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

Action number: CA21126

Grantee name: Ransel Barzaga Guzmán

Details of the STSM

Title: Exploring the IR spectra of PAH-C60 adducts from indene and pentacene: Neutrality vs Charge

Start and end date: 23/07/2026 to 04/08/2026

Description of the work carried out during the STSM

During this STSM, Dr. Ransel Barzaga visited the High Field Magnet Laboratory and Free Electron Lasers for Infrared eXperiments (HFML-FELIX) as part of the beamtime granted from this institution, as part of a competitive call. Samples of PAH-C60 adducts from indene and pentacene were measured under two different experimental setups in order to obtain them in the form of neutral or charged species. Mass spectrometry (MS) was used to track-down the presence of the species and to follow any possible fragmentation routes. Although this required an ion-trap coupled to the mass spectrometer, something that was not available in the setup for neutral species. Consequently, only the fragmentation routes of the PAH-C60 adducts were carried out for the charged species. In this case it is possible to select a specific ion fragment to induce further fragmentations. Exploring the complex path of induced fragmentations allowed us to know whether or not the PAH-C60 adducts breakdown produced any new high reactive species. Once the conditions for the fragmentation routes were stable, we proceeded to measure the infrared (IR) spectrum of the selected species with FELIX. Here it is worth noting, that the IR spectrum can be measured at specific MS signals for all the cases either neutrals or charged. Furthermore, using the ion trap to choose the desired fragments we also recorded the IR spectrum in these specific species. Since all the species were produced under Ultra High Vacuum (UHV) conditions, FELIX measurements guaranteed that IR spectra lacked the matrix effect contributions typically observed in standard-solid state (pellets) IR data.

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[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

The main achievements of the STSM were the identification of the short lifetime of the PAH-C60 adducts under the laser conditions. According to our results it would be necessary less harsh conditions in order to the adduct species to survive. MS data showed that, although the PAH-C60 adducts were present, they were very unstable lasting a very short-time (less 1 min). The former was only observed in the case of charged species, whose experimental setup had a higher sensitivity. In fact, PAH-C60 adducts from pentacene proved to be the best sample to record the data with MS signals of very low intensity. Under these problems, the record of IR spectra with FELIX was hinder by the lifetime span of the PAH-C60 adducts, consequently we were unable to obtain an accurate IR spectrum. Due to the fact that laser conditions were unfavorable, we instead used FELIX to get insight in the proper conditions for these types of samples. Our findings suggested that it is appropriate to initially measure the UV spectra of these species to know with certainty which are the correct excitation conditions. In addition, we find out that as a second strategy the PAH-C60 adducts could be directly produced inside the UHV chamber by ionizing first C60 and then adding the PAH (pentacene) in Ar-flux. Assuming this approach could be second choice, although it would be only available for the charged species setup, for the case of the neutral ones a different strategy will be followed that still requires further study. Since in this STSM non-accurate IR spectra were obtained, we consider that future plans will go in the directions of above-mentioned in situ UHV synthesis of the PAH-C60 adducts. Recording of accurate UV spectra should be another key task moving forward; thus, we also have planned follow-up activities to measure this data in FELIX. Our plan is to cover all the problems that affected our current measurements in a next proposal for HFML-FELIX, including samples with PAH-C60 adducts at different purity which it seems another determinant factor. Nevertheless, our PAH-C60 adducts have been one of the biggest molecular species measured on these conditions, therefore, there are still challenges to be tackled.

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