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Formation of Positive and Negative Ions of Thymine Molecules under the Action of Slow Electrons

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Abstract—The formation of positive and negative molecules of thymine—a base of nucleic acids—under the action of slow electrons is investigated by the method of crossed electron and molecular beams. The method developed makes it possible to measure the molecular beam intensity and determine the energy dependences and absolute values of total cross sections for the formation of positive and negative ions of thymine molecules. It is found that the maximal cross section for the formation of positive ions is reached at an energy of 95 eV and its absolute value is, accordingly, 1.4×10^{-15} cm^2. The total cross section for the formation of negative ions is 8.2×10^{-18} cm^2 at an energy of 1.1 eV. The mass spectra of thymine molecules are measured and the cross sections of dissociative ionization are determined.

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INTRODUCTION

Recently, the number of publications devoted to ionization of biologically important molecules by an electron impact has increased in avalanche-like manner. This phenomenon is explained by the fact that researchers have recognized extraordinary importance of the problem and serious effects of intracellular irradiation of molecules by secondary electrons. Such electrons are produced in large numbers when flows of ionizing radiation penetrate a substance. The majority of the secondary electrons are low-energy (slow) particles with energies ranging from a fraction of an electron-volt to several tens of electron-volts [1]. According to the existing notions, these low-energy electrons account for destructive changes in biological structures on the molecular level, their main targets being genetic DNA and RNA macromolecules. For physical modeling of these changes and estimation of their radiobiological consequences, knowledge of basic characteristics of the processes of electron–molecule interactions, such as absolute values of the cross sections, for the formation of positive and negative ions is required.

Earlier [2, 3], we found the cross sections for the formation of negative and positive cytosine ions by electron impact. In this study, new data concerning the ionization cross sections of a thymine molecule are presented. Thymine, as well as cytosine, adenine, uracil, and guanine, is a nucleotide base, which is an important component of genetic DNA and RNA macromolecules. Note that, in the available literature [4–8], there are rather conflicting data concerning the absolute values of the cross sections of the formation of negative thymine ions; therefore, setting up new investigations by a precision method is necessary.

EXPERIMENTAL

The experiment is based on the method of crossed molecular and electron beams, which we have successfully applied earlier [2, 3]. In this method, the most complex problem is to produce the gaseous phase of molecules and to measure their concentration. In this study, a beam of molecules under investigation was generated using an effusive thermal multichannel source and a system of collimating slits. The needed temperature (405 K) of the source at which the structural changes of thymine are absent was found experimentally. The components of the effusive source are a copper container with the substance under investigation, a resistive heater of the container, a calibrated thermocouple sensor of the temperature in the container, and thermal screens. The container has the form of a hollow cylinder. At one of the ends of the cylinder, an element containing effusive channels (100 channels over a 1.5×1.5 mm^2 area) was mounted. At the other side, the container was closed by a hermetic cover. On the inner surface of the cover, the material under investigation and the temperature sensor were placed. The design of the container ensured a temperature of the element 10°C higher than the temperature of the cover. This prevented blockage of microchannels during the experiments. The material under investigation—thymine ($C_5H_6N_2O_2$)—was obtained from Sigma-Aldrich Co. (purity 99%).