

**THURSDAY MORNING (ROOM 160B)**  
***Microwave & Millimeter-Wave Astrochemistry***  
**I. Gordon, *Presiding***

**8:30** Introductory Remarks.

**8:35 (556).** New instrumental and synthetic developments in rotational spectroscopy: A focus on metal-bearing radicals. **L.M. Ziurys**, D.T. Halfen, M. Burton, J. Keogh, P.M. Sheridan

**9:15 (557).** Millimeter-wave spectroscopy of KO: Metal oxides relevant to astrochemistry. **M. Burton**, B. Russ, P.M. Sheridan, M.P. Bucchino, L.M. Ziurys

**9:35 (558).** Spectroscopic characterization of astrophysical isomers: The relatives of ketene. **M. Martin-Drumel**, K. Lee, O. Pirali, J. Guillemin

**9:55 INTERMISSION**

**10:25 (559).** From weeds to dust: Astrochemical insights by rotational spectroscopy. **A. Steber**

**11:05 (560).** Tracing the origins of nitrogen bearing organics toward Orion KL with ALMA. **B. Carroll**, G.A. Blake

**11:25 (561).** From one to two dimensional interstellar carbon: A synthesis of laboratory, observations, and theory. **B. McGuire**, K. Lee, M.C. McCarthy

**THURSDAY AFTERNOON (ROOM 160B)**  
***Condensed-Phase Astrochemistry***  
**K. Oberg, *Presiding***

**1:30** Introductory Remarks.

**1:35 (588).** Study of morphology, diffusion and ordering kinetics of CO<sub>2</sub> and CO<sub>2</sub>/H<sub>2</sub>O thin film ices. **G. Vidali**, J. He, S. Emtiaz

**2:15 (589).** Some subtle problems of ice-phase astrochemistry and spectroscopy. **R.L. Hudson**, P. Gerakines

**2:35 (590).** Laboratory spectroscopy with a miniature mm-wave cavity spectrometer and coupled laser-ablation source. **A. Raymond**, B. Drouin, M. McCarthy, K. Lee, E. Mazur

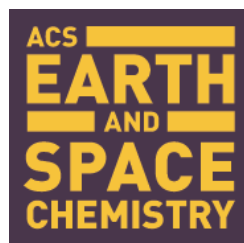
**2:55 INTERMISSION**

**3:25 (591).** Submillimeter spectroscopy of sublimated interstellar ice analogs: A new technique for laboratory astrochemistry. **P. Gerakines**, S.L. Widicus Weaver, S.N. Milam, K. Yocum, H. Smith

**4:05 (592).** Spectroscopic measurements of radicals in outer Solar System ice analogs. **E. Fayolle**, P.V. Johnson, R. Hodyss, X. Zhang, S.P. Sander

**4:25** Concluding Remarks.

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## ACS DIVISION OF PHYSICAL CHEMISTRY

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## NEW SPECTROSCOPIC TECHNIQUES FOR ASTROCHEMISTRY

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**Kyle N. Crabtree**  
**Michael C. McCarthy**  
*Organizers*

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**Boston Convention Center**

**Room 204B**  
(Room 160B on Thursday)

**August 19-23, 2018**

## SUNDAY AFTERNOON

### *Astrochemical Challenges & Opportunities*

K. N. Crabtree, Presiding

1:30 Introductory Remarks.

1:35 (81). Cavity-enhanced millimeter and submillimeter spectroscopy as a probe of reaction dynamics. **S.L. Widicus Weaver**, K. Roenitz, C. Wright, H. Bunn, C. Powers, K. Yocum

2:15 (82). "Grotthuss-like" proton relays in anomalous carbocations dictate spectroscopy, stability and mechanisms: Case studies on small and medium sized non-classical hydrocarbons along with deuterated counterparts.

**S.S. Iyengar**

2:35 (83). Photoelectron-photoion coincidence spectroscopy for laboratory astrochemistry: VUV Photodynamics of radicals, PAHs, sulfur containing compounds and other peculiar molecules. **H.R. Hrodmarsson**, G. Garcia, L. Nahon

2:55 **INTERMISSION**

3:25 (84). Computing rotational, rovibrational, and vibrational spectra for astronomical observations: high accuracy line lists for high temperatures, limited line lists for biosignature molecules, and PAH emission spectra.

**T.J. Lee**

4:05 (85). Utilizing tunable vacuum ultraviolet light for isomer specific detection of complex organic molecules from astrophysical ice analogues: The hydrocarbon chemistry of interstellar ices. **M. Abplanalp**, S. Göbi, R. Kaiser

4:25 (86). Developments in high-resolution spectroscopy of Rydberg states of small molecules. **T. Barnum**, J. Jiang, R. Field

## MONDAY MORNING: *New Experimental Methods*

M. C. McCarthy, Presiding

8:30 Introductory Remarks.

8:35 (132). Terrestrial progress toward infrared spectroscopy/detection of hydrocarbon radicals and molecular ions in the interstellar medium.

**D.J. Nesbitt**

9:15 (133). Preparation, characterization and storage of water vapours highly enriched in its ortho-H<sub>2</sub>O nuclear spin isomer. **P. Ayyotte**, J. Vermette, I. Braud, P. Turgeon, X. Michaut, G. Alexandrowicz

9:35 (134). Sub-THz cavity enhanced absorption with a conventional confocal Fabry-Perot resonator. **K. Truitt**, R. O'Neal, J. Bracewell, **L. Duffy**

9:55 **INTERMISSION**

10:25 Buffer-gas cell and molecular beam sources for chirality-sensitive spectroscopy and population transfer experiments. **C. Perez**, A. Steber, D. Patterson

11:05 (136). AC Stark effect observed in a microwave-(sub)millimeter wave double resonance experiment. **K. Roenitz**, B. Hays, C. Power, M.N. McCabe, H. Smith, S.L. Widicus Weaver, S.T. Shipman

11:25 (137). Determination of the sign of the population difference in a two-level system by frequency-modulation spectroscopy. **J. Jiang**, Z. Du, R. Field

## MONDAY AFTERNOON

### *Optical & Infrared Astrochemistry: Large Molecules*

S. Widicus-Weaver, Presiding

1:30 Introductory Remarks.

1:35 (191). Triple-resonance laser spectroscopy of protonated PAHs.

**T.W. Schmidt**, S. Kable, K. Nauta, O. Krechkivska

2:15 (192). Rotationally-resolved infrared frequency comb spectroscopy of the C<sub>60</sub> fullerene. **M.L. Weichman**, P.B. Changala, T.Q. Bui, K. Iwakuni, J.F. Niedermeyer, K.F. Lee, M.E. Fermann, J. Ye

2:55 **INTERMISSION**

3:25 (193). Interstellar PAHs: From ground to space, expanding spectroscopic frontiers. **F. Salama**

4:05 (194). Infrared spectra of protonated and hydrogenated corannulene (C<sub>20</sub>H<sub>10</sub>) and sumanene (C<sub>21</sub>H<sub>12</sub>) in solid para-hydrogen. **P. Sundararajan**, M. Tsuge, Y. Lee

4:25 (195). Validating the recent identification of interstellar C<sub>60</sub><sup>+</sup> using VLT UVES and a new method for high-signal-to-noise HST STIS spectroscopy.

**M. Cordiner**, N. Cox, R. Lallement, F. Najjarro, J. Cami, T. Gull, B. Foing, H. Linnartz, D. Lindler, C. Proffitt, P. Sarre, S. Charnley, J. Smoker, A. Fahrang, M. Elyajouri, E. Consortium

## TUESDAY MORNING

### *Optical & Infrared Astrochemistry: Small Molecules*

K. L. K. Lee, Presiding

8:30 Introductory Remarks.

8:35 (247). Broad bandwidth laser frequency combs for terrestrial and astronomical spectroscopy. **S. Diddams**

9:15 (248). Purified *para* and *ortho*-water for fundamental physics and chemical reactions. **J. Kupper**

9:35 (249). Probing vibrationally excited states of astrophysically important species by stimulated emission pumping (SEP) spectroscopy. **N. Reilly**

9:55 **INTERMISSION**

10:25 (250). Spectroscopy of an argon-oxygen covalent bond in the ArOH<sup>+</sup> cation. J.P. Wagner, D. McDonald II, **M.A. Duncan**

10:45 (251). Accuracy of spectroscopic constants predicted by explicitly correlated methods. **M. Gronowski**

11:05 Infrared spectrum of H<sub>3</sub><sup>+</sup> as the probe for cosmic rays. **T. Oka**

## WEDNESDAY MORNING

### *Solar System & Planetary Atmospheres*

S. Brünken, Presiding

8:30 Introductory Remarks.

8:35 (309). Spectroscopy and data science in the service of planetary remote sensing: the HITRAN and HITEMP databases. **I. Gordon**, L.S. Rothman, R.V. Kochanov, Y. Tan, C. Hill

9:15 (310). The ExoMol atlas of cool star and exoplanet molecular opacities. **J. Tennyson**, S. Yurchenko

9:35 (311). Novel metalorganic compounds revealed in meteorites.

**A. Ruf**, P. Schmitt-Kopplin

*Winner of Best Dissertation Award from the Astrochemistry  
Subdivision: Alexander Ruf*

9:55 **INTERMISSION**

10:25 (312). Infrared and near-infrared spectroscopy of hot molecules for exoplanets. **P.F. Bernath**

11:05 (313). Inelastic collisions dynamics of optically-centrifuged high-J molecules: Transient spectroscopy beyond the sudden regime.

**A.S. Mullin**

11:25 (314). Pyrolysis and matrix-isolation FTIR spectroscopy for characterization of astrochemically significant radicals. G.J. Brown, M.J. Ellis, **L.R. McCunn**

## WEDNESDAY AFTERNOON

### *Kinetics & Dynamics*

L. M. Ziurys, Presiding

1:30 Introductory Remarks.

1:35 (367). Rotational and vibrational action spectroscopy of reactive hydrocarbon cations: Intermediates in interstellar carbon chemistry.

**S. Brünken**, P. Jusko, O. Asvany, B. Redlich, S. Schlemmer

2:15 (368). Metastable atomic spectroscopy (MAS) of the N(<sup>2</sup>D<sub>j</sub>) atoms using photofragment excitation spectroscopy (PHOFEX) and a slice imaging time of flight mass spectrometer (SI-TOF-MS). Y.C. Chang, K. Liu, K. Kalogerakis, C. Ng, **W.M. Jackson**

2:35 (369). High-resolution photoelectron imaging of C<sub>n</sub>P<sup>+</sup> clusters: Towards their possible detection in the interstellar medium.

**G. Kocheril**, J.G. Czekner, L. Cheung, L. Wang

2:55 **INTERMISSION**

3:25 (370). IR spectroscopy and ice kinetics. **K. Oberg**, J. Bergner, I. Cooke

4:05 (371). Chirped-pulse microwave spectroscopy in uniform supersonic flows: Isomer-specific branching in photodissociation of propargyl radical. **B. Broderick**, N. Suas-David, N. Dias, A.G. Suits  
4:25 (372). Formation of HC<sub>3</sub>N in space environments. M. Fournier, B. Joalland, S. Cheikh Sid Ely, J. Guillemin, S.J. Klippenstein, **I.R. Sims**