Report on the Outcomes of a Short-Term Scientific Mission[1]

Action number: CA20129 Multichem

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Details of the STSM

Title: Electron Beam Irradiation-Induced Dissociative Electron Attachment in Benzothiophene and Dibenzothiophene.

Start and end date: **27/07/2025** to **09/08/2025**

Description of the work carried out during the STSM

The initial working plan and the mission of the STSM were successfully achieved within the scheduled period. Upon arrival at the host institution, I began my work by visiting several laboratories within the Department of Dynamics of Molecules and Clusters at J. Heyrovsky Institute of Physical Chemistry. This initial tour provided valuable insights and significantly impressed me, particularly in highlighting the interdisciplinary nature of modern scientific research. During the STSM, we conducted mass spectrometric studies of benzothiophene, dibenzothiophene, their homogeneous clusters, and clusters with water. The mass spectra were obtained at various energies, including 1.5 eV and range from 0 eV to 10 eV for negative ions and 70 eV, and range from 6 eV to 26 eV, and from 5 eV to 75 eV for positive ions. Throughout the experiments, background spectra were systematically acquired each time there was a change in experimental parameters such as the electron energy, the ion polarity (positive or negative), or the molecular system under investigation (including clusters). This ensured accurate and reproducible data acquisition across all measurements. Over the 14-day period of my stay, I also gained hands-on experience with techniques used to stabilize and promote molecular clustering using inert gases like neon and argon. I became proficient in operating the data acquisition system, converting a series of binary files to ASCII files in Tof50.exe software, and enhancing my understanding of experimental workflow and instrumentation. Furthermore, I had basic training in data analysis techniques using the ELS CLUB software, which allowed us to construct and interpret specialized data matrices

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

Description of the STSM main achievements and planned follow-up activities

Figure 1 presents the mass-to-charge ratio spectra of positive ions of benzothiophene and dibenzothiophene, recorded during interactions with low-energy electrons. We successfully identified and analyzed the resulting ion fragments and clusters. Similarly, we obtained mass spectra for negative ions, including cluster formation at various electron irradiation energies.

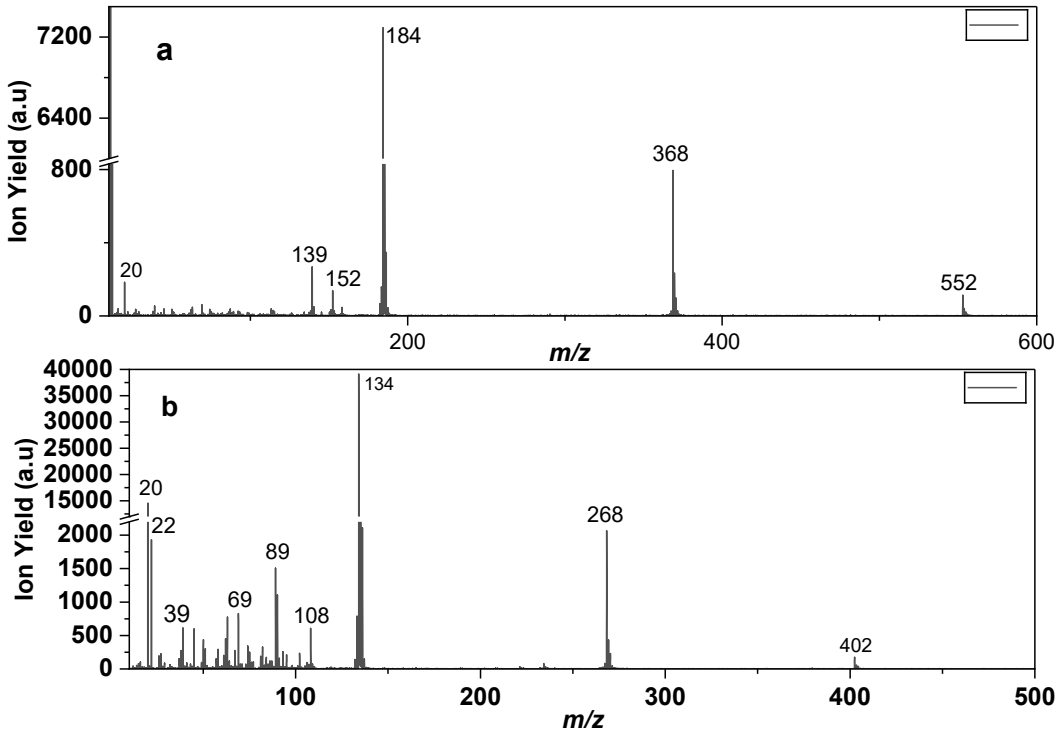

Figure 1. Positive ions mass to charge ratios spectra of benzothiophene (a) and dibenzothiophene (b) at 70 eV electron energy radiation.

In addition to acquiring the mass spectra presented in this report, we initiated analysis of the raw datasets, with particular focus on the mass-to-charge ratios, threshold energies, and energy dependence of the processes. To support this, a matrix of data across a range of electron energies was developed. Although working with ELS CLUB is new to me, I have begun working with the ELS CLUB to investigate energy dependence and threshold energies using the constructed data matrix, using the experience I gained during my stay at the host institution, and I will continue the analysis during the following months

The next step is to complete all the data analysis and prepare a manuscript for publication. Publishing the findings is one of the key objectives of our COST Action group, as disseminating results through peer-reviewed articles ensures a broader impact and contributes to the efficient transfer of fundamental knowledge, particularly in alignment with the objectives of the Working

Group (WG3) of the MultiChem Action. Electron-induced fragmentation data for benzothiophene and dibenzothiophene directly contribute to the objectives of Working Group (WG1), which aims to achieve a fundamental understanding of irradiation-driven chemical transformations under various types of radiation.

We also intend to compare the results obtained during this STSM with complementary experiments conducted at the Laboratory of Experimental Physics (Plasma Physics Group) at Comenius University. This comparative analysis will further strengthen the mission of the STSM by promoting the exchange of knowledge and technological capabilities between research groups. Additionally, the preliminary data analysis shows a possible trend in the thiophene to dibenzothiophene sequence and therefore, we plan to extend the study of the thiophene molecule shortly.

Finally, I plan to present the outcomes of this STSM to my colleagues and the research group at Comenius University to promote internal knowledge sharing and foster further collaboration. Based on the data collected and our preliminary analyses, we believe that our study of electron beam irradiation-induced dissociative electron attachment in benzothiophene and dibenzothiophene will make a meaningful contribution to the scientific community and relevant research databases.