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

Action number: CA21126

Grantee name: Dariusz Piekarski

Details of the STSM

Title: Electron induced reactivity in the ionized clusters of triazole derivatives.

Start and end date: 03/06/2024 to 11/06/2024

Description of the work carried out during the STSM

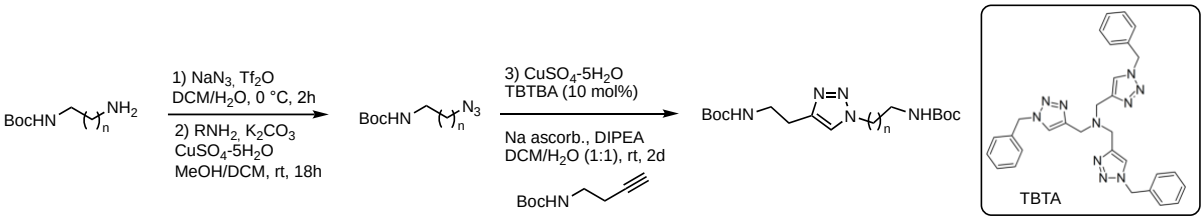


Fig.1. The steps of synthesis of and the structures of NHBoc triazole derivatives for n = 1, 3 and 5, the target molecules are named **1**, **2** and **3**, respectively (prepared by O. García Mancheño).

During the STSM stay we measured time-of-flight spectra of three targets: **1, 3** (see Fig.1.) and 1-OH-benzo-1,2,3-triazole. The slow, and 70 eV electrons were used to ionize the aforementioned molecules, as well as its clusters and nano-solvated water clusters. We checked the temperature effects by slowly heating the samples from RT to 200 Celsius to obtain a good signal-to-background ratio in the fragmentation mass spectra. I had a hands on experience with tuning also other molecular beam parameters, which will be crucial for the development of a similar source in my home laboratory. For example, we tuned the position of the expansion nozzle with respect to the first skimmer (x,y,z directions), the pressure of carrier gases Ne and He (1-3 bars), the position of the deflection planes of the time-of-flight for compensating the kinetic energy gain along the molecular beam axis, the temperature of the nozzle, delay in the extraction pulse and many others. Changing these parameters allows us to improve the signal-to-background ratio. For 1-OH-benzo-1,2,3-triazole, we recorded a strong signal of m/z=17, which was observed in the broad temperature screening (T=140-175). However, even heating up to 199 Celsius did not result in a measurable signal of the parent molecular ions in the spectrum, while the OH signal already disappeared. After opening we found out that the sample was decomposed (black solid state sample) and we concluded that the measurements in the present configuration of the experiment would not be possible.

For 1,3 NHBoc triazole derivatives, we reached measurable signals, even though we needed to heat the samples up to a minimum temperature of 160 Celsius to gain enough signal. In total we recorded approx. 100 spectra including both, fragmentation mass spectra and energy-dependent ion yields for negative ion fragmentation upon

[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.

interaction with low energy electrons (0 to 12 eV) and positive ion fragmentation upon interaction with high energy electrons (5-85 eV).

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

During my STSM stay at Heyrovsky Institute we were able to study the interaction of both low and high energy electrons with two freshly synthetize molecular targets **1** and **3** and 1-OH-benzo-1,2,3-triazole. For these species, we observed charged fragments after single ionization for single molecule and small molecular clusters (dimer and trimer) as well as nano-solvated water clusters. The preliminary spectra are shown in Fig.2.

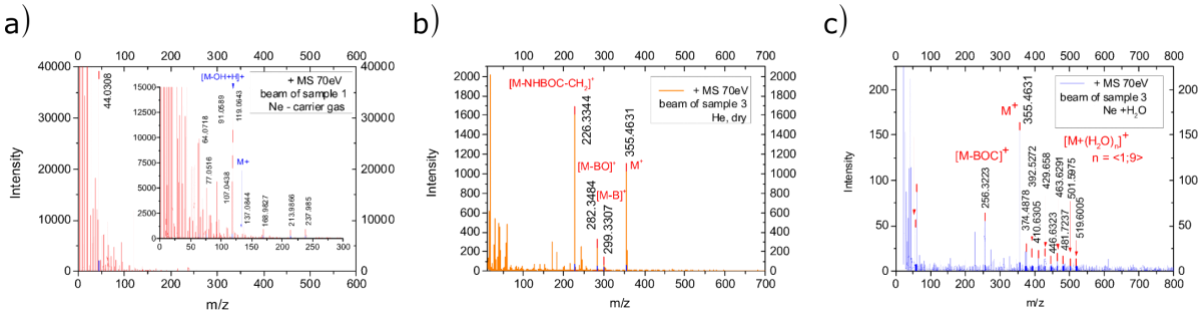


Fig.1. The mass spectra recorded at 70 eV electrons for a) 1-OH-benzo-1,2,3-triazole, b) molecular target **1**, and its c) nano-solvated water clusters.

The aforementioned molecules were challenging targets to introduce to the gas-phase with the current molecular beam generator that operates at high pressures of the expansion gas at CLUB set-up. Moreover, there is no data at NIST to compare with. Thus, the heating procedure was slow and time-consuming to assure that there is no thermal decomposition of the samples.

These results of the experiment will be analysed in detail in the next months and the theoretical calculations are running to understand the experiments and explain the mechanisms of the formation of the observed fragments. We agreed to further collaborate including experiments for the DEA and 70 eV electron collisions with clusters of 1,2,3-triazole and nanosolvated water clusters. It was a great experience and opportunity to visit Heyrovsky Institute, start fruitfully collaboration with Jaroslav Kočišek and Jozef Rakovský, and enjoy the scientific discussion with Juraj Fedor, Pamir Nag, Vitek Svoboda and Michal Farnik. The visit of Jozef Rakovský is planned at Institute of Physical Chemistry, Polish Academy of Sciences in the near future to collaborate on the development of the fs laser induced cross-beam set-up. It will be very helpful to compare the results obtained after electron vs. laser induced fragmentation of much simple targets like 1,2,3-triazole derivatives. A series of joint publications are planned.