Mem. S.A.It. Vol. 95, 15

Memorie della

Extragalactic Astrochemistry

Understanding the molecular gas in external galaxies

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Received: 22 March 2024; Accepted: 14 June 2024

Abstract. Molecules are present in most astrophysical environments within galaxies and, beside having a key role in the formation and shaping of such galaxies, they are also powerful tracers of their physical characteristics and energetics. Robustly interpreting molecular observations, however, requires a systematic methodology involving the coupling of radiative transfer, chemical modelling, statistics and machine learning. In this paper, I will review some of the recent progress in molecular observations and astrochemical modelling in extragalactic star forming regions and active galactic nuclei, in order to demonstrate how important molecules are for our understanding of star and galaxy formation.

Key words. galaxies: ISM; astrochemistry; molecular processes; radiative transfer

1. Introduction

Molecules pervade the cooler, denser parts of every galaxy. For low gas temperatures (< 100 K) and high gas densities (n_H > 1000 cm^{-3}) the gas in galaxies will be mostly in molecular form. Giant Molecular Clouds (GMCs) in nearby starburst galaxies or the dense material around Active Galactic Nuclei (AGNs) have indeed revealed an almost entirely molecular content (e.g. Leroy et al. 2015; Martín et al. 2011). This dense molecular gas is important for our understanding of how galaxies evolve. For example, measuring the mass of this reservoir gas in a galaxy and comparing with the existing stellar mass may give some indication of the evolutionary state of that galaxy. Moreover, feedback will depend on several processes involving the interaction of radiation or of violent processes with cold dense gas; hence molecules, by tracing the dynamics, the physics as well as the chemistry of such dense gas, are excellent probes of the history of a galaxy.

The power of molecules reside in the fact that different species and different transitions within each species can trace different gas components, excitation conditions or evolutionary stages. Observations of the Milky Way, as well as of few nearby galaxies, have shown that several molecules are useful for tracing specific dense gas regions; for example, HCO, HOC^+ and C_2H have in the past been associated with photon-dominated regions (PDRs) (e.g., Gerin et al. 2009; Martín et al. 2009; Cuadrado et al. 2015) while HCN, HNC and CS with dense gas (e.g., Gao & Solomon 2004; Bayet et al. 2008; Aladro et al. 2011). The implication, for extragalactic molecular

observations, is that molecules can be used to "disentangle" multi-gas unresolved components since, even for the nearest galaxies and with our best intereferometers such as ALMA and NOEMA, one can seldom resolve individual molecular clouds, let alone individual star-forming cores. At high redshift, the power of molecules may even become more important because often the beam encompasses the whole galaxy. However, it has also been shown that there is no unique molecular identifier (Kauffmann et al. 2017; Viti 2017; Tafalla et al. 2021). This can be understood by considering that there are several routes of formation and destruction for each molecular species, depending on the dominant "driver(s)" (e.g. cosmic rays and/or UV radiation and/or shocks etc). Hence, individual molecules can be unique tracers of a particular energetic process, but only within specific physical conditions.

In summary, molecules can yield important information about the physical conditions of the gas. However, considering the potential degeneracies and difficulties in the interpretation of the molecular observations, we need a systematic approach that allows us to robustly transform observational results into physically meaningful information.

2. A systematic methodology for the interpretation of molecular observations

In this section we discuss a method for the interpretation of molecular observations and molecular line ratios in nearby extragalactic regions.

There are different methodologies that can be applied to the molecular dara (see Figure 1). One can simply of course derive a rough estimate of a column density of a molecular species by making the assumption that the gas is in Local Thermodynamic Equilibrium (LTE) and, if only one transition is available, assuming a range of plausible temperatures. This is the simplest and most used step, especially if the aim is simply to measure the total average molecular gas mass. While such LTE analyses provide the observer with rough estimates of the density (and temperature, if several transitions of the same molecule are available) of the gas at equilibrium, no further information on the physics and history of the gas can be derived from such analysis. A step further is taken when analysing multiple molecular line observations with a non LTE radiative transfer model, e.g. a Large Velocity Gradient model for example that can be ran for very large ranges of gas densities, temperatures, and column densities of the observed species and a best fit to the observations can lead to constrains on the "on the spot" physical characteristics of the gas traced by the molecules. However, molecular observations can provide much further insight into the physical conditions, as well as the history and dynamics of the gas if interpreted with the right tools. Theoretical abundances and column densities calculated with chemical models where large parameter spaces in gas density, temperature, metallicities, cosmic ray ionization rates, and radiation fields can be used as inputs to radiative transfer codes, which in turn provides the theoretical intensities as well as common line ratios for the parameter space investigated by the chemical models. The best fit parameters can then be derived in a variety of ways, by using Bayesian inference or Monte Carlo techniques and (at least some degree of) the degeneracy inherent in each molecule and each ratio can then be determined (e.g. Holdship et al. 2019).

It is indeed now possible for the observer to use well-established modelling codes to exploit the information contained in the molecular data using the methodology described above. In the next sections, we shall present examples of how one can derive physical information from molecular observations. For most of the work presented here we use the time dependent open source gas-grain code UCLCHEM (https://uclchem.github.io/; Holdship et al. 2017) and the public radiative transfer coed RADEX (van der Tak et al. 2007).

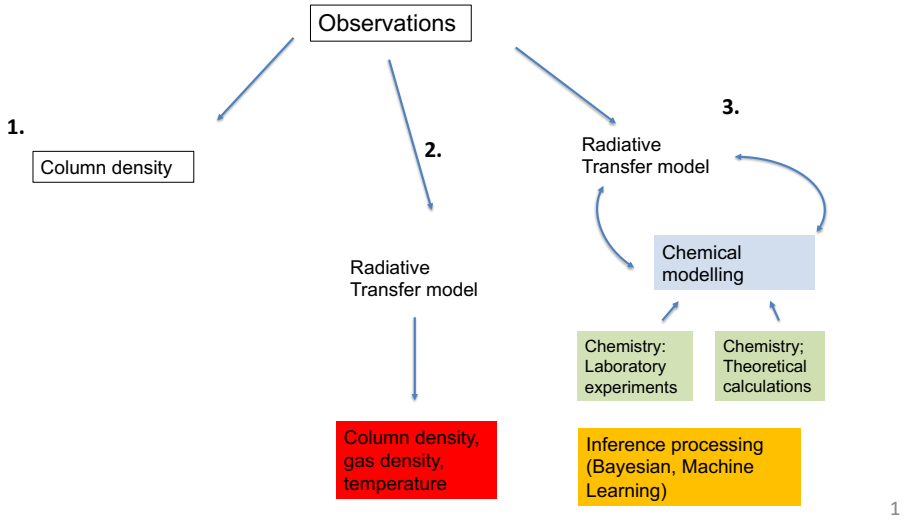

Fig. 1. Schematic of the different methodologies for the interpretation of molecular observations.

3. Characterizing nearby galaxies using molecules

For most galaxies, even with the highest spatial resolution available with the ALMA, the beam usually encompasses emissions from multiple phase gas components in which the spatial and temporal effects are diluted in the beam. Detection of multiple molecules in a galaxy does not necessarily mean that they are emitted from the same gas. This is in fact true even for the nearest galaxies. Below we report examples of how we can still interpret molecular observations and molecular line ratios in nearby extragalactic regions, in particular, starburst and AGN dominated galaxies as these are the most targeted types of galaxies for dense gas studies.

3.1. A case study: the starburst galaxy NGC 253

NGC 253 is one of the best extragalactic astrochemical laboratory to date. It is a nearby (3.5 Mpc) edge on starburst galaxy that has been the subject of multi-wavelength studies since the 70s. In particular, observations in the submillimter continuum and multiple line emission show that NGC 253 hosts several large (~30 pc), and dense (~ 10^5 cm^{-3}) massive giant molecular clouds (GMCs) (e.g., Sakamoto et al. 2011; Leroy et al. 2018). NGC 253 also hosts a starburst driven outflow observed at X-ray wavelengths (Dahlem et al. 1998) as well as in molecular emission (Bolatto et al. 2013; Krieger et al. 2019). In recent years, the ALMA Large Program ALCHEMI (Martín et al. 2021) obtained the most complete extragalactic molecular inventory in the central molecular zone of a starburst galaxy at a spatial resolution of tens of parsecs. The power of a spectral survey is that it provides us with multi-transitions of multi-species at the same spatial resolution which is essential in order to fully trace the dynamics, physics as well as chemistry of dense gas: below we shall see how one can use different species and to trace different gas components, excitation conditions or evolutionary stages.

The methodology described in the previous section has been applied to several ALCHEMI studies. In particular, we wish to locate and characterize the dense molecular gas; the sites of massive star formation; and the outflows and their extensions. For example, take the

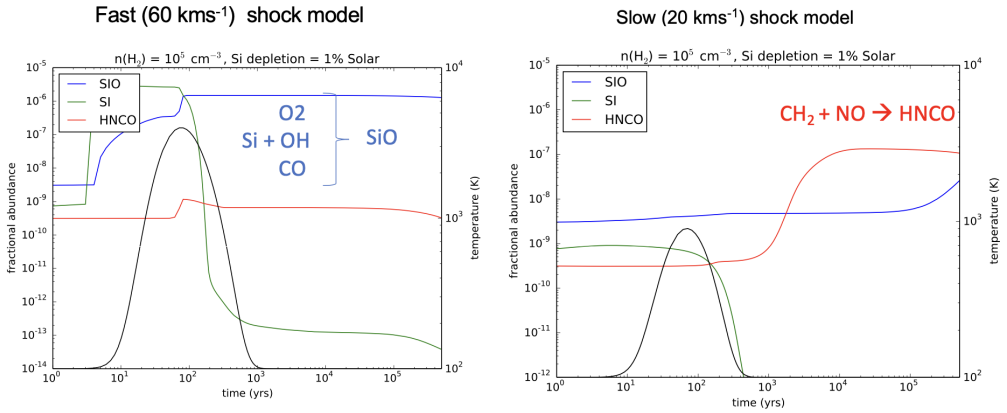

Fig. 2. Chemical evolution of selected species as a function of time for two shock models. Adapted from Kelly et al. (2017).

two molecules: SiO and HNCO, two well known shock tracers (Martín-Pintado et al. 1997; Rodríguez-Fernández et al. 2010). The "coupling" of these two species has been used to trace the shock structure and shock history in NGC 253. As long as the shock is strong enough, Si, depleted in the core of the grains in its initial elemental abundance by a factor of up to 100, is released from the dust grains due to shock sputtering and it then quickly react with oxygen to form SiO (Schilke et al. 1997). HNCO, on the other hand, is believed to form mainly in the icy mantle during a cold phase of the gas evolution and can be then easily released via ice sublimation by the passage of any shock, including slow shocks (see Figure 2. adapted from Kelly et al. 2017). This may imply that these two tracers will trace different types of shocks. In fact in Huang et al. (2023) this scenario was tested: they used a bayesian inference method coupled with radiative and chemical modelling to analyse multiple transitions of both SiO and HNCO from the ALCHEMI dataset (see Figure 3, adapted from Huang et al. 2023) and found that first of all the HNCO and SiO Spectral Line Energy Distributions (SLEDs) differ in shape across the GMCs; secondly the gas properties traced by these two species are substantially different, with SiO always tracing a clearly higher temperature and lower densities than HNCO; and finally it was indeed confirmed that fast shocks are definitely needed to produce the necessary abundance of SiO, while slow shocks can be responsible for the abundance of HNCO.

Another example of the power of multiple transitions of multiple species in characterizing the dense gas in the CND of NGC 253 has been provided by the work of Holdship et al. (2021). They find that the molecule C_2H in the CND of this galaxy traces the *dense* gas of the brightest GMCs (unlike in our own Galaxy) and does not appear to follow the galaxy's starburst driven outflow (unlike the C_2H in the galaxy NGC 1068 - see below). Moreover, such gas must be impacted by enhanced cosmic ray ionization rates but the use of this molecule would not allow the authors to constrain such rate beside finding that it needed to be higher than the galactic value.

More studies using the ALCHEMI data have demonstrated that by using measurements of multiple molecular species and transitions interpreted by chemical and physical models, it is possible to measure the galaxy physical conditions at GMC scales (e.g. Harada et al. 2021; Holdship et al. 2021; Holdship et al. 2022; Behrens et al. 2022; Huang et al. 2023; Bouvier et al. submitted). From this high spatial resolution (GM scales) picture that is coming out of the ALCHEMI survey it is now clear that each GMC has a gradient of densities (10^3

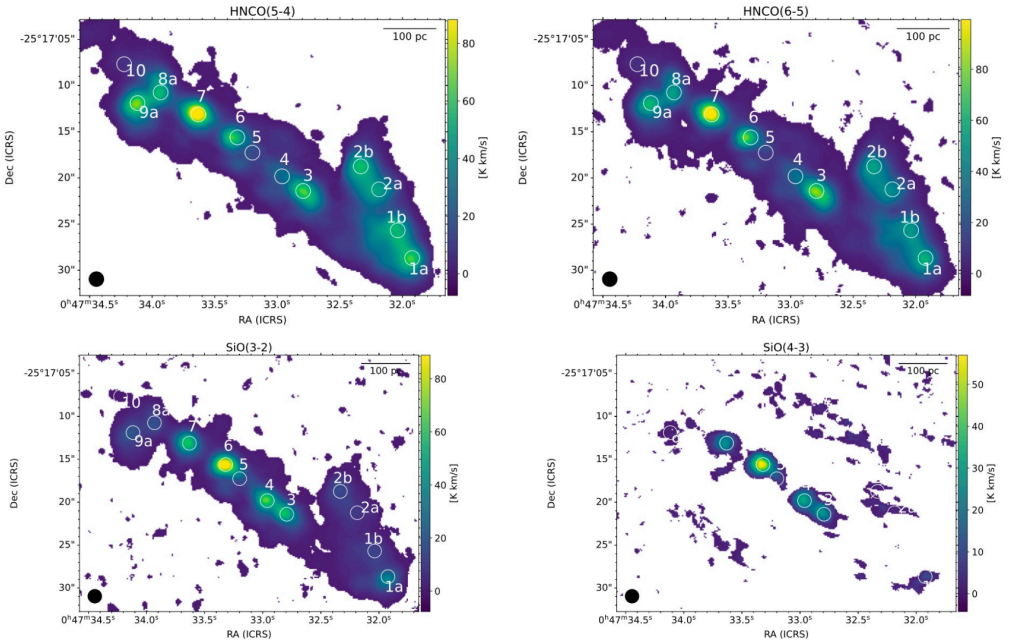

Fig. 3. Extent and distribution of some of the HNCO and SiO transitions in NGC 253 as observed by the Large ALMA Program, ALCHEMI. Adapted from Huang et al. (2023)

to 10^6 cm^{-3}), is impacted by a very high cosmic ray ionization rate, and is host to multiple episodes of slow and fast shocks, likely driven by star formation.

4. A case study: the AGN-dominated galaxy NGC 1068

NGC 1068 is a composite galaxy, dominated by a powerful and obscured AGN and also characterized by active starburst regions (Schinnerer et al. 2000; Garcıia-Burillo et al. (2010). NGC 1068 is another excellent laboratory, this time to study not only the dense gas in its central region (the Circumnuclear Disk or CND) where the AGN dominates but also the interstellar medium that "bridges" the AGN dominated gas with the starburst dominated gas. This galaxy has indeed been studied in multiple wavelengths and at different resolutions. Here we shall concentrate on a similar spatial resolution to the observations in NGC 253 in order to be able to make comparisons.

For this galaxy we can start by looking at how to trace the different regions of dense gas across the CND as well as the starburst. CS is a particularly useful molecule to trace the dense gas due to several transitions in the submmilimeter having a high critical density (Plume, Jaffe & Evans 1992). Bayet et al. (2009), and more recently, using ALMA, Scourfield et al. (2020) show that CS is not however a simple dense gas tracer as it can trace, especially if observed in multiple transitions, different types of regions. This allowed the authors to actually determine the temperature, density and cosmic ray structure across the CND and the starburst rings and found that the temperature in the CND increases from East to West and that the CND is hotter than most of the starburst regions. The cosmic ray follows a similar pattern within the CND but it

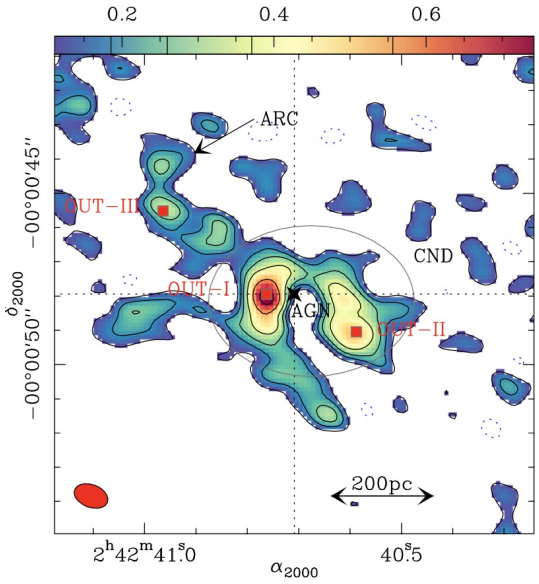

Fig. 4. $C_2H(1–0)$ integrated intensity map obtained with ALMA in the disk of NGC 1068. Adapted from García-Burillo et al. (2017).

is higher in some spots in the rings. Clearly, none of these physical characteristics can be used to distinguish whether the energetics are dominated by the AGN or by the starbursts.

How about the C_2H molecule, which so clearly traced the dense and compact gas in NGC 253? In fact, in NGC 1068, it is much more extended (and abundant) (see Figure 4, from García-Burillo et al. 2017). Chemical modelling shows that this species trace the turbulent dense molecular interfaces along the outflow, unlike in NGC 253 (García-Burillo et al. 2017). Interestingly in our own galaxy C_2H often traces UV irradiated and diffuse gas (e.g. Cuadrado et al. 2015) This is a clear confirmation that there are no unique line tracers: the same molecule can trace different energetics, gas components, and histories of the gas.

4.1. Molecular ratios: their use and challenges

One of the most used "tools" to discern patterns in the energetics and physical structures of galaxies are molecular ratios. Observationally, many studies have shown that molecular line ratios, such as HCO^+/HCN or HCN/CO, differ across different types of galaxies especially between AGN-dominated galaxies and starburst-dominated galaxies

In particular, AGN activity is often traced by looking at the HCN/HCO^+ ratio. This ratio is routinely found to be brighter close to AGN positions (e.g. the CND of NGC 1068, see Butterworth et al. 2022; the nuclei of the Antenna Galaxies, see Schirm et al. 2016) than where star formation is dominant. Yet several studies show no enhancements of HCN/HCO^+ in AGNs or show that enhanced HCN/HCO^+ are not unique to AGN environments but can also be found in systems dominated by star formation (e.g. Costagliola et al. 2011; Privon et al. 2015; Martín et al. 2015; König et al. 2018; Harada et al. 2018). Moreover, the derived abundance ratios for an individual galaxy also highly differ across studies depending on the transitions observed, available resolution, and method used in deriving the column densities. Often well used ratios, for example the HCN(4– 3)/HCO^+(4–3) or the HCN(1–0)/HCO^+(1–0), are the same for several chemical models within the accuracy assumed. It is clear therefore that an understanding of the chemistry behind each molecule and its dependencies on the density and temperature of the gas is essential and this is well depicted by the study of Holdship et al. (2022): we saw earlier how C_2H was able in NGC 253 to hint at high cosmic ray ionization rate but without further constrains. In Holdship et al. (2022) they perform a comprehensive analysis, following a similar methodology as sketched in Figure 1, of the H_3O^+/SO ratio in the CND of NGC 253 and find that it very tightly coupled to the cosmic ray ionization rate (see Figure 5 - adapted from Holdship et al. 2022). They are therefore able to determine that the cosmic ray ionization rate in NGC 253 CND is between 1000 and 100000 higher than the galactic cosmic ray ionization rate.

Clearly molecular ratios can be powerful probes provided that there is enough evidence (e.g. high enough spatial resolution) to assume that the two transitions arise from the same gas.

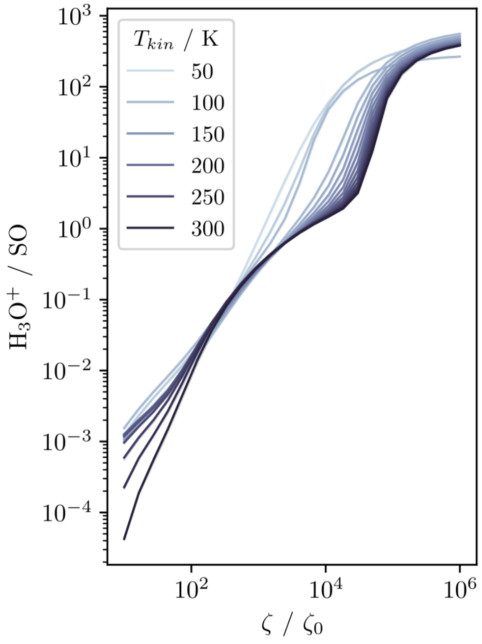

Fig. 5. The tight relationship between the H_3O^+/SO rato and cosmic ray onization rate. The different curves ae models ran at different temperatures. Figure from Holdship et al. (2022).

5. Conclusions

There is no doubt that molecules are ideal tools to trace the wide ranges of gas densities, temperatures and energetics in galaxies, especially the most nearby ones. However, to robustly interpret molecular observations requires an understanding the spectroscopy and chemistry of the molecules observed. In this review article we took a brief tour into methodologies that can be used to fully exploit the power of molecules and we showed examples of applications to two well studied nearby galaxies: NGC 253 and NGC 1068.

Acknowledgements. SV acknowledges support from the European Research Council (ERC) grant MOPPEX ERC-833460.

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