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Statistical description of metastable negative ions' decay

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ABSTRACT

The decay of metastable negative ions resulted from the resonant electron capture by the molecules of acridanoneacetic acid benzyl ester has been studied using the negative ions' mass spectrometry technique. The simple model of metastable decay has been developed on the basis of the statistical Rice–Ramsperger–Kassel–Markus theory (RRKM). Based on the comparative analysis of the experimental and calculated effective yield curves of ions the shape of the internal energy distribution of molecular negative ions has been estimated.

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1. Introduction

The statistical RRKM concept [1] has found a wide application in the mass spectrometry of positive ions. Basing on the structural characteristics and energetic parameters of the molecule, its fragments and specific transition state, this theory can describe quantitatively the mass spectrum of chemical compound. This implies the explanation of the formation of certain groups of ions and prediction of their relative abundance in mass spectrum. Analogous approach has been attempted to the case of negative ion (NI) mass spectra [2,3], but has not been widely accepted. The main difficulties obviously, were caused by the specific features of the formation and decomposition of NIs. Indeed, the latter have several peculiarities not inherent for the case of positive ions formation processes, such as (i) the resonant character of the free electron attachment to the molecule, (ii) the specific selection rules (symmetry, energetic and temporal restrictions) governing the formation and/or mass spectrometric observation of NIs [4,5], and (iii) the presence of nondissociative channel of NI decay by means of electron autodetachment. In this connection, the application of statistical treatment to the case of negative ions is possible only for limited types of monomolecular decay reactions.

In the present article the RRKM theory was applied for the characterization of the fragmentation of metastable negative ions. This choice of the target for the statistical analysis was caused by the following reasons. First, the decaying ions are characterized by a relatively long lifetime ($\tau > 10^{-6}$ s), that facilitates a more complete distribution of an internal energy between active degrees of freedom and, therefore, justifies the application of the statistical approach. Second, the metastable ions have the strict genetic relationship to their parent ions and, accordingly, to the certain dissociation process, that excludes a possibility of the superimposition of several fragmentation pathways leading to yield of the same kind of ions. Third, since the considered ions are formed in the field-free region of a mass spectrometer, it is possible to calculate with adequate accuracy the time interval in which they are generated, that is necessary for quantitative estimations.

The present study is devoted to the metastable decay observed at the dissociative electron capture by the molecules of acridanoneacetic acid benzyl ester (Scheme 1). Derivatives of acridanoneacetic acid are widely used in pharmacology and medicine as drugs possessing antiviral and antitumoral properties [6].

The resonant electron capture by the molecules of acridanone derivatives has been studied previously with the main emphasis on thermochemistry of negative ions formation [7]. At that experiments an abundant broad mass peak with the maximum at noninteger value $m/z \sim 171.9$ have been detected correspondent to the metastable negative ions' fragmentation according the Scheme 1. The latter process was taken as target for elucidation in this work. In line with the molecular NIs (MNIs), for the clearness of the following speculations the fragment ions with $m/z = 252, 208$ and 171.9 will be referred to as parent, daughter, and metastable NIs, respectively.

A simple statistical model was elaborated for the characterization of the fragmentation of NIs. This model is based on the decay rate constant which was calculated on the basis of statistical RRKM theory. The ions' internal energy distribution function was

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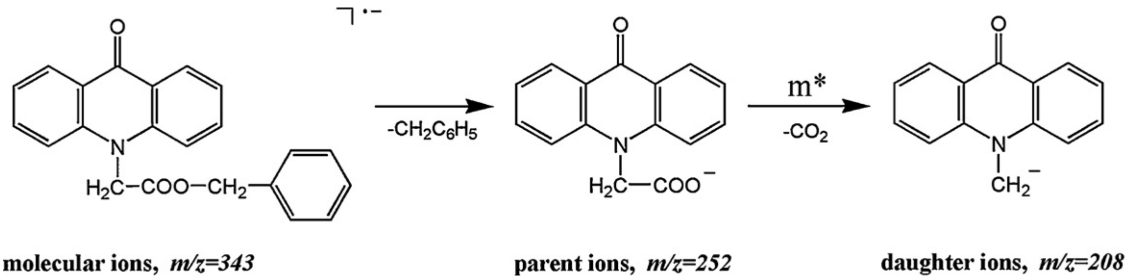

Scheme 1.

approximated by the known analytical function with several variable parameters. The best values for these parameters were found by fitting the calculated data to experimental curves. Similar statistical approach has been applied earlier to the metastable decay processes proceeding in negative ions formed from iron pentacarbonyl [8].

2. Theoretical model

Within the framework of the statistical approach, the process of fragmentation of negative ions is described by a rate constant of the monomolecular decay $k(\varepsilon)$ and ions' internal energy distribution function $f(\varepsilon)$. These functions determine the kinetics of the fragmentation quantitatively allowing the computation of the number of intact and decomposed ions to a definite time moment since the beginning of decay.

We have calculated the rate constant according to the equation of RRKM theory

$$k(\varepsilon)=\frac{\sigma W^{\pm}(\varepsilon-E_a)}{h\rho(\varepsilon)}, \tag{1}$$

where ε is the ions' internal energy, σ is the reaction path degeneracy, $W^{\pm}(\varepsilon-E_a)$ is the sum of states of the activated complex in the energy range from 0 to $(\varepsilon-E_a)$, E_a is the activation energy, $\rho(\varepsilon)$ is the density of states of the active molecule, and h is the Planck's constant. The $W^{\pm}(\varepsilon-E_a)$ and $\rho(\varepsilon)$ functions were calculated using the Stein–Rabinovitch algorithm [9]. The required vibrational frequencies were obtained by quantum chemical calculations of a parent ion ($m/z=252$). The ground state geometry optimization and computation of frequencies were performed at the DFT level using B3LYP functional and the 6-31G* basis set. The stretch of the C—C bond was considered as reaction coordinate, therefore a vibrational mode with frequency 1100 cm^{-1} was excluded from the calculations at evaluation of $W^{\pm}(\varepsilon-E_a)$. The activation energy was found to be $E_a\sim 1.21$ eV on the basis of the thermochemical evaluation using Ref. [7].

In metastable decay under study, the parent ions have a fragment origin. Therefore, the shape of their internal energy distribution function $f(\varepsilon)$ was expressed using the distribution function $F(\varepsilon)$ of molecular ions, precursors for the parent ions. The distribution of MNIs was simulated by the Gaussian function:

$$F(\varepsilon)=C\exp\left[-\frac{(E_M-\varepsilon)^2}{0.36(\Delta E)^2}\right], \tag{2}$$

where C is the normalization factor selected from the condition $\int F(\varepsilon)\,d\varepsilon=1$, E_M is the energy of a distribution maximum, ΔE is the distribution full width at half-maximum. The magnitude of ΔE depends on the initial thermal distribution of molecules in the ionization chamber as well as on the electron energy distribution and, presumably, varies with the increase in electron energy E_e. Therefore, we have approximated it by the following expression:

$$\Delta E=\Delta E_0+aE_e, \tag{3}$$

where ΔE_0 is the distribution full width at half-maximum at $E_e=0$, a is the factor reflecting the possible change in the distribution width with the increase of the electron energy. The ΔE_0 was taken to be equal to a half-width of a function, obtained by the convolution of Boltzmann distribution of molecules at given temperature with the kinetic energy distribution of the electrons captured.

The MNIs are decomposed both by the dissociation of interatomic bonds and by the spontaneous emission (autodetachment) of a captured electron. As a consequence of this mutual competition between accessible decay channels, the shape of energy distribution function of fragment ions differs from that of MNIs. In this connection, at the transition to the parent ions' distribution it is necessary to take into account both the electron autodetachment and the competition between different dissociative channels of the molecular ions which decompose.

Because of electron autodetachment, some part of MNIs does not survive until dissociative decay. This effect was taken into account by introducing the survival factor, i.e., the probability that MNI will not autodetach an electron and will be subjected to fragmentation:

$$P=\exp\left(\frac{-\tau_D}{\tau_{AD}}\right), \tag{4}$$

where τ_D is the time needed for separation of fragmenting parts up to that point, where the electron detachment becomes impossible; τ_{AD} is the MNIs' lifetime with respect to electron autodetachment, which is expressed as $\tau_{AD}=h/\Gamma$. As it is mentioned in Ref. [10], the resonance width Γ increases dramatically (most probably exponentially) with the energy of captured electrons. Therefore with the rise of E_e the process of autodetachment will stronger suppress the dissociative decay channels and their efficiency will drop. This effect results usually in the survival probability shift observed as the displacement of the resonant peaks' maxima towards lower energies with respect to total electron capture cross-section maxima. In our case it should lead to the cutoff of ions' distribution in the high-energy region and consequently to the shift of its maximum to the lower energy. In accordance with Ref. [11] we have accepted $\tau_{AD}\approx\varepsilon^{-0.5}$. Besides, the value τ_D depends on energy as well. We have expressed it as $\tau_D\approx\varepsilon^{0.5}$. Thus, the shape of the distribution of molecular ions survived until dissociation is described as follows:

$$F'(\varepsilon)=F(\varepsilon)\exp(-bE_e), \tag{5}$$

where b is some parameter.

In the general case, the survived (overlived the electron autodetachment) MNIs are subjected to the fragmentation by several parallel competing channels characterized by own rate constants $k_i(\varepsilon)$. The distribution of fragment ions generated in some channel i can be expressed as

$$f_i(\varepsilon)=F'(\varepsilon)\frac{k_i(\varepsilon)}{\sum_{j\neq i}k_j(\varepsilon)}. \tag{6}$$

In the considered energy range (0–4 eV) the molecular ions of acridanoneacetic acid benzyl ester dissociate into parent ions ($m/z=252$) and also into fragment ions with a mass number

$m/z = 194$. However, in the whole mentioned energy range the intensity ratio of these ions is constant and close to 1:4, and the ratio of their effective yield curves (EYC) represents almost a horizontal line. This fact indicates that $k_{252}(\varepsilon)/k_{194}(\varepsilon) \sim 4$ is actual for entire energy range under discussion. So, from (6) it is resulted that $f_{252}(\varepsilon) \sim 0.8F'(\varepsilon)$, i.e., the shape of parent ions' distribution function will be similar to that of MNI survived until a dissociation. Thus, the presence of the second dissociative channel will have no significant effect on the shape of distribution function of parent ions, and the latter can be accepted to be coincident with the distribution function of MNI survived after autodetachment, described by Eq. (5).

The parent ions inherit a part of internal energy of molecular ions as well as some portion of excess energy Q released during MNI fragmentation. The following equation was used for determination of the energy of the $f(\varepsilon)$ distribution function maximum:

$$E_P = \alpha(E_e + E_{vib} + Q), \tag{7}$$

where E_e is the energy of captured electrons and E_{vib} is the vibrational energy of neutral molecules. The expression in brackets describes a total energy distributed among the products of MNI decay, and coefficient α defines the portion of this energy inherited by parent ions. In addition, the part of energy passes into translational energy of fragments. Under the hypothesis of uniformity of energy distribution between fragments, the coefficient α is assumed to be equal to the ratio of degrees of freedom number in the parent and molecular ions. Thus, its value is taken as $\alpha \sim 0.66$. Eq. (7) is well fitted with the results of experiments. In Ref. [10] it was shown, that the kinetic energy of decay products linearly increases with the elevation of electron energy, hence, the internal energy of ions should also demonstrate a linear dependence, which is expressed by Eq. (7).

The vibrational energy value included in (7) was calculated according to the following formula [12]:

$$E_{vib} = \sum_{j=1}^{N} \frac{\sum_{n=0}^{\infty} n\varepsilon_j \exp(-n\varepsilon_j/k_B T)}{\sum_{n=0}^{\infty} \exp(-n\varepsilon_j/k_B T)}, \tag{8}$$

where ε_j is the energy of the jth vibrational mode, N is the total number of vibrations, k_B is the Boltzmann constant, and T is the temperature. The calculated values of vibrational energy for different temperatures were $E_{vib}(114\,^\circ C) = 0.80$ eV, $E_{vib}(233\,^\circ C) = 1.36$ eV, $E_{vib}(288\,^\circ C) = 1.67$ eV. The excess energy of the process of MNI fragmentation into parent ions was calculated from the equation of the energy balance of the decay reaction:

$$Q = \Delta H_f^\circ[\mathrm{ACH_2COOCH_2C_6H_5}] - \Delta H_f^\circ[\mathrm{CH_2C_6H_5}] - \Delta H_f^\circ[\mathrm{ACH_2COO^-}] = 0.86\,\mathrm{eV},$$

where A is acridanone nucleus ($C_{13}H_8NO$). Following thermochemical characteristics were used in calculations: $\Delta H_f^\circ[\mathrm{ACH_2COOCH_2C_6H_5}] = -1.39$ eV, $\Delta H_f^\circ[\mathrm{ACH_2COO^-}] = -4.32$ eV, $\Delta H_f^\circ[\mathrm{C_6H_5CH_2^\bullet}] = 2.07$ eV [7].

Thus, the energy distribution of parent ions is described as follows:

$$f(\varepsilon) = C \exp\left[-\frac{(E_P - \varepsilon)^2}{0.36(\Delta E_0 + aE_e)^2} - bE_e\right], \tag{9}$$

where two parameters a and b are present. Parameter a describes the broadening of the distribution with the elevation of E_e, the parameter b is responsible for process of electron autodetachment by molecular ions. The energy position of a distribution maximum E_P is described by Eq. (7).

We have calculated the number of formed metastable m*, daughter D^-, and parent P^- ions as relations $[m^*]/[P^-]$ and $[D^-]/[P^-]$ in terms of the functions $k(\varepsilon)$ and $f(\varepsilon)$. These ratios allow to eliminate the resonant nature of the formation of negative ions and demonstrate the efficiency of metastable decay depending on the energy of captured electron. The daughter ions are generated inside the ionization chamber in a time interval $t_0 - t_1$ (see Fig. 1); the metastable ions are formed along the first field free region of a mass spectrometer in the time interval $(t_2 - t_3)$; the ions survived until a moment of the exit from magnetic field t_4 were detected as parent ones. To summarize, we have calculated the required relations $[m^*]/[P^-]$ and $[D^-]/[P^-]$ according to following equations:

$$\frac{[m^*]}{[P^-]} = \frac{\int f(\varepsilon)\exp[-k(\varepsilon)t_2]\,d\varepsilon - \int f(\varepsilon)\exp[-k(\varepsilon)t_3]\,d\varepsilon}{\int f(\varepsilon)\exp[-k(\varepsilon)t_4]\,d\varepsilon}, \tag{10}$$

$$\frac{[D^-]}{[P^-]} = \frac{\int f(\varepsilon)\,d\varepsilon - \int f(\varepsilon)\exp[-k(\varepsilon)t_1]\,d\varepsilon}{\int f(\varepsilon)\exp[-k(\varepsilon)t_4]\,d\varepsilon}. \tag{11}$$

The time interval $t_0 - t_1$ of ions extraction from the ionization chamber was estimated using numerical simulation of the electric field distribution in the reaction region. The time of ions' drift in a mass spectrometer $t_1 - t_4$ was evaluated from the known geometrical sizes of the instrument (see Fig. 1) and accelerating potential value.

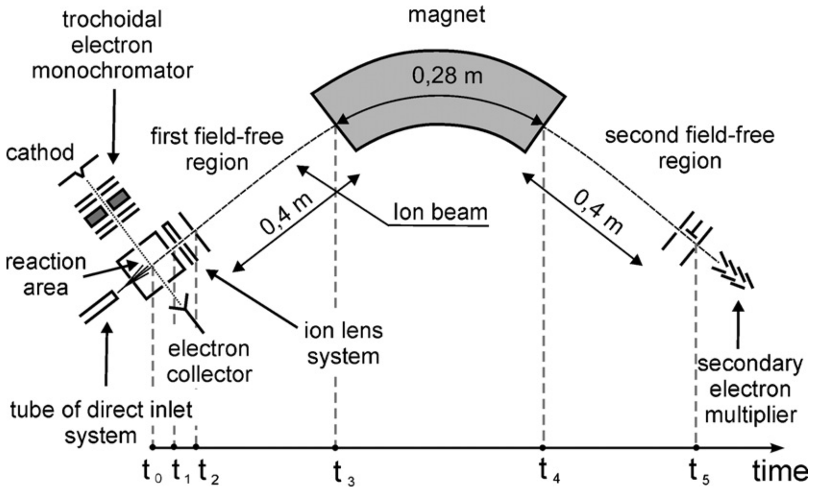

Fig. 1. Schematic diagram of the negative ions mass spectrometer and the time intervals of ions drift in the instrument (bottom).

3. Experimental

The experiments were performed using a commercial single focusing magnetic sector-type mass spectrometer, Model MI-1201V (Sumy, Ukraine) modified for the generation and detection of negative ions, also maintaining the opportunity of the operation with positive ions [13]. The schematic diagram of an instrument is given in Fig. 1. The compound investigated was introduced into the ion source through a tube of a direct inlet preheated up to $t \sim 90\,^{\circ}\mathrm{C}$. The experiments were performed at temperatures of ionization chamber 114, 233 and 288 °C. The pressure measured with an ion gauge near the ionization chamber did not exceed $\sim 10^{-4}$ Pa. In special experiments for testing the influence of collisionally induced dissociation on metastable ions' decay the pressure was increased up to $\sim 10^{-2}$ Pa. It was achieved by partial shutting off the valve of a vacuum pump.

The electron energy scale was calibrated using the maximum of the effective yield curve of SF_6^- from SF_6 (~0 eV). The electron energy resolution (FWHM of the above mentioned SF_6^- peak) was adjusted from the condition of reasonable compromise with the ions' intensities and was $\Delta\varepsilon \sim 0.3$ eV at an electron current $I_e \sim 1\,\mu A$. Ion accelerating voltage was 3.5 kV.

Metastable ions, as a rule, are characterized by a broad mass peak in mass spectra. Its width depends on ions' kinetic energy. To take into account the total number of generated metastable ions, their EYC recorded at peak maximum was multiplied by the correction factor $K_1 \sim 15.6$. This factor is taken to be equal to the ratio of areas under mass peaks of stable and metastable ions.

Amplification factor of the secondary electron multiplier is known to be dependent on mass of ions [14], therefore the relation $[D^-]/[P^-]$ was multiplied by factor $K_2 = (208/252)^{0.5} \sim 0.9$.

4. Results and discussion

Resonant electron capture by the molecules of acridanoneacetic acid benzyl ester appears in a broad energy range 0–12 eV. In the spectrum obtained at thermal energies the mass peak of molecular ions is observed indicating the positive electron affinity of the molecules. The dissociative electron capture mass spectrum is represented by numerous fragment ions generated both by the break of a side chain and by the fragmentation of an aromatic skeleton. Among them two groups of ions with the mass numbers $m/z = 252$ and 194 dominate. Their relative intensity exceeds almost by two orders that for remaining fragment ions. The ions with $m/z = 252$ are formed as a result of benzyl fragment ejection, and ions with $m/z = 194$ correspond to acridanone nucleus remained after removal of the whole side chain. The broad mass peak with noninteger value $m/z \sim 171.9$ observed in a spectrum indicates the instability of ions $m/z = 252$ with respect to the subsequent fragmentation according to Scheme 1.

Fig. 2a shows the effective yield curves of metastable m*, daughter D^-, and parent P^- ions. The considered decay encloses two resonant states with maxima at $E_e \sim 1$ eV and 2 eV. It is rather curious, since metastable ions usually demonstrate single resonant peak disposed in the region of parent and daughter ions' EYCs crossing. In this connection, the problem of the mechanisms of fragmentation in each of the resonances is of interest. Whether these mechanisms are similar or fragmentation takes place following the different scenarios? In Fig. 2b (open circles) the relation of intensities of metastable and parent ions $[m^*]/[P^-]$ is plotted, that allows to eliminate the resonant nature of the formation of negative ions and reflects the efficiency of the decay process depending on the energy of captured electrons. A monotonic rise of a curve with the elevation of electron energy and the absence of noticeable breaks in the region of the transition from one resonance to another is observed. This circumstance provides the reason to suppose that in both cases the unique dissociative process takes place, the efficiency of which determined solely by the internal energy of ions.

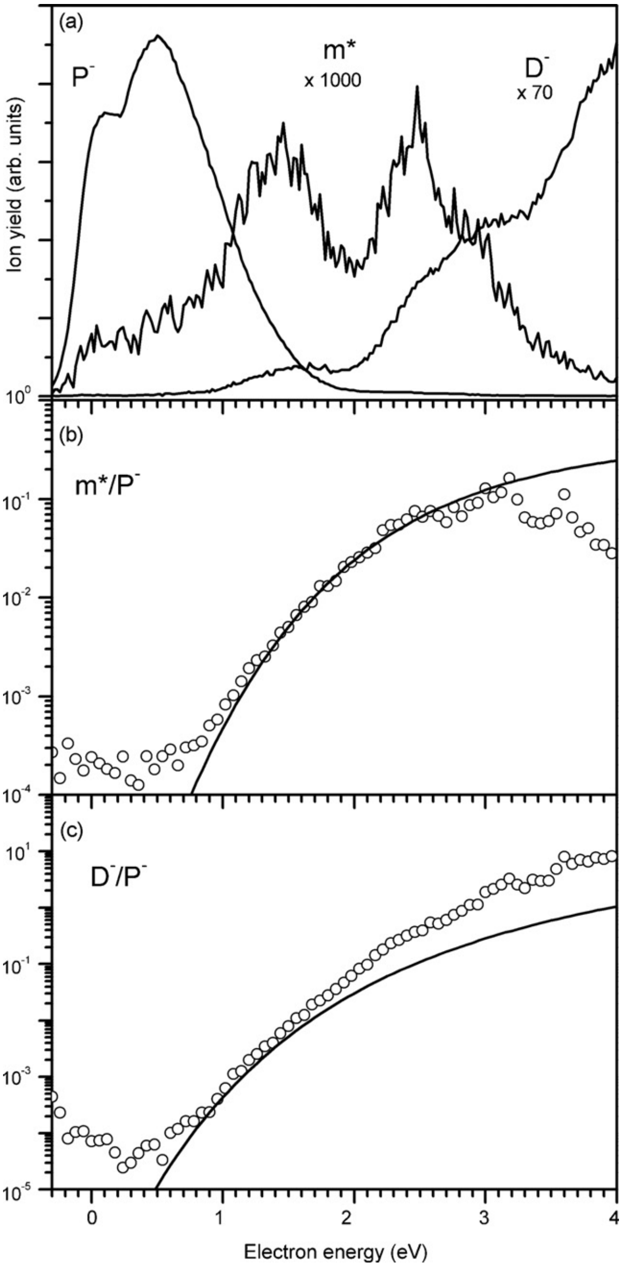

Fig. 2. Effective yield curves of the metastable m*, daughter D^- and parent P^- ions (a), experimental (open circles) and calculated (line) intensity relations of metastable, daughter and parent ions $[m^*]/[P^-]$ (b) and $[D^-]/[P^-]$ (c).

Using the RRKM statistical approach for the metastable decay (see Section 2), we have calculated the relation $[m^*]/[P^-]$. The resulted curve is given in Fig. 2b (line). During the calculation we have fitted the values of parameters a and b, which describe the ions' distribution $f(E)$ in such a way, that the disagreement with the experimental data was minimal. Other parameters were varied insignificantly. It is clear, that the calculated curve reproduces correctly a middle part of the experimental curve. However, there are discrepancies in the thermal and high-energy parts of the curves. Presumably, these discrepancies are caused by the low abundance of metastable ions, that results in the deficiency of the signal-to-noise level of curves and fatal increase of the measurement error, and finally leads to the incorrect reflection of the real processes.

At the same time, the disagreement in behaviour of experimental and calculated curves also could have different explanation. The decay efficiency should monotonously decrease with the diminution of electron energy, since the internal energy of ions becomes insufficient for bond dissociation. The inadequate behaviour of the experimental curve in this region is probably caused by the processes of collisional activation. During the drift in a mass spectrometer tube the accelerated ions interact with molecules of residual gas and are subjected to the fragmentation after gaining an additional energy. Two experimental facts testify to that: (i) the compulsory degradation of vacuum in the instrument results in even greater increasing of the relation $[m^*]/[P^-]$ in zero energy region; (ii) at $E_e \sim 0$ eV the position of the metastable ions' mass peak is slightly shifted with respect to that recorded at higher electron energies. This observation implies that metastable ions formed at thermal electron energies possess a lower kinetic energy which is lost probably due to the collisions of ions with the molecules of background gas.

Another discrepancy of curves is observed at high electron energies, where the experimental relation $[m^*]/[P^-]$ ceases growing with elevation of electron energy. It seems unusual, since the decay rate constant represents a monotonic increasing function and the decay efficiency should rise with the ions' energy. Seemingly, the observed "stabilization" of a relation $[m^*]/[P^-]$ is caused by the suppression of dissociative decay channels owing to the process of autoneutralization of MNI. The high-energy part of the molecular ions' distribution is predominantly droped out by the electron detachment and only ions with a low internal energy survive until the fragmentation. As a result, despite of a high energy of captured electrons, the parent ions have a small internal energy and the dissociative decay efficiency is low.

Using optimal parameters for the relation $[m^*]/[P^-]$, we have plotted the intensities relation for daughter and parent ions $[D^-]/[P^-]$ (Fig. 2c, line). In contrast to metastable ions having a strict relationship to the specific decay, the daughter ions can be formed both from parent ions and by the direct decay of MNI. Therefore, their EYC, probably, contains the contribution from the several dissociative processes, that seemingly explains some discrepancy between the slopes of calculated and experimental $[D^-]/[P^-]$ curves.

We have also performed experiments at different temperatures of an ionization chamber. The temperature elevation leads to the increase in the internal energy of molecules and consequently of molecular ions. Energy distribution $F(\varepsilon)$ becomes broader and its maximum is shifted towards higher energy region. Therefore, at the calculation of curves $[m^*]/[P^-]$ and $[D^-]/[P^-]$ for each temperature, the separate values of a vibrational energy E_{vib} and parameter a (defining the distribution width at half-height at $E_e = 0$ eV) were evaluated. The values of other parameters were not varied. One can see from Fig. 3 the elevation of the temperature leads to the bias of the experimental curves towards lower energies and their slope becomes more mild. The calculated curves also demonstrate similar shift, but the slope is not changed. Apparently, the change of curves' slope originates from the increase of the efficiency of the collisional activation in a mass spectrometer, which is a parasitic process and is not considered within the present model.

Thus, despite of some revealed drawbacks, the simple statistical model of the metastable negative ions' decay presented in this paper is in fairly good agreement with experimental results.

One of the applications of the statistical approach described above is the opportunity of estimation of ions' internal energy distribution $f(\varepsilon)$. The shape of the function $f(\varepsilon)$ cannot be determined directly by any experimental method. In case of positive ions there are some procedures of the indirect evaluation of energy distribution parameters, which are based on the comparison of the efficiency of ions' formation in two competitive processes [15] or in the stepwise fragmentation [16]. However, the application of these approaches for negative ions is problematic because of the reasons mentioned above (see Section 1). In present study we have simulated the distribution of MNI by Gaussian function (2). The distribution of parent ions was modeled by Eqs. (9) and (7). These expressions contain several parameters, the optimal values of which are fitted on the comparison of calculated and experimental data and represented in Table 1. These data infer that the width of the molecular ions' distribution is greater than the thermal distribution of molecules, though this difference is not so significant at thermal electron energies. At the same time, the value of parameter a which is responsible for the dependence of the distribution width on electron energy is obtained to be different from zero ($a = 0.24$). This means that the distribution width increases gradually with the rise in electron energy. On the other hand, this effect can be conditioned not by the electron capture process but by the influence of other factors. One of the possible explanation may be the instrumental electron energy distribution broadening along the electron energy scale, which can take place due to specific construction of an electron monochromator [17].

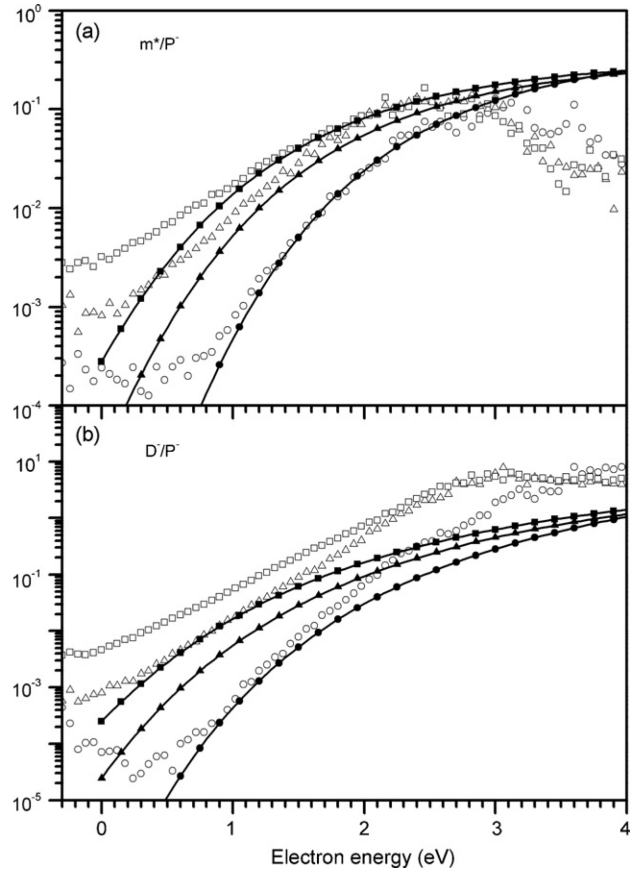

Fig. 3. Experimental (open symbols) and calculated (solid symbols) intensity relations of metastable, daughter and parent ions $[m^*]/[P^-]$ (a) and $[D^-]/[P^-]$ (b) at different temperatures of an ionization chamber (114 °C—circles, 233 °C—triangles, 288 °C—squares).

Table 1
Optimal values of parameters used in model

T (°C)	ΔE_0 (eV)	E_a (eV)	α	Q (eV)	E_{vib} (eV)	a	b
114	0.65	1.21	0.66	0.86	0.8	0.24	4.2
233	0.85	1.21	0.66	0.86	1.36	0.24	4.2
288	0.93	1.21	0.66	0.86	1.67	0.24	4.2

Acknowledgements

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