Excitation of L-valine molecules by electrons and photons

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Abstract

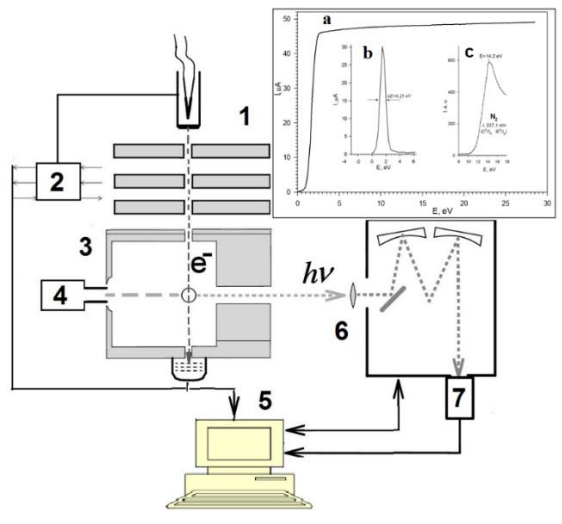
Excitation of L-valine molecules was studied by optical spectroscopy. Optical emission spectra of the L-valine molecule and optical excitation functions of molecular bands and the H_β spectral line were measured in the gas phase using electron impact. In the spectra of optical emission in the wavelength range of 250-500 nm, intense emission bands were found at energies of incident electrons of 30, 50 and 70 eV. Analysis of structural features of the valine molecule suggested a fragmentation scheme with the formation of excited particles in collisions with electrons. A notable feature of the presented optical excitation functions is a different growth dynamics with an increase in the energy of exciting electrons and the presence of a number of features and kinks, which are especially pronounced for λ = 305 nm and λ = 311 nm. The excitation thresholds were determined from the initial sections of the excitation functions of the most intense spectral lines by the least squares method. The photo-luminescence spectra of L-valine were measured for the first time on a Shimadzu RF-6000 spectrofluoro-photometer in the spectral range of 400-800 nm for excitation wavelengths of 250, 275, 333, 351 and 380 nm.

Introduction

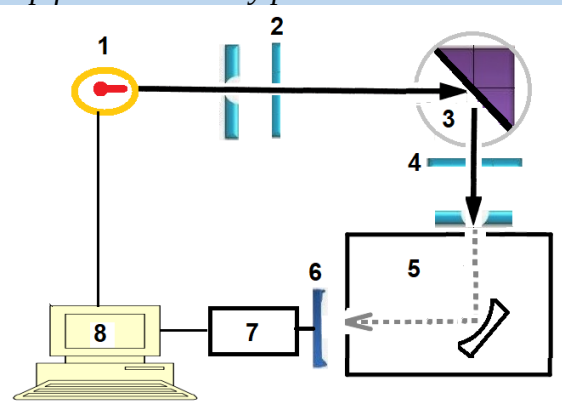
Excitation of atoms, ions and molecules by electron impact is a key elementary process that determines the basic properties of matter in the gas and plasma phases. Excitation of molecules into repulsive states leads to dissociation, which determines the concentration of various atomic particles. In addition, collisions of electrons with molecules are accompanied by vibrational and rotational excitations of molecular energy levels. Similar processes occur when molecules are excited by photons, and photodissociation is the main accompanying process. The energies of photons of visible and ultraviolet radiation are sufficient both to break a chemical bond and to change the structure of an excited molecule.

Experimental setups

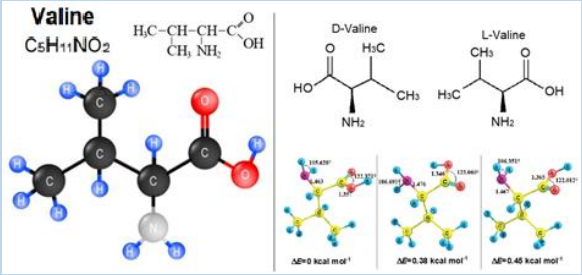
Installation for excitation by electrons



Setup for excitation by photons



Structural 3D and lines formula's of the valine molecule

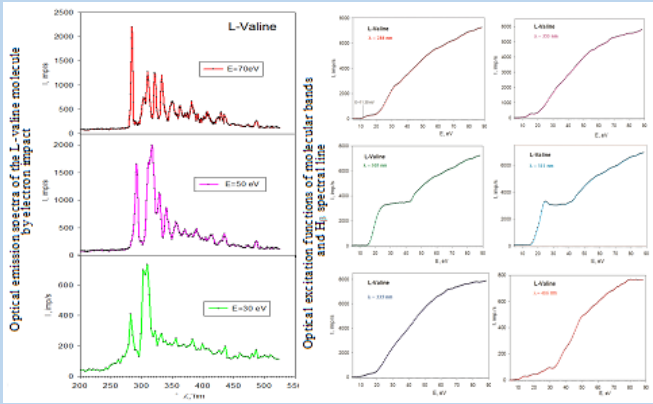


Results and discussion

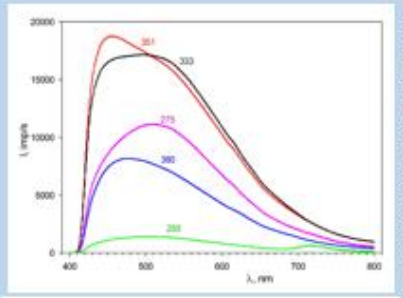
Optical spectra under electron impact

Analyzing the structural diagrams of the valine molecule one can be assume that its fragmentation with the formation of excited particles in collisions with electrons can occur according to the following schemes:

$$C_5H_{11}NO_2 + e^- \rightarrow \begin{cases} C_5H_{10}NO_2 + H^* + e^- & (a) \\ C_5H_{10}NO + OH^* + e^- & (b) \\ C_4H_{10}N + OH^* + CO^* + e^- & (c) \\ C_4H_{10}N + OH^* + CO + e^- & (d) \\ C_4H_{10}N + OH + CO^* + e^- & (e) \end{cases}$$



Photoluminescence spectra



Luminescence spectra of L-valine measured at 250, 275, 333, 351 and 380 nm excitation wavelengths

Conclusions

1. When colliding with electrons, a direct detachment of a hydrogen atom and other mechanisms of fragmentation with the formation of excited neutral molecules occur, which indicates the decay of a valine molecule at the moment of interaction with an electron with corresponding energy.
2. Excitation of valine molecules by electrons in the gas phase leads to the appearance in the emission spectrum of both OH*, CO* molecular bands and spectral lines of the hydrogen atoms. In the electron energy range 30–70 eV, the distribution of radiation intensities between individual bands changes significantly and new molecular emissions appear.
3. A significant part of the processes of fragmentation of L-valine during electron impact occurs with the participation of the carboxyl group COOH, the excitation of which also occurs when interacting with photons.
4. In the luminescence spectrum of L-valine in the wavelength range of 400–800 nm upon excitation with different wavelength we observed emission bands with maxima at λ = 474 nm and λ= 505 nm which related to excitation in the carboxyl group COOH, which plays the main role in the structure of the valine molecule, especially in the processes of inelastic interactions of photons and electrons with aliphatic amino acids.
5. Thresholds of the appearance of excitated hydrogen atoms and excited molecules are different and its possible influence of formation of the negative ions states as a whole molecule of valine as well as fragments of its dissociation.