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THE INFRARED SPECTRUM OF THE ULTRA QUALITY MAIZE HYBRID PREFERABLE FOR HUMAN CONSUMPTION: THE IDENTIFICATION OF ORGANIC MOLECULES AND EXCITED STATE OF FUNCTIONAL GROUPS IN SPECTRAL BANDS OF THE KERNEL, ENDOSPERM, PERICARP AND THE GERM

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Results on the studies of kernels and their structural parts: endosperm, pericarp and the germ of the maize hybrid ZP 633 that is very desirable for human consumption are presented. For the first time, the method of infrared spectroscopy was apply to record and study all spectral bands (of very high, high, low and very low intensity) of the infrared spectrum of maize hybrid kernels, endosperm, pericarp and the germ. Based on performed studies it can be stated that infrared spectra of maize hybrid kernels, endosperm, pericarp and the germ are characterised by all their spectral bands and several parameters: number, intensity, kinetics and the distribution of the site of origin in the wavenumber range of 400—4000 cm⁻¹. These parameters were particularly observed for both kernels and their parts (endosperm, pericap and the germ). Spectral bands of very high and high intensity are also characterised by the stated parameters: the number that usually ranges from 3 to 5, intensity, various kinetic forms, as well as the distribution of their origin within the wavenumber range. These spectral bands make possible the identification of organic compounds, their fragments and molecular structures that determine them. In case of spectral bands for the kernel, endosperm, pericarp and the germ with very high and high intensity, organic compounds can be identified as: proteins, lipids, sugars, esters, amides, ketones, aldehydes, carboxylic acids, ethers, phenols, alcohols, aromatic carbohydrates, acyclic compounds, alkenes, alkanes, and alkynes. Spectral bands of the kernel, endosperm, pericarp and the germ of low and very low intensity are also characterised by the stated parameters: the number that can differ, low intensity, the distribution of sites of their origin, and especially the frequency of vibrations of valence bonds of functional groups of organic molecules.

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Spectral bands of the kernel, endosperm, pericarp and the germ of low and very low intensity, also provide the possibility to identify the excited state of molecular structures and valence bonds of functional groups of organic compounds. The excited state of molecular structures and valence bonds of functional groups of organic compounds is expressee in different forms of vibration movements: symmetric and asymmetric valence vibration (stretching), deformation vibration of valence bonds and molecular structures (scissoring), rocking of valence bonds and molecular structures (wagging), twisting of valence bonds and molecular structures (twisting), trembling of valence bonds and molecular structures (trembling).

Key words: *Zea mays* L., hybrid, kernel, pericarp, endosperm, germ, infrared spectrum, spectral band, organic molecule, functional group, excited state, vibration of chemical bonds.

Today's comprehension of modern biophysical and biophysical-chemical studies of plant systems necessarily implies the inclusion of the method of infrared spectroscopy. This essentially provides the breakthrough in the diagnosis of the state and the function of individual plant organs at the molecular level. By the application of infrared spectroscopy, particularly with the up-to-date techniques, it is possible to identify the vibration characteristics of organic compounds, their fragments and functional groups that originate from the oscillation of chemical bonds of functional groups of organic compounds and vibrations within them. Its successful application provides a number of other relevant results. Of these, the identification of organic compounds, the structure of organic molecules, their properties and other parameters depending on the distribution of spectral bands along the wavenumber, stand out. In addition, the results on the nature, quality and a vital function of plant organs that have been increasingly studied, are important [1—6].

The aim of this study was to develop the methodology for analyses of all spectral bands of very high, high, low and very low intensity, of different shapes and kinetics and the distribution of sites of their origin, in order to identify not only organic compounds, but also functional groups, and to determine the nature of their excited state in the maize hybrid kernel, endosperm, pericarp and the germ.

Materials and Methods

Plant material. Kernels of high yielding, chemically enriched and outstanding quality maize hybrid ZP 633, were used as a material for studying infrared spectra and all spectral bands of different properties: intensity, kinetics and the site of origin. This hybrid is also very suitable for human consumption (standard for nutrition of children, elderly, and in certain cases athletes) [7]. The outstanding quality maize hybrid ZP 633 has been developed at and is the property of the Maize Research Institute, Zemun Polje, Belgrade, Serbia.

Moreover, the structural parts of the maize hybrid kernels, endosperm, pericarp and the germ were used in the studies (Fig. 1). The method of their separation from the kernels was done under laboratory conditions [8], and it was expressed in percents [9]. It was determined that





Fig. 1. The outstanding quality maize hybrid ZP 633 and the structural parts of its kernels: endosperm, pericarp and germ

kernels of the maize hybrid ZP 633 contained 83.80 % endosperm, 11.14 % germ and 5.06 % pericarp.

Agronomic, morphological, chemical and physiological traits of this hybrid, including its relevant breeding and seed production properties, were described more detail in the [7].

Methods. The method of infrared spectroscopy applied to the kernels of maize hybrid, as well as to their parts: endosperm, pericarp and the germ, includes spectrophotometers used in the infrared spectrum region. In principle, they do not differ from spectrophotometers in the ultraviolet-visible spectrum. Specificities exist in the performance of operations of spectrophotometers. Possible differences can occur in the radiation sources, the nature of samples, the principle of the radiation absorption, as well as the use of different thermal and photo-detectors [10, 11].

In recent times, a special type of spectrophotometers, based on the principles of interferometry has been used. Interferometers do not produce the spectrum itself, but an interferogram, which is then processed by a computer into a common spectral shape. This is co-called Fourier transformation, and hence the name Fourier Transform Spectroscopy (FTS). These devices are especially suitable for the use in the far-infrared region and are characterised by good resolution [3, 5].

In order to record the infrared spectrum of the observed maize hybrid kernels, endosperm, pericarp and the germ was done by the use of the ATR-FTIR spectra. They were recorded in an ATR compartment connected to a Thermo Scientific Nicolet iS10 FT-IR spectrometer. Spectra were recorded as an average of 64 scans with 4 cm⁻¹ resolution within the range of 4000—525 cm⁻¹. Diamond was used as the ATR-reflecting element. A background spectrum was taken prior to each sample, using the same settings as for the sample acquisition but with a completely clean stage.

Thirty kernels of the observed hybrid were selected by the method of random sampling. In order to record the infrared spectrum of maize kernel samples and its parts (endosperm, pericarp and germ), kernels were ground and homogenised. Dried sample (1–10 mg) was placed upon the crystal stage of the instrument, ensuring that the entirety of the crystal was covered. In order for the ATR to resemble reference transmission spectra, advanced ATR correction implemented in the Omnic 9.0 software (ThermoScientific, USA) was applied. A refractive index of 1.5 was used

for all the samples. The instrument stage was cleaned with ethanol and dried between samples.

Technical tips. The primary processing of infrared spectra was done by the program package OriginPro, 2017 (OriginLab Corporation, USA).

The calculations were performed using the Microsoft software package Excel 2013 (Microsoft Corporation USA).

The majority of statistical programs were performed using the software package Statistica, vers. 10 (StatSoft, Inc, USA).

Results and Discussion

Infrared spectrum of kernels of the maize hybrid ZP 633. Kernels of the studied high yielding, chemically enriched and outstanding quality maize hybrid, that is also highly desirable for human consumption, were homogenised and prepared to record the infrared spectrum with all spectral bands.

In general, the observed infrared spectrum of kernels of the maize hybrid ZP 633 is characterised by all its 24 spectral bands, which differ from each other in the intensity, kinetic forms and range (400—4000 cm⁻¹). The intensity of spectral bands of kernels of the maize hybrid can be (cm⁻¹): very high (3298, 2925, 1648, 1016), high (1745, 1150, 1077), low (2854, 1540, 1457, 766) and very low (3011, 2162, 1980, 1415, 1364, 1341, 1241, 1211, 930, 863, 711, 607, 576) (Fig. 2, Tables 1 and 2).

Spectral bands of very high and high intensities have been initially observed in our studies [3–5]. However, in this study, in addition to these intensities, spectral bands of low and very low intensities, individual or grouped and often of complex nature, were also recorded in the infrared spectrum of kernels of the maize hybrid ZP 633. Such spectral bands have not been mentioned in the literature nor studied. Due to it, besides very

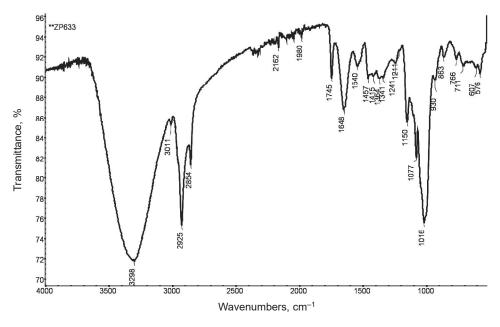


Fig. 2. Infrared spectrum of kernels of the maize hybrid ZP 633 with all spectral bands

TABLE 1. Properties of spectral bands of infrared spectra of kernels of the maize hybrid ZP 633 and their structural parts: endosperm, pericarp and the germ

Sequence of recording spectral bands	Spectral band intensity (%)	Wave number (cm ⁻¹)*	Spectral bands of kernels of very high and high intensity provide the identification of classes of organic molecules (or organic compounds)	Spectral bands of kernels of low and very low intensity provide the identification of excited state of functional groups — forms of vibrations of valence bonds				
1	2	3	4	5				
Features of spectral bands of kernels of maize hybrid ZP 633								
1	20.0	3298	Alkanes,	- Symmetric and asymmetric				
2	0.4	3011	alkenes, alkynes,	valence vibration (stretching),				
3	11.0	2925	acyclic compounds,	- Deformation vibration of valence bonds and molecular				
4	1.9	2854	aromatic carbohydrates, alcohols,	structures (scissoring), - Rocking of valence bonds and molecular structures (rocking),				
5	0.2	2162	phenols,					
6	0.2	1980	ethers, amines,					
7	5.2	1745	nitro compounds,	- Wagging of valence bonds				
8	6.2	1648	aldehydes, ketones,	and molecular structures (wagging),				
9	1.7	1540	amides,	- Twisting of valence bonds				
10	0.2	1457	esters, sugars,	and molecular structures				
11	0.2	1415	proteins,	(twisting),Trembling of valence bonds and molecular structures				
12	0.2	1364	lipids, carboxylic acids					
13	0.2	1341	•	(trembling)				
14	0.1	1241						
15	0.2	1211						
16	2.4	1150						
17	6.2	1074						
18	8.9	1016						
19	0.2	930						
20	0.3	863						
21	0.2	766						
22	0.2	711						
23	0.2	607						
24	0.2	576						
	Features of sp	ectral bands of l	kernel endosperms of mai	ze hybrid ZP 633				
1	18.1	3284	Alkanes,	- Symmetric and asymmetric				
2	5.8	2925	alkenes, alkynes,	valence vibration (stretching), - Deformation vibration of valence bonds and molecular structures (scissoring), - Rocking of valence bonds and molecular structures (rocking), - Wagging of valence bonds and molecular structures (wagging),				
3	6.0	1646	acyclic compounds,					
4	1.1	1534	aromatic carbohydrates, alcohols,					
5	0.2	1413	phenols, ethers,					
6	0.6	1452	amines,					
7	0.2	1249	nitro compounds, aldehydes,					
8	8.0	1208	ketones,					
9	0.2	1149	amides, esters,	- Twisting of valence bonds				
10	6.0	1075	sugars, (twisting).					
11	10.1	1014	proteins,					

1	2	3	4	5
12	0.2	1000	lipids,	- Trembling of valence bonds
13	0.2	924	carboxylic acids	and molecular structures (trembling)
14	1.0	857		
15	0.6	768		
16	0.2	696		
	Features of s	nectral bands of	`kernel pericarps of ma	ize hybrid ZP 633
l	14.0	3343	Alkanes,	- Symmetric and asymmetric
2	5.1	2921	alkenes,	valence vibration (stretching)
3	0.2	2846	alkynes, alcohols,	 Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds
1	5.0	1734	phenols,	
5	2.1	1644	ethers, amines,	
ó	1.1	1517	aldehydes,	
7	0.2	1423	ketones, amides,	
3	1.1	1378	esters, sugars,	
)	0.2	1329	proteins,	
10	2.4	1241	lipids	and molecular structures
11	3.1	1157		(twisting),Trembling of valence bond and molecular structures
12	0.2	1073		
13	4.0	1037		(trembling)
			of kernel germs of maiz	o hybrid 7D 633
	1 catules of	spectral valius (of Kerner germs of maiz	c nyond Zi oss
1	9.1	-	Alkanes	-
1	9.1	3302	Alkanes, alkenes,	- Symmetric and asymmetric
2	6.1	3302 3009	alkenes, alkynes,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of
2	6.1 8.0	3302 3009 2932	alkenes, alkynes, alcohols, phenols,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of
2 3 4	6.1 8.0 6.0	3302 3009 2932 2858	alkenes, alkynes, alcohols,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds
2 3 4 5	6.1 8.0 6.0 12.8	3302 3009 2932 2858 1747	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures
2 3 4 5	6.1 8.0 6.0 12.8 6.0	3302 3009 2932 2858 1747 1649	alkenes, alkynes, alcohols, phenols, ethres, amines,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds
2 3 4 5 6	6.1 8.0 6.0 12.8 6.0 0.6	3302 3009 2932 2858 1747 1649 1544	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures
2 3 4 5 5 6 7 8	6.1 8.0 6.0 12.8 6.0 0.6 3.6	3302 3009 2932 2858 1747 1649 1544 1460	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging),
2 3 4 5 5 6 7 8	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures
2 3 4 5 6 7 8 9	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting),
2 3 4 5 6 7 8 9 10	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bond and molecular structures
2 3 4 5 5 6 7 8 9 10 11	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds
2 3 4 5 5 6 7 8 9 110 111 122	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)
2 3 4 5 6 7 8 9 10 11 11 12	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 1.6 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241 1157 1100	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)
2 3 4 5 6 7 8 9 10 11 12 13 14	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2 1.6 0.2 0.4	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241 1157 1100 1075	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)
2 3 4 5 6 7 8 9 10 11 12 13 14	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2 1.6 0.2 0.4	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241 1157 1100 1075 1045	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)
2 3 4 5 6 7 8 9 10 11 11 12 13 14 15 16	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2 1.6 0.2 0.4 0.2	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241 1157 1100 1075 1045 996	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)
2 3 4 5 6 7 8 9 10 11 12 13 14	6.1 8.0 6.0 12.8 6.0 0.6 3.6 0.2 0.2 0.2 1.6 0.2 0.4	3302 3009 2932 2858 1747 1649 1544 1460 1423 1397 1374 1241 1157 1100 1075 1045	alkenes, alkynes, alcohols, phenols, ethres, amines, aldehydes, ketones, amides, esthers, sugars, proteins,	 Symmetric and asymmetric valence vibration (stretching) Deformation vibration of valence bonds and molecular structures (scissoring), Rocking of valence bonds and molecular structures (rocking), Wagging of valence bonds and molecular structures (wagging), Twisting of valence bonds and molecular structures (twisting), Trembling of valence bonds and molecular structures (twisting)

^{*}Sources: [12], [13], [11], [14].

TABLE 2. Types of vibrations of valence bonds and molecular structures of functional groups of organic compounds in low and very low intensity spectral bands in kernels, endosperms, pericarps and germs of the maize hybrid ZP 633

	Wave num	ber, cm ⁻¹ *	Types of vibrations of valence bonds of	
Kernels	Endosperm	Pericarp	Germ	functional groups of organic molecules
3298	3284	3343	3302	Alcohols (O–H),
3011	2925	2921	3009	amines (N–H), (C–H), alkynes (C \equiv N, C \equiv C),
2925	1646	2846	2932	ketones (=C=O), alkenes (C=C),
2854	1534	1734	2858	ester $(O-CH_2-)$,
2162	1413	1644	1747	lipids (C=O), carbonyl group (C=O) (ester),
1980	1452	1517	1649	amides (N–CH ₂ –, –CO–N=), nitrogen-hydrogen group (–NH–),
1745	1249	1423	1544	primary amines ($-CONH_2$),
1648	1208	1378	1460	carboxylic acids ($-CO_2H$), imides ($-CO-N-CO-$),
1540	1149	1329	1423	acid chlorides ($-COCI$), nitrites ($-C \equiv N$),
1457	1075	1241	1397	amides ($N-CH_2-$),
1415	1014	1157	1374	carbonyl group (C=O) (amide), aliphatic carbon-hydrogen bond,
1364	1000	1073	1241	aldehydes (–CHO)
1341	924	1037	1157	
1241	857	_	1100	
1211	768	_	1075	
1150	696	_	1045	
1074	_	_	996	
1016	_	_	930	
930	_	_	852	
863	_	_	719	
766	_	_	_	
711	_	_	_	
607	_	_	_	
576		_	_	

^{*}Sources: [11], [13], [14].

high and high intensity spectral bands, the attention in this study was also paid to low and very low intensity spectral bands and bands with specific kinetic forms (Fig. 2, Tables 1 and 2).

Infrared spectrum of kernel endosperms of the maize hybrid ZP 633. The endosperm of the maize hybrid kernels, having been extracted and homogenised by the laboratory procedure, was ready for recording the infrared spectrum with all spectral bands.

The recorded spectral bands of kernel endosperms of the maize hybrid, in comparison with spectral bands of kernels of this hybrid, differed in the kinetic form, intensity and their origin. Thus, the intensity of endosperm spectral bands can be (cm⁻¹): very high (3284, 2925, 1646, 1208, 1461, 1014), high (1534, 854, 768), low (1413, 1352, 1249) and very low (1534, 1413, 1352, 1208, 1000, 924, 768, 695) (Fig. 3, Tables 1 and 2).

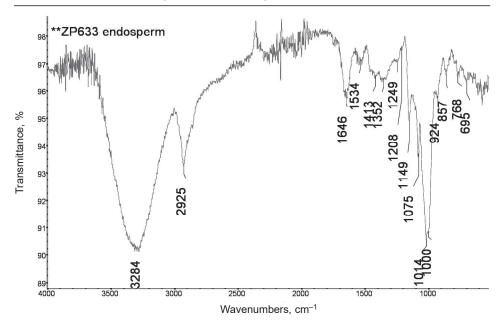


Fig. 3. Infrared spectrum of kernel endosperms of the maize hybrid ZP 633 with all spectral bands

Infrared spectrum of kernel pericarps of the maize hybrid ZP 633. Kernel pericarps of the maize hybrid were prepared according to the identical procedures as those applied in endosperms.

The intensity of spectral bands of kernel pericarp of the maize hybrid ZP 633 ranges from very high (3343, 2921, 1734 and $1241 \,\mathrm{cm^{-1}}$), over high (2846, 1644, 1241, 1157 and $1037 \,\mathrm{cm^{-1}}$), and low (1517 and 1376 $\,\mathrm{cm^{-1}}$) to very low (1423, 1329 and 1073 $\,\mathrm{cm^{-1}}$) (Fig. 4, Tables 1 and 2).

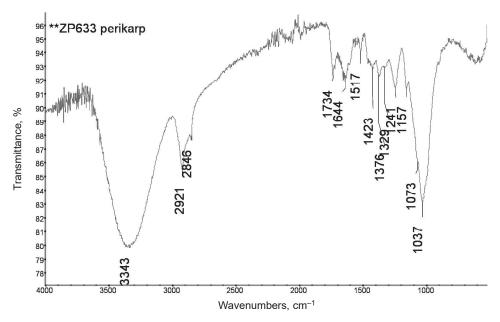


Fig. 4. Infrared spectrum of kernel pericarps of the maize hybrid $ZP\ 633$ with all spectral bands

Infrared spectrum of kernel germs of the maize hybrid ZP 633. Prior to recording the infrared spectrum, kernel germs of the maize hybrid were prepared according to the identical procedures as those applied in endosperms and pericarps. Large differences are immediately noticeable, in terms of intensity, origin and kinetics of the spectral bands of maize hybrid kernel germs.

The intensity of spectral bands of kernel germs of the maize hybrid was (cm⁻¹): very high (3302, 2932, 2858, 1747, 1649, 1544), high (3009, 1544, 1241), low (1374, 1241, 1157, 1045) and very low (1460, 1423, 1397, 1374, 1100, 1075, 1045, 996, 930, 852, 719) (Fig. 5, Tables 1 and 2).

As already stated, spectral bands of very high and high intensity of the maize hybrid ZP 633 kernels including their structural parts: endosperm, pericarp and the germ make the identification of organic compounds and their fragments possible: amines, proteins, lipids, ethers, sugars, ketones, aldehydes and others (Table 1). Since the maize hybrid ZP 633 is desirable for human consumption, the existence of organic compounds is very significant.

On the other hand, the low and very low intensity spectral bands of the maize hybrid ZP 633 kernels and their structural parts (endosperm, pericarp and germ), provide the possibility of identifying the excited state of valence bonds and molecular structures of functional groups of organic compounds (Table 2). This excited state is expressed in different forms of vibration movements:

- Symmetric and asymmetric valence vibration (stretching);
- Deformation vibration of valence bonds and molecular structures (scissoring);
- Rocking of valence bonds and molecular structures (rocking);
- Wagging of valence bonds and molecular structures (wagging);
- Twisting of valence bonds and molecular structures (twisting);
- Trembling of valence bonds and molecular structures (trembling).

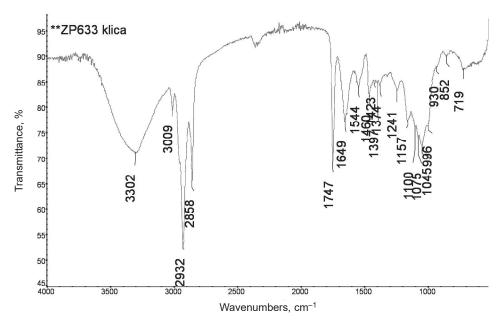


Fig. 5. Infrared spectrum of kernel germs of the maize hybrid ZP 633 with all spectral bands

This last form of vibration movement of valence bonds and molecular structures was initially discovered in medicine. In this study, this form of vibration movement was also observed in low and very low intensity spectral bands of the maize hybrid kernels (Table 2).

Thus, according to our hypothesis, low and very low intensity spectral bands with different kinetic parameters of complex nature, provide the possibility of identifying the unstable (excited) state of functional groups of organic compounds, their fragments, but also biological systems [15—19]. It should not be forgotten that unstable states of biological systems (tissue, cell, membrane) are a consequence of the excited state of organic compounds, molecules, radicals, atoms or ions, and that they are inevitably caused by the occurrence of kinetic energy and their different movement modes (oscillations, vibrations, rotations and translations), which can cause the decrease or increase of spectral bands intensities, and often the unequal kinetic form and different sites of origin. This behaviour is primarily found in the low and very low intensity spectral bands of kernels, endosperm, percarp and the germ. The similar events happen in the process of the ion oscillatory transport through the excited cell membrane [15, 16, 18, 19].

Based on everything stated above, two questions may be posed. First, how to obtain reliable information on the existence of different compounds, and possibly their fragments, whose specific activity causes the occurrence of different spectral bands of kernels, endosperm pericarp and the germ of low and very low intensity, different kinetic form, unequal site of origin, and various vibration movements of valence bonds of functional groups of organic compounds?

The second question would refer to the nature of the creation of the excited state of functional groups, and possibly molecular structures, whose valence bonds are characterised by various vibration movements, which is inevitably transferred to low and very low intensity spectral bands, which occur in certain regions of the infrared spectrum of kernels, endosperms, pericarps and germs. The issue of the distribution of the regions of formation of all spectral bands of very high, high, low and very low intensity, depending on the object (kernels, endosperms, pericarps and germs) of recording of the infrared spectrum can also be analysed. Moreover, the issue of the distribution of regions of the formation of low and very low intensity spectral bands is questionable. It has at least two aspects. The first refers to the functional role of certain structural parts of the kernel that carry out life functions [18], while the second aspect refers to the quality of structural parts of kernels, and finally to the need for human nutrition [7, 19].

Conclusions. For the first time, the method of infrared spectroscopy was used to record and study very high, high, low and very low intensity spectral bands of kernels, endosperms, pericarps, and germs of the maize hybrid. Based on all performed studies, it was possible to determine the following.

Infrared spectra of maize hybrid kernels and their structural parts (endosperm, pericarp and germ) are characterised by all their spectral bands with several parameters: number, intensity, kinetics and the distribution of sites of origin, range of the wavenumber (400—4000 cm⁻¹). These parameters were fully observed for both kernels and their structural parts (endosperm, pericarp and germ).

Spectral bands of high and very high intensity are also characterised by stated parameters: the number that usually ranges from 3 to 5, intensity, various kinetic forms, as well as the distribution of their origin in the wavenumber range. These spectral bands make possible the identification of organic compounds, their determinable fragments and molecular structures. In case of spectral bands for the kernel, endosperm, pericarp and the germ with very high and high intensity, organic compounds can be identified as: proteins, lipids, sugars, esters, amides, ketones, aldehydes, carboxylic acids, ethers, phenols, alcohols, aromatic carbohydrates, acyclic compounds, alkenes, alkanes, and alkynes.

Spectral bands of kernels and their parts (endosperm, pericarp and the germ) of low and very low intensity are also characterised by the stated parameters: the number, different intensity, the distribution of their origin, and especially the frequency of vibrations of valence bonds of functional groups and molecular structures of organic compounds. Spectral bands of kernels, endosperms, pericarps and germs of low and very low intensity, also provide the possibility to identify the excited state of molecular structures and valence bonds of functional groups of organic compounds.

The excited state of molecular structures and valence bonds of functional groups of organic compounds is expressed in different forms of vibration movements: symmetric and asymmetric valence vibration (stretching), deformation vibration of valence bonds and molecular structures (scissoring), rocking of valence bonds and molecular structures (rocking), wagging of valence bonds and molecular structures (wagging), twisting of valence bonds and molecular structures (twisting), trembling of valence bonds and molecular structures (trembling).

The excited state of molecular structures and valence bonds of functional groups of organic molecules can be supported by the following examples: alcohols (O-H), amines (N-H), (C-H), alkynes (C=N, C=C), ketones (=C=O), alkenes (C=C), ester (O-CH₂-), lipids (C=O), carbonyl group (C=O) (ester), amides (N-CH₂-, -CO-N=), nitrogenhydrogen group (-NH-), primary amines (-CONH₂), carboxylic acids (-CO₂H), imides (-CO-N-CO-), acid chlorides (-COCl), nitrites (-C=N), amides (N-CH₂-), carbonyl group (C=O) (amide), aliphatic carbon-hydrogen bond, aldehydes (-CHO).

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ІНФРАЧЕРВОНИЙ СПЕКТР УЛЬТРАЯКІСНОГО ГІБРИДА КУКУРУДЗИ, РЕКОМЕНДОВАНОГО ДЛЯ СПОЖИВАННЯ ЛЮДИНОЮ: ІДЕНТИФІКАЦІЯ ОРГАНІЧНИХ МОЛЕКУЛ І ЗБУДЖЕНОГО СТАНУ ФУНКЦІОНАЛЬНИХ ГРУП У СПЕКТРАЛЬНИХ СМУГАХ ЗЕРНА, ЕНДОСПЕРМУ, ПЕРИКАРПІЮ І ЗАРОДКА

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У роботі представлені результати досліджень зерна та його структурних частин: ендосперму, перикарпію та зародка гібрида кукурудзи ZP 633, що є дуже бажаним для споживання людиною. Вперше метод інфрачервоної спектроскопії був застосований для реєстрації та вивчення всіх спектральних смуг (дуже високої, високої, низької та дуже низької інтенсивності) інфрачервоного спектра гібридних зерен кукурудзи, ендосперму, перикарпію та зародка. На основі проведених досліджень можна стверджувати, що інфрачервоні спектри зерна, ендосперму, перикарпію та зародка характеризуються всіма їхніми спектральними смугами та кількома параметрами: кількістю, інтенсивністю, кінетикою та розподілом місця походження в діапазоні хвильового числа 400—4000 см⁻¹. Ці параметри особливо спостерігались як для зерна, так і для його частин (ендосперму, перикарпію та зародка). Спектральні смуги дуже високої та високої інтенсивності також характеризуються такими параметрами: числом, яке зазвичай коливається від 3 до 5, інтенсивністю, різними кінетичними формами, а також розподілом їх походження в діапазоні хвильового числа. Ці спектральні смуги дають змогу ідентифікувати органічні сполуки, їхні фрагменти та молекулярні структури, які їх визначають. У випадку спектральних смуг із дуже високою й високою інтенсивністю для зерна, ендосперму, перикарпію та зародка органічні сполуки можна ідентифікувати як: білки, ліпіди, цукри, естери, аміди, кетони, альдегіди, карбонові кислоти, етери, феноли, спирти, ароматичні вуглеводи, ациклічні сполуки, алкени, алкани, алкіни. Спектральні смуги зерна, ендосперму, перикарпію та зародка низької й дуже низької інтенсивності характеризуються такими параметрами: кількістю, яка може відрізнятися, низькою інтенсивністю, розподілом місць їх походження, а особливо частотою вібрацій валентних зв'язків функціональних груп органічних молекул. Спектральні смуги зерна, ендосперму, перикарпію та зародка низької й дуже низької інтенсивності також дають можливість ідентифікувати збуджений стан молекулярних структур та валентні зв'язки функціональних груп органічних сполук. Збуджений стан молекулярних структур і валентних зв'язків функціональних груп органічних сполук виражається в різних формах вібраційних рухів: симетричних і асиметричних валентних вібраціях (розтягування), деформаційних вібраціях валентних зв'язків і молекулярних структур (сходження і розходження), розгойдуванні валентних зв'язків і молекулярних структур (коливання), осциляції валентних зв'язків та молекулярних структур (осциляція), скручуванні валентних зв'язків і молекулярних структур (скручування), вібрації валентних зв'язків та молекулярних структур (вібрація).

Ключові слова: Zea mays L., гібрид, зерно, перикарпій, ендосперм, зародок, інфрачервоний спектр, спектральна смуга, органічна молекула, функціональна група, збуджений стан, вібрація хімічних зв'язків.