

Interrelations Between Astrochemistry and Galactic Dynamics

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Mendoza E, Duronea N, Ronsó D, Corazza LC, van der Tak F, Paron S and Nyman L-Å (2021) Interrelations Between Astrochemistry and Galactic Dynamics. Front. Astron. Space Sci. 8:655450. doi: 10.3389/fspas.2021.655450 This paper presents a review of ideas that interconnect astrochemistry and galactic dynamics. Since these two areas are vast and not recent, each one has already been covered separately by several reviews. After a general historical introduction, and a needed quick review of processes such as stellar nucleosynthesis that gives the base to understand the interstellar formation of simple chemical compounds (e.g., H₂, CO, NH₃, and H₂O), we focus on a number of topics that are at the crossing of the two big areas, dynamics and astrochemistry. Astrochemistry is a flourishing field that intends to study the presence and formation of molecules as well as the influence of them on the structure, evolution, and dynamics of astronomical objects. The progress in the knowledge on the existence of new complex molecules and of their process of formation originates from the observational, experimental, and theoretical areas that compose the field. The interfacing areas include star formation, protoplanetary disks, the role of the spiral arms, and the chemical abundance gradients in the galactic disk. It often happens that the physical conditions in some regions of the interstellar medium are only revealed by means of molecular observations. To organize a rough classification of chemical evolution processes, we discuss about how astrochemistry can act in three different contexts, namely, the chemistry of the early universe, including external galaxies, star-forming regions, and asymptotic giant branch (AGB) stars and circumstellar envelopes. We mention that our research is stimulated by plans for instruments and projects, such as the ongoing Large Latin American Millimeter Array (LLAMA), which consists in the construction of a 12 m sub-mm radio telescope in the Andes. Thus, modern and new facilities can play a key role in new discoveries not only in astrochemistry but also in radio astronomy and related areas. Furthermore, the research on the origin of life is also a stimulating perspective.

Keywords: astrochemistry, galaxies: general, ISM: molecules, methods: miscellaneous, history and philosophy of astronomy

1 INTRODUCTION

1.1 Early Impressions on the Milky Way

One of the most fundamental questions of mankind is why there is something rather than nothing (Stavinschi, 2011; Allen and Lidström, 2017); from archaic times, cultures have been intrigued and inspired by the galaxy-in classical Latin via lactea¹—the hazy band that can be visible across a cloudless and unpolluted night sky (Figure 1). The ancient philosophers speculated about what was that luminous band; the Platonist philosopher Plutarch described it as a cloudy circle, from Greek galaxias kyklos, literally the milky circle (kýklos "wheel"). Across the ages, arts and sciences have portrayed the origin and meaning of the galaxy; today, we know that it is the Milky Way seen from inside (Figure 2A); the spiral arm where the Solar System is located is the so-called Orion Arm or Orion Spur (Bok, 1950a; Bok, 1950b). The Milky Way is only one galaxy among hundreds of billions, and a neighbor galaxy is Andromeda (Figure 2B) (Conselice et al., 2016; Urquhart et al., 2018; Boardman et al., 2020).

"Galaxy" and "atom" are examples of words with Greek etymological roots. They are broadly used in contemporary science, but their meanings evolve with time. Various astronomical objects, chemical elements, and molecules also gained their names from Greek. The discovery of the noble gas helium ($h\bar{e}lios$ "sun") constituted a remarkable example in the recent history of astronomy, physics, and chemistry (Kragh, 2009). Today, we know that hydrogen (hydr-, hydro "water") and helium are the lightest and most abundant elements in the universe; they burn in stars forming heavier elements through nuclear reactions. As part of the life cycle of stars, the chemical elements ejected by a dying star will enrich the cloud in which the birth of the next stellar generation will take place; thus, stars are also seen as fossils that preserve the history of their host galaxies (De Silva et al., 2015; Kobayashi, 2016).

As a big question about the universe, Stavinschi (2011) also asked the following: Why is nature comprehensible to humans? How is cosmos related to humanity? Under the perspective of the *Homo sapiens* evolution, various insights can be found since the earliest interpretations about the galaxy. Etymologically, galaxy alludes to the liquid *milk*, the essential food for young mammals. In retrospect, such association is not minor if one considers Charles Darwin's legacy (e.g., Darwin, 1859), since the physiological synthesis of milk and lactation period are aspects that continuously drive the mammals' evolution, whose origins date back 200 million years (Capuco and Akers, 2009; Morgan, 2016).

According to one of the best known stories of the Greek mythology, the galaxy was formed by the milk spilled from the breast of a goddess, when the child Heracles, the famous hero and son of Zeus (Jupiter) and Alcmene, was pushed from Hera's breast (Bertola, 2009). Thus, the whiteness of the milk, secreted

from the breast of a nursing mother, was associated with that of the *Milky Way*. Translated from Greek, ancient texts recorded some thoughts about the galaxy; in Plutarch's Morals,² Parmenides realized it as a mixture of a thick and thin substance whose color resembles milk, Anaxagoras saw it as a shadow produced by the relative movement of the Sun and Earth, and Democritus saw it as a splendor arisen from the coalition of many small bodies (Wintemberg, 1908).

Since the renaissance, modern science revoked ideas such as geocentrism and vitalism, whose origins date back indeed to older ages. The laboratory synthesis of urea (NH₂)₂CO, a molecule found in mammals' urine, recently discovered in the interstellar medium (ISM) (**Figure 3**), see Remijan et al. (2014), established a new paradigm in the so-called organic chemistry. At the beginning of the 19th century, the chemist Friedrich Wöhler wrote to his mentor Jöns Jakob Berzelius: "I must tell you that I can prepare urea without requiring a kidney of an animal, either man or dog" (Yeh and Lim, 2007). For the time being, it was not well known how to transform inorganic substances into organic compounds, so that the production of urea from an aqueous solution of ammonium cyanate, without requiring a "vital force," set a milestone for chemical synthesis, so that not all the carbon compounds derived from living organisms (Forster and Church, 2006; Sumiya and Maeda, 2019).

1.2 The Organic Side of the Galaxy

Hydrogen, carbon, nitrogen, oxygen, sulfur, and phosphorus are essential elements in biomolecules; they are frequently referred to with the acronym CHNOPS (or CHONPS). The chemical evolution of the biogenic elements, from their cosmic origin to their inclusion in living organisms, constitutes a major topic in astrophysics, astrochemistry, and astrobiology (Whittet and Chiar, 1993; Nomoto et al., 2013; Pizzarello and Shock, 2017).

By the fact that they are tangible objects, meteorites have been intensively studied since the 19th century, a period in which a high number of meteorite falls and fireballs were recorded; then, chemists, astronomers, geologists, and meteorologists were among the specialists that initially characterized meteorites (Romig, 1966). In the present day, it is known that amino acids, nucleobases, and phosphates are present in meteorites: in a recent study, Furukawa et al. (2019) identified sugar-related compounds in samples of carbonaceous chondrites. Their results also include evidence for ribose, which is a building block of genetic molecules (e.g., RNA). The presence of organic molecules in comets is also relevant, since they contain and carry materials of the primitive solar nebula. Using remote observations at radio wavelengths, Biver and Bockelée-Morvan (2019) described the identification of organic molecules, such as acetaldehyde (CH3CHO), formamide (NH2CHO), and methyl formate (HCOOCH₃), whose abundances are usually reported with respect to, e.g., water or methanol. Those are aspects that unveiled an extraordinary chemistry in space.

¹Dictionaries and online sources: Cambridge, at https://dictionary.cambridge.org/dictionary/. Oxford, at https://www.oxfordlearnersdictionaries.com/. Merriam-Webster, at https://www.merriam-webster.com/. Online Etymology Dictionary, at https://www.etymonline.com/. Stanford Encyclopedia of Philosophy, at https://plato.stanford.edu/. Ancient History Encyclopedia, at https://www.ancient.eu/.

²Online source: Online Library of Liberty, at https://oll.libertyfund.org/. Plutarch's Morals. Translated from the Greek by Several Hands. Corrected and Revised by William W. Goodwin, with an Introduction by Ralph Waldo Emerson. 5 Volumes. (Boston: Little, Brown, and Co., 1878). Vol. 3. Chapter I.: Of the Galaxy, or the Milky Way. The text is in the public domain.



FIGURE 1 | Panoramic image capturing the Milky Way in a night sky arching over the ALMA Observatory's antennas in the Chajnantor Plateau (Chilean Andes). A cosmic rainbow in ultra HD, credit: ESO/B. Tafreshi (twanight.org).

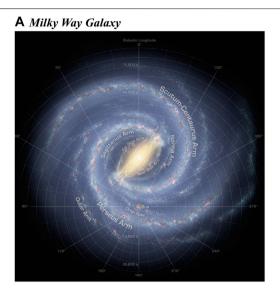




FIGURE 2 | (A) Artistic view of the Milky Way galaxy (diameter ~100 klyr) showing its arms and central bar with respect to the Sun's position, which lies near the so-called Orion Arm, or Orion Spur, between the Sagittarius and Perseus arms (credit: NASA/JPL-Caltech/R. Hurt, SSC/Caltech). (B) The Andromeda Galaxy (diameter ~220 klyr) in a composite image from three parts of the electromagnetic spectrum, the infrared, X-ray, and optical (credit: ESA/Herschel/PACS/SPIRE/J.Fritz, U. Gent/XMM-Newton/EPIC/W. Pietsch, MPE/R. Gendler). The Milky Way and Andromeda are neighboring galaxies expected to collide in a few billion years forming a merge galaxy ("Milkomeda") (Schiavi et al., 2020).

Organic molecules have been detected in different astronomical environments, from objects ranging in size from comets up to external galaxies (Tielens, 2013). Glycine, the simplest amino acid, has been searched for in the ISM, but its detection has been controversial (Kuan et al., 2003; Snyder et al., 2005); the ROSINA³ mass spectrometer provided a more robust result but in the coma of the 67P/Churyumov-Gerasimenko comet, where volatile glycine was confirmed (Altwegg et al., 2016; Hadraoui et al., 2019). In the case of the molecule urea, as was mentioned above, it was detected in the Murchison meteorite (Hayatsu et al., 1975) and has been searched for toward the high-mass star-forming region Sgr B2, Figure 3 (e.g., Remijan et al., 2014; Belloche et al., 2019; Belloche et al.,

2020); the interstellar synthesis of urea has also been computationally studied (Slate et al., 2020).

Why do organic compounds matter? Because they are based on the chemistry of carbon, whose most abundant isotope has an atomic and mass number of 6 and 12 (Z = 6, A = 12), respectively. As it is known by the nature of triple a reactions, elements with $A \ge 12$ are produced by stars, and the origin of C is associated with low- and intermediate-mass AGB stars (Karakas, 2010). Regarding the number of electrons, in the periodic table, carbon occupies a reference cell: it is the first element of the IV A group, in the middle of the I A and VIII A groups, which are headed by hydrogen and helium (Figure 4), so that carbon has a suitable electronic configuration to form multiple and stable covalent bonds. As a consequence, the element is present in the vast majority of (natural and synthetic) molecules known (Friedman, 2012; Wencel-Delord and Glorius, 2013). In the ISM, carbon can be abundantly found as gas CO, or in the condensed phase forming polycyclic aromatic hydrocarbons (PAHs) (Candian et al., 2018). C-bearing molecules are key in chemistry and astrochemistry: from CO, a

³ROSINA - Rosetta Orbiter Spectrometer for Ion and Neutral Analysis. The Mass Spectrometer for the Rosetta Mission. Online resource at https://www.esa.int/Science_Exploration/Space_Science/Rosetta/ROSINA.



FIGURE 3 | (A) Result of the search for urea in Sagittarius B2 (N-LMH); the green line represents a total simulated spectrum including both urea (red line) and methyl formate (dashed blue and dotted magenta lines) (from Remijan et al., 2014). (B) Color-composite image of the galactic center and Sgr B2. Credit: ESO/APEX & MSX/IPAC/NASA.

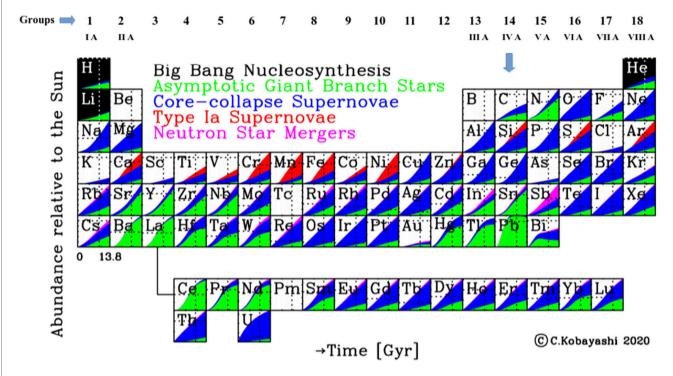


FIGURE 4 | Periodic table indicating the cosmic origin and evolution of the chemical elements [from Kobayashi et al. (2020)]; the group numbers are added in the upper part of the periodic table; they are related with the atomic properties. Credit: Chiaki Kobayashi, 2020.

cosmic diatomic molecule, to deoxyribonucleic acid (DNA), which can have order of 10⁸ carbon atoms, the search and detection of organic molecules in space contribute to our understanding of the emergence of life. Research on molecules such as HNCO, H₂CO, and NH₂CHO has shed light on the interstellar chemistry of pre-biotic molecules and species carrying various biogenic elements (e.g., Saladino et al., 2006; Bisschop et al., 2007; Mendoza et al., 2014; López-Sepulcre et al., 2015; Allen et al., 2020; Jørgensen et al., 2020).

The history around the concept of galaxy is rich; nowadays, astronomy, physics, and chemistry converge in specialized areas to study the Milky Way and other galaxies. In the next sections, we discuss relevant aspects to the subject: astrochemistry and

galactic dynamics (Section 2); the state of the art in methods and techniques (Section 3); a discussion considering different astronomical contexts and objects of study (Section 4); and perspectives on future facilities and final remarks (Section 5).

2 ASTROCHEMISTRY AND GALACTIC DYNAMICS

The essential subject matter of astrochemistry, also known as molecular astrophysics, is the study of the formation, destruction, and excitation of chemical species in astronomical environments and their influence on the structure, dynamics, and evolution of astronomical objects in galaxies (Dalgarno, 2008; van Dishoeck, 2018). To date, more than 200 molecules have been identified in the interstellar and circumstellar media, among which there are hydrocarbons and aromatic, inorganic, organic, and pre-biotic species (McCarthy and Thaddeus, 2001; Tielens, 2013; McGuire, 2018). The detection of the most abundant molecules, such as CO and its isotopologues (e.g., CO and CO), is used to diagnose the properties and the distribution of molecular clouds across the galaxy, which is crucial for our understanding of galactic dynamics (e.g., Heyer and Dame, 2015).

What are the connections between astrochemistry and galactic dynamics, the topic of this collection? Usually, by galactic dynamics, we understand stellar dynamics, basically the study of the orbits of stars. This field of research had impressive progress with the recent release of Gaia results (e.g., Gaia Early Data Release 3, Gaia Collaboration et al., 2021) with determination of distances, proper motion, photometry, and velocity of more than 1 billion stars. From these data, we obtained a much better description of the mass distribution, gravitational forces, and galactic resonances that are acting on the stars, at least within a radius of 2 kpc around the Sun. We must not forget, however, that galactic dynamics also includes hydrodynamics. On a large-scale point of view, the forces acting on the gas are almost the same as those acting on the stars, not only because the mass fraction of the galaxy in the form of gas is small compared to the stellar mass (about 5%; Lequeux, 2005) but also because the mass of the gas is already taken into account in stellar dynamics, like, for instance, in the gravitational potential derived from the rotation curve. The exact nature of the spiral arms is a question of major importance in astrochemistry. In the past, the spiral arms were considered to be large-scale gas shock waves (Roberts, 1969), but the stellar mass content has been a matter of investigation and continuous revisions over the past decades (Lin and Shu, 1964; Kalnajs, 1973; Shu, 2016). The high-resolution HI Nearby Galaxy Survey, THINGS (Walter et al., 2008), revealed the HI gas is strongly concentrated in the spiral arms, which are narrow structures. The fact that, normally, the arms are thin can also be seen in the image of Andromeda (Figure 2B). This reinforces the view that the arms are like grooves in the gravitational potential and that the gas flows along these grooves (Barros et al., 2021; Monteiro et al., 2021). The grooves, or elongated potential wells, are due to the larger density of stars in the arm, as the stellar orbits come close to each other, as in Kalnajs (1973) models, and in the model of our galaxy proposed by Junqueira et al. (2013)—see their Figure 8. The spiral arms are known to be the star-forming machines of the galaxy, as spiral arm tracers are the young and massive stars, like OB stars, young open clusters, and molecular masers associated with massive stars. The OB stars that we observe in the arms of external galaxies are believed to be the tip of the iceberg of clusters

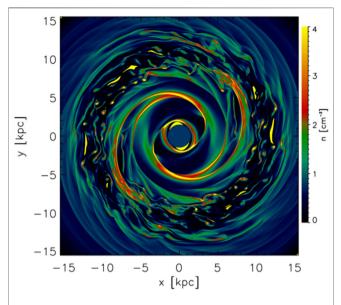


FIGURE 5 | Simulation of the density distribution of the galactic gaseous disk when perturbed by the PERLAS spiral arm potential [from Pérez-Villegas et al. (2015)].

of stars that are not visible to us (Wright, 2020). Falceta-Gonçalves et al. (2015) presented a detailed hydrodynamical simulation of interstellar clouds penetrating in the groove-shaped arms, due to the relative velocity of the galactic material with respect to the arms, showing the generation of turbulence and conditions favorable to star formation. Interestingly, at the end of their paper, Falceta-Gonçalves et al. (2015) made a comparison with another context of star formation in spiral arms, the context of transient arms (Baba et al., 2013). They concluded that, despite the dynamical differences between the two scenarios, the driving mechanisms of turbulence, which are at the origin of star formation, occur similarly.

The molecular content of the cold gas in spiral arms was observed by Greaves and Nyman (1996); they identified various chemical species such as HCO^+ , HCN, HNC, CN, C_2H , C_3H_2 , CS, SiO, N_2H^+ , CH_3OH , and SO, by means of a technique of looking at absorption lines in front of a radio continuum source, which permits to see the coldest components.

The formation of stars represents in some way the life of our galaxy, the means by which the galaxy evolves, and, in particular, how the chemical composition of the galaxy evolves. When we go down in size scales to the star formation cores in the molecular clouds, hydrodynamics is not governed anymore by the general potential of the galaxy, but by very local effects. Observation of molecules has two main roles. Since stars form in the interior of molecular clouds in regions obscured by the ISM, the molecular emission is a tool (together with mm and sub-mm dust emission) that can reveal what is happening inside of them. Therefore, astrochemistry is a powerful tool that allows us to determine densities and temperatures and observe gas flows, so that molecules are not only a tool but also main actors. Although the elements are only synthesized in the interior of stars or in outer layers of stars, in the case of supernovae, the ISM

⁴In line with the Cologne Database for Molecular Spectroscopy, CDMS, we refrain from stating an exact number of molecules as detected, since that status usually generates controversies and divergences in the community. More information at https://cdms.astro.uni-koeln.de/classic/ molecules.

contributes to transporting the elements, in the form of atoms or in the form of molecules or of dust grains, to regions that are distant from the stellar birthplace and distributing them more uniformly, contributing to the formation of smooth metallicity gradients.

A major feature of the galactic structure, related to metallicity gradients, is worth to mention here. There is a gap in the distribution of the ISM, in the form of a ring void of gas, at the corotation radius. Mishurov et al. (2009) called it the "Cassinilike" gap. It was observed in the HI surveys of the galactic disk (Amôres et al., 2009), and it appeared clearly in the hydrodynamic simulations of the galactic disk by Pérez-Villegas et al. (2015) (**Figure 5**). Monteiro et al. (2021) also present a discussion of the gap, including a figure with a toy model to explain its formation.

The fact that the gap is larger than 1 kpc in the radial direction and very deep (the gas density is almost zero in the gap) has enormous consequences. There is no communication between the gas situated in the two parts, inside and outside the corotation radius. So, the disk of the galaxy is divided into two parts that have independent chemical evolution. The outer part has a lower metallicity, since the star formation rate is smaller there, due to the smaller gas density, on average. The transition between the metallicity of the two halves of the galactic disk cannot be called a "gradient"; it is so abrupt across the Cassini-like gap, which we prefer to call the "step" in metallicity. This step was first discovered by Twarog et al. (1997) who presented a plot of [Fe/H] as a function of galactocentric distances of a sample of open clusters, in which we can already see all the important features: a step of -0.3 dex at 10 kpc (their adopted R0), a gap in the cluster density at 10 kpc (clusters cannot be born in the Cassini-like gap where there is no gas), and a flat gradient in the outer half-galaxy. The step in (Fe/H) was further studied and confirmed by Lépine et al. (2011). The existence of this step is evidence for the long-lived nature of the spiral arm structure. The step height is a consequence of the different metallicity enrichment rate on the two halves of the galaxy. If the corotation radius was frequently changing its position according to the intermittent arm models, the metallicity step would not have grown. Lépine et al. (2011) estimated a lower limit of 3 Gyrs for the present spiral arm structure. There are other examples of steps in metallicity at corotation, see, for instance, the step of the (O/H) abundance in M83 seen by Bresolin et al. (2009); in a similar way, it is an argument in favor of long-lived arms in M83. The flat (stellar) gradient of metallicity in the outer part of the galactic disk can be understood as an effect of the gas flow in spiral arms, remembering also that stars can only be born in arms. Another important consequence of this bimodal metallicity in the galactic disk is that it may explain the distribution of O-rich and C-rich AGB stars in the galaxy (a further revision is given in Section 4.3). At this point, it seems to be important to distinguish the high-mass AGB stars with cold circumstellar envelopes (CSEs) from the more common low-mass AGB stars (Omont et al., 1993). The O-rich and C-rich AGB stars with cold CSEs are more clearly separated in the galaxy. There is a belief, at least for the more massive stars, that if they are born in an ISM with low metallicity, they will become, in the AGB phase, C-rich stars, and

if the birthplaces have high metallicity, then the stars will become O-rich in the AGB phase (e.g., Noguchi et al., 2004; Ishihara et al., 2011). One example supporting this concept of the dependence on ambient metallicity is a deep search for OH/IR stars (O-rich AGB stars with cold CSEs) that was performed by Goldman et al. (2018) in the Small Magellanic Cloud (SMC), a low-metallicity galaxy. They made long integration on a dozen of luminous, long-period, large-amplitude variable stars, and no one confirmed to be an O-rich star. We will come back to the discussion of AGB stars in Section 4.3.

The metallicity step is a feature of the ISM that affects young stars. However, there is no obstacle for stars, as soon as they form, to start crossing the corotation gap, since it is a gap of hydrodynamical origin, and the stars have very little interaction with the gas. It is possible to find older stars that were born in the low-metallicity region and are presently in the highmetallicity region, and vice versa (Lépine et al., 2014). The radial migrations turn it more difficult to observe the metallicity step, depending on the sample of stars used; it is better observed using young stars. For instance, the gap at 8 kpc and the difference in metallicity of the inner and outer disks can be noticed in the sample of HII regions (Paladini et al., 2004, see their Figure 4). The authors did not mention the observed feature because this was not understood at that time. Interestingly, none of the major models of chemical evolution of the galaxy mention the important points that we discussed here. Concerning the importance of the corotation resonance being close to the Sun, see also the implications in the solar neighborhood regarding the Hercules stream, discussed in Section 4.4.

3 APPROACHES AND METHODOLOGIES

In view of relevance that astrochemistry has from a microscale to a cosmic scale (**Figure 6**), in this section, we focus on how it integrates observational, experimental, and theoretical approaches (**Figure 7**) to study the physical and chemical conditions of the interstellar gas and dust in galaxies.

3.1 Molecules in Space: Observations From Infrared to Radio Wavelengths

Molecules emit radiation from transitions that are denoted by electronic, vibrational, and rotational quantum levels; thus, the total energy is defined as $E = E_{electronic} + E_{vibrational} + E_{rotational}$. The electronic transitions are typically the most energetic and can stimulate photodissociation processes, such as those that take place in the upper atmosphere (stratosphere and above). Electronic transitions have frequencies ranging from the visible to the UV region of the spectrum; vibrational transitions are typically observed in the infrared range; rotational transitions, which are the weakest in energy, approximately range from submm to cm in the electromagnetic spectrum (Cook, 2003; Wilson et al., 2013).

Astrochemistry has benefited in the past decades from the construction of telescopes to observe interstellar molecules (van

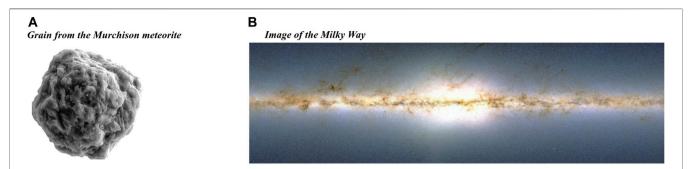
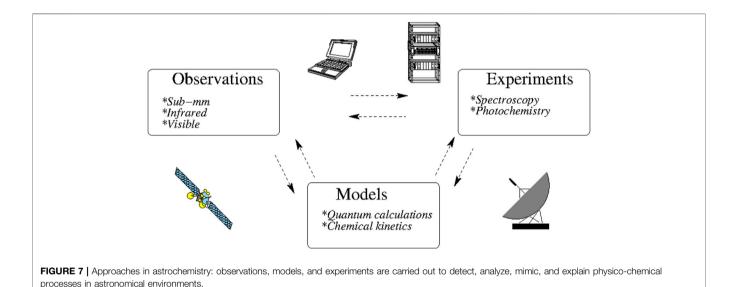


FIGURE 6 | The universe can be explored from a microscale to a cosmic scale: (A) scanning electron microscope image showing the morphology of a presolar silicon carbide (SiC) grain extracted from the Murchison CM2 meteorite [from Heck et al. (2020)]; (B) infrared map of the Milky Way exhibiting the disk, as a plane, and bulge of the galaxy. APOGEE-2 Background (https://www.sdss.org/surveys/apogee-2/apogee-2-background/).



Dishoeck, 2018). Since the early 1960s, with the advent of radio astronomy, molecules have been detected with ground-based facilities such as the NRAO 36 ft, IRAM 30 m, Nobeyama 45 m, and GBT 100 m. Galactic sources such as Sgr B2, IRC+10216, TMC-1, and Orion have recorded a vast number of molecular detections (McCarthy and Thaddeus, 2001; McGuire, 2018). From infrared to radio wavelengths, the latter facilities like the Spitzer Space Telescope, the Herschel Space Observatory, the Stratospheric Observatory for Infrared Astronomy (SOFIA), and the (sub)millimeter telescopes in the Atacama Desert, such as the Atacama Pathfinder Experiment (APEX), the Atacama Submillimeter Telescope Experiment (ASTE), and the Atacama Large Millimeter/submillimeter Array (ALMA), have contributed to the state of the art of observational astrochemistry. In addition to molecular surveys based on abundant species (e.g., CO and CH₃OH), those new facilities have provided results about rare species, such as ArH (Schilke et al., 2014), HeH+ (Güsten et al., 2019; Neufeld et al., 2020), p-H₂D⁺ (Brünken et al., 2014), and complex organic molecules like formamide and N-methylformamide (NH2CHO and CH₃NHCHO), with the latter studied by Belloche et al.

(2017) by combining experiments, modeling, and observations with the ALMA toward Sgr B2(N2).

The interstellar molecules are generally listed by their number of atoms. In the particular case of the so-called complex organic molecules (COMs), with a different connotation, e.g., in organic chemistry or biochemistry, it stands for interstellar molecules containing an organic functional group and usually more than five atoms (Herbst and van Dishoeck, 2009), such as the C₂H₄O₂ isomers methyl formate (HCOOCH₃), glycolaldehyde (CH₂OHCHO), and acetic acid (CH₃COOH), which have been detected in Sgr B2(N) (Xue et al., 2019). Examples of lists of interstellar and circumstellar molecules can also be found at *The Astrochymist*⁵ (D. Woon), in which species are ordered by the first year of reported discovery, also including the astronomical sources, wavelength, and bibliographic information.

Along with the advances about detection of molecules, efficient codes have also been developed to infer the physical

⁵The Astrochymist: http://www.astrochymist.org/astrochymist_ism.html.

and chemical conditions from observations. As part of the data analysis, local thermodynamic equilibrium (LTE) hypotheses are generally evaluated (Goldsmith and Langer, 1999; Roueff et al., 2021); however, collisional rate coefficients and non-LTE calculations are also important to estimate, e.g., gas kinetic temperatures and volume densities. Public programs such as RADEX,6 which is a one-dimensional non-LTE radiative transfer code (van der Tak et al., 2007), permit the estimation of physical conditions from a given observational dataset. The RADEX code is also an alternative tool to the population diagram method (e.g., Goldsmith and Langer, 1999), which relies upon the availability of various optically thin emission lines. Collisional rate coefficients are essential for statistical equilibrium calculations. The Leiden Atomic and Molecular Database (LAMDA)⁷ contains spectroscopic and collisional rate coefficients for a number of astrophysically interesting chemical species, including data for 4 atomic/ionic species and 37 molecules (Schöier et al., 2005). A new revision of LAMDA, including its current status, recent updates, and future plans, is described in van der Tak et al. (2020), where planned updates consider data for noble gas species, extensions of existing collisional data to more transitions, additional collisional partners, and data for molecular isotopologues. This conjunction of theoretical, experimental, and observational methods (Figure 7) represents an example about how astrochemistry is developed nowadays.

3.2 Experimental Astrochemistry: Laboratory Work

Atomic and molecular spectroscopy, gas phase, and ice chemistry are essential subjects to understand the physics and chemistry of the ISM; they are part of the laboratory work that benefits astrochemistry. Regarding spectroscopy, the association of an astronomical spectral signature with a given molecule depends on the availability of rest frequencies and spectroscopic properties that are usually obtained from laboratory data and quantum chemical calculations. The Cologne Database for Molecular Spectroscopy (CDMS) is an exceptional resource founded in 1998 that provides an updated catalog of molecular species (Endres et al., 2016); many of them have been detected and reconfirmed in astronomical sources usually observed in radio wavelengths; however, in particular cases, the catalog contains entries for transitions in the far- and mid-infrared, such as those for species as C₃, C₃O₂, CH⁺, C₂H, HCO⁺, and N₂H⁺. The Splatalogue database for astronomical spectroscopy compiles resources such as the CDMS, the JPL Molecular Spectroscopy Catalogue (Pickett et al., 1998), and the Lovas/NIST list of recommended rest frequencies for observed interstellar molecular microwave transitions (Lovas, 2004).

Although interstellar molecules are generally observed in the gaseous phase, it is well known that the solid state plays an important role in the synthesis of molecules (Boogert et al., 2015;

Linnartz et al., 2015). As part of the life cycle of gas and dust during the stellar evolution, the cold conditions in dark interstellar clouds favor a rich ice chemistry in which molecules are produced in icy dust grains. The Infrared Space Observatory and Spitzer provided important evidence of the composition of interstellar ices (Gibb et al., 2004; Öberg et al., 2011); in particular, as part of the Spitzer ice legacy, Öberg et al. (2011) estimated that the median ice composition H₂O:CO:CO₂: CH₃OH:NH₃:CH₄:XCN (e.g., OCN⁻) is 100:29:29:3:5:5:0.3 and 100:13:13:4:5:2:0.6 toward low- and high-mass protostars, respectively. The ice chemistry is relevant to explain aspects such as the formation of complex organic molecules, e.g., ethylene glycol [H₂C(OH)CH₂OH] (Fedoseev et al., 2015), and isotopic exchange reactions, e.g., H2CO ice analogs in H2O (Ratajczak et al., 2009; Oba et al., 2012), since gas chemical reactions alone cannot explain the presence and abundance of various interstellar molecules.

The study of interstellar ice analogs has also provided clues about how life arose in our planet. Chirality is a property that some molecules exhibit, in which living organisms use lefthanded (L) amino acids in proteins and right-handed (D) sugars in RNA and DNA; the appearance of molecular chirality in meteorites and/or comets might provide clues on the asymmetric evolution of life on Earth (Kondepudi et al., 1990; Evans et al., 2012). In the ISM, McGuire et al. (2016) reported the discovery of the chiral molecule propylene oxide (CH₃CHCH₂O) toward the Sagittarius B2 north molecular cloud. Experiments have demonstrated that ices irradiated with UV circularly polarized light can yield a given stereo-specific photochemistry; in that way, Modica et al. (2014) found an enantiomeric excess during the synthesis of amino acids in ice analogs irradiated at two different photon energies. Among the 16 amino acids identified in the experiment, they found an L-enantiomeric excess in five of them. Based on the known biochemical processes, the search for and study of chiral asymmetry are discussed as a potential bio-signature in the Solar System (Goesmann et al., 2017; Glavin et al., 2020).

3.3 Calculations and Modeling in Astrochemistry

The different conditions and inaccessibility to interstellar regions demand elaborating models to understand the physical and chemical processes in space. Astrochemical models can be used to study the composition and chemical reactions of the ISM and to include gas-solid reactions depending on the evolutionary stage of the interstellar regions. Reactions of astrochemical interest have been experimentally and theoretically investigated by research groups worldwide. The KInetic Database for Astrochemistry (KIDA)⁸ and the UMIST Database for Astrochemistry (UDfA)⁹ are web-based resources providing lists of species and chemical reactions between them; such databases compile rate coefficients from the literature and

⁶RADEX: https://home.strw.leidenuniv.nl/moldata/radex.html.

 $^{^7} LAMDA:\ https://home.strw.leidenuniv.nl/\widetilde{m}oldata/.$

⁸KIDA: http://kida.astrophy.u-bordeaux.fr/.

⁹UMIST RATE12: http://udfa.ajmarkwick.net/index.php.

are continuously updated. McElroy et al. (2013) presented one of the latest releases of the UDfA, which consists in a new reaction network (labeled Rate12) containing 6,173 gas-phase reactions involving 467 chemical species. Among the novelties, various anion chemical reactions, deuterium exchange reactions, and surface binding energies for neutral species are available. Wakelam et al. (2015) presented the 2014 KIDA network for interstellar chemistry (labeled kida.uva.2014), which includes a total of 7,509 reactions involving 489 species. In comparison with previous versions (kida.uva.2011), 446 rate coefficients changed and 1,038 new reactions were added. Comparisons between both databases have been discussed, and McElroy et al. (2013) compared Rate12 with kida.uva.2011 considering a dark cloud model. For instance, among 62 modeled species, considering observations of TMC-1, 38 agree at a time of 2.5×10^5 years. They also discussed differences for O-bearing molecules such as acetaldehyde (CH₃CHO) and formic acid (HCOOH) (Hamberg et al., 2010; Vigren et al., 2010), which are associated with newly measured dissociative recombination rate coefficients for reactions with electrons.

The KIDA also provides astrochemical codes, ¹⁰ such as the Nautilus gas–grain code whose latest version allows to simulate the chemical evolution of the ISM considering three phases, i.e., gas, grain surface, and grain mantles (Iqbal and Wakelam, 2018); the gas chemistry uses the kida.uva.2014 network, and the grain chemical network is that presented in Garrod et al. (2007) and Ruaud et al. (2015). Such types of codes and chemical models find important applications in sources like cold cores, which in conjunction with sub-mm observations might explain the desorption and formation of COMs in icy mantles (Vasyunin et al., 2017).

4 THE OBJECTS OF STUDY: A LARGE AND SPECIAL ISSUE

In order to provide an overview about astronomical objects connecting astrochemistry and galactic dynamics, in this section, we present a discussion from three different perspectives, namely, the chemistry of the early universe and external galaxies, star-forming regions, and evolved stellar objects such as AGB stars. Such topics are also seen in the perspective for future investigations integrating the methodologies described in **Section 3**.

4.1 Chemistry of the Early Universe

After primordial nucleosynthesis, the chemistry started in the recombination era when the ions produced in the Big Bang recombined with free electrons. The first molecules and molecular ions were simple species, such as H_2 , HD, HeH^+ , and LiH. Given the difficulties to observe them, the chemistry of those species is mainly inferred from models (Galli and Palla, 2013). In the case of the helium hydride ion (HeH⁺), **Table 1** lists

chemical equations of formation and destruction reported in the literature.

Miller et al. (1992) presented and discussed evidence for ${\rm H_3^+}$ and ${\rm HeH^+}$ in the envelope of the supernova 1987A. Zinchenko et al. (2011) searched for ${\rm H_3^+}$ and ${\rm HeH^+}$ in a high-redshift quasistellar object. In a recent work, Güsten et al. (2019) identified HeH⁺ in the planetary nebula NGC 7027 using data from the SOFIA airborne observatory and also identified the pure rotational HeH J=1–0 ground-state transition at 149.137 µm. Neufeld et al. (2020) confirmed the discovery of HeH⁺ in NGC 7027 and identified rovibrational lines at 3.51629 and 3.60776 µm using the NASA Infrared Telescope Facility (IRTF) on Mauna Kea.

Heavier chemical elements would start to appear after the formation of the first stars, or Population III stars. Galactic chemical evolution models are important to understand the baryonic matter behavior in galaxies (Pagel, 1997; Matteucci, 2012). As a type of feedback mechanism, molecules such as CO and SiO provide C and Si to produce dust grains, e.g., in the form of amorphous carbon and/or refractory silicate compounds concurrently. The grain surfaces are essential to catalyze the H₂ synthesis, since the gas-phase routes do not account for the H₂ formation and abundance. Marassi et al. (2015) quantified the role of core-collapse supernovae as the first cosmic dust polluters and carried out models about dust formation considering grain species such as amorphous carbon (C), Al₂O₃, Fe₃O₄, MgSiO₃, Mg₂SiO₄, and SiO₂; in the gas phase, they considered reactions involving CO and SiO. Depletion processes are important in dust formation; grains can grow at high accretion rates by condensation of gas molecules such as CO and SiO. In the context of Type II supernovae at redshift $z \ge 5$, Schneider et al. (2004) found that grain condensation starts ~150 days after the explosion, when the temperature of the expanding gas falls from $T \approx 10^4 \,\mathrm{K}$ to $T \approx 500 \,\mathrm{K}$, yielding dust masses in the 0.01–10 M_{\odot} range. Therefore, in such events, dust grows and acts as an effective cooling agent thermalizing the gas phase.

Currently, there are no observational constraints on the Pop III SNe events. However, observational results point to evidence of large amounts of dust at high redshifts. The reddening of background quasars and Ly α systems at high redshift (z > 6) requires large column densities of dust to be explained (Cherchneff and Dwek, 2009). Detection of dust thermal emission appears from high-redshift QSOs from the Sloan Digital Sky Survey (SDSS) out to redshift 6.4. From the IR luminosities of the hyperluminous galaxy SDSS J1148 + 5251 at redshift z = 6.4 (Bertoldi et al., 2003), the amount of dust required to explain the results would be about $2.10^8 M_{\odot}$ (Schneider et al., 2004; Cherchneff and Dwek, 2009). These results cannot be accounted for by processes efficient for dust formation in the local universe such as the winds of AGB and supergiant stars and the colliding winds of Wolf-Rayet stars or the ejecta of core-collapse supernovae, mainly due to their long evolutionary timescales of around a few Gyr. Therefore, the short timescales for supermassive primordial star evolution offer the best explanation for the high amounts of dust found at high redshifts (Schneider et al., 2004; Cherchneff and Lilly, 2008; Cherchneff and Dwek, 2009).

 $^{^{10}\}mbox{KIDA}$ Codes: http://kida.astrophy.u-bordeaux.fr/codes.html.

TABLE 1 | Primordial chemistry of HeH+. Examples of chemical reactions of formation and destruction of HeH+.

Reactions: formation	Туре	References	
$H_2^+ + He \rightarrow HeH^+ + H$	Ion-neutral	Theard and Huntress (1974)	
$H^+ + He \rightarrow HeH^+ + hv$	Radiative association	Zygelman et al. (1998)	
Reactions: destruction	Туре	References	
HeH ⁺ +e ⁻ → He + H	Dissociative recombination	Novotný et al. (2019)	
$H + HeH^{+} \rightarrow He + H_{2}^{+}$	Ion-neutral	Karpas et al. (1979)	

With observatories like the ALMA, new evidence demonstrates the important role of dust in the evolution of galaxies. Dunlop et al. (2017) conducted a deep ALMA imaging in the Hubble Ultra-Deep Field ($z\approx 2.15$) and estimated that ~85% of the total star formation is hidden in dust.

4.1.1 Astrochemistry in Neighboring and More Remote Galaxies

The first observations of molecules in external galaxies were reported in the 1970s; Weliachew (1971) recorded the first detection of a molecular line outside the Milky Way, which was OH identified in the NGC 253 and M82 galaxies. From the abundant H₂ (Thompson et al., 1978) to pre-biotic species such as NH₂CHO (Muller et al., 2013), various molecules observed in the Milky Way have also been found in external galaxies (Viti, 2016).

In the vicinity, the Large Magellanic Cloud (LMC), located at about 50 kpc, is a galaxy that is seen nearly face-on with an inclination angle of 35°. The metallicity in the LMC is $Z \sim 0.5 Z_{\odot}$ (Keller and Wood, 2006), and the gas-to-dust ratio is a factor of 4 higher than that in the Milky Way. This galaxy has many active star-forming and HII regions (e.g., Paron et al., 2016; Ochsendorf et al., 2017). Therefore, the LMC is a unique laboratory for studying the effects of metallicity on molecular gas and star formation at high spatial resolution in an extragalactic medium. Indeed, several complex molecules have been detected toward hot cores in the LMC. Sewiło et al. (2018) reported the first extragalactic detection of the COMs dimethyl ether (CH₃OCH₃) and methyl formate (HCOOCH₃); along with CH₃OH, a chemical precursor, those species were detected toward the N 113 star-forming region in the LMC. Molecular studies like those can shed light on chemical processes in the past universe, where the metallicity was significantly lower than that in the present-day galaxies (see also Shimonishi et al., 2020).

4.2 Astrochemistry in Star-Forming Regions

Interstellar molecules can be found in different conditions and environments, either in nearby objects of our Solar System or in distant galaxies. The study of interstellar molecules has helped to better understand not only the evolutionary stages of stellar formation but also the physical and chemical properties of galactic nebulae and star-forming regions, which are known to be one of the main tracers of the spiral structure of the galaxy (Reid et al., 2019). The molecular spectra may contribute to the determination of important properties such as temperature, density, abundance, and kinematic properties (expanding or collapsing motions, rotations, etc.) of the molecular clouds in

which the molecules are embedded. Although the high-mass star formation is not well understood, it is believed to occur inside giant molecular clouds; the resulting stages in the formation of high-mass young stellar objects (YSOs) can be summarized as follows: 1) Infrared dark clouds (IRDCs), which are massive and cold (T~ 10 K) clouds, where the collapse takes place. 2) Warm/hot (T~ 100–300 K) inner envelopes heated by the central protostar with sizes up to \sim 0.1 pc and densities of 10^{7-8} cm⁻³, known as hot cores (e.g., Kurtz et al., 2000; Tan et al., 2014; Motte et al., 2018; Beaklini et al., 2020). This stage is characterized to be a strong emitter of rotational lines of complex molecular species. In fact, the detection of COMs, which are present in dense and hot gases, is the strongest indicator of the hot core phase and its most distinctive feature. 3) Ultracompact HII region, powered by the newly formed YSO. For the case of low-mass star-forming regions, the phenomena and stages may include 1) molecular outflows, 2) hot corinos, which are the low-mass version of hot cores, and 3) protoplanetary disks (e.g., Ceccarelli et al., 2007; Walsh et al., 2016; Lefloch et al., 2018; Belloche et al., 2020). High-mass protostellar objects also exhibit a complex chemistry, and studies have been dedicated to detect and model the presence of molecules (e.g., CH₃OH, H₂CO, CH₃CN, HNCO, and NH₂CHO) in YSOs, disks, and outflows (Isokoski et al., 2013; Choudhury et al., 2015).

Hot molecular cores and hot corinos are believed to be objects preceding the formation of high-mass and low-mass YSOs, respectively. They are both characterized for being strong emitters of high-energy rotational lines of rare molecular species at mm and sub-mm wavelengths. They will determine the chemical richness of star-forming regions in the galaxy, which, as previously mentioned, are the main tracers of the spiral structure of our galaxy. Then, it is crucial to detect and study complex organic molecules in hot cores and hot corinos, which allows to obtain a better understanding of chemical processes that are taking place on them and to better comprehend the chemical compositions of the spiral structure of the galaxy. In the last few years, several detections of complex molecules were obtained toward a small number of galactic hot cores/corinos (paradigmatic cases are Sgr B2, Orion-KL, W51, NGC 6334I). For these reasons, it is crucial to increase the number of detections of complex molecules in high- and low-mass star-forming regions during the latest phases of star formation.

4.3 Evolved Stars and Circumstellar Envelopes

The AGB stars and their circumstellar envelopes exhibit a rich chemistry in heavy elements, ions (cations and anions), radicals,

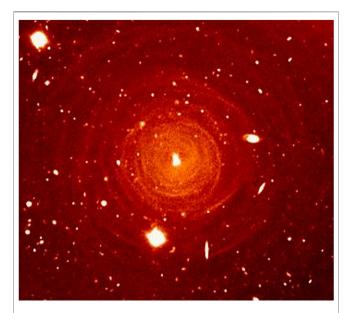


FIGURE 8 | Image of IRC+10216 and its shells. The source is a near C-rich AGB star, and various chemical species including anions (e.g., CN⁻) have been detected in its circumstellar envelope (Agúndez et al., 2010). Image credits: Izan Leao (Universidade Federal do Rio Grande do Norte, Brazil).

and molecules; various chemical species detected in space have been discovered in circumstellar shells (Li et al., 2016). For example, IRC+10216 (**Figure 8**) is one of the nearest and most investigated AGB stars; observational and theoretical studies have unveiled aspects on its chemistry, structure, and evolution (Leão et al., 2006; Cernicharo et al., 2015). AGB stars are classified according to their carbon-to-oxygen abundance ratios; on the one hand, they are defined as carbon-rich (C-rich) AGB stars if C/O > 1; on the other hand, they are defined as oxygen-rich (O-rich) AGB stars if C/O < 1; as an intermediate category, the S-type AGB stars stand for those sources with $C/O \approx 1$ values (Brunner et al., 2018).

In the Milky Way, O-rich AGB stars exhibit silicatedominated circumstellar features. C-rich AGB stars exhibit signatures associated with hydrocarbons and carbonaceous dust. Regarding their galactic distributions, O-rich AGB stars are more concentrated toward the galactic center, while C-rich ones are distributed more uniformly across the galaxy (Le Bertre et al., 2003). Ishihara et al. (2011) confirmed such trends in a study of C- and O-rich AGB stars using a mid-infrared all-sky survey (Figure 9), also proposing that the metallicity gradient with galactocentric distance might be one of the possible factors to explain the spatial distributions of C-rich and O-rich AGB stars; a comprehensive study covering the entire Milky Way is still needed to understand the dependence on the metallicity and galactic environment. Evolved stars are also important in studies about the chemical enrichment of the ISM in galaxies, which can be specially studied in the local group of galaxies where AGB stars are useful to study the structure, chemical enrichment, and galaxy evolution (Javadi and van Loon, 2019). Surveys such as the HERschel Inventory of The Agents of Galaxy Evolution (HERITAGE) (Meixner et al., 2010) have allowed to investigate the presence of evolved star candidates in the LMC and SMC with metallicities of 0.5 and $0.2Z_{\odot}$, respectively (Russell and Dopita, 1992; Jones et al., 2015). Studies highlight the importance of using the ratios between C- and O-rich AGB stars to evaluate the metallicity distribution in galaxies such as the Magellanic Clouds, unveiling that stars in the SMC are, in general, older and poorer in metals than those in the LMC, in line with the fact that the SMC is considered a more primitive and less evolved galaxy than the LMC (Cioni and Habing, 2003; Cioni et al., 2006). We remind here the discussion presented in Section 2 on the two halves of the galactic disk that are separated by an abrupt step in metallicity. The abrupt separation is attenuated for populations of not too young stars, like AGB stars, since part of them might have suffered migration across the corotation gap, which is a barrier only for the gas.

We will now focus on the C-rich AGB stars with thick circumstellar dust envelopes, since these AGB stars or post-AGB stars have the potential to have strong influence on the chemical evolution of the ISM. These stars have quite high mass loss rates, frequently over $10^{-5}M_{\odot}$ per year. Epchtein et al. (1990) made a crude estimate of the number of C-rich AGB stars with thick circumstellar dust envelopes in the galaxy and of their mass loss rates. They reached the conclusion that the total mass returning to the galaxy is $0.5~M_{\odot}$ per year; as a rough estimation, in 2 Gyr, this would amount to $10^9 M_{\odot}$, which corresponds to 20% of the mass of the ISM estimated by Lequeux (2005). One may wonder, therefore, if part of the molecules that are found in the cold ISM did not originate in the winds of AGB stars.

IRC+10216 is considered the prototype of the C-rich stars with thick envelopes. Matthews et al. (2015) discovered the presence of a shell of neutral hydrogen around IRC+10216, with an estimated diameter of 0.8 pc. The authors did their observations in the 21 cm HI line, but based on simple calculations of mass loss rates, they concluded that the bulk of the stellar wind is not only in the form of HI but also in the molecular form. The number of published works on IRC+10216 is enormous. There are results such as the Plateau de Bure and ALMA high-resolution observations, the observations of dust shells, the discovery of a dust lane, and the binary nature of the star. We will only focus on the molecular species that have been discovered. A list of molecules detected in IRC+10216 according to Ziurys (2006) is given in **Table 2**, as well as the molecules reviewed by McGuire (2018). Recently, Cernicharo et al. (2019) discovered the magnesium-bearing species MgC₃N and MgC₄H in the same source.

The fact that many molecules are composed of elements heavier than O, such as Mg, Si, Na, S, Al, P, and Fe, shows that, indeed, the AGB stars are contributing to the chemical evolution of the galaxy. Nyman et al. (1993) compared the molecular abundances of IRAS 15194-5144, another very bright C-rich AGB star, with those of IRC+10216. They performed a survey in the 1.3 and 3 mm bands with the Swedish–ESO Submillimetre Telescope (SEST) and detected 29 transitions of 14 species and some of their isotopologues. Woods et al. (2003) observed a rich and complex chemistry toward a sample of carbon-rich circumstellar envelopes observed in both the

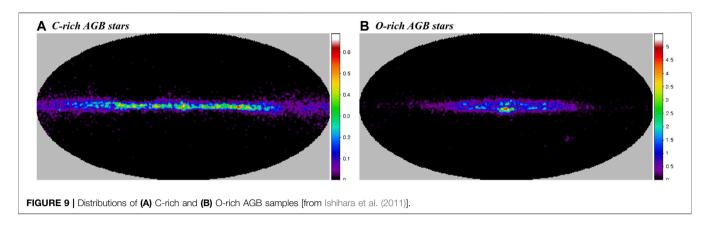


TABLE 2 | List of various molecular identifications carried out in IRC+10216.

Chemical species in IRC+10216							
CO	C ₂ H	HC₃N	C ₂ S	SiO	NaCl		
CS	C ₃ H	HC₅N	C ₃ S	SiS	AICI		
CN	C ₃ O	HC ₇ N	C ₅ S	SiC	KCI		
CN⁻	C ₄ H	HC ₉ N	C ₂ N	SiN	AIF		
HCN	C ₅ H	H_2C_4	C ₃ N	SiC ₂	MgCN		
C_2H_2	C ₆ H	H_2C_6	C ₃ N⁻	SiC ₃	MgNC		
HNC	C ₆ H ⁻	HC ₂ N	C ₅ N	SiCN	MgC ₃ N		
C_2H_4	C ₇ H	NC ₂ P	C ₅ N⁻	SiNC	MgC₄H		
CH ₄	C ₈ H	CH ₃ SiH ₃	HC₄N	SiC ₄	FeCN		
NH_3	C ₈ H⁻	C_3	c-C ₃ H ₂	SiH₄	AINC		
H ₂ S	C_2	C ₅	CH ₃ CN		KCN		
			CP		NaCN		
			C ₂ P				
			PN				
			HCP				

Note: The list was organized considering, e.g., Ziurys (2006), Glassgold (1996), Agúndez et al. (2014), the 2018 Census of molecular detections presented by McGuire (2018), and current detections reported by Cernicharo et al. (2019).

northern and southern skies, for which they used the Onsala Space Observatory 20 m and SEST antenna, respectively. They identified more than 20 chemical species, e.g., CN, C₂H, HC₃N, and CH₃CN, whose chemistry in the outer envelope can be explained through photochemical models. Almost all the species detected in IRC+10216 were also present in IRAS 15194-5144, and there is a good correlation between the abundances. Similarly, Zhang et al. (2009) performed a line survey of the carbon AGB star CIT6 and found that the spectral properties of CIT6 are consistent with those of IRAS+10216. We are allowed, therefore, to consider that the set of molecules in Table 2, at least for the strongest lines, is characteristic of C-rich AGB stars. We now come to the question of the observations of Greaves and Nyman (1996), who made a survey of molecules in "spiral arm clouds" and found HCO+, HCN, HNC, CN, C2H, C3H2, CS, SiO, N2H+, CH₃OH, and SO, which are basically the same species expelled by C-rich AGB stars, except that now there are two new oxygenrich molecules, which could be explained if the line-of-sight crosses regions containing also O-rich AGB stars.

In a recent work, Cristallo et al. (2020) claimed that the majority (90%) of presolar SiC grains found in primitive meteorites (e.g., **Figure 6A**) originate from ancient AGB stars,

whose ejected mass was merged into the Solar System during its formation. Thus, the role of AGB stars in chemical enrichment is significant for producing ^{12,13}C, ¹⁴N, F, ^{25,26}Mg, and ¹⁷O and slow neutron-capture process (s-process) (Kobayashi et al., 2020). Evolved stellar objects are relevant to galactic studies; the similar molecular content of AGB stars' mass loss and in spiral arm clouds is not a sufficient proof that the gas clouds in the arms originate partly from the AGB star, but it suggests that it is a question that merits to be further investigated.

4.4 Dynamics Very Close to the Sun, Moving Groups, and Stellar Streams

It is known that there exist groups of stars situated around and very near the Sun, which have anomalous velocities, with each of these groups forming a kind of "wind" of stars traveling in a given direction. Antoja et al. (2018) presented an historical perspective and an updated list of moving groups. The interest of these groups for astrochemistry is that they offer the opportunity to investigate what was the composition of the gas where the stars were born. Let us take one example, the Hercules stream, which is well studied. According to an investigation of the origin of moving groups by Barros et al. (2020), the Hercules stream could be mostly associated with the 8/1 and 12/1 Lindblad resonances, believed to be strong resonances in a four-arm spiral galaxy. The stellar orbits at these resonances are illustrated in Figure 5 (bottom) of Michtchenko et al. (2018). See Figure 7 of Barros et al. (2020) to follow the discussion on the origin of the stars. Starting from their present position, by integrating their orbits to the past (counter-clockwise in that figure), we should find their birthplaces. The orbits present many loops, but they can be considered to be contained in a kind of torus (a concept much used in dynamics). Since the stars are expected to be born in spiral arms, we should look for the first crossing of the torus (or of the stellar orbits) with an arm. This is situated on the Sagittarius-Carina Arm; we must conclude, therefore, that most stars of the Hercules stream were born in that arm. It must be remembered that the figure represents the arms in their own standard of rest, which rotates with a velocity of the order of 28 km/s/kpc, in the inertial frame. Ramya et al. (2016) performed a detailed study of the stellar population of the Hercules stream. They found an average metallicity of the order of (Fe/H) = 0.15,



which is perfectly compatible with the stellar orbits discussed above, which have a radius a little smaller than that of the Sun. They found an average age of the Hercules stars of about 1.0 Gyrs, which again is compatible, in the order of magnitude, with the travel time between the probable birthplace and the present-day position. There is a small uncertainty in the exact position of the Sagittarius–Carina Arm that is possibly not a perfect spiral. Finally, the surprising velocity of the Hercules stream stars in the LSR frame, with a large component in the galactic radial direction, could be explained by a part of loop situated close to the Sun (see Figure 5, bottom left, of Michtchenko et al., 2018). Note that the ideas presented in this section are not at all a consensus in the literature, see, e.g., Monari et al. (2017) and Asano et al. (2020), among others, with a great variety of proposed models.

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5 FINAL REMARKS AND PERSPECTIVES

Astrochemistry looks like a flourishing area of research, with such an incredible amount of papers published in a few recent years, bringing new molecules, new ideas, and new paths for future research, so that we had to make choices in our presentation. Possibly, our interest in radio astronomy and in particular in the possibilities of the ALMA interferometer had some influence. Most of the authors of the present paper are involved, directly or indirectly, in the LLAMA Argentinian-Brazilian project to construct a 12 m sub-mm radio telescope in the Andes (Figure 10), at 4800 m altitude. The first light will take place in 2022, and the first two receivers will work in band 5 (163-211 GHz) and band 9 (602-720 GHz)-ALMA bands. The cooled receivers are ready and waiting in the NOVA Laboratories in Groningen (NL). These frequency bands are very rich in molecular lines, and certainly, a good fraction of the observing time will be dedicated to astrochemistry. This group is happy to ascertain that there will be no lack of ideas for competitive use of the LLAMA. The association of astrochemistry with galactic dynamics will be an additional source of original ideas and important contributions to science.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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- **Conflict of Interest:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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