

Report on THE ROLE OF LOW-LYING ELECTRONIC STATES IN AMINOPHENOL COMPOUNDS

I was part of an experimental team along with Prof. Paulo Limao-Vieira's group (University of Lisbon) in the Centre for Storage Ring Facilities (ISA) in Denmark from 20th – 26th February 2017. The original aim was to perform VUV photoabsorption experiments of 3-aminophenol to better understand the electronic excitation and ionisation processes aimed to support the interpretations of our previous multi-photon ionisation experiments performed at The Open University in Milton Keynes.

Unfortunately, due to low vapour pressure of 3-aminophenol (even at the maximum temperature of Aarhus experiment) and high water contamination of the sample, the photoabsorption spectra were mainly dominated by water absorption which prevented us from successfully carrying out the photoabsorption experiments on 3-aminophenol. Therefore, we changed focus of our experiments to pyrazine (1,4-diazabenzene), a benchmark system in photochemistry for more than 60 years, and catechol (1,2-dihydroxybenzene) which is a molecule involved in cultivation being a precursor to pesticides as well as naturally present in fruits and vegetables. To the best of our knowledge, there is a lack of VUV photoabsorption studies on catechol and all of the previous VUV photoabsorption measurements on pyrazine in 110-330 nm range were performed with lower resolution especially in the low energy part of the above-mentioned range.

I am very grateful to the Sir John Mason Academic Trust for the financial support which allowed me to carry out the experiments at ISA in Denmark. Although the initial plan to obtain VUV photoabsorption spectra of 3-AP could not be accomplished due to the above-mentioned reasons, I consider the stay at the synchrotron facility to be a really valuable experience for me for the following reasons:

1. I have deepened my knowledge in valence and Rydberg excited state spectroscopies from a highly respected expert in the field: Prof. Limao-Vieira. Furthermore, I have gained experience and learned a lot about the experimental setup from Dr. Jones, who is in charge of the UV beamline.
2. Complications associated with the 3-AP measurements made me think about and understand the mechanisms and limitations of the experiments much deeper, which I exploited directly when doing measurements on catechol (also

contaminated with water, however a bit higher vapour pressure allowed us to do the measurements).

3. In view of our unsuccessful experiments on 3-aminophenol, we have devised a new strategy to study the molecule's electronic excited states. This involves UV absorption measurements in solution (at the OU) and calculations by Prof. Limao-Vieira's collaborator Dr. Duflot, as well the possibility of future gas-phase measurements using a high-temperature system at the University of Aarhus (built for circular dichroism experiments and currently being tested).
4. I had an opportunity to work within a research team at an international research facility and build contacts with scientists in related research areas which is invaluable for me as a young researcher in the field.
5. We have successfully performed photoabsorption measurements on pyrazine and catechol, which will be analysed in cooperation with Prof. Paulo Limao-Vieira's group and reports on these measurements will be published in peer-reviewed journals.

Thank you very much for your support in my studies.

Best regards,

Jana Bocková