

# 249<sup>th</sup> National ACS Meeting

Division of Physical Chemistry

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## Carbon in the Galaxy:

### The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

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Louis J. Allamandola

Timothy J. Lee

Christine Martinez

Organizers

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March 22–26, 2015

Colorado Convention Center

ROOM 502

Sunday Morning (80)

#### *Organic Molecules in Carbon Star Outflows*

Jos Oomens, Presiding

8:00 (8). Lifecycle of cosmic carbon. **A. Tielens**

8:35 (9). Molecular content of carbon-rich evolved stars and the carbon balance from observations at all wavelengths.

**P. Chernicharo**

9:10 (10). Formation of complex organics and carbonaceous grains in the outflow of carbon stars: A laboratory study. **F. Salama**

9:45 *INTERMISSION*

10:15 (11). Synthesis of pure and N-substituted cyclic hydrocarbons (e.g. pyrimidine) via gas-phase ion-molecule reactions. **P.P. Bera**, R.

Peverati, M.P. Head-Gordon, T.J. Lee

10:50 (12). Computational rovibrational spectroscopy and applications to astrochemistry. **R.C. Fortenberry**, X. Huang, W. Morgan, R.A. Theis, T. Crawford, T.J. Lee

11:15 (13). Multiple excited states of PANH anions using informed orbital descriptions. **M.L. Theis**, A. Candian, A. Tielens, T.J. Lee, R.C. Fortenberry

Sunday Afternoon (90)

#### *Organic Molecules in Carbon Star Outflows*

Farid Salama, Presiding

1:30 (67). Observations of organic molecules in carbon-rich proto-planetary nebulae and planetary nebulae. **E. Peeters**

2:05 (68). Dust formation in carbon stars. **I. Cherchneff**

2:40 (69). Ion chemistry of cyclic aromatics and interactions with polar molecules leading to the formation of complex organics in the gas phase and on ice grains. **M. El-Shall**

3:15 *INTERMISSION*

3:45 (70). Laboratory infrared spectroscopy of 'hard-to-get' ionized polyaromatics. **J. Oomens**

4:20 (71). Carbonaceous dust and fullerenes in evolved stars.

**J. Cami**

4:45 (72). Quantum chemical studies of interstellar organic molecules: Formation mechanisms, spectroscopic signatures, and properties. **T.J. Lee**

Monday Morning (70)

#### *Organic Molecules in the Diffuse Interstellar Medium*

Jan Cami, Presiding

8:00 (118). Carbon bearing molecules in interstellar clouds.

**J. Krelowski**

8:35 (119). Molecular laboratory astrophysics: About molecular transients and molecule formation under interstellar conditions.

**H. Linnartz**

9:10 (120). Small Hydrocarbons in Diffuse Clouds and in Photon Dominated Regions. **E. Roueff**

9:45 *INTERMISSION*

10:15 (121). Low temperature formation of polycyclic aromatic hydrocarbons in the Interstellar medium via bimolecular neutral-neutral reactions. **R. Kaiser**

10:50 (122). Angle-resolved PEPICO imaging of the dissociative ionization of methyl azide and methylenimine using a tabletop

high harmonic generation light source. W.K. Peters, **D.E. Couch**, C.W. Hogle, D. Beltran, P. Towstik, D.M. Jonas, H. Kapteyn, M.M. Murnane

11:15 (123). Electronic excited states of interstellar species: Quantum chemical prediction of spectroscopic signatures using quartic force fields. **W.J. Morgan**, R.C. Fortenberry

Monday Afternoon (65)

#### *Organic Molecules in Dense Interstellar Clouds*

Harold Linnartz, Presiding

1:30 (173). Review of the molecular complexity of organic material in the gas-phase ISM. **S.N. Milam**

2:05 (174). Global optimization and broadband analysis software for interstellar chemistry. S.L. Widicus Weaver, **L. Zou**, M. Rad, J. Sanders

2:40 (175). Molecular line lists of carbon-containing molecules for exoplanets and other hot bodies. **J. Tennyson**

3:15 *INTERMISSION*

3:45 (176). Observations of carbon in interstellar and circumstellar ices. **A. Boogert**

4:20 (177). Reliable abundances of extraterrestrial hydrocarbon ices: Interminable quest or end in sight? **R.L. Hudson**, P.A. Gerakines

4:45 (178). Optical properties of Titan haze analogs using photoacoustic and cavity ring-down spectroscopy. **M.S. Ugelow**, K.J. Zarzana, M.A. Tolbert

## Wednesday Morning (65)

### *Organic Molecules in Dense Interstellar Clouds*

**Stefanie N. Milam, Presiding**

**8:00 (271).** Organic molecules in ices and their release into the gas phase. **E. Fayolle**, K. Oberg, R.T. Garrod, E.F. van Dishoeck, M. Rajappan, M. Bertin, C. Romanzin, J. Fillion

**8:35 (272).** Ice chemistry in interstellar dense molecular clouds, protostellar disks, and comets. **S.A. Sandford**

**9:10 (273).** Like a fly and the fire - polycyclic aromatic hydrocarbons (PAHs) in icy environments: A historical perspective. **M.S. Gudipati**

**9:45 INTERMISSION**

**10:15 (274).** Theoretical studies of interstellar ice chemistry involving polycyclic aromatic hydrocarbons and other compounds. **D.E. Woon**

**10:50 (275).** Formation of aromatic heterocycles from the UV-photoirradiation of aromatic hydrocarbons in ices. **C.K. Materese**, M. Nuevo, S.A. Sandford

**11:15 (276).** Infrared spectroscopic properties of polycyclic aromatic nitrogen heterocycles (PANHs): The acridine series. **A.L. Mattioda**, J. Bregman, C. Bauschlicher, A. Ricca, D. Hudgins, L.J. Allamandola

## Wednesday Afternoon (55)

### *Organic Molecules in Dense Clouds and Star and Planet Forming Regions*

**Els Peeters, Presiding**

**1:30 (326).** Complex organic molecules in star-forming regions: Sweet results from ALMA. **E.F. van Dishoeck**

**2:05 (327).** Polycyclic aromatic hydrocarbons as catalysts for interstellar molecular hydrogen formation. **L. Hornekaer**

**2:40 (328).** Modeling grain surface chemistry in dense molecular clouds. **H. Cuppen**, L. Karssemeijer

**3:15 INTERMISSION**

**3:45 (329).** Formation of complex organic molecules in protoplanetary disks. **T. Millar**

**4:20 (330).** Time-domain terahertz spectroscopy of polycyclic aromatic hydrocarbons. **M.A. Allodi**, P. Carroll, S. Ioppolo, B.A. McGuire, G.A. Blake

**4:45 (331).** Tackling the theoretical anharmonic infrared spectra of polycyclic aromatic hydrocarbons. **C. Mackie**, A. Candian, X. Huang, T.J. Lee, A. Tielens

## Thursday Morning

### *PAH-Related Processes*

**Herma Cuppen, Presiding**

**8:35 (564).** Gas phase ion chemistry of complex organic species. **Veronica M. Bierbaum**, C.A. Cole, Z. Wang, T.P. Snow

**9:10 (565).** Tying interstellar PAH emission spectra and (photo)chemistry to local physical conditions in the emission zones. **C. Boersma**

**9:45 INTERMISSION**

**10:15 (566).** Dehydrogenation of PAHs: First steps towards fullerenes in the ISM. **P. Castellanos Nash**, J. Zhen, A. Candian, H. Linnartz, A. Tielens

**10:50 (567).** Photochemical model of the top down formation of fullerenes in the interstellar medium. **O. Berne**, J. Montillaud, C. Joblin

**11:25 (568).** Anharmonic bands in the 3- $\mu\text{m}$  region of acenes: A combined experimental and theoretical study. **A. Petrignani**, E. Maltseva, A. Candian, A. Tielens, J. Oomens, W. Buma

This document was created in a three-column format for printing as a brochure to be distributed at the 249<sup>th</sup> National ACS Meeting. Its format was changed slightly for posting on the Astrochemistry Subdivision's web site (<http://astro.phys-acs.org/>).