MEMORIA DE LA ACTIVIDAD TÉCNICA e INVESTIGADORA. ADECUACIÓN.

SUMMARY ON PROPOSED RESEARCH LINES WHERE THE RESEARCHER DEMONSTRATES HIS/HER COMPETENCE

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1. REPORT SUMMARY

TITLE OF MAIN RESEARCH LINE:: *Prebiotic chemistry in interstellar clouds and the role of complex carbon molecules in the interstellar medium*

KEY WORDS: Interstellar Medium: molecular clouds and protoplanetary discs; Synthesis and Spectroscopy of complex carbon molecules : prebiotic chemistry in space

SUMMARY OF MAIN RESEARCH LINE:
My research activity is focused on the study of complex carbon based molecules (polycyclic aromatic hydrocarbons –PAHs- and fullerenes) in the interstellar medium and in the laboratory with the aim to clarify their contribution to interstellar extinction, diffuse interstellar bands, anomalous microwave emission, and **ultimately investigate how in interstellar clouds and circumstellar environments these molecules may lead to the formation of amino acids and other key molecules in the development of life**. I have carried out theoretical and experimental research on the physical and chemical properties of fullerenes (the new pure carbon molecules discovered in 1985) including synthesis and spectroscopy at the laboratory, studied the role of these molecules on the extinction of radiation in the interstellar medium, the origin of diffuse interstellar bands, and on the origin of the recently discovered anomalous microwave emission. I currently work on the characterization of hydrogenated fullerenes (fulleranes) at the laboratory since their properties are so far poorly known, and plan to perform searches in interstellar (diffuse and molecular) clouds to clarify their potential as carriers of several intriguing astrophysical processes. We are studying the role of these molecules in prebiotic chemistry. I have been PI of proposals approved at VLT, 9m HET, 4.2 m WHT and Galileo. As a result,I have searched and for the first time (after 30 yr of multiple efforts in the field) achieved the identification of optical transitions of specific PAHs (naphthalene and anthracene) in a molecular cloud (Iglesias Groth et al. 2008, Ap J Lett; 2010 MNRAS). Now, I aim to extend these searches to other molecular clouds and to more complex PAHs (with more benzenic rings) for which laboratory spectroscopy is already available in conditions resembling the interstellar medium. Laboratory experiments show that PAHs may lead to the formation of prebiotic material in molecular clouds, in particular amino acids. I aim to study prebiotic material in molecular clouds (including searches and understanding of chemical reaction networks in the physical conditions of the medium) and trace their evolution from molecular clouds to protoplanetary disks.

2.- *CANDIDATE'S TRAJECTORY and ADEQUACY to POSITION*

Before I started my research trajectory I spent several years working under contract by the Canarias Government as Physics and Chemistry lecturer for the Secondary School. I carried out my PhD thesis entitled "Physisorption and Photoabsorption of Fullerenes: physical and astrophysical implications " at the Dept. of Fundamental Physics II of the University of La Laguna, where I spent several years as an external collaborator. During the whole thesis period I simultaneously worked as teacher at Secondary level including pre-University courses. Since I defended my PhD thesis (June 2003) I left the teaching activity and focused on research.

In my PhD thesis I developed semiempirical models of the type Hückel and Pariser-Parr-Popper

which I applied to single and multishell fullerenes to compute polarizabilities, dispersion energies and photoabsorption spectra. The fullerenes (a new form of pure carbon) were discovered in 1985 by Kroto and Smalley when they were trying to reproduce the chemistry in the atmospheres of red giant stars (the discovery of this new molecules had far reaching implications recognized with the award of Nobel Prize on Chemistry). In spite of the intensive work on fullerenes in the last two decades their spectroscopic properties were not well known. I studied fullerene molecules with a number of atoms in the range 60-2000. First, I showed that this type of models reproduce correctly the available laboratory information for the arquetype fullerene C60. Then I extended the computations and for the first time obtained photoabsorption curves for larger fullerenes. Iglesias-Groth et al. (2002; J. Chem. Phys 116, 1064; J. Chem. Phys . 118, 7103) and Iglesias-Groth (2004, ApJ 608, L37) present the key results of my research during the pre-doctoral period. The first two papers report computations of polarizabilities and theoretical photoabsorption spectra for icosahedric fullerenes (single and multishell) with more than 90 carbon atoms, and up to 2000 atoms. The last paper showed that single and multishell fullerenes (buckyonions) can explain the most prominent feature of the interstellar extinction curve, the UV bump at 217.5 nm previously ascribed to graphite particles. I showed that the wavelength, width and general profile of the bump is well fitted by the computed photoabsorption cross sections for fullerenes in the range C60 to C2000. I derived a first estimate of the amount of interstellar carbon that could be locked in fullerenes resulting that these molecules and (as I describe later) their corresponding hydrogenated forms could lock as much interstellar carbon as the more extensively studied polycyclic aromatic hydrocarbons (PAHs).

After my PhD thesis I was awarded a post-doctoral contract at Instituto de Astrofísica de Canarias to carry out work for the Instrument Control Center (ICC) of the submillimeter instrument PACS on board the Herschel satellite of ESA. I have participated in the development of the ICC of PACS, specifically developing scripts for the data reduction, as a consequence I have studied the observational techniques in the infrared relevant to this and other instruments, I am experienced with the calibration methods proposed for PACS and with the software packages developed within the PACS Common Science System (PCSS), in particular with those related to the calibration of the instrument and with the decompression of processed data. I had to learn JAVA programming and also that I carried out frequent working visits to the Max Planck Institute for Extraterrische Physics (Munich). I am also experienced with the Herschel Planning Observation Tool (HSPOT) designed to allow the Herschel observers to prepare observations and the associated AOTS. As developer for the PACS ICC I was a member of the Interactive Analysis Group and had to build myself several functions for the numerical treatment of arrays and matrices of more than three dimensions. I produced 14 jython scripts. I was also responsible for a web page for PACS which provides information to the potential users, including observing modes and the access to the key documents and description on how the instrument works, including user libraries and how to manage HSPOT (www.iac.es /proyectos/herschel/pacs). The technical work carried out for the instrument PACS has allowed me a good knowledge of the instrument essential to write competitive proposals for my own research and access to the open time available at the Herschel satellite.

While I was developing this work for PACS, I carried out research on the role of fullerenes and hydrogenated fullerenes in interstellar space. I showed that hydrogenated fullerenes can be carriers of the anomalous microwave emission. This is a new process (discovered the past decade) of emission of radiation (continuum) in the frequency range 10-60 GHz, in some galactic regions is dominant with respect the well known synchrotron and free-free emission processes. In particular, I explored the potential of these molecules to explain the anomalous microwave emission detected by several Cosmic Microwave Experiments and wrote two papers (Iglesias-Groth 2005 ApJ Lett; 2006 MNRAS) showing how this emission in the Perseus molecular complex and in the dark cloud Lynds 1622 could be accounted by electric dipole radiation of hydrogenated fullerenes.

After my Herschel post-doc, I was awarded a contract at IAC to work on the synthesis and spectroscopic characterization of carbon based molecules of astrophysical interest and to carry out the identification of PAHs and fullerene based molecules in interstellar space. I investigated the hydrogenation processes of molecules with a high number of carbon atoms at ambient temperatures first, and then at very low temperatures to resemble the conditions of various phases of the interstellar medium. I have worked on the design and construction of an instrument that allows the synthesis of these molecules and to measure their properties at temperatures approaching the conditions of diffuse, translucent and dark molecular clouds. This work has been carried out in collaboration with Prof. Franco Cataldo (Actinium Research Laboratory in Rome and Catania Observatory). We have produced hydrogenated fullerenes for C60Hn and C70Hn and obtained their spectra in the 190-900 nm range. We also determined their properties at various temperatures and studied their stability and vaporization to gaseous phase. For larger fullerenes, as the C76, C78 y C84, there was no previous results reported in the literature given the difficulty to obtain macroscopic samples. We have worked on their production from fullerites under conditions of Kratschmer-Huffmann, then I investigated their behaviour against corpuscular and gamma radiation and achieved spectroscopic characterization of these fulleranes for the first time. As main achievements I would note the paper on the action of UV photons on hydrogenated fulleranes C60H36 (Cataldo and Iglesias Groth, 2009 MNRAS 400, 291) which shows experimental measurements of the photoabsorption curve that reproduces very well the UV bump of interstellar extinction. We infer that these molecules could lock a significant fraction of the carbon in the interstellar medium (> 10%). In Cataldo, Strazzulla and Iglesias-Groth (2009, MNRAS) we show experimentally how these molecules survive under gamma radiation and estimate survival rates at the interstellar medium. We concluded that hydrogenated fullerenes are among the most robust carbonaceous molecules which can be built in Nature and therefore may have an important role in various unresolved astrophysics problems: remarkably, to understand the interstellar extinction and in particular the origin of the more than 300 diffuse interstellar bands known by spectroscopy for decades but not yet identified the carrier. Our laboratory work is aimed to characterize hydrogenated fullerenes in the optical and infrared as a path to their identification in the interstellar medium. We have recently edited the book "Fulleranes: The Hydrogenated Fullerenes. " (Cataldo and Iglesias-Groth, Springer 2010) where I am co-author of several chapters describing the current stage of research on this new molecules (the book is prologued by Nobel Prize on Chemistry Harold Kroto).

In the last two years I have been very involved in the search and identification of the most simple PAHs in the interstellar medium. Many searches had previously attempted to identify specific transitions of these molecules without much success. My approach was different to previous ones. Assuming that anomalous microwave emission is produced by electric dipole radiation from fast spinning hydrogenated carbon molecules (an idea originally proposed by Draine at Princeton Univ.) I started a search for PAHs in regions of enhanced anomalous microwave emission. I selected the Perseus molecular complex and undertook high resolution spectroscopy of background or embedded stars in the line of sight. The results led to the paper (Iglesias-Groth et al. 2008 ApJ 685, L55) where we report the first identification of naphthalene (the most simple PAH) in the interstellar medium and first observational evidence supporting that PAHs are carriers of the anomalous microwave radiation. I led this research which is a collaboration of our group at IAC and D.L. Lambert (Director of the Dpt of Astronomy of the Univ. of Texas and one of the most reknown stellar spectroscopists). The goal is now to carry out a systematic search in molecular clouds for bands which agree well with PAH transitions measured in cavity ring down gas phase spectroscopy. I was Invited by Prof. Patt Thaddeus (a pioneer of the research on interstellar molecules) for a working visit in April 2009 at the Molecular Astrophysics group of the University of Harvard to discuss collaborative work on PAHs. During 2009, I have been invited and did working visits to University of Granada (Prof. E. Battaner), University of Valencia (Prof. Vicent Martínez), Univ. of Salamanca (Prof. Fernando Atrio) to carry out and explore collaborative work on topics related to microwave anomalous emission and prebiotic chemistry.

In Iglesias-Groth et al. (2010, MNRAS) we extended the previous PAH work and discovered the anthracene cation in the same Perseus molecular cloud. The anthracene cation transitions have been measured at laboratory via cavity ring down spectroscopy by the Molecular Astrophysics group of the Max Planck Institute for Astronomy (MPIA) at Heidelberg and at Univ. of Jena. I was invited by the Director of the MPIA, Prof. Thomas Henning for a working visit in August 2009 to these two centres. The anthracene molecule, conformed by three benzene-like rings, is the most complex molecule ever detected in the interstellar medium. Associated to this PAH research, I have been PI of several observing proposals that were awarded time for spectroscopy at optical/infrared large telescopes. Among them, the 3.5m Telescopio Nazionale Galileo, the 4.2m William Herschel Telescope, the 8m VLT (Paranal, Chile) and the 9m Hobby-Eberly Telescope (Mc Donald Obs. Texas). I wrote the proposals, prepared the observing blocks and carried out the observations whenever it was required. I led the scientific analysis of the data and the writing of the papers. I have been referee on three occasions for Astrophysical Journal.

I would like to remark that this generic post-doctoral position would be an ideal option to continue this research since it allows the flexibility required to keep my collaborations at Texas and Roma, where I could spend several months every year, while retaining access to the major European Observing Astronomical Facilities (including VLT, Herschel, GTC, in the future ALMA). This combination would work very efficiently for me. Provided I receive some minimum support, I think in the next three years I can solve several important long-standing problems associated with molecules in space, as described below. This, could possibly be done from other institutes in the world but I would very much like to do it from IAC Tenerife Spain, I would feel very proud to do it from the land were I was born.

3.- *RELEVANT RESEARCH LINES*

The main goal of my research is to investigate how in the interstellar medium and circumstellar environments complex hydrocarbon molecules may lead to the formation of amino acids and other key molecules in the development of life. With this aim, I study the physical and chemical properties of hydrocarbons (including fulleranes and PAHs) in conditions resembling molecular clouds with emphasis on the interaction with radiation (extinction and emission processes) and with other chemical species. My research includes synthesis and spectroscopy at the laboratory and dedicated searches in interstellar molecular clouds and protoplanetary discs with optical/(near and far) infrared and millimetre telescopes, to determine the abundances and chemical evolution of these species

1. Prebiotic molecules in molecular clouds and protoplanetary discs

Carbonaceous species are condensed mainly around carbon rich stars which display large mass losses. After injection in the interstellar medium the material begins a cycle from the diffuse medium to dense clouds where several energetic processes contribute to modify the original nature of the material and give rise to new molecular species. The complex evolution of the structural properties of these molecules is determined by the interactions with the gas, radiation, ionic bombardment and shocks. Indeed, an enormous variety of carbon based molecules have been identified in the various phases of the interstellar medium. Polycyclic aromatic hydrocarbons are advocated as a major carbon reservoir in the interstellar medium. Many emission lines in the near infrared can be ascribed to the various CH bending modes but these are not exclusive transitions of PAHs **Only recently the first specific PAHs (naphthalene and anthracene, the two most simple with two and three benzene rings, respectively) have been identified with optical spectroscopy in a molecular cloud of the Perseus complex (Iglesias-Groth et al. 2008, ApJ 685, L55; Iglesias-Groth et al. 2010, MNRAS**). We identified optical transitions previously measured in gas phase spectroscopy at the laboratory in conditions resembling the ISM. The cations of naphthalene and anthracene were measured with colmn densities of order 10^{13} cm^{-2} in a cloud with a column density of H_2 of 6 x 10^{21} cm^{-2}

Recent laboratory experiments (Chen et al. 2008, MNRAS 84, 605) have shown that at least 13 of the amino acids relevant to life are formed as a result of UV irradiation on a mixture of the most simple PAH (naphthalene) with water and ammonia at very low temperatures (15 K). Rosolowsky et al. (2008, ApJS 175, 509) have already shown the presence of ammonia in the same line of sight in the Perseus molecular complex where we detected naphthalene. UV radiation is provided by the A3 V star (Cernis 52) which we have shown it is embedded in the cloud (González-Hernández, Iglesias-Groth et al. 2009, ApJ 706, 866). I have obtained observations of the C2 Phillips (2,0) and (3,0) bands with the 9m HET telescope which allow to determine the excitation temperature of the gas in this cloud. Preliminary results indicate temperatures in the range 20-50 K which would favour the formation of amino acids via the Chen et al. mechanism. The Perseus cloud could meet the conditions for an active amino acid “factory” which would be of extraordinary importance to trace the evolution of prebiotic material in interstellar space. In the immediate future, I plan to carry out a systematic comprehensive study of the physical and chemical properties of this (and other) cloud using optical, near and mid infrared imaging and spectroscopy (WHT; GTC; HET) and submillimeter (Herschel satellite) and millimetre (30m IRAM, ALMA) facilities. We plan to search for amino acids in this line of sight using the 30 m radiotelescope at Sierra Nevada. The laboratory results by Chen et al. suggest that glycine (and other amino acids) could form with a column density which would be detectable with moderate integration times at the 30m telescope with EMIR. **We plan in the immediate feature to measure glycine transitions at 101.3 and 130.4 GHz (5 lines and 4 lines, respectively) and in a second step extend the millimetric search to other amino acids with well known transitions. A proposal to measure glycine with the 30m IRAM was recommended for execution this year and we are awaiting this to be carried out.**

This Perseus molecular cloud is “special” because it is the most intense source of anomalous microwave emission so far detected in the sky by Cosmic Microwave Background experiments (COSMOSOMAS, VSA, RATAN). The anomalous microwave emission is explained as a result of electric dipole radiation from hydrogenated carbon molecules (Draine and Lazarian 1998, ApJ 494, L19; Iglesias-Groth 2005, ApJ 632,L25, Iglesias-Groth 2006, MNRAS 368, 1925). Next year the Planck satellite will provide many more examples of such clouds with anomalous microwave emission. I plan to carry out systematic searches for PAHs and amino acids in these anomalous microwave emission molecular clouds and extend the study **to investigate the properties of these clouds including comparison with (sub)millimetre emission, protostellar content and the presence of the most simple PAHs in protoplanetary disk material.** Using the TNG and the WHT at La Palma, I have started a search for optical transitions associated to the most simple PAHs in protoplanetary discs around nearby stars. The goal is to investigate whether PAHs survive long enough in the interstellar medium to enrich the material that will end in protoplanetary disks, and ultimately form planets and other minor bodies. Successful PAH searches would lead us to seek evidence for formation of the more complex amino acid molecules in protoplanetary disks.

2. Complex carbon based molecules and their impact on interstellar extinction (UV bump and diffuse bands) and microwave anomalous emission

Cataldo (Roma), Stoldt et al. (Berkely Univ., EEUU) and other groups have demonstrated in their laboratory research work that C60 fullerene and its homologues are reactive with hydrogen. In the interstellar medium fullerenes may exist at various degrees of hydrogenation (fulleranes) rather than in its elemental carbon form. Both fullerenes and fulleranes may contribute to the extinction “UV bump” at 217 nm (Iglesias-Groth 2004, ApJ 608, L37; Cataldo and Iglesias-Groth 2009, MNRAS 400, 291) and to the diffuse interstellar bands (Iglesias-Groth 2007, ApJ Lett.) which are interstellar absorptions in the optical and near infrared discovered more than six decades ago for which the carrier has not bee identified yet. Since the 30s, it is well known the existence of interstellar material which causes absorption bands in the spectrum of distant stars. The widths of these bands range from 0.5 to 30 Å . Hundreds of these bands have been detected which do not appear to correspond with any known spectrum of atomic or molecular species. It has been proposed that they could be associated to the very little explored fullerene family. PAHs have been intensively studied in this respect but without concluding results. The theoretical spectra obtained for icosahedric fullerenes and buckyonions (from C60 to C6000) using semiempirical methods (Iglesias-Groth, S., et al. (2002) J. Chemical Phys. 116, 10648; Iglesias-Groth S., et al. (2003) J. Chemical Phys. 118, 7103 provide numerous low-intensity bands in the optical and near-infrared. Several with wavelengths very similar to well known DIBs.

A significant fraction of interstellar carbon (20%) could then reside in fullerene related molecules but demonstration requires first better characterization of these molecules in the laboratory. Prompted by my computations using semiempirical models, I currently work on the **synthesis and spectroscopic characterization at the laboratory of fullerenes and hydrogenated fullerenes of various sizes and various levels of hydrogenation and for amino acids in conditions resembling the interstellar medium. I aim** to measure absorption bands at laboratory of hydrogenated fullerenes and amino acids with wavelength determinations as accurate as possible (0.1 Angstroms in the optical, and 1 Angstrom in the near infrared). We are preparing samples as representative of the conditions of the interstellar medium (typical temperatures are of order 10-100 K and very low densities. This work started recently (see the four papers by Cataldo, Iglesias-Groth and Manchado in vol. 17 of the journal Fullerenes Nanotubes and Carbon Nanostructures 2009). The plan is to carry out a systematic production of hydrogenated fullerenes and perform the spectroscopic characterization which is currently absent in the literature, then we will correlate with available lists of diffuse interstellar bands, or if the laboratory bands take place in a region previously unexplored, we will take data at the optical/infrared telescopes we have access (GTC, WHT, TNG). Available instruments (OSIRIS; ISIS; CANARICAM; SARG) at these telescopes cover from 400 nm to 20 microns with a variety of spectral resolutions. We also plan to investigate at the laboratory the formation of prebiotic material from hydrogenated fullerenes exposing them to gamma, UV and corpuscular radiation in the presence of ammonia and water, always at cryogenic temperatures resembling the ISM. First results on the stability of hydrogenated fullerenes to the action of gamma radiation have been achieved by Cataldo, Strazzulla, Iglesias-Groth, (2009) MNRAS 394, 615. Exploratory studies on the stability of C60H36 and any other reasonably stable fullerene derivative to the action of ultraviolet light in solution and, possibly in the solid state have been made in order to assess whether or not fulleranes may survive the action of high energy photons (Cataldo and Iglesias-Groth S. 2009 MNRAS 400, 291-298) We plan to extend this survival experiments to amino acids.

Anomalous microwave emission. Hydrogenated fullerenes have been proposed as carriers of the anomalous microwave emission recently detected by several experiments on the Cosmic Microwave Background (see Iglesias-Groth 2005 ApJ 632, L25; Iglesias-Groth 2006, MNRAS 368, 1925). Under the physical conditions of the interstellar medium these molecules should have spin rates of several to tens of GHz, if as expected they have a small dipole moment, then they would emit electric dipole radiation in a frequency range very similar to the observed for the anomalous microwave emission . Is there any relationship between the carrier of the anomalous emission and the presence of DIBs and/or Unidentified Infrared Emission Lines? We plan to observe with GTC (OSIRIS) selected hot stars located behind regions where clear anomalous emission have been detected in order to detect optical transitions associated to the carriers of this emission. In addition, with CANARICAM and with PACS (Herschel satellite) we aim to characterize the possible thermal infrared emission lines of the carrier in several dark clouds. The detection of diffuse interstellar bands and thermal infrared lines in regions where anomalous microwave emission is dominant will be key to establish the nature of the responsible particles for this new emission process.