

A STUDY ON THE INFLUENCE OF WATER ON THE L-LEUCINE FRAGMENTATION

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All living organisms are constantly affected by ionizing radiation emitted by natural sources such as cosmic rays and radionuclides contained in rocks from the Earth, food, water, air, etc. Moreover, ionizing radiation exposures also occurs during medical procedures. Low-energy electrons are produced due to ionizing radiation. These low-energy electrons cause damage of biomolecules, including amino acids, e.g., leucine. Data on fragmentation of amino acids in water under impact of ionizing radiation are scarce, although they are relevant to the analysis of processes in living organisms.

Hence, the aim of our research is to determine whether the appearance energies of fragments differ between conditions with and without the influence of water included.

The fragmentation of the L-leucine molecule was theoretically studied by using Becke's three-parameter hybrid functional applying the non-local correlation provided by Lee, Yang and Parr (B3LYP) with the correlation consistent triple zeta basis (cc-pVTZ). The polarized continuum model (PCM) method was used to evaluate the presence of water. We applied Gaussian 03 Rev D.01/09 Rev D.01 program. Fragments for the research were selected on the basis of the experimental data of mass spectrometry.

We determined that cation with mass 86 a.m.u. is $C_5H_{12}N^+$, cation with mass 44 a.m.u. is $C_2H_6N^+$ and cation with mass 30 a.m.u.- CH_4N^+ . The results of our research with and without the influence of water indicate that more energy is needed for the formation of same cations in water.

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