EESTI NSV TEADUSTE AKADEEMIA TOIMETISED. 32. KÖIDE
KEEMIA. 1983, NR. 2

ИЗВЕСТИЯ АКАДЕМИИ НАУК ЭСТОНСКОЙ ССР. ТОМ 32
ХИМИЯ. 1983, № 2

https://doi.org/10.3176/chem.1983.2.06

УДК 677.4+543.422.4

O. KIRRET, Lilja LAHE,
G. RAJALO, Ene KIRJANEN

CHARACTERIZATION AND IDENTIFICATION OF CHEMICAL FIBRES BY INFRARED SPECTROMETRIC METHOD AND COMPUTER*

At present the commercial output of synthetic chemical fibres comprises more than ten types under thousands of trade names. Of them, polyamide, polyester, polyacrylonitrile, modacrylic, polypropylene, polyvinylchloride, polytetrafluoroethylene and polyvinylalcohol (=acetal) are most wellknown. Chemical fibres on the cellulose basis, such as viscose and cellulose acetate fibres are also known under many trade names.

The aim of this work is to characterize and possibly identify chemical

Table 1

Part of absorption bands file KA1 of infrared spectra of fibres

10		17		22	
556	0	550	0	535	1
570	3	730	0	770	1
675	3	795	0	1040	0
720	3	—34	0	1128	0
780	3	—37	0	1170	0
820	0	1020	0	1233	0
860	0	—44	0	1355	1
920	0	1160	0	1365	1
980	3	1170	0	1450	3
1000	0	1408	0	1678	0
1080	0	1450	0	1725	0
1130	0	1463	0	2242	3
1165	3	1502	0	2870	1
1240	3	1529	0	2930	3
1300	0	1550	0		
1325	0	1578	0		
1380	0	1610	0		
1410	3	1630	0		
1430	0	1640	0		
1470	3	1673	0		
1480	0	1690	0		
1505	0	—67	0		
1515	0	2920	0		
1530	3	—72	0		
1550	0				
1610	3				
1642	3				
1660	0				
2855	0				
2925	0				
3060	0				
3320	0				

* Reported at the 6th European Symposium on Polymer Spectroscopy, Aulanko, Hämeenlinna, Finland, August 11—13, 1982.

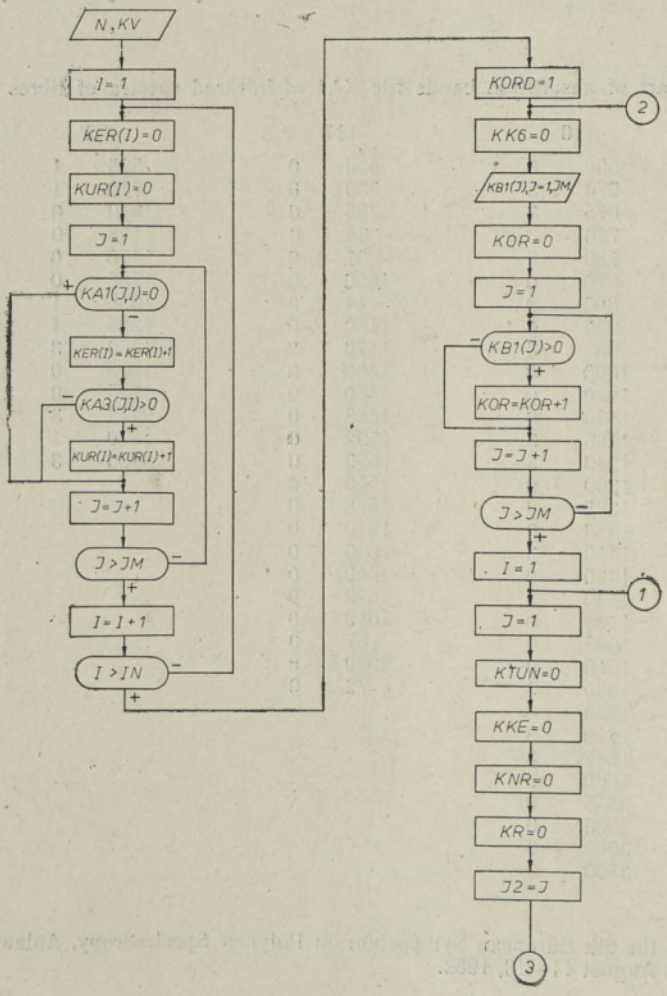
fibres of different chemical structure using infrared spectrometric method and computer. Besides the use of the infrared spectra and computer, elemental analysis of all the fibre samples were made, providing us with valuable additional information.

Infrared spectra were taken on a UR-10 spectrometer using the KBr pellet method. The absorption bands of infrared spectra were investigated in the region 400—4000 cm^{-1}. The fibres were characterized on the basis of the absorption bands of their infrared spectra, of them only the most characteristic, highly intense ones, and those of medium intensity being chosen; in Table 1, besides absorption bands, the relative intensities are given: 3 — very strong, 2 — middle, 1 — intense, 0 — weak.

Fibres identification with computer

The results measured by the authors [1–4] and those to be published later were used for compiling the computer program. The characteristic data on the absorption bands of infrared spectra of fibres are in fair accordance with the results reported by D. O. Hummel [5–6]. In order to facilitate the identification of fibres by a computer, a system of programs has been composed, consisting of three parts.

Flow chart of fibre identification program



1. Data files stored in the disk memory:

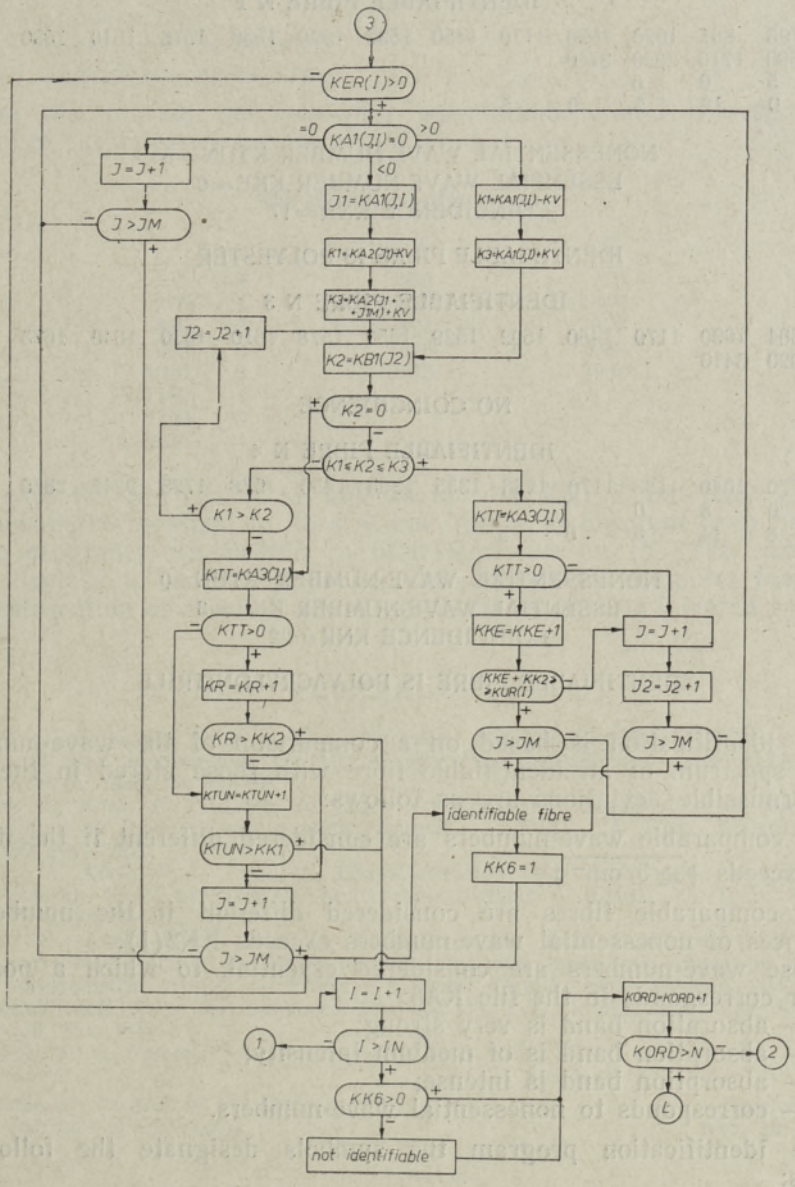
a) the file KA1 contains wave-numbers of the infrared spectra of fibres, the wave-numbers of the spectrum of one fibre being in the increasing sequence in one column;

b) the file KA3 contains weights of the wave-numbers of the infrared spectra of fibres, the weights of wave-numbers of one fibre being in one column;

c) if the wave-number covers some range, the file KA1 contains a negative number instead of the wave-number of the corresponding band, the file KA3 containing the storage positions of the corresponding initial and end numbers of the range.

2. New data recording and the available data updating program.

3. Fibres identification program.



Some examples for identification of chemical fibres (polyamide, polyester, polyacrylonitrile)

IDENTIFIABLE FIBRE N 1

570 675 715 785 820 920 980 1000 1080 1132 1165 1242 1300 1325
1383 1410 1430 1474 1480 1505 1532 1550 1610 1644 1662 2850 2900 2927
3060 3322
10 3 13 0
32 13 30 5 0 5

NONESSENTIAL WAVE-NUMBER KTUN=0
ESSENTIAL WAVE-NUMBER KKE=13
COINCIDENCE KNR=10

IDENTIFIABLE FIBRE IS POLYAMIDE

IDENTIFIABLE FIBRE N 2

730 795 864 1020 1090 1170 1450 1502 1529 1550 1578 1610 1630 1640
1673 1690 1710 2920 3410
17 5 0 0
24 0 19 5 0 5

NONESSENTIAL WAVE-NUMBER KTUN=5
ESSENTIAL WAVE-NUMBER KKE=0
COINCIDENCE KNR=17

IDENTIFIABLE FIBRE IS POLYESTER

IDENTIFIABLE FIBRE N 3

730 864 1090 1170 1450 1502 1529 1550 1578 1610 1630 1640 1673 1690
1710 2920 3410

NO COINCIDENCE

IDENTIFIABLE FIBRE N 4

535 770 1040 1128 1170 1233 1355 1365 1450 1678 1725 2242 2870 2930
22 0 8 0
14 8 14 5 0 5

NONESSENTIAL WAVE-NUMBER KTUN=0
ESSENTIAL WAVE-NUMBER KKE=8
COINCIDENCE KNR=22

IDENTIFIABLE FIBRE IS POLYACRYLONITRILE

The identification is based on a comparison of the wave-numbers of the spectrum of an identifiable fibre with those stored in the file. The permissible deviations are as follows:

a) the comparable wave-numbers are considered different if the difference exceeds $\sqrt{\pm 5\ \text{cm}^{-1}}$;

b) the comparable fibres are considered different if the number of differences of nonessential wave-numbers exceeds KK2(1).

Those wave-numbers are considered essential, to which a positive number corresponds in the file KA3:

3 — absorption band is very strong;
2 — absorption band is of medium intensity;
1 — absorption band is intense;
0 — corresponds to nonessential wave-numbers.

In the identification program the symbols designate the following notions:

N — number of experiments,
KV — permissible deviation,
KA1 (J, I), J=1—JM, I=1—IN — file of absorption bands of infrared spectra of fibres,
KA2 (J1), J1=1—J1M — intermediate file of absorption bands of infrared spectra of fibres,
KA3 (I, J), J=1, JM, I=1, IN — file of essential wave numbers,
IN — number of fibres in files KA1 and KA3,
JM — number of absorption bands in files KA1 and KA3,
J1M — intermediate number of absorption bands in file KA2,
KK1 — number of permissible differences of nonessential wave-numbers,
KK2 — number of permissible differences of essential wave-numbers,
KER(I) — number of bands in column I,
KUR(I) — number of essential wave-numbers in column I,
KB1(J) — identifiable fibre,
KOR — number of bands in identifiable fibre,
KTUN — nonessential,
KKE — essential wave-number,
KNR — coinsidence in column.

Let the file contain the following wave-numbers and corresponding weights of the infrared spectrum of fibre A.

The identifiable fibres are

A		B	C
535	0	530	773
770	1	775	840
840	0	977	990
980	3	1023	1083
1020	2	2943	2938
1180	1		
1750	0		
2940	1		

In case KV=±5 cm^{-1} as well as in case KK1 2 and KK2 1, fibre B is considered identical to fibre A, but fibre C is different from fibre A.

The programs are written in FORTRAN for an EC-1022 computer using displays in the dialog mode. Calculations by computer facilitate the identification of chemical fibres on the basis of their infrared spectra.

REFERENCES

1. *Kirret, O., Pank, M., Lahe, L.* Characterization and identification of polyester fibres and their modifications by infrared spectrometric method. — ENSV TA Toim. Keemia, 1980, **29**, 92—96.
2. *Kirret, O., Koch, P.-A., Lahe, L.* Characterization and identification of polyamide fibres by infrared spectrometric method. — ENSV TA Toim. Keemia, 1981, **30**, 281—287.
3. *Kirret, O., Koch, P.-A., Lahe, L.* Characterization and identification of polyvinylchloride fibres by infrared spectroscopic method. — ENSV TA Toim. Keemia, 1982, **31**, 50—53.
4. *Kirret, O., Koch, P.-A., Lahe, L.* Characterization and identification of polyacrylonitrile fibres and their modifications and modacrylic fibres by infrared spectrometric method. — ENSV TA Toim. Keemia, 1982, **31**, 197—203.
5. *Hummel/Scholl.* Atlas der Kunststoff-Analyse, Bd. I Tl. 1. München, 1968, S. 158—159, 111, 188.
6. *Hummel, D. O.* Polymer Spectroscopy. Weinheim, 1974, 143.

Academy of Sciences of the Estonian SSR,
Institute of Chemistry

Received
Nov. 10, 1982

O. KIRRET, Lilja LAHE,
G. RAJALO, Ene KIRJANEN

KEEMILISTE KIUDAINETE ISELOOMUSTAMINE JA IDENTIFITSEERIMINE INFRAPUNASE SPEKTROMEETRIA JA ELEKTRONARVUTI ABIL

Artiklis on osutatud võimalusele iseloomustada ja identifitseerida keemilisi kiudaineid infrapunase spektromeetria meetodil elektronarvuti abil. Uurimisobjektidena on kasutatud polüamiid-, polüester- ja polüakrüülnitriilkiudaineid.

О. КИРРЕТ, Лилья ЛАХЕ
Г. РАЯЛО, Эне КИРЬЯНЕН

ОПРЕДЕЛЕНИЕ И ХАРАКТЕРИСТИКА ХИМИЧЕСКИХ ВОЛОКОН МЕТОДОМ ИК-СПЕКТРОМЕТРИИ С ПОМОЩЬЮ ЭВМ

Наиболее известны в настоящее время классы следующих волокон: полиамидные, полиэфирные, полиакрилнитриловые, поливинилхлориды, политетрафторэтен, модакриловые, полипропиленовые, поливиниловые спирты (ацетали). Вискозные и ацетатцеллюлозные волокна также имеют сотни различных названий. Поэтому имеет большое значение определение химического состава волокон при их анализе. При помощи ИК-спектров и ЭВМ определены структурные элементы и элементарный состав химических волокон.