

A Vision for the Future of Astrochemistry in the Interstellar Medium by 2050

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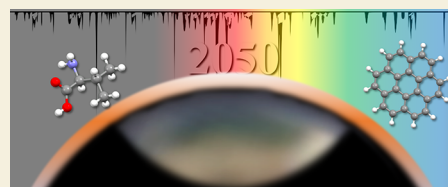
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ABSTRACT: By 2050, many, but not nearly all, unattributed astronomical spectral features will be conclusively linked to molecular carriers (as opposed to nearly none today in the visible and IR); amino acids will have been observed remotely beyond our solar system; the largest observatories ever constructed on the surface of the Earth or launched beyond it will be operational; high-throughput computation either from brute force or machine learning will provide unprecedented amounts of reference spectral and chemical reaction data; and the chemical fingerprints of the universe delivered by those of us who call ourselves astrochemists will provide astrophysicists with unprecedented resolution for determining how the stars evolve, planets form, and molecules that lead to life originate. Astrochemistry is a relatively young field, but with the entire universe as its playground, the discipline promises to persist as long as telescopic observations are made that require reference data and complementary chemical modeling. While the recent commissionings of the *James Webb Space Telescope* and Atacama Large Millimeter Array are ushering in the second "golden age" of astrochemistry (with the first being the radio telescopic boom period of the 1970s), this current period of discovery should facilitate unprecedented advances within the next 25 years. Astrochemistry forces the asking of hard questions beyond the physical conditions of our "pale blue dot", and such questions require creative solutions that are influential beyond astrophysics. By 2050, more creative solutions will have been provided, but even more will be needed to answer the continuing question of our astrochemical ignorance.



KEYWORDS: Astrochemistry, Rotational Spectroscopy, Vibrational Spectroscopy, Telescopic Spectroscopy, Infrared, Microwave

INTRODUCTION

The year 2050 will look like today but not. A veneer of the contemporary will mask the changes underneath, like a remodel of a house undertaken when the mortgage is nearly paid off. The late 1990s are as close to today as 2050. In thinking back to this earlier time, compared to today, many things are the same. Many are different, but the differences are more subtle than Marty McFly would have hoped they should be. As such, in 2050 science, physical chemistry, and even astrochemistry will look the same on the outside, but the inside will have all new developments where many of the "grand questions" will have been answered, while others will remain unsolved. New challenges will have arisen, and the depth of knowledge will be greater.

A back extrapolation of another quarter-century from the turn of the 21st century to the 1970s can be viewed, though, as showing more stark differences in many ways than the late 1990s compared to the early/mid 2020s. In other words, the 1990s looked more like the 2020s than the 1990s did the 1970s. Undoubtedly, the Internet, cable television, email, satellite phones, and most other electronic communications have caused a huge shift in how humans interact and also how science is

performed. However, this shift was more acute from the 1970s to 1990s than over the most recent 25 year span. Consequently, the roughly 50-year lookback from 1970 to now is much more significant than a 25-year lookback and actually encompasses all major aspects of astrochemistry, except for some of the earliest wanderings by Sir William Huggins, Andrew McKellar, and Gerhard Herzberg among others. A vision for 2050 must first begin with a view from the beginning.

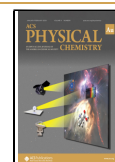
The game-changer for astrochemistry and, specifically, the study of the chemistry of the interstellar medium (ISM) was, without a doubt, the radiotelescope, a technological child of the radar technology pioneered in World War II. Radio emissions from rotating molecules observed from sources all over the immediate galactic neighborhood shifted the paradigm for the presence of molecules in space. Space, and the ISM in particular,

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was thought to be too harsh with high-energy photons and cosmic rays to allow molecules to persist for any observable lifetime. However, observation of these emissions ceased their discussion as purely theoretical or only limited to postulated H₂ and put molecules and chemistry in the regions between stars and even in between galaxies. These observations put the hydroxyl radical,¹ ammonia,² and water³ into the astrochemical molecular census. While CN and CH had been observed through telescopic ultraviolet–visible (UV–vis; the domain of electronic spectroscopy) 30–35 years prior,^{4–6} they were soon confirmed through their rotational emissions in the early 1970s^{7,8} along with carbon monoxide,⁹ formaldehyde,¹⁰ and the first trove of interstellar molecules with strong emission features ranging from methanol (Figure 1)¹¹ to hydrogen cyanide¹² and many others^{13–23} in what should be called the first “golden age” of astrochemistry.

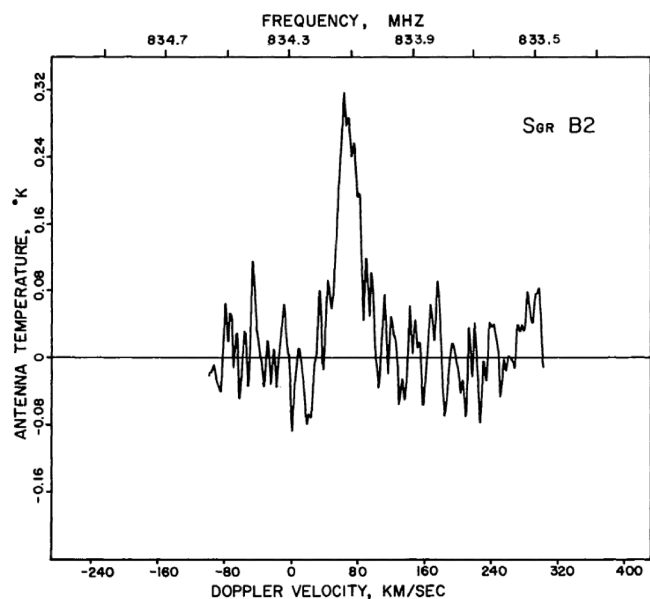


Figure 1. September 1970, 140-foot NRAO radio telescope observed spectrum of Sagittarius B2, leading to the detection of methanol at 834.301 MHz. Reproduced from ref 11 with permission from the authors.

From these radio/millimeter/submillimeter/rotational emission observations, early chemical models began to show the ways in which these molecules could interconvert and then even react to become other chemical species yet to be observed.^{24,25} The detection of these new molecules would require laboratory (or even theoretical) reference data. Many of the predicted species were detected. Many were not. The models were refined. More were detected. The models were refined. More reference data were generated. More observations were made. And again and again and again. Thus, astrochemistry and its interdependent triangle²⁶ of observation, modeling, and reference data production were born.

This process of astromolecular discovery has continued with fits and starts in the time since,^{27,28} but the most recent years have been among the most fruitful with newly developed observational techniques pioneered by many groups producing a census of what is fast approaching 250 novel molecules observed beyond our solar system.^{23,29–31} However, hordes of other molecular species are likely lurking in the same regions as these known molecules, but many lack the pesky dipole moment

required for radiotelescopic observation. These currently unobserved molecules will offer more complete clues about the molecular origins of stars, planets, and likely also life. While molecular probes like CO and N₂H⁺³² have been used for decades as proxies for H₂ and N₂, respectively, direct observation of nonpolar species will require new wavelengths and new observatories. Additionally, while robotic rovers on Mars^{33,34} and probes to the gas giants^{35–37} have provided additional chemical insights into these regions, remote sensing will still play a huge role in astrochemistry.³⁸ Luckily, the *James Webb Space Telescope* (JWST) is here.

■ A NOTE ABOUT THE PRESENT (JWST AND FRIENDS)

JWST has already provided clear detection of benzene in a stellar disk,³⁹ confirming a detection claim from 2001 in the Westbrock Nebula (stellar cocoon CRL 618).⁴⁰ Of course, the radio detection of the related benzonitrile⁴¹ shows clear evidence for benzene, as well, but, again, nothing really compares to direct observation. JWST provides for that.

Benzene is a big deal because, while most of the carbon in the universe is tied up in carbon monoxide, most of the remainder, as much as 20% of the total, is locked in polycyclic aromatic hydrocarbons (PAHs),⁴² basically sheets of benzene rings. Most PAHs do not possess a dipole moment, rendering their observation with radiotelescopes unobtainable. The *Hubble Space Telescope* (HST) could see evidence for them in the near-IR, and the *Spitzer Space Telescope* could, as well, but JWST does it better, a veritable James Bond of observation. It was built to do so. However, even when a dipole moment is not required for observation, the problem with PAHs is that they are too amorphous and likely too ubiquitous.⁴³ They have spectral properties much too similar to one another for incontrovertible unique detections, and like the tar and soot they make here on the Earth, PAHs gunk up infrared (IR) spectra.^{44,45} They are believed to dominate all IR spectra^{46–48} and cloud the observation of arguably more interesting molecules. Hence, the problem with PAHs and JWST is that in order to see what else is out there, the PAH spectra must be removed. While such a process is fairly routine,⁴⁸ no ab initio reference PAH spectra perfectly match the observed JWST spectral features. That sounds like a future problem.

The larger issue at play is that IR spectra are not unique identifiers of molecular properties. For instance, the so-called “fingerprint” region in organic laboratory IR spectra is necessary to provide some semblance of unique identification, but even that is not fully rigorous in many cases since many molecules can have nearly identical vibrational behavior for certain modes. Even so, the IR still possesses the necessary properties that make its use with JWST essential. Most notably, silicates and other minerals that comprise most rocky and dusty particles are more-or-less transparent in the IR, allowing instruments such as NIRSPEC and MIRI onboard JWST to pierce these veils previously hidden. Additionally, even though NMR is nearly fully replacing IR in the organic laboratory for classification, the idea of an NMR telescope is a bit of an oxymoron. Hence, IR is key even if such an instrument has to be outside of the Earth’s atmosphere.

As such, JWST is providing amazing images and insights into regions never before thought imaginable. Clear, directly imaged exoplanetary atmospheric spectra are coming back with the lowest signal-to-noise ever recorded for such observations.^{49,50} JWST has also observed everything from the most-distant

known galaxies to planets within our solar system. The unprecedented chemical data that each observation provides⁵¹ is beyond the previous capabilities of any observatory, but even this is based on designs that are nearly 20 years old or more.⁵² Standard NASA mission protocols will have technology freeze dates three-to-five years before the anticipated mission launch. This ensures that technologies included in the mission are robust, adequately tested, and able to interact with one another so that the technology does not end up like Johnny Cash's Cadillac in "One Piece at a Time." Hence, an initial technology testing date of 2014 actually relied upon parts from pre-2010 that were mostly pre-existing before this.^{51,52} Consequently, the fantastic images provided by JWST could have been even better if the inclusion of more contemporary technology had been possible. The advances in camera technology, largely from smartphones, imply that the future of astrochemistry looks bright provided that the next generation telescopes are funded. However, the 2020 Astronomical Decadal Survey⁵³ specifically calls for such to be funded and built in order to keep pushing astronomy, astrophysics, and, hence, astrochemistry forward; more on this later.

However, there are other wavelengths of light besides UV–vis and the IR. The radio and its observation of rotational lines have been the workhorse of ISM studies for decades, as described above. Unlike the IR, it provides definite identification of molecules due to the unique moments of inertia present in every rotating body, but radioastronomical observation competes with communication frequencies such that most radiotelescopes can operate only in certain ranges. However, some places like the national radio quiet zone around Green Bank, WV and the National Radio Astronomy Observatory's (NRAO) Green Bank Telescope (GBT) along with observatories in the mountains of Arizona, New Mexico, Spain, and France (among others) are less hindered by such windows. Then, beyond all of these, the Atacama Large Millimeter Array (ALMA) stationed in the high desert of Chile has the largest current baseline and the most individual nodes in its interferometer and is in one of the most remote regions of the world, guaranteeing the highest sensitivity of any telescope of any kind ever built, thus far. Additionally, while HST could be serviced from orbit, ALMA is on the ground even if it is in a remote region. Hence, driving a truck to the Atacama Desert to repair one of its dishes is orders of magnitude less expensive than launching a now-defunct space shuttle to service the HST. Worse than HST, the JWST is not serviceable at all and has a finite lifetime based on its fuel tanks. Hence, ALMA stands a good chance to be operational for generations provided there is enough regular maintenance performed and there is a desire to do so.

In all cases, the current status of astrochemistry, especially as it applies to the study of the ISM, is really in its second "golden age" with JWST and ALMA filling in the gaps and far exceeding the capabilities of their predecessors. Observers have the most amazing telescopes ever constructed, and the laboratory/theoretical reference data developers and astrochemical modelers have more data from observation than they know what to do with at the moment. To this point for pushing toward 2050, the gathering of astrochemical spectral data is not the limiting factor. The parsing and unique determination of molecular data are where the new confusion limit resides. Observation will not and should not slow; the other two branches must catch up. Hence, the future of astrochemistry lies in our ability to reduce the time required to go from observation to characterization. This is just now opening up even as the

future of observatories is exceptionally exciting for astrochemical applications.

■ THE 2050 HORIZON

Observation by 2050

In keeping with radio/millimeter/submillimeter/rotational emission observations, the allure of deterministic spectral characterization will not fade any time soon, even in the days of JWST. Additionally, the easiest means of producing even higher sensitivity and a larger frequency range for radio telescopes is simply to build an interferometer with more observing units over a longer baseline. The 2050 horizon in this regard is dominated by the square kilometer array (SKA) currently under construction in South Africa and Australia with work scheduled to proceed in earnest for the next decade and continuing improvements likely to progress for another decade after that, putting its "completion" (a mostly arbitrary choice of definition for something so large) nearer to 2050 than 2030. Its tens of thousands (yes, tens of thousands) of antennas will be spread over a distance of 3,000 km with a collecting area of roughly 1 km² (hence, the name). While each of the individual receivers for SKA will be paltry compared to those for ALMA, the sheer number of them spread between these two countries will make pixel resolution the smallest swaths of the sky ever conceived.

Similar to the SKA is the next generation very large array (ngVLA), another radiotelescope array that is building upon the existing VLA hosted by the National Radio Astronomy Observatory at its high desert site in New Mexico. The upgraded ngVLA has larger individual dishes at 18 m than SKA but will cover a smaller area of roughly 1000 km stretched over Arizona, Mexico, Texas, and New Mexico at an average altitude of roughly 2100 m. Hence, ngVLA will augment SKA and ALMA and provide an unprecedented resolution of astronomical (and hence astrochemical) observations.

In either case of the SKA or ngVLA, more fine spectral and chemical details will be teased out like never before. The chemical census of certain bands of protoplanetary disks may yet be uniquely characterized, such that the chemical evolution for the molecules that lead to life could be identified as they form in certain regions. What ALMA did for spectral resolution, SKA and ngVLA will do for spatial resolution and, like ALMA, SKA and ngVLA can be modified, updated, expanded, and maintained for as long as interest and the associated funding allow.

Along a similar vein but for higher light frequencies, one of the next space observatories supported by the 2020 Decadal Survey is for a telescope that would effectively combine the HST with the JWST and then ramp up both. The *Large UV/Optical/IR Surveyor* (LUVOR; Figure 2) is JWST's much larger offspring and potential successor considering that the next generation telescope is proposing to be built along nearly the same engineering strategy (i.e., individual movable hexagonal mirrors, folding portions, solar orbit at L2, etc.). For instance, JWST's mirror is 6.5 m in diameter; LUVOR's is proposed to be a whopping 15 m. JWST has 18 mirrors while LUVOR Architecture A is proposing 120! This Architecture A will require solar orbital insertion via the Space Launch System (SLS) from NASA which has not been fully developed for launch, yet. Architecture B (Figure 2C) is roughly half the diameter as well as half the number of mirrors but could fit in modern rockets for launch. In either case, JWST data will be

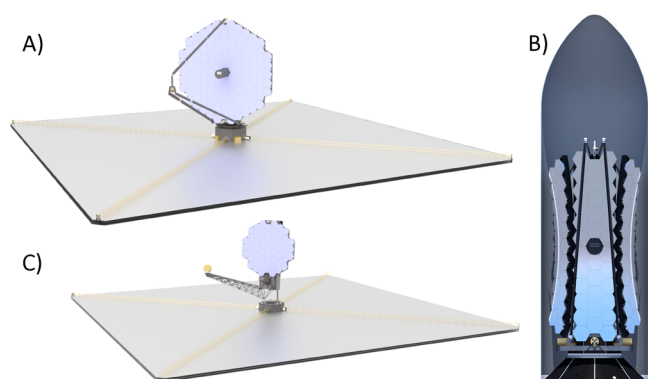


Figure 2. Concept designs for the LUVOIR telescope in the A) Architecture A configuration, B) Architecture A folded into the as-of-yet unfinished SLS launch fairing, and C) smaller Architecture B configuration. All images are reproduced with permission from NASA/GSFC.⁵⁴

comparable to 16th century maps of the Earth's Western Hemisphere in regards to what LUVOIR promises to produce. It will also be able to combine multiple wavelengths of light in a single observation with its various instruments, providing a complete spectral picture of specific astrophysical regions at the same time. Such timestamps will reduce uncertainty and give large band analysis like never before. LUVOIR is scheduled to launch in the late 2030s if it is selected for development. However, with JWST delayed by more than a decade, LUVOIR probably will not launch for at least a similar delay (and may be combined with the *Habitable Exoplanets Observatory* creating the *Habitable Worlds Observatory*, or HWO, still observing the same UV/optical/IR wavelengths), implying that it will be coming online close to 2050 and will only begin providing astrophysical insights then.

Reference Benchmarking by 2050

In consideration of SKA, ngVLA, and LUVOIR (or HWO) combined with the ongoing influx of JWST data for another decade or so and the possible perpetuity of ALMA, the amount of astronomical spectral data to be produced is staggering. Again, the characterization of such data will be key in moving forward. The most promising emerging technology to be able to handle such is not unique to astrochemistry in any way: computational analysis, specifically via machine learning (ML) and artificial intelligence (AI). Such ideas are actually not new, even in

astrochemistry. For all of the benefits of radiotelescopic observation, broadband rotational spectroscopy has had its challenges in attribution since it began. Any observation is a forest of lines with different species growing to different heights in different locations. Determination of such is like a game of pickup sticks played in the dark. For example, a simulated rotational spectrum in Figure 3 is composed of only five molecules at 10 K, the average temperature of TMC-1. Hundreds of lines are present and stretch across ALMA bands 1–7 with the highest density in bands 1, 2, and 3. A much higher density of lines will certainly be present when more than five molecules contribute. While some patterns are clearly visible in this sample spectrum and eagle-eyed, trained graduate students can pick this out and pull useful data from such observations, this is tedious and filled with trial and error, a procedure that computers should be able to handle much better than people.

Computers are supposed to be good at completing large numbers of redundant tasks. Picking out one line in the radiotelescopic rotational emission spectrum, comparing to others, finding a pattern, and matching that pattern to a known standard^{56,57} should be relatively straightforward to any computationally minded programmer. Some attempts have been made to provide such programs including AUTOFIT⁵⁸ and the Global Optimization and Broadband Analysis Software for Interstellar Chemistry (GOBASIC),⁵⁹ but work in this area has focused on providing spectral explanations based on known standards. By 2050, predictions of the molecular carriers should be based solely on the analyzed spectrum itself.

In a nutshell, such a computer program would be able to select a rotational line and find all of the associated lines that would comprise a full, unique molecular spectrum. It would have to compare how that line would match with those to whom it was being paired based on various factors and how the pairing of those lines predicted and matched third, fourth, and higher lines. If this could be accomplished, molecular spectra could be pulled from broadband data, and rotational constants could be produced from it. Such a method would then produce a set of molecular properties that could then be further analyzed through high-level quantum chemistry or cutting-edge laboratory experimentation in order to find a closest match.

The computational problem with such a broadband analysis comes down to the number of permutations and combinations that are possible for line pairing. This is actually similar to the classic traveling salesman problem (TSP) from computer

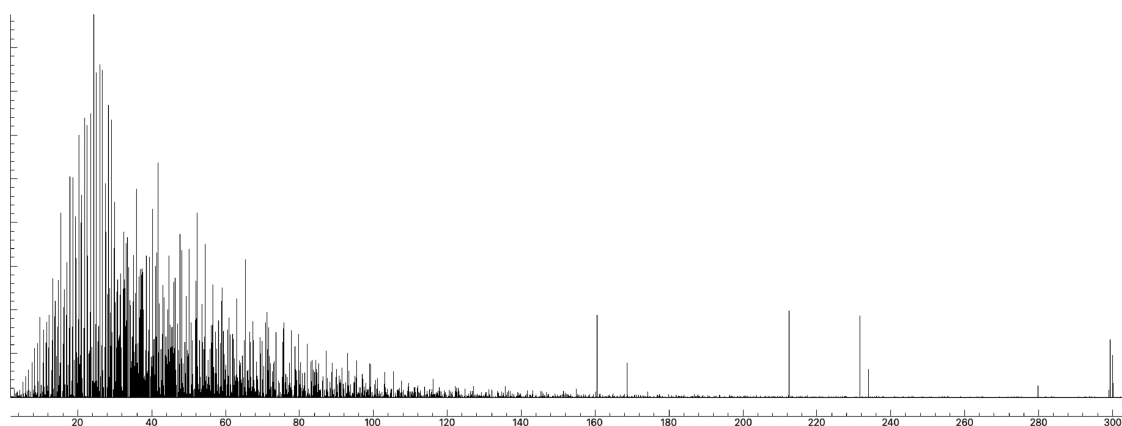


Figure 3. Sample rotational spectrum (in GHz) for five molecules at 10 K comprising arbitrarily chosen near-prolate, near-oblate, asymmetric top, and high mass sets of rotational constants. Image created by the author via PGopher.⁵⁵

science and optimization research: what is the shortest distance that can be traveled between a given set of destinations? However, here, the distance between spectral lines then begets a prediction for the position of other lines, unlike TSP where the distances are arbitrary based on simple geography. The rotational line version makes the problem somewhat simpler in that a sampling of two or so distances (differences in transition frequencies) will provide immediate feedback as to whether those three lines giving the two distances are related to a fourth line. However, this last part also makes the problem more difficult to solve in that additional criteria have to be predicted and tested for comparison before the end of the run, which takes computational time. However, the growth in computer hardware along with the needed algorithms to take advantage of such things is simply a product of the need to develop and make use of what is currently available. Graphical processing units (GPUs) can process large amounts of data quickly thanks to the growth in the video game industry, and these combined with computational buzzwords such as ML will enhance the throughput that such methods would require.

Broadband analysis of this type is still very open-ended, but cracking this type of spectral prediction would be a game changer for radioastronomical observation. Analyzing by hand or with current reference-based computer programs of such broadband rotational spectral data as that provided by ALMA or, later, SKA or ngVLA is intractable for the amount of data that is currently being produced and is not predictive in giving quantum chemists and laboratory astrophysicists clear targets for matching molecular properties. Even with the removal of known lines, new, unassigned lines crop up in every observation. What programs like that outlined above promise is to be able to parse spectra and provide good estimates for rotational constants that define the spectral features, which can then lead to the detection of new molecules. If there are no quality candidates to explain the lines from known benchmarks, the rotational constants themselves combined with the nature of quantum mechanical rotational behavior give a clear indication for the type of molecule present. Hence, this will not only reduce the guessing from spectral characterization but also provide an additional means of finding new molecules in space.

The alternative of analyzing the spectrum to produce rotational constants is to produce rotational constants from high-throughput analysis for direct comparison to observations. No other means of data production can easily and quickly generate novel molecular structures and spectra, quite like quantum chemical computations. In fact, comparison to theory is now expected for the determination of rotational constants in radiotelescopic observation,²⁷ but this has only emerged recently for vibrational spectra as would be needed by JWST or LUVOIR.^{60,61}

Automation of quantum chemical computations for various, “big hammer” chemical applications is not a new idea,⁶² but further complexities arise for vibrational spectroscopy more than what method and basis set to use, which itself is an important choice. Anharmonicity is essential for accurate predictions, but how should that be modeled: explicitly or heuristically? If explicitly, then, is perturbation theory sufficient or are variational methods needed? In either case, which flavor of those and how large does the potential energy surface need to be? Each choice is based on a balance between time and accuracy.⁶³ Recent work has shown that density functional theory (DFT), scaled harmonic vibrational frequencies can provide broad-strokes IR data for thousands of molecules in a small amount of time on a

standard high-performance computing cluster.⁶¹ Such an approach promises to provide more data than ever before within the time frame of a JWST data release. This is getting closer to the throughput needed to conjoin efficiently with observation.

Again, as hardware like GPUs and even quantum computing technology develops, dedicated, stochastic approaches could “brute force” their way through thousands of molecules in a similar fashion especially through the use of dedicated backbones and functional groups linked together with SMILES strings⁶⁴ which can construct molecules with single-line computational syntax. Of course, larger molecules like PAHs will require even lower-levels of theory than DFT can provide in order to reach the needed level of throughput for scratching the surface of JWST (much less LUVOIR) data, and ongoing work is parametrizing semiempirical methods to this effect through automated, explicitly anharmonic computations trying to solve the future problem of PAHs as alluded to previously.^{65–67}

By the time we approach 2050, however, high-throughput quantum chemical analysis will become routine. Reference papers will contain dozens to hundreds and even thousands of molecules with near-spectroscopic quality. This will be enhanced by experimental analysis to fine-tune the results, and more molecules will be handed to modelers and observers to grow the chemical inventory like never before.

Modeling by 2050

While ML and AI are the current buzzwords in computer science, by 2050 they will either have been forgotten completely or be so ubiquitous and commonplace such that they will have taken on a completely different meaning in pop culture much like “drive,” “fax,” or “tweet” have over the previous half-century. ML is actually not a new idea itself, with versions of this coming from the dawn of computer science in the post-World War II era (much like radioastronomy that begat modern astrochemistry in its first “golden age”). However, modern computer hardware finally has the resources necessary to effectively utilize such ML and AI algorithms for chemically meaningful problems. In astrochemical modeling, having a more efficient means of predicting the needed quantities for observational characterization and how that influences the overall reaction network of a given astronomical region is key to pushing our understanding forward.

ML offers an elegant computational means of producing such data in novel ways. Recent work has provided estimates of column densities (a measure of molecular abundance) in the dark molecular cloud TMC-1 found in the constellation Taurus.⁶⁸ Such a body is relatively stagnant in its ongoing chemistry, but other bodies are more dynamic and have shorter timeframes related to how the chemical environment changes. ML techniques have been brought to bear on modeling such environments in the case of protostars. Novel molecular targets have now been predicted in reaction networks providing impetus for subsequent observation.⁶⁹ Additionally, ML has shown that it competes with traditional modeling needed to provide column densities (and, hence, emission peak heights) in the detection of $C_{10}H^-$, the first interstellar anion observed in more than a dozen years.^{70,71}

As such, the ML appears to be on the cusp of securing a place in how chemical reaction networks are processed. This is also true in many other areas of chemistry, but the column densities of molecules are essential for pinning down as narrow of a range as possible in the concentration portion of the Beer–Lambert

Law such that the observed telescopically observed emission signal can be tied to a molecular carrier. As such algorithms develop, they may or may not supersede traditional methods of modeling molecular abundances, but they are allowing for new pathways of corroboration if not dominance in how modeling is undertaken.

■ THE STATE OF ASTROCHEMISTRY IN 2050

The future of astrochemistry comes down to determining the carriers of telescopic spectral features and then understanding how these observed molecules will react. The fundamental understanding of the chemical censuses of different regions will inform astronomers, planetary scientists, and astrobiologists of the chemical stockpiles available to form planets, produce stars, and even create life. However, this problem of spectral characterization is not new for the present and will not be new for 2050. As shown previously, it will be even more difficult. This is most easily showcased in visible spectroscopy where, potentially, LUVOIR or other space telescopes like the upcoming *Nancy Grace Roman Space Telescope* could provide novel insight. Here, will the “grand questions” of astrochemistry be answered by 2050? Yes, in part but never completely.

Diffuse Interstellar Bands

While PAHs are believed to be the cause for a majority of observed IR emission transitions,^{44,72–75} the exact cause of their UV-to-visible (likely electronic) absorption transition counterparts remains a mystery. These so-called “diffuse interstellar bands” (DIBs) stretch from wavelengths of roughly 4,000 Å to nearly 10,000 Å,^{43,76–78} and some may be linked to PAHs⁷⁹ while others likely are not. Several reviews are available for these features,^{80–84} but they have often been called longest-standing problem in spectroscopy since they went unattributed for nearly a century.^{24,85} Even though “there is no better way to lose a scientific reputation than to speculate on the carrier[s] of the [DIBs],”^{24,86,87} C₆₀⁺ now has few obstacles to its claim as carrier for at least four of these features.^{88–91} More carriers must be forthcoming.

By 2050, slightly more than 25 years from now, more of these DIBs will be linked to molecular carriers. While it took more than five years before C₆₀⁺ was widely accepted for its role in DIBs, the first attribution is always the hardest. Since HST confirmed C₆₀⁺ as this first DIB carrier,⁸⁹ LUVOIR (or HWO) should be able to assist with future attribution claims after it launches. Additionally, once the DIB code is cracked, the carriers will begin falling into place in much the same way molecules were observed via radiotelescopic characterization in the 1970s. The past will likely be repeated. Certainly, there are untold radioastronomical rotational lines that are still unattributed, but the molecules being uniquely detected in those regimes now are in what used to be the noise for earlier generations of telescopes. Such will be the case with the DIBs, as well. Hence, the broadest, tallest, and most correlated DIB features should be attributed by 2050, and many more unattributed DIBs will be added. Novel understanding of chemical reactions via modeling (potentially using ML) aided by both laboratory and quantum chemistry will likely and clearly show that already known molecules from rotational emission are producing some of the DIBs, and these will likely then explain many emission features in the IR. Such cross-wavelength correlation has largely been lacking in astrochemistry, but once it takes place, the depths of knowledge for the chemical cosmos will have unprecedented contiguity.

Such holistic provision will then provide clear molecular holes in the chemical reaction networks that have to be explained. The chemical inventory of certain regions will increase. The roles that these new molecules play in reaction networks and in observations will be firmly established. Multiwavelength characterization should happen by 2050. Then, after 2050 when SKA, ngVLA, and LUVOIR have come into their own, these observatories will lower the noise limit once more, providing for even more molecules to be classified, observed, and placed in reaction pathways. Different astronomical regions and even subregions (via SKA/ngVLA) will have definitive variations showcasing once more how astrochemistry is the fingerprint of astrophysics. This will provide unprecedented stepwise progression in observing the evolution of exoplanets, protoplanetary disks, and stars.

Amino Acids

When such large, coordinated spectral characterization and links are established, the molecular inventory at that point must include what are considered to be the molecular origins of life, amino acids. Amino acids have been directly observed in core samples of meteors,⁹² and laboratory simulations of interstellar ices form them routinely.^{93–98} In fact, the thermodynamic product of interstellar ices with some molecular source of nitrogen (often ammonia) and carbon (methanol) beyond oxygen in water appears to be amino acids, but their gas phase formation pathway is currently incomplete. This discrepancy between their presence in solar system bodies from in situ measurements⁹⁹ and a lack of gas phase, remote observation almost certainly points to shortcomings in the latter. Claims for remote amino acid detections have already been given without confirmation from the community¹⁰⁰ while other searches have turned up empty-handed,¹⁰¹ but several prebiotic precursors have been observed directly^{102,103} including an isomer of glycine¹⁰⁴ giving reason to believe that amino acids should be present and potentially observable in various astrophysical regions.

The number of conformers for amino acids reduces the overall signal for each of their possible IR or radio emission, but high quality quantum chemical computations for conformer energetics¹⁰⁵ and new resolutions across multiple spectral regimes should change how these are observed. Such combinations will be most ideal with SKA/ngVLA/ALMA interacting with LUVOIR (or HWO) after 2050, but this should happen before that with ALMA and JWST. Hence, once the models based on the presumed chemistry of known, less floppy amino acid precursors show exactly where (astronomically and chemically) amino acids should be found, they will be found. To stake a claim in a prediction, a few amino acids (likely alanine, serine, valine, and potentially proline) will be observed remotely either within or beyond our solar system before 2050. More will come later. Again, once the code is cracked, their detections will become nearly commonplace and we will wonder why it ever was so difficult to find them in the first place.

■ CONCLUSIONS

A significant number of DIBs explained, remote detection of amino acids, ML and exascale computations employed. 2050 will have taken this current, 2020s second golden age of astrochemistry and will earnestly fill in the biggest gaps in the biggest questions of the chemistry of the ISM. However, just like telescopic resolution, the “noise” limit will have been pushed down, and new questions will arise. More complicated problems

will crop up. Challenges that defy conventional chemistry continue to confound us. Even so, these future questions that cannot be fully contemplated today will be met with the diligence and passion that astrochemistry creates in its practitioners. Plus, the serendipity of addressing these difficulties will spin off new technologies in currently unfathomable ways much like buckyballs and carbon nanotubes originated with astrochemical questions^{106–108} for instance. What those will be, naturally, has yet to be determined. In any case, the answering of difficult questions leads to novel solutions. Where those solutions take us, makes the future even more exciting. As such, the world will be a better place because some chemists have their heads in interstellar clouds. The astrochemistry of 2050 will be recognizable compared to that today, but it will be much more informed and deal with much more specific questions than we do today in the 2020s. Such is the nature of science, and 2050 is an exciting horizon for which astrochemists should look forward.

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Notes

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REFERENCES

- (1) Weinreb, S.; Barrett, A. H.; Meeks, M. L.; Henry, J. C. Radio Observations of OH in the Interstellar Medium. *Nature* **1963**, *200*, 829–831.
- (2) Cheung, A. C.; Rank, D. M.; Townes, C. H.; Thornton, D. D.; Welch, W. J. Detection of NH₃ Molecules in the Interstellar Medium by Their Microwave Emission. *Phys. Rev. Lett.* **1968**, *21*, 1701–1705.
- (3) Cheung, A. C.; Rank, D. M.; Townes, C. H.; Thornton, D. D.; Welch, W. J. Detection of Water in Interstellar Regions by Its Microwave Radiation. *Nature* **1969**, *221*, 626.
- (4) Swings, P.; Rosenfeld, L. Considerations Regarding Interstellar Molecules. *Astrophys. J.* **1937**, *86*, 483–486.
- (5) McKellar, A. Evidence for the Molecular Origin of Some Hitherto Unidentified Interstellar Lines. *Publ. Astron. Soc. Pac.* **1940**, *52*, 187–192.
- (6) Adams, W. S. Some Results with the COUDE Spectrograph of the Mount Wilson Observatory. *Astrophys. J.* **1941**, *93*, 11–23.
- (7) Rydbeck, O. E. H.; Ellder, J.; Sume, A.; Irvine, W. M.; Hjalmarsen, A. Radio astronomical determination of ground state transition frequencies of CH. *Astron. Astrophys.* **1974**, *34*, 479–482.
- (8) Jefferts, K. B.; Penzias, A. A.; Wilson, R. W. Observation of the CN Radical in the Orion Nebula and W51. *Astrophys. J.* **1970**, *161*, L87–L89.
- (9) Wilson, R. W.; Jefferts, K. B.; Penzias, A. A. Carbon Monoxide in the Orion Nebula. *Astrophys. J.* **1970**, *161*, L43–L44.
- (10) Snyder, L. E.; Buhl, D.; Zuckerman, B.; Palmer, P. Microwave Detection of Interstellar Formaldehyde. *Phys. Rev. Lett.* **1969**, *22*, 679–681.
- (11) Ball, J. A.; Gottlieb, C. A.; Lilley, A. E.; Radford, H. E. Detection of Methyl Alcohol in Sagittarius. *Astrophys. J.* **1970**, *162*, L203–L210.
- (12) Snyder, L. E.; Buhl, D. Observations of Radio Emission from Interstellar Hydrogen Cyanide. *Astrophys. J.* **1971**, *163*, L47–L52.
- (13) Turner, B. E. Detection of Interstellar Cyanoacetylene. *Astrophys. J.* **1971**, *163*, L35–L39.
- (14) Snyder, L. E.; Buhl, D. Detection of Several New Interstellar Molecules. *Ann. N.Y. Acad. Sci.* **1972**, *194*, 17–24.
- (15) Zuckerman, B.; Morris, M.; Palmer, P.; Turner, B. E. Observations of CS, HCN, U89.2, and U90.7 in NGC 2264. *Astrophys. J.* **1972**, *173*, L125–L129.
- (16) Wilson, R. W.; Penzias, A. A.; Jefferts, K. B.; Kutner, M.; Thaddeus, P. Discovery of Interstellar Silicon Monoxide. *Astrophys. J.* **1971**, *167*, L97–L100.
- (17) Penzias, A. A.; Solomon, P. M.; Wilson, R. W.; Jefferts, K. B. Interstellar Carbon Monosulfide. *Astrophys. J.* **1971**, *168*, L53–L58.
- (18) Solomon, P. M.; Jefferts, K. B.; Penzias, A. A.; Wilson, R. W. Detection of Millimeter Emission Lines from Interstellar Methyl Cyanide. *Astrophys. J.* **1971**, *168*, L107.
- (19) Jefferts, K. B.; Penzias, A. A.; Wilson, R. W.; Solomon, P. M. Detection of Interstellar Carbonyl Sulfide. *Astrophys. J.* **1971**, *168*, L111–L113.
- (20) Rubin, R. H.; Swenson, G. W.; Benson, R. C.; Tigelaar, H. L.; Flygare, W. H. Microwave Detection of Interstellar Formamide. *Astrophys. J.* **1971**, *169*, L39–L44.
- (21) Woon, D. E. The Astrochymist. 2023; <http://www.astrochymist.org>; accessed on 11/10/2023.
- (22) McGuire, B. A. 2018 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules. *Astrophys. J. Suppl. Ser.* **2018**, *239*, 17.
- (23) McGuire, B. A. 2021 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules. *Astrophys. J. Suppl. Ser.* **2022**, *259*, 30.
- (24) Herbst, E. Chemistry in the Interstellar Medium. *Annu. Rev. Phys. Chem.* **1995**, *46*, 27–53.
- (25) Herbst, E.; Green, S.; Thaddeus, P.; Klemperer, W. Indirect Observation of Unobservable Interstellar Molecules. *Astrophys. J.* **1977**, *215*, 503–510.
- (26) Fortenberry, R. C.; Kaiser, R. I.; McMahon, R. J. 10 Years of the ACS PHYS Astrochemistry Subdivision. *J. Phys. Chem. A* **2022**, *126*, 6571–6574.
- (27) Fortenberry, R. C. Quantum Astrochemical Spectroscopy. *Int. J. Quantum Chem.* **2017**, *117*, 81–91.
- (28) Fortenberry, R. C. The Case for Gas-Phase Astrochemistry without Carbon. *Mol. Astrophys.* **2020**, *18*, 100062.
- (29) Burkhardt, A. M.; Long Kelvin Lee, K.; Bryan Changala, P.; Shingledecker, C. N.; Cooke, I. R.; Loomis, R. A.; Wei, H.; Charnley, S. B.; Herbst, E.; McCarthy, M. C.; McGuire, B. A. Discovery of the Pure Polycyclic Aromatic Hydrocarbon Indene (c-C₉H₈) with GOTHAM Observations of TMC-1. *Astrophys. J. Lett.* **2021**, *913*, L18.
- (30) Changala, P. B.; Gupta, H.; Cernicharo, J.; Pardo, J. R.; Agúndez, M.; Cabezas, C.; Tercero, B.; Guélin, M.; McCarthy, M. C. Laboratory and Astronomical Discovery of Magnesium Dicarbide, MgC₂. *Astrophys. J. Lett.* **2022**, *940*, L42.
- (31) Cernicharo, J.; Agúndez, M.; Kaiser, R. I.; Cabezas, C.; Tercero, B.; Marcelino, N.; Pardo, J. R.; de Vicente, P. Discovery of Benzynes, o-C₆H₄, in TMC-1 with the QUIJOTE Line Survey. *Astron. Astrophys.* **2021**, *652*, L9.

- (32) Green, S.; Montgomery, J. A.; Thaddeus, P. Tentative Identification of U93.174 as the Molecular Ion $N_2^+ H^+$. *Astrophys. J.* **1974**, *193*, L89–L91.
- (33) Sharma, S.; et al. Diverse Organic-Mineral Associations in Jezero Crater, Mars. *Nature* **2023**, *619*, 724–732.
- (34) Fornaro, T.; Brucato, J. R.; Poggiali, G.; Corazzi, M. A.; Biczysko, M.; Jaber, M.; Foustoukos, D. I.; Hazen, R. M.; Steele, A. UV Irradiation and Near Infrared Characterization of Laboratory Mars Soil Analog Samples. *Frontiers in Astronomy and Space Sciences* **2020**, *7*, 539289.
- (35) Waite, J. H., Jr.; et al. Ion Neutral Mass Spectrometer Results from the First Flyby of Titan. *Science* **2005**, *308*, 982–985.
- (36) Vuitton, V.; Yelle, R. V.; Anicich, V. G. The Nitrogen Chemistry of Titan's Upper Atmosphere Revealed. *Astrophys. J.* **2006**, *647*, L175–L178.
- (37) Coates, A. J.; Cray, F. J.; Lewis, G. R.; Young, D. T.; Waite, J. H., Jr.; Sittler, E. C., Jr. Discovery of Heavy Negative Ions in Titan's Ionosphere. *Geophys. Res. Lett.* **2007**, *34*, L22103.
- (38) Cordiner, M. A.; Palmer, M. Y.; Nixon, C. A.; Irwin, P. G. J.; Teanby, N. A.; Charnley, S. B.; Mumma, M. J.; Kisiel, Z.; Serigano, J.; Kuan, Y.-J.; Chuang, Y.-L.; Wang, K.-S. Ethyl Cyanide On Titan: Spectroscopic Detection and Mapping Using ALMA. *Astrophys. J.* **2015**, *800*, L14.
- (39) Tabone, B.; et al. A Rich Hydrocarbon Chemistry and High C to O Ratio in the Inner Disk around a Very Low-Mass Star. *Nat. Astron.* **2023**, *7*, 805–814.
- (40) Cernicharo, J.; Heras, A. M.; Tielens, A. G. G. M.; Pardo, J. R.; Herpin, F.; Guélin, M.; Waters, L. B. F. M. Infrared Space Observatory's Discovery of C_4H_2 , C_6H_2 , and Benzene in CRL 618. *Astrophys. J.* **2001**, *546*, L123–L126.
- (41) McGuire, B. A.; Burkhardt, A. M.; Kalenskii, S.; Shingledecker, C. N.; Remijan, A. J.; Herbst, E.; McCarthy, M. C. Detection of the Aromatic Molecule Benzonitrile ($c-C_6H_5CN$) in the Interstellar Medium. *Science* **2018**, *359*, 202–205.
- (42) Allamandola, L. J. In *PAHs and the Universe: A Symposium to Celebrate the 25th Anniversary of the PAH Hypothesis*; Joblin, C., Tielens, A. G. G. M., Eds.; EAS Publication Series: Cambridge, UK, EAS Publication Series, Vol 46, 2011; Toulouse, France, 31 May–04 June, 2010.
- (43) Hansen, C. S.; Peeters, E.; Cami, J.; Schmidt, T. W. Open Questions on Carbon-Based Molecules in Space. *Chem. Commun.* **2022**, *5*, 94.
- (44) Allamandola, L. J.; Tielens, A. G. G. M.; Barker, J. R. Interstellar Polycyclic Aromatic Hydrocarbons: The Infrared Emission Bands, the Excitation/Emission Mechanism, and the Astrophysical Implications. *Astrophys. J. Suppl. Ser.* **1989**, *71*, 733–775.
- (45) Berné, P.; et al. PDRs4All: A JWST Early Release Science Program on Radiative Feedback from Massive Stars. *Publ. Astron. Soc. Pacific* **2022**, *134*, No. 054301.
- (46) Peeters, E.; Hony, S.; Van Kerckhoven, C.; Tielens, A. G. G. M.; Allamandola, L. J.; Hudgins, D. M.; Bauschlicher, C. W. The Rich 6 to 9 μm Spectrum of Interstellar PAHs. *Astron. Astrophys.* **2002**, *390*, 1089–1113.
- (47) Boersma, C.; Bauschlicher, C. W., Jr.; Ricca, A.; Mattioli, A. L.; Peeters, E.; Tielens, A. G. G. M.; Allamandola, L. J. Polycyclic Aromatic Hydrocarbon Far-infrared Spectroscopy. *Astrophys. J.* **2011**, *729*, 64.
- (48) Maragkoudakis, A.; Boersma, C.; Temi, P.; Bregman, J. D.; Allamandola, L. J. Linking Characteristics of the Polycyclic Aromatic Hydrocarbon Population with Galaxy Properties: A Quantitative Approach Using the NASA Ames PAH IR Spectroscopic Database. *Astrophys. J.* **2022**, *931*, 38.
- (49) Coulombe, L.-P.; et al. A Broadband Thermal Emission Spectrum of the Ultra-Hot Jupiter WASP-18b. *Nature* **2023**, *620*, 292–298.
- (50) Miles, B. E.; et al. The JWST Early-release Science Program for Direct Observations of Exoplanetary Systems II: A 1 to 20 μm Spectrum of the Planetary-mass Companion VHS 1256–1257 b. *Astrophys. J. Lett.* **2023**, *946*, L6.
- (51) Rigby, J.; et al. The Science Performance of JWST as Characterized in Commissioning. *Publ. Astron. Soc. Pacific* **2023**, *135*, No. 048001.
- (52) Birkmann, S. M.; et al. The Near-Infrared Spectrograph (NIRSpec) on the James Webb Space Telescope - IV. Capabilities and Predicted Performance for Exoplanet Characterization. *Astron. Astrophys.* **2022**, *661*, A83.
- (53) National Academies of Sciences, Engineering, and Medicine *Pathways to Discovery in Astronomy and Astrophysics for the 2020s*; The National Academies Press: Washington, DC, 2021.
- (54) National Aeronautics and Space Administration. *Large UV/ Optical/IR Surveyor*. 2023; <https://asd.gsfc.nasa.gov/luvoir/resources/>; accessed on 11/14/2023.
- (55) Western, C. M. PGOPHER: A Program for Simulating Rotational, Vibrational and Electronic Spectra. *J. Quant. Spectrosc. Rad. Trans.* **2017**, *186*, 221–242.
- (56) Gamache, R. R.; et al. Total Internal Partition Sums for 166 Isotopologues of 51 Molecules Important in Planetary Atmospheres: Application to HITRAN2016 and Beyond. *J. Quant. Spec. Rad. Trans.* **2017**, *203*, 70–87. HITRAN2016 Special Issue
- (57) Müller, H. S.; Schlöder, F.; Stutzki, J.; Winnewisser, G. The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists. *J. Mol. Struct.* **2005**, *742*, 215–227.
- (58) Seifert, N. A.; Finneran, I. A.; Perez, C.; Zaleski, D. P.; Neill, J. L.; Steber, A. L.; Suenram, R. D.; Lesarri, A.; Shipman, S. T.; Pate, B. H. AUTOFIT, an Automated Fitting Tool for Broadband Rotational Spectra, and Applications to 1-Hexanal. *J. Mol. Spectrosc.* **2015**, *312*, 13–21.
- (59) Rad, M. L.; Zou, L.; Sanders, J. L.; Widicus Weaver, S. L. Global Optimization and Broadband Analysis Software for Interstellar Chemistry (GOBASIC). *Astron. Astrophys.* **2016**, *585*, A23.
- (60) Biczysko, M.; Bloino, J.; Puzzarini, C. Computational Challenges in Astrochemistry. *WIREs Comput. Mol. Sci.* **2018**, *8*, e1349.
- (61) Zapata Trujillo, J. C.; Pettyjohn, M. M.; McKemmish, L. K. High-Throughput Quantum Chemistry: Empowering the Search for Molecular Candidates behind Unknown Spectral Signatures in Exoplanetary Atmospheres. *Mon. Not. R. Astron. Soc.* **2023**, *524*, 361–376.
- (62) Bera, P. P.; Sattelmeyer, K. W.; Saunders, M.; Schaefer, H. F.; v. R. Schleyer, P. Mindless Chemistry. *J. Phys. Chem. A* **2006**, *110*, 4287–4290.
- (63) Fortenberry, R. C.; Lee, T. J. Computational Vibrational Spectroscopy for the Detection of Molecules in Space. *Ann. Rep. Comput. Chem.* **2019**, *15*, 173–202.
- (64) Santaloci, T. J.; Meador, W. E.; Wallace, A. M.; Valencia, E. M.; Rogers, B. N.; Delcamp, J. H.; Fortenberry, R. C. Automated Generation and Theoretical Predictions for Dye Sensitized Solar Cell Molecular Dyes. *Digital Discovery* **2023**, *2*, 1269–1288.
- (65) Kerkeni, B.; García-Berete, I.; Rigopoulou, D.; Tew, D. P.; Roche, P. F.; Clary, D. C. Probing Computational Methodologies in Predicting Mid-Infrared Spectra for Large Polycyclic Aromatic Hydrocarbons. *Mon. Not. R. Astron. Soc.* **2022**, *513*, 3663–3681.
- (66) Westbrook, B. R.; Layfield, J. P.; Lee, T. J.; Fortenberry, R. C. Reparameterized Semi-Empirical Methods for Computing Anharmonic Vibrational Frequencies of Multiply-Bonded Hydrocarbons. *Electronic Struct.* **2022**, *4*, No. 045003.
- (67) Westbrook, B. R.; Fortenberry, R. C. pbqff: Push-Button Quartic Force Fields. *J. Chem. Theory Comput.* **2023**, *19*, 2606–2615.
- (68) Lee, K. L. K.; Patterson, J.; Burkhardt, A. M.; Vankayalapati, V.; McCarthy, M. C.; McGuire, B. A. Machine Learning of Interstellar Chemical Inventories. *Astrophys. J. Lett.* **2021**, *917*, L6.
- (69) Fried, Z. T. P.; Lee, K. L. K.; Byrne, A. N.; McGuire, B. A. Implementation of Rare Isotopologues into Machine Learning of the Chemical Inventory of the Solar-Type Protostellar Source IRAS 16293–2422. *Digital Discovery* **2023**, *2*, 952–966.
- (70) Remijan, A.; et al. Astronomical Detection of the Interstellar Anion $C_{10}H^-$ toward TMC-1 from the GOTHAM Large Program on the Green Bank Telescope. *Astrophys. J. Lett.* **2023**, *944*, L45.

- (71) Fortenberry, R. C. Interstellar Anions: The Role of Quantum Chemistry. *J. Phys. Chem. A* **2015**, *119*, 9941–9953.
- (72) Léger, A.; Puget, J. Identification of the 'Unidentified' IR Emission Features of Interstellar Dust? *Astron. Astrophys.* **1984**, *137*, L5–L8.
- (73) Puget, J. L.; Leger, A. A New Component of the Interstellar Matter: Small Grains and Large Aromatic Molecules. *Annual Rev. Astron. Astrophys.* **1989**, *27*, 161–198.
- (74) Allamandola, L. J.; Hudgins, D. M.; Sandford, S. A. Modeling the Unidentified Infrared Emission with Combinations of Polycyclic Aromatic Hydrocarbons. *Astrophys. J.* **1999**, *511*, L115.
- (75) Peeters, E.; Mackie, C.; Candian, A.; Tielens, A. G. G. M. A Spectroscopic View on Cosmic PAH Emission. *Acc. Chem. Res.* **2021**, *54*, 1921–1933.
- (76) Heger, M. L. The spectra of certain class B stars in the regions 5630Å–6680Å and 3280Å–3380Å. *Lick Observatory Bulletin* **1922**, *10*, 146.
- (77) Merrill, P. W. Unidentified Interstellar Lines. *Publ. Astron. Soc. Pacific* **1934**, *46*, 206–207.
- (78) Merrill, P. W. Stationary Lines in the Spectrum of the Binary Star Boss 6142. *Astrophys. J.* **1936**, *83*, 126–128.
- (79) Salama, F.; Galazutdinov, G. A.; Krelowski, J.; Allamandola, L. J.; Musaev, F. A. Polycyclic Aromatic Hydrocarbons and the Diffuse Interstellar Bands: A Survey. *Astrophys. J.* **1999**, *526*, 265–273.
- (80) Douglas, A. E. Origin of Diffuse Interstellar Lines. *Nature*. **1977**, *269*, 130–132.
- (81) Smith, W. H. *The Diffuse Interstellar Bands*; Kluwer: Dordrecht, Netherlands, 1995; pp 3–12.
- (82) Herbig, G. H. The Diffuse Interstellar Bands. *Annu. Rev. Astrophys.* **1995**, *33*, 19–73.
- (83) Sarre, P. J. The Diffuse Interstellar Bands: A Major Problem in Astronomical Spectroscopy. *J. Mol. Spectrosc.* **2006**, *238*, 1–10.
- (84) Hobbs, L. M.; York, D. G.; Snow, T. P.; Oka, T.; Thorburn, J. A.; Bishof, M.; Friedman, S. D.; McCall, B. J.; Rachford, B.; Sonnentrucker, P.; Welty, D. E. A Catalog of Diffuse Interstellar Bands in the Spectrum of HD 204827. *Astrophys. J.* **2008**, *680*, 1256–1270.
- (85) McCall, B. J.; Drosback, M. M.; Thorburn, J. A.; York, D. G.; Friedman, S. D.; Hobbs, L. M.; Rachford, B. L.; Snow, T. P.; Sonnentrucker, P.; Welty, D. E. Studies on the Diffuse Interstellar Bands. IV. The Nearly Perfect Correlation between $\lambda\lambda 6196.0$ and 6613.6 . *Astrophys. J.* **2010**, *708*, 1628–1638.
- (86) Exarhos, G. H.; Mayer, J.; Klemperer, W. Chemical Processes in the Interstellar Medium: On the Nature of the Carrier of the Diffuse Interstellar Bands. *Philos. Trans. R. Soc. London A* **1981**, *303*, 503–511.
- (87) Fortenberry, R. C.; Crawford, T. D. Electronically Excited States in Interstellar Chemistry. *Annu. Rep. Comput. Chem.* **2011**, *7*, 195–214.
- (88) Campbell, E. K.; Holz, M.; Gerlich, D.; Maier, J. P. Laboratory Confirmation of C_{60}^+ as the Carrier of Two Diffuse Interstellar Bands. *Nature* **2015**, *523*, 322–324.
- (89) Cordiner, M. A.; Linnartz, H.; Cox, N. L. J.; Cami, J.; Najarro, F.; Proffitt, C. R.; Lallement, R.; Ehrenfreund, P.; Foing, B. H.; Gull, T. R.; Sarre, P. J.; Charnley, S. B. Confirming Interstellar C_{60}^+ Using the *Hubble Space Telescope*. *Astrophys. J. Lett.* **2019**, *875*, L28.
- (90) Lykhin, A. O.; Ahmadvand, S.; Varganov, S. A. Electronic Transitions Responsible for C_{60}^+ Diffuse Interstellar Bands. *J. Phys. Chem. Lett.* **2019**, *10*, 115–120.
- (91) Linnartz, H.; Cami, J.; Cordiner, M.; Cox, N.; Ehrenfreund, P.; Foing, B.; Gatchell, M.; Scheier, P. C_{60}^+ as a Diffuse Interstellar Band Carrier; A Spectroscopic Story in 6 Acts. *J. Mol. Spectrosc.* **2020**, *367*, 111243.
- (92) Cronin, J. R.; Pizzarello, S. Enantiomeric Excesses in Meteoritic Amino Acids. *Science*. **1997**, *275*, 951–955.
- (93) Sorrell, W. H. Origin of Amino Acids and Organic Sugars in Interstellar Clouds. *Astrophys. J.* **2001**, *555*, L129–L132.
- (94) Munoz Caro, G. M.; Meierhenrich, U. J.; Schutte, W. A.; Barbier, B.; Arcones Segovia, A.; Rosenbauer, H.; Thiemann, W. H.-P.; Brack, A.; Greenberg, J. M. Amino Acids from Ultraviolet Irradiation of Interstellar Ice Analogues. *Nature*. **2002**, *416*, 403–406.
- (95) Bernstein, M. P.; Dworkin, J. P.; Sandford, S. A.; Cooper, G. W.; Allamandola, L. J. Racemic Amino Acids from the Ultraviolet Photolysis of Interstellar Ice Analogues. *Nature*. **2002**, *416*, 401–403.
- (96) Lee, C.-W.; Kim, J.-K.; Moon, E.-S.; Minh, Y. C.; Kang, H. Formation of Glycine on Ultraviolet-Irradiated Interstellar Ice-Analog Films and Implications for Interstellar Amino Acids. *Astrophys. J.* **2009**, *697*, 428–435.
- (97) Materese, C. K.; Nuevo, M.; Bera, P. P.; Lee, T. J.; Sandford, S. A. Thymine and Other Prebiotic Molecules Produced from the Ultraviolet Photoirradiation of Pyrimidine in Simple Astrophysical Ice Analogs. *Astrobiology* **2013**, *13*, 948–962.
- (98) Sandford, S. A.; Nuevo, M.; Bera, P. P.; Lee, T. J. Prebiotic Astrochemistry and the Formation of Molecules of Astrobiological Interest in Interstellar Clouds and Protostellar Disks. *Chem. Rev.* **2020**, *120*, 4616–4659.
- (99) Altwegg, K.; Balsiger, H.; Bar-Nun, A.; Berthelier, J.-J.; Bieler, A.; Bochsler, P.; Briois, C.; Calmonte, U.; Combi, M. R.; Cottin, H.; et al. Prebiotic Chemicals—Amino Acid and Phosphorus—in the Coma of Comet 67P/Churyumov-Gerasimenko. *Science Advances* **2016**, *2*, e1600285.
- (100) Iglesias-Groth, S. A Search for Tryptophan in the Gas of the IC 348 Star Cluster of the Perseus Molecular Cloud. *Mon. Not. R. Astron. Soc.* **2023**, *523*, 2876–2886.
- (101) Carl, T.; Wirstrom, E. S.; Bergman, P.; Charnley, S. B.; Chuang, Y.-L.; Kuan, Y.-J. Deep Search for Glycine Conformers in Barnard 5. *Mon. Not. R. Astron. Soc.* **2023**, *524*, 5993–6003.
- (102) Zeng, S.; Quénard, D.; Jiménez-Serra, I.; Martín-Pintado, J.; Rivilla, V. M.; Testi, L.; Martín-Doménech, R. First Detection of the Pre-Biotic Molecule Glycolonitrile (HOCH_2CN) in the Interstellar Medium. *Mon. Not. R. Astron. Soc.* **2019**, *484*, L43–L48.
- (103) Rodríguez-Almeida, L. F.; Rivilla, V. M.; Jiménez-Serra, I.; Melosso, M.; Colzi, L.; Zeng, S.; Tercero, B.; de Vicente, P.; Martín, S.; Requena-Torres, M. A.; Rico-Villas, F.; Martín-Pintado, J. First Detection of C_2H_5NCO in the ISM and Search of Other Isocyanates towards the G+0.693–0.027 Molecular Cloud. *Astron. Astrophys.* **2021**, *654*, L1.
- (104) Rivilla, V. M.; et al. First Glycine Isomer Detected in the Interstellar Medium: Glycolamide ($\text{NH}_2\text{C}(\text{O})\text{CH}_2\text{OH}$). *Astrophys. J. Lett.* **2023**, *953*, L20.
- (105) Barone, V.; Biczysko, M.; Pazzarini, C. Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules. *Acc. Chem. Res.* **2015**, *48*, 1413–1422.
- (106) Kroto, H. The Spectra of Interstellar Molecules. *Int. Rev. Phys. Chem.* **1981**, *1*, 309–376.
- (107) Kroto, H. W.; Heath, J. R.; O'Brien, S. C.; Curl, R. F.; Smalley, R. E. C_{60} : Buckminsterfullerene. *Nature* **1985**, *318*, 162–163.
- (108) Terrones, M.; Hsu, W. K.; Kroto, H. W.; Walton, D. R. M. In *Fullerenes and Related Structures*; Hirsch, A., Ed.; Springer: Berlin, 1999; pp 189–234.