
M.I. MYHOVICH, V.A. KELMAN

Institute of Electron Physics, Nat. Acad. of Sci. of Ukraine
(21, Universytets'ka Str., Uzhgorod 88017, Ukraine; e-mail: m_migovich@rambler.ru)

THEORETICAL AND EXPERIMENTAL STUDY OF SPECTROSCOPIC CHARACTERISTICS OF AROMATIC AMINO ACIDS

PACS 78.40.Me

Photoluminescence spectra of aromatic amino acids, which are prepared in the form of microcrystalline powders and their aqueous solutions and are excited by laser radiation, are studied. Luminescence spectral regions and the maxima of luminescence intensity are determined. The spectral dependences of the molar extinction coefficients are measured for the aqueous solutions of amino acids. The electronic absorption spectra of aromatic amino acids and the charge distribution in the corresponding molecules are calculated, by using the quantum-chemical Hartree-Fock method with the application of the semiempirical PM3 and ZINDO/S approximations. The electronic absorption spectra are analyzed.

Keywords: aromatic amino acids, photoluminescence, absorption spectra, quantum transitions, HOMO (highest occupied molecular orbital), LUMO (lowest unoccupied molecular orbital), charge distribution.

1. Introduction

To understand the processes in biological systems, it is necessary to know the spectral characteristics of important organic molecules, which can be obtained on the basis of measurements of molecular absorption and luminescence spectra. Those spectra make it possible to determine the positions of electron levels for the ground and excited states [1] and to study the energy interaction between molecules.

The most important complex organic molecules include the molecules of amino acids, which together with others form the basis of life. Amino acids are organic compounds, which include carboxyl ($-\text{COOH}$) and amine ($-\text{NH}_2$) functional groups. The properties of proteins are governed by the characteristics of their amino acid components [2], which participate together with nucleic acids, carbohydrates, and lipids in all vital processes. In aqueous solutions, amino acids are in the form of amphoteric (zwitter-) ions. The structure of proteins includes only α -amino acids, in which the carboxyl and amine groups are attached to the same carbon atom.

Aromatic amino acids are the brightest chromophores among all amino acids. The structures of tryptophan (Trp), tyrosine (Tyr), and phenyl alanine (Phe) molecules are illustrated in Fig. 1. Proteins contain Trp, Tyr, and Phe amino-acid residues, which give

a contribution to the ultra-violet photoluminescence spectrum. Luminescence of the majority of proteins is associated, first of all, with the residues of Trp, whose indole ring is a sensitive and complicated fluorophore. However, it was found in work [3] that the fluorescence spectra of capsid proteins of the mosquito iridescent virus do not coincide with the corresponding spectra of aromatic amino acids that enter the structure of those proteins, which can testify to the interaction between closely located aromatic amino acids in the protein macromolecule.

The ground state and the first excited singlet one take part in all photophysical processes [4, 5]. Electron transitions from the ground state are responsible for the absorption spectra, and those from the first excited state into the ground one generate luminescence spectra [6]. For today, we know the general form of absorption spectra for aromatic amino acids. They are composed of wide smeared bands, but the spectroscopic classification of separate elements in those spectra remains obscured.

The luminescence spectra of the solutions of three aromatic amino acids and five proteins at room and low (down to -160°C) temperatures were studied in work [7]. As the temperature decreased, the fluorescence bands were found to shift into the short-wave region. The absorption and luminescence spectra of aromatic amino acids and a significant number of proteins were also studied in works [8, 9]. In work [8], it

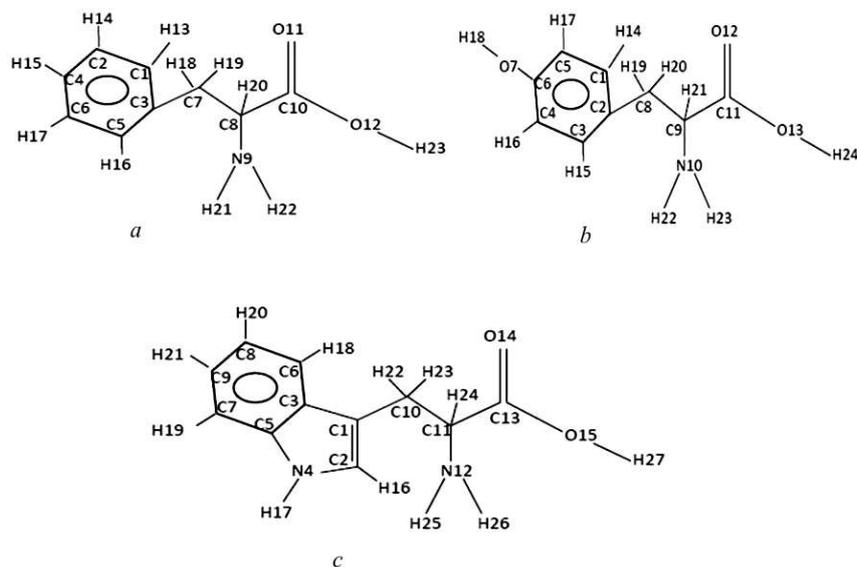


Fig. 1. Structures of (a) phenyl alanine, (b) tyrosine, and (c) tryptophan molecules

was shown for the first time that the absorption and excitation spectra of Trp and Tyr residues do not coincide, and the photoluminescence intensities of those two fluorophores are proportional to the excitation intensity, but not to the absorption at the excitation wavelength.

The influence of pH of a solution on the luminescence properties of aromatic amino acids was examined in works [9, 10]. In work [10], it was found that a low pH creates a positive amine charge and, thereby, increases the probability of the electron transfer from the indole ring to the protein chain, so that the luminescence quantum yield decreases. At a high pH level, on the contrary, the luminescence quantum yield grows, because a negative charge is formed on the carboxyl group, which gives rise to a reduction of the electron transfer probability. The two-photon excitation of luminescence in the solutions of aromatic amino acids and in crystalline L-tryptophan was studied in works [11, 12]. Similarly to the case of one-photon luminescence, the maximum position was found to depend on the pH of a solution.

The spectroscopic characteristics of complicated organic molecules can be estimated theoretically on the basis of quantum chemical calculations. For this purpose, various software packages are used, e.g., the software package HyperChem, in which all modern methods of computer chemistry were implemented,

including non-empirical and semiempirical quantum chemical methods [13]

The structural properties of amino acids are also the subject of intense researches. The geometrical parameters, dipole moments, charge distribution over the atoms of some amino acids, results of calculations of vibrational components in the absorption spectra with the use of semiempirical and non-empirical quantum chemical methods are presented in works [14–18]. In work [15], it was found that, although the charge distributions among the atoms calculated by the CNDO, AM1, and PM3 methods are different, the characters of charge distributions described by those methods are similar. For the absorption spectra of complicated molecules to be simulated more adequately, the Gauss curves can be applied for the approximation of vibrational components of various electron transitions [17]. The theoretical estimations of the process of intermolecular electron transfer in the tyrosine–tryptophan complex with the help of quantum chemical methods were made in work [19]. It was established that the transition $LUMO + + 2(\text{Tyr}) \rightarrow LUMO + 2(\text{Trp})$ can be used to simulate the intermolecular transfer.

This work is devoted to the study of photoluminescence spectra emitted by the microcrystalline powders of aromatic amino acids and their aqueous solutions. We also made quantum-mechanical calcula-

tions of the electronic absorption spectra and compared them with experimentally obtained absorption spectra.

2. Materials and Methods

2.1. Experimental part

For experimental researches, we used the powders of aromatic amino acids of 99.4% (Trp), 99.8% (Tyr), and 99.5% (Phe) purities supplied by Sigma Aldrich. Photoluminescence in the tryptophan, tyrosine, and phenyl alanine powders and their aqueous solutions was excited by laser radiation. For this purpose, we used a wavelength-tunable solid-state titanium-sapphire laser CF 131A (the third harmonic, $\lambda = 253.3$ nm). The laser pulse duration amounted to 10 ns, the repetition frequency to 10 Hz, and the laser pulse energy to 20 μ J.

The spectra of fluid specimens were registered with the use of cuvettes 4 cm in depth. The cuvette was illuminated from above with unfocused exciting radiation. Solutions were prepared to such a concentration that the absorption of exciting laser radiation at a wavelength of 4 cm was insignificant, and the brightness along the photoluminescence zone in the form of a luminescence thread oriented vertically was uniform. The corresponding concentrations amounted to 0.0009 M (Trp), 0.0037 M (Tyr), and 0.0024 M (Phe). In addition, the very photoluminescence zone was made adjacent to the input window of a cuvette in order to eliminate the reabsorption effects. The photoluminescence spectra of powder specimens were registered in the reflection geometry.

With the use of a quartz lens with the focal distance $f = 75$ mm, the non-scaled image of the luminescence zone was projected onto the entrance slit of a monochromator MS 7504i with a diffraction grating of 150 g/mm and with an inverse dispersion of 8.78 nm/mm. The spectral resolution amounted to 2 nm. The luminescence spectra of amino acids, integrated in time, were registered using a CCD-chamber HS 101H and a personal computer. All measurements were carried out at room temperature.

In order to measure the absorption spectra of aqueous-solution specimens in the near UV region, a DDS-30 deuterium lamp was used.

2.2. Quantum Chemical Calculations

Quantum chemical calculations were carried out using the software package HyperChem, which includes

various methods and approximations for molecular simulation, the optimization of a molecular geometry and an electron structure, and the determination of spectroscopic and energy parameters.

The geometry of tryptophan, tyrosine, and phenyl alanine molecules was optimized by the semiempirical PM3 method. The Fletcher-Reeves algorithm with the limiting absolute value of gradient equal to 0.01 kcal/A/mol was used. The smaller the limiting absolute value of gradient, the higher was the accuracy of the result. For the indicated maximum gradient value, we obtained data that remained invariable if the gradient decreased further [20]. The PM3 method provided a sufficient accuracy of reproduced results [21].

Semiempirical computational techniques are based on the Hartree-Fock method and the linear combination of atomic orbitals approximation for the calculation of molecular orbitals (the valence approximation), i.e. only the valence electrons are taken into account, whereas the inner ones are considered to be localized on atomic orbitals. In all semiempirical methods, the differential overlapping is neglected, i.e. while calculating the optimum geometry, the Coulomb repulsion integrals are not taken into consideration. Certainly, the non-empirical methods provide a higher accuracy of the results obtained; however, they require powerful computation facilities.

The electron spectra were calculated in the framework of the ZINDO/S spectral approximation. This is a parametrized technique for the reconstruction of UV and visible optical transitions taking the configuration interaction (CI) into account. While calculating the quantum transitions, the configuration interaction between 10 occupied and 10 vacant molecular orbitals was taken into consideration.

3. Results and Discussion

The initial stage of the photobiophysical process consists in the light absorption by a chromophore group accompanied by the electron transition from the occupied molecular orbital onto a vacant one and the formation of an electron-excited state. In Fig. 2, the spectral dependences of the molar extinction coefficients for the tryptophan, tyrosine, and phenyl alanine aqueous solutions are shown. The extinction coefficients were calculated by the relation $\xi = \frac{1}{cl} \ln \tau$, where $\tau = I/I_0$ is the transmission coefficient, c

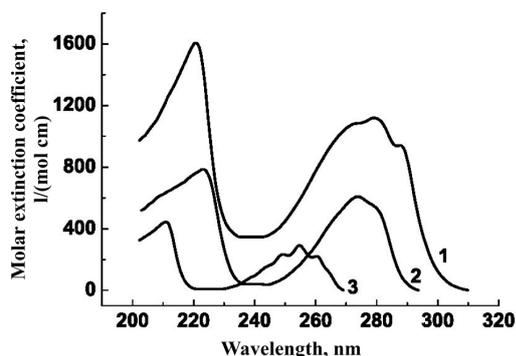


Fig. 2. Spectral dependences of the molar extinction coefficients for aqueous solutions of the aromatic amino acids: (1) tryptophan, (2) tyrosine, and (3) phenyl alanine

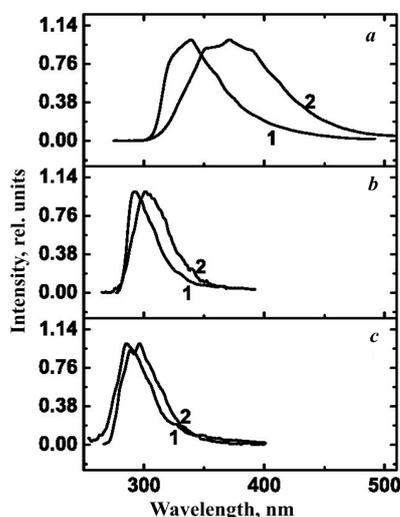


Fig. 3. Normalized fluorescence spectra of (a) tryptophan, (b) tyrosine, and (c) phenyl alanine: (1) powder specimens and (2) aqueous solutions

the concentration of a corresponding specimen in the solution (mol/l), l the cuvette thickness (cm), and I and I_0 are the radiation intensities after passing through the cuvette with and without the solution, respectively.

Under the action of UV radiation, the electron shells of molecules become excited, which is associated with the transition of valence σ - and π -electrons, as well as unpaired n -electrons that do not participate in the bond formation, from the ground state into the excited one. A contribution to the absorption by amino acids in the UV range is given not only by $\pi \rightarrow \pi^*$ transitions, but also by $n \rightarrow \pi^*$ ones. The latter transitions are related to the facts

that the chromophore of amino acids is the carbonyl group C=O, and the p -orbital of oxygen (the n -level) contains an unshared pair of electrons that do not participate in the formation of a bond with carbon, so that the electron from this unshared pair finds itself on the antibinding π^* -orbital. The molecules of aromatic amino acids, which, besides conjugated double bonds, have also heteroatoms (the nitrogen atom in the indole ring), manifest two absorption maxima, which agree well with the data of works [8, 9]. As was noted in work [9], the absorption maxima at 280 (Trp), 274 (Tyr), and 254 nm (Phe) result from the absorption by the aromatic ring part of their structure. The parameters of absorption spectra—the wavelength of absorption maximum, $\lambda_{\max}(\text{abs.})$, and the corresponding value of molar extinction coefficient, ξ^{\max} —are quoted in Table 1. Note that the spectral resolution gives rise to a good coincidence of absorption maximum positions in all research results listed in Table 1.

The measured photoluminescence spectra of aromatic amino acids are depicted in Fig. 3. The observed photoluminescence bands correspond to the transitions from the excited singlet π^* -state onto vibrational levels of the ground π -state. Some differences are observed between the spectra obtained for those substances in aqueous solutions and in powders. The main maxima and the short- and long-wave band edges in the photoluminescence spectra of aqueous solutions are shifted toward the long-wave region, which is especially noticeable in the fluorescence spectrum of tryptophan. The fluid specimens also demonstrate a wider emission band. This circumstance may probably be explained by the fact that every molecule in the solution is surrounded by several solvent molecules, the dipole moments of which

Table 1. Parameters of the experimental absorption spectra of aromatic amino acids

N	Amino acid	$\lambda_{\max}(\text{abs.}), \text{nm}$			$\xi^{\max},$ 1/(mol×cm)
		Our data	[9]	[8]	
1	Tryptophan	220	225	–	1606
		280	280	282	1108
2	Tyrosine	223	227	–	782
		274	274	277	605
3	Phenyl alanine	210	212	–	442
		544	257	–	291

Table 2. Parameters of the photoluminescence spectra

N	Amino acid	λ_{\max} , nm				Half-height width, nm		$E(S_1)$, eV
		Powder	Solution			Powder	Solution	
			Our data	[8]	[9]			
1	Tryptophan	340	370	360	348	47	82	4.1
2	Tyrosine	300	305	303	303	23	32	4.4
3	Phenyl alanine	285	296	–	290	31	36	4.7

create local electric fields, and the dipole moment of the excited state is larger in comparison with that in the ground state. In the presence of an external electric field, the energies of electron transitions are changed, and the corresponding shift of levels results in the frequency shift of radiative optical transitions toward long waves. The parameters of photoluminescence spectra – the wavelength of the emission maximum λ_{\max} , half-height width, and energy of first excited singlet state $E(S_1)$ – are quoted in Table 2. The energy $E(S_1)$ was determined as the abscissa of the intersection point between the long-wave edge of the absorption curve and the short-wave edge of the photoluminescence curve.

The calculated electronic absorption spectra are shown in Fig. 4. The tryptophan specimens demonstrate a wide absorption band formed by the transitions at 246, 248, 250, 255, 263, 271, 279, and 287 nm (see Table 3). The main maximum is observed at 279 nm, which means that the main contribution to this absorption band is given by the corresponding HOMO–LUMO transition. In the short-wave region, one can observe a more intensive absorption band formed by the contributions of the transitions at 207, 217, 221, 223, 228, and 231 nm, with the main maximum being observed at 223 nm (HOMO–1 \rightarrow LUMO+4). The oscillator strengths for the corresponding transitions are quoted in Table 3.

Two absorption bands are also observed in the electron spectrum of a tyrosine molecule. The long-wave band is formed by the transitions at 252, 257, 265, 270, and 280 nm. The absorption maximum is observed at 270 nm, i.e. the first excited state can be described by the wave function consisting of the configuration HOMO \rightarrow LUMO. The short-wave band is formed by the transitions at 215, 225, 231, 235, and 243 nm. The main contribution is given by the transition at 225 nm, i.e. HOMO–1 \rightarrow LUMO+2.

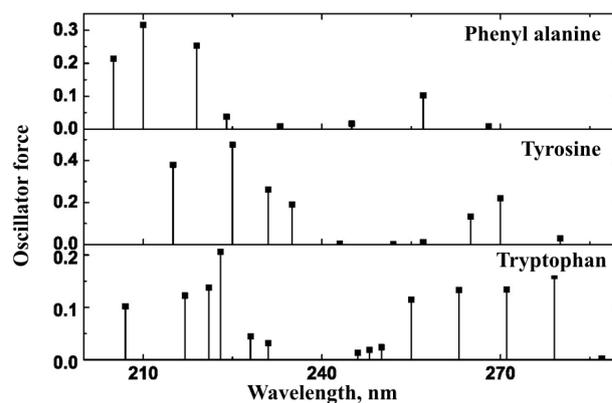


Fig. 4. Electronic absorption spectra of aromatic amino acids

For the phenyl alanine molecule, three transitions are observed in the long-wave band: at 245, 257, and 268 nm. The most probable transition at 257 nm is described by the wave function composed of two configurations, HOMO \rightarrow LUMO and HOMO \rightarrow LUMO+2. In the short-wave region, the spectral maxima are observed at 205, 210, 219, 224, and 233 nm, with the main maximum being located at 210 nm, which corresponds to the transition HOMO–1 \rightarrow LUMO+2.

The calculated absorption spectra are in good agreement with the results of works [17, 19]. For instance, in work [19], the energies of main transitions amount to 4.25 eV (292 nm), 4.3 eV (288 nm), 5.1 eV (243 nm), 5.4 eV (230 nm), 5.6 eV (221 nm), and 5.9 eV (210 nm) for Trp, and 4.45 eV (278 nm) and 5.7 eV (217 nm) for Tyr. The electronic absorption spectrum of tryptophan calculated in work [17] using a non-empirical *ab initio* method in the interval of 200–280 nm is formed by the transitions at 214, 280, and 300 nm. Comparing the calculated absorption spectra with the experimental ones, we come to

Table 3. Calculated parameters of the electronic absorption spectra of aromatic amino acids

Molecule	Wavelength, nm	Oscillator strength	Quantum transitions	
Tryptophan	287	0.0025	HOMO → LUMO	
	279	0.1599	HOMO → LUMO	
	271	0.1337	HOMO - 1 → LUMO	
	263	0.1332	HOMO → LUMO + 5	
	255	0.1148	HOMO → LUMO + 5	
	250	0.0240	HOMO → LUMO + 6	
	248	0.0186	HOMO → LUMO + 6	
	246	0.0135	HOMO → LUMO + 6	
	231	0.0315	HOMO → LUMO + 6	
	228	0.0448	HOMO - 1 → LUMO + 3	
	223	0.2059	HOMO - 1 → LUMO + 4	
	221	0.1377	HOMO - 1 → LUMO + 4, HOMO - 2 → LUMO + 2	
	217	0.1225	HOMO → HOMO + 10, HOMO - 3 → LUMO + 1	
	207	0.1021	HOMO - 1 → LUMO + 5	
	Tyrosine	280	0.0289	HOMO → LUMO
		270	0.2214	HOMO → LUMO
		265	0.1329	HOMO → LUMO + 2, HOMO - 1 → HBMO
257		0.0111	HOMO → LUMO + 3	
252		0.0018	HOMO → LUMO + 3	
243		0.0051	HOMO → LUMO + 3	
235		0.1907	HOMO - 1 → HOMO + 1, HOMO - 2 → LUMO	
231		0.2614	HOMO - 1 → LUMO + 1, HOMO - 2 → LUMO	
225		0.4755	HOMO - 1 → LUMO + 2	
215		0.3804	HOMO - 1 → LUMO + 2	
Phenyl alanine	268	0.00852	HOMO → LUMO, HOMO → LUMO + 2	
	257	0.1025	HOMO → LUMO, HOMO → LUMO + 2	
	245	0.0167	HOMO → LUMO + 3	
	233	0.0089	HOMO - 2 → LUMO	
	224	0.0378	HOMO - 2 → LUMO	
	219	0.2528	HOMO - 1 → LUMO + 2	
	210	0.3164	HOMO - 1 → LUMO + 2	
	205	0.2143	HOMO → LUMO + 5	

a conclusion that, in general, they agree well with respect to the spectral positions of long- and short-wave absorption bands and to the ratio between their intensities. Moreover, the calculated gap widths ΔE (see Table 4) practically coincide with the $E(S_1)$ -values (see Table 2).

Table 4. Physico-chemical parameters of aromatic amino acid molecules

Parameter	Tryptophan	Tyrosine	Phenyl alanine
Gap width ΔE , eV	4.3	4.4	4.6
μD	2.631	2.258	2.480

Table 5. Effective charges on the atoms of aromatic amino acid molecules

Tryptophan		Tyrosine		Phenyl alanine	
Atom	Charge, e	Atom	Charge, e	Atom	Charge, e
C1	-0.025471	C1	-0.028624	C1	-0.034478
C2	0.006139	C2	-0.002337	C2	-0.013357
C3	-0.012825	C3	-0.028762	C3	0.012642
N4	-0.239152	C4	-0.025032	C4	-0.026190
C5	0.078701	C5	-0.033104	C5	-0.035892
C6	-0.040701	C6	0.142464	C6	-0.015700
C7	-0.035301	O7	-0.351323	C7	0.012997
C8	-0.037676	C8	0.013071	C8	0.130131
C9	-0.023500	C9	0.130271	N9	-0.371873
C10	0.022335	N10	-0.371891	C10	0.488662
C11	0.139619	C11	0.488921	O11	-0.538793
N12	-0.375094	O12	-0.539308	O12	-0.319473
C13	0.486689	O13	-0.319160	H13	0.022443
O14	-0.543992	H14	0.024360	H14	0.021982
O15	-0.307715	H15	0.020116	H15	0.020571
H16	0.044365	H16	0.030168	H16	0.018043
H17	0.165326	H17	0.024650	H17	0.020182
H18	0.040780	H18	0.219275	H18	0.022162
H19	0.022486	H19	0.021288	H19	0.014113
H20	0.016206	H20	0.013851	H20	0.040754
H21	0.019009	H21	0.039712	H21	0.145826
H22	0.021652	H22	0.145970	H22	0.143299
H23	0.010764	H23	0.143336	H23	0.241949
H24	0.032615	H24	0.242086		
H25	0.151275				
H26	0.141582				
H27	0.241883				

The analysis of the calculated charge distributions among the atoms (Fig. 1) testifies that the total charge of each molecule strictly equals zero (Table 5). This fact evidences a high quality of calculations in the framework of used approximations. The carboxyl and amine groups do not contain consider-

able charges ($0.08 \div 0.1$ e) for all three amino acids, whereas the charges on separate atoms are rather substantial (up to 0.54 e). Therefore, the charge becomes redistributed within each group.

In the combined groups containing the carboxyl and amine groups together with the linking carbon atom and the adjacent hydrogen one, the total charge is also not substantial, amounting to $0.03 \div 0.04$ e. In those parts of molecules that are not included into combined groups, the attention is attracted by the concentration of a considerable negative charge on atom N4 that is located in the indole ring (tryptophan) or on atom O7 adjacent to the benzene ring (tyrosine).

On the basis of the obtained charge distributions, the dipole moments μ of aromatic amino acid molecules were calculated (see Table 4), which make it possible to estimate their polarity. The tryptophan molecule turned out to be the most polar in comparison with the tyrosine and phenyl alanine ones. It seems that just this circumstance can explain why the photoluminescence spectra for the powder and solution specimens are the most different for tryptophan.

4. Conclusions

Photoluminescence spectra of aromatic amino acids – tryptophan, tyrosine, and phenyl alanine – have been studied and analyzed. The photoluminescence spectra of aqueous solutions turned out to be wider and with the main emission maximum shifted toward long waves in comparison with those of powders, which is associated with the influence of a solvent on the amino acid molecules. By determining the abscissa of the intersection point between the long-wave edge of the absorption curve and the short-wave edge of the fluorescence one, the energy of the first excited singlet state of examined molecules was found to equal 4.1 eV for tryptophan, 4.4 eV for tyrosine, and 4.7 eV for phenyl alanine.

With the use of quantum chemistry methods, the electronic absorption spectra of aromatic amino acids are calculated, which are in good agreement with experimental data. The long-wave absorption band associated with the excitation of the first singlet state is found to mainly result from the transitions from the highest occupied molecular orbital onto the lowest un-

occupied one. As a whole, those data determine the origin and the detailed structure of absorption bands.

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Received 10.09.13.

Translated from Ukrainian by O.I. Voitenko

М.І. Мигovich, В.А. Кельман

ТЕОРЕТИЧНЕ
ТА ЕКСПЕРИМЕНТАЛЬНЕ ВИВЧЕННЯ
СПЕКТРОСКОПІЧНИХ ХАРАКТЕРИСТИК
АРОМАТИЧНИХ АМІНОКИСЛОТ

Резюме

Досліджено спектри фотолюмінесценції порошоків мікрокристалів ароматичних амінокислот та їх водних розчи-

нів, збуджених дією лазерного опромінення. Визначено спектральні області та максимуми інтенсивності люмінесценції. Виміряно спектральні залежності коефіцієнтів молярної екстинкції водних розчинів амінокислот. Квантово-хімічним методом Хартрі–Фока з використанням напівемпіричних наближень RM3 та ZINDO/S розраховано електронні спектри поглинання ароматичних амінокислот та розподіл електричних зарядів в молекулах. Проведено аналіз електронних спектрів поглинання.