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Special Issue Preface

10 Years of the ACS PHYS Astrochemistry Subdivision

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The Astrochemistry Subdivision of the PHYS Division of the American Chemical Society recently celebrated its 10th anniversary. This interdisciplinary field of chemists, astronomers, and astrophysicists existed well before the subdivision was created, but the gathering of like-minded scientists into an associated group has truly fostered exceptional growth in this area. The ACS PHYS Astrochemistry Subdivision, along with our sister organization, the Laboratory Astrophysics Division of the American Astronomical Society, has provided a meeting place of ideas for researchers who previously were often isolated from one another across geographic and even disciplinary boundaries.

In the ten years since its founding, the subdivision has sponsored 14 symposia at ACS national meetings and many others at regional and even international meetings. The subdivision started with dedicated leadership from Ralf Kaiser of the University of Hawaii and Arthur Suits, then of Wayne State University (now at the University of Missouri−Columbia), as well as a strong membership of more than 100 individuals that has now grown to nearly 700, roughly half of whom are undergraduate or graduate students, in recent years. The list of ACS Astrochemistry Subdivision Chairs has included experimental, observational, and theoretical chemists in junior, midcareer, and senior scientist positions, showing the breadth of the field.

Astrochemistry is typically thought of as an interdependent triangle consisting of observation, modeling, and laboratory/theoretical insights. Each of these legs informs the others, making practitioners of this field consummate chemists, conscientious collaborators, and capable communicators. As a result of the demands that nonterrestrial conditions place on the nature of the research, astrochemists have pushed research technology to new depths. For instance, they have developed and interfaced new experimental techniques beyond the traditional, but still powerful residual gas analyzer−infrared spectroscopy approach to space simulation chambers. These include molecular beam experiments, photoionization techniques, and microwave spectroscopy connected to ice simulation experiments. These experiments and their complementary theoretical predictions are imperative to provide data on formation mechanisms and absolute production rates of new molecules in extreme environments rather than speculating on formation processes from astronomical observations alone. Consequently, well-defined and better-refined reaction data can be incorporated into astrochemical models, and these models, along with experimental and/or theoretical spectral benchmarks, drive subsequent observations showcasing the interdependency of three prongs of astrochemistry research. Furthermore, emerging technologies and insights have enabled astrochemists to question instances of the often-utilized phrase "It is well established that ..." Very often, nothing is "well established." Concepts such as polycyclic aromatic hydrocarbon (PAH) formation at high temperatures, ion−molecule dominated interstellar chemistry, and solely grain-surface chemistry were often speculated (and extrapolated) and carried over from one generation of students to the other without questioning them. However, the establishment of the ACS Astrochemistry Subdivision has (at least partly) provided a forum where these misconceptions can be openly questioned and discussed. Such corroboration between the apexes of the astrochemistry triangle and fresh analysis of previously held concepts, both fostered by ACS Astrochemistry, has significantly pushed astrochemistry forward in the past decade to fully classify newly observed molecules in deep space driven by physical chemistry.

This virtual special issue is a celebration of astrochemistry. It showcases novel and, yet, quintessential cutting-edge astrochemistry research highlighting the interdisciplinary, cooperative, and forward-looking nature of this field. The contributions to this issue are largely from speakers involved in two symposia that took place during 2021: "Elucidating the Interstellar Chemistry of Silicon" held during the 2021 ACS Fall Meeting and "Misconceptions in Astrochemistry" as part of the 2021 Pacifichem meeting. Broadly speaking, this issue encompasses three areas of ongoing astrochemistry research reminiscent of the astrochemistry triangle. These include the creation and analysis (and astronomical search) for molecules new to science, experimental exploration and modeling of novel chemical reactions, and advances in spectral characterization techniques and unique molecular treatments. Multiple manuscripts overlap several of these three areas, but each has a unique role to play in informing various astrophysical insights ranging from the chemical inventory of the observable universe to how meaningful spectra can be produced and even to how molecules

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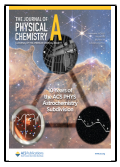

combine with one another in space in order to produce new chemistry and chemical reactions.

To start, two manuscripts in this work focus, at least in part, on the observational portion of astrochemistry. One is an extension of the GOTHAM project where a search for heterocyclic species containing nitrogen, oxygen, and sulfur does not return any new detections in the Taurus Molecular Cloud.[1] Similarly, a radioastronomical search for methoxyacetone and methyl methoxyacetate does not find any correlating spectral features in Sagittarius B2(N), a giant molecular cloud found close to the center of the Milky Way Galaxy, even though new laboratory data are produced for comparison.[2] In spite of the negative results of these searches, these studies are providing new spectral data and exploring the possible natural formation of molecules with little previous impetus to examine.

This virtual special issue also contains other studies employing exceptionally creative experimental techniques and equally inventive synthetic approaches in order to provide a complete picture of additional, novel molecules. Most notably, one manuscript reports that silicon carbide grains in conditions like those found in late-stage circumstellar envelopes will produce buckyballs and nanotubes,[3] confirming in large part Nobel Laureate Sir Harry Kroto's original idea about the astrophysical formation of these carbon allotropes. Examples of other novel molecules with potential astrochemical significance include 2-aza-1,3-butadiene,[4] the C_7H_5 radical,[5] functionalized buckyballs in the form of $C_{60}O^+$ and $C_{60}OH^+$,[6] the 1-quinolinium ($C_9H_7NH^+$) cation along with its corresponding neutral and hydrogenated radicals,[7] cyano-cyclopentadiene ions,[8] the simplest aminooxycarbene in aminohydroxymethylene ($H_2N-\ddot{C}-OH$),[9] 1-cyanocyclobutene (C_5H_5N),[10] monocyclic carbon ring cations of the form C_{2n}^+,[11] the phenalenyl radical,[12] and isomers of the PAH $C_{16}H_{10}^+$.[13] Purely theoretical studies are providing characterization for other unique molecules including glycolic acid,[14] pyridyl radicals,[15] and diazirine along with its cyclic isomers.[16] Additionally, the molecular structure and spectra of noncovalent interactions are also characterized through a mixture of theory and experiment for glycerol−water clusters,[17] HCN and CH_3Cl clusters,[18] and complexes of $NH_3\cdots CO$.[19]

The extreme conditions of various astrophysical environments also open novel chemistry. However, such reactions can only be interrogated through the use of emerging and cutting-edge experimental and theoretical techniques. Of particular note is the formation of prebiotic molecules (such as acetaldehyde, urea, and, tentatively, glycine) from water, ammonia, and carbon dioxide ices.[20] However, this is hardly the only novel result. In this virtual special issue, N_2O is reacted with $C(^3P)$, producing rate coefficients for such chemical processes,[21] and a similar study on fluoromethane and calcium atomic cations is also reported.[22] Additionally, the deuterated ethynyl radical is reacted with propylene producing a wealth of hydrocarbons,[23] NO + the propargyl radical generates branching ratios for eight common astrochemical products,[24] furan + H_2 reactions generate various c-C_4H_xO (x = 4−8) species,[25] myriad nitrous oxides are synthesized in H_2O-N_2O/N_2 ice mixtures,[26,27] dinitriles are shown to be produced from gas-phase reactions of cyano radicals and cyanoethane,[28] and porous amorphous solid water appears to catalyze interstellar organic chemistry.[29] From theory, the earliest molecule in the universe (HeH^+) is most efficiently rotationally excited by collisions with H_2,[30] H_2CCS and HCCSH are likely not detected since they are destroyed through barrierless reactions with atomic hydrogen,[31] and MgNC reacts with water clusters to produce the known HMgNC molecule along with other Mg-containing species.[32] Even large molecules are explored in this work where five-membered rings can be produced in PAHs subsequent to their functionalization,[33] and water is shown to stick better to PAH clusters as the number of monomers in the cluster increases.[34]

Spectral characterizations and techniques necessary for subsequent astrochemical experiments, modeling, and observation are also provided in this virtual special issue. Non-minima conformers of carbonic acid clusters appear to be required for producing experimentally-observed UV spectra,[35] while the mid-IR spectrum of methane ice shows that the thickness of methane ice layers plays a role in its phase characterization.[26] Furthermore, new vibronic spectral features of N-heterocyclic PAHs are established,[36] the far-IR spectrum of *syn*-vinyl alcohol is recorded in detail,[37] the C−D stretches and C−H stretches in phenylacetylene (ethynyl benzene) are established,[38] the theoretically computed cascade IR emission spectra of PAHs are shown to exhibit red-shaded wings while the C−H stretches are affected by resonance interactions,[39] the rovibrational spectral features of MgC_3 isomers are reported,[40] CO_2 dimers are suggested to play a vital role in greenhouse effects for thick planetary atmospheres like Venus from IR analysis,[41] and small silicate clusters are found to heat up more than previously realized potentially affecting future infrared observations.[42] Similar relationships between deuterated methanol and temperature in Orion KL are also reported.[43] One manuscript in this virtual special issue shows that resistively heated silicon carbide microreactors have little-to-no rovibrational cooling in the expansions, but the chemical composition of the background likely will differ from that of the molecular beam emanating directly from the reactor.[44] Finally, two spectral databases are also reported in order to provide large amounts of spectral data for many molecules[45] and rich spectral characterization of CO_2.[46] All of these considerations for spectral analysis certainly enhance inferences that can be gleaned from these types of experiments and theoretical computations informing future astrochemical observations.

As the topics, results, and insights from this virtual special issue highlight, the establishment of the ACS PHYS Astrochemistry Subdivision provides a community where astrochemists with backgrounds from a breadth of traditional disciplines can present new data and even question long-held speculations and assumptions. In either case, such developments provide an underlying chemical knowledge that will drive future science for the next decade and into the future. The new methods and chemical insights presented in this special issue will not remain solely within astrochemistry; these approaches, born out of a need to ask difficult chemical questions from beyond our terrestrial veil, showcase the power of human creativity and stand to influence astronomy, biochemistry, materials science, and beyond.

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Notes

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