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INFLUENCE OF PARAMETERS OF AN ELECTRON BEAM ION SOURCE ON THE FRAGMENTATION PROCESS OF DEUTERATED PROPANE (C_3D_8)

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Abstract

In this work, the electron beam ion source (EBIS) was used to study the molecular fragmentation of the deuterated propane C_3D_8 molecules. The experiments were performed in the Kielce EBIS facility at Jan Kochanowski University (Kielce, Poland). During the measurements, the EBIS operated in the so-called leaky mode, which guaranteed a wide spectrum of fragmented ions with a constant value of the beam current. The molecular fragments produced in the source were charge-separated using a dipole magnet and detected with a Faraday cup connected to a high-sensitivity electrometer. The measured mass spectrum exhibited a variety of possible molecular fragments, including CD_x ($x = 0 - 3$), C_2D_x ($x = 0 - 5$), and C_3D_x ($x = 0 - 8$). Systematic tests were performed to illustrate the influence of working gas pressure and current of the electron beam on the intensity of individual fragmentary ions.

Keywords: electron beam ion source, deuterated propane, electronic ionisation, mass spectrometry, molecular fragmentation.

1. Introduction

The *electron beam ion source* (EBIS) is a universal device for producing, trapping, and extracting ions in high-charge states. The EBIS can also be used for production of low-charged molecular ions by fragmentation of complex molecules in a high-energy dense electron beam [1–4]. The study of fragmentation processes at high electron energies is an interesting field of research in the context of the description of fragmentation phenomena, as well as interactions of fragmentation products with surfaces [5,6]. Molecular fragmentation is defined as the dissociation of energetically unstable molecular ions formed from molecules in the ionisation chamber [5–9] into various

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fragmentary ions. These ions, detected using mass spectrometry, form a pattern called mass spectrum, which can be used to determine the structure of the produced fragments, study fragmentation processes, and gas production efficiency [10–12]. The ionisation process can occur through collisions with electrons (*electronic ionisation* EI), reactive gas ions (*chemical ionisation* CI), fast atoms (*fast atom bombardment* FAB) or fast ions (*secondary-ion mass spectrometry* SIMS) as well as in *field desorption processes* (FD) and *field ionisation* (FI).

In electron ionisation (EI) of a molecular gas, the [AB] molecule is excited (gains internal energy) in collisions with the electron beam e^-, which can lead to the ejection of one of its electrons and conversion of the molecule into a $[AB]^{+\cdot}$ positive molecular ion:

$$[AB] + e^- \rightarrow [AB]^{+\cdot} + 2e^- . \tag{1}$$

Smaller or greater excess of energy in the molecular ion can cause its dissociation into fragments, i.e. fragmentary ions and molecule, atom or radical:

$$[AB]^{+\cdot} \rightarrow A^+ + B^\cdot \quad \text{or} \quad [AB]^{+\cdot} \rightarrow A^\cdot + B^+ . \tag{2}$$

An example of the fragmentation process is illustrated in Fig. 1, which shows the process of electron ionisation of a deuterated propane molecule C_3D_8 in an electron beam ion source. Fragmentation in this type of source is a result of the process of consecutive EI. At the top of the scheme, the dissociation of the deuterated propane C_3D_8 molecule into charged and neutral molecule fragments is depicted. At the bottom, the diagram shows only the ionised deuterated propane C_3D_8 molecule (that has not dissociated) [8].

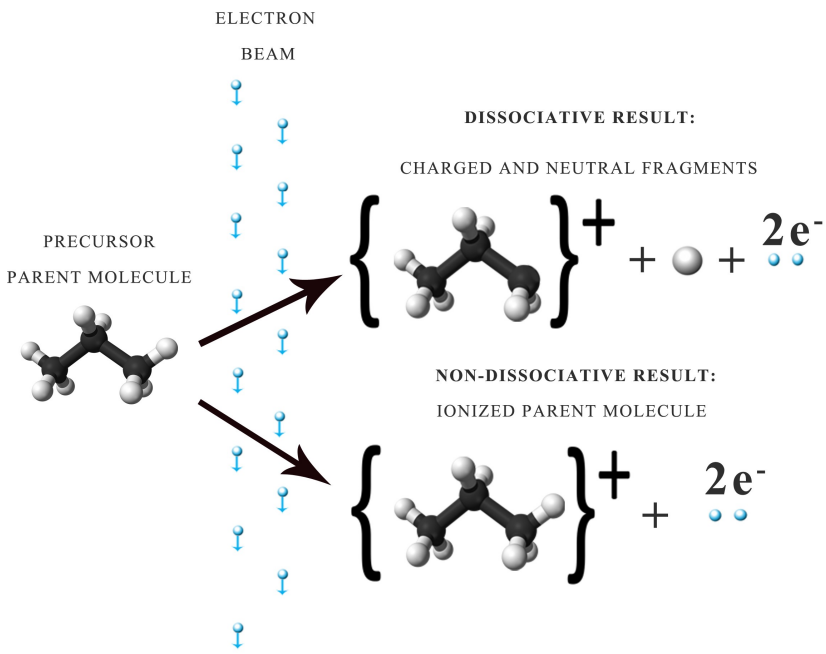

Fig. 1. Electron ionisation (EI) of a deuterated propane C_3D_8 molecule. Firstly, a molecular ion $[C_3D_8]^+$ is produced which then dissociates in various ways to form more fragmentary ions such as $[C_yD_x]^+$, C^+, D^+ and others, including those with a higher charge state (x, y are the number of individual atoms in the molecule).

In this paper, we present the results of the first test experiment carried out using the Kielce EBIS facility, located at the Institute of Physics of Jan Kochanowski University in Kielce. In the experiment, we studied the process of fragmentation of deuterated propane molecule C_3D_8. The aim of the experiments was to determine the influence of parameters of the ion source (Dresden EBIS-A) of the facility, such as the pressure of the working gas and the current of the electron beam, on the intensity of the C_3D_8 molecule fragmentation products.

2. Experimental setup

The Kielce EBIS facility comprises several key components (see Fig. 2), including the EBIS-A ion source equipped with an integrated Electron Gun (EG), a dipole magnet for separating ion beams based on the charge-to-mass ratio, and the target chamber. Beam geometry adjustment is achieved with einzel lenses (EL A&B), 2-axis deflectors (DF A&B), and a 4-jaw Slit System (SS). The ion beam current is measured using Faraday Cups (FC A&B) that are connected to a highly sensitive Keithley electrometer.

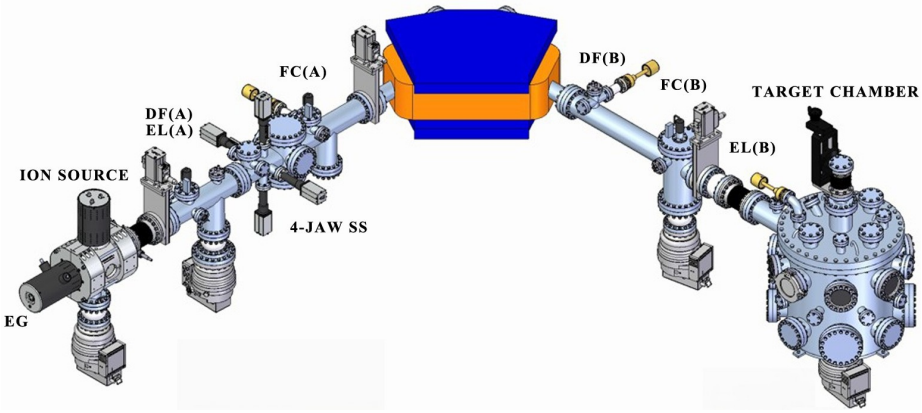

Fig. 2. Scheme of the EBIS facility. EG – electron gun, DF – deflectors, EL – einzel lenses, FC – Faraday cups, 4-JAW SS – four-jaw slit system.

The source provides a diverse range of slow, highly charged ions, starting from bare ions of light elements to Ne-like and Ar-like ions of high-Z elements. The maximum electron energy and current available for ionizing the trapped ions are 25 keV and 200 mA, respectively. The produced ions can be extracted either in a pulsed mode, with pulse widths ranging from 2 s to 40 s, or in the continuous "leaky" (DC) mode [13–15].

For the purpose of the experiment, propane (D8, 98%) from Cambridge Isotope Laboratories Inc. was used as the working gas. The gas was injected into EBIS-A source through a precision thermally controlled UDV 046 valve. The initial pressure, measured before dosing the working gas, was $p = 4\times10^{-10}$ mbar, while the injection pressure ranged from $p = 3\times10^{-9}$ mbar to 1.5×10^{-8} mbar. Within the source, the molecules of gas are radially confined by the combined effects of the space charge of the electron beam and the magnetic field generated by permanent magnets, while axially trapped by electrostatic barriers (traps) defined by three drift tubes of the source.

During the measurements presented, the EBIS was operated in the "leaky mode", which ensured a wide spectrum of fragmentation ions with a constant value of the beam current. In this configuration, the trap potential in the direction to the extraction is lower than on the other side.

The molecules stay in the trap for a short time, preventing their excessive fragmentation (observed also in [1]). The electric potentials in the EBIS ion trap are shown in Fig. 3, and parameters of the ion source used in the experiments are summarised in Table 1.

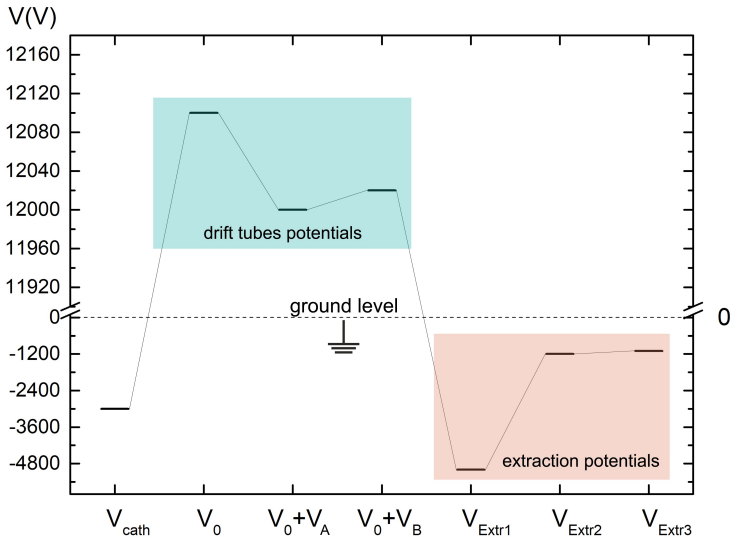

Fig. 3. Diagram of electric potentials in the EBIS ion trap, including the main adjustable electrical parameters. The selection of individual potential values affects, among others, the electron energy value and the operating mode of the trap (leaky or pulsed).

Table 1. EBIS-A parameters during measurements.

Parameter	**Value**
Cathode potential V_{cath}	–3 kV
Drift tube potential V_0	12.1 kV
Trap potential V_A	–100 V
Trap potential V_B (trap open)	–80 V
Extraction potentials	$V_{\text{Extr1}} = -5$ kV, $V_{\text{Extr2}} = -1.2$ kV, $V_{\text{Extr3}} = -1.1$ kV
Current of the electron beam I_e	30 mA, 50 mA, 70 mA, 90 mA
Working gas pressure p	1.5×10^{-8} mbar – 3×10^{-9} mbar (five values)

Then, the ion beam is extracted from the trap using three extraction potentials ($V_{\text{Extr1,2,3}}$). In the region between the trap and the mass-to-charge separator, preliminary diagnostics and beam focusing are performed. The selection of the main trapping parameters (V_0, V_A, V_B, $V_{\text{Extr1,2,3}}$) is verified based on the signal intensity observed in FC(A). At this stage, it is also possible to focus the beam using a three-segment einzel lens, which generates an electric field capable of compressing or expanding the passing ion beam depending on the applied polarisation. The X-Y beam positioning is controlled via the integratedPodziekowania deflector, featuring a 30 mm aperture. The deflection voltages can be set in the range ±1250 V. The fragmentary ions produced and extracted from the source were then directed to the mass-to-charge separation section.

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A Danfysik dipole magnet with a 50 mm pole gap was powered by a high-stability (10 ppm) power supply. The bending angle and bending radius of the magnet are 90 degrees and 461 mm, respectively.

After passing through the field of the dipole magnet, the ion beam undergoes bending and separation depending on the mass and charge of its components. Next, the separated ions enter the FC(B), where their total charge is measured using a Keithley 6517B electrometer operating in the range of 200 pA and 2 nA, with a resolution of 0.001 pA and 0.01 pA, respectively. A precise scan of the magnetic field in the range of 20.5–256.4 mT, with a step size of 0.028 mT, allowed for the registration of the fragmentary ions generated during the fragmentation process and the quantitative determination of the contribution of individual components. In order to investigate the influence of the parameters of the EBIS-A ion source on the products of the fragmentation process, we conducted systematic tests for different measurement configurations: working gas pressure and current of the electron beam. For all of these configurations, the intensity of individual fragments was recorded, and the stoichiometric ratios were calculated.

3. Experimental results

3.1. Ion mass spectrum calibration

By conducting a precise scan across a broad magnetic field range, we successfully obtained mass spectra of deuterated propane C_3D_8. An example of such spectrum is presented in Fig. 4.

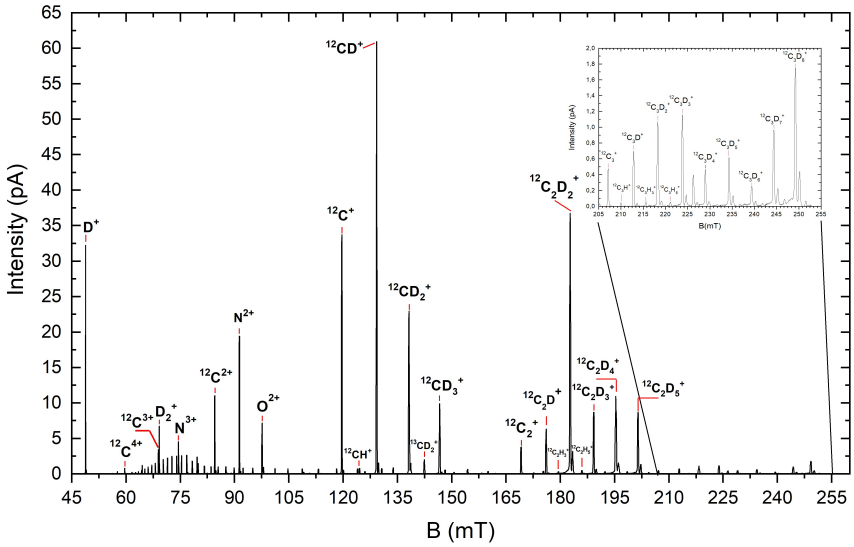

Fig. 4. Mass spectrum of deuterated propane C_3D_8 measured in the leaky mode. The electron beam energy was set at 15 keV with electron current $I_e = 30$ mA and working gas pressure $p = 6 \times 10^{-9}$ mbar. For a better visualisation of $C_3D_x^+$ low intensity lines, the inset graph was added.

The spectrum was measured for an electron beam energy of 15 keV and the electron beam current of $I_e = 30$ mA. The operating gas pressure was maintained at $p = 6 \times 10^{-9}$ mbar. This general spectrum encompassed a wide range of fragmentary ions, beginning with the deuterium D^+, D_2^+, carbon in different charge states, going through groups of CD_x^+ ($x = 0 - 3$), $C_2D_x^+$ ($x = 0 - 5$),

and $C_3D_x^+$ ($x = 0 - 8$) (where $x$is number of deuterium atoms). In addition, some molecular ions of hydrocarbons - $C_nH_m^+$ ($n = 1 - 3$, $m = 1 - 5$) were also identified in the spectra, along with ionised rest gas atoms and highly charged xenon remnants (from previous experiments).

The theoretical values of magnetic induction corresponding to individual fragments of the molecule present in the mass spectrum were calculated using the basic equation of mass spectrometry:

$$\frac{m}{q} = \frac{B^2 r^2 e}{2U}, \tag{3}$$

where: m – ion mass, q – ion charge, e – elementary charge, r – bending radius of the magnet ($r = 0.4575$ m), U – accelerating voltage.

The raw experimental spectra were corrected using eight calibration peaks covering the entire area of the recorded spectrum. An example spectrum is shown in Fig. 5.

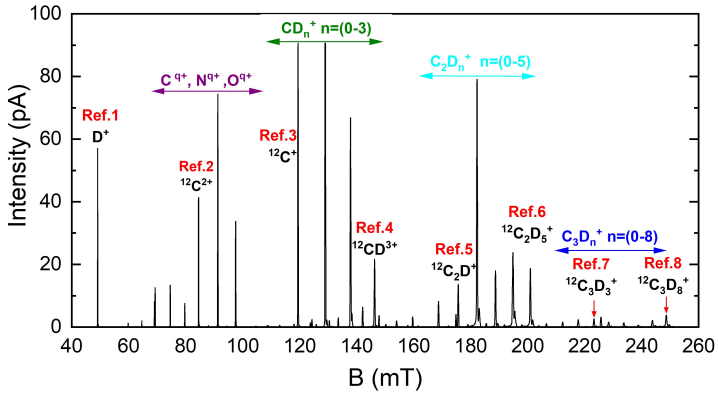

Fig. 5. Mass spectrum of deuterated propane C_3D_8 measured in the leaky mode with eight calibration peaks covering the entire area of the recorded spectrum. The electron beam energy was set at 15 keV with electron current $I_e = 70$ mA and working gas pressure $p = 6 \times 10^{-9}$ mbar.

The list of selected peaks along with the corresponding theoretical, experimental, and calibrated magnetic field induction values for these peaks is presented in Table 2 [16]. The calibration carried out in this way allowed for the unambiguous identification of other unknown peaks in the mass spectrum.

Table 2. Reference line of magnetic induction B values for selected fragmentary ions, for pressure $p = 6 \times 10^{-9}$ mbar and electron current $I_e = 70$ mA.

Ref. No.	Ion	$B_{\text{theor.}}$ (mT)	$B_{\text{exp.}}$ (mT)	$B_{\text{calibrated}}$ (mT)
1	D^+	48.974	49.128	48.975
2	C^{2+}	84.528	84.570	84.523
3	C^+	119.541	119.452	119.558
4	CD_3^+	146.579	146.318	146.548
5	C_2D^+	176.008	175.699	176.045
6	$C_2D_5^+$	201.427	200.978	201.389
7	$C_3D_3^+$	223.754	223.339	223.773
8	$C_3D_8^+$	249.115	248.695	249.112

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3.2. Dependence of molecular ion intensity on the gas pressure

A series of measurements was conducted, while maintaining a constant electron energy of 15 keV and an electron beam current I_e of 30 mA, to study the influence of variation of working gas pressure on the intensity of fragmentation products. The range of these pressure changes was 1.5×10^{-8} mbar to 3×10^{-9} mbar. The mass spectrum acquisitions were performed after stabilizing the pressure value in the source. The results of these measurements, which contained information on the intensities of individual fragmentary ions recorded in the spectrum, were compiled in the form of Figs. 6 and 7. A clear increase in intensity can be observed as a function of the increase in working gas pressure for the individual molecular ions in the groups: $C_3D_x^+$, $C_2D_x^+$, CD_x^+ and also for C^{q+} ions. Moreover, we can see that for such source configuration, some molecular ions are clearly preferred in the fragmentation process (*e.g.*, $C_2D_2^+$).

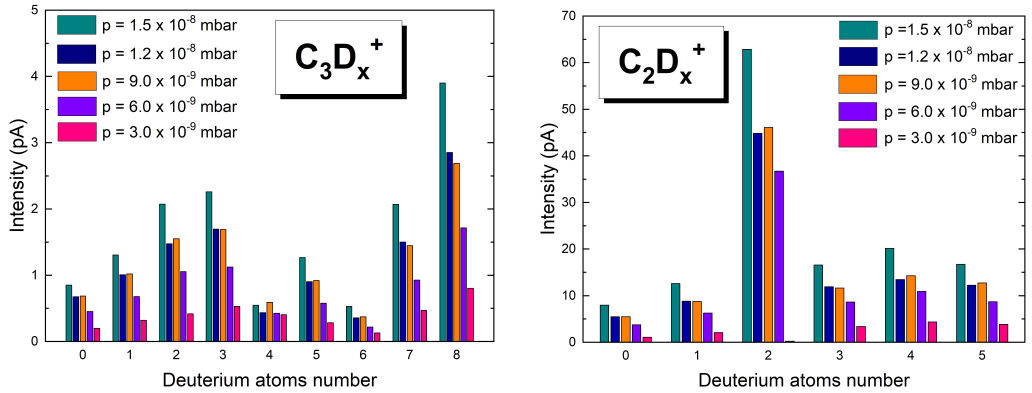

Fig. 6. Influence of the pressure of the working gas on the intensity of individual molecular ions in the $C_3D_x^+$ (left) and $C_2D_x^+$ (right) groups, E_e = 15 keV and I_e = 30 mA.

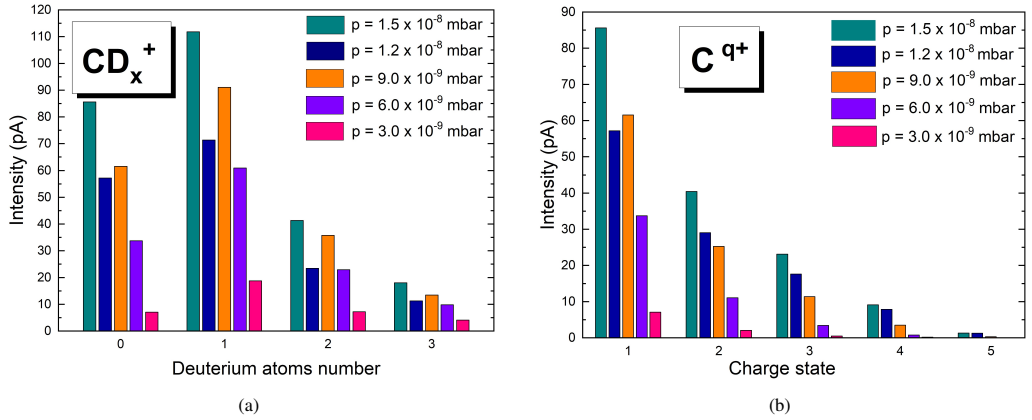

Fig. 7. Influence of the pressure of the working gas on the intensity of individual molecular ions in the CD_x^+ group (left) and the effects of the pressure on the observed intensity of various charge states of carbon C^{q+} (right), E_e = 1;keV and I_e = 30 mA.

A comparison of results obtained from two measurements conducted at two different working gas pressures, namely 1.5×10^{-8} mbar and 3×10^{-9} mbar, and constant electron beam current equal to 30 mA, is presented in Fig. 8. The data show a clear increase in the intensity of individual spectrum components with increasing gas pressure. The increase for the $C_3D_x^+$ group is slightly lower compared to the other two groups, while among components of the ($C_2D_x^+$) group, the $C_2D_2^+$ fragment stands out, with its intensity increasing more than 240 times.

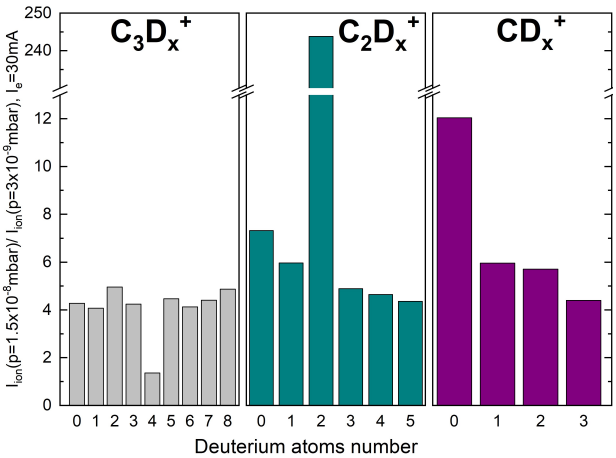

Fig. 8. Effect of the change in working gas pressure on the intensity of the peak of a given fragmentation ion in the mass spectrum. Individual bars express the ratio of the intensity of the given peak in relation to the working gas pressure ratio: 1.5×10^{-8} mbar/3×10^{-9} mbar. The measurements were performed for an electron energy of 15 keV and an electron current equal to 30 mA.

3.3. Dependence of molecular ion intensity on the electron beam current

The series of results obtained for measurements carried out for various electron current values in the range of 30–90 mA show several interesting relationships (Figs. 9 and 10). For the heaviest fragment ions (in the area of the $C_3D_x^+$ group), the dominant fragments are $C_3D_8^+$ and $C_3D_7^+$. In their case, the intensity saturation effect is noticeable for a current value of 70 mA. At the value of 90 mA, there is a slight decrease in intensity – for these two fragments. A similar saturation effect is observed for the $C_3D_6^+$ and $C_3D_5^+$ fragments. For the remaining fragments in this group, the current intensity associated with a given fragment ion increases with an increase in the intensity of the electron beam. Interestingly, for ions in the range: C_3D^+–$C_3D_6^+$, the $C_3D_3^+$ ion is distinguished in terms of intensity. In the group of molecular ions containing two carbon atoms ($C_2D_x^+$), the increase in the intensity of individual ions is consistent with the increase in the intensity of the electron current. In the case of elements of this group, we observe the molecular fragment $C_2D_2^+$ distinguished by its intensity.

The current intensities obtained associated with the presence of these ions exceed the typical intensities obtained for other fragments in this group by three times. In the CD+ group, we again observe an increase in the intensity of individual fragment ions as a function of the electron current. The intensity of the current associated with fragmented ions CD^+ is distinguished for the remaining elements of this group and is almost twice as high as that obtained for the remaining fragments in this group. The last graph (Fig. 10 on the right) shows the influence of intensity of the electron beam on the obtained intensities of unbound carbon ions (with different charge states).

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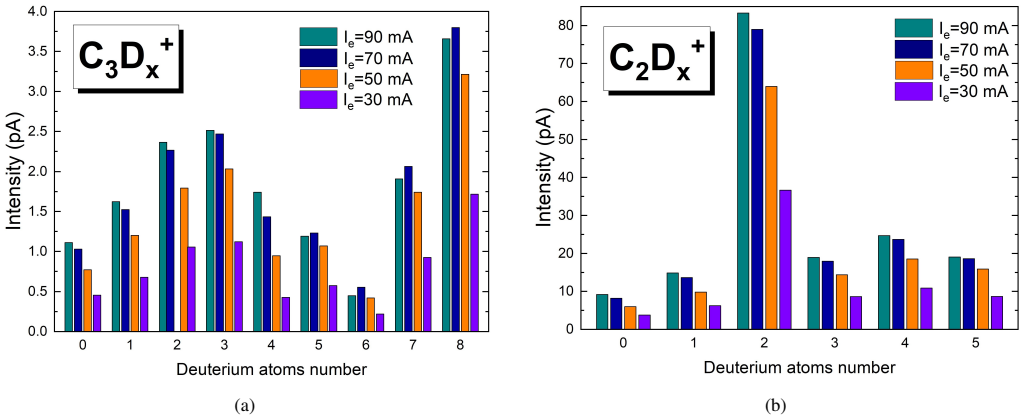

Fig. 9. Influence of the electron current on the intensity of individual molecular ions in the $C_3D_x^+$ (left) and $C_2D_x^+$ (right) groups, $E_e = 15$ keV and $p = 6 \times 10^{-9}$ mbar.

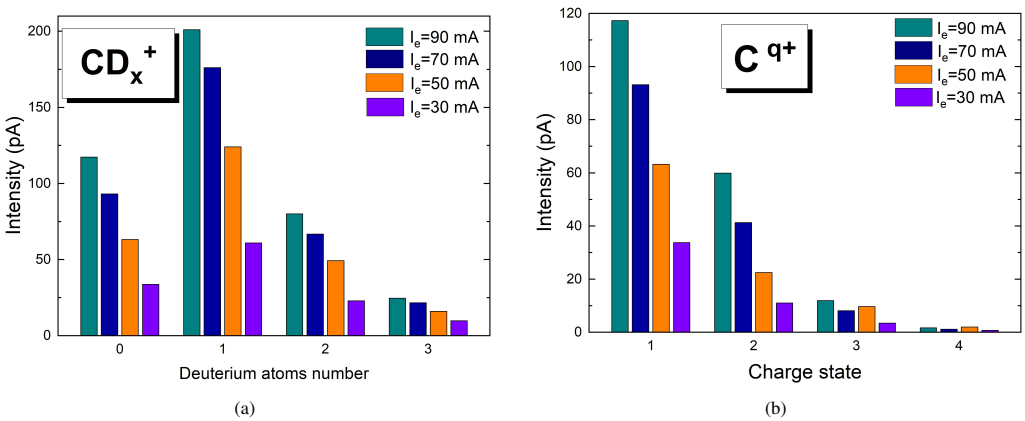

Fig. 10. Influence of the electron current on the intensity of individual molecular ions in the CD_x^+ group (left) and on the observed intensity of various charge states of carbon C^{q+} (right), $E_e = 15$ keV and $p = 6 \times 10^{-9}$ mbar.

The intensity of the ion current decreases rapidly as the charge state increases. For charge states $q = 1$ and $q = 2$, we see an increase in the intensity of the ion beam current as the electron current increases. However, this relationship is disturbed for the C^{3+} and C^{4+} ions.

After a detailed analysis of the spectra, the intensity of the lines of the groups $C_3D_x^+$, $C_2D_x^+$ and CD_x^+ was studied for four different electron beam currents $I_e = 30$ mA, 50 mA, 70 mA and 90 mA and for the constant pressure value of 1.2×10^{-8} mbar. Exemplary intensity ratios for selected molecular ions measured for beam currents of 90 mA and 30 mA are shown in Fig. 11. The measurements were performed at an electron energy of 15 keV.

The intensities of the extracted fragments of the deuterated propane molecule at a gas pressure of 1.2×10^{-8} mbar for the 90 mA electron beam intensity are about 3–7 times higher than in the case of the 30 mA electron beam current. The authors of the study [1], examining such a relationship for propane gas, obtained values 2.5–7. Interestingly, in this case, the component ($C_3D_x^+$) with four deuterium atoms is much more intense than the others in this group (contrary to the previous case).

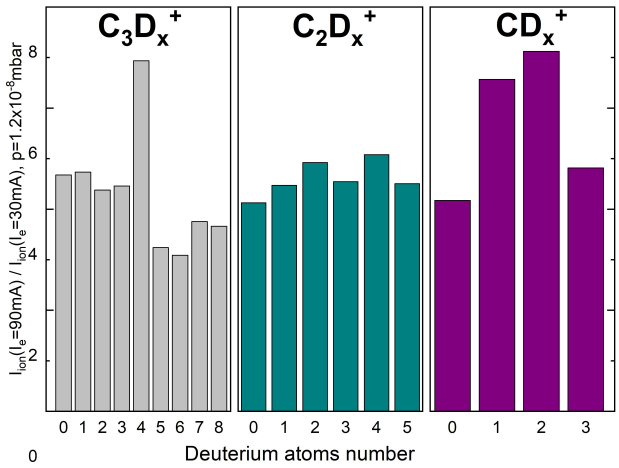

Fig. 11. Effect of the change in electron beam current I_e on the intensity of the peak of a given fragmentation ion in the mass spectrum. Individual bars express the ratio of the intensity of the given peak in relation to the electron current ratio: 90 mA/30 mA at a given pressure equal to 1.2×10^{-8} mbar. The measurements were performed at an electron energy of 15 keV.

4. Theoretical calculations

Quantum chemical calculations were performed to confirm the experimental results. The structural parameters of the C_3D_8 were first optimised using several approaches based on the wavefunction and the density functional theory. The final optimised geometry was calculated at with a second-order Møller–Plesset perturbation theory (MP2) using a correlation-consistent polarised basis set of Dunning (cc-pVTZ) [17]. The electronic structure calculations were performed using the Gaussian 16 software package [18]. The Quantum Chemical Mass Spectrometry (QCxMS) method, recently proposed by Grimme [19, 20] in order to automate the particle–molecule mass spectra calculation for small molecules was applied. It combines elements of statistical theory with *molecular dynamics* (MD) and enables the calculations of EI with the computed charge assignments on the resulting spectrum. A comparison of the computed EI mass spectra with the experimental spectra reveals that QCxMS is able to predict some of the main peaks correctly, while other peaks are missing or their intensities are too small compared to the experiment. Explaining the significant discrepancies observed between the experimental and simulation results requires further detailed analyses, which are currently in progress.

5. Conclusions

In this article, we described an experiment whose aim was to determine the effect of ion source parameters (Dresden EBIT-A) for the high electron beam energy E_e = 15 keV on the process of fragmentation of deuterated propane molecules (C_3D_8). By selecting suitable parameters for trapping the molecules, extracting, and guiding the fragmentary ion beam, we were able to obtain a measurable signal on FC(B). A magnetic dipole was employed for the process of mass separation, resulting in the acquisition of a comprehensive mass spectrum. Within this spectrum, all potential fragments of the $C_3D_8^+$ molecular ion were clearly identified. Detailed analysis of the spectrum also revealed the presence of fragmentation ions formed from the $C_3H_8^+$ molecular ion, likely resulting from the limited purity of the working gas. Additionally, residual gases and highly-charged xenon

remnants were detected in the mass spectrum. The intensities of individual peaks in the spectrum were measured and compared for different ionisation conditions in the EBIS-A. These conditions included different pressures of the molecular gas and electron beam currents. Based on these investigations, it was observed that the intensity of individual fragmentation peaks in the $C_3D_x^+$, $C_2D_x^+$, CD_x^+ groups exhibited a proportional increase in response to pressure changes within the range of 3×10^{-9} mbar to 1.5×10^{-8} mbar. A similar proportional increase was observed for carbon in different charge states. Notably, the $C_2D_2^+$ fragmentation peak demonstrated a rapid increase in intensity with changes in both pressure and electron beam current. The electron current significantly affects the intensity of the fragment ions, with notable differences depending on the type of ions. Some ions exhibit saturation of intensity at higher current values, while others show a consistent increase in intensity as the current increases. Characteristic fragments such as $C_2D_2^+$ and CD^+ stand out with significantly higher intensity values within their groups. These observations highlight the complex relationship between the parameters of the electron beam and the characteristics of the resulting fragment ions. In conclusion, the conducted experiments allowed us to determine the possibilities of the EBIS-A ion source in the context of molecular fragmentation studies, and the obtained results will be helpful for other groups using a similar device.

Additionally, preliminary quantum chemical calculations were performed using the density functional theory and MP2 methods. These results, obtained using quantum chemical mass spectrometry (QCxMS), provide valuable insight into the mechanisms of C3D8 fragmentation under high-energy electron impact compared to experimental data. Although some discrepancies remain, the combined approach demonstrates the potential of EBIS-based ion sources for detailed molecular fragmentation studies.

The experimental and theoretical results obtained will allow us to plan more complex experiments in which fragmentation of molecules in the EI process for high electron beam energies will be studied.

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References

[1] Kreller, M., Zschornack, G., Kentsch, U., & Heller, R. (2008). Molecule fragmentation at the Dresden EBIS-A. *Review of Scientific Instruments*, *79*(2). https://doi.org/10.1063/1.2804864

[2] Currell, F., & Fussmann, G. (2005). Physics of electron beam ion traps and sources. *IEEE Transactions on Plasma Science*, *33*(6), 1763–1777. https://doi.org/10.1109/tps.2005.860072

[3] Shirkov, G. D., & Zschornack, G. (1996). Electron Beam Ion Sources. In *Electron Impact Ion Sources for Charged Heavy Ions* (pp. 90–122). https://doi.org/10.1007/978-3-663-09896-6_4

[4] Zschornack, G., Schmidt, M., & Thorn, A. (2013) Electron Beam Ion Sources. *CAS – CERN Accelerator School : Ion Sources (pp.* 165–201). https://doi.org/10.5170/CERN-2013-007.165

[5] Kęcki Z.This work was co-financed by the Minister of Science of the Republic of Poland under the ”Regional Excellence Initiative” programme (project no.: RID/SP/0015/2024/01). The functioning of the

facility is supported by the Polish Ministry of Education and Science (project 28/489259/SPUB/SP/2021). The calculations were performed at Gdańsk University of Technology and the Academic Computer Centre in Gdańsk (CI TASK). (2013). *Fundamentals of Molecular Spectroscopy*. PWN Scientific Publishers

[6] Anbar, M., & Aberth, W. H. (1974). Field ionisation mass spectrometry: a new tool for the analytical chemist. *Analytical Chemistry*, *46*(1), 59A–64A. https://doi.org/10.1021/ac60337a712

[7] Dass, C. (2006). *Fundamentals of Contemporary Mass Spectrometry*. https://doi.org/10.1002/0470118490

[8] Gross, J. H. (2011). Mass spectrometry. In *Springer eBooks*. https://doi.org/10.1007/978-3-642-10711-5

[9] Lattimer, R. P., & Schulten, H. R. (1989). Field ionisation and field desorption mass spectrometry: past, present, and future. *Analytical Chemistry*, *61*(21), 1201A–1215A. https://doi.org/10.1021/ac00196a001

[10] Huang, Z., Jiang, Y., Dai, X., Zhou, M., & Fang, X. (2024). Improving the efficiency of soft electron ionisation by using the oscillatory movement of electrons. *Metrology and Measurement Systems*, 31(2), 353–367. https://doi.org/10.24425/mms.2024.149696

[11] Wei, F., Huang, Z., Dai, X., Fang, X., & Jin, S. (2023). Quantitative analysis of reaction gases or exhaust using an online process mass spectrometer. *Metrology and Measurement Systems*. 32(2) 337–352. https://doi.org/10.24425/mms.2023.144874

[12] Dantus, M. (2024). Tracking Molecular Fragmentation in Electron–Ionisation Mass Spectrometry with Ultrafast Time Resolution. *Accounts of Chemical Research*, *57*(6), 845–854. https://doi.org/10.1021/acs.accounts.3c00713

[13] This work was co-financed by the Minister of Science of the Republic of Poland under the "Regional Excellence Initiative" programme (project no.: RID/SP/0015/2024/01). The functioning of the facility is supported by the Polish Ministry of Education and Science (project 28/489259/SPUB/SP/2021). The calculations were performed at Gdańsk University of Technology and the Academic Computer Centre in Gdańsk (CI TASK). Dreebit, *Instruction Manual for Ion Irradiation Facility L*. Version: 1.0.

[14] Banaś, D., Braziewicz, J., Semaniak, J., & Pajek, M. (2010). The physics program at the Kielce EBIS-A facility. *Journal of Instrumentation*, *5*(09), C09005. https://doi.org/10.1088/1748-0221/5/09/c09005

[15] Banaś, D., Jabłoński, Ł., Jagodziński, P., Kubala-Kukuś, A., Sobota, D., & Pajek, M. (2014). EBIS-A facility for the studies of X-ray emission from solids bombarded by highly charged ions. *Nuclear Instruments and Methods in Physics Research. Section B Beam: Interactions with Materials and Atoms*, *354*, 125–128. https://doi.org/10.1016/j.nimb.2014.11.107

[16] McLafferty, F. W., & Turecek, F. (1993). *Interpretation of Mass Spectra*. 4th Edition. University Science Books.

[17] Dunning, T. H. (1989). Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *The Journal of Chemical Physics*, *90*(2), 1007–1023. https://doi.org/10.1063/1.456153

[18] Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H. & at al., *Gaussian 16 and Revision C.01. Gaussian and Inc. and Wallingford CT*. https://gaussian.com/gaussian16/

[19] Grimme, S. (2013). Towards first principles calculation of electron impact mass spectra of molecules. *Angewandte Chemie International Edition*, *52*(24), 6306–6312. https://doi.org/10.1002/anie.201300158

[20] Bauer, C. A., & Grimme, S. (2016). How to Compute Electron Ionisation Mass Spectra from First Principles. *The Journal of Physical Chemistry A*, *120*(21), 3755–3766. https://doi.org/10.1021/acs.jpca.6b02907

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