THE COUPLING OF DYNAMICS AND MOLECULAR CHEMISTRY IN GALAXIES

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Abstract. While the best tracer of the molecular component and its dynamics in galaxies is the CO molecule, which excitation is revealed by its isotopic and (2-1)/(1-0) ratios, the denser gas is revealed by molecules such as HCN, HNC, HCO$^+$ or CN, which are now widely used to probe star formation regions, or to quantify the impact of the nuclear activity on the interstellar medium. This paper reviews recent observations in nearby galaxies, where these molecular line ratios serve as diagnostic tools of the physical conditions of the gas and also of its chemical properties. Those differ significantly according to the proximity of an AGN or of a starburst. The origin of the differences is not yet well known and could be due to different densities, temperatures, chemical abundances or non-collisional excitation of the gas (e.g. Aalto et al 2007, Krips et al 2007).

HCN or HNC line enhancements can be caused not only by higher gas densities/temperatures, but also UV/X-ray radiation, and global IR pumping. The chemistry can be dominated by PDR regions near a starburst, or X-ray dominated in a molecular torus surrounding an AGN (XDR regions). The molecular line ratios expected in those regions vary according to the different models (Meijerink et al. 2007).

In the last decade, a large progress has been made in our knowledge of various molecules other than CO in external galaxies. A wide molecular survey has been carried out in the nearby starburst galaxy NGC 253 (Martin et al 2006), and 35 (4 tentative) new species have been detected, with in addition 13 (+2) isotopic substitutes (cf Table 1).

1 Shocks and Chemistry in Galaxies

The silicon monoxide molecule (SiO) is well established as a good tracer of high temperatures and/or shock chemistry in molecular clouds. For shock velocities larger than 40 km/s, grain destruction becomes important, and Si and SiO can be released to the gas phase. SiO abundance is enhanced in star-forming regions, supernovae remnants, but not in clouds or PDR (photon dominated regions).

SiO emission is intense in the Seyfert 2 prototype NGC1068, and also in the starburst galaxy NGC253 (may be because of the bar shocks), but 50 times less in the starburst disk of M82 (Garcia-Burillo et al 2001; Usero et al 2007).
### Table 1. Extragalactic Molecules

| 2 atoms | 3 atoms | 4 atoms | 5 atoms | 6 atoms | 7 atoms |
|---------|---------|---------|---------|---------|---------|
| H$_2$   | H$_2$O  | H$_2$CO | c-C$_3$H$_2$ | CH$_3$OH | CH$_3$CCH |
| OH      | HCN     | H$_2$CS | HC$_3$N    | CH$_3$CN  |         |
| CO      | HNC     | NH$_3$  | CH$_2$NH   |         |         |
| CH      | HCO     | HNCO    | NH$_2$CN   |         |         |
| CS      | HCO$^+$ | C$_3$H  |         |         |         |
| CH$^+$  | H$_2$S  | HOCO$^+$|         |         |         |
| CO$^+$  | SO$_2$  |         |         |         |         |
| NO      | C$_2$H  |         |         |         |         |
| CN      | HOC$^+$ |         |         |         |         |
| NS      | C$_2$S  |         |         |         |         |
| SiO     | N$_2$H$^+$|       |         |         |         |
| SO      | OCS     |         |         |         |         |
| LiH     | H$_3^+$ |         |         |         |         |

1.1 Outflows and chimneys

Two distinct features are observed in the disk-halo interface in M82. The associated large-scale shocks are traced by SiO emission, extending out of the galaxy plane, in a chimney (essentially to the North, see Fig 1) and a supershell (mainly to the South).

In the SiO chimney, the molecular filament extends out to 500pc in size above the plane, the SiO abundance is estimated to (2-4)$\times$10$^{-10}$, and the corresponding H$_2$ mass at M(H$_2$)$\sim$ 6x10$^6$ M$_\odot$ (Garcia-Burillo et al 2001). The SiO supershell is the boundary of a cavity filled by ionised gas around a supernova remnant, well identified in the disk of M82. The supershell, of size 150pc, is still closed towards the south (while it is broken towards the north). It is associated to a supercluster of young stars. The estimated H$_2$ mass is M(H$_2$) $\sim$ 1.6x10$^7$ M$_\odot$.

1.2 Shocks and bars

The intense SiO emission in NGC253 could appear like a surprise, since there is no AGN nor large chimneys and associated shocks, although there exists a hot galactic wind entraining some molecular gas (Garcia-Burillo et al 2000). However, it seems that large-scale shocks due to the bar, more precisely the crowding of clouds in resonant structures (inner Lindblad resonances mainly), enhance cloud-cloud collisions and heat the dust/gas to produce the SiO signature. Most of the SiO emission comes from a 600 x 250pc circumnuclear disk (CND) with a double ringed structure. The inner ring, of radius 60pc, hosts the nuclear starburst; the outer pseudo-ring opens out as a spiral-like arc, in response to the barred potential. The SiO abundance in the CND ($\sim$ 10$^{-9}$) is about one order of magnitude larger than what is expected in a PDR.

High excitation level NH$_3$ lines reveal that there is a large fraction of warm (T=150K) gas in NGC 253, probably heated by C-shocks in cloud-cloud collisions, while the gas is relatively cooler in M82 (Mauersberger et al 1996, 2003).
Fig. 1. The contours of SiO(v=0,J=2-1, at 87 GHz) emission are superposed on the 4.8GHz radiocontinuum emission image in gray-scale, in the central region of M82. The location of the radiocontinuum filament (RC) is highlighted by an arrow, it delimits the chimney and the ejection of ionized gas, towards the north. The supershell is to the south. The outer circle represents the IRAM PdB primary beam (55″), while the synthesized beam (5.9″ × 5.6″) is shown at the bottom left. The major axis of the galaxy is traced by the white line. From Garcia-Burillo et al (2001).

2 PDR versus XDR

2.1 PDR chemistry in the starburst galaxy M82

The M82 disk can be considered as a giant PDR of 600 pc in size (Mao et al 2000; Garcia-Burillo et al 2002; Fuente et al 2005). The strong UV field due to the compact starburst influences in depth the chemistry. Widespread HCO emission is detected with IRAM-PdB (Garcia-Burillo et al 2002), and there are indications that PDR chemistry is propagating outward in the disk of the galaxy. Global HCO abundances are comparable or even higher than PDR in the Milky Way, X(HCO)~ 4x10^{-10} (Hollis & Churchwell, 1983; Snyder et al 1985; Schilke et al 2001). This high abundance of HCO in M82 puts the current PDR chemistry models into difficulties. The formation of HCO is thought to be due to photo-destruction of grains to produce H2CO, followed by a photodissociation of this molecule in the gas phase. But this process predicts an abundance X(HCO)~ 10^{-11}, at least 10 times lower. In a similar way, PDR models cannot account for the high abundance of CO^+, HOC^+ or c-C3H2. The latter abundance, as well as other small hydrocarbons, has been tentatively attributed to the desctruction of PAH, but this dust grain chemistry is not yet fully included in the PDR chemistry models.
2.2 XDR chemistry in the Seyfert 2 galaxy NGC 1068

X-rays are suspected to heavily influence molecular gas chemistry in the nuclear disks of AGN (Tacconi et al 1994, Maloney et al 1996). While UV radiation is stopped by a column density of $10^{21} \text{ cm}^{-2}$, hard X-rays of energy 2-10kev can penetrate much further, up to $10^{24} \text{ cm}^{-2}$. The first evidence of a highly different chemistry in extra-galactic XDR was obtained from the high HCN/CO ratio ($\approx 1-10$) in NGC 1068 (Tacconi et al 1994), leading to a high HCN abundance. This abnormally high abundance could be due to oxygen depletion due to X-rays, yielding a depletion of all oxygen-bearing molecules, and in particular CO. Another possibility is that the X-rays enhance the ionisation, itself enhancing the abundance of HCN, CN and molecular ions. Alternatively, the X-rays could destroy small dust grains, and enhanced the frozen-in molecules, and in particular SiO. The multi-species observations of NGC 1068 by Usero et al (2004) have shown that oxygen-bearing molecules are not depleted, ruling out the first hypothesis. SiO has been observed in the circum-nuclear disk (CND) to be at least ten times higher than normal, supporting the X-induced sputtering of dust grains (cf Fig 2). One surprising result is the high HOC$^+$/HCO$^+$ ratio in the CND. This supports also the scenario of a high ionisation towards the nucleus, and confirms that the central part of NGC 1068 can be considered as a giant XDR.

![Emission spectra of the 2–1 and 3–2 lines of SiO detected in the inner 3 kpc of NGC 1068. The regions observed are indicated on the CO(1–0) integrated intensity map of Schinnerer et al. (2000). The central offset coincides with the position of the AGN, while offsets at North, South and East probe the SiO emission over the starburst ring. From Usero et al (2004).](image)

As for NGC 1068, NGC 1097 has an active nucleus, a Seyfert 1. HCN is enhanced in the center, and has been derived to be a tracer of AGN (Kohno et al 2003). While the HCN/CO emission ratio is equal to 0.1 in the nuclear star-forming ring, it is 0.35 in the nucleus.
2.3 Dynamics and chemistry in NUGA: NUclei of GAlaxies

Observations at high spatial resolution with the IRAM interferometer have been done towards a dozen nearby galaxies, with an active nucleus (NUGA). The CO gas morphology has been used to infer the gravitational torques due to the bar on the gas, and derive the efficiency of AGN fueling (Garcia-Burillo et al 2005). Statistically, the phase of fueling is not encountered frequently, suggesting that the fueling is a short transient phase.

Some galaxies have also been observed in multi-species, in order to test the influence of the AGN or starburst on the chemistry (e.g. Krips et al 2007). HCN(1-0), (2-1), (3-2), and HCO$^+$ (1-0), (3-2) have been observed at IRAM and also the submillimeter array (SMA). It is frequent that both an AGN and a starburst are simultaneously present in the galaxy centers, the starburst being a nuclear ring encircling the nucleus. Spatial resolution is therefore required to separate them.

Differences are indeed found in the line ratios between AGN and starbursts. There is a higher HCN emission, a lower HCO$^+$ emission and higher temperatures in AGN than in the starburst regions. Similarly to NGC 1068, this might result from a higher HCN abundance in the centre due to an X-ray dominated gas chemistry, but a higher gas density/temperature or additional non-collisional excitation of HCN cannot be entirely ruled out. Indeed, a new result comes from the J=2-1, J=3-2 lines of HCN and HCO$^+$. The HCN/CO ratio decreases with J in AGN, while it remains constant in starbursts.

Low HCO$^+$ emission in AGN suggests that IR pumping is not important (however it might be important for HNC in ULIRGs, Guerin et al 2007, Aalto et al 2007).

The excitation ratios HCN(2-1)/HCN(1-0), or HCN(3-2)/HCN(1-0) and HCO$^+$(3-2)/HCO$^+$(1-0) are found to be clear discriminators between AGN and starbursts, the latter being more excited (Krips et al 2007, in prep). The excitation could come from a higher density and/or higher temperature. A modelisation through LVG models confirms that there is relatively more dense gas in star-forming regions. The $\text{H}_2$ density in regions around the AGN is then relatively low, which may explain the low HCO$^+/\text{HCN}$ in those XDR.

A prototypical example of the separation between AGN and starburst is the galaxy NGC 6951 (Fig 3). It is a barred spiral, with a ring of CO emission at the inner Lindblad resonance. This nuclear ring (400pc radius) is a clumpy starburst, while the central component is AGN influenced. There appears to be a molecular torus of 50pc in size, which could be the obscuring component required by the AGN unification model for this Seyfert 2. The HCN/CO ratio is about 0.02 in the nuclear ring, while it is $>0.4$ in the torus (Krips et al 2007).

2.4 PDR and XDR models

The differences between starburst and AGN chemistry and physical conditions have been predicted by several models, with sometimes non converging results (e.g. Maloney et al 1996; Meijerink & Spaans 2005). Starbursts create regions dominated by UV photons (6-13.6ev) from O & B stars, e.g. PDR; they illuminate the surface of clouds, in the nuclear regions on scales $<1$pc, where higher HCO$^+$ is expected (from supernovae and associated cosmic rays). Around AGN, molecular clouds are X-ray irradiated (1-100kev); X-ray penetrate more deeply into clouds of the circum-nuclear disk CND. The radiation has then a volume effect, instead of a surface effect in PDR.
Fig. 3. Integrated HCN(1–0) emission (black contours) overlaid on CO(2–1) (color scale) in natural (left) and uniform weighting (right); the CO emission has been smoothed to the same spatial resolution as the HCN. The black line (left) indicates the major axis of the bar (PA=100°) and the grey line the major axis of the galaxy (PA=130°). From Krips et al (2007).

The higher HCN/CO ratio in AGN, due to the XDR, is indeed a prediction of models, but only for high (column) density gas, with columns in excess of $10^{23}$ cm$^{-2}$ and densities larger than $10^4$ cm$^{-3}$. Otherwise, the HCN/CO ratio is lower in XDR than in PDR.

In recent models (e.g. Meijerink et al 2007) there is no oxygen depletion in AGN, and CO emission is even enhanced with respect to PDR, since the volume in which CO is excited is much wider. Contrary to the observations, models predict a low HCN/HCO$^+$ ratio at high density in the XDR, i.e. when the HCN/CO ratio is high. The contrary is expected to be true at low density. According to density and irradiation strength, it should be possible to find HCN/HCO$^+$ enhanced in XDR. On the other hand, CO(1-0)/H$_2$ is predicted to be lower in XDR, since the CO molecule is warmer, and high-J levels are excited, which could also explain the HCN/CO(1-0) ratio.

2.5 Is the HCN/CO ratio a star formation indicator?

It is now well established that, while the HCN/CO ratio is about 0.1 or less in normal galaxies, it is enhanced to values larger than 0.3 and even up to 1 towards the nuclei of AGN (Kohno et al 1999, Usero et al 2004).

There is however another observation of boosted HCN emission towards starburst galaxies, and in particular ultraluminous in the infrared: there is in particular a good correlation between HCN and IR due to star formation (Gao & Solomon 2004). This correlation is not likely due to infrared pumping through UV/X-ray heated dust, since there is no correlation between X-ray and MIR.

The far infrared luminosity is thought to be one of the best tracers of star formation, and the fact that it is better correlated to HCN than to CO is interpreted as a correlation with dense gas (HCN being here a dense gas tracer essentially).
While the relation between the star formation rate and CO is non-linear, it is linear with the HCN(1-0) emission. The SFR is directly proportional to the dense gas, and it is to the latter that the Schmidt law is related.

We are therefore left with a degeneracy, towards the central parts of ULIRGs: either the HCN is a tracer of dense gas, and therefore of star formation (Gao & Solomon 2004), or the importance of the AGN is highly increasing at high infrared luminosity (as has been already observed, Tran et al 2001, Veilleux et al 2002), and most of the HCN emission could come from abundance effects due to an XDR.

HCO$^+$, which is also a dense gas tracer, might help to raise the degeneracy. The problem is complex however, since not only density, but also temperature, excitation and physical effects play a role, and in starbursting galaxies, the nucleus activity is often symbiotic to the star-forming region. According to the low HCO$^+$/CO ratio observed in ULIRGs by Gracia-Carpio et al (2006), cf Fig 4, and the correlation found between the HCN/HCO$^+$ ratio and the IR luminosity of the galaxy (LIR), the HCN enhancement in ULIRG could be due only to the XDR chemistry, and not to the dense gas and star formation.

**Fig. 4.** Variation of the HCN(1–0)/CO(1–0) (top) and HCO$^+$(1–0)/CO(1–0) (middle) luminosity ratios from normal galaxies ($L_{IR} < 10^{11} L_\odot$) to LIRGs and ULIRGs ($L_{IR} > 10^{11} L_\odot$). The HCO$^+$(3–2) /CO(1–0) ratio (bottom) is about constant for LIRGs and ULIRGs. From Gracia-Carpio et al (2006).
3 Conclusions

The abundant observations of many different chemical and density tracers in external galaxies have shown that chemistry is indeed coupled to dynamics, via shocks, bars, galactic outflows.

Chemical and density tracers could help to discriminate between starburst and AGN as the source of molecular emission. In particular, photodissociation regions (PDR) and X-ray dominated regions (XDR) bear different diagnostics in HCN, CO and HCO+ ratios.

The fact that the HCN abundance is enhanced in XDR, brings a degeneracy in the HCN/CO tracer of dense gas and of star formation rate. In nuclei of galaxies, other tracers should be also searched for in parallel. In all cases, enhanced spatial resolution is required to raise the degeneracy.

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