
The Developed Computer IR-Spectroscopic “Spectrum” Application

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ABSTRACT

*The use of a computer for processing of the data of infrared spectroscopy of the tumors of the bones permits not only to simplify the labour of the treating doctor- oncologists, but to achieve of the central objective - the identification of the diagnosis and conducting of studies of the physical chemistry mechanism of the formation of the tumor. In connection with this the fundamentally new computer IR- spectroscopic “**Spectrum**” application was developed. This application permits to carry out in the regime of real time the diagnostics of tumors on the basis of the quantitative analysis of the structures of the molecules of the inorganic and organic part of the bone and changes, which incoming in it with the development of pathologic process among the patients. The essence of the use of developed application consists in the establishment of the basic physical chemistry reasons for the appearance of disease, the implementation of the prognosis of its outcome, the selection of the optimum methods of treatment.*

Keywords: *Modeling; IR-Spectroscopy; Programming; Application; Cancer; Quantative Analysis.*

INTRODUCTION

The use of a computer for processing of the database of infrared spectroscopy of tumors [1-3] allows not only to simplify the work of the attending oncologist, but also to solve the main problem - the diagnosis and research of the physic-chemical mechanism of tumor formation. In this regard, a computer application “Spectrum” was developed, which allows diagnosing bone tumors using an infrared spectroscope [4]. Based on the results of the program, the basic principles of computer infrared spectroscopic diagnostics, classification and prediction of methods for treating bone tumors were formulated.

MATERIALS

As test materials were taken blood, biopsy and ash sample of cancer patients bone.

METHOD AND RESULTS

The essence of work of developed application “Spectrum”, implemented on the computer and minicomputer EC1033, CM-4, and today on the personal computer, for use in the clinical practice, is reduced to the following algorithm (figure 1):

- 1) The composition of the data base on all inputting patients is produced in the form, compatible with the means of the information input to the personal computer. The principle of the construction of these forms is based on the coding, i.e., the conditional assigning to each observed patient and each investigated symptom of their number. The qualitative assessments of the investigated symptoms are inputted in the digital form. The

majority storages data are computer's oriented medical documents - the spectra of the nonashing and ashing samples of the bones of the investigated patients, the ambulant cards and the histories of disease.

Figure 2 presents the printout and graphical presentation on the personal computer screen of nonashing sample spectrum 1 data input (the base absorption and absorption lines according to the wave numbers).

Figure 3 presents the printout and graphical presentation on the personal computer screen of ashing sample spectrum 1 data input (the base absorption and absorption lines according to the wave numbers).

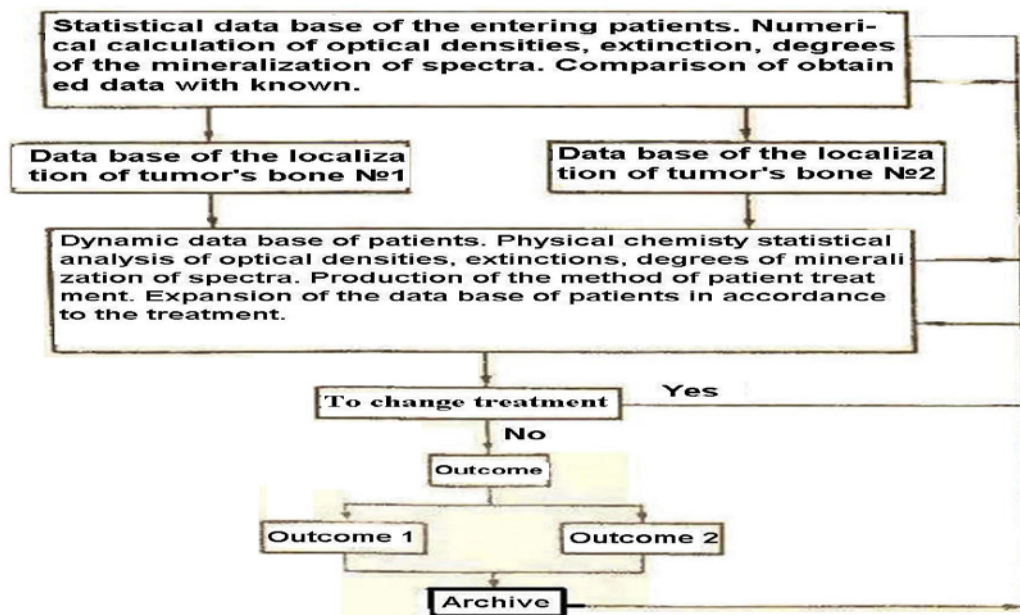


Fig.1: Algorithm of the developed application "Spectrum"

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NONASHESING SPEKTR N 1

NUMBER	WAVE NUMBER	ABSORPTION LINE	BASIS LINE
1	100	0.100	1.000
2	200	0.200	1.200
3	300	0.300	0.770
4	400	0.400	1.800
5	500	0.500	0.880
6	0	0.600	0.500
7	0	0.900	0.700
8	0	1.000	0.700
9	0	1.400	0.900
10	0	1.300	1.000
11	0	1.000	1.000
12	0	0.600	0.600
13	0	0.500	0.900
14	0	0.100	0.600

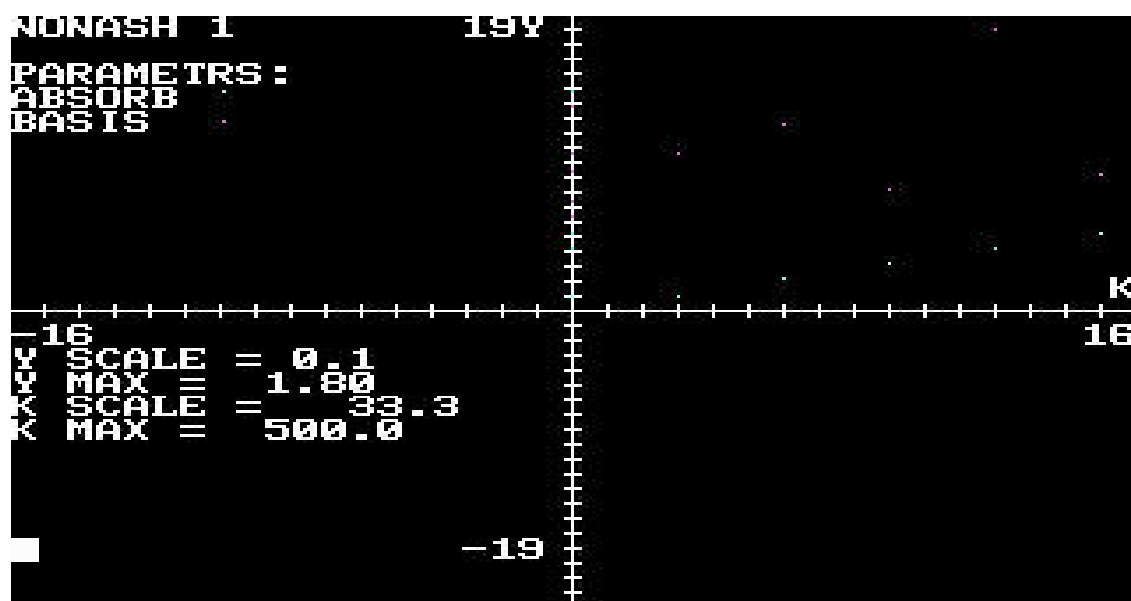


Fig. 2: Printout and graphical presentation of nonashing sample spectrum 1 data input (the base absorption and absorption lines according to wave numbers).

ASHESING SPEKTR N 1				
NUMBER	WAVE LINE	ABSORPTION LINE	BASIS LINE	
1	100	0.100	1.000	
2	200	0.200	1.000	
3	300	0.300	0.890	
4	400	0.400	1.000	
5	500	0.500	1.000	
6	600	0.600	1.000	
7	700	0.500	1.000	
8	800	0.400	1.000	
9	900	0.300	1.000	
10	1000	0.400	1.000	
11	1100	0.500	1.000	
12	1200	0.600	1.000	
13	1300	0.500	1.000	
14	1400	0.400	1.000	
15	1500	0.300	1.000	



Fig. 3: Printout and graphical presentation of ashesing sample spectrum 1 data input (the base absorption and absorption lines according to wavenumbers).

The information input was produced on the magnetic storages of the personal computer. The computer program "Spectrum", implemented on the computer's language C, was capable to load the information, in the dialog regime, to the data base of magnetic storages.

2) The numerical calculations of the coefficients of the optical densities, of the extinction, of the degrees of the mineralization, of the initial spectra are completed using the basic formulas of molecular infrared spectroscopy:

$$T = \frac{FFON}{F0FON} \quad (1)$$

$$D = \log_{10} \frac{1}{T} \quad (2)$$

$$E = \frac{\pi \cdot D \cdot L^2}{4M} \quad (3)$$

$$SM = \frac{D}{D_1} \quad (4)$$

Where T - the coefficient of passing, FFON - the line of the absorption, F0FON - the base line of the absorption, D1 - the coefficient of the optical density of the organic and inorganic part of the spectrum, D - the coefficient of the optical density of the inorganic part of the spectrum, E - extinction coefficient, SM – the degree of the mineralization, M - the mass of the sample, L - the diameter of the sample. Figure 4 presents the results of calculation of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient, according to the wave numbers, for nonashing sample spectrum 1.

The graphical representation of the obtained values of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient depending on the wave numbers is illustrated in graphs 5, 6 and 7. Figure 8 presents the results of calculation of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient, according to the wave numbers, for ashing sample spectrum 1. The graphical representation of the obtained values of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient depending on the wave numbers is illustrated in graphs 9, 10 and 11. Figure 12 graphically illustrates the general dependence of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient on the wave numbers for ashing sample spectrum 1.

Listing 1 presents the printout of mineralization matrix. The analytical and graphic dependences of the calculated values on the wave numbers are made using the specially developed computer program of optimum interpolation.

3) The tumors of the bones are characterized such relationship of inorganic and organic substance, which easily and simply can be discovered by the method of infrared spectroscopy.

The previously conducted investigations showed that the healthy, benign and malignant tissues of the bones have the characteristic group of wave numbers on the infrared spectrum of the ashing sample: 570, 610, 880, 1050, 1080, 1120, 1430, 1460 cm⁻¹. The differences between them consist in the different values of the degree of mineralization. So, the degree of the mineralization of benign tumors regarding its value is lower than the degree of the

mineralization of healthy tissues. The degree of the mineralization of malignant tumors is, in turn, lower than the degree of the mineralization of benign tumors. In connection with this, the complete information about all known spectra of healthy, benign, malignant bone tissues and also corresponding to them degrees of mineralization with the commentaries was written on the magnetic storage of the personal computer (hard drive, USB driver). The initial data of the investigated patients, extended by the spectra of optical densities, extinction, by the degrees of mineralization, are compared with the data of the magnetic storage of personal computer. Under the coincidence of initial data with the standards, the typical, corresponding to precisely diagnosis symptom, the text of the diagnosis of the patient from the magnetic storage, was printed on the screen of computer.

- 4) On the basis of obtained during of the process of diagnostics of data the construction of the data base of infrared spectroscopy and formalized histories of the disease of the bones investigated patients on the concrete localizations of tumors is produced, using the computer.

It should be noted, that this data base is not isolated from the data base of the inputting patients. It is its path.

NONASHESING SPEKTR N 1		
COEF.OF PASSING	OPTICAL DENSITY	EXTINSION
0.100	2.303	1.808
0.167	1.792	1.407
0.390	0.943	0.740
0.222	1.504	1.181
0.568	0.565	0.444
1.200	-0.182	-0.143
1.286	-0.251	-0.197
1.429	-0.357	-0.280
1.556	-0.442	-0.347
1.300	-0.262	-0.206
1.000	0.000	0.000
1.000	0.000	0.000
0.556	0.588	0.462
0.167	1.792	1.407
0.308	1.179	0.926

Fig.4: The results of calculation of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient, according to the wave numbers, for nonashing sample spectrum 1.

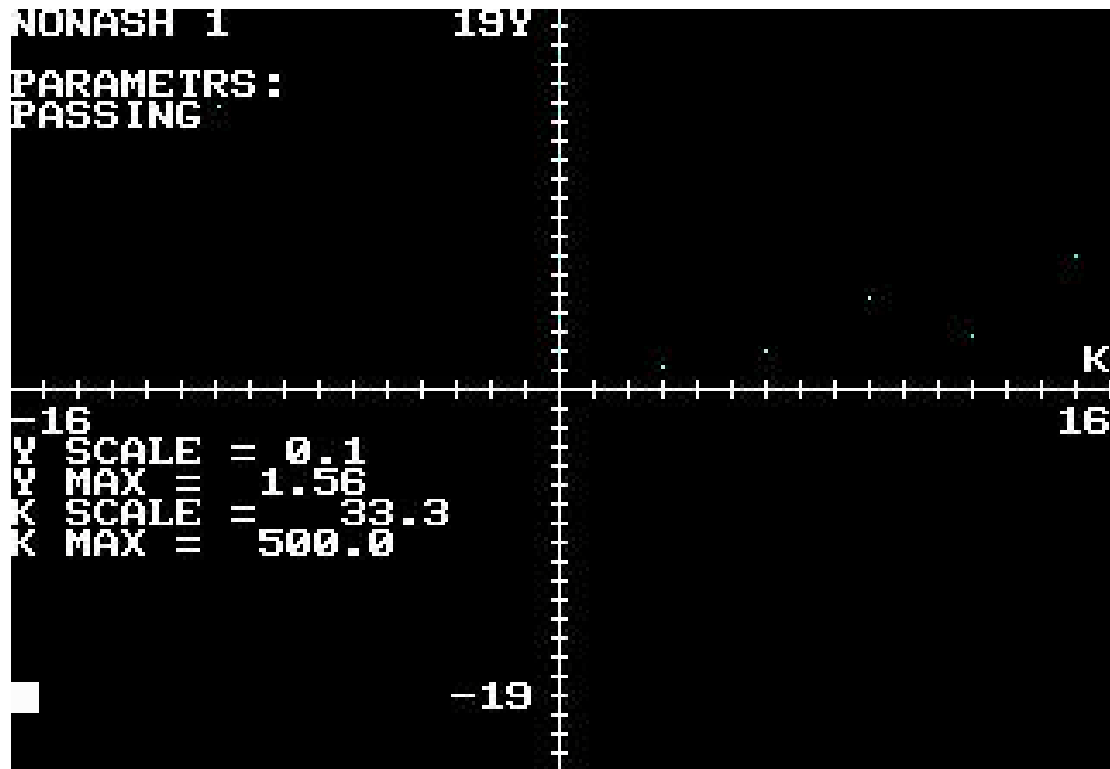


Fig. 5: The graphical representation of the obtained values of the coefficient of passing depending on the wave numbers for nonashing sample spectrum 1.

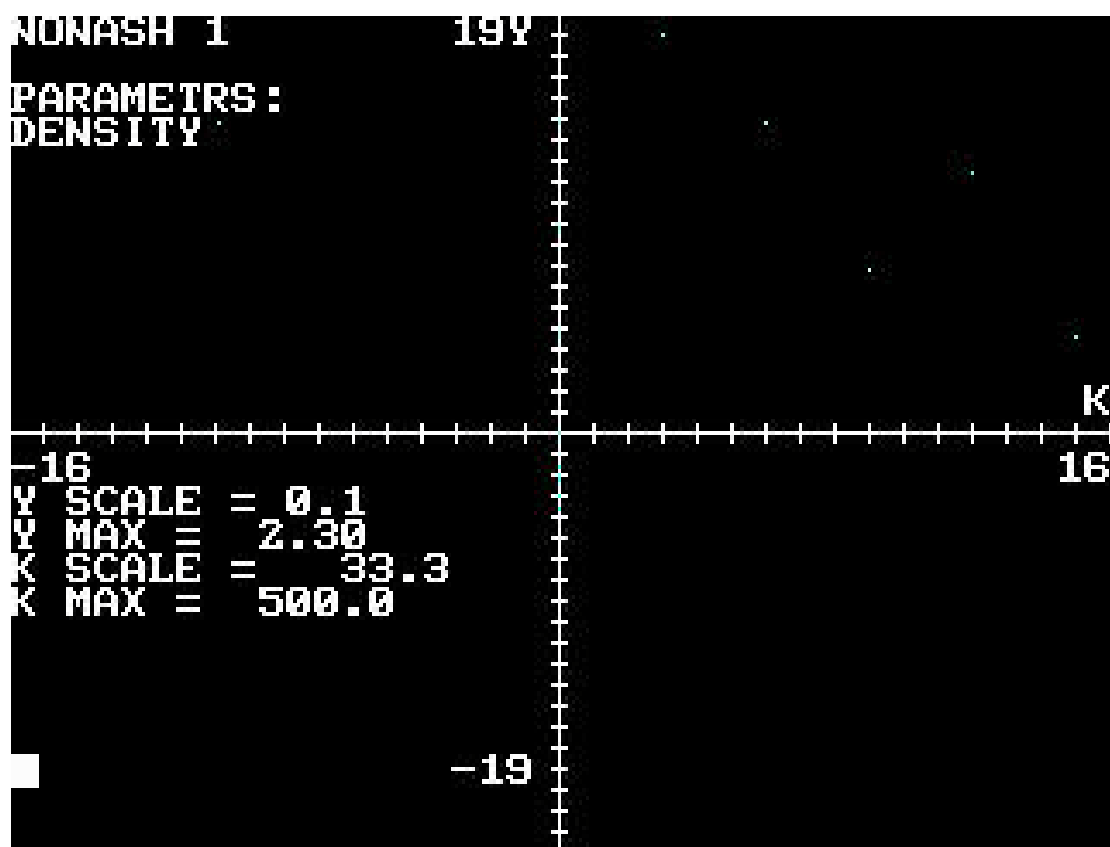


Fig. 6: The graphical representation of the obtained values of the coefficient of the optical density depending on the wave numbers for nonashing sample spectrum 1.

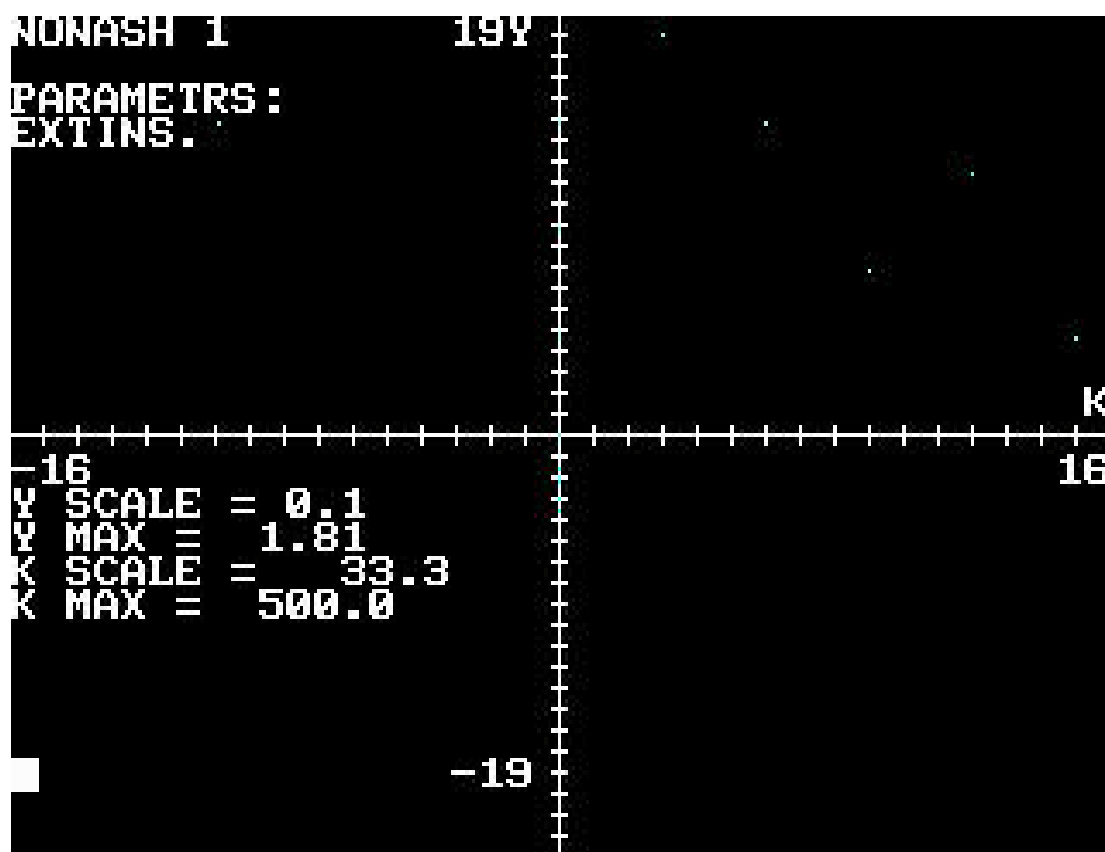


Fig. 7: The graphical representation of the obtained values of the coefficient the extinction depending on the wave numbers for nonashing sample spectrum1.

ASHESING SPEKTR N 1		
COEF.OF PASSING	OPTICAL DENSITY	EXTINSION
0.100	2.303	1.808
0.200	1.609	1.264
0.337	1.087	0.854
0.400	0.916	0.720
0.500	0.693	0.544
0.600	0.511	0.401
0.500	0.693	0.544
0.400	0.916	0.720
0.300	1.204	0.946
0.400	0.916	0.720
0.500	0.693	0.544
0.600	0.511	0.401
0.500	0.693	0.544
0.400	0.916	0.720
0.300	1.204	0.946

Fig. 8: The results of calculation of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient, according to the wave numbers, for ashing sample spectrum 1.

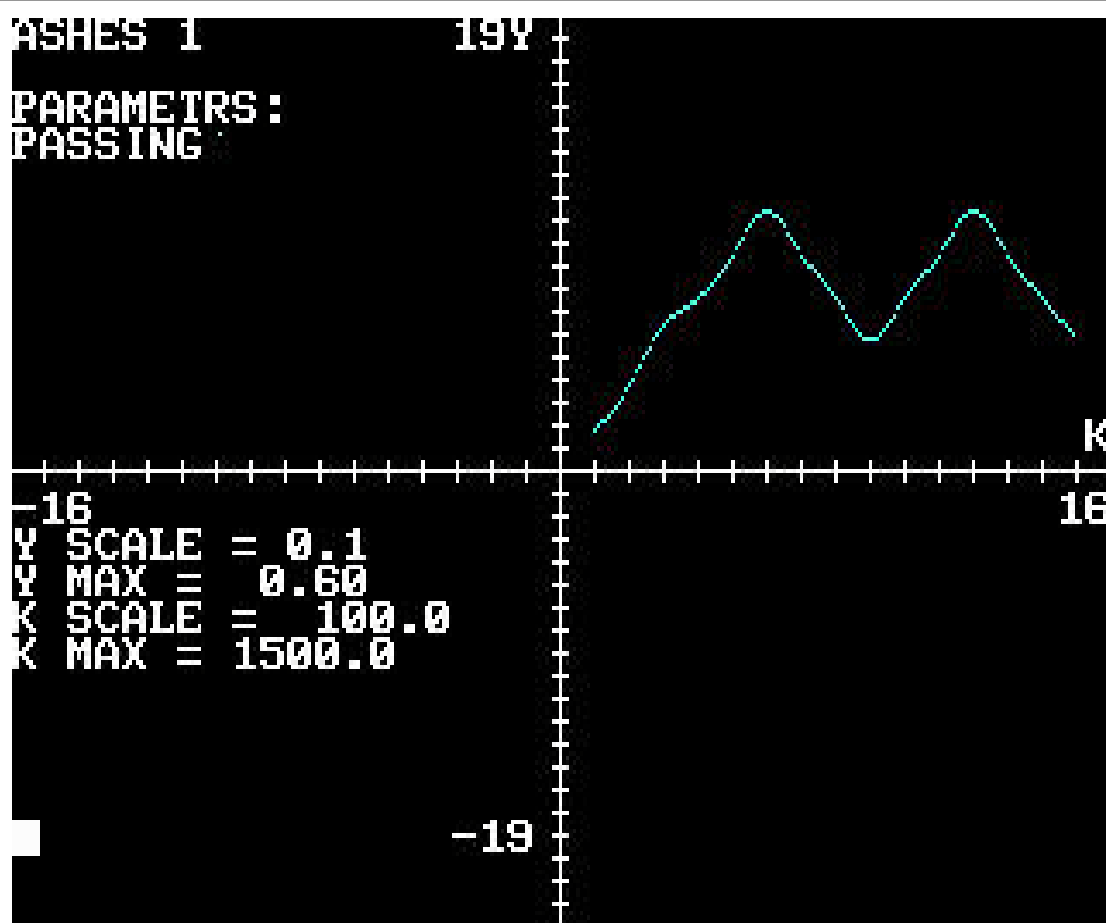


Fig. 9: The graphical representation of the obtained values of the coefficient of passing depending on the wave numbers for ashesing sample spectrum 1.

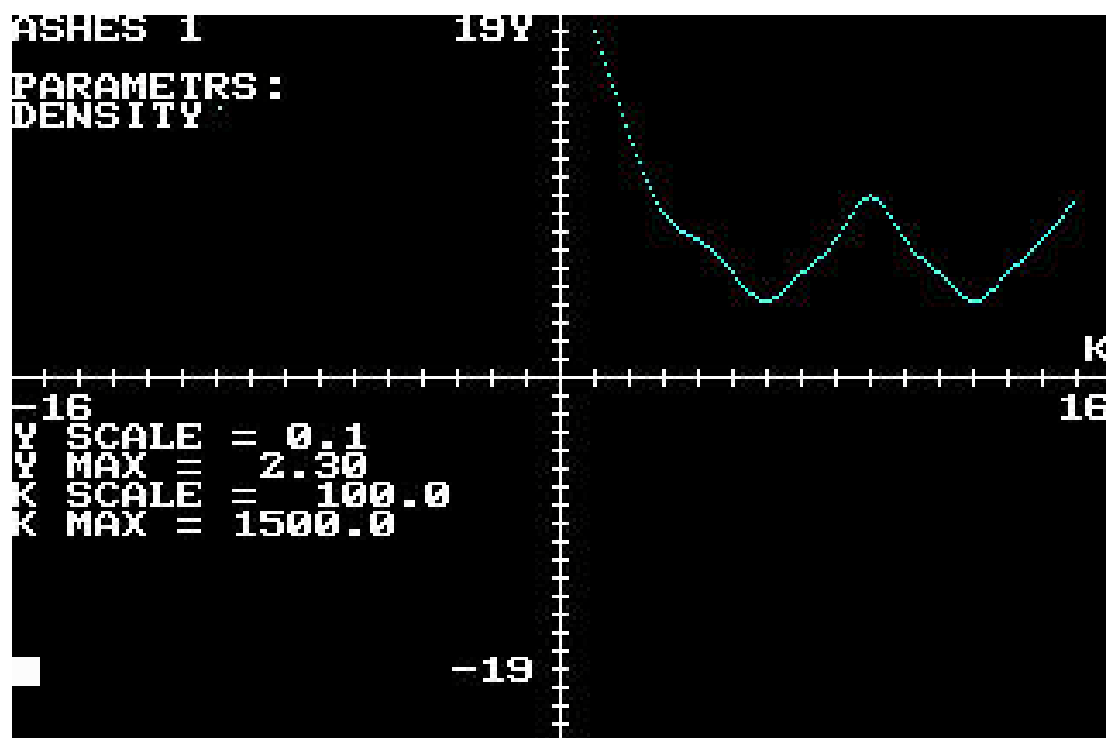


Fig. 10: The graphical representation of the obtained values of the coefficient of the optical density depending on the wave numbers for ashesing sample spectrum 1.

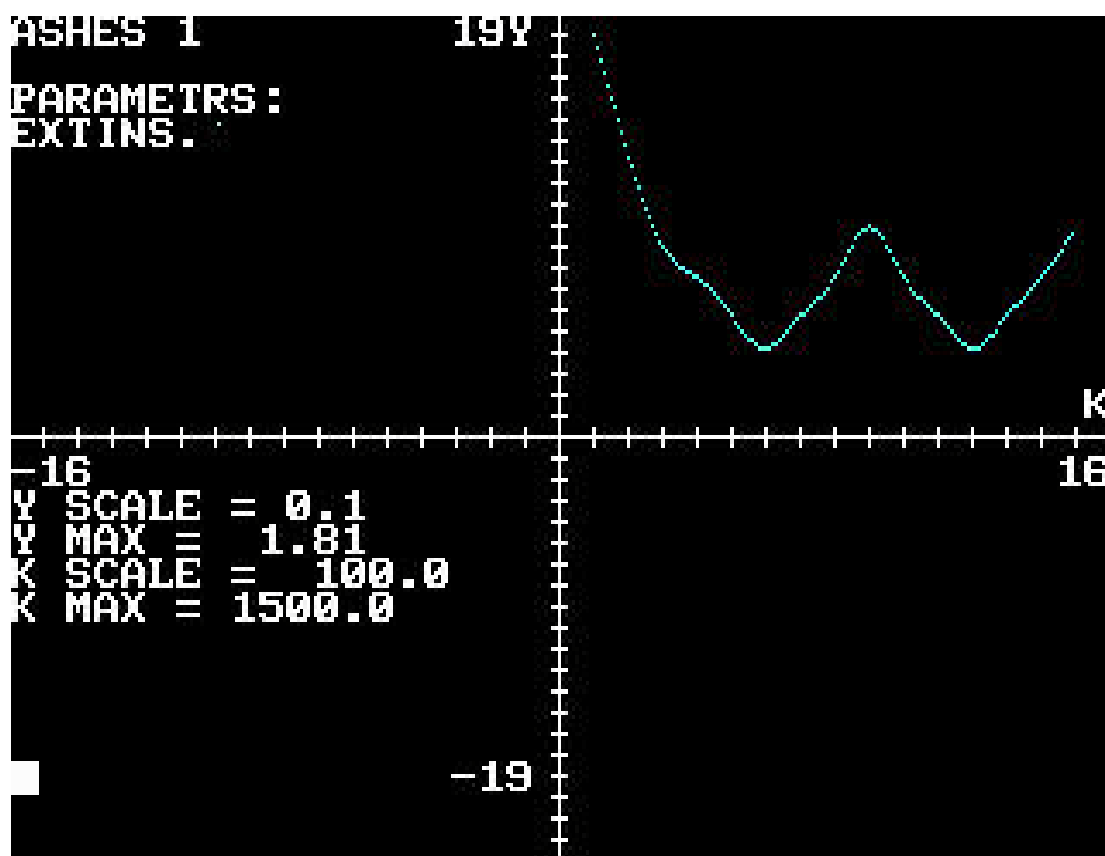


Fig. 11: The graphical representation of the obtained values of the coefficient the extinction depending on the wave numbers for ashing sample spectrum 1.

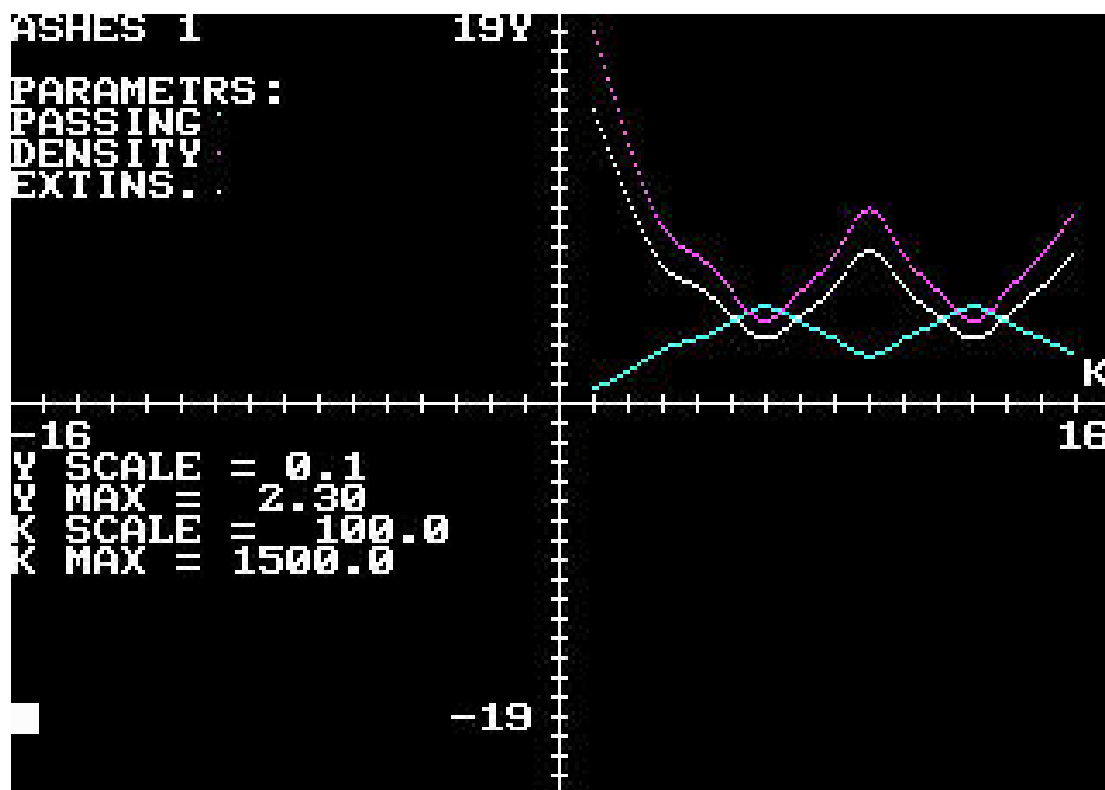


Fig. 12: The general dependence of the coefficient of passing, of the coefficient of the optical density and the extinction coefficient on the wave numbers for ashing sample spectrum 1.

Listing 9. The mineralization matrix printout

MINERAL DEGREES			
K (1) =	100	WITH K (1) =	100 MINERAL DEGREE = 1.000
K (2) =	200	WITH K (1) =	100 MINERAL DEGREE = 0.778
K (3) =	300	WITH K (1) =	100 MINERAL DEGREE = 0.409
K (4) =	400	WITH K (1) =	100 MINERAL DEGREE = 0.653
K (5) =	500	WITH K (1) =	100 MINERAL DEGREE = 0.246
K (6) =	0	WITH K (1) =	100 MINERAL DEGREE = -0.079
K (7) =	0	WITH K (1) =	100 MINERAL DEGREE = -0.109
K (8) =	0	WITH K (1) =	100 MINERAL DEGREE = -0.155
K (9) =	0	WITH K (1) =	100 MINERAL DEGREE = -0.192
K (10) =	0	WITH K (1) =	100 MINERAL DEGREE = -0.114
K (11) =	0	WITH K (1) =	100 MINERAL DEGREE = 0.000
K (12) =	0	WITH K (1) =	100 MINERAL DEGREE = 0.000
K (13) =	0	WITH K (1) =	100 MINERAL DEGREE = 0.255
K (14) =	0	WITH K (1) =	100 MINERAL DEGREE = 0.778
K (15) =	0	WITH K (1) =	100 MINERAL DEGREE = 0.512
K (1) =	100	WITH K (2) =	200 MINERAL DEGREE = 1.431
K (2) =	200	WITH K (2) =	200 MINERAL DEGREE = 1.113
K (3) =	300	WITH K (2) =	200 MINERAL DEGREE = 0.586
K (4) =	400	WITH K (2) =	200 MINERAL DEGREE = 0.935
K (5) =	500	WITH K (2) =	200 MINERAL DEGREE = 0.351
K (6) =	0	WITH K (2) =	200 MINERAL DEGREE = -0.113
K (7) =	0	WITH K (2) =	200 MINERAL DEGREE = -0.156
K (8) =	0	WITH K (2) =	200 MINERAL DEGREE = -0.222
K (9) =	0	WITH K (2) =	200 MINERAL DEGREE = -0.275
K (10) =	0	WITH K (2) =	200 MINERAL DEGREE = -0.163
K (11) =	0	WITH K (2) =	200 MINERAL DEGREE = 0.000
K (12) =	0	WITH K (2) =	200 MINERAL DEGREE = 0.000
K (13) =	0	WITH K (2) =	200 MINERAL DEGREE = 0.365
K (14) =	0	WITH K (2) =	200 MINERAL DEGREE = 1.113
K (15) =	0	WITH K (2) =	200 MINERAL DEGREE = 0.732
K (1) =	100	WITH K (3) =	300 MINERAL DEGREE = 2.117
K (2) =	200	WITH K (3) =	300 MINERAL DEGREE = 1.648
K (3) =	300	WITH K (3) =	300 MINERAL DEGREE = 0.867
K (4) =	400	WITH K (3) =	300 MINERAL DEGREE = 1.383
K (5) =	500	WITH K (3) =	300 MINERAL DEGREE = 0.520
K (6) =	0	WITH K (3) =	300 MINERAL DEGREE = -0.168
K (7) =	0	WITH K (3) =	300 MINERAL DEGREE = -0.231
K (8) =	0	WITH K (3) =	300 MINERAL DEGREE = -0.328
K (9) =	0	WITH K (3) =	300 MINERAL DEGREE = -0.406
K (10) =	0	WITH K (3) =	300 MINERAL DEGREE = -0.241
K (11) =	0	WITH K (3) =	300 MINERAL DEGREE = 0.000
K (12) =	0	WITH K (3) =	300 MINERAL DEGREE = 0.000

K (13) = 0 WITH K (3) = 300 MINERAL DEGREE = 0.541
K (14) = 0 WITH K (3) = 300 MINERAL DEGREE = 1.648
K (15) = 0 WITH K (3) = 300 MINERAL DEGREE = 1.084

K (1) = 100 WITH K (4) = 400 MINERAL DEGREE = 2.513
K (2) = 200 WITH K (4) = 400 MINERAL DEGREE = 1.955
K (3) = 300 WITH K (4) = 400 MINERAL DEGREE = 1.029
K (4) = 400 WITH K (4) = 400 MINERAL DEGREE = 1.641
K (5) = 500 WITH K (4) = 400 MINERAL DEGREE = 0.617
K (6) = 0 WITH K (4) = 400 MINERAL DEGREE = -0.199
K (7) = 0 WITH K (4) = 400 MINERAL DEGREE = -0.274
K (8) = 0 WITH K (4) = 400 MINERAL DEGREE = -0.389
K (9) = 0 WITH K (4) = 400 MINERAL DEGREE = -0.482
K (10) = 0 WITH K (4) = 400 MINERAL DEGREE = -0.286
K (11) = 0 WITH K (4) = 400 MINERAL DEGREE = 0.000
K (12) = 0 WITH K (4) = 400 MINERAL DEGREE = 0.000
K (13) = 0 WITH K (4) = 400 MINERAL DEGREE = 0.641
K (14) = 0 WITH K (4) = 400 MINERAL DEGREE = 1.955
K (15) = 0 WITH K (4) = 400 MINERAL DEGREE = 1.286

K (1) = 100 WITH K (5) = 500 MINERAL DEGREE = 3.322
K (2) = 200 WITH K (5) = 500 MINERAL DEGREE = 2.585
K (3) = 300 WITH K (5) = 500 MINERAL DEGREE = 1.360

K (4) = 400 WITH K (5) = 500 MINERAL DEGREE = 2.170
K (5) = 500 WITH K (5) = 500 MINERAL DEGREE = 0.816
K (6) = 0 WITH K (5) = 500 MINERAL DEGREE = -0.263
K (7) = 0 WITH K (5) = 500 MINERAL DEGREE = -0.363
K (8) = 0 WITH K (5) = 500 MINERAL DEGREE = -0.515
K (9) = 0 WITH K (5) = 500 MINERAL DEGREE = -0.637
K (10) = 0 WITH K (5) = 500 MINERAL DEGREE = -0.379
K (11) = 0 WITH K (5) = 500 MINERAL DEGREE = 0.000
K (12) = 0 WITH K (5) = 500 MINERAL DEGREE = 0.000
K (13) = 0 WITH K (5) = 500 MINERAL DEGREE = 0.848
K (14) = 0 WITH K (5) = 500 MINERAL DEGREE = 2.585
K (15) = 0 WITH K (5) = 500 MINERAL DEGREE = 1.700

K (1) = 100 WITH K (6) = 600 MINERAL DEGREE = 4.508
K (2) = 200 WITH K (6) = 600 MINERAL DEGREE = 3.508
K (3) = 300 WITH K (6) = 600 MINERAL DEGREE = 1.845
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K (8) = 0 WITH K (6) = 600 MINERAL DEGREE = -0.698
K (9) = 0 WITH K (6) = 600 MINERAL DEGREE = -0.865
K (10) = 0 WITH K (6) = 600 MINERAL DEGREE = -0.514

K (11) =	0 WITH K (6) =	600 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (6) =	600 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (6) =	600 MINERAL DEGREE =	1.151
K (14) =	0 WITH K (6) =	600 MINERAL DEGREE =	3.508
K (15) =	0 WITH K (6) =	600 MINERAL DEGREE =	2.307

K (1) =	100 WITH K (7) =	700 MINERAL DEGREE =	3.322
K (2) =	200 WITH K (7) =	700 MINERAL DEGREE =	2.585
K (3) =	300 WITH K (7) =	700 MINERAL DEGREE =	1.360
K (4) =	400 WITH K (7) =	700 MINERAL DEGREE =	2.170
K (5) =	500 WITH K (7) =	700 MINERAL DEGREE =	0.816
K (6) =	0 WITH K (7) =	700 MINERAL DEGREE =	-0.263
K (7) =	0 WITH K (7) =	700 MINERAL DEGREE =	-0.363
K (8) =	0 WITH K (7) =	700 MINERAL DEGREE =	-0.515
K (9) =	0 WITH K (7) =	700 MINERAL DEGREE =	-0.637
K (10) =	0 WITH K (7) =	700 MINERAL DEGREE =	-0.379
K (11) =	0 WITH K (7) =	700 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (7) =	700 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (7) =	700 MINERAL DEGREE =	0.848
K (14) =	0 WITH K (7) =	700 MINERAL DEGREE =	2.585
K (15) =	0 WITH K (7) =	700 MINERAL DEGREE =	1.700

K (1) =	100 WITH K (8) =	800 MINERAL DEGREE =	2.513
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K (2) =	200 WITH K (8) =	800 MINERAL DEGREE =	1.955
K (3) =	300 WITH K (8) =	800 MINERAL DEGREE =	1.029
K (4) =	400 WITH K (8) =	800 MINERAL DEGREE =	1.641
K (5) =	500 WITH K (8) =	800 MINERAL DEGREE =	0.617
K (6) =	0 WITH K (8) =	800 MINERAL DEGREE =	-0.199
K (7) =	0 WITH K (8) =	800 MINERAL DEGREE =	-0.274
K (8) =	0 WITH K (8) =	800 MINERAL DEGREE =	-0.389
K (9) =	0 WITH K (8) =	800 MINERAL DEGREE =	-0.482
K (10) =	0 WITH K (8) =	800 MINERAL DEGREE =	-0.286
K (11) =	0 WITH K (8) =	800 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (8) =	800 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (8) =	800 MINERAL DEGREE =	0.641
K (14) =	0 WITH K (8) =	800 MINERAL DEGREE =	1.955
K (15) =	0 WITH K (8) =	800 MINERAL DEGREE =	1.286

K (1) =	100 WITH K (9) =	900 MINERAL DEGREE =	1.912
K (2) =	200 WITH K (9) =	900 MINERAL DEGREE =	1.488
K (3) =	300 WITH K (9) =	900 MINERAL DEGREE =	0.783
K (4) =	400 WITH K (9) =	900 MINERAL DEGREE =	1.249
K (5) =	500 WITH K (9) =	900 MINERAL DEGREE =	0.470
K (6) =	0 WITH K (9) =	900 MINERAL DEGREE =	-0.151
K (7) =	0 WITH K (9) =	900 MINERAL DEGREE =	-0.209
K (8) =	0 WITH K (9) =	900 MINERAL DEGREE =	-0.296

K (9) =	0 WITH K (9) =	900 MINERAL DEGREE =	-0.367
K (10) =	0 WITH K (9) =	900 MINERAL DEGREE =	-0.218
K (11) =	0 WITH K (9) =	900 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (9) =	900 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (9) =	900 MINERAL DEGREE =	0.488
K (14) =	0 WITH K (9) =	900 MINERAL DEGREE =	1.488
K (15) =	0 WITH K (9) =	900 MINERAL DEGREE =	0.979

K (1) =	100 WITH K (10) =	1000 MINERAL DEGREE =	2.513
K (2) =	200 WITH K (10) =	1000 MINERAL DEGREE =	1.955
K (3) =	300 WITH K (10) =	1000 MINERAL DEGREE =	1.029
K (4) =	400 WITH K (10) =	1000 MINERAL DEGREE =	1.641
K (5) =	500 WITH K (10) =	1000 MINERAL DEGREE =	0.617
K (6) =	0 WITH K (10) =	1000 MINERAL DEGREE =	-0.199
K (7) =	0 WITH K (10) =	1000 MINERAL DEGREE =	-0.274
K (8) =	0 WITH K (10) =	1000 MINERAL DEGREE =	-0.389
K (9) =	0 WITH K (10) =	1000 MINERAL DEGREE =	-0.482
K (10) =	0 WITH K (10) =	1000 MINERAL DEGREE =	-0.286
K (11) =	0 WITH K (10) =	1000 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (10) =	1000 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (10) =	1000 MINERAL DEGREE =	0.641
K (14) =	0 WITH K (10) =	1000 MINERAL DEGREE =	1.955
K (15) =	0 WITH K (10) =	1000 MINERAL DEGREE =	1.286

K (1) =	100 WITH K (11) =	1100 MINERAL DEGREE =	3.322
K (2) =	200 WITH K (11) =	1100 MINERAL DEGREE =	2.585
K (3) =	300 WITH K (11) =	1100 MINERAL DEGREE =	1.360
K (4) =	400 WITH K (11) =	1100 MINERAL DEGREE =	2.170
K (5) =	500 WITH K (11) =	1100 MINERAL DEGREE =	0.816
K (6) =	0 WITH K (11) =	1100 MINERAL DEGREE =	-0.263
K (7) =	0 WITH K (11) =	1100 MINERAL DEGREE =	-0.363
K (8) =	0 WITH K (11) =	1100 MINERAL DEGREE =	-0.515
K (9) =	0 WITH K (11) =	1100 MINERAL DEGREE =	-0.637
K (10) =	0 WITH K (11) =	1100 MINERAL DEGREE =	-0.379
K (11) =	0 WITH K (11) =	1100 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (11) =	1100 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (11) =	1100 MINERAL DEGREE =	0.848
K (14) =	0 WITH K (11) =	1100 MINERAL DEGREE =	2.585
K (15) =	0 WITH K (11) =	1100 MINERAL DEGREE =	1.700

K (1) =	100 WITH K (12) =	1200 MINERAL DEGREE =	4.508
K (2) =	200 WITH K (12) =	1200 MINERAL DEGREE =	3.508
K (3) =	300 WITH K (12) =	1200 MINERAL DEGREE =	1.845
K (4) =	400 WITH K (12) =	1200 MINERAL DEGREE =	2.944
K (5) =	500 WITH K (12) =	1200 MINERAL DEGREE =	1.107
K (6) =	0 WITH K (12) =	1200 MINERAL DEGREE =	-0.357

K (7) =	0 WITH K (12) = 1200 MINERAL DEGREE =	-0.492
K (8) =	0 WITH K (12) = 1200 MINERAL DEGREE =	-0.698
K (9) =	0 WITH K (12) = 1200 MINERAL DEGREE =	-0.865
K (10) =	0 WITH K (12) = 1200 MINERAL DEGREE =	-0.514
K (11) =	0 WITH K (12) = 1200 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (12) = 1200 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (12) = 1200 MINERAL DEGREE =	1.151
K (14) =	0 WITH K (12) = 1200 MINERAL DEGREE =	3.508
K (15) =	0 WITH K (12) = 1200 MINERAL DEGREE =	2.307

K (1) =	100 WITH K (13) = 1300 MINERAL DEGREE =	3.322
K (2) =	200 WITH K (13) = 1300 MINERAL DEGREE =	2.585
K (3) =	300 WITH K (13) = 1300 MINERAL DEGREE =	1.360
K (4) =	400 WITH K (13) = 1300 MINERAL DEGREE =	2.170
K (5) =	500 WITH K (13) = 1300 MINERAL DEGREE =	0.816
K (6) =	0 WITH K (13) = 1300 MINERAL DEGREE =	-0.263
K (7) =	0 WITH K (13) = 1300 MINERAL DEGREE =	-0.363
K (8) =	0 WITH K (13) = 1300 MINERAL DEGREE =	-0.515
K (9) =	0 WITH K (13) = 1300 MINERAL DEGREE =	-0.637
K (10) =	0 WITH K (13) = 1300 MINERAL DEGREE =	-0.379
K (11) =	0 WITH K (13) = 1300 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (13) = 1300 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (13) = 1300 MINERAL DEGREE =	0.848

K (14) =	0 WITH K (13) = 1300 MINERAL DEGREE =	2.585
K (15) =	0 WITH K (13) = 1300 MINERAL DEGREE =	1.700

K (1) =	100 WITH K (14) = 1400 MINERAL DEGREE =	2.513
K (2) =	200 WITH K (14) = 1400 MINERAL DEGREE =	1.955
K (3) =	300 WITH K (14) = 1400 MINERAL DEGREE =	1.029
K (4) =	400 WITH K (14) = 1400 MINERAL DEGREE =	1.641
K (5) =	500 WITH K (14) = 1400 MINERAL DEGREE =	0.617
K (6) =	0 WITH K (14) = 1400 MINERAL DEGREE =	-0.199
K (7) =	0 WITH K (14) = 1400 MINERAL DEGREE =	-0.274
K (8) =	0 WITH K (14) = 1400 MINERAL DEGREE =	-0.389
K (9) =	0 WITH K (14) = 1400 MINERAL DEGREE =	-0.482
K (10) =	0 WITH K (14) = 1400 MINERAL DEGREE =	-0.286
K (11) =	0 WITH K (14) = 1400 MINERAL DEGREE =	0.000
K (12) =	0 WITH K (14) = 1400 MINERAL DEGREE =	0.000
K (13) =	0 WITH K (14) = 1400 MINERAL DEGREE =	0.641
K (14) =	0 WITH K (14) = 1400 MINERAL DEGREE =	1.955
K (15) =	0 WITH K (14) = 1400 MINERAL DEGREE =	1.286

K (1) =	100 WITH K (15) = 1500 MINERAL DEGREE =	1.912
K (2) =	200 WITH K (15) = 1500 MINERAL DEGREE =	1.488
K (3) =	300 WITH K (15) = 1500 MINERAL DEGREE =	0.783
K (4) =	400 WITH K (15) = 1500 MINERAL DEGREE =	1.249

K (5) =	500	WITH K (15) =	1500	MINERAL DEGREE =	0.470
K (6) =	0	WITH K (15) =	1500	MINERAL DEGREE =	-0.151
K (7) =	0	WITH K (15) =	1500	MINERAL DEGREE =	-0.209
K (8) =	0	WITH K (15) =	1500	MINERAL DEGREE =	-0.296
K (9) =	0	WITH K (15) =	1500	MINERAL DEGREE =	-0.367
K (10) =	0	WITH K (15) =	1500	MINERAL DEGREE =	-0.218
K (11) =	0	WITH K (15) =	1500	MINERAL DEGREE =	0.000
K (12) =	0	WITH K (15) =	1500	MINERAL DEGREE =	0.000
K (13) =	0	WITH K (15) =	1500	MINERAL DEGREE =	0.488
K (14) =	0	WITH K (15) =	1500	MINERAL DEGREE =	1.488
K (15) =	0	WITH K (15) =	1500	MINERAL DEGREE =	0.979

- 5) In the process of treatment of the oncological patients a dynamic change data, entering to the computer from spectra of the ashy and dried tests and corresponding to these tests information from the ambulant cards and the histories of disease, occurs. The dynamic change data concerns the results of treatment of primary tumor and its metastases, of the change in the stages of disease, of the condition of patient, which coming during the process of the surgical, radiation, medical and combined treatment. In connection with this the expansion of the primary data base due to the fixation, using the infrared spectrophotometer and the computer, of all stages of the treatment of the patients and continuous completion of the data base by these data is provided. Consequently, the transformation of the statistical data base to the dynamic data base occurs.
- 6) The statistical physical chemistry analysis of optical densities, extinction and degrees of the mineralization of the spectra of patients samples, obtained as a result of diagnostic examination and treatment of malignant new formations, is conducted concerning the characteristic wave numbers on the basis of using of the methods of mathematical modeling.

These methods include the programs of optimum interpolation and approximation, correlation and regression analysis, intended for establishing the functional connections between pair or group IR- spectroscopic of the investigated parameters of the patients samples, that correspond to the specific wave numbers and plotting the analytical and graphic dependences of optical densities, extinction, degrees of mineralization on the characteristic wave numbers.

On the basis of this conducted analysis, subsequently, the classification of the tumors of the bones for the identification of the diagnosis of tumors and a study of the mechanism of formation and development of tumor were refined and implemented.

- 7) The expansion of the data base of the oncological patients due to fixation, using the computer's spectrophotometer, the spectra of patient's samples that correspond to the used methods of treatment, and information obtained in the process of observation of the patients in the period of treatment.
- 8) The construction of the archive of the survival of patients and a constant completion it by the information about the patients, discharged from the medical organization after the carried out treatment.

Listing 10 presents the printout of the developed application “Spectrum”, implemented on the computer language Turbo basic. The developed application permits to use the modern methods of physical chemistry analysis and mathematical modeling in diagnostics, treatment and management of the oncological patients. The computer infrared spectroscopic “Spectrum” application permits to implement work in the regime of real time, *i.e.*, to obtain information about the patient on the stage of examination, treatment and observation within a few seconds. The developed application gives possibility, using a computer spectrophotometer, to study the physical chemistry mechanism of the formation of tumor, and also actively to participate in the process of treatment of malignant new formations. The essence of the use of a computer in this case consists in the establishment of the basic physical chemistry reasons for the appearance of disease, the implementation of the prognosis of its outcome, the selection of the optimum methods of treatment. The obtained results give the possibility to clinician to use a number of new tests, schemas, which remarkably increase the effectiveness of diagnostics, and to select the method of treatment. The developed computer infrared spectroscopic “Spectrum” application permits to diagnose, classify and predict of the methods of treatment of the tumors of the bones that can be successfully applied to any cancer tumor under research of a biopsy of this tumor, which is not only in a solid, ashing state, as it is required for cancer bone tumors, but also in a liquid or gaseous state.

CONCLUSION

Thus, the developed computer infrared spectroscopic “Spectrum” application permits to carry out in the regime of real time the diagnostics of tumors on the basis of the quantitative analysis of the structures of the molecules of the inorganic and organic part of the bone and changes, which incoming in it with the development of pathologic process among the patients.

The essence of the use of developed application consists in the establishment of the basic physical chemistry reasons for the appearance of disease, the implementation of the prognosis of its outcome, the selection of the optimum methods of treatment.

The developed computer infrared spectroscopic “Spectrum” application permits to diagnose, classify and predict of the methods of treatment of the tumors of the bones that can be successfully applied to any cancer tumor under research of a biopsy of this tumor, which is not only in a solid, ashing state, as it is required for cancer bone tumors, but also in a liquid or gaseous state.

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