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THE EXPERT SYSTEMS FOR ANALYSIS OF ATOM AND MOLECULE THRESHOLD SPECTRA

I. PETROVIĆ, V. BOČVARSKI and V. PETROVIĆ
Faculty of Science, R. Domanovića 12, 34000 Kragujevac, Serbia

Abstract. In this paper is presented development of the expert systems for threshold spectra analysis, starting from firstly developed expert system for atom threshold spectra analysis, up to the expert system for analysis more complex molecule threshold spectra (firstly two-atomic and then tree-atomic molecules). The goal of the expert systems application is to automate, speed up and improve process of spectra analysis. Interest for threshold spectra originates from the fact that, by studding them, it is possible obtained information about processes which happened on energies near reaction threshold. Also, in these spectra can be seen peaks that correspond to forbidden transitions and which can't be seen in the optical spectroscopy. For testing of the expert systems, we used the threshold spectra for the He atom, and N_2 and SO_2 molecules. All these spectra are obtained on threshold spectrometer which is situated in Institute for Physics in Zemun.

1. INTRODUCTION

The main characteristic of threshold spectra is possibility to detect electrons with low energy i.e. electrons which are loosed almost of their incident energy in collisions with atoms or molecules. Advantage of this method in relation to optical spectroscopy method, is possibility for detections and studying optical forbidden transitions.

The spectra used for development and testing of the expert system are obtained by using threshold method spectroscopy which is developed by Cvejanovic and Read (1974). This method is known as method of "field penetration". The essence of this method is penetration of external electrical field in the area where is performed collision between electron and atom or molecule beams. Aforementioned electrical field creates, in the center of area such potential, which can extract electrons with zero energy. Threshold spectra used for development and testing of expert systems are result of detection of these electrons. All mentioned spectra are obtained on threshold spectrometer that is situated in Institute for Physics in Zemun.

2. EXPERT SYSTEMS

The expert systems used for threshold spectra analysis and described in this paper, are developed by using expert system building tool I2+, which in conclusion process enables the backward changing method. The advantage is avoiding of conflict resolution, which can be very complicated factor in process of practical exploitation of an

expert system. The knowledge is presented in form of production rules with structure IF-THEN-ELSE.

The first expert system is developed with aim to automate the process of atom threshold spectra analysis (Petrović and Bočvarski 2003). Actually, we used He atom threshold spectra, but it should be emphasized that the expert system can be adapted to make spectra analysis of the other atoms. Beside identification of states, which is necessary step in process of analysis, the additional task for expert system is identification of resonances in these spectra. Resonances are non stable, short-lived states created by electron capture by atom or molecule, and they are characteristic for threshold spectra. After the short time the electron leaves atom or molecule and gives contribution to peak of other state. In this way, in the case of atom spectra, these electrons are disturbing the rule that the peaks which correspond to states of one group (peaks that have been determined with same value of principal quantum number form one group) must form a growing array, looking from a point of view of peak intensity. Deviations in spectra are consequence of resonance influence on some states. Because of that, detection of this influence on a peak of state is one of the most important steps in process of spectra analysis. On Figure 1 is given a part of characteristic spectrum of He atom. This spectrum represents a second group of peaks, which is determined by a value of principal quantum number $n = 2$, and where can be seen the aforementioned deviation.

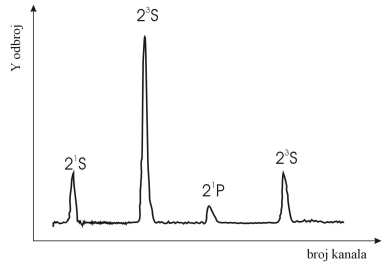

Figure 1: The second group of characteristic spectrum of He.

Application of the expert system in process of the threshold spectra analysis has fulfilled our expectations, and enabled us to upgrade an expert system for analysis of more complex spectra, i.e. the molecule threshold spectra.

Besides peaks which arise from discrete states and resonances, in molecule threshold spectrum is characteristic an appearance of vibrational level peaks. Vibrational movement in molecules is consequence of oscillation of atoms around position of equilibrium which represents the most probable distance between atoms. This is the reason why in the total sum of molecular energy there is always an oscillation energy, i.e. energy of vibrational movement.

Vibrational levels can be observed on almost all peaks which correspond to electronical transitions. For vibrational levels is characteristic that they appear on almost identical energy distances. In the first phase we limited ourselves on two-atomic molecule spectra, actually on molecules of nitrogen (Petrović and Bočvarski 2005).

On the Figure 2 is given characteristic threshold spectrum of N_2 molecule. In the structure of this spectrum it can be seen that the every state has exactly determined

number of vibrational levels. On the higher energies, overlapping of vibrational levels forms the complex structures. Qualitative improving of process analysis can be seen at those structures where the peaks can't be separated and where they are often in form of "shoulders" on higher energy side of most intense peaks of states. Such appearance of spectra makes their analysis and states identification very difficult by classical methods.

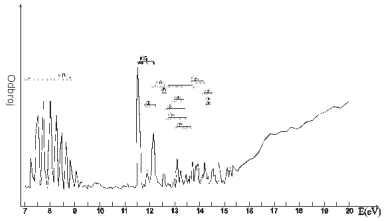

Figure 2: Characteristic threshold spectrum for N_2 molecules.

Molecules of N_2 are chosen for development and testing of an expert system because their spectra are very well examined. Because of that they can be used for checking the same ideas and principles which were necessary in the process of searching a correct methodology for analysis of polyatomic molecules by expert system. For development and testing of the expert system for polyatomic molecules we used the SO_2 molecules threshold spectra (Petrović and Bočvarski 2007). On the Figure 3 is given part of characteristic threshold spectrum for SO_2 molecules.

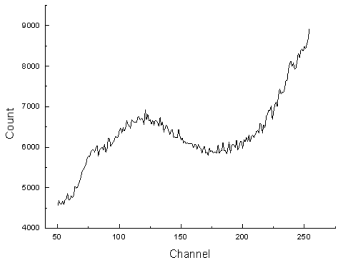

Figure 3: Characteristic threshold spectrum for SO_2 molecules (energy range 5,5 - 8 eV).

For those spectra is characteristic non existence or very small existing of determined structures which are necessary for calibration process.

In order for expert system to work, beside energy levels tables of atom and molecule states, we also formed tables of energy levels of corresponding vibrational levels and resonances.

After the input of initial data, calibration of energy scale and estimation of resolution, the expert system starts with identification and classification of peaks of states, and by the same principle makes identification of vibrational levels (Petrović and Bočvarski 2003, 2005, 2007).

In the process of calibration and identification, each peak obtains corresponding mark, depending of its nature. Aforementioned marks will be written by expert

system, in collaboration with appropriate Pascal program, in corresponding field in the table with spectrum.

Where atom and two-atom spectra are concerned, the process of analysis is finished.

However, in tree-atom molecule spectra, regarding of density and overlapping of peaks, especially at higher energy intervals, it is necessary to make some additional analyses.

Additional analysis should solve two problems. First problem originates from fact that the number of vibrational levels isn't always known. Second problem is consequence of the fact that the distance between vibrational levels isn't always known also. Additional problem is disturbance of equidistance between vibrational levels that originates from different influences. Development of the expert system should show if, on base the known minimum data, the expert system can generate spectrum which will correspond, in principle, to experimentally obtained spectrum.

These problems have been solved by using the process of peak generation in form of a Gaussian, after identification of peak of states and separated vibrational levels. The parameters for Gaussian are obtained based on the characteristic peak which represents structure the most intense and defined in spectrum. Generating is performed by using the Pascal program on the channels at which the expert system positioned itself, based on the characteristic number of channels. After the correction of peak intensity, the expert system checks the position of peaks and, if necessary, moves a spectrum on left or right side. After that, the expert system generates additional peaks with aim to obtain overlapping structures which, in principle, correspond to real spectrum. The Figure 4 illustrates aforementioned processes.

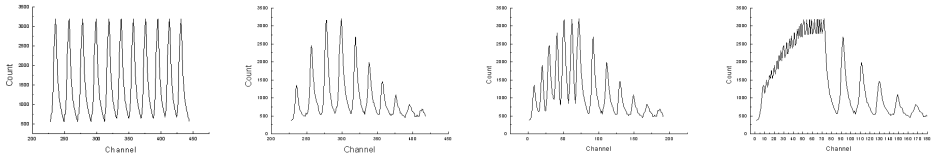

Figure 4: Generating of peaks of vibrational levels on equal distance, correction of peak intensity, and addition of peaks.

3. CONCLUSION

Application of expert system in processes of spectra analysis gave expected results. Quantitatively and qualitatively, improvement of analysis process completely vindicated a further work on development of expert systems which would find their application in processes of spectra analysis.

References

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