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Mass Spectrometric Study of the First Ionization Potential of Guaiazulene

Pomiar pierwszego potencjału jonizacji guajazulenu

Измерение ионизационного потенциала молекул гуаязулена

ABSTRACT

The first ionization potential of Guaiazulene has been measured by the surface ionization method using one-filament ion source of the mass-spectrometer. The measurements were carried out on oxidized tungsten filament as an ionizing surface. The thermal dependence of the ion currents produced for molecular mass M and for some dissociation fragments has been measured at a temperature range of about 650 to 1000 K. The presented results, obtained by the mass spectrometer, are the first contribution to the knowledge of the first ionization potential of Guaiazulene molecule.

INTRODUCTION

The measurements of the ionization potentials for the organic molecules by the surface ionization method have been rather scarce. As a general feature, the ionization potentials for most of the organic molecules show high values, and therefore, a high work function of the ionizing surface is needed. Tungsten filaments are often preferred as support materials. Moreover, it is well known that an oxygen adsorption on the

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filament considerably increases the work function [1]. It has been found out that the maximum work function [1, 2, 3] of tungsten, presumably covered by oxygen, is about 6.3 eV and decreases to 4.5 eV for the clean tungsten surface.

In view of the importance of an ionization potential in the study of molecular structure, the method of surface ionization is applied to Guaiazulene molecule in the present work. An estimation of the first ionization potential for Guaiazulene molecule has been reported by T. G o w o r e k [4] who used the positron annihilation method.

THEORY

The ion current density during evaporation of a material of ionization potential V, taking place on a surface of work function $e\varphi$ at absolute temperature T, is given by the following equation:

$$J^+ = a \, n \, e \, g^+/g^0 \, \exp\left[\frac{e(\varphi - V)}{kT}\right] \qquad (1)$$

where:

a — coefficient depending on the geometry of the ion source,

n — number of molecules reaching the ionizing surface per second, g^+ and g^0 — the statistical weights of the ground states of the ions and neutral atoms, respectively.

One may see from the equation (1) that the ion current density, produced at a particular temperature, varies very rapidly as an exponential function of $(\varphi - V)$ reaching the highest value for the surface of the high work function and the materials of the low ionization potentials. Substances of high ionization potentials, for instance, organic compounds provide small ion current density as the value $(\varphi - V)$ becomes negative. Equation (1) can be rewritten in a more applicable form:

$$J^+ = A \, \exp\left[\frac{11600}{T}(\varphi - V)\right] \qquad (2)$$

where A is a constant at any temperature and it may be expressed by the partition function of ions and neutral atoms. A logarithmic plot of the ion current density against $11600/T$ displays a straight line of a slope depending on the difference $(\varphi - V)$.

EXPERIMENTAL

The measurements in the present work are performed by means of the mass-spectrometer of type MI-1201 with one filament ion source. Since the ionization potential of the organic materials is relatively high,

an oxidized tungsten filament is used. Guaiazulene used in this experiment was in a crystalline form. Guaiazulene crystals are heated to the melting point. A constant pressure is established in the mass spectrometer by means of a special-inlet system connected with a quartz capillary tube adjacent to the ionizing support in the ion source. The filament is oxidized at the temperature of the order of 900 K at a residual oxygen pressure starting from 10^{-1} to 10^{-3} torrs for 20 minutes. The temperature dependence of the ion current density of the masses M, M-1, $M+1$ is measured at a temperature of 650 to 1000 K, where M is molecular weight of Guaiazulene.

RESULTS AND DISCUSSION

In the present work, the ionization potentials of masses M-1, M, $M+1$ were determined by using an oxidized tungsten surface only, since the ion current produced by the clean surface is relatively very small. The most important part of the mass-spectrum of Guaiazulene which contains the molecular beam of mass M of the highest intensity is shown in Fig. 1. The temperature dependence of the ion current of the three masses, mentioned above, covering a temperature range from 650 to 1000 K is shown in Fig. 2. Through the experimental points in Fig. 2 the regression
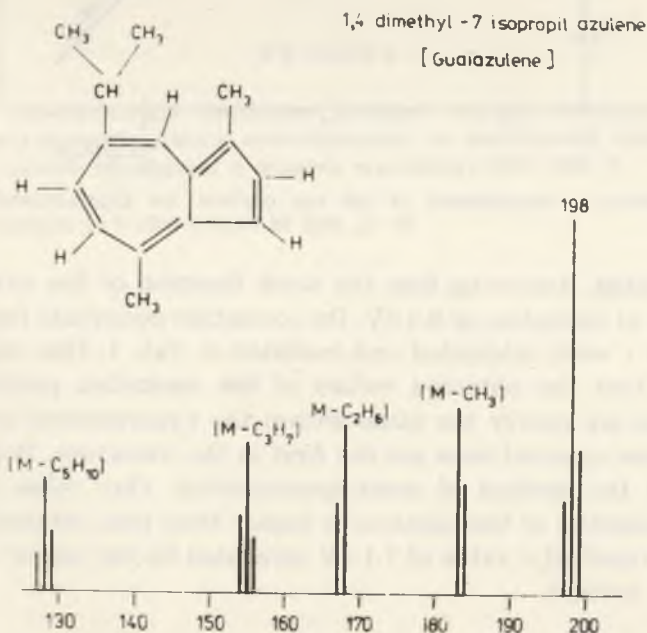

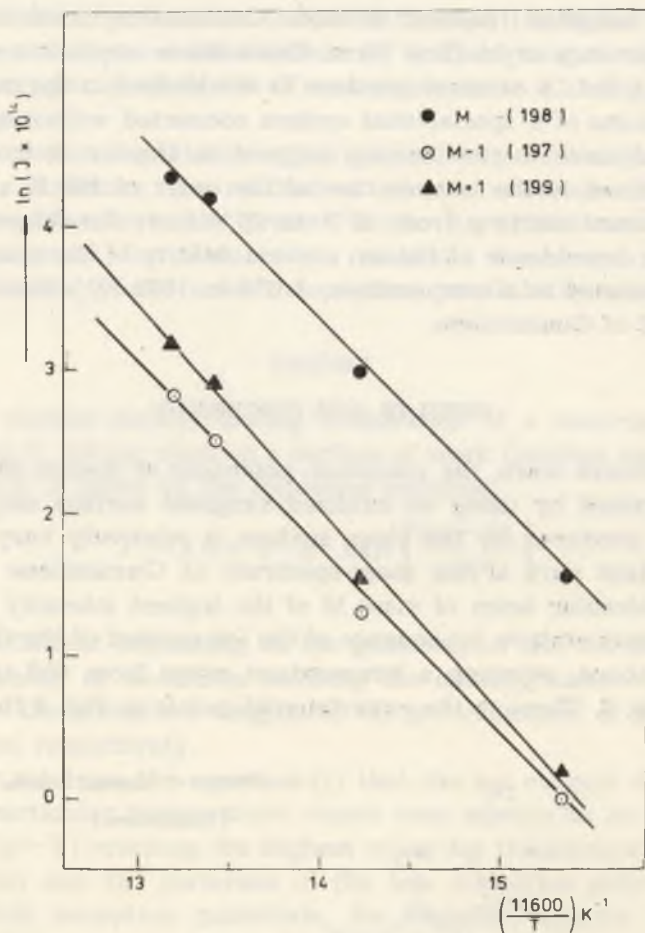Fig. 1. A typical part of the mass spectrum of Guaiazulene at 850°K

Fig. 2. Temperature dependence of the ion current for Guaiazulene and masses
M−1, and M+1

line was plotted. Assuming that the work function of the oxidized tung-
sten surface of ionization is 6.3 eV, the ionization potentials for the masses
M-1, M, M + 1 were calculated and included in Tab. 1. One may see from
the Tab. 1 that the obtained values of the ionization potential of the
three masses are nearly the same within the experimental error.

The values reported here are the first in the literature, that have been
obtained by the method of mass spectrometry. Our value of the first
ionization potential of Guaiazulene is higher than that obtained by T. Go-
worek who reported a value of 7.1 eV estimated by the use of the positron
annihilation method.

Tab. 1. Values of the ionization potential of Guaiazulene
$C_{15}H_{18}$

M	Ionization potential
197 (M−1)	7.49 ±0.04
198 (M)	7.52 ±0.04
199 (M+1)	7.59 ±0.08

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STRESZCZENIE

Za pomocą spektrometru mas zaopatrzonego w termoemisyjne źródło jonów wyznaczono pierwszy potencjał jonizacji guajazulenu.

Stosowano metodę jonizacji powierzchniowej na utlenionym wolframie w zakresie temperatur 650 ÷ 1000 K.

РЕЗЮМЕ

Методом поверхностной ионизации измерен первый потенциал ионизации молекул гуаязулена. Измерения производились на окисленной поверхности поликристаллического вольфрама в области температур 650÷1000 К.