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Innsbruck, 09th May 2022

Beneficiary: Farhad Izadi, Universität Innsbruck (AT)

Host: Dr. Jaroslav Kocisek, J. Heyrovsky Institute of Physical Chemistry Dolejskova 3, 18223 Prague 8, Czech Republic (CZ)

Period: from 24/04/2022 to 08/05/2022

Place: Prague 8, Czech Republic (CZ)

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SCIENTIFIC REPORT

PURPOSE OF VISIT

Sanazol (AK-2123) is a hypoxic radiosensitizer and is specifically used in the treatment of stage III cervical cancer. In the other hand, 2-bromo-1-(3,3-dinitroazetidin-1-yl)ethan-1-one (RRx-001), is a NO donor and has been studied in hypoxic tumors. Since reduction of the agents in cells may be a relevant process, knowledge about the reactions of free low-energy electrons (LEEs) with these compounds is crucial. It is unknown to what extent and by what mechanism LEEs may contribute to the action of electron-affinic radiosensitisers used in hypoxic tumor radiotherapy. Therefore, the findings of dissociative electron attachment to sanazol and RRx-001 in the gas phase will provide relevant information about the possible fragmentation pathways and mechanisms of anion formation upon DEA. The information gained in these experiments, we studied electron attachment to the title compounds at micro-hydrated conditions in order to gain knowledge about the effect of molecular environment on the electron attachment. The study has been carried out in cooperation with Dr. Jaroslav Kocisek at the Heyrovsky Institute of Physical Chemistry, Department of Dynamics of Molecules and Clusters, in Prague, Czech Republic, from 24th of April 2022 until 8th of May for two weeks. The aim of the present STSM to the Institute was to perform mixture of humidified buffer gas and the compounds, M (Sanazole or RRx-001), resulting in the formation of $M(H_2O)_n$ clusters then all anions will be analysed with each extraction pulse and recorded as mass spectrum at variable electron energies.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

During this STSM, it was possible to study electron attachment and electron ionization to the title compounds (Sanazole and RRx-001) at dry, low and high micro-hydrated conditions with the CLUster Beam (CLUB) apparatus in order to gain knowledge about the effect of molecular environment on the positive electron ionization mass spectrum (Fig. 1). Anion mass spectra for both compounds at different hydration conditions are depicted in Figure 2. So $M(H_2O)_n$, has been observed. The anion formation has a resonant character as can be seen from Figure 3, which shows electron energy dependent ion yields. Therefore, we are showing cumulative

spectra, which are obtained by summing individual spectra taken at different energies. The top panel of Figure 2, left, represents “dry” conditions when pure Helium, without humidification, was used as a buffer gas as well as Figure 2, right, related to pure Neon used as a buffer gas.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

RRx-001 compound has been measured in the CLUB setup and the energy integrated mass spectra, energy-mass matrices, peak intensities, and DEA spectra have been taken which we used helium and neon gas that humidified by a Pergo gas humidifier, to produce clusters.

Regarding Sanazole, signal and background mass spectra with Helium and Neon buffer gas (hydrated) have been measured in negative mode signal and background mass spectra at 2.0 and 3.0 eV beside positive mode signal and background mass spectra at 70 eV and DEA spectra which all were hydrated.

FUTURE COLLABORATION WITH HOST INSTITUTION

The mission also served to exchange and expand knowledge between the two laboratories, where a strong and particularly fruitful collaboration has been established between Innsbruck and Prague. In addition to the measurements obtained during this visit, will hopefully result in a joint publication to be submitted to an international peer review journal.

Innsbruck, 09th May 2022

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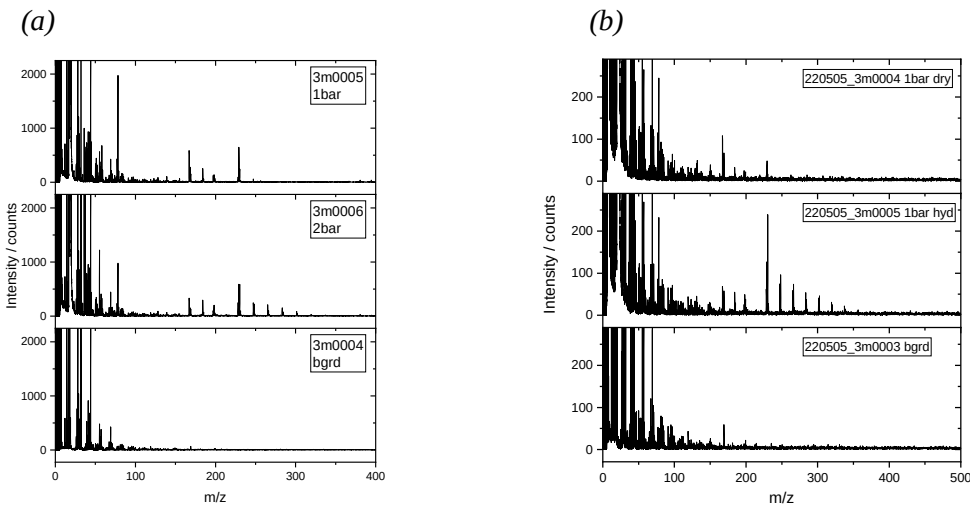

Fig. 1. Positive mode signal and background mass spectra at 70 eV. All hydrated. (a) and Positive mode signal and background mass spectra at 70 eV (b) for Sanazole compound.

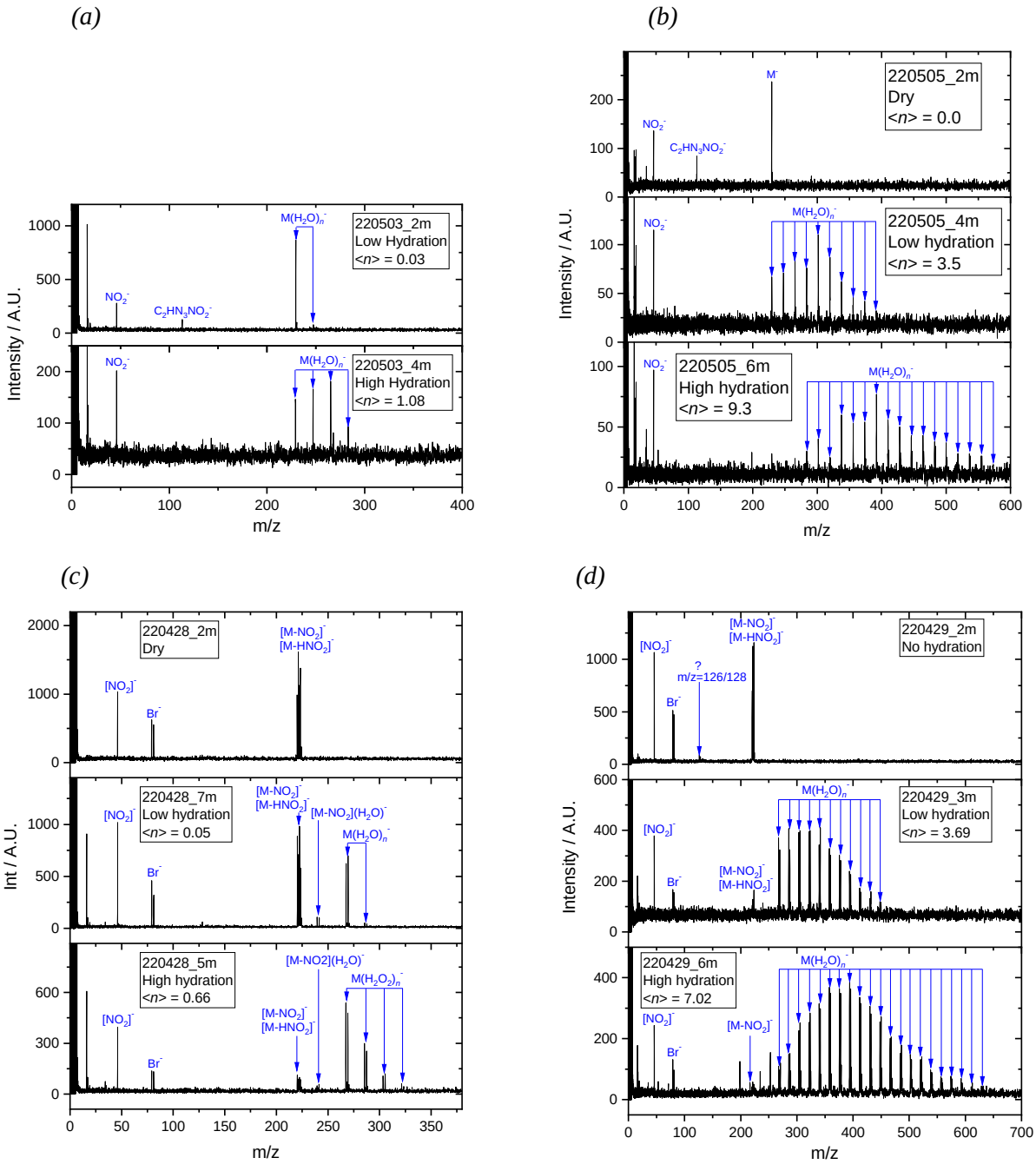

Fig. 2. Negative ion mass spectra to the compound Sanazole which Helium (a) Neon (b) buffer gases.

Negative ion mass spectra to the compound RRx-001, Helium (c) Neon (d) buffer gases. Both compounds measured in the conditions dry, low hydration and high hydration.

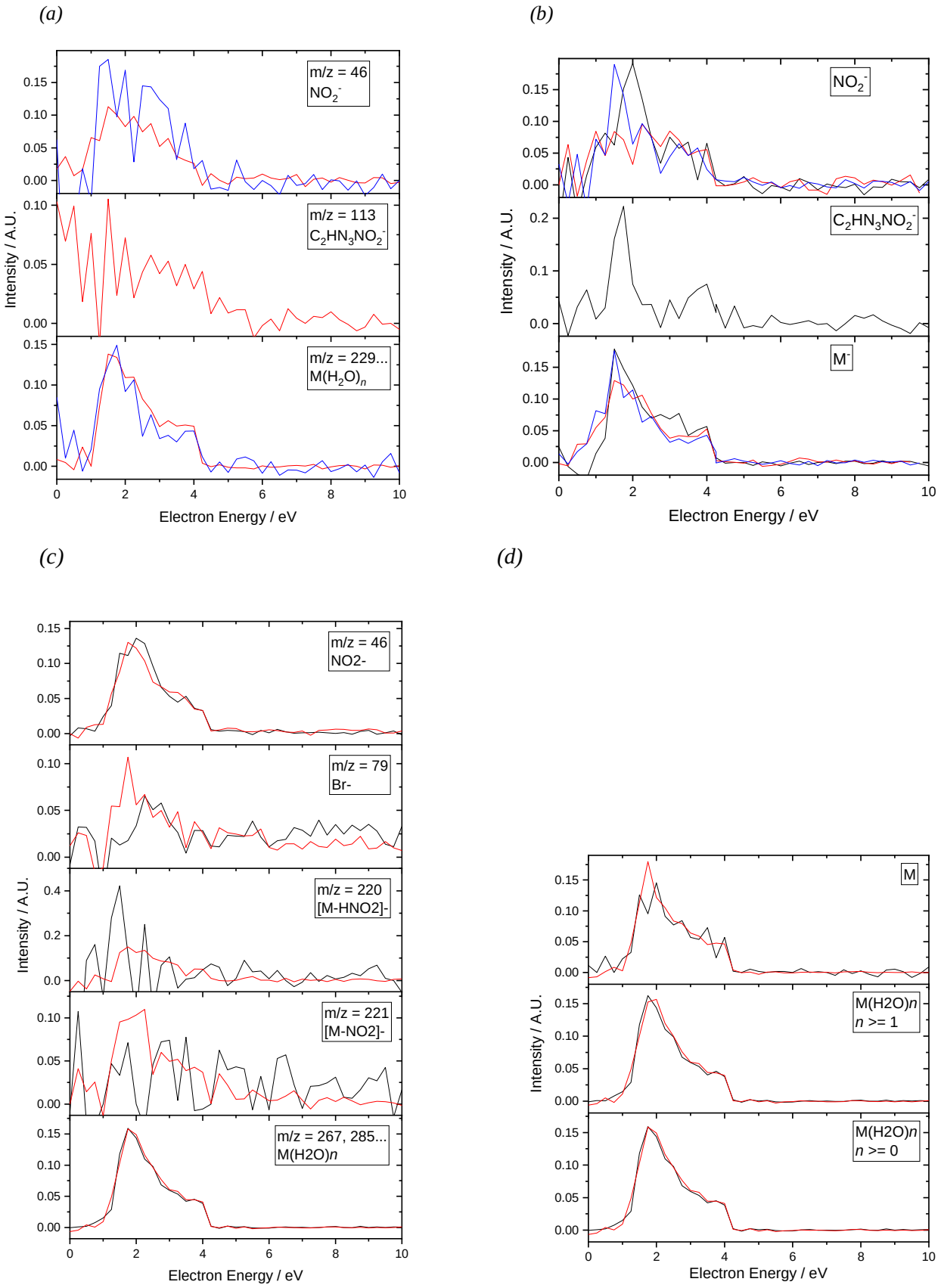

Fig. 3. DEA spectra to the Sanazole anion fragments m/z 46 and 113 besides parent anion m/z 229 thus Helium (a) and Neon (b) as seed gases. Black line represents dry condition as well as red line low hydration and blue for high hydration.

In addition, DEA spectra to the RRx-001 DEA spectra for the most intense species, which black line represents high hydration and red for medium hydration (c) and DEA spectra of the parent ion, both dry and hydrated(d).