

THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

H_2S and dense gas in luminous infrared galaxies and their outflows

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Artist's impression of galactic outflows. Copyright: ESA/AOES Medialab

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With reverence for those who defy the sole infinity.

Abstract

Luminous infrared galaxies (LIRGs) are dusty galaxies that are going through an important and likely transient phase in their evolution. They experience rapid growth through bursts of star formation or an accreting supermassive black hole, an Active Galactic Nucleus (AGN). Radiative feedback from the AGN or starburst is absorbed by the dust and re-emitted in the infrared. Mechanical feedback in the form of outflows can effectively expel gas and dust from the central regions of the LIRGs. Thus, studying the physical processes and conditions of outflows is one of the key elements for a complete understanding of galaxy evolution. Especially molecular outflows are significant because cold and dense gas, that normally participates in star formation, can be highly affected by the presence of the central energy source. In some cases, the gas may even be accelerated to velocities over 1000 km s^{-1} . Many fundamental questions about the formation or physical processes of these feedback mechanisms still remain to be answered.

In this thesis, I put my attention to one molecule, hydrogen sulphide (H_2S), as a new diagnostic tool to probe the physical conditions in the dense molecular gas in dusty galaxies and their outflows. One aim is to investigate if H_2S can be used to study the outflow driving mechanisms. The observations with the Atacama Pathfinder Experiment (APEX) telescope and the IRAM Northern Extended Millimeter Array (NOEMA) are described in Paper I. In this paper, we present new detections of ground state H_2S line emission in a sample of LIRGs, and compare intensities to other lines, such as HCN and HCO^+ 2–1. At the observed resolution, we do not find any H_2S abundance enhancements linked to the outflows. Instead, we find a possible relation between the dense gas reservoir and the properties and evolution of the molecular feedback. Another point we discuss is the similar infrared-correlation coefficient between H_2S and H_2O which may indicate a similar origin of their emission. For example from warm gas in shocks or in gas irradiated by star formation or an AGN.

The next step is to look into the dense dusty galaxy nuclei with higher spatial resolution, and to proceed to radiative transfer modelling using multi-transition lines of several molecular gas tracers, including H_2S .

Keywords: Galaxies:ISM - ISM: molecules - ISM: outflows.

List of Publications

This thesis is based on the following publications:

[A] **M. T.Sato**, S. Aalto, K. Kohno, S. König, N. Harada, S. Viti, T. Izumi, Y. Nishimura, and M. Gorski, “APEX and NOEMA observations of H₂S in nearby luminous galaxies and the ULIRG Mrk 231”. Accepted by *Astronomy & Astrophysics*, 2022.

Other publications by the author, not included in this thesis, are:

[B] N. Falstad et al., **M. Sato**, “CON-quest Searching for the most obscured galaxy nuclei”. *Astronomy & Astrophysics* 649, A105, 2021.

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CHAPTER 1

Introduction

Galaxies are the largest building blocks of the Universe. Many of them go through an evolutionary phase of rapid, dust-enshrouded growth, constituted by intense star formation (=starburst) and black hole feeding (accretion) in their centres. The nuclear activity gives feedback through radiation (that is absorbed and re-emitted by dust), and in the form of powerful outflows. This mechanical feedback expels gas from galaxy centres, and in some cases the ejected gas can reach as far as inter-galactic space. Understanding the physical conditions, mass, velocity and morphology of the outflows is key in giving them their right place in the puzzle of galaxy evolution.

1.1 (Ultra) Luminous Infrared Galaxies ((U)LIRGs)

General references: Sanders & Mirabel (1996), Pérez-Torres et al. (2021)

Discovery and classification of (U)LIRGs

The first all-sky survey at far-infrared wavelengths (carried out in 1983 by the Infrared Astronomical Satellite (IRAS)) resulted in the detection of tens of thousands of galaxies, the majority of which were too faint to have been included in previous optical catalogues. Here started the identification of a class of "infrared galaxies", objects that emit more energy in the infrared ($\sim 5\text{--}500\ \mu\text{m}$) than at all other wavelengths combined. Among them, luminous and ultra-luminous infrared galaxies ((U)LIRGs) are defined by having excessive infrared luminosities ($L_{\text{IR}} > 10^{11} L_{\odot}$ and $> 10^{12} L_{\odot}$, respectively). Recent studies show that most (U)LIRGs are part of close interactions or are mergers of molecular gas-rich spirals. When galaxies interact with each other, large masses of gas and dust are funnelled to their central regions. This leads to a dense, dusty and molecular-rich region in the centre of the galaxy. The dust absorbs uv emission from young stars or from the accretion onto a supermassive black hole (SMBH) - a so called Active Galactic Nucleus (AGN). This emission is then re-radiated as infrared emission. There is an ongoing debate if star formation, or an AGN, dominates the thermal infrared emission.

Gao & Solomon (2004b) presented a tight correlation between the infrared luminosity (L_{IR}) and the luminosity of the hydrogen cyanide 1-0 line emission (L_{HCN}) as evidence of star formation being the main power source of the (U)LIRGs. This can be argued, assuming that L_{IR} is a measure of the star formation rate (SFR), and L_{HCN} indicates the mass of the dense molecular gas. Gao & Solomon (2004b) find that this correlation is valid in normal spiral galaxies, LIRGs, and ULIRGs alike (fig.1.1).

Compact Obscured Nuclei (CONs)

Since (U)LIRGs are in general highly dust-enshrouded objects, the dust hides very active evolutionary phases of nuclear growth. Some (U)LIRGs host extremely compact ($r < 100\text{ pc}$) and dust obscured nuclei with visible extinction $A_V \gg 1000$ (corresponding to $N_{\text{H}_2} > 10^{24}\text{cm}^{-2}$). These regions are categorised as Compact Obscured Nuclei (CONs, Aalto et al. (2015b)).

At these high levels of extinction, the large amount of obscuring material hampers optical, mid- and near-infrared and X-ray observations and one has to use far-infrared and/or sub-mm/mm lines and continuum to probe the activity within these most enshrouded galaxy nuclei.

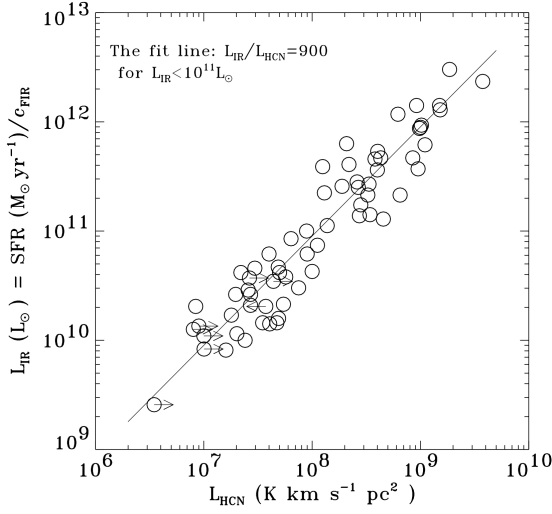


Figure 1.1: Correlation between HCN and IR luminosities in 65 galaxies (Gao & Solomon 2004b)

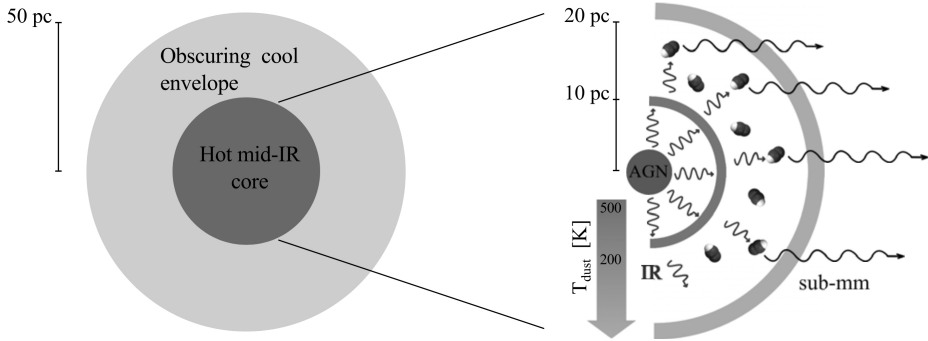


Figure 1.2: Schematic drawing of CON (credit: F.Costagliola). It shows how HCN molecules absorb buried mid-infrared emission and then re-radiates this emission at longer wavelengths.

For regions where column densities are above 10^{24} , but below 10^{25}cm^{-2} , radiatively excited molecular emission lines of e.g., H_2O and OH are good probes of the nuclei in the far-infrared. At longer radio wavelengths OH mega-masers are commonly seen in ULIRGs, and also H_2O masers are found associated with AGN accretion discs or in post-shock gas along nuclear jets (See a review by Lo (2005)). Several CONs have $N(\text{H}_2)$ in excess of 10^{25}cm^{-2} and in some cases column densities may reach extreme values of $> 10^{26}\text{cm}^{-2}$. The nearby LIRG-CON, NGC 4418, is likely one example and an $N(\text{H}_2)$ in excess of 10^{26}cm^{-2} has been suggested for the LIRG IC860 and for the ULIRG Arp220 (e.g., Aalto et al. 2019; Scoville et al. 2017).

The intense infrared radiation arising from warm dust (100-300 K) in these sources can provide a significant fraction of the bolometric luminosity of the galaxy and is prone to excite vibrational levels of molecules such as HCN. Sakamoto et al. (2010) firstly reported the detection of strong line emission from the rotational transitions of the vibrationally excited $v_2=1$ state of HCN (HCN-vib) in external galaxies at (sub) millimetre wavelengths. HCN-vib requires a mid-IR surface brightness of over $5 \times 10^{13} L_\odot/\text{pc}^2$ to be excited (Aalto et al. 2015b). For an illustration of HCN absorbing buried mid-infrared emission and re-emitting it at longer wavelengths, see fig.1.2. The large H_2 column density in the CON regions will also result in luminous dust emission in the mm- and submm-range (for a discussion between the link between HCN-vib and the mm-continuum surface brightness see Falstad et al. (2021)). The emitting region should be either an extremely compact opaque starburst, or an obscured AGN.

Falstad et al. (2021) defined CONs as galaxies with strong HCN-vib $l = 1f, J = 3 - 2$ transition line emission ($\Sigma_{\text{HCN-vib}} > 1 L_\odot \text{pc}^{-2}$) from a region with radius $r > 5$ pc. A CON is also defined as having a lower limit of $L(\text{HCN-vib})/L(\text{IR}) > 10^{-8}$. Falstad et al. (2021) found CONs in almost 40% of a volume limited sample of ULIRGs, and in 20 % of the LIRGs. No CONs were found in a local sample of sub-LIRGs with $L(\text{IR})$ of $10^{10} L_\odot$. This ALMA survey (CONquest) was limited to a total of 38 galaxies and a larger survey is important for a full census of CONs. There have been several observations searching for CONs, but so far, luminous HCN-vib line emission has primarily been found in ULIRGs and in LIRGs that appear to be early type spirals (e.g., Aalto et al. 2015a,b, 2016, 2019; Falstad et al. 2021; Imanishi, Nakanishi, & Izumi 2016; Imanishi & Nakanishi 2013; Martín et al. 2016).

Inflows and outflows in CONs

The central regions of CONs show evidence of reversed P-Cygni profiles in molecular and atomic lines - indicating inflowing gas (e.g., Aalto et al. 2015a, 2019; Costagliola et al. 2013; Falstad et al. 2021; González-Alfonso et al. 2012; Sakamoto et al. 2013). Therefore, there has been a suggestion that CONs may represent a short phase in the galaxy's evolution which is occurring before the feedback from the starburst/AGN becomes important, before an outflow develops enough to be detected (see Falstad et al. (2019) for a discussion). However, recent mm- and cm-wave studies of some LIRG- and ULIRG-CONs reveal fast outflows - for example the collimated outflow in Arp220 (Barcos-Muñoz et al. 2018). More studies of the morphology and extent of outflows are necessary to understand what role the outflows play in CONs.

1.2 Feedback: outflows

General references: Veilleux et al. (2020), Veilleux, Cecil, & Bland-Hawthorn (2005)

Overview of galactic outflows

Galaxy centres can be fed with gas and dust during mergers or more distant interactions with other galaxies. On the other hand, they also expel part of the material of which they are constituted (like gas and dust) in large-scale galactic outflows. (There are also some reports about expelled stars and dark matter from a galaxy (e.g., Fensch et al. 2019; Koposov et al. 2020)). Such mechanisms of accretion and feedback of mass, momentum and energy regulate the physical processes which occur within galaxies, which in turn determine important parameters such as star formation rate, chemical composition, and stellar populations. For example, star formation could be quenched due to the mass-loss occurring as a result of an outflow. Mass-loss from a galaxy nucleus also has an impact on the black-hole growth. Consequently, by studying the processes of inflowing and outgoing gas and dust, including the mass and physical conditions of the out- and inflows, it is possible to understand the evolutionary state of a galaxy.

The role of outflows as a mechanism of feedback is of particular impor-

tance because they can transfer and distribute mass, energy and momentum from small to large scales. Outflowing gas is commonly seen from a variety of galaxies, which include (U)LIRGs hosting a starburst and/or an AGN. Outflows can occur on different size scales in a galaxy. There is also observational evidence of large-scale narrow-angle/jet-like outflows from several Seyfert galaxies, which might be mainly AGN-driven, as suggested from their morphology and orientation.

Outflows have been identified at different wavelengths: optical, infrared, radio, UV and X-rays, suggesting that outflows are multi-phase with both hot and cool gas components. For example Mrk 231, a nearby ULIRG and quasar, has a neutral gas outflow observed in the molecular and atomic phases on scales of a few hundreds of parsecs (e.g. Cicone et al. 2012; Morganti et al. 2016). NGC1365, a barred spiral Seyfert galaxy, has an outflow of ionised gas on scales extending over a few kiloparsecs (Venturi et al. 2017, 2018). Gao et al. (2021) reported a high-resolution CO 1–0 map of NGC1365, showing noncircular motion of molecular gas, reaching a velocity of up to 100 km s^{-1} , which is comparable to that of the ionised gas.

Molecular outflows

Winds and feedback often occur in the form of molecular outflows that carry large amounts of cold molecular gas out from the centre of galaxies. A large fraction of ULIRGs are observed to have wide angle molecular outflows that are detectable using the median velocities of far-infrared OH absorptions (Veilleux et al. 2013). It is believed that these outflows help to regulate the growth of galaxy nuclei. A large fraction of the gas mass in outflows may reside in molecular (H_2) clouds. Indeed, molecular line studies have delivered very high H_2 mass-loss rates of several $100 M_\odot \text{ yr}^{-1}$ (Cicone et al. 2014, also fig.1.3), which may therefore have a large impact on the star formation in the host galaxy.

Since molecular outflows may evict significant masses of gas out of the galaxy, or the gas may return to the system to fuel another growth spur (see e.g. Aalto et al. (2020)), they are important to our understanding and modelling of galaxy evolution. There has been a discussion of the origin of the molecular gas in the outflows: is it carried out in molecular form from the disk and nucleus, or is it formed in situ in the outflow through instabilities in the hot gas? One proposed scenario of molecules forming in outflows is presented

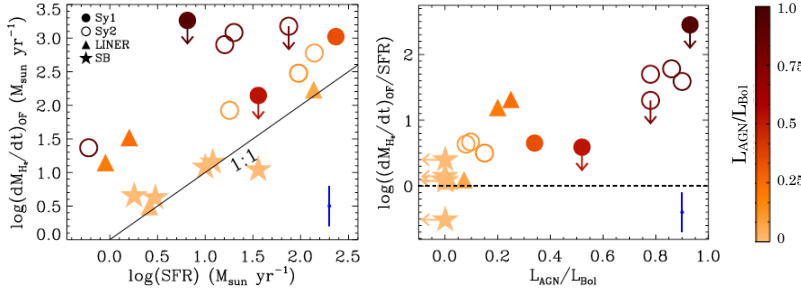


Figure 1.3: *left:* outflow mass-loss rate as a function of the star formation rate for the extended sample of galaxies. Filled and open circles represent unobscured and obscured AGNs, respectively. LINERs are plotted as upward triangles and "pure" starburst galaxies as stars. Symbols are colour-coded according to the fraction of bolometric luminosity attributed to the AGN (L_{AGN}/L_{Bo1}). The black dashed line represents the 1:1 correlation between SFR and outflow mass-loss rate. *right:* this plot indicates a positive correlation between the outflow mass loading factor ($\dot{M}_{H_2,OF}/SFR$) and L_{AGN}/L_{Bo1} that emerges from the diagram in the left panel. (fig.8 of Cicone et al. 2014)

in Richings & Faucher-Giguère (2018). This will be discussed further in chapter 3.

Energy sources

Here I would like to describe a rough structure of the physical processes related to the galactic outflows. Possible energy sources for the molecular outflows are starburst or AGN.

There are several stellar processes which inject mass, momentum and energy into the surrounding environment, which may affect the rate of star formation. The most important processes are supernova remnants (SNR) and hot stellar winds from young massive stars. When a star with a mass over $8 M_{\odot}$ ends its life, its core collapses and ejects $\sim 1-10 M_{\odot}$ of material with kinetic energy $E_{SN} \simeq 10^{51} \text{ erg} \equiv E_{51}$ and momentum $p_{SN} = \sqrt{2E_{SN}M_{SN}}$, where M_{SN} is the mass of the ejected material per SN. (Other stellar processes include proto-stellar outflows, type Ia supernovae, and stellar winds from old stars, which seem not play an important role in driving the cool outflows in starburst and

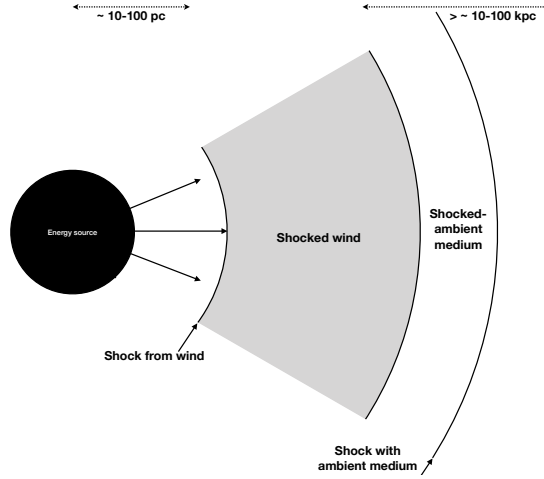


Figure 1.4: A schematic drawing of outflow driving mechanism (adapted from Faucher-Giguère & Quataert (2012)).

active galaxies.)

In the case of an AGN, the primary energy source to drive outflows is accretion onto the central SMBH. The gravitational potential energy released by the accreted material is transformed into thermal energy and partly to radiation.

There are two modes in AGN feedback: *radiative* and *kinetic*, depending on the accretion rates. The radiatively efficient AGN gives feedback in "radiative" (or "quasar") mode. This type of AGN has a high accretion rate, and the feedback can often be seen as wide-angle outflow. A radiatively inefficient AGN gives feedback in "kinetic" or "radio" mode. This type of AGN has a lower accretion rate, which gives rise to radio jets.

Driving mechanisms

Both starbursts (SBs) and AGNs can exert their energy into the surrounding medium in multiple forms. The radiation from the central energy source can create a pressure to push the immediate surroundings outwards. The kinetic energy can directly push the medium as well. It also heats up the medium to create hot winds. Finally, cosmic rays can also contribute to move the gas

outwards. Furthermore, AGNs can also carry the ambient medium through jet entrainment.

Molecular outflows may be *energy-driven* when radiative losses are negligible, or *momentum-driven* when radiative losses are not negligible. They are difficult to distinguish observationally because often both mechanisms are at work.

Fig.1.4 is a simple sketch to explain the impact given from the energy sources to the ambient medium. The central energy source, an SB or an AGN (or both of them) drives a wind from the surface of the region. The small scale wind experiences a wind shock with the immediate surrounding medium and the bulk kinetic energy of the wind is converted into thermal energy. The thermal energy inflates a bubble of very hot gas which can push the interstellar medium in the galaxy outwards. The swept up gas will pile up and be observed in molecules with an area of a few kiloparsec, which drives a second shock at the outer radius with the ambient medium.

Whether a large-scale outflow is energy-driven or momentum-driven depends on the conditions of the hot bubble region (the grey-coloured region in fig.1.4). If the cooling time in the hot bubble is shorter than the time it takes for the wind to expand in the galaxy, it loses its support of thermal pressure, and the momentum of the gas that was swept up at the outer edges is basically just what was put in by the central engine. On the other hand, if the gas in the hot bubble remains hot, the thermal energy is trapped and can be used to do work on the swept up ambient medium. That work can give momentum to the swept up gas, thus can be said, energy-driven.

If the outflow is energy-driven, the energy injected in the ambient gas (thermal energy, E_{th}) is transformed into the kinetic energy (E_{kin}) of bulk motion at a rate $\dot{E}$, which is proportional to $\dot{M}v_{\text{out}}^2$. Whilst if the outflow is momentum-driven, the energy injected in the ambient gas is due to the momentum that was put in by the central energy source, thus $\dot{E} \propto \dot{M}v_{\text{out}}$. Therefore, Murray, Quataert, & Thompson (2005) argued that estimating the mass loss rate of outflows is a way to distinguish between the two driving mechanisms.

Tracers and observations of molecular outflows are discussed further in chapter 3.

CHAPTER 2

Molecular Lines

General references: Veilleux et al. (2020), Solomon & Vanden Bout (2005)

(U)LIRGs are rich in molecular gas, which feeds star formation and AGN activity. Several observations have shown that (U)LIRGs also often have molecular outflows (See Sect. 1.2). Tracer molecules are required to probe the mass, dynamics and distribution of the molecular gas (see Sec. 2.2). Millimetre and sub-millimetre wave techniques can provide direct estimates of the luminosity, kinematics, and morphology of the molecular emission. This information can be converted into estimates of the physical properties of the molecular clouds, for example column- and volume density, mass, momentum and energy. There are a large number of molecular transitions in the millimetre/sub-millimetre-wave window. This means that observations provide a unique view of the chemistry and excitation in the outflowing gas.

To investigate the energy source and driving mechanism of molecular outflows in galaxies, we need a combination of molecules that trace the full extent of the outflow, from its launch point and out to its outer edge. These molecules should have transitions that are excited in such a way that we can locate where the emission comes from. Molecular line emission (and contin-

uum) is also important to probe the central rotating discs of dusty galaxies to determine physical conditions, dynamics and enclosed mass.

But, some of the (U)LIRGs (for example the CONs) are so dusty and dense in their central region that traditional tracers of dense gas (such as HCN and HCO⁺) can not penetrate to reach our eyes. It is therefore important to explore more tracers that go beyond the standard ones.

2.1 Brightness temperature, flux density and luminosity

Measurements obtained with single-dish radio telescopes are usually expressed in Rayleigh-Jeans brightness temperature units of Kelvins, corresponding to $T_B = I_\nu c^2 / 2k\nu^2$, where I_ν is the specific intensity, k is the Boltzmann constant and ν is the frequency of the line. In interferometers, the measurements are usually expressed in flux density units. The conversion between temperature surface brightness units and flux density is

$$T_B = 1360 \text{K} \frac{\lambda^2}{\theta^2} S_\nu, \quad (2.1)$$

where T_B is the Rayleigh-Jeans brightness temperature in K, θ is the full-width at half-maximum of the Gaussian beam of the observation in arcseconds, λ is the wavelength of the observation in cm, and S_ν is the flux density in Jy beam⁻¹. The Rayleigh Jeans brightness temperature can be expressed with the excitation temperature of the transition through

$$T_B = \frac{h\nu}{k} (1 - e^{\tau_J}) \left(\frac{1}{e^{\frac{h\nu}{kT_{\text{ex},J}} - 1}} - \frac{1}{e^{\frac{h\nu}{kT_{\text{cmb}}} - 1}} \right), \quad (2.2)$$

where the cosmic microwave background temperature T_{cmb} is the background against which the emission is measured and J is the upper-level of the transition. The last term is usually a small correction for $z \sim 0$, and it is frequently neglected.

Luminosities are frequently expressed in units of K km s⁻¹ pc², and when using these units they may be noted as L' . In general,

$$L' = 3.25 \times 10^7 S_\nu \Delta\nu \nu_{\text{obs}}^{-2} (1+z)^{-3} D_L^2, \quad (2.3)$$

where S_ν is the flux density in Jy, Δv is the line width in km s^{-1} , ν_{obs} is the observed frequency in GHz, z is the source redshift, and D_L is its luminosity distance in Megaparsec (Solomon & Vanden Bout 2005).

2.2 CO as reservoir tracer

Over a very wide variety of conditions, the brightest transitions from molecular gas at millimetre/sub-millimetre wavelengths are the rotational transitions of carbon monoxide (CO), $^{12}\text{C}^{16}\text{O}$. These transitions of CO are excited mostly through collisions with H_2 molecules. Radiative trapping will play an important role in the excitation if the transition is optically thick, which is easy to achieve since CO is an abundant molecule that is frequently the largest reservoir of carbon in the gas phase. CO is also the most abundant molecule after H_2 , and $X(\text{CO})$ may reach 10^{-4} (in relation to H_2). The low- J transitions of CO mainly trace the bulk of the gas including more diffuse (unbound) phases. Low- J CO line emission probes different gas conditions than the dense gas tracers trace. The critical density of CO $J=1-0$ can be as low as $n_{\text{crit}} \sim 10^2 \text{ cm}^{-3}$ (see below), and it can probe gas with relatively low number density.

CO emission lines are used to calculate the molecular mass because it is the next abundant molecule in the clouds, including in outflows. The observed CO luminosity is converted to the molecular mass using a CO-to- H_2 conversion factor, α_{CO} . There is a continuing discussion on this factor, though, since this includes assumptions on cloud physical conditions and self-gravitation that are often difficult to verify. For example, the CO luminosity depends on the optical depth effects, including kinematics and excitation temperature, of the emitting molecular gas which introduces non-trivial effects on the conversion of the line luminosity to the molecular gas mass (see for example the discussion in Veilleux et al. (2020)). Cicone et al. (2018) used an alternative method to estimate the molecular mass of the outflow of NGC 6240, using the neutral atomic carbon line (CI 1-0).

2.3 Dense molecular gas and HCN, HCO^+

HCN is one of the most abundant H_2 mass tracers after CO. HCN $J=1-0$ line emission traces molecular gas at densities $n(\text{H}_2) \gtrsim 3 \times 10^5 \text{ cm}^{-3}$ which is three orders of magnitude higher than CO $J=1-0$ (Gao & Solomon 2004a).

HCN has a high dipole moment ($\mu_{10} = 2.98$ D for HCN J=1–0) compared to that of CO ($\mu_{10} = 0.11$ D for CO J=1–0), which makes its lower transitions excellent tracers of dense molecular gas in galaxies. This is because critical densities of rotational transitions are proportional to the square of the dipole moment, $n_{\text{crit}} \propto \mu^2 \nu_{J+1J}^3$ (for optically thin lines at frequency ν_{J+1J}) (Papadopoulos 2007), and the excitation is such that bright emission usually requires densities that are similar to or larger than n_{crit} . Critical densities of HCN 1–0 and CO 1–0 emission lines, for example, are calculated $\sim 10^5 \text{ cm}^{-3}$ and $\sim 10^2 \text{ cm}^{-3}$, respectively at $T = 50$ K. HCO^+ rotational lines are also considered as a dense gas mass tracer due to the same reason, i.e. high dipole moment ($\mu_{10} = 3.92$ D for HCO^+ J=1–0) leading to its higher critical density ($n_{\text{crit}} \sim 10^4 \text{ cm}^{-3}$ at $T = 50$ K).

A HCN molecular line intensity is the results of the excitation and/or its abundance. HCN can be excited either collisionally or being pumped by infrared continuum. The collisional excitation is affected by the abundance, which may be enhanced by high temperature and shock chemistry. On the other hand, HCO^+ abundance is less affected by shocks (Tafalla et al. 2010), therefore it is valuable to obtain both dense gas tracers.

Line intensity ratios of those dense gas tracers to CO (such as HCN/CO and HCO^+/CO), are employed as, to first order, indicators of density, or dense gas content. However comparison among molecular species can be affected by their relative abundances which are determined by the chemistry. There can be more than one collisional partner to excite some molecules. For example, HCN and HCO^+ have a 10^5 and a 10^4 times larger cross-section to collisions with electrons than with hydrogen molecules, respectively. This may affect their use as density tracers in regions where electrons are abundant (Goldsmith & Kauffmann 2017). More importantly, infrared radiative excitation and pumping may affect those molecules, which can impact the interpretation of the rotational transition molecular line emission.

In general the presence of bright emission from one of the high-dipole moment species like HCN or HCO^+ is taken to suggest that the volume density is similar to or higher than the critical density of the transition. A full treatment of the gas density requires solving the detailed balance equation to establish the population of each rotational level. This can provide simultaneous constraints on volume density, column density, and temperature.

However, in the extremely dense regions of CONs, even the emission from

those traditional dense gas tracers can not escape. This is because the large opacities and temperature gradients give rise to effects of self-absorption in the line emission. The molecules also absorb continuum emission from the nuclear dust source. As briefly mentioned in Sect.1.1, the HCN-vib emission line can be used in those cases.

2.4 H_2S

Sulphur (S) is one of the most abundant elements in the universe. However, the abundances of sulphur-bearing species derived from observations are much lower than expected in the ISM. The observed low abundances are thought to be mainly due to depletion inside molecular clouds during the cold collapse phase. While it is expected that most sulphur-bearing molecules in dense cores are locked on the ice mantle around grains, they can be released into the gas phase in hot cores or in the regions affected by strong shocks. However, even in the Orion KL hot core ($T = \sim 100\text{-}300\text{ K}$), the observed H_2S fluxes (Wakelam et al. 2004) can be best reproduced with an initial sulphur abundance of 0.1 times the sulphur solar abundance, suggesting that 90 % of the sulphur solar abundance has been depleted (Crockett et al. 2014; Esplugues et al. 2014).

Depleted Sulphur may form sulphur-bearing molecules, then those molecules come out in gas-phase by desorption from icy grain mantle through several processes. Most of the Sulphur that is locked on the ice mantles is a component of the molecule hydrogen sulphide (H_2S). Thus, since this molecule is thought to be one of the main reservoirs of sulphur it has received special attention by astrochemists. H_2S can be formed through hydrogenation of a sulphur atom on grain surfaces, which can then be (i) thermally desorbed by shocks or by infrared radiation, (ii) photodesorbed by UV radiation, (iii) desorbed after cosmic-ray impacts, or (iv) sputtered by shocks (Fig.2.1, Sato et al. 2022, and references therein). Chemical desorption could be also efficient enough to release H_2S into the gas phase (e.g. Navarro-Almaida et al. 2020; Oba et al. 2019). Hydrogenation of sulphur is also possible in the gas phase if the kinetic temperature is higher than a few thousand Kelvin (Mitchell 1984).

Detection of H_2S line emission means that there is a significant abundance of this molecule in the gas phase. The ground state transition line of H_2S was first detected in cold dark clouds in the Milky Way in 1972 (Thaddeus et al. 1972), followed by several other detections from Galactic sources (e.g.,

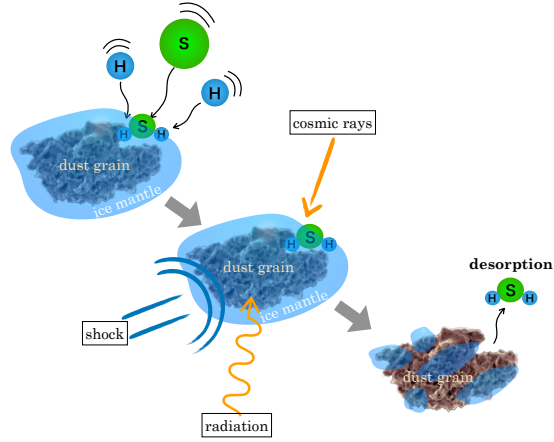


Figure 2.1: Schematic picture on the formation and desorption of H₂S molecule. (Credit:D.Tafoya)

Herpin et al. 2009; Minh et al. 1990; Navarro-Almaida et al. 2020). Minh et al. (1990) reported that H₂S abundances were enhanced by a factor of 1000 ($X_{\text{H}_2\text{S}} \sim 10^{-6}$) in the regions affected by outflows and have elevated temperatures relative to quiescent clouds. Pineau-desForets et al. (1993) explained that the high abundance of H₂S found toward Orion KL hot cores (Minh et al. 1990) can be best reproduced when you assume a shock passage with a shock velocity over 25 km s⁻¹ and a weak pre-shock value of the magnetically induced B field (around 70 μ G), through a medium with hydrogen density above 10⁵ cm⁻³.

The first extragalactic detection was reported in 1999 towards the Large Magellanic Cloud (LMC) (Heikkilä, Johansson, & Olofsson 1999). There were three more extragalactic detections before my work that I report here, toward NGC 253 (e.g. Martin et al. 2005), Arp 220 (e.g. Martín et al. 2011), and IRAS17208-0014 (Aalto et al. 2015b). Aalto et al. (2015b) detected strong higher transition line of H₂S toward IRAS17208-0014 (Fig.2.2). There are two lines (ortho-H₂S 3_{2,1}-3_{1,2} and para-H₂S 4_{3,1}-4_{2,2}) at 369 GHz with only 26 MHz between them, so the lines are blended into one line. They discussed that H₂S might be generated in relation to the energetic activities like outflows, starbursts in dense gas.

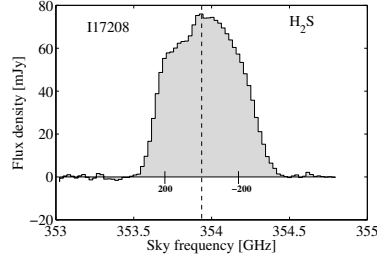


Figure 2.2: ALMA H_2S spectrum of IRAS17208-0014. The x axis is sky frequency in GHz. The velocity relative to the systemic velocity of IRAS17208-0014 ($cz = 12\,834 \text{ km s}^{-1}$) is shown in the axis at Flux Density = 0 mJy.

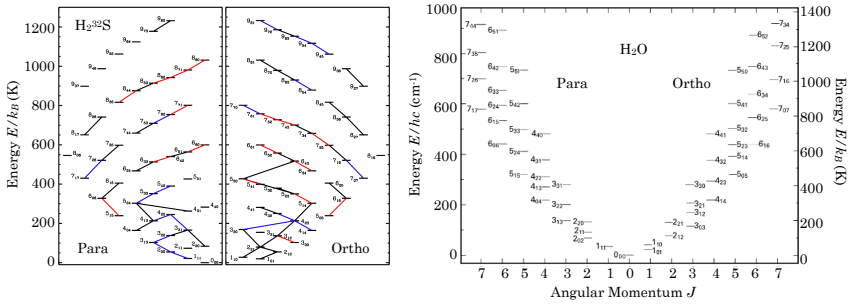


Figure 2.3: Energy-level diagrams of H_2^{32}S (left, Crockett et al. (2014)) and H_2O (right, Banzatti (2013)).

Another importance of H_2S molecule comes from its chemical similarity to the water molecule (fig.2.3). This leads to both of them having similar formation processes including grain chemistry processes. From the above discussion, H_2S may serve both as a shock tracer and a water proxy. The benefit of H_2S compared to H_2O is that its ground-state line is observable by ground-based telescopes for nearby galaxies. We have a discussion in relation to this in my paper I.

CHAPTER 3

Molecular probes of cool outflows

3.1 CO

Molecular outflows in dusty galaxies may be detected in absorption in far-infrared transitions of OH (see Veilleux et al. (2020) for a review), but to get the full extent and morphology it is important to image the outflows. The most common molecular line used for this is the $J=1-0$ transition of CO.

Following the first extragalactic detection by Nakai et al. (1987), toward the luminous starburst galaxy M 82, CO emission has been detected in many more starburst galaxies - for example NGC 2146, NGC 1808, NGC 3628, VII Zw 31, NGC 1614, NGC 3256 (fig. 3.1), ESO 320-G 030 and NGC 4945 (e.g. García-Burillo et al. 2015; Henkel et al. 2018; Leroy et al. 2015; Pereira-Santaella et al. 2016; Sakamoto et al. 2014; Salak et al. 2016; Tsai et al. 2009, 2012).

AGN galaxies with known CO outflows include Mrk 231, M 51, IRAS 13120, IRAS 17208-0014, NGC 1433, NGC 1068, IC 5063, Circinus, Mrk 273, NGC 1266 and NGC 1377 (e.g. Aalto et al. 2012a; Aalto et al. 2012b; Aalto et al. 2016, 2017, 2020; Aladro et al. 2018; Alatalo et al. 2011; Alatalo 2015; Cicone et al. 2012; Combes et al. 2014; Dasyra et al. 2016; Feruglio et al. 2010; García-Burillo et al. 2014; Matsushita et al. 2015; Morganti et al. 2015;

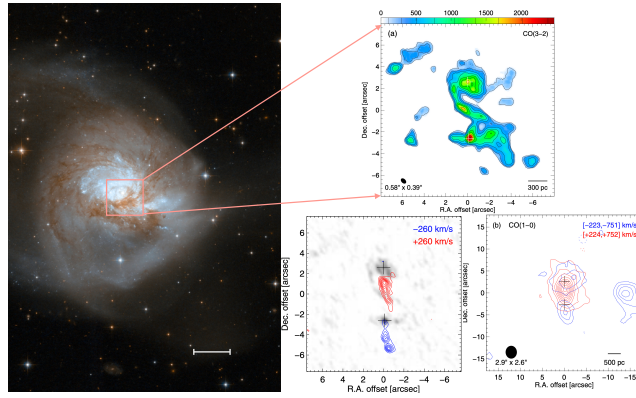


Figure 3.1: Molecular outflow traced by CO at NGC 3256. *Top:* CO(3-2) moment 0 map. *Bottom left:* CO(3-2) channel map of high-velocity emission at $0''.5$ resolutions. *Bottom right:* CO(1-0) map of high-velocity emission at around $3''$ resolution. (Sakamoto et al. 2014). *left:* HST image of NGC 3256 (NASA/ESA/A.Evans).

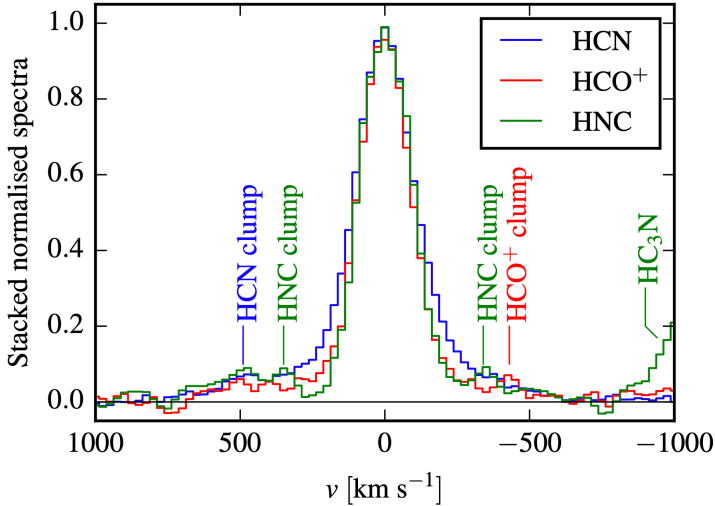


Figure 3.2: HCN 1–0, 2–1, and 3–2 lines; the HCO⁺ 1–0 and 2–1 lines; and the HNC 1–0 line of Mrk 231 observed with IRAM PdBI, are shown normalised, riggridded, and stacked weighted by the S/N to show the variations in line profile between the species. (Lindberg et al. 2016)

Oosterloo et al. 2017; Privon et al. 2017; Zschaechner et al. 2016). There are also galaxies that experience a combined AGN- and SB-driven outflow, for example NGC 6240 (Feruglio et al. 2013; Saito et al. 2018).

The low- J CO line may trace the full extent of the outflow (that shows a variety of morphology) and is often used as a tracer of molecular mass (See, Sect.2.2).

3.2 HCN, HCO⁺, CN

It is often found that emission from dense gas molecular tracers (such as HCN and HCO⁺ which trace $n(\text{H}_2) \gtrsim 3 \times 10^4 \text{ cm}^{-3}$, or CN ($n(\text{H}_2) \gtrsim 1 \times 10^6 \text{ cm}^{-3}$)) are enhanced in galactic outflows (e.g. Aalto et al. 2012a, 2015a; Barcos-Muñoz et al. 2018; Ciccone et al. 2020; Falstad et al. 2018; García-Burillo et al. 2014; Harada et al. 2018; Impellizzeri et al. 2019; Michiyama et al. 2018; Walter et al. 2017). Lindberg et al. (2016) studied the outflow features in the HCN, HCO⁺ and HNC emission lines in Mrk 231 and discussed the velocity structure in

terms of shocks in the outflow (Fig.3.2). Cicone et al. (2020) found extremely luminous CN emission in the same outflow and studied this in terms of UV irradiation and star formation.

It is possible that the higher compression of the gas in some outflows makes the dense phase of the molecular gas more prevalent than in galactic discs of the host galaxy, or the diffuse molecular phase is more easily evaporated and destroyed, or probably both phenomena are at work. Studying the dense gas phase in the outflow - using a combination of tracers - is key to the understanding of the physical conditions and evolution of the outflow, and how it relates to the driving mechanism of the outflow and the properties of the host galaxy.

3.3 Outflows from CONs

As discussed in Sect.1.1, molecular outflows are seen in (U)LIRGs that are CON-hosts. These outflows are not obvious in the far-infrared OH lines (see Falstad et al. (2019) for a discussion), but can be detected at mm-wavelengths in for example CO or HCN emission. Barcos-Muñoz et al. (2018) reported a fast molecular outflow detected in HCN (fig.3.3). Other examples include an outflow detected in the cm-wave OH-line in the LIRG Zw 049.057 (Falstad et al. 2018), a fast CO-outflow in the ULIRG-CON IRAS17208-0014 by García-Burillo et al. (2014), and nuclear feedback in the LIRG-CON IC 860 (Aalto et al. 2019). In CONs, both in- and outflows seem to be occurring at the same time (Falstad et al. 2021).

3.4 Origin of the H₂

The origin and the fate of the molecular gas in the galactic outflows are still not well understood. One question is whether the gas was formed in the host galaxy and has being swept up from its circumnuclear disc, or it is formed in the outflow from the precursory atoms, ions or molecules (e.g. Ferrara & Scannapieco 2016; Richings & Faucher-Giguère 2018). Another question is whether the molecular gas in the outflow spreads and evaporates, or whether it condenses to form stars (Maiolino et al. 2017). It is also poorly known what fraction of the gas is expelled from the galaxy by the driving force of the outflow, and what fraction returns to fuel another cycle of activity in the

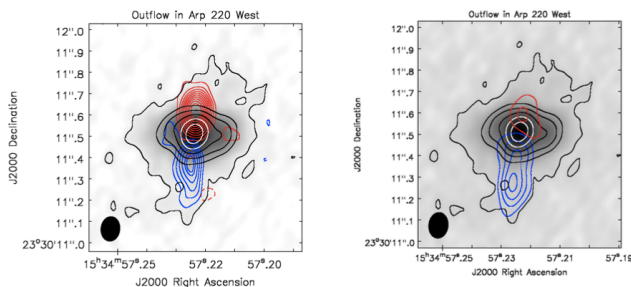


Figure 3.3: HCN (1-0) (left) and CO (1-0) (right) emission of the integrated intensity map are shown in red- and blue contours for redshifted and blueshifted channels, respectively. Greyscale: 92 GHz continuum image of the western nucleus of Arp 220 with its black ($3, 24, 48$ and $96 \times \sigma_{92\text{GHz}}$) and white ($192, 384 \times \sigma_{92\text{GHz}}$) contours. (fig.3 of Barcos-Muñoz et al. 2018)

same galaxy (e.g. Lutz et al. 2020; Pereira-Santaella et al. 2018).

A good estimate of the molecular mass is critical for the questions above, but it is also a challenge to determine the mass. Molecular hydrogen, H_2 , is the most abundant ($\sim 99\%$) molecule but typically is not observed¹. One of the reasons is that it has no permanent electric dipole moment, meaning the transitions tends to be relatively weak in emission. Another reason is that the temperature of the typical galactic molecular clouds are lower than that necessary to excite H_2 rotationally ($T_{\text{min}} = 510 \text{ K} \gg T_{\text{GMC}}$). Instead, CO emission lines are used to calculate the molecular mass (see sect.2.2 for a brief discussion on this.).

¹Richings & Faucher-Giguère (2018) suggested in their simulations that most H_2 is warm and observable in infrared rotational lines in outflows. This might explain the warm H_2 excess found by Spitzer in ULIRGs (Hill & Zakamska 2014)

CHAPTER 4

Observations and data reduction

The molecular lines discussed in this thesis are found in the mm-submm range as well as in the radio regime. We require radio telescopes with appropriate sizes for the wavelength of the molecular line which we aim to observe. The angular resolution is determined by the diameter of a telescope D and the observing wavelength λ as $\approx \lambda/D$. On the other hand, The sensitivity of the observations depend on the collecting area of the telescope ($\propto D^2$), on the observing time as well as on the spectral resolution (the channel width of the spectrum).

4.1 Single-Dish telescope

A *single dish* radio telescope (usually consisting of a parabolic antenna) is an instrument that operates as a single entity - to be distinguished from an *interferometer*, which contains multiple antennas observing simultaneously towards a target source.

The radio (or mm) emission from the source is collected by the parabolic antenna and goes through the horn to a spectrometer or a bolometer, converted into an electric signal to be detected and recorded.



Figure 4.1: A picture of APEX telescope at Chajnantor plateau, Chile. (Photo credit: D.Tafoya).

The Atacama PathFinder EXperiment (APEX)

For this thesis, the APEX telescope has been used for observations (fig.4.1).

APEX started as a collaboration among the Max-Planck-Institut für Radioastronomie (MPIfR), the Onsala Space Observatory (OSO) and the European Southern Observatory (ESO).

This millimetre and sub-millimetre observatory is located at the Chajnantor plateau in Chile, which was chosen for its high elevation (around 5000 m above sea level) and low-humidity environment, minimising the effect of water vapour on observations. The dish of the telescope has a diameter of 12 metres, the frequency coverage currently ranges from 157 GHz to 850 GHz.

One of the receivers is the SEPIA180, which covers the frequency range from 159 to 211 GHz (Belitsky et al. 2018). This is suitable to start observations with the lower transition lines of several molecules including some of the dense gas tracers such as HCN, HCO^+ , HNC and other molecules such as CH_3OH , SO, and H_2S . The SEPIA180 channel is a dual polarisation 2SB receiver built to the specifications of ALMA Band 5 (it is based on the pre-production version of this receiver). The instrument was built by the Group for Advanced Receiver Development (GARD) at OSO. The SEPIA180 receiver has two IF outputs per polarisation, upper sideband (USB) and lower sideband (LSB), each covering 4-8 GHz, adding up a total of 16 GHz instantaneous IF bandwidth. The central frequencies of the two sidebands are separated by 12 GHz. The full width at half maximum (FWHM) of APEX at the SEPIA180

frequencies is in the range of 30 - 39 arcseconds.

APEX data reduction

Calibrations

The APEX raw data are stored in the MBFITS data format. For heterodyne observations, these raw data are calibrated online by the apexOnlineCalibrator program, which writes the calibrated spectra (in antenna temperature (T_A^*) scale) into a CLASS -format data file. The data can be further reduced and analysed using the CLASS, GREG and MAPPING packages included in the GILDAS software.

Data reduction

CLASS was used for further treatment of the data. For example, the continuum was removed by subtracting a baseline of a polynomial of order 1 for individual scans and spectral smoothing. Gaussian fitting to each line gives a peak intensity and line width. The integrated line intensity is calculated using the formula,

$$I_{\text{line}} = \sum_i I_i dv, \quad (4.1)$$

where I is the intensity at each velocity and dv is the velocity resolution. The line-free frequency range in a spectrum gives its root mean square (rms) error for each sideband.

Error calculation

The error for the integrated line intensity is calculated using the formula,

$$\Delta I_{\text{line}} = \sqrt{(\Delta I_L)^2 + (\Delta I_B)^2} = \sqrt{(\sigma v_{\text{res}} \sqrt{N_L})^2 + (\sigma v_{\text{res}} N_L / \sqrt{N_B})^2}, \quad (4.2)$$

where σ is the rms noise level, v_{res} is the velocity resolution, N_L is the number of channels that contribute to the line, and N_B is the number of channels that are outside the emission line.

4.2 NOEMA description (used for paper I)

The IRAM Northern Extended Millimeter Array (NOEMA) is an interferometer with 11 antennas located on the Plateau de Bure at 2550 m altitude in the French Alps. Powerful dual-polarisation receivers for the 3 mm and 1 mm observing bands were installed in 2006, and extended to the 2 mm observing band in late 2007, and to the 0.8 mm band at the end of 2010. The antennas of the NOEMA interferometer can move on rail tracks up to a maximum separation of currently 760 m in the East-West direction and 368 m in the North-South direction, corresponding to a resolution of 0.5 arcseconds at an observing wavelength of 1.3 mm (230 GHz).

For the observations included in the paper I, the 2 mm band receivers were tuned to 161.934 GHz to cover the $\text{H}_2\text{S } 1_{10}-1_{01}$ line in the 3.6 GHz bandwidth of the wide-band correlator (WideX). Calibration sources are MWC 349 as flux calibrator, 3C 454.3 as bandpass calibrator, and J1418+546 and J1300+580 as phase calibrators.

Data reduction and analysis was performed using the CLIC and MAPPING software packages within GILDAS and AIPS.

CHAPTER 5

Outlook and future works

5.1 Summary of paper I

In this paper, we report the observation of the $\text{H}_2\text{S } 1_{10}-1_{01}$ emission line towards 12 nearby galaxies. The observations were executed using the APEX single dish telescope. Our aim was to find out how luminous the H_2S ground state emission is in dusty, luminous galaxies and if this can be related to the prevalence and properties of outflows. To further investigate the origin and distribution of H_2S emission, we also observed the $\text{H}_2\text{S } 1_{10}-1_{01}$ emission line at higher spatial resolution towards the ULIRG Mrk 231 using the NOEMA interferometer.

We detected the $\text{H}_2\text{S } 1_{10}-1_{01}$ emission line in 10 out of 13 galaxies (including in Mrk 231 with NOEMA). This supports the notion that ground state H_2S line emission is relatively common in U/LIRGs. We compared the $\text{H}_2\text{S}/\text{HCN}$ line intensity ratio among the galaxies in our sample and did not find any increase of the H_2S abundance (in relation to HCN) associated with the existence of outflows in the galaxies. On the other hand, when we compare H_2S , HCN, HCO^+ (as dense gas tracers) and CO (as a global molecular mass tracer), the line luminosity of the H_2S has a stronger correlation with

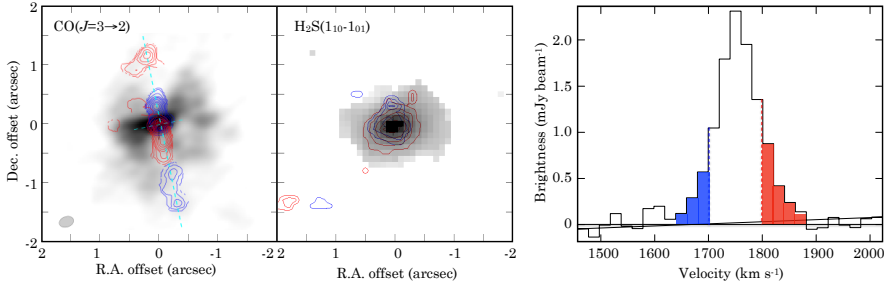


Figure 5.1: *left:* The image of the molecular jet of NGC 1377 in CO 3-2 at 0."25 resolution (Aalto et al. 2020). Red- and blue-shifted emissions are indicated with red- and blue-coloured contours, respectively. *middle:* Same as the left map but in H₂S 1₁₀-1₀₁ at 0."5 resolution (in prep), observed with ALMA. *right:* The H₂S spectrum from the central 1" of NGC 1377. The x axis is the systematic velocity in km s⁻¹.

the molecular mass of outflows than CO in the sample galaxies. We discuss that this indicates the direct relation of the H₂S molecule in outflows and the host galaxy reservoir. We also compared the $L(\text{H}_2\text{S})$ - $L(\text{IR})$ correlation to that previously found between higher excitation H₂O and IR (Yang et al. 2013), and found them to be similar.

5.2 Future work

High resolution

In order to further investigate the physical conditions, origin and fate of molecular gas in outflows, we have obtained high-resolution ($\sim 0."$ 5) ALMA H₂S data toward five galaxies with known molecular outflows, and with single dish H₂S detections (NGC 3256, NGC 1266, NGC 1377, IR17208-0014, and NGC 4418). Preliminary results show that one of them, NGC 1377, has compact H₂S emission with both red- and blue-shifted line wings (fig.5.1). We speculate that the nuclear H₂S emission traces the launch region of the collimated molecular outflow previously detected (e.g. Aalto et al. 2016, 2020). We expect to be able to distinguish different regions in the centre of the five galaxies with our new, high-resolution H₂S data.

Multi transition

To further study the physical conditions, such as number density n or kinetic temperature T_k , in the molecular gas in the galaxy centres and outflows, it is important to have lines of multiple transitions of H_2S , but also of other molecules such as HCN , HCO^+ , CN , HNC . We plan to fit several lines from several tracers to a non-LTE radiative transfer model to constrain key properties of the outflows from dusty, luminous galaxies.

Archival ALMA data have been found for all five target galaxies of which we have obtained ALMA H_2S data: at least one more H_2S transition for all five galaxies, HCN 1–0 and 3–2 for four galaxies. NGC 1377 has CO , ^{13}CO , C^{18}O at Band 6, and CO 6–5 at Band 9 archival data in addition to H_2S and HCN .

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