

247th National ACS Meeting

Division of Physical Chemistry

Chemistry in the Interstellar Medium: New Frontiers in Laboratory, Theory, and Observations

Eric Herbst

Ralf I. Kaiser

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Organizers

Dallas Convention Center

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Sunday Morning, ROOM C154

Molecular Observations

Susanna Widicus Weaver, *Presiding*

8:30 (39). Probing the interstellar origin of carbon and nitrogen-bearing organics in our solar system. [Edwin A. Bergin](#), Nathan R. Crockett, Geoffrey A. Blake

9:05 (40). New carbon-chain chemistry found in solar-type star-forming regions. [Nami Sakai](#), Satoshi Yamamoto

9:40 (41). Interstellar ice diffusion and desorption. [Karin I. Oberg](#)

10:15 INTERMISSION

10:45 (42). Protoplanetary disks: A unique laboratory for astrochemistry. [Catherine Walsh](#), Tom J Millar, Hideko Nomura, Susanna Widicus Weaver, Eric Herbst, Ewine F van Dishoeck

11:20 (43). Chemical tracers of episodic accretion bursts in embedded protostars. [Ruud Visser](#), Jes K Jorgensen, Edwin A Bergin

11:40 (44). Unraveling the identity of B11244 ($L\text{-C}_3\text{H}^+/\text{C}_3\text{H}^-$): An observational approach. [Brett A McGuire](#), P Brandon Carroll, Geoffrey A Blake, Anthony J Remijan

Sunday Afternoon, ROOM C154

Ice and Surface Chemistry

Ralf Kaiser, *Presiding*

1:30 (87). Non-thermal desorption from icy grain mantles: Is hydrogen bonding important? Mark P Collings, [Martin R S McCoustra](#)

2:05 (88). Oxygen chemistry on stardust. [Gianfranco Vidali](#), Jiao He, Dapeng Jing

2:40 (89). Diffusion of hydrogen atom on amorphous solid water: Thermal or tunneling? [Naoki Watanabe](#), Kazuaki Kuwahata, Tetsuya Hama, Akira Kouchi

3:15 INTERMISSION

3:45 (90). Formation of complex organic molecules in astrophysical ice analogs: A mechanistic approach. [Fabrice Duvernay](#), Vassilissa Vinogradoff, Gregoire Danger, Patrice Theulé, Thierry Chiavassa

4:05 (91). Surface formation of water in interstellar ice analogs. [Thanja Lamberts](#), Sergio Ioppolo, Herma Cuppen, Gleb Fedoseev, Fabrizio Puletti, Harold Linnartz

4:25 (92). Quantifying IR spectral measurements of icy solids of the ISM and the outer solar system: A new spectral database. [Reggie L Hudson](#), Marla H Moore, Robert F Ferrante, Perry A Gerakines, Mark J Loeffler

Monday Morning, ROOM C154

Large Molecules in Space

Els Peeters, *Presiding*

8:30 (129). Chemistry in nano and outer space. [Harold Kroto](#)

9:05 (130). Astronomical polycyclic aromatic hydrocarbons: Yesterday, today, and tomorrow. [Louis J Allamandola](#)

9:40 (131). Cosmic fullerenes. [Jan Cami](#)

10:15 INTERMISSION

10:45 (132). Infrared spectra of protonated coronene and its neutral counterpart in solid parahydrogen: Implications for the unidentified interstellar infrared emission bands. Mohammed Bahou, Yu-Jong Wu, [Yuan-Pern Lee](#)

11:20 (133). Low temperature pathways of PAH formation in the interstellar medium. [Ralf I Kaiser](#)

11:40 (134). Organism/organic exposure to orbital stresses (O/OREOS) satellite: Radiation exposure in LEO and supporting laboratory studies. [Andrew Mattioda](#), Amanda Cook, Richard Quinn, Andreas Elsaesser, Pascale Ehrenfreund, Alessandra Ricca, Nykola C. Jones, Søren Hoffmann, Antonio Ricco

Monday Afternoon, ROOM C154

Chemical Kinetic Simulations

Eric Herbst, *Presiding*

1:30 (174). Eta Carinae: Astrochemistry in an extreme environment. [T J Millar](#), M A Cordiner, S B Charnley, S N Milam, T R Gull

2:05 (175). 3D off-lattice Monte Carlo simulations of interstellar grain chemistry and ice structure. [Robin T Garrod](#)

2:40 (176). Kinetic Monte Carlo simulations of interstellar grain surface chemistry. [Herma M. Cuppen](#), Thanja Lamberts, Xander de Vries

3:15 INTERMISSION

3:45 (177). Atomic-scale simulations of atomic and molecular mobility in models of interstellar ice. [Stefan Andersson](#), Bethmini Senevirathne, W. M. C. Sameera, Pavel Elkind, Gunnar Nyman

4:05 (178). Nested sampling for parametric chemical models: Constraining nitrogen chemistry and physical conditions in diffuse clouds. [Richard Rollins](#), Jonathan Rawlings, Serena Viti, Filipe Abdalla, Sreekumar Balan

4:25 (179). Formation mechanisms of PAHs by gas phase and intracluster ion-molecule reactions. [M. Samy S El-Shall](#)

Wednesday Morning, ROOM C154

Gas Phase Chemistry

Stephan Schlemmer, *Presiding*

8:30 (229). Laboratory studies of gas phase ion chemistry relevant to the interstellar medium. Veronica M. Bierbaum

9:05 (230). Combining experimental techniques for comprehensive astrophysical case studies. Holger Kreckel, Florian Grussie, Aodh P. O'Connor, Arno Becker, Philipp Herwig, Claude Krantz, Oldřich Novotný, Stephen Vogel, Andreas Wolf

9:40 (231). Ion traps for the laboratory study of extreme environments: Kinetics at low temperatures and pressures. Mark A. Smith

10:15 INTERMISSION

10:45 (232). Exotic chemistry in circumstellar environments: Laboratory and astronomical studies. Lucy M Ziurys

11:20 (233). HF formation from the $F(^2P_1) + H_2$ reaction at very low temperatures. Meryem Tizniti, Sébastien D Le Picard, François Lique, Coralie Berteloite, André Canosa, Millard Alexander, Ian R Sims

11:40 (234). High-resolution IR spectra of trans and cis-HOCO and H_5^+ using MULTIMODE and ab initio potential and dipole moment surfaces. Joel Bowman, Stuart Carter, Yimin Wang

Wednesday Afternoon, ROOM C154

Theory; Joel Bowman, *Presiding*

1:30 (274). Recent advances in electronic structure methods with applications to hydrocarbon association and growth mechanisms. Martin Head-Gordon, Roberto Peverati, Partha Bera, Timothy J. **2:05 (275).** Applications of quantum chemistry to astrochemistry: Spectroscopic signatures, properties, and formation mechanisms. Timothy J Lee

2:40 (276). Theory of radiative electron attachment to molecules: Benchmark study of CN^- . Viatcheslav Kokoouline, Nicolas Douguet, Samantha Fonseca dos Santos, Olivier Dulieu, Maurice Raoult, Ann Orel

3:15 INTERMISSION

3:45 (277). Polarizing and electrons charge effects for the formation of CH_2O on surfaces of water icy dust particles. Albert Rimola, Mariona Sodupe, Piero Ugliengo, Cecilia Ceccarelli

4:05 (278). Comparing astrochemical reactions in the gas phase and on icy grain mantles: $C^+ + H_2O$. David E Woon

4:25 (279). Electronically excited states of interstellar anions. Ryan C Fortenberry

Thursday Morning, ROOM C147

Spectroscopy

Frank De Lucia, *Presiding*

8:30 (453). Centimeter-wave rotational spectroscopy: A stepping-stone to the FIR and beyond. Michael McCarthy

9:05 (454). High-precision and high-accuracy rovibrational spectroscopy of astrochemically important molecular ions. James N. Hodges, Adam J. Perry, Benjamin J. McCall

9:40 (455). Detection of aldehydes, ketones and alcohols via reflectron time-of-flight mass spectroscopic analysis of astrophysically relevant ices exposed to ionization radiation. Brant M Jones, Surajit Maity, Ralf Kaiser

10:15 INTERMISSION

10:45 (456). Cold ion chemistry in space and laboratory. Stephan Schlemmer

11:20 (457). THz time-domain spectroscopy of interstellar ice analogs. Sergio Ioppolo, Marco A. Allodi, Brett A. McGuire, Geoffrey A. Blake

11:40 (458). Investigation of prebiotic molecules using $O(^1D)$ insertion reactions. Brian M Hays, Althea A. M. Roy, Nadine Wehres, Jake C. Laas, Bridget A. DePrince, Susanna L. Widicus Weaver

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Wednesday Evening Poster Session

Hall F; 6:00 to 8:00 PM

(286). Effects of water on sulfur chemistry in planetary atmospheres. Jay A Kroll, Veronica Vaida

(287). Analyses of volatile organic compounds and organic refractory residues coming from the heating of cometary/interstellar ice analogs: An insight in complex astrophysical chemistry. Gregoire Danger, Ninette Abou Mrad, Aurelien Fresneau, Fabrice Duvernay, Thierry Chiavassa

(288). Role of quantum tunneling for the formation of H_2O by reaction of H_2 with OH on interstellar grains. Yasuhiro Oba, Naoki Watanabe, Tetsuya Hama, Kazuaki Kuwahata, Hiroshi Hidaka, Akira Kouchi

(289). Calculations of rotationally inelastic scattering cross sections of hydrogen molecules by helium atoms using mixed quantum/classical theory. Alexander Semenov

(290). Interstellar anion states: Experiment theory and correlations. Edward C M Chen, Reece Rosenthal, Tristan Lim, Spencer Chang, Edward S. Chen

(291). WITHDRAWN

(292). Low-energy electron-induced chemistry of condensed methanol: Implications for the interstellar synthesis of prebiotic molecules. Mavis D Boamah, Katie Shulenberg, Michael Boyer, Karen Atkinson, Chris Arumainayagam

(293). Dynamics of adsorbed CO on amorphous and crystalline water ices. Leendertjan Karssemeijer, Herma Cuppen

(294). Reaction mechanisms between CH ($X^2\Pi$) and CH_4 , C_2H_2 , C_2H_4 , and C_2H_6 : An ab initio study. Joao Marcelo L Ribeiro, Alexander Mebel

(295). Electronic structure of vanadium monochloride cation (VCl^+): At the crossroads of experimental and computational astrochemistry. Nathan J. DeYonker, DeWayne T. Halfen, Lucy M. Ziurys, Wesley D. Allen

(296). Critical influence of ionization in protoplanetary disks on the process of deuterium fractionation. Ilse Cleeves, Edwin A Bergin, Fujun Du

(297). Mass-analytical tool for reactions in interstellar ices (MATRIICES). Daniel M Paardekooper, Jean-Baptiste Bossa, Karoliina Isokoski, Harold. Linnartz. Mourad Frites, Shahed U. M Khan

(298). Porosity measurements of interstellar ice mixtures using optical laser interference and extended effective medium approximations. Jean-Baptiste Bossa, Karoliina Isokoski, Paardekooper M Daniel, Maelle Bonnin, Ellen P van der Linden, Thomas Triemstra, Stephanie Cazaux, Alexander G. G. M. Tielens, Harold Linnart