

Galaxies and Galaxy Nuclei: From Hot Cores to Cold Outflows

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Abstract. Studying the molecular phase of the interstellar medium in galaxies is fundamental for the understanding of the onset and evolution of star formation and the growth of supermassive black holes. We can use molecules as observational tools exploiting them as tracers of chemical, physical and dynamical conditions. In this short review, key molecules (e.g. HCN, HCO⁺, HNC, HC₃N, CN) in identifying the nature of buried activity and its evolution are discussed including some standard astrochemical scenarios. Furthermore, we can use IR excited molecular emission to probe the very inner regions of luminous infrared galaxies (LIRGs) allowing us to get past the optically thick dust barrier of the compact obscured nuclei. We show that the vibrationally excited lines are important probes of nuclei where lines of CO, HCN and HCO⁺ in their vibrational ground state ($\nu=0$) may be self-absorbed. Finally, molecular outflows are briefly discussed - including the new ALMA discovery of a highly collimated (jet-like) reversed molecular outflow in the lenticular, extremely radio-quiet galaxy NGC1377.

1. Extragalactic astrochemistry

Molecular emission and absorption lines are very useful tools to study the nature and evolution of luminous ($L_{\text{FIR}} = 10^{10} - 10^{11} L_{\odot}$) and ultraluminous ($L_{\text{FIR}} \gtrsim 10^{12} L_{\odot}$) infrared galaxies (LIRGs). Molecular gas serves as fuel for the evolution of galaxies through star formation and the growth of SMBHs. Molecular, mm and submm emission can penetrate highly obscured regions allowing us to probe the dusty nuclei of LIRGs and ULIRGs revealing the nature of the buried activity. In addition, the starbursts and AGNs power massive large-scale molecular outflows that can help regulate the growth of the galaxy - both in the nucleus and on larger scales.

The CO 1–0 line is often used to trace H₂ mass (e.g. Paglione et al. 2001; Wada & Tomisaka 2005; Narayanan et al. 2012) and gas dynamics. The line intensity ratio between CO and the polar molecule HCN is a popular measure of the mass fraction of dense ($n > 10^4 \text{ cm}^{-3}$) molecular gas (e.g. Gao & Solomon 2004). Astrochemistry offers an additional new tool to study galaxy evolution - in particular in deeply dust-obscured objects. We can study both the radiative and dynamical impact on the gas properties and its chemistry and hence develop scenarios for the evolution of molecular gas in galaxies. There are a number of standard scenarios often referred to when we discuss extragalactic astrochemistry (for a longer account see Aalto (2013)): **Photon (or Photo) dominated region (PDR)** Regions affected by far-ultraviolet photons ($h\nu=6 - 13.6 \text{ eV}$) with large surface temperatures (300 - 1000 K) and moderate (20 - 50 K) bulk temperatures (due to the layered structure of the PDR) . The chemistry is dominated by

photo-chemistry (e.g. Hollenbach & Tielens 1997); **X-ray dominated region (XDR)** are affected by X-rays with $h\nu=1\text{--}100$ keV with larger penetration depth than in PDRs. Thus XDRs are signified by large bulk temperatures > 100 K and a chemical structure typical of the special ion-neutral chemistry triggered by the irradiation of X-rays. (e.g. Maloney et al. 1996; Lepp & Dalgarno 1996; Meijerink & Spaans 2005); **Cosmic ray dominated region (CDR or CRDR)** are regions of elevated ($> 10^3 \times$ Galactic value) cosmic ray energy density (e.g. Suchkov et al. 1993; Meijerink et al. 2011; Bayet et al. 2011) primarily originating from supernovae; **Dense shielded regions** Hot core-like chemistry can dominate in warm, shielded regions with temperatures ranging from 50 to 500 K (e.g. Nomura & Millar 2004; Viti 2005). Icy grain mantles are released affecting chemistry and the intense infrared (IR) radiation fields impact the molecular excitation (Costagliola & Aalto 2010; Sakamoto et al. 2010); **Mechanically dominated region** The chemistry reflects the speed of the shock and thus the level of grain processing (e.g. Usero et al. 2007; Viti et al. 2011; Kazandjian et al. 2012). Milder shocks results in evaporation of icy mantles and in more violent shocks the grain cores may be affected. Combining molecular species and transitions with spatial resolution and sensitivity will enable us to disentangle chemical scenarios and to separate effects of excitation and radiative transfer from those of chemistry. There will be a mixture of scenarios in galaxies even at high spatial resolution and it is a challenge to identify dominant conditions and key tracers.

2. Some useful molecular emission lines and ratios

By 2014 at total of 60 species have been detected in external galaxies (see <http://www.astro.uni-koeln.de/cdms/molecules>). Intensity ratios of emission lines between species are often used to identify various astrochemical scenarios and/or physical conditions in the gas. Below is a short list of a few popular molecular lines and ratios (for a longer account see Aalto (2013)).

HCN and HCO^+ : In the molecular cores around some AGNs elevated HCN/ HCO^+ 1–0 intensity ratios have been found (e.g. Kohno 2003; Imanishi et al. 2009) and also in some ULIRGs (Graciá-Carpio et al. 2006). It is not clear if the HCO^+ abundance is suppressed or enhanced relative to HCN in XDRs (e.g. Maloney et al. 1996; Meijerink & Spaans 2005), but HCN is expected to be enhanced in warm and shocked environments (e.g. Aalto et al. 2007a; Kazandjian et al. 2012). *Thus, it is possible that HCN/ HCO^+ 1–0 ratios are generally enhanced in compact molecular regions towards galaxy nuclei - regardless off the nature of the buried activity. Recently, the detection of self-absorbed HCN and HCO^+ towards compact obscured nuclei shows that the line ratio may be difficult to interpret in environments with steep temperature gradients and large $N(\text{H}_2) > 10^{24} \text{ cm}^{-2}$ (Aalto et al. 2015a).*

HNC In cold ($T < 24$ K) gas HNC/HCN abundance ratios are expected to be greater than unity while in dense, warmer gas and in shocked gas $X(\text{HCN}) > X(\text{HNC})$ (Schilke et al. 1992). However, in XDRs and PDRs $X(\text{HCN}) \gtrsim X(\text{HNC})$ also in warm gas (Meijerink & Spaans 2005) which complicates the use of the HCN/HNC abundance ratio as a tracer of gas temperature. Surveys reveal that global HCN/HNC 1–0 intensity ratios in luminous galaxies often range between 1 and 6 (e.g. Aalto et al. 2002; Baan et al. 2010), but there are cases where the HNC/HCN 3–2 intensity ratio exceeds unity (Aalto et al. 2007b, 2009). The cause for this "overluminosity" of HNC (e.g. in Arp 220) has

been suggested to be either due to XDR chemistry or effects of IR-pumping of HNC. Studies of isotopomers of HCN and HNC in Arp220 suggest that HNC is really underabundant and its overluminosity is due to excitation and radiative transport effects (Tunnard et al. 2015).

HC₃N Surveys have revealed a subset of luminous galaxies with unusually bright HC₃N 10–9 emission compared to HCN 1–0 (Lindberg et al. 2011a; Costagliola et al. 2011). HC₃N is destroyed by UV and particle radiation and in the Galaxy it can be found in high abundance in hot cores and in general in dense and shielded gas. Interestingly, luminous HC₃N emission has also been found near AGN nuclei such as Mrk231 (Aalto et al. 2012a).

CN In contrast to HC₃N, enhancement of CN is expected in XDRs and in PDRs (e.g. Aalto et al. 2002; Baan et al. 2010; Meijerink & Spaans 2005). CN is also chemically linked to HCN via photodissociation. The abundance enhancement of CN over HCN is greater in an XDR (factors 40 - 1000) than in a PDR (CN/HCN abundance ratio range from 0.5 to 2) (Lepp & Dalgarno 1996; Meijerink & Spaans 2005).

SiO, H₂O, HNCO, CH₃OH Shocks can form SiO through the sputtering of Si from silicate grain cores, followed by reactions between the released Si and O₂ or OH (Guillet et al. 2009). The shock must therefore be strong enough to get the Si off the grains while species such as H₂O, HNCO, CH₃OH can be released in milder events resulting in mantle evaporation.

3. Global line ratios and spectral scans

There are a large number of studies using global molecular line ratios to attempt to classify galaxies in terms of nuclear activity and evolutionary status (e.g. Aalto et al. 1995; Paglione et al. 2001; Aalto et al. 2002; Gao & Solomon 2004; Graciá-Carpio et al. 2006; Krips et al. 2008; Baan et al. 2010; Papadopoulos et al. 2010; Lindberg et al. 2011b) Although effects of radiative transfer and excitation are difficult to account for in these surveys, they are useful in identifying trends and searching for correlations. These relations may then be further explored with multi-transition observations as well as higher resolution studies. The new broadband receivers allow several lines to be measured simultaneously improving the accuracy of the line ratios. One such example is the EVOLUTION study of (U)LIRGs with the EMIR receiver at the IRAM 30m telescope (Costagliola et al. 2011). Simultaneous observations of HCN, HCO⁺, HNC, HC₃N, C₂H, SiO and CO, ¹³CO, C¹⁸O, CN were correlated with nature of activity, PAH EW and silicate strength (using the diagnostic diagram of Spoon et al. (2007)). Another recent EMIR study of LIRGs is the HCN/HCO⁺ 1–0 survey of GOALS galaxies by Privon et al (2015 submitted).

Combining many lines simultaneously in a *spectral scan* will give a more complete (and complex) picture of the chemical status of a galaxy. This includes emission from rarer species with clearer diagnostic value. Spectral scans of the nearby starburst galaxies NGC253 and M82, and the starburst/Seyfert NGC1068 have been carried out at 1, 2 and 3 mm wavelength by the IRAM 30m and the Nobeyama 45m telescopes (e.g. Martín et al. 2006; Nakajima et al. 2011; Aladro et al. 2011, 2012) and NGC253 recently with ALMA (Meier et al. 2015). Aladro et al (2015) have carried out single dish 3mm scans of M82 ,M83, M51, NGC1068, NGC7469, Arp220 and Mrk231. The ULIRG Arp220

has been surveyed in the 1mm band by the SMA interferometer (Martín et al. 2011) and the chemical composition seems consistent with an ISM heated by a young starburst and chemically enriched by consecutive bursts of star formation. An ALMA spectral scan of the LIRG NGC4418 (band 3,6,7) (Costagliola et al 2015, submitted) reveal a rich spectrum dominated by vibrationally excited species of e.g. HCN and HC_3N (Aalto et al. 2007a; Costagliola & Aalto 2010; Sakamoto et al. 2010, 2013; Costagliola et al. 2013).

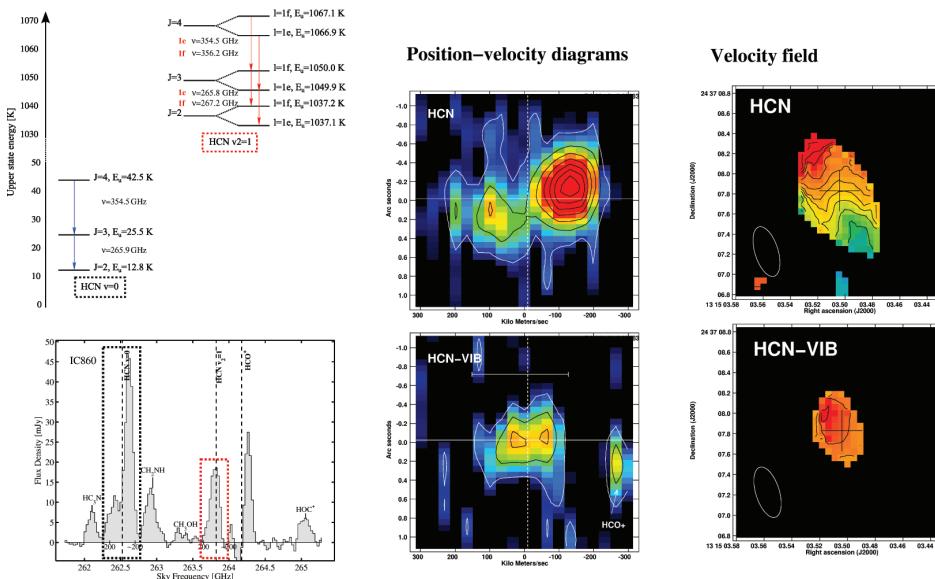


Figure 1. Top left: HCN energy diagram with the HCN $v=0$ and $v_2=1$ $J=4,3,2$ levels marked. The split of the $v_2=1$ rotational levels into e and f is also shown. The energy levels are not to scale which is illustrated by the dashed y-axis. The transitions are indicated with arrows. Lower left: IRAM 1mm spectra of IC860 showing the incredibly luminous HCN-VIB lines and the self-absorbed double-peaked lines of HCN and HCO^+ in their vibrational ground state. The HCN-VIB line is marked with a red- and the HCN with a black box. Luminous emission from CH_2NH , CH_3OH and HOC^+ is also shown (Aalto et al 2015b). Center: Position velocity diagrams of HCN (top) and HCN-VIB (bottom) showing that the HCN-VIB line peak near systemic velocity where the HCN line has a minimum due to self-absorption Right: Velocity fields of HCN and HCN-VIB. The HCN field is severely distorted by the effects of the self-absorption while the HCN-VIB velocity field is not resolved in our IRAM PdBI beam.

4. Molecular excitation - IR pumping of molecules

When we interpret mm and submm molecular spectra from external galaxies we usually assume that the excitation is dominated by collisions with H_2 . However, there are also other possible mechanisms including IR radiative excitation where molecules absorb IR continuum which affects the excitation of the rotational levels in the vibrational ground state. Thus, to correctly interpret the molecular emission we must examine its excitation. For example, HCN can absorb IR-photons to the bending mode (its first

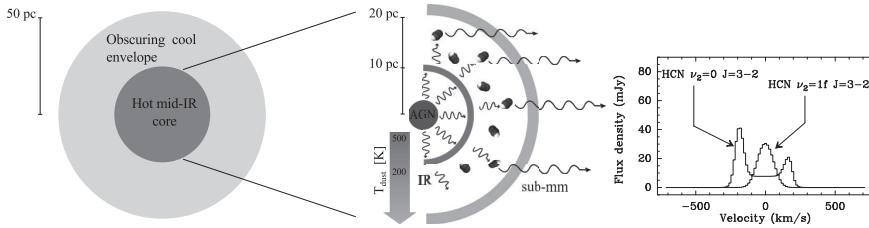


Figure 2. *Left:* Left: Cartoon Illustrating the effect of self-absorption. Right: A model spectrum of IC860: A double peak self-absorbed HCN line is shown together with the unabsorbed HCN-VIB line (Aalto et al 2015b, Gonzalez-Alfonso in prep).

vibrational state) and then it decays back to the ground state via its P-branch ($\nu = 1-0$, $\Delta J = +1$) or R-branch ($\nu = 1-0$, $\Delta J = -1$). In this way, a vibrational excitation may produce a change in the rotational state in the ground level and can be treated (effectively) as a collisional excitation in the statistical equations. For HCN the mode occurs at $\lambda = 14 \mu\text{m}$ (713.5 cm^{-1}), energy level $h\nu/k = 1027 \text{ K}$ and the pumping may start to become effective when the IR background reaches an optically thick brightness temperature of $T_B \gtrsim 100 \text{ K}$.

Furthermore, recent results toward dust obscured galaxies show the presence of rotational lines from vibrationally excited HCN, HC₃N and HNC (Aalto et al. 2007a; Costagliola & Aalto 2010; Sakamoto et al. 2010; Martín et al. 2011; Sakamoto et al. 2013; Costagliola et al. 2013; Aalto et al. 2015b,a) and Costagliola et al (submitted). *These lines appear near the lines in the vibrational ground state (see Fig. 1 left) and can be used to probe inside the optically thick dust cocoons in the nuclei of deeply obscured galaxies.* Therefore, vibrationally excited lines open up a new interesting avenue to gain access to the most obscured AGNs and starbursts.

4.1. Vibrationally excited HCN in extremely obscured nuclei.

High resolution IRAM PdBI and ALMA mm and submm observations of the (Ultra) Luminous Infrared Galaxies ((U)LIRGs) IRAS17208-0014, Arp220, IC860 (see Fig.1) and Zw049.057 show intense line emission from vibrationally excited ($\nu_2=1$) $J=3-2$ and $4-3$ HCN (Aalto et al. 2015a). The emission is emerging from buried, compact ($r < 17-70 \text{ pc}$) nuclei that have very high implied mid-infrared surface brightness $> 5 \times 10^{13} \text{ L}_\odot \text{ kpc}^{-2}$. These nuclei are likely powered by accreting supermassive black holes (SMBHs) and/or hot ($> 200 \text{ K}$) extreme starbursts. Vibrational, $\nu_2=1$, lines of HCN are excited by intense $14 \mu\text{m}$ mid-infrared emission and are excellent probes of the dynamics, masses and physical conditions of (U)LIRG nuclei when H₂ column densities exceed 10^{24} cm^{-2} . Vibrationally excited HCN acts as a proxy for the absorbed mid-infrared emission from the embedded nuclei, which allows for reconstruction of the intrinsic, hotter dust SED. *In contrast, the ground vibrational state ($\nu=0$), $J=3-2$ and $4-3$ rotational lines of HCN and HCO⁺ fail to probe these highly enshrouded, compact nuclear regions due to strong self- and continuum absorption.*

4.2. Astrochemistry at high spatial resolution

Interferometric studies provide both spatial resolution and sufficient pointing accuracy to allow us to separate regions of different dominant chemical processes. For example, high resolution studies of IC 342 and Maffei 2 (Meier & Turner 2005, 2012) show that

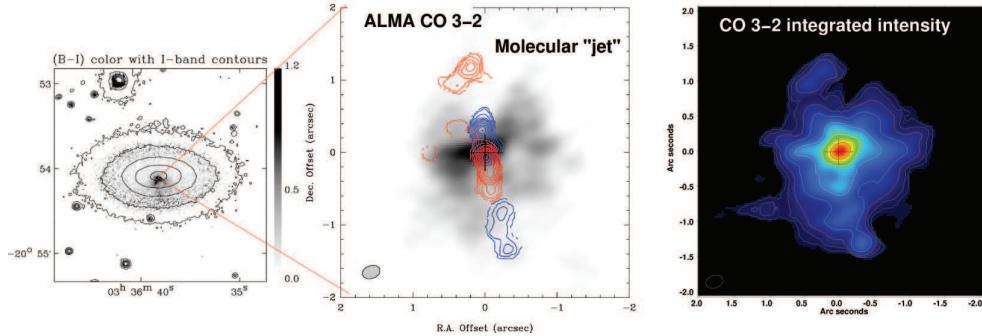


Figure 3. Left: Optical (B-I) image from Roussel et al (2006) showing a southern outflow dust feature. Center: ALMA Cycle2 $0.0''24 \times 0.0''17$ CO 3-2 data where emission at systemic velocity is shown in gray scale and the high velocity emission in red and blue contours. It has a jet-like morphology and seems to occupy a cavity in the systemic emission. Remarkably the emission reverses direction near the nucleus. Right: Integrated CO 3-2 emission.

the HNCO, and CH₃OH emission follow the molecular bar arms, especially the bar ends. This is probably caused by the spiral and bar shocks resulting in evaporation of the icy grain mantles. the nearby Seyfert/starburst NGC1068 (García-Burillo et al. 2014; Viti et al. 2014; Takano et al. 2014; Nakajima et al. 2015). Many of the results are presented elsewhere in this volume. It is interesting to note that the HCN/HCO⁺ 4–3 line ratio is high throughout the CND, but shrinks again close to the AGN. This may be an effect of increased HCO⁺ abundances near the AGN, excitation effects, and/or line opacities. This result is important for our calibration of the HCN/HCO⁺ line ratio as a diagnostic tool.

4.3. Molecular outflows

Outflows driven by AGNs and/or starbursts represent a strong and direct mechanism for feedback that may clear central regions of fuel for star formation or black hole (BH) growth. Many galactic winds and outflows carry large amounts of molecular gas and dust with them and there is a growing list of examples of molecular gas in outflows in nearby galaxies (e.g. Nakai et al. 1987; Greve et al. 2000; García-Burillo et al. 2000, 2001; Walter et al. 2002; Sakamoto et al. 2006; Baan 2007; Tsai et al. 2009; Fischer et al. 2010; Feruglio et al. 2010; Alatalo et al. 2011; Chung et al. 2011; Sturm et al. 2011; Aalto et al. 2012a; Cicone et al. 2012; Aalto et al. 2012b; Bolatto et al. 2013; Sakamoto et al. 2014; Veilleux et al. 2013; Cicone et al. 2014; García-Burillo et al. 2014; Matsushita et al. 2015; Aalto et al. 2015b), Studying the physical and chemical conditions of the outflowing molecular gas will help us understand the driving mechanism, origin of the gas and its fate in the wind. *Interestingly, the Mrk231 outflow has very bright HCN emission* (Aalto et al. 2012a, 2015b) and recent PdBI imaging shows that the broad line wings are also present in the HCN 3–2 spectrum (Aalto et al. 2015b). This can be explained by the presence of dense ($n > 10^4 \text{ cm}^{-3}$) gas in the outflow and with an elevated HCN abundance (possibly due to shocks). HCN enhancements have also been seen in other AGN-driven outflows such as M51 (Matsushita et al. 2015); NGC1068 (García-Burillo et al. 2014), NGC7469 (Izumi et al submitted). Re-

cently, emission from the CN radical is found to be luminous in the NGC3256 outflow (Sakamoto et al. 2014) and in Mrk231 (Cicone, priv. com.).

With the high resolution, high sensitivity capacity of ALMA it is possible to image molecular outflows in unprecedented detail (e.g. NGC253 (Bolatto et al. 2013)). With ALMA Cycle 2 CO 3–2 imaging we have discovered an extremely collimated, 200 pc scale, molecular outflow in the nearby (21 Mpc ($1''=102$ pc)), moderate luminosity ($4.3 \times 10^9 L_\odot$) lenticular galaxy NGC1377. *Remarkably, the outflow reverses direction near the nucleus* - apparently along the same line of sight (Fig. 1). Lower velocity gas outlines a cone-like structure with a wide opening angle, but the relation between the cone and the high speed highly collimated outflow is not clear. There is no immediate explanation for the velocity-reversal, but a molecular bipolar "jet" rotating around an axis perpendicular to the line of sight could tentatively reproduce observations. An alternative is that there are two molecular jets due to a binary black hole with opposite spins and two accretion disks.

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