

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

Division of Physical Chemistry

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## Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability & Spectroscopic Signatures

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**Ryan C. Fortenberry**  
**M. Samy El-Shall**

**Organizers**

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**Boston Convention Center**

**ROOM 257A**

**August 16-20, 2015**

**Sunday Morning (35)**

*What Astrochemistry Has Taught Chemists*

**Ryan C. Fortenberry, Presiding**

**8:00** Introductory Remarks.

**8:10 (40)**. How astrochemists add to our knowledge of chemistry. **E. Herbst**

**9:00 (41)**. Computing the spectroscopic signatures of molecules in various astrophysical environments: Rotational, rovibrational, and electronic spectroscopy. **T.J. Lee**, X. Huang, P. Bera, R.C. Fortenberry, C. Mackie, A. Candian, A. Tielens

**9:35 INTERMISSION**

**10:05 (42)**. Curious case of NH<sub>2</sub>OH: Hunting a direct amino acid precursor species in the interstellar medium. **B. McGuire**, B. Carroll, K. Dollhopf, G.A. Blake, A. Remijan

**10:40 (43)**. Interplay between ice chemistry and desorption in the dense interstellar medium. **E. Fayolle**, K. Oberg, J. Bergner, D. Graninger, M. Rajappan, M. Bertin, J. Fillion, X. Michaut, C. Romanzin, R. Garrod, E. van Dishoeck

**11:05 (44)**. Formation pathways, reactivity, stability, and structure of astrophysically relevant organic ions. **M.S. El-Shall**

**Sunday Afternoon (35)**

*Inorganic Astrochemistry*

**Brett A. McGuire, Presiding**

**1:30 (93)**. Crossed molecular beams and computational study on the formation of organosilicon molecules in the interstellar medium. **R. Kaiser**, T. Yang, B.B. Dangi, L. Bertels, M.P. Head-Gordon

**2:05 (94)**. Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology? **N.J. Deyonker**, T.N. Brown, K.O. Brown

**2:40 (95)**. Laser detection and characterization of transient gas phase silicon species. **D. Kokkin**, T. Steimle

**3:15 INTERMISSION**

**3:45 (96)**. Spectroscopic and photochemical properties of the nitrogen oxide sulfide (SNO) radical and its isomer. **J.S. Francisco**, R.C. Fortenberry

**4:20 (97)**. Spectroscopic, structural, and energetic analysis of noble gas cations. R.C. Fortenberry, **R.A. Theis**

**Monday Morning (45)**

*Laboratory Techniques*

**M.S. El-Shall, Presiding**

**8:00 (150)**. Selected-ion infrared spectroscopy of small organic cations. **M.A. Duncan**

**8:35 (151)**. Silicon and sulfur analogs of well-known astronomical molecules: Exploring chemistry beyond the first row. **M. McCarthy**, S. Thorwirth

**9:10 (152)**. Laser spectroscopy of interstellar molecules in the laboratory. **T. Schmidt**

**9:45 INTERMISSION**

**10:15 (153)**. Electronic spectroscopy of astrophysically relevant silicon-containing species: Si-terminated carbon chains SiC<sub>n</sub>H (n=3-5), rhomboidal Si<sub>3</sub>C, and Si<sub>2</sub>C. N.J. Reilly, **D. Kokkin**, P.B. Changala, J. Baraban, R.C. Fortenberry, M. Steglich, T. Crawford, J. Maier, J. Stanton, M. McCarthy

**10:50 (154)**. Ultrafast dynamics of methyl azide photodissociation in the far UV. **W.K. Peters**, D.E. Couch, H. Kapteyn, M.M. Murnane

**11:15 (155)**. CUPF: Chirped-pulse microwave spectroscopy in uniform supersonic flows to probe molecular reaction dynamics and photochemistry under astrophysical conditions. **L.N. Zack**, C.S. Abeysekera, N. Ariyasingha, B.Y. Joalland, B. Park, R. Field, I.R. Sims, A.G. Suits

**Tuesday Morning (40)**

*Large Molecules*

**Edith Fayolle, Presiding**

**8:00 (269)**. Spectral features and nanostructuring of soot as analog of the carbonaceous cosmic dust. **T. Pino**, T. Le, L. Gavilan, I. Alata, D. Deldicque, J. Rouzaud, E. Dartois

**8:35 (270)**. Tackling the anharmonic spectrum of polycyclic aromatic hydrocarbons.

**A. Candian**

**9:10 (271)**. PAH clusters and the interstellar infrared emission bands. **J. Roser**, A. Ricca Bauschlicher

**9:45 INTERMISSION**

**10:15 (272)**. Search for sugars and related compounds in residues produced from the UV irradiation of astrophysical ice analogs. **M. Nuevo**, S.A. Sandford, C.K. Materese, G.W. Cooper

**10:50 (273)**. Activation of two weak IR fundamentals of solid methane: The importance of amorphous ices. **R.L. Hudson**, P. Gerakines, M. Loeffler

**Wednesday Morning**  
*Advances in Theory*  
Timothy J. Lee, Presiding

8:00 (352). WITHDRAWN

8:35 (353). Unraveling intermolecular interactions using electronic structure calculations: Theory and applications to polycyclic aromatic hydrocarbon ion molecule complexes. **M.P. Head-Gordon**, R. Peverati

9:10 (354). Deep hydrogen tunneling as an isomerization mechanism in organic species of astrochemical significance. **W.D. Allen**

9:45 INTERMISSION

10:15 (355). Diffusion Monte Carlo approaches for studying rotation/vibration couplings astrochemical ions. **A.B. McCoy**, J.E. Ford, Z. Lin, M. Marlett, A.S. Petit

10:50 (356). Equation-of-motion coupled-cluster methods for metastable electronic states. **T.C. Jagau**, A. Krylov

11:15 (357). Photionization/photodetachment spectroscopy and Dyson orbitals: Theoretical tools to aid experimental studies. **A. Gunina**, S. Gozem, A. Krylov

**Wednesday Afternoon**  
*Spectroscopy*  
William K. Peters, Presiding

1:30 (415). THz time-domain spectroscopy of interstellar ice analogs. **S. Ioppolo**, B. McGuire, X. de Vries, B. Carroll, M.A. Allodi, G.A. Blake

2:05 (416). Structural studies of reactive molecules by rotational spectroscopy: HOON, HOCOH, and C<sub>6</sub>H<sub>5</sub>. **K.N. Crabtree**, C. Womack, O. Martinez, J. Stanton, M. McCarthy

2:40 (417). Rotational effects in the reactions of OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> with H<sub>2</sub> and D<sub>2</sub>. **N. Shuman**, S.G. Ard, O. Martinez, A.A. Viggiano

3:15 INTERMISSION

3:45 (418). Rotational spectroscopy and radio observations of exotic species created via novel laboratory synthesis. **D.T. Halfen**, L.M. Ziurys

4:20 (419). Large amplitude motions and feasible proton permutations in the spectroscopy and dynamics of H<sub>3</sub><sup>+</sup>. **Z. Lin**, A.B. McCoy

**Thursday Morning**  
*Charged Species*  
Reggie L. Hudson, Presiding

8:00 (640). WITHDRAWN

8:35 (641). Reactions of negative ions of astrochemical relevance. **Z. Wang**, C. Cole, T. Snow, V.M. Bierbaum

9:10 (642). Photodestruction and reactive processes of interstellar carbon chain anions. **R. Wester**

9:45 INTERMISSION

10:15. Panel Discussion: *The Future Challenges and Goals of Astrochemistry*  
**R.C. Fortenberry** and **R.L. Hudson**

10:50 (644). Role of low-energy (< 20 eV) electrons in astrochemistry.  
**C.R. Arumainayagam**

11:15 (645). Growth of computational chemistry from the needs of astrochemistry. **R.C. Fortenberry**, R. Thackston, W. J. Morgan



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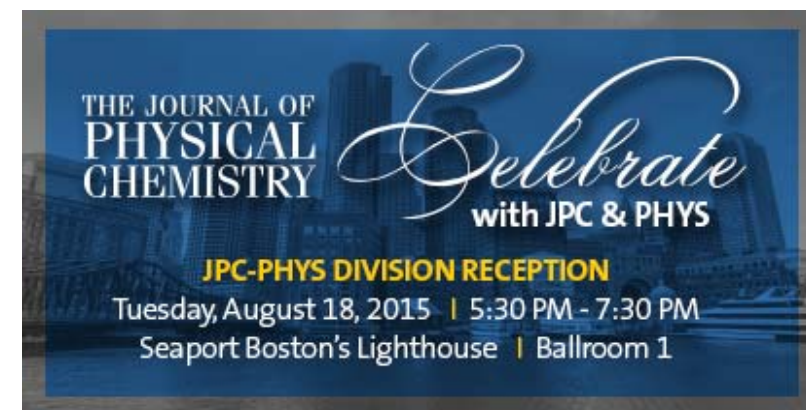
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