed with the step $h = \Delta\omega_{\min}/M$, where $\Delta\omega_{\min}$ is the minimum halfwidth of spectral line in the examined spectral interval and the integer M is preset by the user (default number is $M = 10$). But the theoretical spectrum does not coincide with the experimental one observed with the help of a real device. The latter $I'(\omega)$, as a rule, has a lower resolution and is related to the theoretical spectrum $I(\omega)$ by the formula¹⁵

$$I'(\omega) = \int_{-\infty}^{+\infty} A(\omega - \omega') I(\omega') d\omega', \quad (2)$$

where $I(\omega)$ describes the dependence of the received power density on the wave number, $A(\omega - \omega')$ is the instrumental function of the spectral instrument. Various instrumental functions were studied in Ref. 15. It is easy to show that the coefficients of absorption derived from the measured and theoretical spectra are related by the formula similar to Eq. (2). In this paper for calculating the coefficients of absorption of the low-resolution spectra $k_i(\omega)$ we used the iterative formula

$$k_i(\omega) = \int_{-\infty}^{+\infty} A(\omega - \omega') k_{i-1}(\omega') d\omega',$$

where i is the total number of iterations. The quantity $k_0(\omega)$ corresponds to the coefficients of absorption of the high-resolution spectra.

Iterative process is introduced to smooth the functions while the total number of iterations determined empirically depends on the spectral resolution. One of the program options corresponds to the simplest instrumental function in the form of the rectangular slit of width r_0

$$A(\omega) = \begin{cases} 1/r_0, & |\omega| \leq r_0/2, \\ 0, & |\omega| > r_0/2. \end{cases}$$

Figure 2 shows the ozone spectrum calculated in such a way with 2 cm⁻¹ resolution against the background of the high-resolution spectrum. The above-described method enables one to predict the results of measurements by the spectral instruments with various resolutions in the real atmosphere.

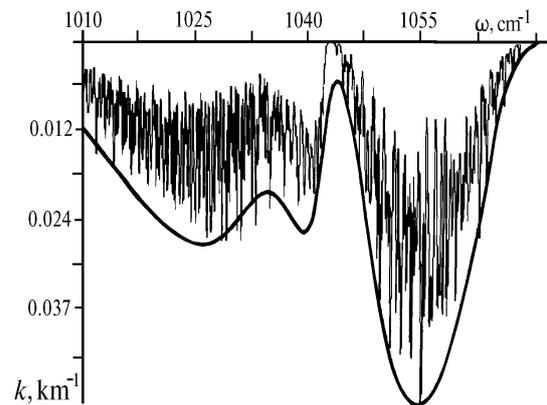


FIG. 2. The ozone spectrum of low resolution (~ 2 cm⁻¹) against the background of the high-resolution spectrum for the concentration being equal to $5 \cdot 10^{-8}$ in the interval 1010–1070 cm⁻¹. The lower threshold of the intensity was equal to $0.5 \cdot 10^{-20}$ cm/mol at $T = 296$ K.

TRANSPARENCY MICROWINDOWS

The graphical system especially vividly searches for the transparency microwindows in the atmosphere for sounding of its components by a concrete laser. For this purpose the shape of the absorption line of the component of interest to us is displayed against the background of absorption by all the rest of the components of the atmosphere taking into account the preset concentrations and external conditions. The lines of lasing of CO₂ or CO lasers are also displayed on the screen. This method is particularly useful for sounding of the gases by the method of differential absorption. Figure 3 shows the transparency microwindow for the ozone sounding in the standard atmosphere.

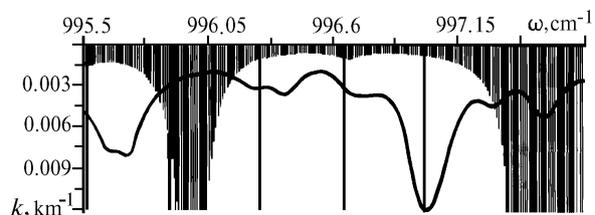


FIG. 3. The transparency microwindow for the ozone sounding (solid curve) against the background of absorption by the rest of the components of the atmosphere (black background) at $T = 296$ K. The vertical lines denote the wave numbers of radiation generated in the CO₂-laser medium.

To simplify the search for the transparency microwindows in long spectral intervals, the special option EXPRESS WINDOW is provided in the system for the gross atmospheric spectrum to be displayed (in linear scale). In this case the lines of the component being sounded are displayed by an individual color against the background of the other lines. For remote control it is important to estimate the maximum sounding range, and the special option is provided for this purpose in order to display in real time the function of spectral transmission for the radiation frequency of an employed laser and for the path length L . Thereby we exclude the spectral regions of very strong absorption of a substance being sounded from consideration, even if they are formally the transparency windows. The above-mentioned option enables one to select correctly the mutual arrangement of a source of radiation and receiver for various atmospheric situations.

PROGRAM IMPLEMENTATION OF THE SYSTEM

The computer program is written in PASCAL (TURBO-PASCAL, version 6.0). To develop the program service, we have widely used the TURBO PROFESSIONAL 4.0 being an extended version of TURBO-PASCAL, which contains the subprograms providing the menu systems, screen windows for input of the parameters, output of error messages, etc. Moreover, we have developed the special computer facilities for displaying the screen windows and loading the data in the graphics mode of the display that allows us to remove switches from the graphics mode of the display to the text one and *vice versa*, retardating the work, and in general provides an improved service and display quality. In our opinion, the use of the screen windows is most suitable and promising for the information and service computer systems.

In conclusion let us point out basic specifications of the computer system and main peculiarities of its operation. For calculating and subsequent displaying the spectroscopic functions initial data in the selected spectral interval (line centers, intensities, and halfwidths) are put into a specially selected segment of the random-access memory. The maximum number of lines which may be loaded depends on the volume of free memory, the DOS version, and, generally speaking, the graphics option.

For the computer with 540 Kbyte random-access memory, approximately 18500 lines may be loaded for display of the high-resolution spectra. For display of the low-resolution spectra or the transparency windows this number is less because the part of the computer memory is used to store the results of calculations of the coefficient of absorption which then are displayed on the screen. The time required to display a spectrum depends on the length of the spectral interval, the number of loaded lines, and the type of a computer. For example, to display the coefficient of absorption of the atmosphere with high resolution in the spectral interval 920–930 cm^{-1} on IBM PC AT-286 with coprocessor, it takes about 2 min, while to display the spectral absorption function, it takes about 3 min.

Few words about the requirements on a computer. The system can be used on IBM PC AT/XT or on IBM-

compatible computers provided with the VGA, EGA CGA, or HERCULES videoadapters. Reliable work requires no less than 280–300 Kbyte free random-access memory.

In our opinion, these systems have practically unlimited possibilities for their development. In particular, in the next versions new options will be included: along with molecular absorption we suppose to study attenuation of radiation by aerosol for various aerosol models. Of special interest is the possibility of determination of the concentrations of the atmospheric components by experimental absorption spectrum processing. The other operational modes may be included as an option.

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