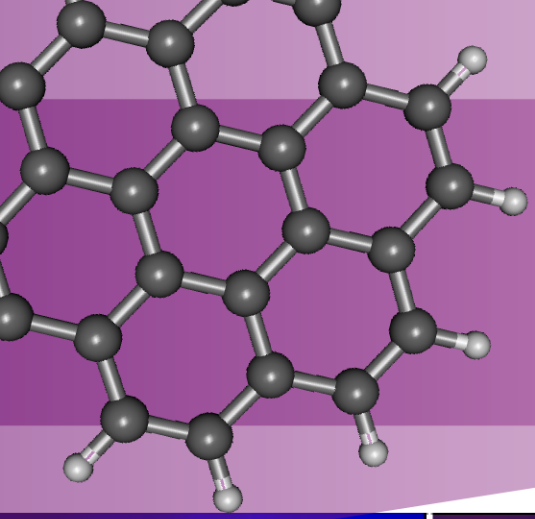
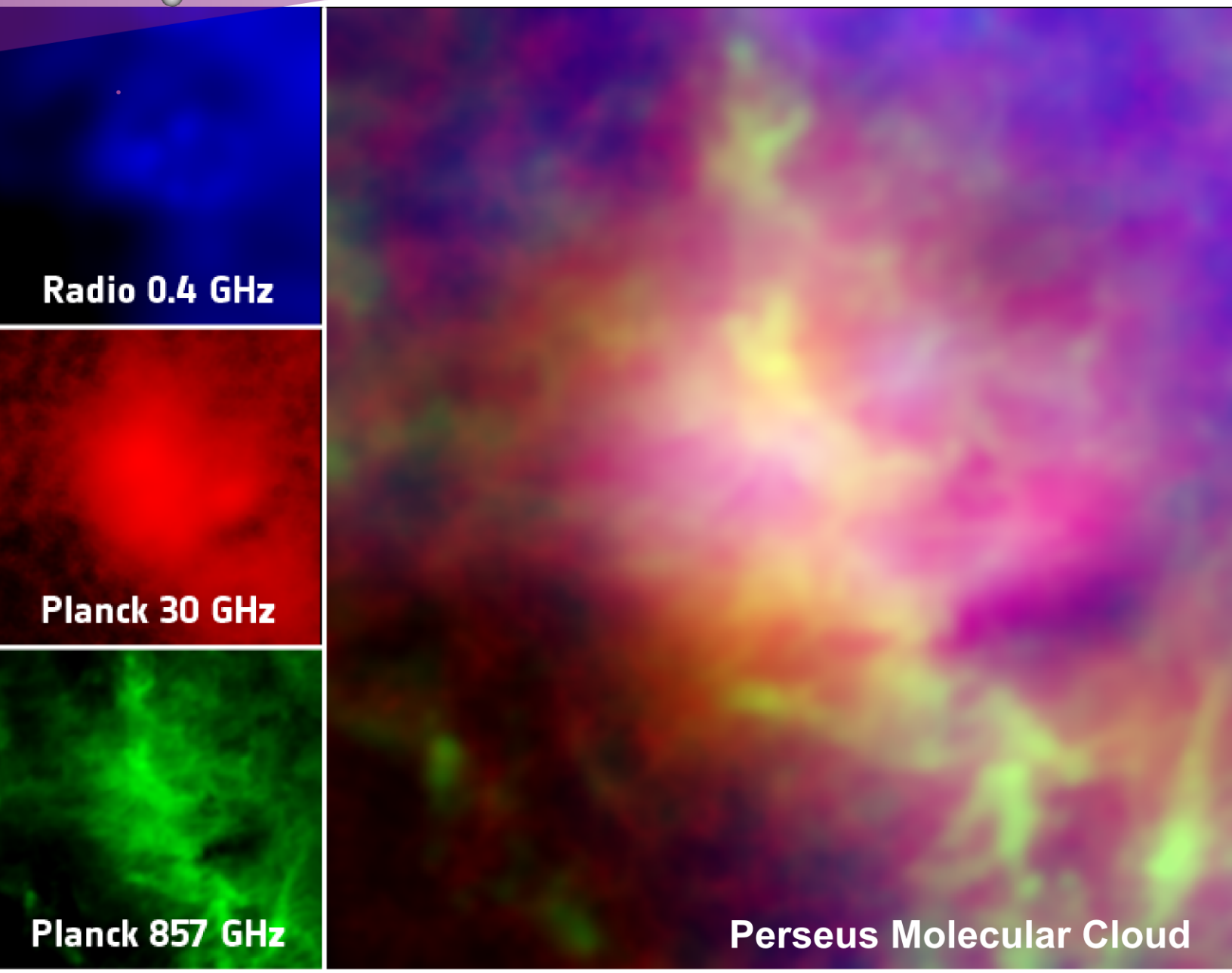


AstroPAH

A Newsletter on Astronomical PAHs

Issue 15 | February 2015



Editorial

Dear Colleagues,

After a break in January, we are starting the year with our 15th release. We are happy to present to you a wide range of contributions covering far infrared to visible spectroscopy, gas phase to ice chemistry, from observations to theory to experiments. Our *Picture of the Month* is the Perseus molecular cloud highlighting emission in the sub-mm to the radio domain and *In Focus* is the International Conference on Interstellar Dust, Molecules and Chemistry that took place in December 2014 in Tezpur, India. In our abstracts section, you can find papers describing studies on low-temperature formation of PAHs, rotational signatures of PAHs, the visible DIBs, and more observations of PAHs in molecular clouds.

We would like to draw your attention to the symposium ”30 Years of Photodissociation Regions”, in honour of David Hollenbach, which will be held in California, USA, early summer (http://pdr30.strw.leidenuniv.nl). Students can apply for a small number of grants (kindly supported by the Stratospheric Observatory for Infrared Astronomy, SOFIA) available to help students attending the symposium until 20 February 2015.

We thank you all for your contributions and please keep them coming. You can send us your contributions anytime. For publication in March, see the deadlines below. Would you like to see your picture as *Picture of the Month*, your project featured in our *In Focus*, or distribute your latest paper or upcoming event amongst our community, we encourage you to contact us.

The Editorial Team

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

Contents

PAH Picture of the Month

Three-colour composite image of the Perseus molecular cloud (displayed on the right) is based on the three individual maps (shown on the left) of the complex, taken at 0.4 GHz by Haslam et al. (1982), and 30 and 857 GHz by Planck (corresponding to wavelengths of 75 cm, 1 cm, and 350 μm, respectively). The colour composite highlights the correlation between the anomalous microwave emission at 30 GHz (in red), most likely due may be due to rotational emission from large molecules such as PAHs and/or from spinning nano grains and the thermal dust emission at 857 GHz (in green).

Credits: ESA/Planck Collaboration

CONTACT
astropah@strw.leidenuniv.nl

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Design by Isabel Aleman

International Conference on Interstellar Dust, Molecules and Chemistry (IDMC-2014)

15-18 December, 2014

by Shantanu Rastogi & Amit Pathak

The International Conference on Interstellar Dust, Molecules and Chemistry (IDMC) in India was organized jointly by IUCAA, Pune and Tezpur University as a sequel to the one organized at IUCAA in November 2011. The conference was aimed to provide a platform for expert discussions and presentations with ample opportunities for the young researchers to interact and take up challenging problems in this field. There were 82 participants including 24 from abroad, representing 11 countries. The sessions consisted of 15 reviews, 18 contributory talks and 38 poster presentations. The presentations included **observational, theoretical and experimental studies of dust, molecules and chemistry in a wide range of astrophysical environments – from galaxies to stars: circumstellar and interstellar, planets and even comets.**

A good fraction of the deliberations focused on PAHs and carbonaceous content of the ISM. The inaugural review by Christine Joblin on ”Interstellar PAHs: combining the astronomer and molecular physicist views” covered details of our current understanding of the excitation and

relaxation processes in PAHs and the importance of mid-IR features as probe for molecular processes in the ISM. The synergy between astrophysicists and molecular physicists in all aspects of PAH photo-physics, relaxation and formation chemistry described the perspective of the Nanocosmos project funded by the European Research Council (ERC). Theoretical study of the IR features from different families and derivatives of PAHs were discussed. A. Candian showed correlation of the 12.7 μm Aromatic Infrared Band (AIB) with the 6.2 μm feature, associated with ionized PAHs, and discussed the possible contribution of armchair edge PAHs to the 12.7 μm band. Studies on PAHs with vinyl and phenyl substitutions were discussed by S. Rastogi to address the problem of suitable fitting of the 6.2 μm AIB. A. Pathak considered deuterated and deuteronated PAHs for their contribution towards the observed 4.4 and 4.65 μm features and also for possible DIBs correlation. The carbon chemistry in evolved carbon rich stars was discussed by J. Cernicharo taking the example of IRC+10216.

Ground and space observations, over a wide spectral range using ISO, Herschel, ALMA etc., showed the molecular complexity and indicated towards different chemical networks. Graphene etching on SiC grains towards formation of PAHs and the experiments under the Nanocosmos project were also discussed. J. Cami presented astronomical observations of fullerenes and laboratory experiments indicating the possible conditions for their formation in the ISM. Experimental study of benzene formation by irradiation of interstellar ices containing propargyl alcohol was discussed by B. Sivaraman and cosmic ray exposure experiments on carbonaceous solids on board the International Space Station were described by I. Sakon. Theoretical simulation of agglomeration of carbon dust from PAHs in circumstellar envelopes was presented by J. Bhatt. T. Onaka reviewed observations from AKARI, Herschel etc. of different regions and the use of PAH band ratio diagnostics towards understanding of dust processing in the ISM. B.G. Anandarao discussed infrared spectral observations of AGB/post-AGB stars and Y.C. Minh discussed observational studies of molecular emissions and dust related processes in star forming regions.

A significant number of talks were also centred on dust and dust extinction within the galaxy and in external galaxies. U.J. Sofia reviewed UV observations, abundances and pointed to the importance of sulphur as dust component. J. Murthy considered GALEX data for 3-D modelling of dust in the Galaxy and R. Gupta reviewed circumstellar dust extinction models. S.K. Pandey and N. Brosch reviewed dust in external galaxies and A. Mahabal proposed software filters for mapping dust in galaxies from images available in various survey catalogues. Fractal growth and porosity in model dust grains was discussed by R. Botet and N. Katyal. Laboratory study simulating the growth of dust grains in ISM was reported by G. Rouillé and laboratory setup for the simulation of light scattering by ISM dust analogues was presented by A. Gazi. A. Sen, U.C. Joshi and S. Ganesh discussed cometary dust and polarimetric observations.

Eric Herbst reviewed the progress in chemical simulations of regions of star formation. Interconnection between observations, laboratory and simulations is needed for improved understanding. He also summarized the deliberations of the conference commending much of the progress in such an interdisciplinary area and reflected upon the growing complexity of molecular evolution. His poser to the community was ”Can each DIB belong to a different molecule?” Then one-line identification may have no meaning. For PAHs he observed ”Will it be possible to identify PAHs from THz spectra?”

The poster sessions had more detailed discussions on specific topics that included studies on dusty plasma. The beautiful campus of Tezpur University and nice weather added to the frequency and quality of one-to-one discussions. A cultural evening showcasing the various

dance forms of North-East India and a special lecture on Thirty Meter Telescope, of which India is now an official partner, by Prof. A.K. Kembhavi added to the content of the conference.

The deliberations of the conference are available on the website:

http://www.iucaa.ernet.in/∼idmc2014

Shantanu Rastogi *is a Professor in the Department of Physics at the DDU Gorakhpur University, Gorakhpur, India. E-mail: shantanu_r@hotmail.com.*

Amit Pathak *is a Professor in the Department of the Physics at Tezpur University, Tezpur, India. E-mail: amit@tezu.ernet.in.*

Abstracts

Rotational spectroscopy of interstellar PAHs

Yacine Ali-Haïmoud[1]

[1] Institute for Advanced Study, Einstein Drive, Princeton, New Jersey 08540

Polycyclic aromatic hydrocarbons (PAHs) are believed to be ubiquitous in the interstellar medium. Yet, to date no specific PAH molecule has been identified. In this paper, a new observational avenue is suggested to detect individual PAHs, using their rotational line emission at radio frequencies. Previous PAH searches based on rotational spectroscopy have only targeted the bowl-shaped corannulene molecule, with the underlying assumption that other polar PAHs are triaxial and have a complex and diluted spectrum unusable for identification purposes. In this paper the rotational spectrum of quasi-symmetric PAHs is computed analytically. It is shown that the asymmetry of planar, nitrogen-substituted symmetric PAHs is small enough that their rotational spectrum, when observed with a resolution of about a MHz, has the appearance of a ”comb” of evenly spaced stacks of lines. The simple pattern of these ”comb” spectra allows for the use of matched-filtering techniques, which can result in a significantly enhanced signal-to-noise ratio. Detection forecasts are discussed for regions harboring ”anomalous microwave emission”, believed to originate from the collective PAH rotational emission. A systematic search for PAH lines in various environments is advocated. If detected, PAH ”combs” would allow to the conclusive and unambiguous identification of specific, free-floating interstellar PAHs.

E-mail: yacine@jhu.edu

MNRAS, 437, 2728 (2014)

http://mnras.oxfordjournals.org/content/437/3/2728.full.pdf
http://arxiv.org/abs/1309.2636

Search for PAHs in the Perseus molecular cloud with the Green Bank Telescope

Yacine Ali-Haïmoud[1,2], **Laura M. Pérez**[3], **Ronald J. Maddalena**[4], **D. Anish Roshi**[5]

[1] Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

[2] School of Natural Sciences, Institute for Advanced Study, Einstein Drive, Princeton, NJ 08540, USA

[3] National Radio Astronomy Observatory, PO Box O, Socorro, NM 87801, USA
[4] National Radio Astronomy Observatory, PO Box 2, Green Bank, WV 24944, USA
[5] National Radio Astronomy Observatory, Green Bank and Charlottesville, VA 22903, USA

Polycyclic Aromatic Hydrocarbons (PAHs) are believed to be the small-size tail of the interstellar carbonaceous dust grain population. Their vibrational emission is the most widely accepted source of the aromatic near-infrared features, and their rotational radiation is a likely explanation for the dust-correlated anomalous microwave emission (AME). Yet, no individual interstellar PAH molecule has been identified to date. It was recently recognized that quasi-symmetric planar PAHs ought to have a well identifiable comb-like rotational spectrum, and suggested to search for them in spectroscopic data with matched-filtering techniques. We report the results of the first such search, carried out with the Green Bank Telescope, and targeting the star-forming region IC348 in the Perseus molecular cloud, a known source of AME. Our observations amounted to 16.75 hours and spanned a 3 GHz-wide band extending from 23.3 to 26.3 GHz. Using frequency switching, we achieved a sensitivity of 0.4 mJy per 0.4 MHz channel (1σ). The non-detection of comb-like spectra allowed us to set upper bounds on the abundance of specific quasi-symmetric PAH molecules (specified uniquely by their moments of inertia) of approximately 0.1% of the total PAH abundance. This bound generically applies to PAHs with approximately 15 to 100 carbon atoms.

E-mail: yacine@jhu.edu
MNRAS, 447, 315 (2015)
http://mnras.oxfordjournals.org/content/447/1/315.full.pdf
http://arxiv.org/abs/1411.0691

Reaction Dynamics in Astrochemistry: Low-Temperature Pathways to Polycyclic Aromatic Hydrocarbons in the Interstellar Medium.

Ralf I. Kaiser[1], Dorian S.N. Parker[1] and Alexander M. Mebel[2]

[1] Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii 96822
[2] Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199

Bimolecular reactions of phenyl-type radicals with the C4 and C5 hydrocarbons vinylacetylene and (methyl-substituted) 1,3-butadiene have been found to synthesize polycyclic aromatic hydrocarbons (PAHs) with naphthalene and 1,4-dihydronaphthalene cores in exoergic and entrance barrierless reactions under single-collision conditions. The reaction mechanism involves the initial formation of a van der Waals complex and addition of a phenyl-type radical to the C1 position of a vinyl-type group through a submerged barrier. Investigations suggest that in the hydrocarbon reactant, the vinyl-type group must be in conjugation with a -C≡CH or HC=CH_2 group to form a resonantly stabilized free radical intermediate, which eventually isomerizes to a cyclic intermediate followed by hydrogen loss and aromatization (PAH formation). The

vinylacetylene-mediated formation of PAHs might be expanded to more complex PAHs, such as anthracene and phenanthrene, in cold molecular clouds via barrierless reactions involving phenyl-type radicals, such as naphthyl, which cannot be accounted for by the classical hydrogen abstraction-acetylene addition mechanism.

E-mail: ralfk@hawaii.edu

Annu. Rev. Phys. Chem., 66, 43 (2015)
http://www.annualreviews.org/doi/abs/10.1146/annurev-physchem-040214-121502

The 11.2 μm emission of PAHs in astrophysical objects

A. Candian[1,2] and P.J. Sarre[2]

[1] Leiden Observatory, Niels Bohrweg 2, Leiden, The Netherlands

[2] School of Chemistry, The University of Nottingham, Nottingham, UK

The 11.2 μm emission band belongs to the family of the 'Unidentified' Infrared (UIR) emission bands seen in many astronomical environments. In this work we present a theoretical interpretation of the band characteristics and profile variation for a number of astrophysical sources in which the carriers are subject to a range of physical conditions. The results of Density Functional Theory (DFT) calculations for the solo out-of-plane (OOP) vibrational bending modes of large polycyclic aromatic hydrocarbon (PAH) molecules are used as input for a detailed emission model which includes the temperature and mass dependence of PAH band wavelength, and a PAH mass distribution that varies with object. Comparison of the model with astronomical spectra indicates that the 11.2 μm band asymmetry and profile variation can be explained principally in terms of the mass distribution of neutral PAHs with a small contribution from anharmonic effects.

E-mail: candian@strw.leidenuniv.nl

Accepted for pubblication on MNRAS
http://arxiv.org/abs/1501.06811

Dusting off the diffuse interstellar bands: DIBs and dust in extragalactic Sloan Digital Sky Survey spectra

Dalya Baron[1], Dovi Poznanski[1], Darach Watson[2], Yushu Yao[3] and J. Xavier Prochaska[4]

[1] School of Physics and Astronomy, Tel-Aviv University, Tel Aviv 69978, Israel

[2] Dark Cosmology Centre, Niels Bohr Institute, University of Copenhagen, Juliane Maries Vej 30, DK-2100 Copenhagen, Denmark

[3] Lawrence Berkeley National Lab, 1 Cyclotron Road, Berkeley, CA 94720, USA

[4] Department of Astronomy and Astrophysics and UCO/Lick Observatory, University of California, Santa Cruz, CA 95064, USA

Using over a million and a half extragalactic spectra we study the properties of the mysterious diffuse interstellar bands (DIBs) in the Milky Way. These data provide us with an unprecedented sampling of the skies at high Galactic latitude and low dust column density. We present our method, study the correlation of the equivalent width of eight DIBs with dust extinction and with a few atomic species, and the distribution of four DIBs - 5780.6, 5797.1, 6204.3, and 6613.6 Å- over nearly 15 000 deg ^{2}. As previously found, DIBs strengths correlate with extinction and therefore inevitably with each other. However, we show that DIBs can exist even in dust-free areas. Furthermore, we find that the DIBs correlation with dust varies significantly over the sky. DIB under- or overdensities, relative to the expectation from dust, are often spread over hundreds of square degrees. These patches are different for the four DIBs, showing that they are unlikely to originate from the same carrier, as previously suggested.

E-mail: dovi@tau.ac.il

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http://mnras.oxfordjournals.org/content/447/1/545.full.pdf
http://arxiv.org/abs/1406.7006

Photochemistry of Polycyclic Aromatic Hydrocarbons in Cosmic Water Ice: The Role of PAH Ionization and Concentration

Amanda M. Cook[1] , Alessandra Ricca[2], Andrew L. Mattioda[1], Jordy Bouwman[3], Joseph Roser[1], Harold Linnartz[4], Jonathan Bregman[1], Louis J. Allamandola[2]

[1] NASA Ames Research Center, PO Box 1, M/S 245-6, Moffett Field, CA 94035, USA

[2] SETI Institute, 189 North Bernardo Avenue, Mountain View, CA 94043, USA

[3] Radboud University Nijmegen, Institute for Molecules and Materials, Toernooiveld 5, 6525 ED Nijmegen, The Netherlands

[4] Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, PO Box 9513, NL2300 RA Leiden, The Netherlands

Infrared spectroscopic studies of ultraviolet (UV) irradiated, water-rich, cosmic ice analogs containing small polycyclic aromatic hydrocarbons (PAHs) are described. The irradiation studies of anthracene:H_2O, pyrene:H_2O, and benzo[ghi]perylene:H_2O ices (14 K) at various concentrations reported by Bouwman et al. are extended. While aromatic alcohols and ketones have been reported in residues after irradiated PAH:H_2O ices were warmed to 270 K, it was not known if they formed during ice irradiation or during warm-up when reactants interact as H_2O sublimes. Recent work has shown that they form in low temperature ice. Using DFT computed IR spectra to identify photoproducts and PAH cations, we tentatively identify the production of specific alcohols [PAH(OH) n] and quinones [PAH(O) n] for all PAH:H_2O ices considered here. Little evidence is found for hydrogenation at 14 K, consistent with the findings of Gudipati & Yang. Addition of O and OH to the parent PAH is the dominant photochemical reaction, but PAH erosion to smaller PAHs (producing CO_2 and H_2CO) is also important. DFT spectra are used

to assess the contribution of PAH-related species to interstellar absorption features from 5 to 9 μm. The case is made that PAH cations are important contributors to the C2 component and PAH(OH) $_n$ and PAH(O) $_n$ to the C5 component described by Boogert et al. Thus, interstellar ices should contain neutral and ionized PAHs, alcohols, ketones and quinones at the 2%-4% level relative to H_2O. PAHs, their photoproducts, and ion-mediated processes should therefore be considered when modeling interstellar ice processes.

E-mail: amanda.m.cook@nasa.gov

ApJ, 799, 14 (2015)

http://iopscience.iop.org/0004-637X/799/1/14

Dissociative Photoionization of Quinoline and Isoquinoline

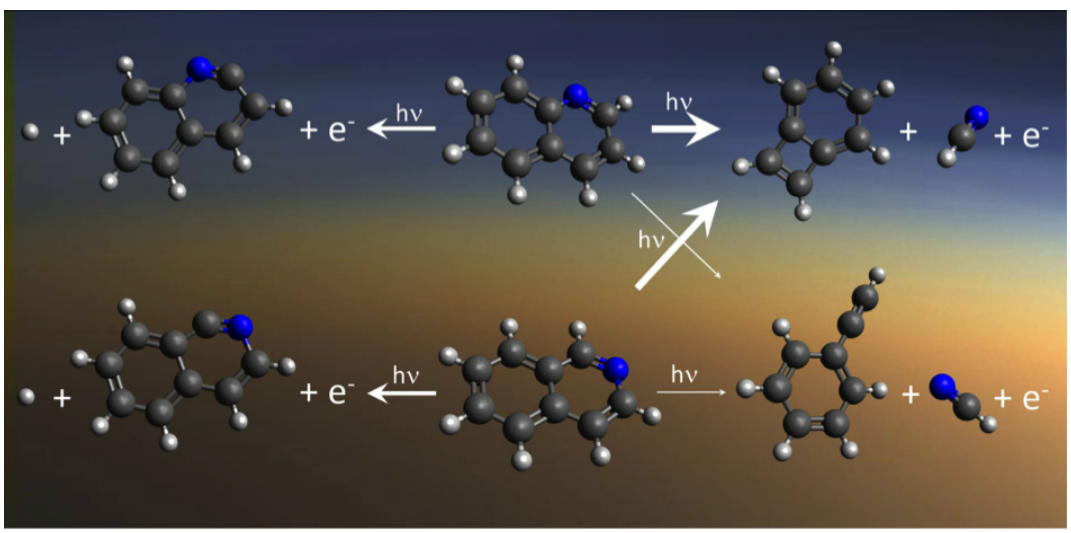
Jordy Bouwman[1], Balint Sztaray[2], Jos Oomens[1,3], Patrick Hemberger[4] and Andras Bodi[4]

[1] Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Laboratory, Toernooiveld 7c, NL-6525 ED Nijmegen, The Netherlands

[2] Department of Chemistry, University of the Pacific, Stockton, CA 95211, USA

[3] van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, NL-1098 XH Amsterdam, The Netherlands

[4] Molecular Dynamics Group, Paul Scherrer Institut, 5232 Villigen, Switzerland



Two nitrogen-containing polycyclic aromatic hydrocarbon isomers of C_9H_7N composition, quinoline and isoquinoline, have been studied by imaging photoelectron photoion coincidence spectroscopy at the VUV beamline of the Swiss Light Source. High resolution threshold photoelectron spectra have been recorded and are interpreted applying a Franck-Condon model. Dissociative ionization mass spectra as a function of the parent ion internal energy are analyzed with the use of breakdown diagrams. HCN-loss and H-loss are the dominant dissociation paths for both $C_9H_7N^{\cdot+}$ isomers at photon energies below 15.5 eV. Computed $C_9H_7N^{\cdot+}$ potential

energy surfaces suggest that the lowest energy path leading to HCN-loss yields the benzocyclobutadiene cation. A statistical model is used to fit the breakdown diagram and in order to account for the kinetic shift the time-of-flight mass spectra that reveal the dissociation rates. We have derived appearance energies of 11.9 ± 0.1 (HCN-loss) and 12.0 ± 0.1 (H-loss), as well as 11.6 ± 0.2 (HCN-loss) and 12.1 ± 0.2 (H-loss) eV for the dissociative ionization of quinoline and isoquinoline, respectively. The results are compared to a recent study on the dissociative ionization of naphthalene. Implications for the formation and destruction of nitrogenated PAHs in the interstellar medium and in Titans atmosphere are highlighted.

E-mail: j.bouwman@science.ru.nl

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Studies of Anomalous Microwave Emission (AME) with the SKA

Clive Dickinson[1], Y. Ali-Haïmoud[2], R. J. Beswick[1], S. Casassus[3], K. Cleary[4], B. T. Draine[5], R. Genova-Santos[6], K. Grainge[1], T. C. Hoang[7], A. Lazarian[8], E. J. Murphy[9], R. Paladini[9], M. W. Peel[1], Y. Perrott[10], J.-A. Rubiño-Martin[6], A. Scaife[11], C. T. Tibbs[9], L. Verstraete[12], M. Vidal[1], R A. Watson[1], N. Ysard[13]

[1]Jodrell Bank Centre for Astrophysics, The University of Manchester, UK

[2]Institute for Advanced Study, Einstein Drive, Princeton, New Jersey 08540, USA

[3]Departamento de Astronomía, Universidad de Chile, Casilla 36-D, Santiago, Chile

[4]Cahill Center for Astronomy & Astrophysics, Caltech, Pasadena CA, 91125, USA

[5]Princeton University Observatory, Princeton, NJ 08544-1001, USA

[6]Instituto de Astrofiśica de Canarias, 38200 La Laguna, Tenerife, Canary Islands, Spain

[7]Institut für Theoretische Physik, Lehrstuhl IV: Weltraum- und Astrophysik, Bochum, Germany

[8]Department of Astronomy, University of Wisconsin, Madison, WI 53706, USA

[9]IPAC, Caltech, Pasadena CA, 91125, USA

[10]Astrophysics Group, Cavendish Laboratory, University of Cambridge CB3 0HE, UK

[11]School of Physics & Astronomy, University of Southampton, Southampton, SO17 1BJ, UK

[12]IAS, CNRS, Université Paris-Sud 11, Orsay, France

[13]Department of Physics, PO Box 64, FI-00014 University of Helsinki, Finland

In this chapter, we will outline the scientific motivation for studying Anomalous Microwave Emission (AME) with the SKA. AME is thought to be due to electric dipole radiation from small spinning dust grains, although thermal fluctuations of magnetic dust grains may also contribute. Studies of this mysterious component would shed light on the emission mechanism, which then opens up a new window onto the interstellar medium (ISM). AME is emitted mostly in the frequency range $\sim$10 – 100 GHz, and thus the SKA has the potential of measuring the low frequency side of the AME spectrum, particularly in band 5. Science targets include dense molecular clouds in the Milky Way, as well as extragalactic sources. We also discuss the possibility of detecting rotational line emission from Polycyclic Aromatic Hydrocarbons (PAHs), which could be the main carriers of AME. Detecting PAH lines of a given spacing would allow for a

definitive identification of specific PAH species.

E-mail: Clive.Dickinson@manchester.ac.uk

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http://arxiv.org/pdf/1412.5054v1.pdf

Titan Aerosol Analog Absorption Features Produced from Aromatics in the Far Infrared

Joshua A. Sebree[a,b], Melissa G. Trainer[b], Mark J. Loeffler[b], Carrie M. Anderson[b]

[a] University of Northern Iowa, Department of Chemistry and Biochemistry, Cedar Falls, IA 50614, USA

[b] NASA Goddard Space Flight Center, Solar System Exploration Division, Greenbelt, MD 20771, USA

We present results on the formation of Titan aerosol analogs produced via far-UV irradiation of five aromatic precursors: benzene, naphthalene, pyridine, quinoline and isoquinoline. This is the first reported evidence of far-IR emission features observed below 200 cm^{-1} in laboratory-created Titan aerosols. These laboratory studies were motivated by recent analyses of Cassini Composite Infrared Spectrometer (CIRS) spectra that show a broad aerosol emission feature in the far-IR spectral region centered near 140 cm^{-1}, which is unique to Titans photochemically-produced aerosol (Anderson and Samuelson, 2011). We find that all three of the aerosol analogs formed from nitrogen-containing aromatics have similar broad emission features near that of the observed CIRS far-IR aerosol spectral feature. In addition, the inclusion of 1.5% methane to that of trace amounts of benzene also gives rise to an aerosol with a weak far-IR emission feature located below 200 cm^{-1}.

E-mail: joshua.sebree@uni.edu

Icarus, 236, 146 (2014)

http://www.sciencedirect.com/science/article/pii/S0019103514001651

Press Release

NASA Experiments Recreate Aromatic Flavors of Titan

Benzene formation on interstellar icy mantles containing propargyl alcohol

B. Sivaraman, R. Mukherjee, K. P. Subramanian, and S. B. Banerjee

Space and Atmospheric Sciences Division, Physical Research Laboratory, Ahmedabad, India

Propargyl alcohol ($CHCCH_2OH$) is a known stable isomer of the propenal (CH_2CHCHO) molecule that was reported to be present in the interstellar medium (ISM). At astrochemical

conditions in the laboratory, icy layers of propargyl alcohol grown at 85 K were irradiated by 2 keV electrons and probed by a Fourier Transform InfraRed spectrometer in the mid-infrared (IR) region, 4000-500cm^{1}. Propargyl alcohol ice under astrochemical conditions was studied for the first time; therefore, IR spectra of reported amorphous (85 K) and crystalline (180 K) propargyl alcohol ices can be used to detect its presence in the ISM. Moreover, our experiments clearly show benzene (C_6H_6) formation to be the major product from propargyl alcohol irradiation, confirming the role of propargyl radicals (C_3H_3) formed from propargyl alcohol dissociation that was long expected based on theoretical modeling to effectively synthesize C_6H_6 in the interstellar icy mantles.

E-mail: Bhala@prl.res.in

ApJ, 798, 72 (2015)

http://iopscience.iop.org/0004-637X/798/2/72/article

Meetings

30 Years of Photodissociation Regions:
A Symposium to Honour David Hollenbach's Lifetime in Science

Asilomar, Pacific Grove, USA
28 June - 3 July 2015
http://pdr30.strw.leidenuniv.nl/

We are happy to announce the conference 30 YEARS OF PHOTODISSOCIATION REGIONS: A SYMPOSIUM TO HONOR DAVID HOLLENBACH'S LIFETIME IN SCIENCE. The goal of this meeting is to overview the state of the art in theoretical PDR studies, to review the processes that control the physical and chemical conditions in PDRs and their emission characteristics, to compare and contrast these models with recent observations of PDRs obtained with the Spitzer Space Telescope, the Herschel Space Observatory, the Stratospheric Observatory For Infrared Astronomy, and the Atacama Large Millimeter Array, to connect studies of dense PDRs in regions of star formation to the studies of the evolution of the interstellar medium of galaxies over the history of the Universe, and to link and compare and contrast studies of PDRs to those of regions dominated by X-rays, by turbulence, by shocks, and by cosmic rays. In addition, we take this occasion to celebrate the contributions to this field of one of the pioneers, David Hollenbach.

The scientific topics of this meeting include:

- The Physics and Chemistry of PDRs,
- Models of PDRs,
- Observations PDRs in the galactic environment,
- PDRs & star and planet formation,
- PDRs & the ISM of galaxies, and
- PDRs in starburst, (U)LIRG, and high-z environments.

The format of the meeting will consist of invited reviews, invited talks, contributed papers, and poster papers. A list of invited speakers is available on the website.

VENUE: The Asilomar conference center is a California State Park (http://www.visitasilomar.com) beautifully situated on the coast of the Monterey peninsula in a very quiet and serene setting that we hope will be very conducive to a highly interactive meeting.

SOFIA GRANT: SOFIA has generously provided support for deserving students to defer their room and board during the meeting. Students who wish to be considered for a SOFIA travel grant have to send a letter of motivation plus a supporting letter from their supervisor. Details can be found on the website.

REGISTRATION: Registration is now open. Early registration is encouraged, as the number of participants will be limited to approximately 150.

IMPORTANT DATES:

- **Student grant requests:** February 20th, 2015
- **Registration and Abstract submission deadline:** April 2nd, 2015

We are looking forward to an exciting meeting and hope to welcome you in Asilomar,

SCIENTIFIC ORGANIZING COMMITTEE:

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AstroPAH Newsletter

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astropah@strw.leidenuniv.nl

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Submission deadline: 6 March 2015