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Fragmentation of tyrosine by high-energy electron impact

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Abstract. The experimental mass spectra of the tyrosine molecule measured at different microtron accelerator-induced high-energy electron irradiation doses (i.e., 0, 5, and 20 kGy) have been identified and analyzed. The experimental investigation was carried out along with the theoretical study performed by Becke's three-parameter hybrid density functional approach without and with the inclusion of electric and magnetic fields. It has been shown that high-energy (11.5 MeV) electrons cause irreversible changes in the structure and energy parameters of the molecule under study. The study revealed the importance of proton transfer for fragment formation of the irradiated and non-irradiated tyrosine.

1 Introduction

It is well known that exposure to ionizing radiation leads to the formation of covalent cross-links between DNA and proteins [1]. For example, di-tyrosine bridges are formed due to peptides or proteins containing tyrosine, one of the most sensitive residues, and damage occurred as a result of mimic stress (UV light, gamma rays, metal-catalyzed oxidation, etc.) [2–4]. These di-tyrosine bridges are found in many structural proteins and are evidenced in many pathological cases. However, only currently the variety of di-tyrosine bridges was established in the case of a protein and a peptide, and tyrosine dimers for the amino acid [4]. This variety indicates different ways of the di-tyrosine bridge formations that could be the result of the decomposition of peptides and, more precisely, tyrosine due to radiation. Gatin et al. state that the bridge structure elucidation is important considering its crucial role in oxidative stress [4]. On the other hand, the knowledge of the formation of di-tyrosine and its dimers could shed some light on the processes occurring as the result of mimic stress in biological systems. In this line, the data on the cleavage of amino acids are urgently needed in order to propose di-tyrosine and its dimer formation pathways to prevent pathological cases. Here, we report on the recent results of studying both non-irradiated and irradiated by high-energy (11.5 MeV) electrons tyrosine fragmentation aiming to suggest the mechanisms of the processes described above. We have measured the mass spectra of non-irradiated and irradiated tyrosine molecule and performed a theoretical study with the aim to explain the experimental results. Computational simulations provide a reliable way to study the fragmentation patterns of various species, providing detailed knowledge of their composition at the atomic level [5–7]. To model irradiation that corresponds to the condition in our experiment, an electric dipole field from 0.1 to 0.6 a.u. was applied taking into account that the electric field influence on the molecule fragmentation is more significant than that of the magnetic field, since the chemical bond strength would change due to electron density variation. The approach we used described well the processes which occurred due to the high-energy electron irradiation [8]. However, the magnetic field effect could be crucial for the proton and/or electron transfer processes [9]. Thus, some correction of the basis set was used in addition, in order to incorporate the influence of the magnetic field on the molecular wave functions. The latter allowed us to study the specific features of the mass spectra of the above both non-irradiated and irradiated amino acid molecules and to predict the influence of the magnetic and electric fields on them.

2 Experimental

The experimental apparatus used in our investigation is a typical crossed-beam setup based on a $MI1201$ magnetic mass spectrometer. Its main characteristics are analyzed in our previous papers (see e.g., [10]). The $MI1201$ operating mass range is $m/z = 1 - 600$ (m/z

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being the mass-to-charge ratio of the ions under study); it provides high ion detection sensitivity ($\sim 10^{-16}$ Å) and mass resolution (±0.25 a.m.u.; however, it is lower in the region of $m/z > 100$) allowing the fragmentation products to be effectively detected and identified. The tyrosine (NOW FOODS, 98% purity) molecular beam having a $\sim 10^{10}$ molecule/cm^3 density was produced by an effusion source operating within the temperature range not exceeding 150 °C, thus excluding possible thermal degradation of the molecule under study. A three-electrode electron gun was applied to produce an electron beam with a current of 30–50 μA. When determining the ion fragment appearance energies, the incident electron energy was varied from 7 to 30 eV allowing the energy dependences of the different ion fragment yields to be measured. The electron energy scale was calibrated against the Ar and N_2 ionization thresholds providing accuracy not worse than ±0.2 eV. First, the not-irradiated tyrosine molecule mass spectrum was recorded in an automatic PC-controlled mode at fixed electron energy (70 eV, typical for mass spectrometric measurements). The accuracy of measuring the appearance energies for the most intense ion fragments was not worse than ±0.2 eV as well.

Afterwards, the irradiated at the above doses amino acid samples were brought to the $MI1201$ magnetic mass-spectrometric apparatus. Then, the above-described mass-spectra measuring procedure was repeated for them in succession. It should be noted that the overall time interval between the moment of molecule irradiation at the microtron and the moment of the initiation of measuring the mass spectra at the magnetic mass spectrometer exceeded at least 300 hours. Such a large time gap allowed any reversible changes in the molecular structure to relax, with no final effect on the mass spectra measured.

3 Theoretical

Our theoretical approach was described in our recent papers [11–13]. The most stable conformer obtained by us was used along with optimization without any symmetry constraints (all bonds length, angles and dihedral angles are changed) with and without the dipole electric field influence. The strength of the dipole electric field was increased gradually by 0.05 a.u. from 0.05 to 0.7 a.u. Additionally, the simulation was performed in the 0.31 a.u. strength field to fix the decomposition of the tyrosine due to the electric field. The Becke's three-parameter hybrid functional approach with non-local correlation provided by Lee, Yang, and Parr ($B3LYP$) and the $cc-pVTZ$ basis set implemented in a GAUSSIAN package was applied in our recent studies [14,15]. This approach described well the geometric and electronic structure of various molecules and their derivatives [16–24]. The vibrational analysis was performed to be sure that the equilibrium point was found.
When an atom/molecule is placed in electromagnetic field, the perturbation to the energy levels is caused by both the electric and the magnetic fields; however, the effects of the electric field are larger by a factor of $1/\alpha$ ($\alpha = 1/137$ is the fine-structure constant). This is due to the fact that the linear Stark shift in energy is $\Delta E_{\text{Stark}} \sim e\varepsilon a_0 \sim e\varepsilon\hbar/mc\alpha$, while in the Zeeman effect it is $\Delta E_{\text{Zeeman}} \sim eB\hbar/2m \sim e\varepsilon\hbar/2mc$. Thus, as a first approximation in our investigations, we neglect the terms of the oscillating magnetic field in the Hamiltonian. The effects of the magnetic field have been accounted for only by using the method of anisotropic Gaussian-type orbital ($AGTO$) basis, first introduced by Schmelcher and Cederbaum [25] and later developed by Zhu and Trickey [26]. The meaning of the AGTO method is that an anisotropy is introduced in the wave function in order to describe the elongation of electron orbitals and densities along the magnetic field direction. Zhu and Trickey have developed an iteration $AGTO$ construction scheme outlined in [26], which we have followed in order to calculate the values of the correction coefficients to the Gaussian exponent. We repeated the process for the H, C, O, and N atoms in the electric field range $E = 0.1 - 0.6$ a.u. and its corresponding magnetic field in the range $B = 7.296 \cdot 10^{-6} - 43.775 \cdot 10^{-6} a.u.$ For simplicity in our calculations, we have taken into account only the orbitals with $m = 0, 1$ (m represents the magnetic quantum number), since they are the predominant ones and for the case of many-electron atoms we have neglected such effects as screening of the nuclear potential, as well as the repulsion between the electrons.

Due to the small values of the radiation magnetic field, we found that the correction coefficients are independent of the type of atom or orbital (e.g., s or p) and are equal to $\alpha_1 = \beta_1 = 0.0539737$. These correction coefficients were included in the basis set in order to perform the numerical calculations of the effects of the magnetic radiation field on the tyrosine molecule. We implemented two modified basis sets, the first one, in which both the s- and p-orbitals are modified by the magnetic field and the second one, where the correction coefficients enter only in the wave-functions of the $p-$ orbitals.

4 Results and discussion

A detailed study of the tyrosine molecule fragmentation by low-energy electrons is presented in [27]. Thus, here we present a brief description of the features that are important for fragmentation of tyrosine under high-energy electron impact:

- This amino acid decomposition could start directly during ionization;
- The intramolecular hydrogen migration confirmed experimentally is crucial for the $m/z = 107$ and 108 fragment formation.

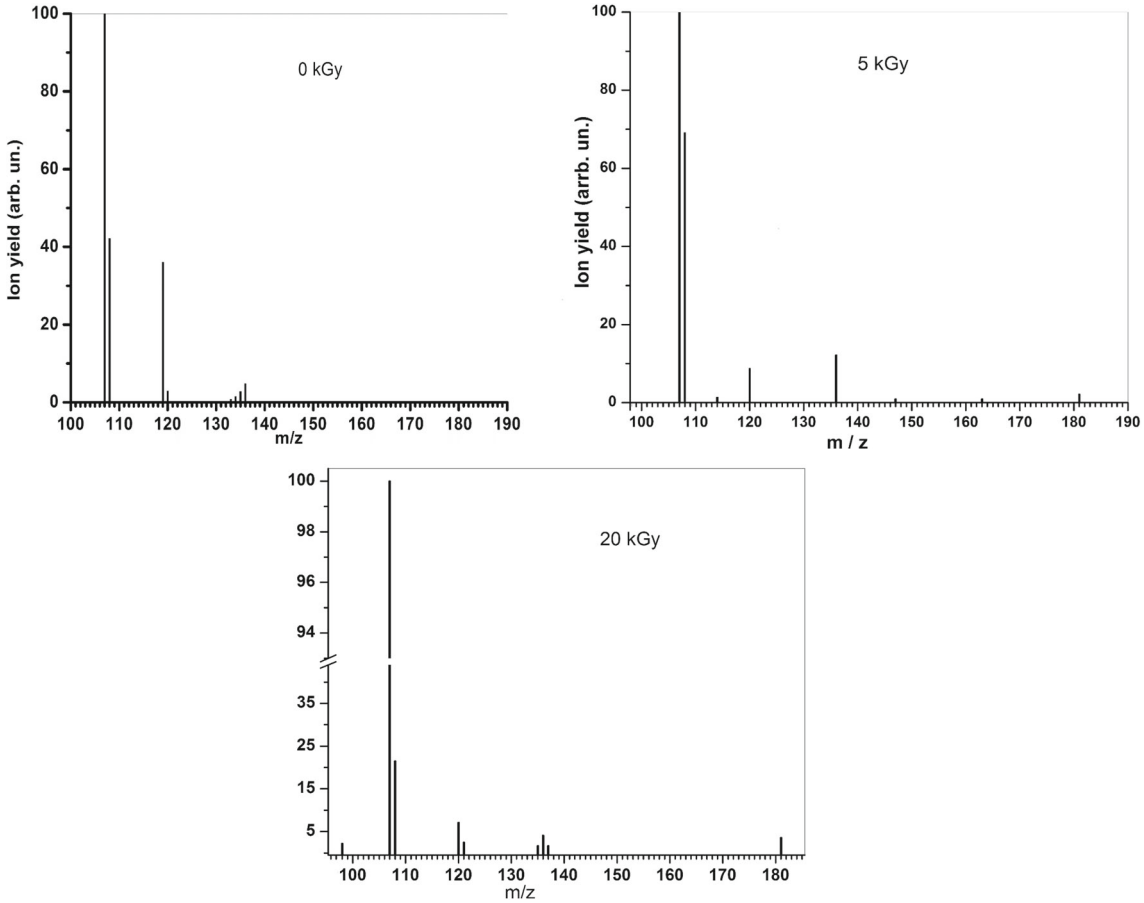

Fig. 1 Comparison of the mass spectra of non-irradiated and electron-irradiated (at the 5 kGy and 20 kGy doses) tyrosine molecules measured at the 70 eV incident electron energy in the mass range 100–190 a.m.u

As it is mentioned above, we measured the mass spectrum of tyrosine after its interaction with a high-energy ($11.5MeV$) electron beam (at the 5 and 20 kGy irradiation doses). The obtained mass spectra within the $m/z = 100 - 140$ mass range were compared to that of the initial non-irradiated sample (Fig. 1). For correct comparison, the intensities of the parent main ion peaks in the above spectra were reduced to the same value.

On the whole, the mass spectra of the irradiated sample are similar to the initial one, i.e., no new intense lines appear in the spectra. However, the intensities of some peaks are (in some cases, significantly) greater or smaller than those without irradiation. As can be seen from Fig. 1, the intensity of the $m/z = 108$ and 136 fragments increases at 5 kGy and decreases at 20 kGy. The peak representing the $m/z = 119$ fragment at 5 kGy disappeared, and a remarkable lower peak at $m/z = 120$ occurs at 5 kGy and 120 kGy.

To explain the experimental results obtained in our studies, the geometric and electronic structures of tyrosine were investigated theoretically with the inclusion of a finite electric field. The strength of this field was changed from 0.05 to 0.7 a.u. We observe significant differences in the geometrical structure of the molecule with and without the inclusion of an electric field (Fig. 2), where the rotation and bending of COOH–CH–NH_2 with respect to the phenol ring are seen.

It is interesting that the increase in the electric dipole field strength from 0.1 to 0.3 a.u. leads to the similar structural changes, although the decomposition of the molecule to COOH, H, and C_8H_9NO is revealed in the 0.31 a.u. and larger dipole electric field. The splitting to COOH and C_8H_9NO is also predicted based on the simulations performed at the inclusion of the dipole electric field with the field strength equal to 0.7 a.u. Our theoretical investigation was repeated with the inclusion of the effects of the magnetic field to be sure that it does not influence formation of the above fragments. The obtained results indicate slightly different consequences of tyrosine splitting in the electromagnetic field, i.e., CO_2, C_8H_9NO, and two H atoms could be formed. These results give a better match with the experimental spectra as we will explain below.

Hence, referring to the results obtained, we may predict the increase of a number of conformers that are less stable and expect more intense formation of C_7H_7O through the $C_\alpha - C_\beta$ bond break with the elimination of the cation side-chain fragment, while the appearance of protons due to irradiation could also facili-

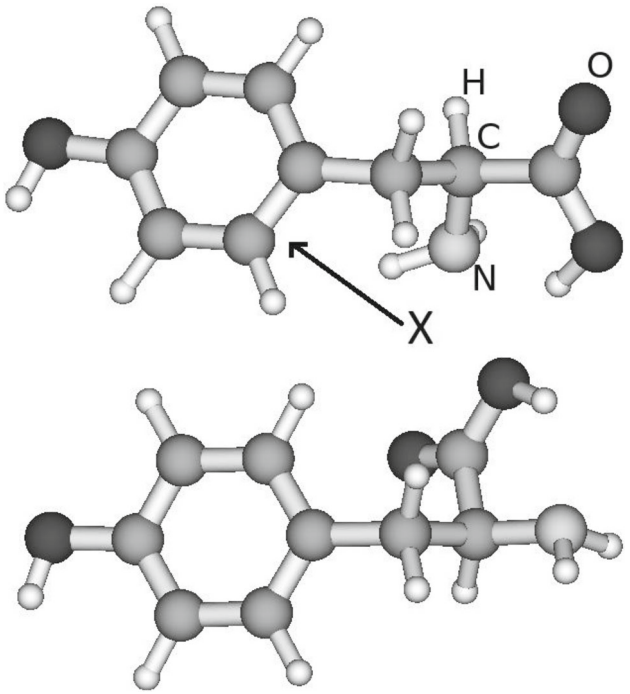

Fig. 2 The view of the most stable conformer of tyrosine obtained without (on the top) and with (on the bottom) the inclusion of the dipole electric field

tate the formation of $m/z = 107$ when C_7H_6O binds the H atom [27,28]. There is no possibility to check the amount of the $m/z = 107$ fragment formed with and without irradiation; thus, it is difficult to speculate about the intensities of these processes and about the particular pathways of this fragment formation that could be dominant when the irradiation dose increases. We also could not conclude whether formation of this fragment under irradiation quenches other processes, i.e., the other fragmentation processes could not be realized because of tyrosine splitting. However, some interesting findings follow from the analysis of intensities of the $m/z = 108$ peaks of both non-irradiated and irradiated at different doses tyrosine (Fig. 1). Earlier we suggested that this fragment is C_7H_8O and it is formed when C_7H_7O binds with the H atom, i.e., a intramolecular hydrogen migration occurs. We can assume that under the influence of high-energy electrons on the micro-powder sample, some of the tyrosine molecules are degraded losing the gaseous COO and CNH_3 ($H_2C{=}NH$) with the formation of a stable paramethyl phenol (C_7H_8O, $m/z = 108$ a.m.u.). These molecules, while remaining stable for a long time after irradiation, make an additional contribution to peak $m/z = 108$ a.m.u. in the mass spectrum. The increase of the intensity of this peak at 5 kGy indicates the facilitation of the intramolecular hydrogen migration process, while the intensity decrease at $20kGy$ indicates the opposite outcome. Referring to these and the abovementioned theoretical results, it is obvious that the electromagnetic field strength influences the intramolecular hydrogen migration process. This finding is confirmed by the presence of the $m/z = 119$ and 120 fragments in the spectra obtained under the different irradiation doses. According to the results of our investigation, the $m/z = 119$ and 120 fragments correspond to C_8H_7O and C_8H_8O, respectively. Both of these fragments could be formed when tyrosine lost COOH, NH_2, and, in the case of $m/z = 119$, a proton, as a consequence of the $C-C$ bond break. The results of our simulations indicate that the total energy of the $HO{-}C_6H_4{-}CH_2{-}C$ positively charged ion is equal to -383.995 a.u., while that of $O{-}C_6H_4{-}CH_2{-}CH$ cation is -383.937 a.u. The comparison of these values of the total energies indicates that $HO{-}C_6H_4{-}CH_2{-}C$ is more stable than $O{-}C_6H_4{-}CH_2{-}CH$. Thus, the $m/z = 120$ peak is formed at various irradiation doses because the C−H bond break is quenched and, as a consequence, this peak appeared instead of the $m/z = 119$ one. The intensity of this peak is significantly lower than that of $m/z = 119$ at $5kGy$ irradiation dose since formation of $m/z = 108$ becomes dominant over that for $m/z = 119$. This finding is based on the increase of the peak intensity of $m/z = 108$ leading to a decrease of that for the $m/z = 119(120)$ fragments.

The $m/z = 136$ fragment was identified as $C_8H_{10}NO$ being formed due to a loss of CHO_2 that is the main process of other amino acid fragmentation [29,30]. This fragment could appear due to electromagnetic field impact as it is exhibited by the results obtained with the inclusion of the dipole electric field within quenched O–H break. This could be a reason for the increase of the $m/z = 136$ peak intensity in the mass spectrum measured at the 5 kGy dose. We have to pay attention to the decrease of this peak intensity in the case of the 20 kGy irradiation dose and perform a simulation with the inclusion of the 1.0 a.u. dipole electric field. The results of this study revealed that along with the above decomposition of tyrosine to $COOH$ and the rest of the fragments, one of them (the C_8H_9NO fragment) is destructed to the C_7H_8N, CO, and H fragments. The latter allows us to suggest that increasing the field strength decreases the possibility of formation of the $m/z = 136$ fragments. It is worth noting that in the numerical simulations the decomposition of the C_8H_9NO fragment takes place both with and without the inclusion of the magnetic field effects. However, the obtained splitting is different in these two cases, e.g., taking into account the magnetic field leads to the formation of different fragments. We can conclude that in our studies the inclusion of the magnetic field influence provides a better fitting to the experimentally obtained spectra and, therefore, gives a useful tool for accurate prediction of the future experimental outcomes.

5 Conclusion

In this paper, we report on the results of studying both non-irradiated and irradiated by high-energy electrons tyrosine molecule fragmentation. The mass spectra of non-irradiated and irradiated tyrosine were mea-

sured and analyzed by an applied theoretical approach. Results of our investigation revealed that the same intense lines are present in the mass spectra of both irradiated and non-irradiated tyrosine, although the intensities of some peaks are significantly different. Referring to the results of our investigation we may state that the geometrical structure of the molecule could be changed due to the presence of an electric field. So, the less stable conformers are formed when a rupture requires less amount of energy in comparison with that for the most stable conformers. This statement is supported by the fact that the molecule could decompose in an electric field, which strength is higher than 0.31 a.u. We also have found that electromagnetic radiation field is capable of facilitating the intramolecular hydrogen migration, quenching, at the same time, some fragmentation processes in the tyrosine molecule. The inclusion of the effect of the magnetic radiation field in our theoretical studies showed the possibility for further decomposition of the fragments and indicated that magnetic field effects are crucial for the intramolecular hydrogen migration and/or electron transfer processes.

Author contributions

LR, VV and AS designed and performed all of the experiments. Theoretical investigations were performed by TK and JT. The results were interpreted by the experimental team in Ukraine together with JT. All authors contributed to writing the manuscript to different extents.

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Data Availability Statement This manuscript has associated data in a data repository. [Authors' comment: All data included in this manuscript are available upon request by contacting the corresponding author.]

Declarations

Conflict of interest Not applicable.

Ethics approval Not applicable.

Consent to participate Not applicable.

Consent for publication Not applicable.

Code availability Not applicable.

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