

## STUDIES ON CHEMICAL COMPOSITION OF WOOD ON THE BASIS OF INFRARED SPECTROSCOPY

### I. Relation between Wood Chemical Composition and Absorbance of Individual Bands of the IR Spectrum within the Range 700 - 1900 $\text{cm}^{-1}$

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Relation between the absorbance of the IR bands of wood to the holocellulose and lignin content was expressed in form of a linear equation. The measured and calculated absorbances were presented in form of a criterion of relative standard deviation ( $u_i$ ). On the basis of such a criterion the tested absorbance bands were arranged in series according to their usefulness for quantitative determinations of holocellulose and lignin in wood. From these series of  $u_i$  values results, that the most useful IR absorption bands for calculation of holocellulose and lignin content are: 1515  $\text{cm}^{-1}$  for pine wood and 1510  $\text{cm}^{-1}$  for beech wood.

### INTRODUCTION

Investigations of chemical constituents of wood by means of the infrared spectroscopy method begun in the 40-ties of this century. First works on cellulose were done by: Ellis and Bath (1940), Rowen et al., (Liang, Marchessault 1959), and Nikitin W. N. (1962). Spectroscopic investigations in infrared range on the lignin were initiated by Jones (1948) and then by Schubert, Nord, Kudzin and by the Freudenberg's school (Kratzl, Tschamler 1952).

As a result of first investigations by means of infrared (IR) spectroscopy basic relations between absorbance of IR spectrum bands and the highmolecular structure of cellulose was obtained (Mann, Marrinan, 1956, O'Connor, Du Pree, Mitcham 1958, Žbankov 1972). There were also developed some methods of lignin investigation by the application of differential spectra (Töppel 1958, Kolboe, Ellefsen 1962, Bolker, Somerville 1963) as well as a spectral analysis

of model compounds (Sarkanen, Chang, Ericsson 1967, Schweers, Faix 1973, Faix, Schweers 1974). There was also conducted an analysis of particular absorption bands of the IR spectrum of wood (Tschamler et al. 1953, Liang et al. 1960, Harrington et al. 1964, Mitchel et al.). Greatest interest was devoted to the range from 700 - 1900  $\text{cm}^{-1}$  of the IR spectrum. A multiple survey and interpretations of particular absorption bands has made within this range. Some of those bands were proposed for quantitative determinations of lignin. The choice of such bands was made until this time on the basis of qualitative comparisons.

The scope of the present work is a quantitative comparison of absorption of IR bands with respect to their use for holocellulose and lignin determinations basing on one common criterion.

## MATERIAL AND METHODS

### EXPERIMENTS

Investigations were made on the Scots Pine (*Pinus silvestris*) and beech (*Fagus sylvatica*) wood, which was submitted to decomposition processes by: cooking in NaOH, hydrolysis in  $\text{H}_2\text{SO}_4$ , fungal decay by *Polystictus versicolor* and *Coniophora puteana*. Following substances were determined in the decomposed wood: solubles in 0.1  $\text{mol/dm}^{-1}$  NaOH, lignin, holocellulose as well as the heat of combustion. A detailed description of the performed experiments was described in the paper (Dziurzyński, Supiński 1986).

Method of obtaining IR spectra. The dried sawdust was ground in a vibrator M. v Ardenne C. Z. Jena. The batch of 400 mg of roasted in an oven in 550°C KBr and  $2.00 \pm 0.05$  mg of ground wood were twice homogenised in the said vibrator 2 minutes each time. The 200.0 mg sample of homogenised mixture was then tableted in a PW-20 tableter with the use of a hydraulic press DP-36 C. Z. Jena under a pressure of 100 kp in the time of 10 minutes. The spectra were recorded on the pallets of 12 mm diameter with the use of spectrophotometer UR-20 C. Z. Jena. The recording parameters of spectra were: slit width 3.6, excitation 16, diaphragm 3%, speed of paper shift 20 mm/100  $\text{cm}^{-1}$ , speed of spectrum shift 64  $\text{cm}^{-1}/\text{min}$ . A minimum at 1880  $\text{cm}^{-1}$  was taken as spectrum basis. Permeability of this minimum was established as 95%. Relative moisture content of the air in laboratory at work was 37%.

### CALCULATIONS

Absorbance calculations of the *i*-band of IR spectrum are based on the assumptions: a) the total of chemical constituents content ( $x_j$ ) *in situ* in a wood sample amounts 100%.

$$\sum_j (x_j)_{in\ situ} = 100. \quad (1)$$

b) Absorbances of wood constituents form a total in an additive way according to the Beer's law (Kössler 1966). Thus, the wood absorbance ( $A_i$ ) may be described

by a weighted mean equation:

$$A_i = \frac{1}{100} \sum_j (a_{ij} x_j)_{in\ situ}, \quad (2)$$

where

- $A_i$  – absorbance of the  $i$ -band of IR spectrum of wood,  $A_i = \log(I_0/I)_i$ ;
- $a_{ij}$  – absorbance of the  $i$ -band of IR spectrum of the  $j$ -chemical constituent of wood,  $a_{ij} = \log(I_0/I)_{ij}$ ;
- $x_j$  – content of the  $j$ -chemical constituent of wood in percents (%);
- $i$  – index of band: 780, 840, 900, ..., 1510, 1600, 1743  $\text{cm}^{-1}$ ;
- $j$  – index of chemical constituent of wood: holocellulose, lignin.

In the case when two constituents of wood: holocellulose ( $x_h$ ) and lignin ( $x_l$ ) are determined, the equation (2) becomes as follows:

$$A_i = \frac{1}{100} (a_{ih} x_h + a_{il} x_l)_{in\ situ}. \quad (3)$$

A total of chemical wood constituents determined in a laboratory differs practically from 100%.  $\sum_j x_j \neq 100$ . It results from the incomplete selectiveness of methods of their determination. In the processes of biological decay of wood a partial depolymerisation of carbohydrates takes also place (Rypáček 1977). Therefore the equation (3) is to be normalized in form

$$A_i = \frac{1}{x_h + x_l} (a_{ih} x_h + a_{il} x_l). \quad (4)$$

The most exact results of calculations of absorbance can be obtained by using an inside standard. The best inside standard in IR spectrum of wood is the band 1378  $\text{cm}^{-1}$  (Vodnansky, Slabina, Schneider 1963). The absorbance of this band depends low on the changes of holocellulose and lignin content. Therefore in this paper the following equation is applied

$$\frac{A_i}{A_{1378}} = \frac{1}{x_h + x_l} \left[ \left( \frac{a_i}{a_{1378}} \right)_h x_h + \left( \frac{a_i}{a_{1378}} \right)_l x_l \right]. \quad (5)$$

## RESULTS AND DISCUSSION

The chemical composition of the tested wood samples is tabulated in table 1. The holocellulose and lignin contents presented in this table are arithmetic means of determinations made on the basis of chemical methods and the heat of combustion measurements (Dziurzyński, Supiński 1986). The IR spectra bands absorbances of the tested wood are presented in tables 2 and 3. Two first lines of those tables contain the absorbances of holocellulose and lignin isolated from original wood. Absorbance of holocellulose and lignin preparations have different values for par-

ticularin dividual bands. Those bands can be gathered into two groups. The group of bands: 900, 1035, 1065, 1163 and 1743 (1745) shows a dominant absorbance of holocellulose while in the group of bands: 780, 840, 1230, 1250, 1270, 1330, 1425, 1460 (1465),

Table 1

Arithmetic means of determinations of holocellulose and lignin percentages in pine and beech wood made on the basis of chemical methods and heat of combustion measurements  
Średnie arytmetyczne zawartości procentowej holocelulozy i ligniny w drewnie sosny i buka oznaczonych na podstawie metod chemicznych oraz pomiarów ciepła spalania

Sample Próbka	Pine - Sosna			Beech - Buk			
	mass loss $\Delta m$ (%) ubytek masy	holocellulose (%) holoceluloza	lignin (%) lignina	mass loss $\Delta m$ (%) ubytek masy	holocellulose (%) holoceluloza	lignin (%) lignina	
Original wood - Drewno wyjściowe	0	67.42	27.64	0	69.49	23.51	
Degraded wood Drewno zdegradowane	NaOH	21.0	66.65	28.53	25.5	66.30	24.96
		33.3	75.63	24.86	52.0	88.74	6.65
		47.8	91.22	10.52	58.5	95.54	0.12
	H <sub>2</sub> SO <sub>4</sub>	10.2	63.74	30.01	13.8	62.04	25.33
		22.6	61.89	33.85	24.0	61.77	28.50
		31.6	57.86	36.91	42.7	59.93	33.71
	<i>Polystictus versicolor</i>	6.0	70.40	21.82	3.0	67.21	21.98
		14.0	69.30	21.48	24.0	66.46	22.30
		28.7	67.58	21.82	33.0	66.40	20.89
	<i>Coniophora puteana</i>				63.0	67.50	18.55
		12.0	59.54	26.15	2.5	64.28	21.76
		23.0	57.46	28.32	16.0	55.36	19.43
		38.0	52.38	31.20	23.0	53.08	19.85
		63.0	18.96	44.16	36.0	51.26	19.55
				57.0	33.46	26.40	

1515 (1510), 1606 (1600) dominates the absorbance of lignin. A particular attention is to be paid to the 1378 cm<sup>-1</sup> band in which the values of absorbance of holocellulose, lignin as well as of natural wood are very close. For that reason this band has been selected as an internal standard (Vodnansky, Slabina, Schneider 1963) table 2 and 3.

Calculations of absorbance of the investigated IR band were made on the basis of equation (5). The difference between calculated and experimental absorbances,  $(A_i/A_{1378})_{\text{calc}} - (A_i/A_{1378})_{\text{exp}}$ , depends on the following factors:

- structural differences between the constituents of wood *in situ* and *in vitro*,
- methodical simplifications of determination of chemical composition of wood and its low selectiveness,
- not identical parameters in course of obtaining the IR spectra.

The main source of differences between absorbances calculated from equation (5) and the experimental ones is the fact that constants  $a_{ih}$  and  $a_{il}$  used for calculations (tab. 2 and 3) are derived from the spectra of holocellulose and lignin preparations *in vitro*. Those preparations differ in their structure from the native holocellulose and lignin *in situ*. Preparations *in vitro* differ each to other in dependence on the method of their isolation both in case of lignin (Čupka et al. 1969, Adamski,

Table 2

Absorbance  $A_i$  of IR spectrum bands of Pine wood degraded by chemical and biotical agents  
 Absorbancja  $A_i$  pasm widma IR drewna sosny zdegradowanego czynnikami chemicznymi i biotycznymi

Sample Próbka	Mass loss $\Delta m$ (%) Ubytek masy	$A_i$																
		780	840	900	1035	1065	1120	1163	1220	1230	1250	1270	1330	1378	1425	1460	1515	1606
Holocellulose Holoceluloza	—	0.080	0.075	0.160	0.612	0.618	0.526	0.432	0.237	0.265	0.249	0.251	0.279	0.244	0.183	0.091	0.045	0.180
Lignin	—	0.139	0.187	0.136	0.501	0.458	0.430	0.367	0.509	0.457	0.568	0.376	0.258	0.348	0.459	0.531	0.307	0.097
Original wood Drewno wyjściowe	0	0.111	0.109	0.154	0.779	0.790	0.589	0.481	0.293	0.317	0.359	0.258	0.283	0.265	0.230	0.225	0.116	0.096
NaOH	21.0	0.130	0.139	0.188	0.910	0.936	0.670	0.545	0.309	0.288	0.369	0.295	0.325	0.350	0.325	0.283	0.190	0.048
	33.3	0.152	0.139	0.207	1.048	1.075	0.782	0.626	0.322	0.310	0.365	0.334	0.359	0.382	0.348	0.255	0.192	0.056
$\text{H}_2\text{SO}_4$	47.8	0.120	0.103	0.204	1.200	1.306	0.871	0.662	0.280	0.287	0.313	0.320	0.373	0.404	0.354	0.193	0.143	0.038
	10.2	0.134	0.128	0.173	0.906	0.944	0.657	0.566	0.327	0.317	0.394	0.300	0.312	0.298	0.263	0.256	0.159	0.076
$\text{P. versicolor}$	22.6	0.126	0.136	0.185	0.768	0.771	0.596	0.501	0.323	0.296	0.376	0.293	0.296	0.296	0.270	0.287	0.139	0.043
	31.6	0.140	0.154	0.208	0.965	0.969	0.706	0.576	0.378	0.346	0.442	0.331	0.336	0.336	0.317	0.346	0.169	0.047
<i>C. puteana</i>	6.0	0.089	0.103	0.160	0.851	0.867	0.628	0.511	0.336	0.348	0.398	0.280	0.302	0.284	0.249	0.217	0.144	0.154
	14.0	0.125	0.143	0.208	0.854	0.871	0.682	0.543	0.351	0.381	0.424	0.327	0.357	0.330	0.294	0.257	0.183	0.190
Degradowane zdegradowane	28.7	0.101	0.121	0.180	0.735	0.740	0.566	0.482	0.335	0.338	0.378	0.280	0.302	0.290	0.263	0.234	0.160	0.176
	12.0	0.120	0.147	0.179	0.747	0.774	0.576	0.470	0.334	0.326	0.387	0.288	0.293	0.270	0.256	0.253	0.172	0.180
Degradowane zdegradowane	23.0	0.114	0.139	0.188	0.871	0.877	0.643	0.543	0.380	0.368	0.451	0.328	0.328	0.309	0.291	0.305	0.167	0.195
	38.0	0.103	0.140	0.175	0.750	0.768	0.586	0.496	0.376	0.349	0.435	0.307	0.307	0.297	0.293	0.315	0.185	0.185
	63.0	0.136	0.190	0.183	0.793	0.747	0.616	0.563	0.576	0.531	0.722	0.398	0.371	0.410	0.425	0.580	0.344	0.220

Table 3

Absorbance  $A_i$  of IR spectrum bands of Beech wood degraded by chemical and biotical agents  
 Absorbancja  $A_i$  pasm widma IR drewna buka zdegradowanego czynnikami chemicznymi i biotycznymi

Sample Próbka	Mass loss $\Delta m$ (%) Ubytek masy	$A_i$																	
		780	840	900	1035	1065	1120	1163	1230	1250	1270	1330	1378	1428	1465	1510	1600	1745 ( $\text{cm}^{-1}$ )	
Holocellulose Holoceluloza	—	0.048	0.055	0.165	0.699	0.711	0.587	0.459	0.309	0.389	0.282	0.258	0.302	0.245	0.212	0.094	0.032	0.257	
Lignin Lignina	—	0.132	0.167	0.146	0.454	0.511	0.780	0.397	0.639	0.492	0.506	0.521	0.325	0.431	0.585	0.575	0.397	0.103	
Original wood Drewno wyjściowe	—	0.061	0.086	0.138	0.790	0.787	0.639	0.469	0.365	0.459	0.352	0.286	0.320	0.279	0.266	0.211	0.161	0.241	
Degraded wood Drewno zdegradowane	NaOH	25.5	0.080	0.116	0.203	0.829	0.841	0.689	0.514	0.329	0.298	0.305	0.334	0.314	0.356	0.339	0.278	0.218	0.055
		52.0	0.075	0.093	0.241	1.069	1.064	0.844	0.635	0.294	0.299	0.302	0.299	0.359	0.325	0.301	0.173	0.125	0.043
		58.7	0.057	0.074	0.226	1.064	1.091	0.817	0.614	0.264	0.275	0.269	0.313	0.340	0.335	0.314	0.172	0.080	0.039
	$\text{H}_2\text{SO}_4$	13.8	0.092	0.112	0.162	0.851	0.888	0.706	0.518	0.407	0.389	0.357	0.330	0.316	0.319	0.303	0.263	0.195	0.159
		24.0	0.067	0.097	0.168	0.787	0.813	0.665	0.501	0.376	0.338	0.337	0.339	0.312	0.333	0.326	0.268	0.213	0.122
		42.7	0.107	0.133	0.205	1.053	1.069	0.827	0.599	0.414	0.353	0.386	0.408	0.350	0.357	0.380	0.328	0.221	0.069
	<i>P. versicolor</i>	3.0	0.058	0.093	0.157	0.635	0.662	0.549	0.364	0.373	0.401	0.347	0.268	0.288	0.260	0.248	0.203	0.163	0.234
		24.0	0.072	0.107	0.188	0.921	0.936	0.746	0.546	0.529	0.515	0.459	0.354	0.375	0.349	0.325	0.250	0.202	0.306
		33.0	0.070	0.102	0.184	0.819	0.847	0.671	0.520	0.473	0.466	0.418	0.331	0.358	0.313	0.295	0.243	0.195	0.286
	<i>C. puteana</i>	63.0	0.088	0.118	0.202	1.059	1.103	0.827	0.607	0.527	0.546	0.505	0.390	0.418	0.380	0.350	0.270	0.222	0.349
		2.5	0.071	0.114	0.186	0.796	0.802	0.659	0.501	0.418	0.486	0.446	0.332	0.353	0.319	0.314	0.258	0.200	0.295
		16.0	0.072	0.108	0.172	0.662	0.672	0.568	0.436	0.425	0.430	0.379	0.310	0.319	0.296	0.294	0.266	0.205	0.292
	Degraded wood	23.0	0.078	0.111	0.171	0.965	1.033	0.807	0.566	0.601	0.550	0.486	0.398	0.407	0.381	0.378	0.311	0.255	0.383
		36.0	0.075	0.116	0.162	0.720	0.722	0.634	0.478	0.481	0.461	0.423	0.361	0.349	0.335	0.345	0.316	0.251	0.328
		57.0	0.111	0.152	0.165	0.807	0.838	0.772	0.534	0.596	0.532	0.523	0.449	0.397	0.419	0.454	0.431	0.367	0.339

Kwaśniewski 1978); and holocellulose (Płonka, Surewicz 1967). Differences between the holocellulose and lignin structure in situ and in vitro became greater with the degree of wood degradation. Proportions between the cellulose and particular hemicelluloses in the holocellulose of degraded wood are varying from sample to sample. Each of those components has got its individual intensities of bands of the IR spectrum, (Žbankov 1972). Thus the IR spectrum of holocellulose changes depending on its composition.

Differences between the calculated and experimental wood absorbance are of individual character for particular absorption bands. Standard deviation ( $\rho_i$ ) of mentioned differences was calculated for each  $i$ -band of absorption spectrum

$$\rho_i = \frac{1}{n} \sum_t^n \left[ \left( \frac{A_i}{A_{1378}} \right)_{\text{calc}} - \left( \frac{A_i}{A_{1378}} \right)_{\text{exp}} \right]_t^2, \quad (6)$$

where

$t$  — index of sample of wood degraded by chemical or biotic agent — mass losses (tab. 2 and 3);

$n$  — sum of samples of wood degraded by chemical or biotic agent.

Similarly, the differences between absorbances of the holocellulose and lignin preparation,  $\left( \frac{a_i}{a_{1378}} \right)_h - \left( \frac{a_i}{a_{1378}} \right)_l$ , are also of individual character. Both kinds of differences can be compiled in form of a criterion of relative standard deviation between the calculated and experimental absorbances ( $u_i$ )

$$u_i = \frac{\rho_i}{\left| \left( \frac{a_i}{a_{1378}} \right)_h - \left( \frac{a_i}{a_{1378}} \right)_l \right|} 100(\%). \quad (7)$$

Values of standard deviation ( $\rho_i$ ) and relative standard deviation ( $u_i$ ) are tabulated in table 4. From this table results, that IR absorption bands of pine and beech wood can be arranged in series — on the basis of the criterion  $u_i$ . These series are as follows:

for pine:  $u_{1515} < u_{1270} < u_{840} < u_{1606} < u_{1230} < u_{1460} < u_{780} < u_{1250} < u_{1330} < u_{900} < u_{1743} < u_{1120} < u_{1163} < u_{1065} < u_{1035}$ ;

for beech:  $u_{1510} < u_{1465} < u_{1330} < u_{780} < u_{1428} < u_{1230} < u_{1600} < u_{1270} < u_{1163} < u_{1120} < u_{1035} < u_{1745} < u_{1065} < u_{1250} < u_{900}$ .

From these series of  $u_i$  values results, that the most useful IR absorption band for calculations of holocellulose and lignin content is the 1515 (1510)  $\text{cm}^{-1}$  one. The sequence of remaining absorption bands in pine and beech series is however not identical. Band 1465 (1460) in the beech series has second and in the pine series sixth position. Those differences are caused by the specific degradation of both wood species at the conducted processes. The band 1270  $\text{cm}^{-1}$  in the pine series has second and in the beech series ninth position. Various positions of 1270  $\text{cm}^{-1}$  band in pine and beech wood are resulting from the differences in lignin structure of these wood species. Absorbance of the 1270  $\text{cm}^{-1}$  band caused by C—H bands of aromatic

Table 4

Statistical characteristics of differences between calculated and experimental absorbances of tested material  
 Charakterystyka statystyczna różnic między obliczoną i eksperymentalną absorpcją badanego materiału

Wood species Gatunek drewna	Statistical value* Wielkość statystyczna		Differences of absorbances — Różnice absorpcji																
	$\rho_i$	$u_i$	780	840	900	1035	1065	1120	1163	1220 1230	1250	1270	1330	1378	1425	1460	1515 1510	1606 1600	1743 1745 ( $\text{cm}^{-1}$ )
Pine	0.041	0.030	0.030	0.030	0.563	0.657	0.212	0.157	0.118	0.150	0.083	0.120	0	0.076	0.130	0.027	0.077	0.222	
Sosna	16.3	6.6	65.2	223.4	149.3	97.2	124.6	10.5	18.3	6.3	21.5	0	16.0	11.6	1.6	7.5	82.5		
Beech	0.025	0.046	0.158	0.398	0.399	0.184	0.120	0.123	0.154	0.169	0.069	0	0.053	0.082	0.088	0.193	0.272		
Buk	10.1	13.9	162.9	43.4	51.0	40.4	40.3	13.0	68.1	27.1	9.2	0	10.3	7.5	6.0	17.3	50.9		

\* Results for samples of wood decomposed in all four investigated processes,  $n=14$  for pine,  $n=16$  for beech

\* Wyniki dla próbek rozłożonych we wszystkich czterech badanych procesach,  $n=14$  dla sosny,  $n=16$  dla buka



rings is in the guaiacyl rests higher than in the siringyl ones (Kawamura 1964, Sarkanen, Chang, Ericsson 1967, Sarkanen, Chang, Allan 1967). It is to be stated that  $1270\text{ cm}^{-1}$  band has the highest absorbance among all tested IR bands of the pine lignin. This band is used for determination of methoxyl groups in lignin (Faix, Schweers 1974) and for distinguishing of wood lignines from various climatic zones (Kawamura, Shinoda, Nonomura 1974). Changes of the positions of the band  $1330\text{ cm}^{-1}$  are reciprocal with the band  $1270\text{ cm}^{-1}$ . The band  $1330\text{ cm}^{-1}$  has in beech series third, and in pine series ninth position. Various positions of this band are also caused by the differences in lignin structure resulting from various C—O bands contents of methoxyl groups. In the beech lignin consisting mainly from siringyl rests the band  $1330\text{ cm}^{-1}$  absorbs more strongly than in the pine lignin containing guaiacyl rests (Hergert 1972, Karklin 1981). Near position in the series of  $u_i$  values have also the bands  $780$ , and  $840\text{ cm}^{-1}$ , which absorbances are mainly caused by the lignin content.

Bands  $1065$ ,  $1035$ ,  $743$  and  $900\text{ cm}^{-1}$  are at the end of the presented series. Absorbances of the bands  $1065$  and  $1035$  are characterized by highest values ( $A_{1035}$  and  $A_{1065} \approx 1$ ) and therefore their dispersions are the greatest ones (Kössler 1966). Absorbance in the  $1743$  ( $1745$ ) band is caused by the bonds C=O of the carboxyl groups (Kratzl, Tschamler 1952, O'Connor et al. 1957 and carbonyl Marton, Adler E., Persson 1961). Those are the most reactive functional groups in wood and their absorbance changes to a high degree even when influenced by weak chemical impulses (Karklin et al. 1971). A far position in the  $u_i$  series is occupied by the  $900\text{ cm}^{-1}$  band. It can be explained by small difference of absorbances of holocellulose and lignin preparations in that band and a rather great variability of it (Nikitin, Levdič 1965). Absorbance of the  $900\text{ cm}^{-1}$  band increases for instance in the mercerization process of cellulose. It was observed on the cellulose mercerized in an alkaline (Hurtubise, Krassig 1960, Blackwell 1971, Žbankov 1972) as in acidic environment (Liang, Marchessault 1959, Marchessault, Liang 1960). Various tendencies of changes of the  $900\text{ cm}^{-1}$  band in pine and beech wood decayed by fungi (table 2 and 3) are caused rather by specificity of the action of fungi on hemicelluloses (Rypáček 1977). Particular hemicelluloses are differing in absorbance in the  $900\text{ cm}^{-1}$  band (Žbankov 1972). The  $900\text{ cm}^{-1}$  band is unsuitable for a quantitative determination of the holocellulose and lignin in wood, although is used in the cellulose structure investigations. Changes in the IR spectrum of wood can be also caused by the differences in crystallinity degree of the cellulose contained in it. It was established by determining the crystallinity degree of cellulose of various origin processed by chemical agents (Mann, Marrinan 1956), and also in grinding process (O'Connor, Du Pree Mitcham 1958).

The repeatability of the measurements of IR spectra absorbance was checked on 4 pellets of beech wood degraded by  $\text{H}_2\text{SO}_4$  with the mass loss ( $\Delta m$ )  $13.8\%$ . It results from those measurements that the mean value of standard deviation ( $\frac{1}{17} \sum_i \rho_i$ ) of  $A_i$  absorbances is 1.7 times greater than the same mean value when the absorbance with the inside standard ( $A_i/A_{1378}$ ) is applied. Mean values of relative standard

deviation ( $\frac{1}{17} \sum u_i$ ) of absorbances of these 4 pellets are without inside standard 39.1% and with it 4.9%. For the band  $1510 \text{ cm}^{-1}$   $u_{1510}$  values are 5.8% and 1.5% respectively.

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BADANIA SKŁADU CHEMICZNEGO DREWNA NA PODSTAWIE  
SPEKTROSKOPII W PODCZERWIENI

I. ZALEŻNOŚĆ MIĘDZY SKŁADEM CHEMICZNYM DREWNA A ABSORBANCJĄ  
INDYWIDUALNYCH PASM WIDMA IR W OBSZARZE 700 - 1900 CM<sup>-1</sup>

Streszczenie

Określono zawartość procentową holocelulozy i ligniny oraz absorbancję widma spektroskopowego w podczerwieni od 700 do 1900 cm<sup>-1</sup> w drewnie sosny i buka w różnym stopniu zdegradowanym czynnikami chemicznymi i biotycznymi. Zależność między absorbancją drewna w podczerwieni a zawartością holocelulozy i ligniny ujęto w formę równania liniowego:

$$\frac{A_i}{A_{1378}} = \frac{1}{x_h + x_l} \left[ \left( \frac{a_i}{a_{1378}} \right)_h x_h + \left( \frac{a_i}{a_{1378}} \right)_l x_l \right],$$

gdzie

$A_i$  — absorbancja  $i$ -tego pasma widma IR drewna;

$A_{1378}$  — absorbancja IR drewna w pasmie 1378 cm<sup>-1</sup> (standard wewnętrzny);

$(a_i)_h, (a_i)_l$  — absorbancja  $i$ -tego pasma widma IR preparatów holocelulozy ( $(a_i)_h$ ) i ligniny ( $(a_i)_l$ );

$(a_{1378})_h, (a_{1378})_l$  — absorbancje preparatów holocelulozy i ligniny w pasmie 1378 cm<sup>-1</sup> (standardy wewnętrzne);

$x_h, x_l$  — zawartości procentowe holocelulozy ( $x_h$ ) i ligniny ( $x_l$ ) w drewnie;

$i$  — wskaźnik pasma absorpcji IR: 780, ..., 1743 cm<sup>-1</sup>.

Absorbancje zmierzone oraz obliczone przedstawiono w postaci kryterium względnego odchylenia standardowego ( $u_i$ ). Na podstawie tego kryterium uszeregowano pasma absorpcji widma IR pod kątem ich przydatności do ilościowych oznaczeń holocelulozy i ligniny w drewnie. Z wielkości kryterium  $u_i$  wynika, że najbardziej przydatnymi do obliczeń zawartości holocelulozy i ligniny są pasma absorpcji: 1515 cm<sup>-1</sup> w drewnie sosny i 1510 cm<sup>-1</sup> w drewnie buka.

ИССЛЕДОВАНИЯ ХИМИЧЕСКОГО СОСТАВА ДРЕВЕСИНЫ НА  
ОСНОВЕ ИНФРАКРАСНОЙ СПЕКТРОСКОПИИ

I. ВЗАИМОЗАВИСИМОСТЬ ХИМИЧЕСКОГО СОСТАВА ДРЕВЕСИНЫ  
И ПОГЛОЩЕНИЯ ИНДИВИДУАЛЬНЫХ ПОЛОС ИК-СПЕКТРА  
В ОБЛАСТИ 700 - 1900 CM<sup>-1</sup>

Резюме

Определено процентное содержание холоцеллюлозы и лигнина, а также поглощение инфракрасного спектра от 700 до 1900 см<sup>-1</sup> в древесине сосны и бука, подвергшейся в разной степени деградации химическими и биотическими факторами. Взаимозависимость инфракрасного поглощения древесины и содержания холоцеллюлозы и лигнина представлена в форме линейного уравнения:

$$\frac{A_i}{A_{1378}} = \frac{1}{x_h + x_l} \left[ \left( \frac{a_i}{a_{1378}} \right)_h x_h + \left( \frac{a_i}{a_{1378}} \right)_l x_l \right],$$

в котором

$A_i$  — поглощение  $i$ -ой полосы ик-спектра древесины,

$A_{1378}$  — ик-поглощение древесины в полосе 1378 см<sup>-1</sup> (внутренний стандарт),

$(a_i)_h, (a_i)_l$  — поглощение  $i$ -ой полосы спектра IR preparatów холоцеллюлозы ( $(a_i)_h$ ) и лигнина ( $(a_i)_l$ ),

$(a_{1378})_h, (a_{1378})_l$  — поглощение preparatów холоцеллюлозы и лигнина в полосе 1378 см<sup>-1</sup> (внутренние стандарты),

$x_h, x_l$  — процентные содержания холоцеллюлозы ( $x_h$ ) и лигнина ( $x_l$ ) в древесине,  
 $i$  — показатель полосы ик-поглощения: 780, ..., 1743  $\text{cm}^{-1}$ .

Измеренные и исчисленные поглощения представлены в форме критерия относительно стандартного отклонения ( $y_i$ ). На основе этого критерия полосы поглощения ик-спектра были систематизированы с точки зрения их пригодности для количественных определений холоцеллюлозы и лигнина в древесине. Из величины критерия  $y_i$  вытекает, что наиболее пригодными для расчетов содержания холоцеллюлозы и лигнина являются полосы поглощения: 1515  $\text{cm}^{-1}$  в древесине сосны и 1510  $\text{cm}^{-1}$  в древесине бука.

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