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ANALYSIS OF SOFTWARE PRODUCTS FOR PROCESSING THE RESULTS OF SPECTROSCOPY

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ABSTRACT

Currently, structurometric methods of analysis play an important role in information support of monitoring in nature management and geological exploration. Any kind of spectroscopy implies the availability of software for obtaining and processing the results of research. This article is of an overview and analytical nature. Software products are considered that are used to process the results of spectroscopy or are potentially suitable for analyzing the results of the relevant studies. The article presents an overview of software applications for processing the results of spectroscopic studies developed over the past few years. The main directions of software modernization for this type of research have been described. A comparative analysis of the most widely used software of domestic and foreign developers has been carried out. The main properties, advantages and disadvantages of software applications have been presented. Based on the comparative analysis, a conclusion has been made about the possibility of applying particular software functional for spectroscopic studies in the structurometric analysis in geology.

Keywords: Spectrometric analysis, Software products, Monitoring, Software packages, Structocrometric analysis, Spectra library.

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1. INTRODUCTION

In the exploration of mineral raw materials, hydrocarbons, as well as in the identification and monitoring of zones of increased geological risk, structurometric analysis plays an important role. Structural elements may serve as indicators of potential oil and gas fields, characterizing both the subsurface geometry of rock formations, and deformation and stress of the earth's crust in the local area.

Among the main directions of using structurometric analysis methods in geology are the following: forecasting of minerals, structural and meta-structural analysis of the Earth's surface; analysis of local and global geological anomalies; geological study of areas and compilation of geological maps; geoecological monitoring of exogenous geological processes, analysis and mapping of relief; lithology; geobotany; infrastructure of the environment; planetary cartography [1-2].

One of the main methods for studying the structure of the lithosphere are spectrometric ones. It serve as a base for finding and analyzing a variety of search signs. For this purposes it is customary to use the correlation of possible mineral deposits with the change of the phototone of the soil, the vegetation cover, the color of the water of the inner water areas, thermal fluxes fixed in the IR and thermal ranges [3]. These methods require careful pre-processing of the source material (radiometric correction, interchannel color transformation, contrast enhancement, noise suppression, etc.) as well as the presence of a spectra library for comparing the spectra obtained during the analysis. There are a number of spectra libraries, mostly prepared by foreign developers. One of them is the ASTER library prepared by Johns Hopkins University (JHU) Spectral Library [4]. It contains a description of more than 2400 spectral responses of natural minerals, soils, vegetation and artifacts.

With the development of geochemical and also volcanological research, the main task of analysts is to develop methods of spectra analysis that provide high performance and the required accuracy with simultaneously determining the content of a large number of elements in samples of variable composition. In geochemical studies, the analyzed material is very diverse and there is often no preliminary data on the composition of the test samples. In this case, the use of direct atomic-emission spectral analysis, which in it richness and reliability of the simultaneously obtained information, is not inferior to many modern methods [5].

2. REVIEW OF EXISTING SOFTWARE PRODUCTS FOR SPECTROSCOPIC RESEARCH

Spectroscopic research occupies a wide place in modern science and industry. Along with the structurometric analysis, the analysis of the composition of the substance, and also the analysis of petroleum products and their wastes, spectrometric studies are widely used in determining the degree of radioactive contamination of the environment by analyzing gamma-ray spectra [6,7]. Currently, new software was developed as well as the already developed software is being modernized which are both dedicated to the study in this area. [8,9]. The problem of developing optimal software for processing the result spectroscopic studies in different areas of environmental management and monitoring does not cease to be relevant in the last decade [10].

The “VMK-Optoelectronics” academics together with the laboratory of analytical geochemistry of the Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences mastered the technology of hybrid assembly of crystals by means of polyamide stubs. Possession of hybrid assembly technology allowed placing crystals on a given curved surface with minimal technological gaps. Photoreceptor cassettes with different number of photodiode array crystals have been developed and manufactured for the modernization of most popular spectrometers [11]. The name of this device is the analyzer of multichannel atomic emission spectra (the analyzer of the MAES). It converts the received optical signals and transmits them for further processing, and the “Atom” software provides the whole complex of actions necessary for recording and decoding spectra, constructing calibration dependencies, calculating statistical parameters, storing and visualizing the analysis results. [12].

The program “Difference” for the automatic processing of IR spectra was created at the Institute of Catalysis of the SB RAS, Novosibirsk [13]. The program allows calculating the area of the IR absorption band of a substance under conditions of interfering influence of other substances with absorption bands in close ranges. The program is intended for companies and specialists solving problems in the field of analysis of varnishes and paints, oil products, pharmacological preparations, gases and air compositions.

The issue of reducing oil pollution of the soil and water resources is relevant nowadays. [14,15]. Thus, in Samara State Technical University was carried out the identification of the content of oil hydrocarbons in various types of oil-containing wastes, including contaminated soils after purification, according to reflection spectra in the multidimensional data analysis software package. The diffusion reflection spectra of each sample were obtained by scanning using a submerged probe on a spectrometer TIDAS P. For multidimensional data analysis was used a package of mathematical programs UNSCRAMBLER of firm CAMO [16].

The “FSpec” base software, complete with the FSM-1201 device, is provided by the company Infraspek. The main features of this software package: obtaining interferograms, converting them into a spectrum, working with a Fourier spectrometer, processing, transforming, displaying data in a graphical form, and creating a spectral database [17].

“Thermo Nicolet” company has developed OMNIC software designed to control all FT-IR and Raman spectrometers manufactured by Thermo Nicolet. It is a 32-bit software running on a Windows operating system. The OMNIC program provides all the necessary functions for controlling the device, recording and processing spectra, performing substance identification and product quality control, forming and printing a report [18].

At the Don State Technical University was carried out a comparative analysis of using MS EXCEL and MATLAB software packages for spectral analysis. Fourier analysis techniques were compared in complexity of obtaining the required values, constructing a histogram and analyzing the data obtained [19].

At Peter the Great St. Petersburg Polytechnic University was developed software, which can be used for quantitative and qualitative analysis. The software was written in Java in the Netbeans development environment. The graphical interface is implemented using the Swing library. Swing - a set of tools for creating graphical interfaces for Java-programs. The Swing application uses a top-level window (JFrame), which contains the necessary elements: buttons, tables, graphs, etc. When the button is clicked, the corresponding handler is triggered and the specified actions are performed, such as opening a new window, populating the data, or directly qualitative/quantitative analysis. For displaying IR spectra was used the JFreeChart. This library is often used in Java applications in order to create different types of graphs. With the help of this library it is possible to build histograms, diagrams, linear graphs and basic types of 3d and 2d graphs. JFreeChart makes it possible to create images of the following formats: SVG, JPEG, PNG and others. The library is provided for free with open source code, which makes it easy to use it [20].

The Horace software package was designed to work with large sets of multiple measurement data collected with neutron spectrometers equipped with arrays of position-sensitive detectors. The software allows conducting research in four dimensions of the inverse space and excitation energy, visualizing multidimensional subsets, performing algebraic manipulations, modeling and fitting data [21].

At St. Petersburg State University of Industrial Technology and Design was carried out a research of the interaction of aluminum complexes with high molecular weight natural polymers based on the results of spectroscopy obtained with the help of the program for processing and adding differential spectra "DIF". This program allows adding the experimental spectra of

individual components of the system and comparing them with the spectrum of the mixture of components [22].

3. ANALYSIS OF THE MAIN FUNCTIONAL CHARACTERISTICS OF SOFTWARE APPLICATIONS

When analyzing software products, it is necessary to have a clear idea of what kind of spectroscopy it can be used for. Based on the specifics of geological studies of both the lithosphere surface and the structure of various materials, it can be said that the inverse task of spectroscopy, that is, the determination of the characteristics of a substance by the properties of its spectrum, is more relevant. By kinds and methods, atomic spectroscopy is most applicable in this area, in particular atomic emission and mainly infrared molecular spectroscopy. Therefore, to analyze and evaluate this software product is necessary in accordance with its applicability for a particular type of analysis.

For fully understanding of the results of the comparative analysis, it is necessary to dwell on some of the functions and properties of each software application under study

Software «Atom». Despite the fact that the first versions of this package appeared more than 10 years ago, its improvement and expansion of opportunities is constantly, which allows using this package in modern studies. First, the program implemented the main tasks of quantitative multi-element atomic emission spectral analysis, including the implementation of all necessary measurements and calculations. The modern version of the program contains both basic formulas and expanded versions of calculations, with corrections for inter-elementary influence. The application of this software package allows ensuring the independence of different stages of data processing:

a) After registration of spectra, repeatedly repeat the calculations, changing individual parameters and achieving the best metrological parameters.

b) Implement different options for statistical processing and monitoring of results in accordance with algorithms and analysis techniques.

c) Offer flexible options for compact and extended presentation of results, saving in the database and transferring it to other programs.

When assessing the possibility of using this product, it is necessary to take into account that it is not universal according to the types of spectroscopic studies; it is applicable only for atomic-emissive spectral analysis. In addition, there is a binding of the software to the specific developer's hardware. Therefore, its application is associated with certain limitations, although it is quite acceptable to perform tasks related to the simultaneous determination of the content of a large number of elements in samples of variable composition.

The software product Difference is designed to process the results of IR-spectroscopy in studies of a wide range of directions in the petrochemical, paint and pharmacological industry. The processing can be performed both in manual mode for a separate spectrum, or in an automatic mode for a series of spectra. The result of calculations is displayed in a graphic and text forms. Based on this program, in the same organization was developed the SPEAN program, which does not have a binding to a specific spectrometer; allows automatically processing the spectra of complex systems; performs automatic intermediate counting of the current experiment; can integrate with automated systems.

UNSCRAMBLER - a software product for the analysis of multidimensional data used in the calibration phase. This software was developed in 1986 by Harald Martens, and later was supported by CAMO Software. Unscrambler was one of the first to use the method of regression of partial least squares. Among other mathematical methods is also used the analysis of the main components, 3-variant PLS, multidimensional resolution of the curve. In addition to

spectroscopy, this software package is used in chromatography, data processing in scientific research, non-destructive quality control systems in the pharmaceutical industry, sensory analysis and the chemical industry.

The FSpec software of the domestic company "Infraspek" is designed for controlling a Fourier spectrometer, receiving and processing IR spectra. It allows receiving interferograms, converting them into a spectrum by means of phase correction by the Mertz method and apodization, testing and tuning of the Fourier spectrometer, primary processing of spectra and its transformation, displaying data in a graphical form (spectrum) on the monitor screen or printing on a printer, databases on different media.

OMNIC - along with the managing of spectrometers manufactured by Thermo Nicolet, registers and processes the spectra obtained. The software package fully complies with ISO requirements. OMNIC includes the following products:

- Data Collection, Data Analysis - contain all operations for registration and processing of spectra, including baseline correction, spectrum smoothing, mathematical processing of spectra, addition and subtraction of spectra, derivation of different orders and introduction of various corrections;
- Search – qualitative analysis and identification of an unknown sample from IR spectra libraries, the ability of creating their own user libraries;
- Spectral Library Collection – a set of several demo libraries containing more than 600 IR spectra of organic substances;
- Data Converters provides full compatibility of the program with the spectral formats JCAMP, ASCII, CSV, PC-IR, Galactic (Grams), Perkin-Elmer (Spectrum), LabControl (Spectra-cle);
- Quality Control - A unique tool that allows easily and quickly monitoring various samples in quality control laboratories. By pressing one QC Compare key, the sample composition is compared with the standard and the result is reported to the operator;
- Correction H_2O, CO_2 allows adjusting the spectrum by the bands, which are due to the presence of water vapor and carbon dioxide. Such correction reduces the influence of the atmosphere and improves the quality of the spectrum, which makes it possible to search the IR spectra libraries with a higher convergence result;
- Report Notebook in accordance with GLP, creates an uneditable notebook with all operator reports, while the archived spectral data can be downloaded to the OMNIC program and analyzed again. Allows creating reports, which contain spectral data, chemical structures, text and other fields. A unique feature of OMNIC is the filling of fields in automatic mode after creating a report template.
- On-line Tutorials – interactive manuals on all aspects of software, the work of the FT-IR spectrometer and attachments, the theory of IR spectroscopy and sample preparation.
- In addition, when working with this software package, it is possible to diagnose all components of the optical system in on-line mode, which allows controlling the operation of each component at any time.

The peculiarity of all Thermo Nicolet systems is the availability of Smart technologies; The E.S.P-protocol allows the creation of a fully integrated system including an FT-IR spectrometer, OMNIC software, add-on devices and additional devices. Smart T technology provides recognition of the optical elements of the system and consoles, automatically sets the parameters of the experiment, conducts the testing of the add-on devices in automatic mode, monitors the

quality of the spectra during the accumulation of data. Thanks to Smart technology, only Thermo Nicolet systems have such a high level of automation.

Analyzing biomedical information is one of the ways of applying the mathematical package MATLAB for processing the results of spectroscopy. For instance, as the main method of automatic computer analysis of EEG (Electroencephalography), there is used spectral analysis based on Fourier transform - representation of the EEG picture as a set of a set of sinusoidal oscillations that differ in frequency and amplitude. The Fourier transform (FS) is a complex frequency function, describing the distribution of the amplitudes and phases of these waves. If there is any characteristic rhythm in the analyzed EEG segment, it will cause a splash on its spectrum. Since the FS is a complex function, there is often used a square of the PF module (power spectrum), and the square root of this quantity is the rms (root mean square) voltage [23].

Working with the MS EXCEL package does not require special programming skills [24,25]. To perform spectral analysis in any area, there is only need to select the necessary functions and correctly fill in the arguments, as well as connect the necessary add-ins [26]. In the MS Excel program, the original data must be translated into complex numbers using the function "Fourier analysis" in the built-in package "Data analysis". The resulting complex numbers are transformed into absolute numbers modulo. Based on the calculated values, graphs are constructed to visually evaluate the spectra obtained. The full spectrum of the signal is constructed on the graph, although only half is sufficient for analysis. However, for the formulation of competent conclusions it is necessary to translate the values of the abscissa axis from the samples to the frequency, which will require some additional calculations.

It should be noted that the Matlab package has a much greater set of mathematical analysis functions than MS Excel; it is used most often in research and educational institutions [27]. This software product is much more powerful in terms of building models of various systems. For spectral analysis in Matlab program loads the digitized data and writes a program that automatically builds graphs for visual analysis of the spectra obtained at a predetermined interval. In Matlab, the program code is easy to write, and the resulting graphics have an informative part without a "mirror" repetition. In addition, the program written in the Matlab environment can be used for almost any data.

The standard mathematical packages MS EXCEL and MATLAB can be downloaded and processed data obtained in any research area [28]. Their application is possible both in the field of monitoring and in geological exploration [29].

4. RESULT AND DISCUSSION

For the modern level of industrial development and especially for the mineral-raw complex, the desire for a high degree of automation is characteristic. The search for new deposits is characterized by ever-increasing difficulties associated with geological exploration in new regions that are more complex in geological and natural climatic terms. Therefore, a number of specific requirements for accessibility, versatility and functionality are presented to methods, hardware and software.

As a result of the analysis of software products, one can compare their functionality and applicability for various types of research and industries. The main parameters of several software products of domestic and foreign manufacturers have been selected, according to which it is possible to judge the optimal degree of the choice of a specific software package.

«Atom»

- Accessibility - **low**: available from the developer, is not in a free access.

- Universality - **low**: atomic-emissivity spectral analysis, binding to a specific spectrometer.
- Functionality - **high**: spectra registration, repetition of calculations, optimization of metrological indicators, statistical processing and monitoring of results, presentation, storage and transmission of results.
- Application area - any area of research where it is necessary to perform tasks related to the simultaneous determination of the content of a large number of elements in samples of variable composition.

«Difference»

- Accessibility - **medium**: the developer is a patent holder, a commercial product.
- Universality - **high**: IR spectroscopy, no binding to a specific spectrometer, integration with automated complexes is available.
- Functionality - **high**: manual and automatic processing mode, output of results in, processing of spectra of complex systems.
- Application area - petrochemical, paint, varnish, and pharmacological industries.

«Unscrambler»

- Accessibility - **high**: commercial product, sale on the developer's site and from partner companies.
- Universality - **high**: various types of spectroscopy and chromatography.
- Functionality - **high**: analysis at the calibration stage analysis of the main components, 3-variant PLS, multidimensional resolution of the curve.
- Application area - pharmaceutical, chemical industry, sensory analysis.

«FSpec»

- Availability - **high**: commercial product, sale on the developer's site and from partner companies.
- Universality - **low**: IR spectroscopy. It is designed to control Fourier spectrometers manufacturer.
- Functionality - **high**: obtaining and converting the interferogram, and apodization, testing and tuning of the Fourier spectrometer, primary processing of spectra and its transformation, displaying the data in a graphical form (spectrum) on the monitor screen or printing on a printer, the option of creating a spectral base.
- Application area - chemical, pharmaceutical, food, textile, coal, electric power.

«OMNIC»

- Availability - **high**: commercial product, sale on the developer's site and from partner companies.
- Universality - **high**: IR spectroscopy, no binding to a specific spectrometer.
- Functionality is **high**: registration and processing of spectra, sample analysis and its identification, creation of libraries, ensuring compatibility in all spectral formats, monitoring samples and adjusting the spectrum, creating an integrated system of hardware and software.
- Application area - any area associated with using of IR spectroscopy.

«Ms Excel+ Matlab»

- Accessibility - **high**: the most popular applications, solving mathematical tasks in particular.
- Universality - **high**: processing data, which is obtained by various methods of research using mathematical analysis
- Functionality - **low**: data loading and its processing, plotting of spectra graphics and system models.Application area - any area of scientific research, where obtained data is amenable to download.
- Based on the results of the comparative analysis, the following conclusions can be drawn.

All software packages being investigated can be used to process the results of spectroscopy and in particular are applicable to geological studies and various types of monitoring. However, depending on the nature of the research and the level of equipment of the research laboratories, preference should still be given to more universal programs not tied to specific equipment, such as UNSCAMBLER or OMNIC, in addition to their high flexibility they are available and have sufficiently high functionality. If you have certain equipment, it's certainly better to contact the developer software, such as FSpec, which has high functionality and relatively low cost. The use of office or mathematical applications is advisable in conditions of research in universities or in research student works, since, despite their availability and versatility, they do not possess high functionality and are unacceptable for large-scale industrial research.

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