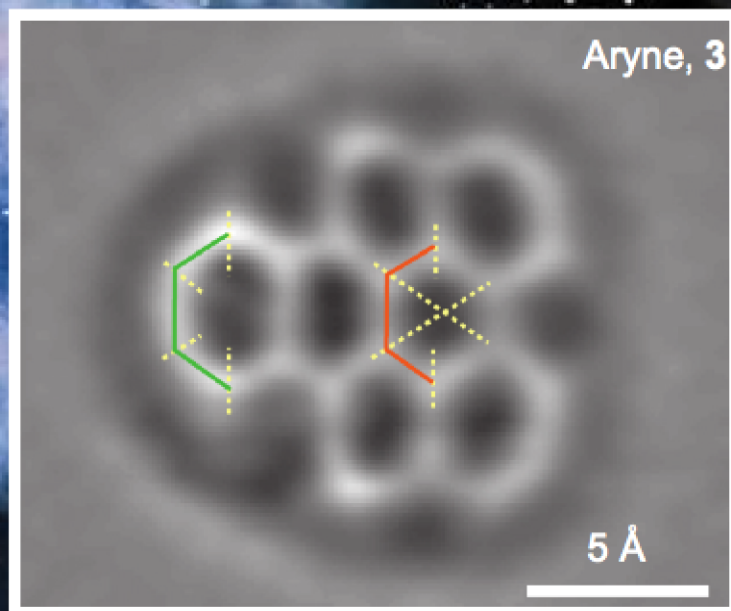
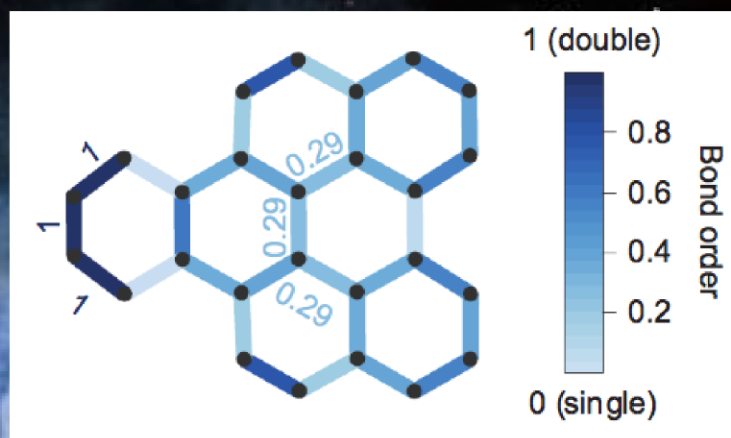


AstroPAH

A Newsletter on Astronomical PAHs

Issue 22 | October 2015



Editorial

Dear Colleagues,

With this 22nd issue, we celebrate our second Anniversary! We hope you have enjoyed the AstroPAH contents in this last revolution around the Sun as much as we did. Thank you for following us and for your contributions. We look forward to another year bridging the small and large scales of astrochemistry.

... And these different scales are what you see in our cover: an innovative study of bond lengths in dehydrogenated PAHs on top of NGC 7023, a PAHs and C₆₀-containing reflection nebula.

In this issue, we have a double *In Focus*. You will read about an exciting experimental study to obtain the rotationally-resolved spectrum of C₆₀ and the summary of the Focus Meeting 12 at IAU.

We also present abstracts of five interesting recent papers, as well as several announcements: the new IAU commission on Laboratory Astrophysics, the future Chemistry and Physics at Low Temperature conference, the new AstroChemical Newsletter, the opening ceremony of the FELIX Laboratory and its associated workshop, and five job positions.

We welcome contributions for any of our sections. They will reach more than 250 subscribers (researchers in correlated fields) plus the visitors of our website.

Best regards,

The Editorial Team

**Next issue: 17 November 2015.
Submission deadline: 6 November 2015.**

AstroPAH Newsletter

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PAH Picture of the Month

Top panel: Colour coded C-C bond order for the Kekulé depiction of the aryne molecule.

Bottom panel: Atomic force microscope image of the double dehydrogenated naphthoperylyne molecule (aryne). Green lines show the length of the C-C bonds in the dehydrogenated part, red lines do the same for the central ring of the aromatic structure. The aryne has three C-C double bonds (cumulene), rather than a short C-C triple bond connected to two long single C-C bonds (alkyne) as previously thought.

Background: A view of NGC 7023, a well-studied source of interstellar PAHs and C₆₀.

Credits: (Top and bottom panels) Reproduced with permission from Pavlíček et al., 2015. (Background) Jean-Charles Cuillandre (CFHT), Hawaiian Starlight.

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Newsletter Design: Isabel Aleman

Background image: NASA, ESA, and the Hubble Heritage Team (STScI/AURA)

Progress towards a rotationally-resolved spectrum of C_{60}

by Nicole C. Koeppen, Bradley M. Gibson, and Benjamin J. McCall

Buckminsterfullerene (C_{60}) was first discovered back in 1985 by Kroto et al.^[1] while they were simulating carbon star chemistry in the laboratory and noticed that carbon clusters comprised of 60 carbon atoms dominated other even number clusters. The presence of these molecules in the outflows of stars was confirmed in 2010, when it was detected in the planetary nebula Tc1^[2]. Also during this time C_{60} was detected in the interstellar medium (ISM) through infrared (IR) emission transitions from reflection nebulae. Although its presence in these environments was confirmed, the exact amount of C_{60} present remains a mystery because of uncertainties in its ultraviolet absorption cross-section^[3]. Obtaining an absorption spectrum would allow the amount of C_{60} to be determined without relying on this value.

Out of the four IR active bands of C_{60} , the $F_{1u}(3)$ band is centered around 1185 cm^{-1} ^[4], and in the region of an atmospheric transmission window. This allows for observations of this band from ground-based telescopes, which makes collecting a high-resolution absorption spectrum of C_{60} in this region even more valuable. To pursue this goal, we have built a continuous-wave external-cavity quantum cascade laser (cw-EC-QCL) cavity ring-down (CRD) instrument. The EC-QCL, shown in **Figure 1**, allows us to achieve a tuning range of $1135 - 1220\text{ cm}^{-1}$. Highly reflective mirrors form the cavity and light is allowed to build up to a user-defined intensity, at which point it is quickly shuttered. The amount of time it then takes the light to ringdown is related to the absorption of any species present within the laser path. This technique has the advantages of a large pathlength for the detection of small number densities, as well as being independent of any intensity fluctuations from the laser. By implementing

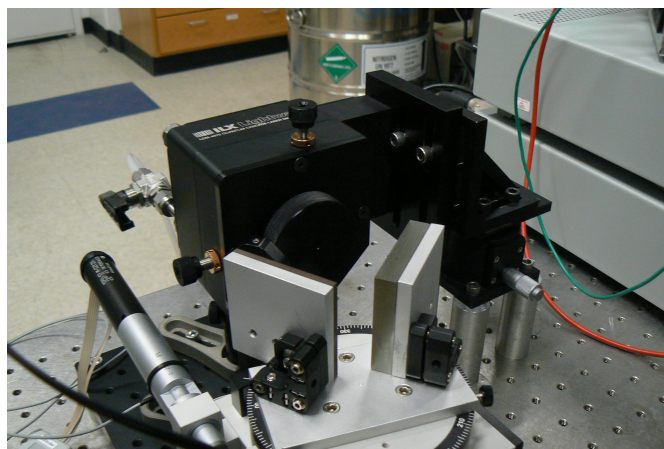


Figure 1 - The cw-EC-QCL used in our system. The resulting light is centered around $8.5\text{ }\mu\text{m}$ and allows for a scanning range of $\sim 100\text{ cm}^{-1}$. Picture adapted from <http://bjm.scs.illinois.edu/laboratory/c60.php>.

a side-of-fringe locking setup to our system^[5], we are able to achieve sensitivities on the order of $10^{-9} \text{ cm}^{-1} \text{ Hz}^{-1/2}$ and laser frequency stability on the order of $\sim 1 \text{ MHz}$. The system has recently been utilized to obtain a gas phase spectrum of the molecule 1,3,5-trioxane^[6]. A detailed diagram of the system is presented in **Figure 2**.

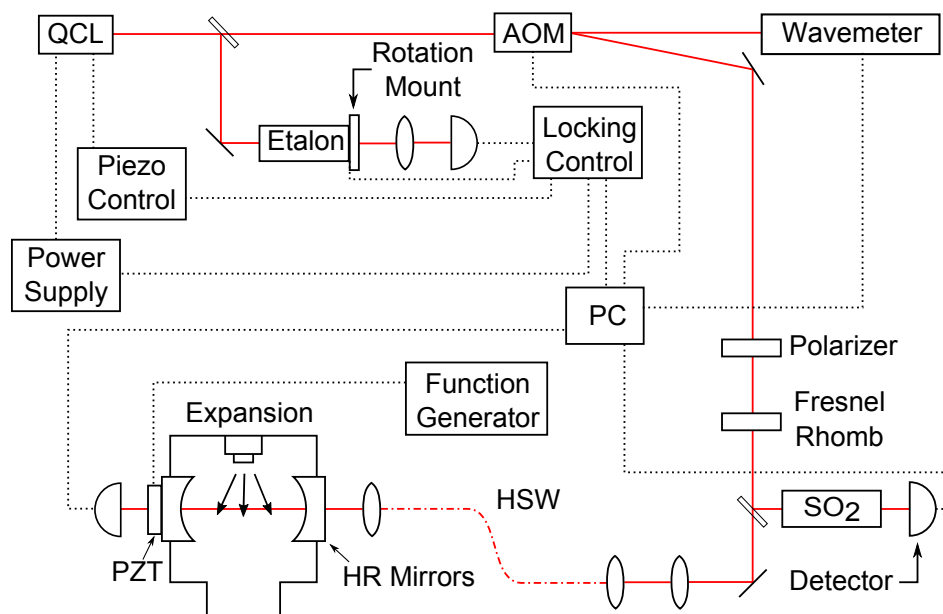


Figure 2 - Experimental layout of our EC-QCL CRD system. For details on the laser path or locking electronics, readers are directed to references [6] and [5], respectively. Figure adapted from reference [6].

The first step towards obtaining a spectrum of C_{60} was to look at a smaller PAH, in this case pyrene^[7]. Pyrene's ν_{68} band was observed between 1182.77 and 1185.06 cm^{-1} (see **Figure 3**) with a slightly older version of our system, which relied on a Fabry-Perot QCL with a tuning range of only $1180 - 1200 \text{ cm}^{-1}$. In order to obtain cooled gas phase pyrene, solid pyrene was heated in an oven to around 420 K and supersonically expanded, using argon as the carrier gas, through a slit and into the path of the laser. By comparing simulations to the observed spectrum, a rotational temperature of around 23 K was determined and the vibrational temperature was estimated to be between 23 and 111 K .

The first attempt to observe gas phase C_{60} was completed in a similar fashion to pyrene^[8]. However, since C_{60} has negligible vapor pressure at room temperature, it must be heated to much higher temperatures than pyrene in order to vaporize a significant amount. C_{60} was thus heated up to $\sim 955 \text{ K}$ and supersonically expanded through a slit using a number of different expansion conditions and a mass flow rate of ~ 2 grams per hour. Although these conditions give a predicted S/N of ~ 130 for the strongest transitions, as can be seen in **Figure 4**, a spectrum was never observed with our setup. A large factor in the ability to observe a spectrum is having a significant portion of the population in the ground state. Since we start at a relatively high temperature of the gas, C_{60} must be efficiently cooled in the expansion in order to achieve this. One difficulty with C_{60} is that it has 174 vibrational modes, which results in a large partition function even at relatively low temperatures. In addition, the lowest excited vibrational mode lies 267 cm^{-1} above the ground state. This is much higher than most PAHs and since the cooling efficiency of collisions decreases as the energy gap increases, it becomes more difficult to completely cool these modes with a similar number of collisions.

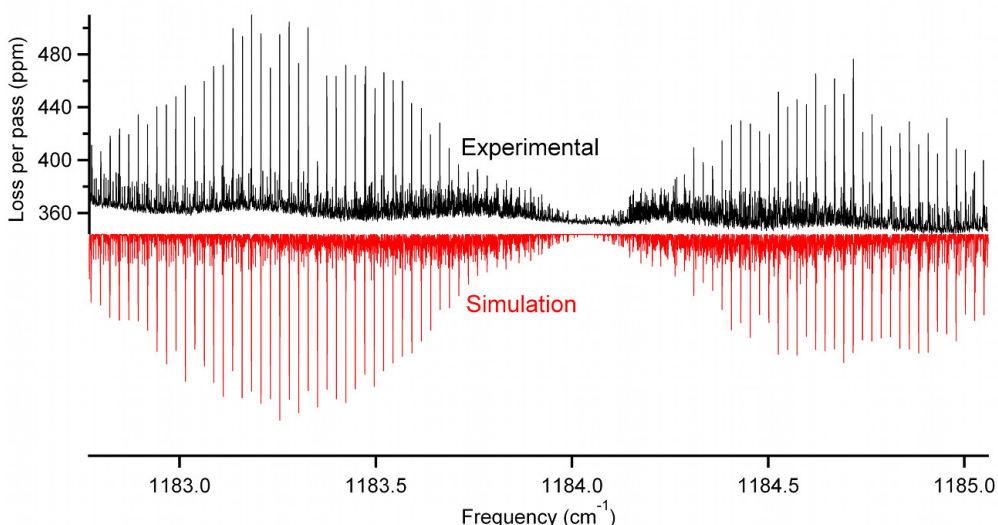


Figure 3 - Experimental and simulated spectrum of the ν_{68} band of pyrene. Figure adapted from reference [7].

The results and analysis from the oven-heated supersonic expansion of C_{60} showed that a new approach was going to be needed if a spectrum was to be observed. To this end, we designed a supercritical fluid (SCF) source based on designs for SCF chromatography by Sin et al.^[9] This allows for the production of C_{60} vapor at much lower temperatures which decreases the partition function. A SCF mixture of CO_2 and toluene was chosen since CO_2 alone is a poor solvent for C_{60} but pure toluene has a high critical temperature of 592 K. By creating a 7:3 mole fraction ratio (CO_2 :toluene), the mixture only needs to be heated to a critical temperature of 445 K.^[10] One iteration of the SCF expansion source has already been tested with D_2O in SCF CO_2 ^[11] and a second-generation source, pictured in **Figure 5**, has recently been built to fix a few minor problems we found with the first one. With this, we have already observed 1,3,5-trioxane dissolved in a CO_2 :toluene (7:3 v/v) SCF mixture. Based on the solubility of C_{60} in these mixtures, we estimate that we will see a mass flow rate of a few milligrams of C_{60} per hour^[9].

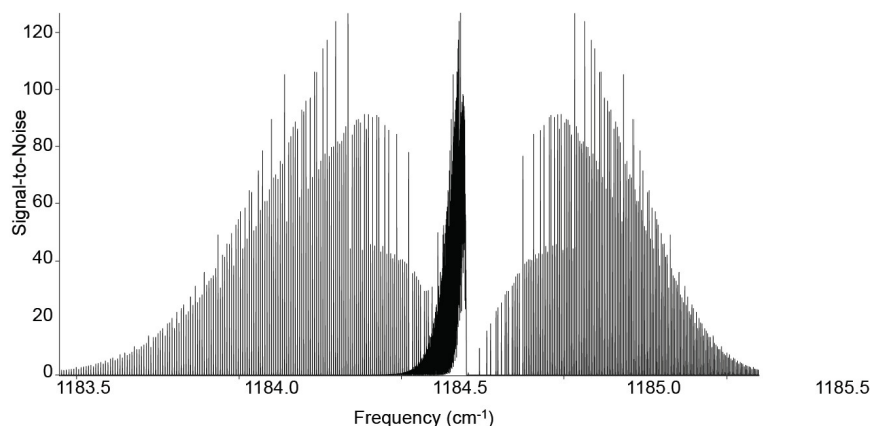


Figure 4 - The expected S/N of the different transitions in the $F_{1u}(3)$ band of C_{60} based on the mass flow rate of C_{60} and the sensitivity of the instrument. Figure adapted from reference [8].

Since the number density of C_{60} in our expansion will be much lower than previous attempts, we will have to increase the sensitivity of our instrument. Currently the intensity of light for ringdown is built up by dithering one of the cavity mirrors by greater than one free spectral range (FSR), which allows for the cavity to be on-resonance with the laser twice per pass. By locking the laser frequency to our cavity with the Pound-Drever-Hall technique, we can achieve almost continual constructive interference of the light since the cavity will be on-resonance with the frequency of the laser. Since sensitivity is based in part on the ringdown rate, increasing ringdown events from 100 Hz to over 10 kHz will allow us to do high-repetition rate ringdown and provide an increase in sensitivity of at least 10-fold to $\sim 10^{-10} \text{ cm}^{-1} \text{ Hz}^{-1/2}$. This sensitivity and the ability to average over many ringdown events should allow us to observe a spectrum of C_{60} even with the decrease in mass flow rate.

Although obtaining an absorption spectrum of C_{60} poses some difficult challenges, the sample introduction and improvements to our instrument make this an attainable goal in the near future. The implementation of a SCF source for C_{60} will encourage vibrational cooling of the molecule; and the addition of high-repetition rate ringdown should make up for loss from the lower mass flow rate. These factors in combination with each other should allow a rotationally-resolved absorption spectrum of C_{60} to finally be observed in the laboratory, and the results will be extremely helpful in the continual search for C_{60} in other regions of the ISM from ground-based telescopes.

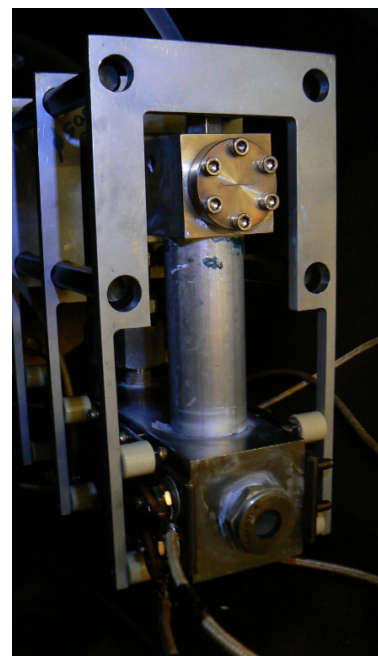


Figure 5 - The second-generation SCF expansion source built for the observation of C_{60} vapor.



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In Focus

A Focus Meeting on Bridging Laboratory Astrophysics and Astronomy at the IAU General Assembly

by Farid Salama (NASA ARC) on behalf of the SOC of FM12

Laboratory astrophysics is the Rosetta stone that enables astronomers to understand and interpret the cosmos. The [IAU Commission 14](#), the predecessor of the new [IAU Laboratory Astrophysics Commission C. B5](#) (Editor note: See the announcement in the corresponding section below) and the AAS Laboratory Astrophysics Division ([LAD](#)) decided to coordinate their efforts this summer to hold a joint meeting at the [IAU General Assembly](#). This joint effort was in the form of a Focus Meeting (<http://astronomy2015.org/focus.meeting.12>) that helped bridge Laboratory Astrophysics and Astrochemistry with Astronomy by bringing together expert providers and users of laboratory and astronomical data. This multidisciplinary meeting brought together astronomers with theoretical and experimental chemists and physicists to discuss the state-of-the-art research in their respective disciplines and how their combined expertise address important open questions in astronomy and astrophysics. Attendees were encouraged to bring and to discuss their data needs to improve the interpretations of astronomical phenomena.

The [Focus Meeting 12, "Bridging Laboratory Astrophysics and Astronomy"](#), discussed the strong interplay between astronomy, astrophysics, astrochemistry and planetary science with theoretical and experimental studies of the chemical and physical processes that drive our Universe. The meeting was divided into seven topical sessions that discussed atomic and molecular data, dust and ices, plasma, nuclear, and particle physics and their application to astronomy and astrophysics/astrochemistry. Twenty-five invited talks were presented, distributed between eleven in-depth reviews of the field, twelve topical presentations that focused on recent, hot topics and two summary talks that concluded the meeting. In addition, close to 70 research contributions were presented at the meeting, distributed between 12 oral presentations and 57 posters. A rich discussion resulted from this wide variety of topics as illustrated in the program of the sessions detailed below.

All presentations were very well received and the meeting ended on a general discussion of the future directions for laboratory astrophysics. Given the current major development of next-generation facilities and projects, the Focus Meeting stressed how laboratory studies can best address the needs of astronomy and stimulate new observations and discussed open questions to be solved in the next decade. All the presentations that were made at the meeting will be included in the new Proceedings series of the IAU, entitled "Focus on Astronomy".

FM 12: Bridging Laboratory Astrophysics and Astronomy

Room 316C, Hawaii Convention Center

Monday, 3 August 2015

FM12.1: Atoms, 10:30 am - 12:30 pm (Session Chairs: Lyudmila Mashonkina and Beatriz Barbuy)

10:30 am - 10:35 am	Farid Salama	SOC opening remarks	FM12.1.00
10:35 am - 11:05 am	Christopher Alan Sneden (Invited Review)	Atomic Data for Stellar Nucleosynthesis	FM12.1.01
11:05 am - 11:35 am	Jelle S. Kaastra (Invited Review)	Atomic processes in optically thin plasmas	FM12.1.02
11:35 am - 11:50 am	Karin Lind (Invited Topical)	Modelling cool star spectra with inadequate input physics	FM12.1.03
11:50 am - 12:05 pm	Michael Thomas Murphy (Invited Topical)	Quasar searches for variations in fundamental constants: the need for laboratory spectroscopy	FM12.1.04
12:05 pm - 12:20 pm	Natalie Hell (Contributed)	K-shell transitions in L-shell ions with the EBIT calorimeter spectrometer	FM12.1.05
12:20 pm - 12:35 pm	Norbert Przybilla (Contributed)	Quantitative spectroscopy of hot stars: accurate atomic data applied on a large scale as driver of recent breakthroughs	FM12.1.06

FM12.2: Molecules I, 2:00 pm - 3:30 pm (Session Chair: Steve Federman)

2:00 pm - 2:30 pm	Ewine van Dishoeck (Invited Review)	The molecular universe: from astronomy to laboratory astrophysics and back	FM12.2.01
2:30 pm - 3:00 pm	Svetlana Berdyugina (Invited Review)	Molecules in Magnetic Fields	FM12.2.02
3:00 pm - 3:15 pm	Leen Katrien Els Decin (Contributed)	Evolved stars as complex chemical laboratories – the quest for gaseous chemistry	FM12.2.03
3:15 pm - 3:30 pm	Annemieke Petrignani (Contributed)	Anharmonicity and infrared bands of Polycyclic Aromatic Hydrocarbon (PAH) molecules	FM12.2.04

Tuesday, 4 August 2015

FM12.3: Molecules II and Dust and Ices I, 10:30 am - 12:30 pm (Session Chair: Harold Linnartz)

10:30 am - 10:45 am	Ralf I Kaiser (Invited Topical)	Probing the Formation of Complex Organic Molecules in Interstellar Ices - Beyond the FTIR - RGA Limitation	FM12.3.01
10:45 am - 11:00 am	James Lyons (Contributed)	CO isotopologue ratios in the solar photosphere	FM12.3.02
11:00 am - 11:30 am	Karin I Oberg (Invited Review)	Laboratory constraints on ice formation, restructuring and desorption	FM12.3.03
11:30 am - 12:00 pm	Anthony Peter Jones (Invited Review)	Interstellar dust: interfacing laboratory, theoretical and observational studies	FM12.3.04
12:00 pm - 12:15 pm	Pascale Ehrenfreund (Contributed - Withdrawn)	Organics in Space: Results from SPace Exposure Platforms and Nanosatellites	FM12.3.05
12:15 pm - 12:30 pm	Gianfranco Vidali (Contributed)	Nitrogen chemistry on dust grains: the formation of hydroxylamine, precursor to glycine	FM12.3.06

FM12.4: Dust and Ices II and Planetary I, 2:00 pm - 3:30 pm (Session Chairs: Gianfranco Vidali and Farid Salama)

2:00 pm - 2:15 pm	Adwin Boogert (Invited Topical)	Telescope Observations of Interstellar and Circumstellar Ices: Successes of and Need for Laboratory Simulations	FM12.4.01
2:15 pm - 2:30 pm	Takashi Onaka (Invited Topical)	AKARI near-infrared spectroscopy of interstellar ices	FM12.4.02
2:30 pm - 3:00 pm	Dominique Bockelee-Morvan (Invited Review)	Comets and Laboratory Astrophysics	FM12.4.03
3:00 pm - 3:15 pm	Athena Coustenis (Invited Topical)	Laboratory and theoretical work in the service of planetary atmospheric research	FM12.4.04
3:15 pm - 3:30 pm	Robert M. Nelson (Contributed)	Laboratory Simulations of Planetary Surfaces: Understanding Regolith Physical Properties from Astronomical Photometric Observations	FM12.4.05

Wednesday, 5 August 2015**FM12.5: Planetary II and Plasma I, 10:30 am - 12:30 pm (Session Chairs: Helen Fraser and Daniel Savin)**

10:30 am - 10:45 am	Peter Jenniskens (Invited Topical)	Meteorites	FM12.5.01
10:45 am - 11:00 am	Ella Sciamma-O'Brien (Contributed)	The THS: Simulating Titan's atmospheric chemistry at low temperature	FM12.5.02
11:00 am - 11:30 am	William Fox (Invited Review)	Magnetic field generation, Weibel-mediated collisionless shocks, and magnetic reconnection in colliding laser-produced plasmas	FM12.5.03
11:30 am - 11:45 am	Frederico Fiuza (Invited Topical)	Generation of collisionless shock in laser-produced plasmas	FM12.5.04
11:45 am - 12:15 pm	James F. Drake (Invited Review)	The emerging understanding of magnetic reconnection through laboratory experiments, theory and modeling and in situ satellite measurements	FM12.5.05
12:15 pm - 12:30 pm	Michael Hahn (Contributed)	Influence of Multiple Ionization on Charge State Distributions	FM12.5.06

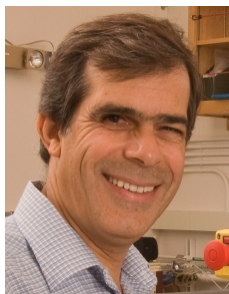
FM12.6: Plasma II and Nuclei and Particles I, 2:00 pm - 3:30 pm (Chairs: Lyudmila Mashonkina, Xiaowei Liu)

2:00 pm - 2:15 pm	Jan Egedal (Invited Topical)	The Wisconsin Plasma Astrophysics Laboratory (WiPAL): A New Experimental User Facility	FM12.6.01
2:15 pm - 2:30 pm	Maëlle Le Pennec (Contributed)	Testing stellar opacities with laser facilities	FM12.6.02
2:30 pm - 3:00 pm	Weiping Liu (Invited Review)	Progress of Jinping Underground laboratory for Nuclear Astrophysics experiment JUNA	FM12.6.03
3:00 pm - 3:15 pm	Elisabete de Gouveia Dal Pino (Invited Topical)	Cherenkov Telescope Array: Unveiling the Gamma Ray Universe and its Cosmic Particle Accelerators	FM12.6.04
3:15 pm - 3:30 pm	Yong-Zhong Qian (Invited Topical)	Neutrinos, Nuclei, and Nucleosynthesis: Implications for Chemical Evolution of the Early Galaxy	FM12.6.05

FM12.7: Nuclei and Particles II and Summary, 4:00 pm - 6:00 pm

(Session Chairs: Steve Federman and Farid Salama)

4:00 pm - 4:30 pm	Kei Kotake (Invited Review)	Multi-D Core-Collapse Supernova Models and the Multi-messenger Observables	FM12.7.01
4:30 pm - 4:45 pm	Rubén López-Coto (Contributed)	MACHETE: A transit Imaging Atmospheric Cherenkov Telescope to survey half of the VHE gamma ray sky	FM12.7.02
4:45 pm - 5:00 pm	Marie-Lise Dubernet (Invited Topical)	Atomic and Molecular Databases, VAMDC (Virtual Atomic and Molecular Data Centre)	FM12.7.03
5:00 pm – 5:25 pm	Beatriz Barbuy (Invited Summary)	Summary & outstanding questions	FM12.7.04
5:25 pm - 5:50 pm	Alexander Tielens (Invited Summary)	Summary & outstanding questions	FM12.7.05
5:50 pm – 6:00 pm	Farid Salama	SOC closing remarks	FM12.7.06



Dr. Farid Salama of NASA's Ames Research Center in Moffett Field, California, is the Chair of the Laboratory Astrophysics Division of the American Astronomical Society (AAS) and the founding President of the newly launched IAU Commission on Laboratory Astrophysics (Commission B5). E-mail: farid.salama@nasa.gov.

Abstracts

The $\lambda 6614$ diffuse interstellar absorption band: evidence for internal excitation of the carrier

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An analysis of absorption profiles of the $\lambda 6614$ diffuse interstellar band recorded along the lines of sight towards HD 179406 (20 Aql) and HD 147889 is described. The difference in band shape is attributed to the degree of internal excitation of the carrier, which is principally due to vibrational hot bands although an electronic component may also be present. The results are discussed with respect to other models of diffuse band spectral line shape.

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MNRAS, 2015, 453 (4): 3912-3917

DOI: 10.1093/mnras/stv1838

<http://mnras.oxfordjournals.org/content/453/4/3912.full>

Modeling dust in the Magellanic Clouds

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We model the extinction profiles observed in the Small and Large Magellanic clouds with a synthetic population of dust grains consisting by core-mantle particles and a collection of free-flying polycyclic aromatic hydrocarbons (PAHs). All different flavors of the extinction curves observed in the Magellanic Clouds (MCs) can be described by the present model, that has been previously (successfully) applied to a large sample of diffuse and translucent lines of sight in the Milky Way. We find that in the MCs the extinction produced by classical grains is generally larger than absorption by PAHs. Within this model, the non-linear far-UV rise is accounted for by PAHs, whose presence in turn is always associated to a gap in the size distribution of

classical particles. This hints either a physical connection between (e.g., a common cause for) PAHs and the absence of middle-sized dust particles, or the need for an additional component in the model that can account for the non-linear far-UV rise without contributing to the UV bump at ~ 217 nm, e.g., nanodiamonds.

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ApJ, 810, 70 (2015)

<http://iopscience.iop.org/article/10.1088/0004-637X/810/1/70/pdf>

<http://fr.arxiv.org/abs/1507.08550>

Mid-infrared spectroscopy of the Andromeda galaxy

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We present *Spitzer*/Infrared Spectrograph (IRS) 5–21 μm spectroscopic maps towards 12 regions in the Andromeda galaxy (M31). These regions include the nucleus, bulge, an active region in the star-forming ring, and 9 other regions chosen to cover a range of mid-to-far-infrared colours. In line with previous results, PAH feature ratios (6.2 μm and 7.7 μm features compared to the 11.2 μm feature) measured from our extracted M31 spectra, except the nucleus, strongly correlate. The equivalent widths of the main PAH features, as a function of metallicity and radiation hardness, are consistent with those observed for other nearby spiral and starburst galaxies. Reprocessed data from the ISOCAM instrument on the *Infrared Space Observatory* agree with the IRS data; early reports of suppressed 6–8 μm features and enhanced 11.3 μm feature intensity and FWHM apparently resulted from background-subtraction problems. The nucleus does not show any PAH emission but does show strong silicate emission at 9.7 μm . Furthermore, different spectral features (11.3 μm PAH emission, silicate emission and [NeIII] 15.5 μm line emission) have distinct spatial distributions in the nuclear region: the silicate emission is strongest towards the stellar nucleus, while the PAH emission peaks 15 arcsec north of the nucleus. The PAH feature ratios at this position are atypical with strong emission at 11.2 μm and 15–20 μm but weak emission at 6–8 μm . The nucleus itself is dominated by stellar light giving rise to a strong blue continuum and silicate emission.

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MNRAS 454, 818830 (2015)

DOI: 10.1093/mnras/stv2001

<http://adsabs.harvard.edu/abs/2015arXiv150905781H>

An early detection of blue luminescence by neutral PAHs in the direction of the yellow hypergiant HR 5171A?

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We re-examined photometry (VBLUW, UB_V, uvby) of the yellow hypergiant HR 5171A made a few decades ago. In that study no proper explanation could be given for the enigmatic brightness excesses in the L band (VBLUW system, $\lambda_{\text{eff}}=3838 \text{ \AA}$). In the present paper, we suggest that this might have been caused by blue luminescence (BL), an emission feature of neutral polycyclic aromatic hydrocarbon molecules (PAHs), discovered in 2004. It is a fact that the highest emission peaks of the BL lie in the L band. Our goals were to investigate other possible causes, and to derive the fluxes of the emission. We used two-colour diagrams based on atmosphere models, spectral energy distributions, and different extinctions and extinction laws, depending on the location of the supposed BL source: either in Gum48d on the background or in the envelope of HR 5171A. False L-excess sources, such as a hot companion, a nearby star, or some instrumental effect, could be excluded. Also, emission features from a hot chromosphere are not plausible. The fluxes of the L excess, recorded in the data sets of 1971, 1973, and 1977 varied (all in units of $10^{-10} \text{ W m}^{-2} \mu\text{m}^{-1}$) between 1.4 to 21, depending on the location of the source. A flux near the low side of this range is preferred. Small brightness excesses in uv (uvby system) were present in 1979, but its connection with BL is doubtful. For the L fluxes we consider the lowest values as more realistic. The uncertainties are 20-30 %. Similar to other yellow hypergiants, HR 5171A showed powerful brightness outbursts, particularly in the 1970s. A release of stored H-ionization energy by atmospheric instabilities could create BL emitted by neutral PAHs.

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Accepted for publication by A&A

<http://arxiv.org/abs/1509.07421>

High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons: the realm of anharmonicity

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We report on an experimental and theoretical investigation of the importance of anharmonicity in the 3 μm CH stretching region of Polycyclic Aromatic Hydrocarbon (PAH) molecules. We present mass-resolved, high-resolution spectra of the gas-phase cold ($\sim 4\text{K}$) linear PAH molecules naphthalene, anthracene, and tetracene. The measured IR spectra show a surprisingly high number of strong vibrational bands. For naphthalene, the observed bands are well separated and limited by the rotational contour, revealing the band symmetries. Comparisons are made to the harmonic and anharmonic approaches of the widely used Gaussian software. We also present calculated spectra of these acenes using the computational program SPECTRO, providing anharmonic predictions enhanced with a Fermi-resonance treatment that utilises intensity redistribution. We demonstrate that the anharmonicity of the investigated acenes is strong, dominated by Fermi resonances between the fundamental and double combination modes, with triple combination bands as possible candidates to resolve remaining discrepancies. The anharmonic spectra as calculated with SPECTRO lead to predictions of the main modes that fall within 0.5% of the experimental frequencies. The implications for the Aromatic Infrared Bands, specifically the 3 μm band are discussed.

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Accepted for publication in The Astrophysical Journal

<http://arxiv.org/abs/1510.04948>

Meetings

CPLT 2016: Chemistry and Physics at Low Temperature

**Biarritz, France
3 - 8 July 2016**

It is with great pleasure that we invite you to attend the 2016 international conference on Chemistry and Physics at Low Temperature, to be held in Biarritz, France, July 3-8.

CPLT 2016 brings together around one hundred specialists from twenty countries working at the interface between physics and chemistry in various fields related to the use of very low temperatures. In addition to studies of structure, dynamics, and reactivity in cryogenic solids, CPLT 2016 will address interstellar and atmospheric chemistry, spectroscopy and dynamics of aggregates.

The scientific topics include cryogenic matrices and quantum hosts, reaction intermediates and unstable species, spectroscopy and dynamics at low temperature, astrophysics, astrochemistry and atmospheric science, biological systems, cryocrystals and clathrates.

The meeting will consist of plenary and keynote lectures, invited talks, contributed talks, posters and opportunities for discussions. There will be awards for the best poster and oral presentation by a young researcher. Registration will open in December 2015 (deadline: 15 May 2016). Abstract submission deadline is 31 January 2016 for oral presentations and 3 May 2016 for posters.

We hope to see you in Biarritz in July 2016!

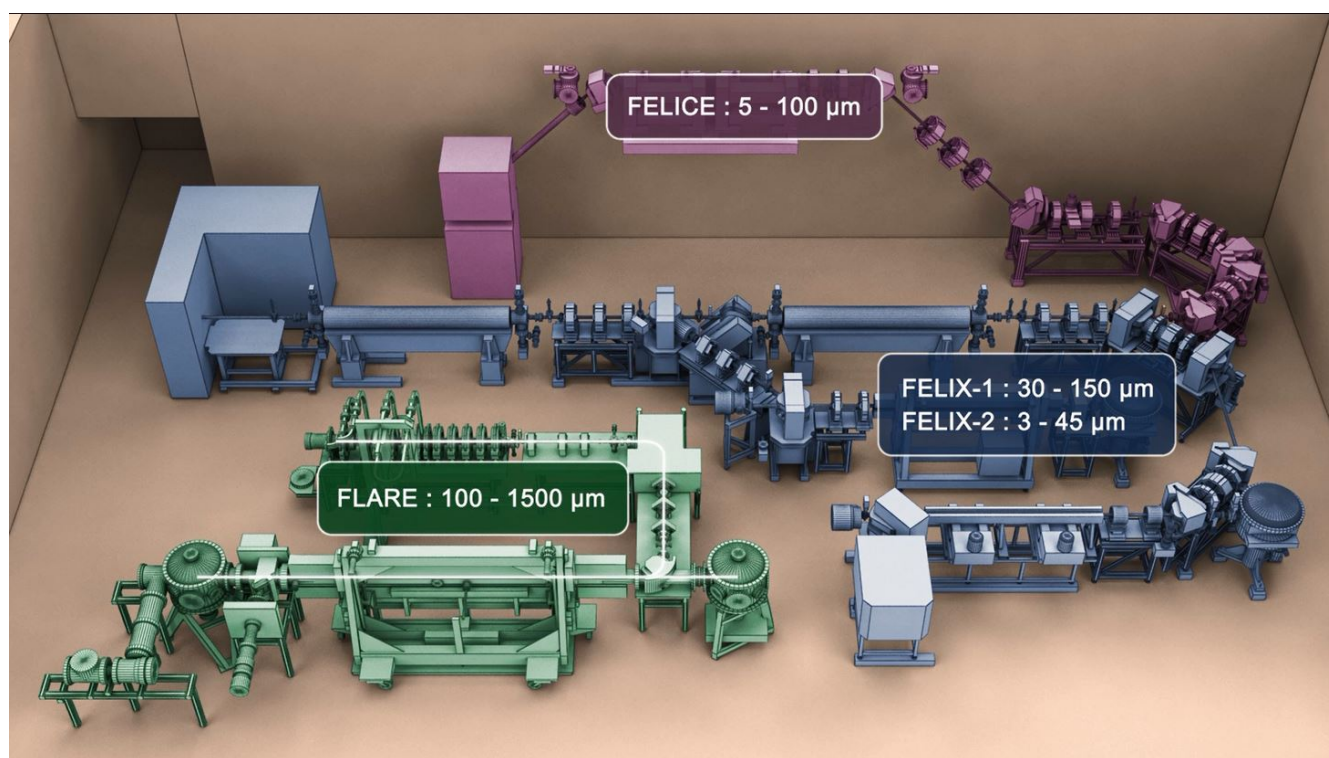
Dr. Joëlle Mascetti (chair, University of Bordeaux)

Dr. Claudine Crépin-Gilbert (co-chair, University of Paris-Sud)

Dr. Stéphane Coussan (co-chair, Aix-Marseille University)

E-mail for contact: info@cplt16.com

Webpage: www.cplt16.com



Enlightened Science - Official opening of the FELIX Laboratory -

**Radboud University, Nijmegen, The Netherlands
Friday October 30, 2015**

On October 30, Sander Dekker - State Secretary for Education, Culture and Science - will officially open the Experimental Garden and the FELIX Laboratory. In the FELIX Laboratory, very intense radiation in the infrared and THz regime of the electromagnetic spectrum is generated and exploited for spectroscopy. Together, the laboratory's unique free electron lasers FELIX, FLARE and FELICE provide the worlds most complete coverage of the infrared and THz spectrum ranging from 3 -1500 micrometer.

Research using the FELIX lasers contributes significantly to the understanding of properties of new materials and molecules, and allows scientists to study the structure and dynamics of a broad class of materials. The research covers a wide range of subjects including condensed matter physics, nanomaterials, spintronics, ion chemistry, cluster science, gas-phase biomolecular studies and astrochemistry.

Its wide and facile wavelength tunability makes FELIX a laser source for laboratory IR spectroscopic studies par excellence. Methods have been developed to obtain spectra for extremely dilute species, such as in particular gaseous mass-selected molecular ions and clusters. In addition to small molecular ions and metal clusters of astrochemical interest, IR spectra for a variety of ionized PAHs (and PANHs) have been obtained, including radical cation, protonated, H-deficient and hydrogenated cations, as well as anionic PAHs.



Registration for the Official Opening:

<http://www.ru.nl/registreren/felix/enlightened-science/>

In connection to the Official Opening, a workshop is organized for current and future FELIX users:

<http://www.ru.nl/felix/news-0/events/felix-user-meeting/>

Announcements

A New Home for Laboratory Astrophysics at the IAU!

Dear Colleagues,

A new Commission on Laboratory Astrophysics, C. B5 (http://www.iau.org/science/scientific_bodies/commissions/B5/), was launched at the IAU XIX General Assembly in Honolulu, this summer.

The goal of the newly formed Commission is to advance our understanding of the Universe through the promotion of fundamental theoretical and experimental research into the underlying processes that drive the cosmos.

The Laboratory Astrophysics Commission is a strongly cross-disciplinary commission with the aim to assist all IAU members in providing the data needed to interpret and understand astronomical observations and to promote Laboratory Astrophysics.

We would like to encourage you to show your support for Laboratory Astrophysics by joining the 130 of your colleagues who have already joined the new commission. As an IAU member you can sign up electronically to join the commission. If you are not an IAU member, you need first to apply to become an IAU member (see instructions at <http://www.iau.org/administration/membership/individual/qualification/>).

Your support is important for the success of the new commission!

Thank you for your support!

Farid Salama and the Organizing Committee of Commission B5

Commission B5 Organizing Committee:

Farid Salama (President), NASA Ames Research Center, United States
Helen J. Fraser (Vice-President), The Open University, United Kingdom
Paul S. Barklem, Uppsala University, Sweden
Thomas Henning, Max-Planck-Institute for Astronomy, Germany
Harold Linnartz, Leiden Observatory, Netherlands
Gianfranco Vidali, Syracuse University, United States
Feilu Wang, National Astronomical Observatories, China Nanjing

Three postdoctoral positions at the University of Hawai'i at Manoa

Advertised by Prof. Ralf Kaiser

The Reaction Dynamics Group, Department of Chemistry, University of Hawai'i at Manoa, invites applications for three postdoctoral positions. The appointment period is initially for one year, but can be renewed annually based on availability of funds and satisfactory progress. The salary is competitive and commensurate with experience. Successful applicants should have a strong background in one or more of the following: experimental reaction dynamics, molecular beams, low temperature condensed phase, soft matter, UHV technology, pulsed laser systems. Programming experience in labview is desirable. A description of our current research group can be found at <http://www.chem.hawaii.edu/Bil301/welcome.html>.

Position I: Reaction Dynamics. The prime directive of the experiments is to investigate the formation of carbonaceous and silicon-bearing molecules in extreme environments ranging from combustion flames, CVD processes, and interstellar/circumstellar environments exploiting the crossed molecular beams method.

Position II: Soft Matter & Material Sciences. The main objective of these experimental studies is to explore the fundamental mechanisms and electron transfer processes involved in the reaction and ignition of prototype boron-based energetic ionic liquids (EILs) doped with passivated nanoparticles in levitated droplets.

Position III: Planetary Chemistry. The goal of these experiments is to probe the formation of water and/or hydroxyl radicals via interaction of the solar wind particles such as keV protons and deuterons with silicates at lunar temperatures. Reaction products will be probed via condensed phase spectroscopy and photoionization of the subliming molecules.

Solid communication skills in English (written, oral), a publication record in internationally circulated, peer-reviewed journals, and willingness to work in a team are mandatory. Only self-motivated and energetic candidates are encouraged to apply. Please send a letter of interest, three letters of recommendation, CV, and publication list to Prof. Ralf I. Kaiser (contact information below). Applicants must demonstrate their capability to prepare manuscripts for publications independently.

The review of applications started October 15, 2015, and will continue until the position is filled.

Contact: Prof. Ralf Kaiser
Department of Chemistry
University of Hawai'i at Manoa
Honolulu, HI 96822-2275, USA
E-mail: ralfk@hawaii.edu

PhD & Postdoctoral position in Laboratory Astrochemistry

Advertised by Dr. Annemieke Petrignani & Prof. Wybren Jan Buma

UvA Faculty of Science – Van 't Hoff Institute for Molecular Sciences

Application deadline: 15 January 2016.

Location: The Van 't Hoff Institute for Molecular Sciences (HIMS) is one of the eight research institutes of the University of Amsterdam Faculty of Science. HIMS performs internationally recognized chemistry research, curiosity driven as well as application driven. This is done in close cooperation with chemical, flavour & food, medical and high-tech industries. Research is organised into four themes: Sustainable Chemistry, Analytical Chemistry, Computational Chemistry and Molecular Photonics.

The **Molecular Photonics** group is active in various areas of photophysical and photochemical research. One of the special areas is astrochemistry, aimed to enhance the interplay between chemistry and astronomy research by bringing state-of-the-art chemistry research to astronomical applications.

Project description: Aromatic hydrocarbons are important molecules in many fields such as photochemical research, environmental physics, and nanophysics. They are also of major importance in astrochemistry or the chemistry in interstellar matter, where they play a key role in the formation of planets and are possible precursors of life. Although they are ubiquitous, little is known about their inventory in space. In this project, state-of-the-art spectroscopic laboratory techniques will be applied and new approaches will be developed to investigate the spectral signatures of Polycyclic Aromatic Hydrocarbon (PAH) species. Specifically, the project targets the spectral characteristics of gas-phase, small to large, neutral and ionic, PAH species in the near infrared (NIR) to far infrared (FIR) and aims to help interpret current and future ground-breaking astronomical observations and identify possible fingerprints needed to determine the shapes and sizes of PAHs in space and thereby the role they play in interstellar chemistry.

Further information: The intended start date is in the spring of 2016. For further information on the respective vacancies and requirements, please check the following links:

PhD position: [Phd-candidate-in-laboratory-astrochemistry](#)

Or: www.academictransfer.com/30419

Postdoc position: [Postdoctoral-researcher-in-laboratory-astrochemistry](#)

Or: www.academictransfer.com/30418

Launch of the AstroChemical Newsletter

Dear colleagues,

We are announcing the launch of the AstroChemical Newsletter, a monthly compilation of recently accepted publications and announcements in the field of astrochemistry (astrophysical observations and modeling as well as theoretical and experimental chemical-physics related to astronomical environments).

You can subscribe to the newsletter and submit abstracts by going to the AstroChemical Newsletter website: <http://acn.obs.u-bordeaux1.fr/>

You can also share your latest astrochemistry news on the AstroChemical Newsletter Facebook page: <https://www.facebook.com/AstrochemicalNewsletter> and follow @AstroChemNews on Twitter.

The Editors:

Pierre Gratier
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Mathieu Bertin
Edith Fayolle
Valentine Wakelam

AstroPAH Newsletter

<http://astropah-news.strw.leidenuniv.nl>
astropah@strw.leidenuniv.nl

Next issue: 17 Nov. 2015
Submission deadline: 6 Nov. 2015