**University of Leicester**

**Chemistry GTA Studentship Project 2022**

**Section 1 – *Supervisor Information***

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| **First Supervisor (Name and Title)** | Professor Andrew M. Ellis |
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**Section 2 – *Project Information***

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| **Project Title** | Energetic processing of polyaromatic hydrocarbons in interstellar space | |
| **Project Highlights:** | 1. | Using helium droplets to combine polyaromatic hydrocarbons with small molecule, and especially H2, CO and H2O, and explore their ion chemistry initiated by electron ionization. |
| 2. | Identify spectroscopic signatures and structures of PAH cations tagged with small molecules, in order to elucidate their possible contribution to unidentified IR bands (UIRBs) in the interstellar medium. |
| 3. | Correlate the findings with UIRB data. |
| **Project Overview** | | |
| The source of the unidentified infrared bands (UIRBs) in the interstellar spectrum is a longstanding puzzle in astrochemistry [1,2]. It is thought that polyaromatic hydrocarbons (PAHs) are responsible for many of the UIRBs but no assignment to specific PAHs has proved possible. This may be the consequence of the combination of the PAH with other molecules in space and/or the processing of those PAHs by energetic collisions (photons, electrons, ions), leading to long-lived intermediate ionic products.  This project aims to tackle both of the above challenges. Phase 1 will focus on the energetic processing of PAHs, both alone and tagged with molecular species. This will be carried out jointly with collaborators at the Centre of Astrophysics and Planetary Science at the University of Kent (Dr Jon Tandy and Prof. Nigel Mason) but will primarily be using facilities here at UoL (see below). This study will focus on small PAHs, both alone and in combination with abundant molecules in the interstellar medium (ISM), and particularly H2, H2O and CO. Essentially, complexes between a PAH and the respective small molecule will be pre-formed in a helium droplet and then subjected to energy injection by electron ionization of the helium droplet. The resulting positive ions will be ejected into the gas phase and can be detected using mass spectrometry. The real strength of this approach is the ability to bring the PAH and the small molecule into contact and at low temperature prior to energy injection, mimicking the situation in the ISM.  In the second part of the project, we will use IR spectroscopy to identify ionic products from the above energetic processing to see how these fit with the UIRBs. The technique needed to do this is described below and has been developed in our laboratory in the past couple of years [3,4].  We are looking to support this project through a Leverhulme Trust project grant application in 2022, but can cross-subsidise the consumables element from existing grants (EPSRC, LT) in the event of this being unsuccessful. | | |
| **Methodology** | | |
| The methods required for this work are already established in our laboratory. We are equipped with two helium nanodroplet systems for this type of work, one of which can be dedicated to the mass spectrometry experiments while the other will be used for the IR spectroscopy. Adding a PAH to a helium nanodroplet requires evaporation at high temperature but we have this capability. The experiment is designed so that molecules can be added sequentially to make complexes inside the droplets and they are then subjected to electron ionization, which initially generates a He+ ion. This ion can roam the droplet and when it finds the dopant complex it transfers over the positive charge along with energy, typically 10-15 eV, which is sufficient to initiate chemistry and so mimics the energetic processing in the ISM.  A similar approach will be used for the IR spectroscopy but there we explore the ionic products by illuminating them with IR radiation from a laser. By selecting the appropriate ion mass, we can record the IR spectrum of a specific ion at low temperature, mimicking the ISM (where the temperature is often close to 10 K | | |
| **Further Reading:** | 1. PAH Products and Processing by Different Energy Sources, G. A. Cruz-Diaz, S. E. Erickson, E. F. da Silveira, A. Ricca, A. L. F. de Barros, C. A. P. da Costa, R. C. Pereira, A. L. Mattioda, *Astrophys. J.* **882**, 44 (2019).  2. Effect of molecular structure on the infrared signatures of astronomically relevant PAHs, J. Bouwman, P. Castellanos, M. Bulak, J. Terwisscha van Scheltinga, J. Cami, H. Linnartz, A. G. G. M. Tielens, *Astron. Astrophys*. 621, A80 (2019).  3.“Infrared Spectroscopy of a Small Ion Solvated by Helium: OH Stretching Region of HeN-HOCO+ ”, J. A. Davies, N. A. Besley, S. Yang, A. M. Ellis, *J. Chem. Phys.* **151**, 194307 (2019).  4.“Probing Elusive Cations: Infrared Spectroscopy of Protonated Acetic Acid”, J. A. Davies, N. A. Besley,S. Yang, A. M. Ellis, *J. Phys. Chem. Lett.* **10**, 2108-2112 (2019). | |