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Biography

Jelena T has completed her PhD in 2000 at the Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania. She is a senior research fellow at the Vilnius University, Lithuania. She has more than 150 publications that have been cited over 200 times, and her publication H-index is 7.

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ELECTRON-IMPACT FRAGMENTATION OF THE GLUTAMINE AMINO ACID MOLECULE: EXPERIMENTAL AND THEORETIC STUDIES

The results on the mass-spectrometric studies of the glutamine molecule ($C_5H_{10}N_2O_3$) fragmentation are presented to show the simplest theoretical approach to predict the products of the fragmentation reactions under the low (<150 eV) energy electron impact. This approach allowed us to identify the chemical composition of the most abundant glutamine molecule fragments, evaluate their absolute appearance energies E_{ap} and find the most probable pathways of their formation. For example, among a series of ionic fragments identified, the absolute appearance energy E_{ap} of the m/z=41 a.m.u. fragment was found by us for the first time both experimentally and theoretically. The experimental appearance energy E_{ap} obtained using the Marquardt-Levenberg fitting procedure was found to be 12.2 eV. Our theoretical DFT-calculation for different conformers of the $C_2H_3N_+$ and C_2HO^+ ions having the above mass has shown that in the near-threshold electron energy region the most probable is production of the CHCHNH$^+$ (i.e. $C_2H_3N^+$) ion with the appearance energy E_{ap} of 10.34 eV, when this fragment is directly formed from the parent glutamine molecule. The details of the approach and the results of the quantum-chemical analysis of the possible ion production pathways for glutamine will be presented at the Conference. This study is closely related to the 'Mass Spectrometry in Metabolomics' and 'Mass Spectrometry in Drug Discovery' research programmes.

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