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EXPERT SYSTEMS FOR THE TREATMENT OF COLLISIONAL SPECTRA



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- Expert system – definition and structure (in general sense)
- Advantages in using ES for spectra analysis
- Expert system for threshold spectra analysis
- Conclusion
- References

Expert system-definition and structure (in general sence)

- Expert systems are developed in order to solve those problems which cannot be solved by using procedural programs (languages).

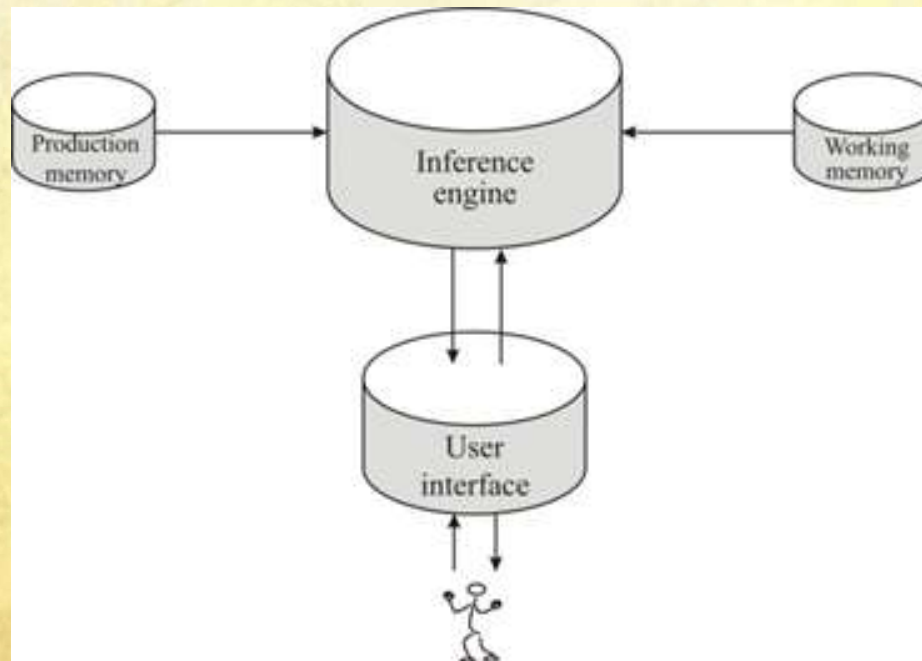


Fig. 1. The basic structure of an expert system 3

Advantages in using ES for spectra analysis

Using the ES in the area of processing experimental data:

- Significantly speeds up data processing,
- Enables various kinds of reviewing of data
- Qualitatively and quantitatively improves obtained results

Additionally, the ES enables:

Absence of subjectivity

Possibility to analysis of large amount of data

And especially, possibility to analyze these parts of spectra which can not be analyzed by classical methods.

Expert system for threshold spectra analysis

- In the area of experimental data analysis the basic task which an expert system has to fulfill is to speed up, automate, and improve the interpretation of experimental results, by simulating activities of the expert.
- We developed couple expert systems for discrete spectra analysis obtained **in the electron method spectroscopy experiments** which consist in detection of very low energy electrons formed in electron - atom (molecules) collisions.

Developed expert systems:

- Expert system for threshold spectra analysis of He atom,
 - Expert system for threshold spectra analysis of N₂ molecules,
 - Expert system for threshold spectra analysis of SO₂ molecules.
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- For the development of aforementioned expert systems we used the expert system building tools, The Insight 2+, which, in the process of conclusion, use the backward chaining, i.e., the mechanism which starts from goal and goes to the facts.
 - All spectra for development and testing of the expert systems are obtained from the threshold spectrometer situated at the Institute of Physics in Belgrade, using the modified method developed by Cvejanovic and Read.

- Although both, atomic and molecular spectra, are discrete important difference among them lies in the fact that the molecular spectra contain vibrational states characteristic for molecules. This causes not only the increase of a number of peaks, but also, because of their overlapping, makes spectral analysis more difficult.

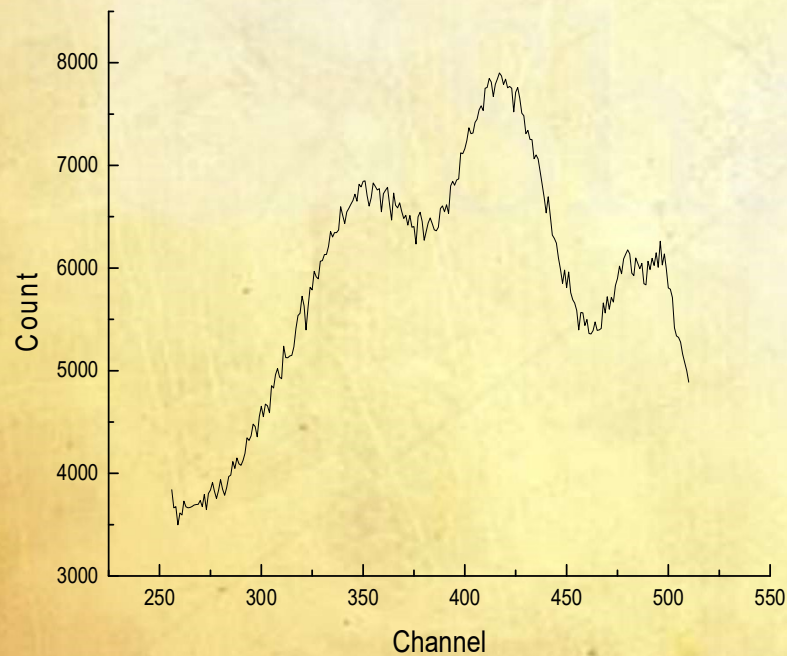


Fig. 2. The part of threshold spectrum of SO_2 molecule

All developed ES have a common (same) thread and also differences caused by a specific problem that should be solved. This thread is incorporated through the following steps of analysis:

- Data input
- Finding and extracting all peaks
- Estimation of signal/noise ratio
- Finding the referents peaks and corresponding energy levels
- Energy scale calibration
- Resolution estimation
- Identification and classification of peaks
- Recording data obtained by spectrum analysis
- Review of the analyzed data
- Calling the programs for numerical calculation

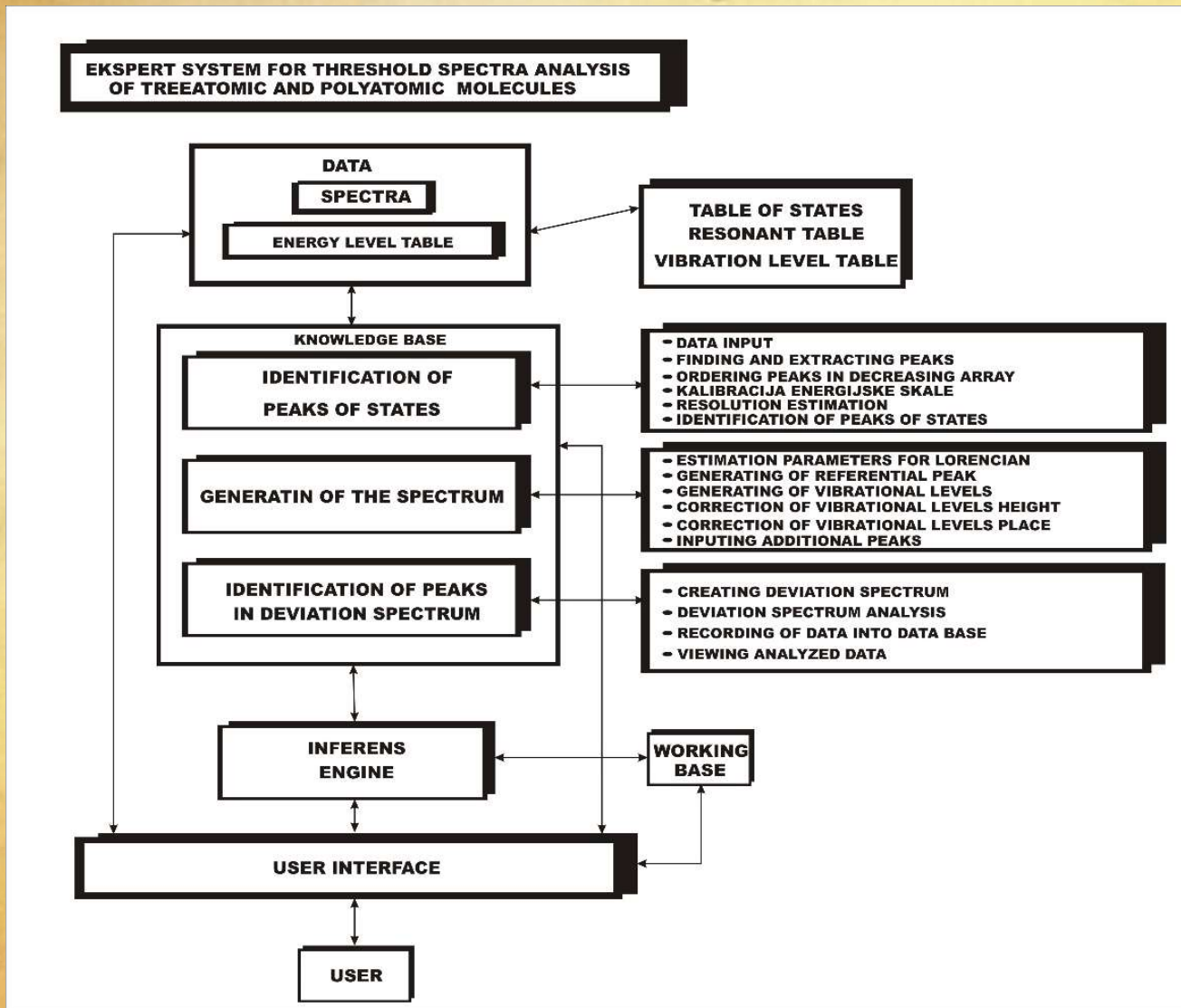


Fig. 3. The structure of the expert system for analysis of SO₂ molecules.

First step – data input

- On the beginning of the ES work, the user inputs some necessities data.
- Those data are usually the name of file with spectrum, and also with upper and lower energy limit.
- Also, it is necessary to direct the ES to tables which are consisted from different data and combination of data which the ES uses in the some phase of work.
- After receiving of initial data, the ES starts with the threshold spectrum analysis.

All spectra are recorded in the form of two integer arrays: one which represents the number of channels and second is a count i.e. the number of events on the given channel.

Second step – Finding and extracting all peaks

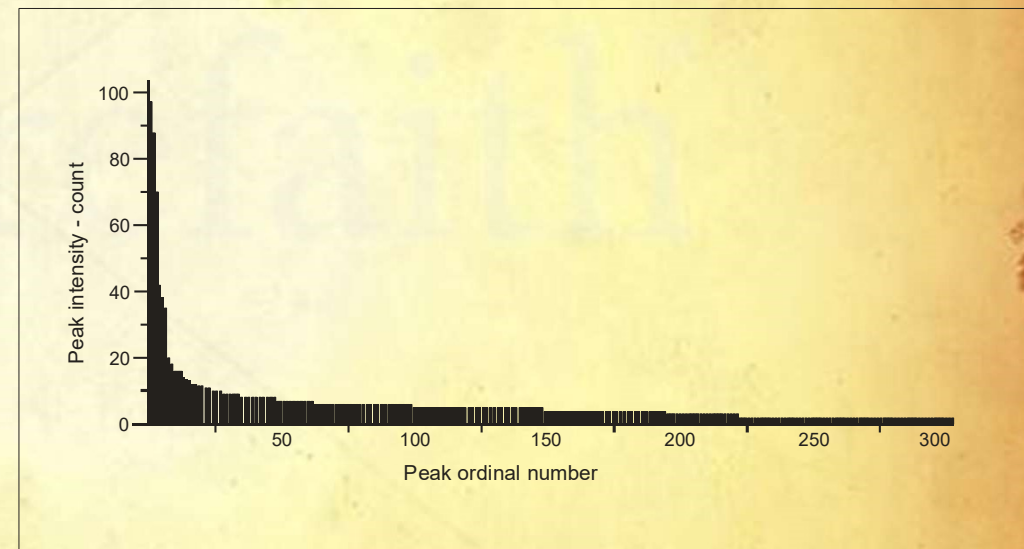
ES, with assistance of Pascal program, marks all peaks in the spectrum.

$$O_{n-1} \leq O_n \geq O_{n+1}$$

Estimation of signal/noise ratio

- As many of peaks arise from noise, one of the first tasks of ES is to separate those peaks from peaks which arise from excited states, vibrational levels and resonances, and to eliminate them from further process of analysis.

The ES create non-decreasing array (from) of the peaks, based on assumption that the most intensive peak, in the spectrum, arise from discrete energetic level, not from noise



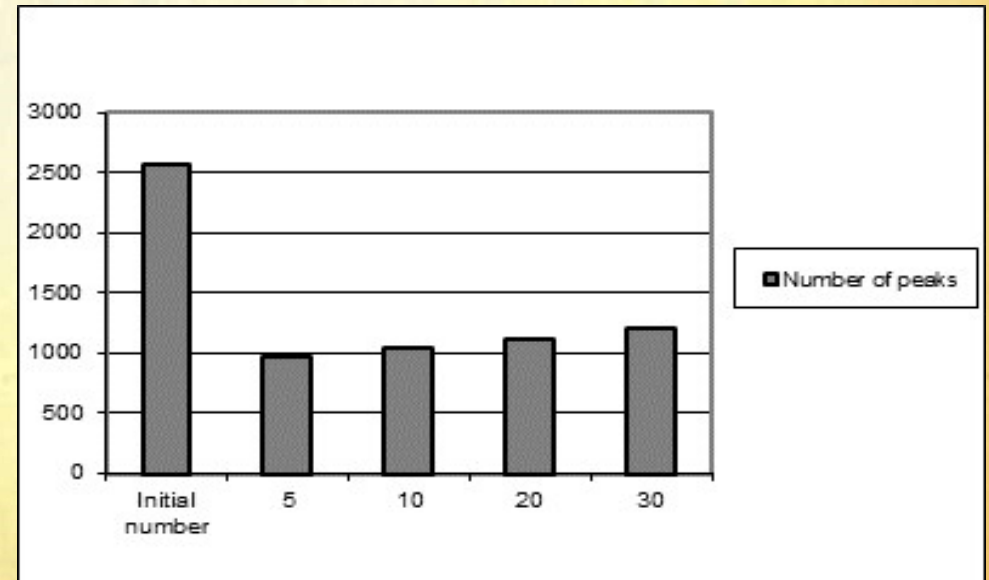
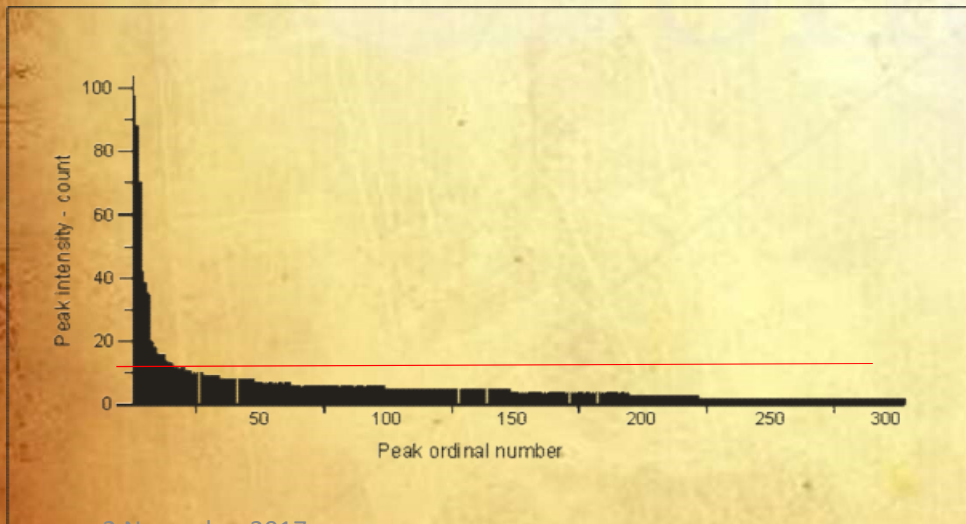
Estimation of signal/noise ratio

$$D(k) = \frac{\sum_{i=N-k+1}^N C_i}{\sum_{i=1}^k C_i}$$

N – the total number of peaks in spectrum

K – chosen number of peaks for estimation of $D(k)$

	Number of peaks	Peaks for analysis %	Reducing the number of peaks for analysis %
Initial number of peaks	2568	100%	0%
Chosen number of peaks			
5	968	38%	62%
10	1042	41%	59%
20	1121	44%	56%
30	1199	47%	53%



Calibration and Referential peak

- Calibration - The calibration of energy scale is very important part of the process of spectral analysis. This is precondition for well-done energy positioning and identification of peaks.
- Calibration can be done in two ways, depending on experimental conditions.
- Calibration can be performed under assumption that the highest peak is not generated by noise, based on its energy position, and by knowing energy interval between channels.
- After the calibration of the energy scale, the expert system starts with estimation of equipment resolution.
- The resolution is defined as smallest energy distance at which a two neighboring peaks are observed as separated.

Identification and classification of peaks

- Identification of peak is next step in process of spectrum analysis.
- The expert system analyses every single peak separately.
- Based on the calibration of energy scale and on energy value of channel, the expert system calculates correspondent energy for a peak.
- This value the expert system compares, using external Pascal program, with values in the table of energy levels of N_2 molecule states. If this value exists, the peak is classified as concrete state and it gets a classification number

Twoatomic molecules

- The presence of vibrational levels and resonances is characteristic
- We know the energy distance between vibrational levels
- Peaks have normal distribution
- We had idea to generate whole spectrum, on entire energy range
- To do this, ES needs the parameters for referential peak
- We used the Lorentzian form as a form of referential peak

Referential peak

$$y = y_0 + \frac{2A}{\pi} \frac{w}{4(x - x_0)^2 + w^2}$$

- Parameters for referential peak from Origin-a



$$X \rightarrow x_0 - \frac{\Delta x}{2}, \dots, x_0 + \frac{\Delta x}{2}$$

Function INIT

Deviation from characteristic symmetrical shape of peak can occur due to a presence of vibrational levels that arose from certain states that are on lower energy values, or because of resonances or because of noise.

Identification and marks

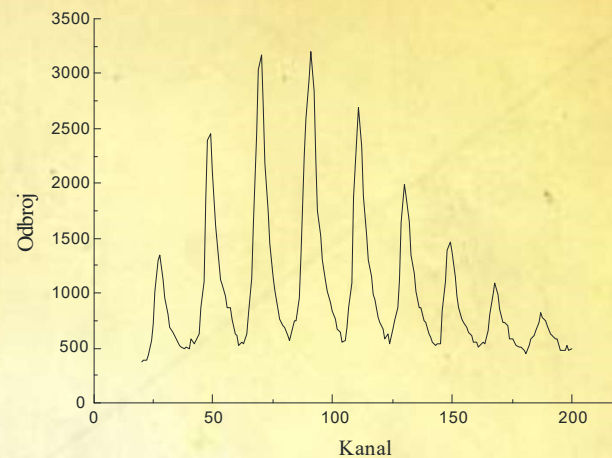


2. Vibrational level 3. Resonance 4. Overlapping state and vibrational level 5. Noise

Twoatomic molecules

- It starts with positioning on the channel which corresponds to the first state of the energy interval.
- Based on known characteristic distance value between vibrational levels, the ES calculates the channels which correspond to vibrational levels for examined state.
- On those channels, the ES, using Pascal program, generates peaks based on referential peak in form of Lorentzian.
- ES forms the DEVIATION spectrum
- ES repeats procedures for this spectrum

Chann el	Count_S	Counts_L	Deviation	Peak	Origine
13	1991	2215	-224	0	0
14	3318	3132	186	1	3
15	4274	4299	-25	0	0
16	4778	4914	-163	1	1
17	4237	4299	-26	0	0
18	3278	3132	146	1	3
19	2349	2215	134	0	0
20	1818	1627	191	1	3
21	1380	1260	120	0	0
22	1101	1024	77	0	0
23	929	866	63	0	0
24	796	757	39	0	0
25	795	679	116	1	3
26	730	621	109	0	0
27	677	577	100	0	0
28	637	543	94	0	0
29	636	517	119	1	3
30	584	495	89	0	0
31	597	397	200	0	0
...
42	1035	1198	-163	1	2



N_2 molecule, the state $\text{B}^3\Pi_g$
(7eV - 9,5eV)

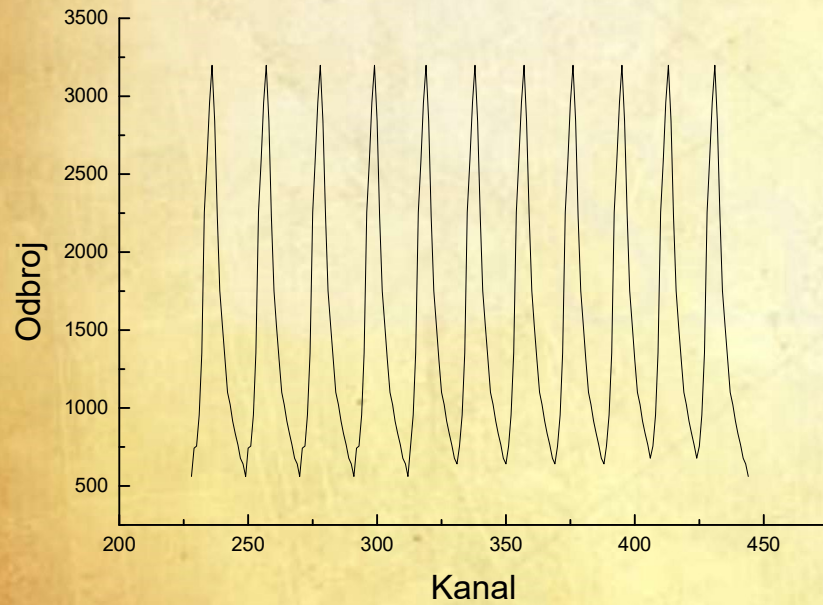
Filled table (after analysis)

Triatomic molecules

- In the threshold spectra of triatomic molecules clearly defined structures almost don't exist
- In triatomic spectrum exists complex, compound structures, because of peaks overlapping.
- The energy value between the vibrational levels is unknown. Often only between the state and the first vibrational level is known.
- However, the ES can make the analysis even in the case if the exact value of concrete energy distance is unknown, because all energy distances have to lie in the interval around some characteristic value.

Triatomic molecules

First step:

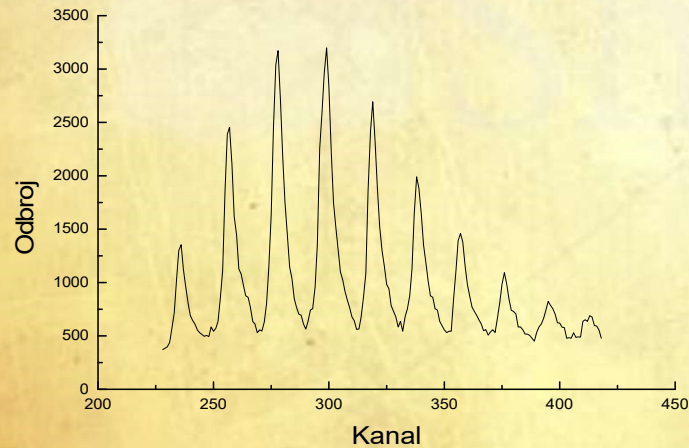


All vibrational levels have the same count and all are equidistant.

Second step: correction of peaks count

The ES, for each peak separately, defines coefficient which presents the ratio between the maximal count value of referential peak and the maximal count value of vibrational level peak.

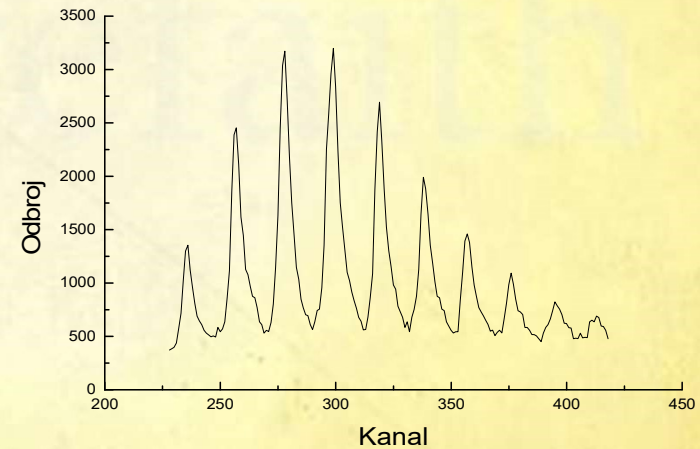
$$k = \frac{O_{\text{refmax}}}{O_{\text{max}}}$$



Generated spectrum

The ES calculates modified value of count for each channel as ratio between referential value of count and calculated value of coefficient for concrete peak using relation:

$$O = \frac{O_{\text{ref}}}{k}$$



Real spectrum

Due to different influences, vibrational levels are not completely equidistant. Because of that, it is necessary to show that by moving peaks in certain interval of energies left or right, can be obtained a spectrum at which the position of vibrational levels almost completely correspond to positions in real spectrum.

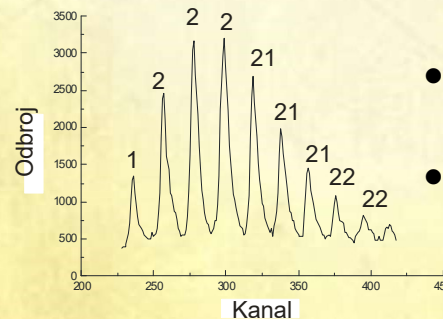
Also, by inputting of additional levels, it is necessary to show that is possible to obtain the spectrum which, on the best way, reproduce the look of the real spectrum,

Our aim was to show that the complex structure of those spectra can be interpreted as sum of large number of vibrational levels that belong to given states.

Third step:

Channel	Count	Count	Deviation	Peak	Origin	Pass
...
253	1858	1572	1286	1	5	
254	2388	2142	1246	0	0	
255	2454	2454	1000	0	2	2
256	2110	2142	968	0	0	
...
312	2694	2694	1000	0	2	21
313	2335	2352	983	0	0	
314	1884	1726	1158	0	0	
315	1526	1230	1296	0	0	
316	1303	911	1392	0	0	
317	1157	710	1447	1	5	
...
332	1646	1738	908	0	0	
333	1991	1991	1000	0	2	22
334	1884	1738	1146	0	0	
...

The ES starts with movement of peak, for one channel in the direction to the right. If, after this movement, the checking of position shows that the peak isn't positioned at the right place, then the ES moves peak for one channel to the left and again performs the check. Movement for one channel either to the left or to the right is called first pass, for two channels a second and for three a third pass.



- 2 - peaks which are overlapping before any movement
- 21, 22, 23 - peaks which are overlapping after first, second and third pass.

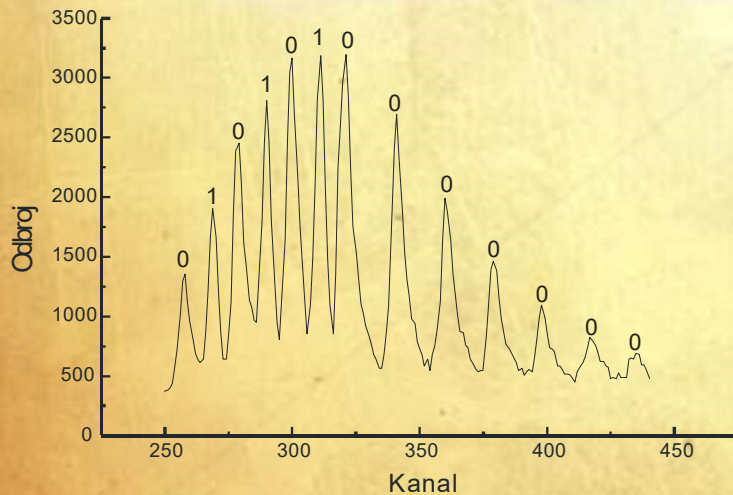
Second, very important thing, which the ES must to check, is possibility to simulate real look of spectrum which contains large number of mutually close vibrational levels.

Idea is putting additional peaks between each two already existing peaks. The channels, in which additional peaks have been put, have been calculated as arithmetic mean value of channels between they have been put

$$x = \frac{x_1 + x_2}{2}$$

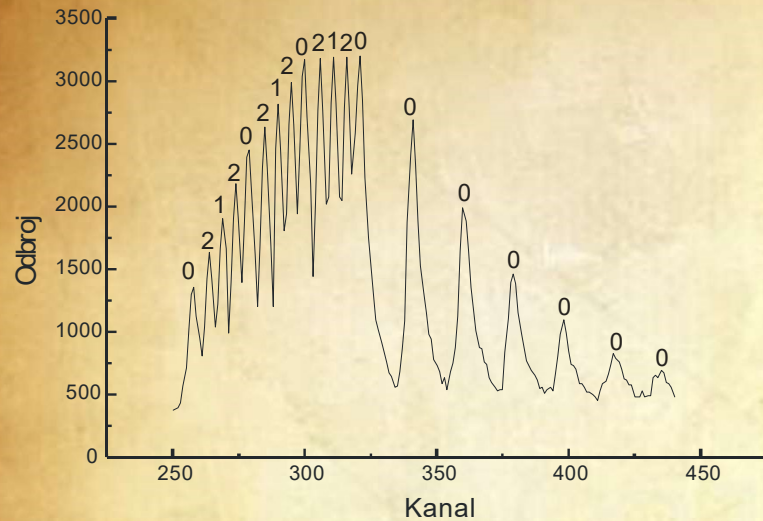
Count of new peaks has been calculated according to the same principle

$$O = \frac{O_1 + O_2}{2}$$

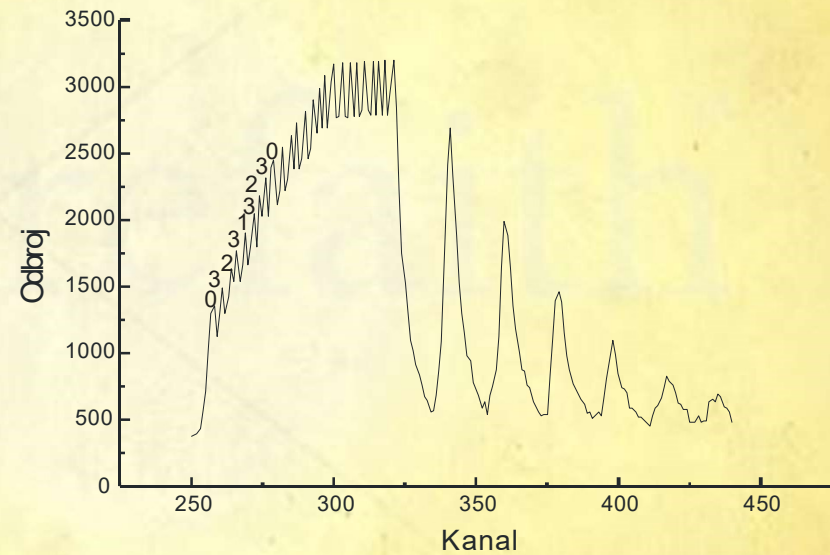


Peak of state or v. level \longrightarrow 0

The peaks of first generation \longrightarrow 1



The third generation peaks



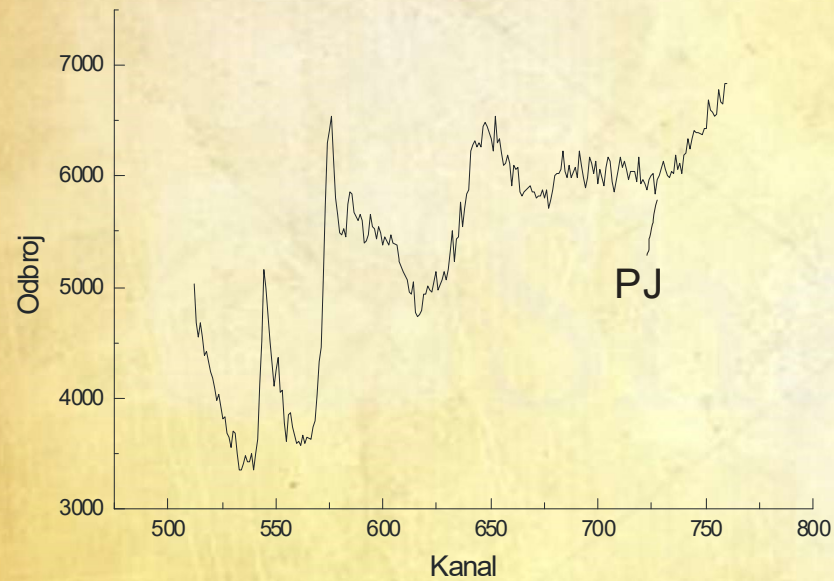
The second generation peaks



On this way, we are checking an assumption that the complex spectrum we can observe like sum of large number of peaks which mostly arise from vibrational levels.

The ES developed on this way enables detailed and very exact analysis of electron spectra of triatomic and polyatomic molecules.

A part of threshold spectrum of SO₂ which is recorded at energies that lie between 9.5 eV and 12.5 eV



Channel	Count	Count_L	Deviation	Peak	Origin e	Pass
...
574	6546	6546	1000	0	1	
...						
578	5651					
579	5483					
580	5480	4829	1651	0		
581	5535	5535	1000	0	2	22
582	5454	4829	1625	0		
583	5758	5115	1643	0		
584	5859	5859	1000	0	2	2
585	5850	5115	735	0		
586	5673	3754	1919	1	5	
587	5596	4941	345	0		
588	5660	5660	1000	0	2	21
589	5607	4941	666	0		
590	5394	3627	1767	0		
591	5415	3623	1792	1	5	
592	5475	4936	593	0		
593	5654	5654	1000	0	2	2
594	5542	4936	606	0		
595	5546	3623	1923	1	5	
596	5543	4851	692	0		
597	5556	5556	1000	0	2	21
...
733	5992	3938		0	6	

Memories



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