Thursday Morning
Modeling: ISM/Clouds & (Exo)Planetary Atmospheres
Herma Cuppen, *Presiding*

8:30: (626). Help is needed: Some current astrochemical problems. **E. Herbst**
9:05: (627). Astrochemical kinetic models of dark molecular clouds: Statistical methods and TMC-1. **D. Maffucci**, E. Herbst
9:25: (628). Deuterium fractionation from molecular clouds to protoplanetary disks: Modeling and observation. **L. Majumdar**
9:45: (629). The unusual dynamics and chemistry in planetary nebulae. **L.M. Ziurys**, D. Schmidt, L.N. Zack, N. Woolf
10:05: (630). Modeling the chemistry in the complex outflows of supergiant stars. **D. Schmidt**, G. Adande, L.M. Ziurys
10:25 Intermission.
10:45: (631). Atmospheric chemistry on Venus: An overview of unresolved issues. **F. Mills**, E. Marcq, Y. Yung, C. Parkinson, K. Jessup, A. Vandaele
11:20: (632). Modeling exoplanet atmospheric chemistry in the era of the James Webb Space Telescope. **S. Horst**

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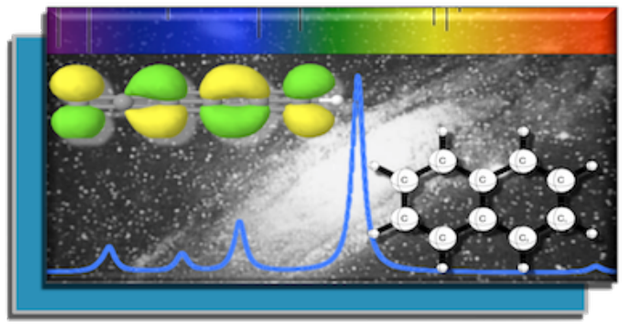

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ACS DIVISION OF PHYSICAL CHEMISTRY

Quantum Chemistry, Dynamics and Reaction Modeling for Molecules and Materials in Astrophysical Environments

David Woon
Herma Cuppen
Organizers

Morial Convention Center
Room 225

March 18-22, 2018

Cosponsored by CATL, ENFL, and INOR

Sunday Afternoon
Spectra & Properties
David. E. Woon, *Presiding*

1:30 Introductory Remarks.
1:35 (86). Accurate structure and spectroscopy of small molecular systems of astrophysical interest. T. Trabelsi, **J.S. Francisco**
2:10 (87). Quantum-chemical needs from the viewpoint of the Cologne Database for Molecular Spectroscopy. **H.S. Müller**
2:45 (88). Spectroscopic characterization of key aromatic and heterocyclic molecules: A route toward the origin of life. **C. Puzzarini**, V. Barone, J. Bloino, N. Tasinato
3:05 Intermission.
3:25 (89). Answering unique spectroscopic and astrochemical problems through quantum chemistry. **R.C. Fortenberry**, K.A. Kloska, J.P. Layfield, C.M. Novak, T.J. Lee
4:00 (90). Exploring the rotational and far infrared spectra of non-rigid species using highly correlated ab initio methods. **M.S. Senent**
4:35 (91). Infrared spectra of interstellar complex organic molecules: accurate energies and intensities by an anharmonic perturbative treatment. **J. Bloino**, A. Baiardi, C. Puzzarini, V. Barone
4:55 (92). Chocolate molecules in space: Utilizing tunable vacuum ultraviolet light for isomer specific detection of complex organic molecules from astrophysical ice analogues. **M. Abplanalp**, S. Góbi, A. Bergantini, A.M. Turner, R. Kaiser

Monday Morning
Spectra & Properties/Gas-Phase Collisions
Ryan C. Fortenberry, *Presiding*

8:30 (134). Spectroscopic, theoretical, and observational study of aminomethanol, a predicted interstellar precursor to glycine. **S.L. Widicus Weaver**, B. Hays, M. McCabe, C. Powers, J. McMillan, S. Zinga
9:05 (135). Probing magnetic fields with methanol masers and ro-vibrational collision rates for modeling protoplanetary disks. **G.C. Groenenboom**, B. Lankhaar, A. van der Avoird
9:40 (136). Exploration of the structure and spectrum of CH_5^+ using diffusion Monte Carlo. **A.B. McCoy**, M.E. Fore
10:00 (137). Inorganic computational astrochemistry: Rovibrational quartic force fields. **N.J. Deyonker**, R.C. Fortenberry, Q. Cheng
10:20 (138). Diffuse interstellar bands and the pseudo-Jahn-Teller distortion in C_{60}^+. S. Ahmadvand, A.O. Lykhin, **S.A. Varganov**
10:40 Intermission.
11:00 (139). Computing collisional energy exchange: Theory, old and new, and comparison with experiments. **L. Wiesenfeld**
11:35 (140). Full-dimensional quantum dynamics of CO, CN, SiO, and CS in collisions with H_2. **B. Yang**, P. Zhang, C. Qu, P. Stancil, J.M. Bowman, B. Naduvalath, R. Forrey
12:10 (141). Mixed quantum/classical theory of molecular collisions: Applications to rotational-vibrational Inelastic scattering in astrophysical environments. **D. Babikov**

Monday Afternoon
Gas-Phase Reactions
Dahbia Talbi, *Presiding*

1:30 (188). High accuracy ab initio kinetics as a tool for astrochemistry. **S.J. Klippenstein**
2:05 (189). Nonadiabatic dynamics in warm dense matter and small molecules. **A.V. Akimov**
2:25 (190). State-of-the-art thermochemical and kinetic computations for complex organic molecules: Gas-phase formation routes in cold interstellar clouds. **V. Barone**, N. Tasinato, J. Bloino, D. Skouteris, C. Puzzarini
2:45 (191). Kinetic measurements of CO^+ and CO_2^+ reactions with N and O atoms for models of planetary atmospheres and the interstellar medium. J. Tenewitz, T. Le, S.G. Ard, N. Shuman, A.A. Viggiano, **J. Melko**
3:05 Intermission.
3:25 (192). Reaction mechanisms and rate constants of PAH growth in astrophysical environments. **A.M. Mebel**
4:00 (193). Dynamics of pure and N-substituted cyclic aromatic hydrocarbon formation in the gas-phase. **P. Bera**, T. Stein, M.P. Head-Gordon, T.J. Lee
4:35 (194). Modelling dehydrogenation in interstellar PAHs. P. Castellanos, **A. Candian**, H. Linnartz, X. Tielens

Tuesday Morning
Gas-Phase Reactions
Stephen J. Klippenstein, *Presiding*

8:30 (254). Withdrawn
9:05 (255). Nonadiabatic dynamics of silicon chemistry. **A.H. Chang**, R. Kaiser
9:40 (256). Reaction rates and mechanism for the reaction of electronically excited sulfur dioxide with alkanes. **J.A. Kroll**, V. Vaida
10:00 (257). Theoretical investigation of possible formation routes of interstellar SiS. M. Rosi, L. Mancini, N. Balucani, N. Faginas Lago, C. Ceccarelli, B. Le Floch, **D. Skouteris**, L. Podio, C. Codella, F. Fontani
10:20 Intermission.
10:40 (258). How to obtain accurate diabatic surfaces governing the dissociative recombination of astrophysical ions. **D. Talbi**, D. Kashinski, P. Hickman
11:15 (260). High accuracy thermochemistry and kinetics of the HCN/HNC system. **K. Lee**, M.C. McCarthy
Note that abstract 259 (Largo) was withdrawn

Wednesday Morning
Surface Interactions/Grain Chemistry
Thanja Lamberts, *Presiding*

8:30 (308). Off-lattice microscopic Monte Carlo kinetics models of interstellar and laboratory ices. **R.T. Garrod**
9:05 (309). A hybrid QM/MM approach to calculate binding energies of radical species on crystalline water ice. **W.C. Sameera**, B. Senevirathne, S. Andersson, G. Nyman
9:40 (586). Detailed study of the formation of sugar derivatives produced by the UV irradiation of astrophysical ice analogs. **M. Nuevo**
10:00 (311). Simulations of energy dissipation and non-thermal desorption on amorphous solid water. **A. Fredon**, H. Cuppen
10:20 Intermission.
10:40 (312). Role of grain surfaces in astrochemical processes. **A. Rimola**, P. Ugliengo, C. Ceccarelli, **N. Balucani**, **M. Sodupe**
11:15 (313). Experimental studies on the surface reaction of hydrogen sulfide with deuterium atoms on amorphous solid water at 10 K. **Y. Oba**
11:50 (314). Reaction experiments on H exposure of solid methanol at low temperatures. **Y. Yarnall**, H. Hidaka, Y. Oba, T. Hama, A. Kouchi, N. Watanabe

Wednesday Afternoon
Grain Chemistry / Modeling: Protostellar Disks
Robin T. Garrod, *Presiding*

1:30 (359). Reactivity of atoms and molecules on interstellar ice analogs at low temperatures. **T. Lamberts**, J. Kästner
2:05 (360). Methanol-containing ice mantle on collision with OH^-: A dust grain reaction through quantum *ab initio* molecular dynamic. **N. Inostroza**
2:40 (361). Mechanisms of SiO oxidation: Implications for dust formation. **S. Andersson**
3:00 (587). Quantum chemical calculations on the metal-bearing dicarbines and experimental verification. **D. Halfen**
3:20 Intermission.
3:40 (363). New constraints on the chemistry of planet formation. **E. Bergin**
4:15 (364). Gaining insights into protoplanetary disk conditions from chemistry. **U. Gorti**