Can Molecular Ratios be used as Diagnostics of AGN and Starburst activity? The Case of NGC 1068.

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ABSTRACT

Context. Molecular line ratios, such as HCN(1-0)/HCO$^+$(1-0) and HCN(4-3)/CS(7-6) are routinely used to identify AGN activity in galaxies. Such ratios are however hard to interpret as they are highly dependent on the physics and energetics of the gas and hence can seldom be used as a unique unambiguous diagnostic

Aims. We use the composite galaxy NGC 1068 as a "laboratory", to investigate whether molecular line ratios between HCN, HCO$^+$ and CS are useful tracers of AGN-dominated gas and determine the origin of the differences in such ratios across different types of gas. Such determination will allow a more rigorous use of such ratios.

Methods. We first empirically examine the aforementioned ratios at different angular resolutions to quantify correlations. We then use LTE and non-LTE analyses coupled with Markov Chain Monte Carlo (MCMC) sampling in order to determine the origin of the underlying differences in ratios.

Results. We propose that at high spatial resolution (< 50 pc) the HCN(4-3)/CS(2-1) is a reliable tracer of AGN activity. Finally we find that the variations in ratios are not a consequence of different densities or temperature but of different fractional abundances yielding to the important result that it is essential to consider the what chemical processes are at play when drawing conclusions from radiative transfer calculations.

Conclusions. Upon analysis at varying spatial scales previous proposed as well as a new molecular line ratio have been shown to have varying levels of consistency. We have also determined from investigation of radiative transfer modelling of our data that it is essential to consider the chemistry of the species when reaching conclusions from radiative transfer calculations.

Key words. Interstellar medium (ISM): molecules, galaxies: active – Seyfert - starburst - ISM, astrochemistry.

1. Introduction

The gas and dust present in the interstellar medium (ISM) within galaxies is not homogeneous; star formation, supernovae events, as well as AGN activities may all greatly alter the ISM (e.g. Meijerink & Spaans 2005; Bayet et al. 2009; Watanabe et al. 2014). In particular, recent studies of nearby external galaxies have shown that the molecular ISM varies at a parsec, as well as, at kiloparsec scales, with evidence of different gas components traced by different molecular species or rotational transitions (Scourfield et al. 2020). The non-homogeneity of the ISM has been observed in galaxies of different types such as: Starbursts (Meier et al. 2015), AGN-Dominated (Audibert, A. et al. 2019) and ULIRG (Imanishi et al. 2018a) galaxies.

Molecular line ratio diagnostics are often used to investigate the physics and chemistry of the ISM in all of these environments. For example, as the gas chemistry located in the central/nuclear regions of galaxies is believed to be dominated by X-rays produced by the AGN, the molecular content of the ISM surrounding such nuclei will greatly differ from that in starburst regions (Usero et al. 2004; García-Burillo et al. 2010). Hence line ratios of specific molecules have been proposed as indicators of certain energetic or physical processes, for example HCN/HCO$^+$ as a tracer of AGNs (Loenen et al. 2007); HCN/HNC as a mechanical heating tracer (Hacar et al. 2020); HCN/CO as a density tracer (Leroy et al. 2017). In particular, the “submm-HCN diagram”, first proposed in (Izumi et al. 2013) and later expanded upon in (Izumi et al. 2016), is a very notable example of the use of molecular line ratios as a probe of AGN-galaxies; this diagram makes use of two line ratios, HCN(4-3)/HCO$^+$(4-3) and HCN(4-3)/CS(7-6), where all of the molecules involved are considered tracers of dense gas. Izumi et al. (2016) observed a clear trend that AGNs, including Seyfert composite galaxy NGC 1068, tend to show higher HCN/HCO$^+$ and/or HCN/CS than in SB galaxies as long as the observations were at high enough spatial resolutions to separate energetically discrete regions. Izumi et al. (2016) propose a scenario where it is the high temperature that is responsible for the HCN enhancement whereby neutral-neutral reactions with high reactions barriers are enhanced (Harada et al. 2010), thus leading to possible enhancement of HCN and depletion of HCO$^+$ via newly available formation and destruction paths, respectively. However, while of course higher gas temperatures are expected in AGN-dominated regions, these are not unique to these environments as starburst regions and/or regions where outflows dominate, can each harbour high enough temperatures for such enhancement to occur. Additionally, the higher temperatures could increase HCN excitation, relative to HCO$^+$ and CS, without necessarily changing their relative abundances (Imanishi et al. 2018a). Finally infrared radiative pumping is also a possible explanation of the HCN intensity enhancement relative to HCO$^+$.
and CS. Infrared pumping is a result of the emission of 14 μm infrared photons due to the presence of hot dust around AGNs. These photons vibrationally excite HCN to the ν2 = 1 state. Upon de-exciting from this state back to the vibrational ground state, ν = 0, the HCN line intensities are thus pumped to higher fluxes (Imanishi et al. 2018a). However we note that it is also not unlikely that the 12 μm infrared photons can similarly vibrationally excite HCO+, thus nullifying the extent of this effect (Imanishi et al. 2016).

In fact, while Miyamoto et al. (2017) observed a similar variation consistent with the submm-HCN diagram between the CND and Star-forming ring of the Seyfert 2 galaxy NGC 613, indicating that the enhancement of HCN may indeed be more prominent in AGN-dominated gas, some studies have observed HCN/HCO+ enhancements in starburst galaxies similar to those observed in AGNs (Harada et al. 2018; König et al. 2018). Furthermore, a statistical study by Privon et al. (2020) surveying a sample of 58 local luminous and ultraluminous infrared galaxies, concluded that an enhancement in the HCN/HCO+ (1-0) line ratio could not be shown to be correlated to the AGN activity. They also concluded that HCN/HCO+ ratios are not a dependable method to find AGN regions in galaxies. Finally, from a chemical point of view the HCN/HCO+ ratio has been shown to be highly dependent on numerous factors, such as density, temperatures and radiation fields and can not alone be used a a unique diagnostic of AGN-dominated galaxies (Viti 2017).

It is clear that for a meaningful analysis of molecular line ratios one first needs to answer the following questions: 1) Are there unique molecular ratios at a specific spatial resolution that trace distinct types of gas and energetics associated with AGN- and starburst dominated galaxies? 2) Do molecular ratios obtained at different spatial resolutions yield different trends?

In order to tackle these questions we perform a multi-scale investigation into the use of molecular line ratios as tracers particularly of AGN versus SB activity by using the galaxy NGC 1068 as a "laboratory". NGC 1068 is a Seyfert 2 barred spiral galaxy; it is also the archetypal composite AGN/SB galaxy. Its close proximity (~14 Mpc) and significant brightness (LBol ≈ 2.5 – 3.0 × 10^11 L_☉ (Bland-Hawthorn et al. 1999; Bock et al. 2000)) allow studies at many different resolutions, down to parsec scales, with 1″ corresponding to ~70pc for reference (Garcia-Burillo et al. 2014, 2016, 2019; Viti et al. 2014; Gallimore et al. 2016; Imanishi et al. 2018b; Impellizzeri et al. 2019; Imanishi et al. 2020). In Section 2 we provide a summary of the data collated for this study. Section 3 presents an analysis of various molecular ratios at both high and low spatial resolution. In Section 4 we perform an LTE and non-LTE analysis of the line intensities used for the ratios in Section 3 in order to determine whether such analysis is consistent with the trends implied by the ratios. We summarize our findings in Section 5.

2. Data

Despite the plethora of available published data focused on NGC 1068, within this study we focus on the dense gas tracers: HCN, HCO+ and CS. This focus is in an effort to validate previously proposed ratios and diagrams rather than suggest new ones. We therefore searched published data for observations of these molecules in NGC 1068 and a summary of all of the data utilized within this study is provided in Table 1. Observations from multiple instruments have been used including interferometric observations from ALMA and PdBI and single dish observations from the 15m diameter James Clerk Maxwell Telescope (JCMT).

To supplement these data, we also re-analysed previously published data (Sánchez-García et al. 2022) of HCN (1-0) and HCO+ (1-0) emission observations. Both lines were observed with the ALMA's Band 3 receiver during cycle 2 (project-ID: 2013.1.00055.S; PI: S. García-Burillo).

The phase tracking centre was set to α2000 = 02h42m40.771s, δ2000 = −00°00’47.94” (J2000 reference system, as used throughout the paper) in each case, the position of the galaxy’s centre in the SIMBAD Astronomical Database, from the Two-Micron All-Sky Survey (2MASS) survey Skrutskie et al. (2006). This is offset relative to the galaxy AGN at α2000 = 02h42m40.710s, δ2000 = −00°00’47.94” by < 1″, and corresponds to a peak in CO emission (García-Burillo et al. 2014). Initial reduction of the data was carried out using the ALMA reduction package CASA (McMullin et al. 2007), and then exported to PYTHON for plotting, making use of the matplotlib and Astropy. The 1σ threshold was determined in CASA by calculating the rms of the signal over an area towards the centre of the galaxy in a channel with no line detection. The angular resolution obtained using uniform weighting was ~0.7° × 0.5° at a position angle of ~56° in the data cube. The conversion factor between Jy beam$^{-1}$ and K is 32 K Jy$^{-1}$ beam.

2.1. Moment 0 maps

Figures 1 and 2 show the velocity integrated maps at the original spatial resolution for HCO+(1-0) and HCN(1-0), respectively. As can be seen in these two Figures, HCN(1-0) is observed to be significantly more prominent in the CND regions, than the equivalent HCO+(1-0) emission.

The structure of the CND ring as observed in previous observations (García-Burillo et al. 2014, 2019) at similarly high resolution in CO, CS, and higher J-transitions of HCN and HCO+ is observed in these intensity maps, with the East and West knots showing particularly prominent emission in these lines. The two knots are connected by ’bridges’ of emission, within which the CND-N and CND-S regions are located. Emission in these ’bridges’ is seen to be significantly more prominent in HCN(1-0) rather than HCO+(1-0).

Within the SB ring regions however, HCO+ is observed to be most prominent, the notable exception being NSB-c at which significant HCN emission is seen to dominate over the respective HCO+ emission; the implications of this will be further elaborated upon in the following section.

As both lines were taken from the same data set at the same resolution their respective rms are equivalent at σ = 16 K km s$^{-1}$ at this resolution.

Moment 0 maps for the remaining high resolution data can be found in the following papers: the CS(2-1) moment 0 map in Figure A1 of Scourfield et al. (2020); CS(7-6) in Figure A3 of Scourfield et al. (2020); HCO+(4-3) in Figure 8 of García-Burillo et al. (2014); a zoomed-in moment 0 map of HCN(4-3) is presented in Figure 8 of García-Burillo et al. (2014), with a zoomed-out equivalent also available in the appendix of this paper, in Section B.1 with an accompanying HCO+(4-3) plot in Section B.2.

2.2. Comparison between observations

The range of transitions from multiple studies will allow us to approach the analysis of NGC 1068 from both a large scale view, using the low spatial resolution detections of single dish instruments, and a more zoomed-in one provided to us via inter-
ferometric instruments. The different spatial resolutions make it necessary to ensure that only similarly obtained detections are compared. This is especially true for the higher resolution observations which cover only a small area of the galaxy. For those observations, the variance over even small distances can be large. An example of such small scale variation in emission can be seen in the CND in Fig 1.

We therefore grouped our data in two ways. Firstly, the archival data were grouped by spatial resolution. Within these groupings, there are variations of resolution of up to a factor of two. Therefore, we deconvolve the intensities by assuming the observation with the lowest resolution is the source size and using the equation,

\[
I_{\text{Source}} = \frac{\left( \theta_s^2 + \theta_b^2 \right)}{\theta_b^2} I_{\text{Beam}}
\]

where \(I_{\text{Source}}\) is the source averaged peak intensity, \(\theta_s\) is the source size (as defined by the lowest resolution observation in the category), \(\theta_b\) is the beam size and \(I_{\text{Beam}}\) is the original intensity as defined in the archive/paper. This is similar to the approach taken in Kamenetzky et al. (2011); Aladro et al. (2013, 2015) in order to account for the effect of beam dilution.

The high resolution data was then further separated by the sub-region on which they were focused. For the low resolution data, this was not a concern as each observation contained many sub-regions. We list each sub-region in Table 2. The regions in the CND and SB ring observed within this report are consistent with those observed in Scourfield et al. (2020), with the exception of the region known as NSB-b, as none of the ratios investigated within this report have been observed at a consistent resolution for this region. We note that not all sub-regions listed in Table 2 and shown in Figures 1 and 2 have been observed at all resolutions for all molecules. As a result, some ratios in some regions are missing at certain resolutions, see Figure 3. The region NSB-c possesses fewer observed ratios than the other regions, with just a single high resolution observation, see Table 3. As a result it is not included in the RADEX fitting discussed later in this paper.

### 3. Molecular line ratios

In this section, we take an in depth look at these ratios across the resolution and sub-region groupings in order to determine which relationships stand up to scrutiny.

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**Table 1: Studies**

| Transition   | Spatial resolution | Average spatial resolution (pc) | Instrument   | Study |
|--------------|--------------------|---------------------------------|--------------|-------|
| HCN(1-0)     | 0.7" × 0.5" (49 pc × 35 pc) | 42 ALMA Band 3 | 1             |
| HCN(1-0)     | 2" × 0.8" (140 pc × 56 pc)  | 98 PdBI               | 2             |
| HCN(4-3)     | 0.6" × 0.5" (42 pc × 35 pc) | 39 ALMA Band 7 | 3,4           |
| HCN(4-3)     | 14"                | 980 JCMT 15m | 5             |
| HCN(4-3)     | 14"                | 980 JCMT 15m | 6             |
| HCO+ (1-0)   | 0.7" × 0.5" (49 pc × 35 pc) | 42 ALMA Band 3 | 1             |
| HCO+ (1-0)   | 2" × 0.8" (140 pc × 56 pc)  | 98 PdBI               | 2             |
| HCO+ (4-3)   | 0.6" × 0.5" (42 pc × 35 pc) | 39 ALMA Band 7 | 3,4           |
| HCO+ (4-3)   | 14"                | 980 JCMT 15m | 5             |
| HCO+ (4-3)   | 14"                | 980 JCMT 15m | 6             |
| CS (2-1)     | 0.75" × 0.51" (~ 53 pc × ~ 36 pc) | ~ 44 ALMA Band 3 | 7             |
| CS (2-1)     | 4.2" × 2.4" (294 pc × 168 pc) | 231 ALMA Band 3 | 8             |
| CS (2-1)     | 6.6" × 3.2" (464 pc × 224 pc) | 343 ALMA Band 3 | 9             |
| CS (7-6)     | 0.6" × 0.5" (42 pc × 35 pc)  | 39 ALMA Band 7 | 3,4,7         |
| CS (7-6)     | 4.2" × 2.4" (294 pc × 168 pc) | 231 ALMA Band 7 | 10            |
| CS (7-6)     | 14"                | 980 JCMT 15m | 11            |

Table 1: Studies, 1 - This study/(Sánchez-García et al. 2022), 2 - García-Burillo et al. (2008), 3 - García-Burillo et al. (2014), 4 - Viti et al. (2014), 5 - Pérez-Beaupuits et al. (2009), 6 - Tan et al. (2018), 7 - Scourfield et al. (2020), 8 - Takano et al. (2014), 9 - Tacconi et al. (1997), 10 - Nakajima et al. (2015), 11 - Bayet et al. (2009).
HCN and HCO$^+$ are both dense gas tracers, with HCN(1-0) and HCO$^+$(1-0) having critical densities of $\sim 10^5$ cm$^{-3}$ and $\sim 5 \times 10^4$ cm$^{-3}$ (at $\sim 10$ K, Shirley (2015)), respectively.

The HCN(1-0)/HCO$^+$(1-0) and HCN(4-3)/HCO$^+$(4-3) ratios have both been proposed as tracers of AGN activity (Kohno 2005; Izumi et al. 2013). Therefore, in this section, we discuss each ratio in turn with a particular focus on how well the ratio separates AGN regions from starburst regions. All the ratios for NGC 1068 are presented in Figures 4 and 3.

3.1. HCN/HCO$^+$

An enhancement of HCN(1-0) relative to HCO$^+$(1-0) or CO(1-0) has been proposed as an indicator of AGN activity (Imanishi et al. 2007; Krips et al. 2008; Davies et al. 2012). In fact, Kohno et al. (2001) proposed the HCN diagram; a diagnostic diagram to identify AGN galaxies using this line ratio and the ratio of HCN(1-0)/CO(1-0). However, as detailed in the Introduction, some studies find high HCN(1-0)/HCO$^+$(1-0) ratios in SB galaxies (Costagliola et al. 2011) and low values of this ratio in AGNs (Sani et al. 2012) which casts doubt on the use of this ratio to trace AGN activity. In the high resolution archival
Table 2: Names and coordinates of the sub-regions of interest across the CND and SB Ring.

| Sub-Region name | RA       | Declination |
|-----------------|----------|-------------|
| E Knot          | 02°42'40''.771 | -00°00'47''.84 |
| W Knot          | 02°42'40''.630 | -00°00'47''.84 |
| AGN             | 02°42'40''.710 | -00°00'47''.94 |
| CND-N           | 02°42'40''.710 | -00°00'47''.09 |
| CND-S           | 02°42'40''.710 | -00°00'49''.87 |
| NSB-a           | 02°42'40''.840 | -00°00'33''.00 |
| NSB-c           | 02°42'39''.820 | -00°00'39''.26 |
| SSB-a           | 02°42'40''.317 | -00°01'01''.84 |
| SSB-b           | 02°42'39''.820 | -00°00'52''.79 |
| SSB-c           | 02°42'39''.870 | -00°00'55''.32 |

Similar to the enhancement of HCN relative to HCO+ observed in their respective J=1-0 transitions, Izumi et al. (2013) found a similar trend for the J=4-3 transitions. This ratio has advantages over the J=1-0 ratio as higher resolution imaging is more easily achievable, it can be observed to higher distances (up to z ∼ 3 with ALMA) and the transitions have higher critical densities resulting in lower contamination by foreground or other extended emission (Izumi et al. 2016). HCN(4-3) and HCO+(4-3) possess high and similar critical densities of $n_{\text{crit}}$, HCN(4-3) ≈ 8.5 × 10^6 cm^{-3} and $n_{\text{crit}}$, HCO+(4-3) ≈ 10^6 cm^{-3} (at ~ 10 K, Shirley (2015)), which means that they are more likely to trace the same component of the dense gas in any observed region.

Figure 3 seems to imply that this ratio does separate AGN and non-AGN regions in our high resolution data. Moreover, once low resolution data is included, the ratio continues to distinguish between regions (Figure 4) albeit with a smaller gap between the two types of region. It must be noted, however, that for region NSB-c both HCN(4-3) and HCO+(4-3) emission is below the 3 σ threshold necessary to derive a reliable intensity ratio, hence we cannot be sure whether in NSB-c this ratio follows the same trend as the HCN(1-0)/HCO+(1-0).
Table 3: The values and uncertainties of the ratio values for the respective ratios displayed in Figures 3, 4 and 5 with the corresponding sub-regions given for each ratio value. Data used in Figure 5 added for clarity.

| Ratios | Ratios error | Location   |
|--------|--------------|------------|
| High resolution (≈ 40 pc) HCN(1-0)/HCO\(^+\)(1-0) |
| 1.01   | 0.14         | AGN        |
| 1.9    | 0.27         | CND-N      |
| 3.64   | 0.51         | CND-S      |
| 2.01   | 0.28         | E Knot     |
| 0.62   | 0.09         | NSB-a      |
| 3.09   | 0.44         | NSB-c      |
| 0.44   | 0.06         | SSB-a      |
| 0.74   | 0.11         | SSB-b      |
| 0.91   | 0.13         | SSB-c      |
| 2.19   | 0.31         | W Knot     |
| High resolution (≈ 40 pc) HCN(4-3)/CS(2-1) |
| 5.83   | 1.86         | CND-N      |
| 5.02   | 3.04         | CND-S      |
| 3.14   | 0.31         | E Knot     |
| 0.5    | 0.07         | NSB-a      |
| 0.55   | 0.09         | SSB-a      |
| 0.47   | 0.08         | SSB-b      |
| 0.69   | 0.15         | SSB-c      |
| 3.61   | 0.56         | W Knot     |
| Low resolution (≥ 100 pc) HCN(4-3)/CS(7-6) |
| 5.39   | 0.97         | SSB-a      |

Table 3: Continued.

| Ratios | Ratios error | Location   |
|--------|--------------|------------|
| High resolution (≈ 40 pc) HCN(4-3)/CS(7-6) |
| 11.02  | 1.81         | AGN        |
| 20.3   | 4.51         | CND-N      |
| 7.82   | 0.93         | E Knot     |
| 1.27   | 0.18         | NSB-a      |
| 4.44   | 1.96         | SSB-a      |
| 3.6    | 1.83         | SSB-b      |
| 7.12   | 3.63         | SSB-c      |
| 11.04  | 1.46         | W Knot     |
| Low resolution (≥ 100 pc) HCN(4-3)/CS(7-6) |
| 20.92  | 4.44         | AGN        |
| 17.09  | 3.62         | CND-N      |
| 10.97  | 2.33         | CND-S      |
| 77.41  | 16.42        | E Knot     |
| 44.64  | 9.47         | W Knot     |
| 9.93   | 3.73         | AGN (≈ 1000 pc scale) |

3.2. HCN/CS

CS is also a commonly used dense gas tracer; CS(1-0) has a critical density of \(n_{\text{crit}} \approx 10^4\text{ cm}^{-3}\) (Shirley 2015). In Izumi et al. (2013) they present the use of CS as opposed to HCO\(^+\) as the molecule with which the HCN enhancement should be measured because earlier studies had shown that the CS abundance varies little between active regions (e.g. near the AGN in the CND) and those in SB regions (Martín et al. 2008, 2009). For these reasons, the HCN/CS ratio has been proposed as a possible starburst/AGN tracer. Under XDR conditions, the CS abundance should be unchanged but the HCN abundance is enhanced, leading to an enhancement in the ratio (Krieger et al. 2020).

3.2.1. HCN(4-3)/CS(7-6)

Izumi et al. (2013) states that the intensity ratio between HCN(J=4-3) to CS (J=7-6) was found to be high in AGN galaxies (> 12.7). HCN(4-3) has an excitation temperature of 42.53K, and a critical density of \(\approx 10^7\text{ cm}^{-3}\). CS(7-6) has an excitation temperature of 65.8K, and a critical density of \(\approx 10^6\text{ cm}^{-3}\) (at \(\approx 10\text{ K}\), Shirley (2015)). Audibert et al. (2020) observed results consistent with those proposed by the Izumi papers, in NGC 1808. Despite this, we find that even at high spatial resolution, this ratio does not clearly distinguish the CND from the SB regions. Considering the uncertainty in the ratios we calculated, there is significant overlap between the ratio values at positions in each region. Thus, one would not be able to reliably separate an unusually large SB ratio due to random error from a large ratio due to the CND enhancement.

One possible reason for the failure of this ratio given its previous success is that Izumi et al. (2013); Izumi et al. (2016) used lower resolution observations than those used here. Hence they may be tracing more extended regions. We indeed also typically find that the highest values for this ratio are obtained from the lower resolution observations in our data. This point is shown quite clearly in Figure 5, which is a recreation of the submm-HCN Diagram from Izumi et al. (2016) of the HCN(4-3)/HCO\(^+\)(4-3) and the HCN(4-3)/CS(7-6) ratios.

3.2.2. HCN(4-3)/CS(2-1)

We further investigated the HCN(4-3)/CS(2-1) ratio. For NSB-c, as before, we do not have a strong enough detection for HCN(4-3), as such we can not derive this ratio for this region. Taking a
Table 3: Continued.

| Ratios | Ratios error | Location |
|--------|--------------|----------|
| High resolution (≈40 pc) HCN(4-3)/HCO+(4-3) | | |
| 1.49 | 0.19 | AGN |
| 2.34 | 0.3 | CND-N |
| 8.19 | 1.01 | CND-S |
| 2.54 | 0.33 | E Knot |
| 0.48 | 0.07 | NSB-a |
| 0.74 | 0.11 | SSB-a |
| 0.81 | 0.11 | SSB-b |
| 0.67 | 0.09 | SSB-c |
| 2.91 | 0.37 | W Knot |
| Low resolution (≥100 pc) HCN(4-3)/HCO+(4-3) | | |
| 2.11 | 0.45 | AGN |
| 2.24 | 0.47 | CND-N |
| 2.73 | 0.58 | CND-S |
| 2.55 | 0.54 | E Knot |
| 1.0 | 0.21 | SSB-a |
| 2.84 | 0.6 | W Knot |
| 3.66 | 0.64 | AGN (~1000 pc scale) |

Fig. 5: A recreation of the submm-HCN Diagram from Izumi et al. (2016) using various resolution data across various sub-regions in NGC 1068. The shape of each marker denotes the region it corresponds to and the colour denotes the resolution. 3σ upper limit for the HCN(4-3) in this sub-region, we obtain an upper limit for the HCN(4-3)/CS(2-1) ratio of ~ 1.4 which is significantly lower than the those observed in the CND regions. Considering all the remaining regions, we find at high spatial resolution, a clear distinction can be made between the CND and SB regions as shown in Figure 3.

This is not surprising if we consider the difference in the lines. The HCN (4-3) transition has an upper state energy of 43 K and a critical density of ~ 8.5 x 10^6 cm^{-3} whilst the CS (2-1) transition has an upper state energy of 7 K and critical density of 8 x 10^5 cm^{-3}. Since the two transitions are likely to be excited under very different gas conditions, this ratio should be able to discriminate between SB and CND regions.

However, Fig. 4 shows that once lower resolution observations are included, this ratio becomes less reliable. In particular, including low resolution data adds a SB observation that is the second highest observation of this ratio.

4. Physical and chemical properties of NGC 1068

We have found that the ratio between HCN (4-3) and HCO^+(4-3) clearly separates SB and AGN regions in our data. We also found that the ratio between HCN (4-3) and CS (2-1) is reliable at high resolution. However, these are observed correlations with as yet undetermined underlying physical or chemical cause. In this section, we attempt to find that cause so that these ratios can be more robustly used to probe AGN regions.

To achieve this, we use radiative transfer modelling to infer the gas conditions and molecular column densities at each location for each resolution. We can then determine whether there are physical differences in excitation conditions between locations, differences in the underlying chemical abundances, or even a combination of the two as a result of shocks, X-ray or Cosmic Ray processing. If it is the former, these ratios may only distinguish between regions insofar as the gas temperature and density are typically different. If it is the latter, more detailed chemical modelling is required to determine the cause of the chemical distinction.

4.1. LTE analysis

Using the observed line intensities from the archival data, we were able to estimate the column densities by assuming LTE and by using the same groupings of observations as discussed earlier, devolved to the lowest resolution of that group. The upper state column density of a molecular transition can be approximated to

\[ N_u = \frac{8\pi k T}{h c^2 A_{ul}} \left( \frac{\Delta \Omega_s}{\Omega_s} \right) \frac{1}{1 - e^{-\tau}} \]  

where \( W \) is the integrated line intensity, \( A_{ul} \) is the Einstein A-coefficient, and \( \tau \) is the optical depth which we include as a correction factor for saturated lines. \( \Omega_s \) and \( \Delta \Omega_s \) are the solid angles of the antenna and the source, respectively, and together give the beam filling factor. Since we are investigating the regions themselves, we make the assumption that the source completely fills the beam, such that \( \frac{\Delta \Omega_s}{\Omega_s} = 1 \).

We can then use these transition column densities to approximate the total column density of the emitting molecule, \( N \), by using

\[ N = \frac{N_u Z(T)}{g_u e^{E_u/kT}} \]  

where \( Z(T) \) is the partition function, \( g_u \) is the statistical weight of level \( u \), and \( E_u \) is the excitation energy of level \( u \). To compute the partition function we make use of molecular data from The Cologne Database for Molecular Spectroscopy (CDMS) (Endres et al. 2016). We combine Eq. 2 and 3 to produce an estimate of the column density for each molecule. We use temperatures...
in order to compare goodness of fit. Where $R_o$ and $R_m$ are the observed and modelled ratios respectively and $\sigma$ is the uncertainty in the observed ratio propagated from the uncertainty in the individual intensities. Assuming a uniform prior, sampling this distribution gives the posterior probability distribution of the parameters.

Our MCMC sampler uses 12 walkers each performing 100000 steps to sample possible parameter combinations. We do this for all combinations of regions and resolutions with at least 2 of the investigated ratios. The joint posterior distributions of temperature and density is shown in Figure A.1 for each of the available regions at the highest resolution (~40 pc scale). Table 5 summarises the parameters of the MCMC fitting of the RADEX models over the entire parameter space for 9 of the 10 regions studied in Scoufield et al. (2020), with NSB-c being excluded due to a lack of observed ratios, as stated in Section 2.2. Neither the CND nor the SB ring regions can be reasonably constrained in the temperature or density planes, at least with regards to showing distinguishing qualities within these parameters. The only two regions in the CND where strong constraints on the gas density can be drawn are the E and W knots regions (5.3$^{+0.2}_{-0.3}$ and 5.1$^{+0.35}_{-0.23}$ respectively). Similarly the SB ring region, NSB-a, has a relatively highly constrained density of 5.0$^{+0.02}_{-0.17}$.

The impact of resolution when it comes to the determination of temperature, density and linewidth with regards to each region is negligible as a result of the fact that these parameters are not reasonably constrained at any resolution. Though it must be noted that the density becomes extensively less constrained for all regions as the resolution is diminished; this can be seen in Figure A.2. Despite the lack of strong constraints, it is clear from this that the best fit gas densities and temperatures are generally quite similar between the CND and SB. This is strongly suggesting that we cannot link the difference in ratios between SB and CND regions to either of these quantities. While the results for the temperature are relatively unconstrained, it is notable that the median values (at high resolution) for the SB region appear to be higher than those located in the CND, particularly those in the CND-N and CND-S. However, while typically the CND regions, by virtue of being located closer to the AGN, would be expected to have higher temperatures, it is possible to imagine a scenario of high starburst activity that could lead to average temperatures on the order of ~300K (typical of galactic hot cores, e.g. Kaufman et al. (1998)). On the other hand, we also note that there is significant uncertainty in these obtained temperature values.

Figures A.3 to A.5 display the 1 sigma ranges of the posterior distributions for the column densities of HCN, HCO$^+$ and CS as a result of the ~40 pc and ~100 pc data. While there is some general trends towards lower (for HCN) or higher (for HCO$^+$ and CS) column densities in the SB ring regions with respect to the CND regions, especially at ~40 pc scale, there is a significant overlap between the regions.

To account for the fact that the total H$_2$ column density varies across individual regions, and hence may be obscuring an underlying HCN enhancement, we compute the posterior probability distributions of the ratios of the column densities. We do this by taking the ratio of the chains of column density samples for each region and resolution. The resulting 16th and 84th percentile limits of the 3 ratio distributions are shown in Figure A.6. What we observe at our highest resolution is that the best fitting RADEX models typically have higher abundances of HCN relative to both HCO$^+$ and CS within the AGN-dominated CND regions when compared to the best fitting models of the SB-dominated SB ring regions. This distinction is maintained somewhat in the lower resolution (~100 pc scale) data for HCN relative to HCO$^+$.

### Table 4: Lower and upper limits of column density calculated for each molecule assuming LTE.

| Molecule | $N_{\text{min}}$ (cm$^{-2}$) | $N_{\text{max}}$ (cm$^{-2}$) |
|----------|-------------------------------|-------------------------------|
| CS       | 3.34E+12                      | 2.44E+16                     |
| HCO+     | 1.73E+11                      | 3.43E+16                     |
| HCN      | 2.62E+13                      | 7.38E+17                     |

The gas density and kinetic temperature ranges on previous studies of NGC 1068 (Viti et al. 2014; Izumi et al. 2016) while the column density ranges are taken from the LTE analysis in Sect. 4.1. In addition to these parameters, we try three line widths that cover range of typical line widths observed in the SB regions (50 km s$^{-1}$) and the CND regions (150 km s$^{-1}$) (Scoufield et al. 2020).

We use the resulting line intensities to compute the ratios which we have explored in this paper, namely: HCN(1-0)/HCO$^+$(1-0), HCN(4-3)/HCO$^+$(4-3), HCN(4-3)/CS(7-6), and HCN(4-3)/CS(2-1). We then fit these modelled ratios to their observed values by Markov Chain Monte Carlo (MCMC) sampling the $\chi^2$ distribution of the parameters. For all parameter combinations, we compute the $\chi^2$ statistic,

$$\chi^2 = \sum_{i=1}^{4} \frac{(R_o - R_m)}{\sigma^2}$$  \hspace{1cm} (4)

1. https://spectralradex.readthedocs.io

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but is not for HCN with respect to CS. The abundances of CS and HCO\(^+\) appear to cover relative similar ranges regardless of the region observed.

It is therefore the underlying ratio of the HCN/HCO\(^+\) and the HCN/CS abundances that determine the processes characteristics of an AGN versus a starburst: hence line ratios are only useful in so far as they probe the column density differences and therefore multi-line multi-species observations coupled with chemical modelling will always be a more powerful, if not essential, method to discriminate and characterize different types of galaxies, while minimizing degeneracy in radiative transfer modelling.

5. Summary and conclusion

By taking NGC 1068 as a "laboratory", we have investigated whether molecular line ratios are useful tracers of AGN-dominated gas. More importantly we determined the origin of the differences in such ratios across different types of gas. Our main conclusions are the following:

- For the ratios HCN(1-0)/HCO\(^+\)(1-0) and HCN(4-3)/CS(7-6) ratios we observe an overlap in the observed ranges of these ratios between AGN-dominated and SB-dominated regions. For HCN(4-3)/CS(7-6) specifically, we observe that the range of values observed in each of the two types of regions overlapped significantly even at the highest spatial resolution.

- The HCN(1-0)/HCO\(^+\)(1-0) ratio first proposed in Kohno (2005) and then put into question by Privon et al. (2020) does appear to show an enhancement in the CND with respect to the SB ring regions for the majority of sub-regions; however we found an "outlier" in at least one SB region. (NSB-c).

- HCN(4-3)/HCO\(^+\)(4-3) on the other hand seems to be distinctively higher in all the regions closer to the AGN position, at least at higher spatial resolution. This distinction is even maintained when the ratio is viewed at lower resolutions scales, though the separation does decrease. Note, however, that for NSB-c the HCN(4-3) and HCO\(^+\)(4-3) lines are too weak and hence we can not confirm whether this ratio in this region conforms to the trend stated above.

- When observed at high spatial resolution, we propose a new ratio as a reliable tracer of AGN activity: the HCN(4-3)/CS(2-1).

- We investigate the origin of the differences in ratios and found that differences in gas densities and temperatures are not the cause of the differentiation. Upon computing the relative fractional abundances of HCN, HCO\(^+\) and CS we in fact determine that these differences are a consequence of differences in chemical abundances and hence it is essential to consider the chemistry of the species (i.e. what chemical processes lead to such abundances) when drawing conclusions from radiative transfer calculations (Viti 2017).

- As also noted in García-Burillo et al. (2014) and Viti et al. (2014) the elevated HCN(1-0)/HCO\(^+\)(1-0) and HCN(4-3)/HCO\(^+\)(4-3) ratios observed throughout the CND can be attributed to the molecular outflow observed in this region. As such the contribution of mechanical heating and possible shock chemistry in CND could be possible contributors to the observed HCN enhancement (Kelly et al. 2017; Huang et al. 2022).
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References

Aladro, R., Martin, S., Riquelme, D., et al. 2015, A&A, 579, A101
Aladro, V., Viti, S., Bayet, E., et al. 2013, A&A, 549, A39
Audibert, A., Combes, F., García-Burillo, S.-a., et al. 2020, arXiv e-prints, arXiv:2011.09133
Audibert, A., Combes, F., García-Burillo, S., et al. 2019, A&A, 632, A33
Bayet, E., Viti, S., Williams, D. A., Rawlings, J. M. C., & Bell, T. 2009, The Astrophysical Journal, 696, 1466
Blum, H.-A., Haworth, J., Gallimore, J. F., Tacconi, L., J., et al. 1997, Astrophysics and Space Science, 248, 9
Bock, J. J., Neugebauer, G., Matthews, K., et al. 2000, The Astronomical Journal, 120, 2904
Costagliola, Aalto, S., Rodríguez, M. J., et al. 2011, A&A, 528, A30
Davies, Mark, D., & Sternberg, A. 2012, A&A, 537, A133
Endres, C. P., Schlemmer, S., Schilke, P., Stutzki, J., & Müller, H. S. 2016, Journal of Molecular Spectroscopy, 327, 95, new Visions of Spectroscopic Databases, Volume II
Gallimore, J. F., Elitzur, M., Maiolino, R., et al. 2016, ApJ, 829, L7
García-Burillo, S., Usero, A., Fuente, A., et al., 2010, A&A, 519, A2
García-Burillo, S., Combes, F., Graciá-Carpio, J., Usero, A., & Guélin, M. 2008, Ap&SS, 313, 261
García-Burillo, S., Combes, F., Ramos Almeida, C., et al. 2019, A&A, 632, A61
Harada, N., Herbst, E., & Wakelam, V. 2010, The Astrophysical Journal, 721, 1570
Harada, N., Sakamoto, K., Martin, S., et al. 2018, The Astrophysical Journal, 855, 49
Huang, K. Y., Viti, S., Holdship, J., et al. 2022, arXiv e-prints, arXiv:2202.05005
Imanishi, M., Nakajima, T., & Izumi, T. 2016, AJ, 152, 218
Imanishi, M., Nakajima, T., & Izumi, T. 2018a, ApJ, 856, 143
Imanishi, M., Nakajima, T., Izumi, T., & Wada, K. 2018b, ApJ, 853, L25
Imanishi, M., Nakajima, K., Tamura, Y., Oi, N., & Kohno, K. 2007, The Astronomical Journal, 134, 2366
Ishii, M., Nguyen, D. D., Wada, K., et al. 2020, ApJ, 902, 99
Izumi, T., Kohno, K., Aalto, S., et al. 2016, ApJ, 818, 42
Izumi, T., Kohno, K., Martin, S., et al. 2013, Publications of the Astronomical Society of Japan, 65, 100
Kamenetzky, J., Glenn, J., Maloney, P. R., et al. 2011, 731, 83
Kaufman, M. J., Hollenbach, D. J., & Tielens, A. G. G. M. 1998, ApJ, 497, 276
Kelly, G., Viti, S., García-Burillo, S., et al. 2017, A&A, 597, A11
Kohno, K. 2005, in American Institute of Physics Conference Series, Vol. 783, The Evolution of Starbursts, ed. S. Hüttemeister, E. Meijerink, M. Roman-Duval, & K. Weis, 203–208
Kohno, K., Matsushita, S., Vila-Vilaró, B., et al. 2001, in Astronomical Society of the Pacific Conference Series, Vol. 249, The Central Kiloparsec of Starbursts and AGN: The La Palma Connection, ed. J. H. Knapp, J. E. Beckman, I. Shlosman, & T. J. Mahoney, 672
König, Aalto, S., Muller, S., et al. 2018, A&A, 615, A122
Krieger, N., Bolatto, A. D., Leroy, A. K., et al. 2020, ApJ, 897, 176
Krips, M., Neri, R., García-Burillo, S., et al. 2008, The Astrophysical Journal, 677, 262
Lefloch, B., Busquet, G., Viti, S., et al. 2021, MNRAS, 507, 1034
Leroy, A. K., Usero, A., Schruba, A., et al. 2017, ApJ, 835, 217
Loenen, A. F., Baan, W. A., & Spaans, M. 2007, in Astrophysical Masers and their Environments, ed. J. M. Chapman & W. A. Baan, Vol. 242, 462–466
Liu, Z., Martin-Pintado, J., & Mauersberger, R. 2009, ApJ, 694, 610
Martin, S., Requena-Torres, M. A., Martin-Pintado, J., & Mauersberger, R. 2008, ApJ, 678, 245
McMullin, J. P., Waters, B., Schiebel, D., Young, W., & Golap, K. 2007, in Astronomical Society of the Pacific Conference Series, Vol. 376, Astronomical Data Analysis Software and Systems XVI, ed. R. A. Shaw, F. Hill, & D. J. Bell, 127
Meier, D. S., Walter, F., Bolatto, A. D., et al. 2013, The Astrophysical Journal, 801, 63
Meyerink & Spaans. 2005, A&A, 436, 397
Miyamoto, Y., Nakai, N., Seta, M., et al. 2017, Publications of the Astronomical Society of Japan, 69, 83
Nakajima, T., Takano, S., Kohno, K., et al. 2015, Publications of the Astronomical Society of Japan, 67, 8
Pérez-Beaupuits, J. P., Spaans, M., van der Tak, F. F. S., et al. 2009, A&A, 503, 459
Privon, G. C., Ricci, C., Aalto, S., et al. 2020, ApJ, 893, 149
Sánchez-García, M., García-Burillo, S., Pereira-Santaella, M., et al. 2022, A&A, 660, A83
Sani, E., Davies, R. I., Sternberg, A., et al. 2012, Monthly Notices of the Royal Astronomical Society, 424, 1963
Schöier, F. L., van der Tak, F. F. S., van Dishoeck, E. F., & Black, J. H. 2005, A&A, 432, 369
Scourfield, M., Viti, S., García-Burillo, S., et al. 2020, Monthly Notices of the Royal Astronomical Society, 496, 5308
Shirley, Y. L. 2015, 127, 299
Skrutskie, M. F., Cutri, R. M., Stiening, R., et al. 2006, AJ, 131, 1163
Sobolev, V. I. 1960, Moving envelopes of stars
Tacconi, L. J., Gallimore, J. F., Genzel, R., Schinnerer, E., & Downes, D. 1997, Ap&SS, 248, 59
Takano, S., Nakajima, T., Kohno, K., et al. 2014, Publications of the Astronomical Society of Japan, 66, 75
Tan, Q.-H., Gao, Y., Zhang, Z.-Y., et al. 2018, ApJ, 860, 165
Usero, García-Burillo, S., Fuente, A., Martín-Pintado, J., & Rodríguez-Fernández, N. J. 2004, A&A, 419, 897
van der Tak, F. F. S., Black, J. H., Schöier, F. L., Jansen, D. J., & van Dishoeck, E. F. 2007, A&A, 468, 627
Viti, S. 2017, A&A, 607, A118
Viti, S., García-Burillo, S., Fuente, A., et al. 2014, Astronomy & Astrophysics
Watanabe, Y., Sakai, N., Sorai, K., & Yamamoto, S. 2014, ApJ, 788, 4

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Appendix A: Additional figures

Fig. A.1: The resulting joint posterior distributions for temperature and density as produced for the high resolution (∼ 40 pc scale data) for the 9 regions which have enough ratios to fit. The temperature and density values shown in Table 5 are from distributions visualised in this plot. It must be noted that the median values of these distributions, as shown in Table 5, do not always correspond to the most densely populated areas of the corresponding plot. This is due to the extent of the posterior distribution in the temperature plane.
Fig. A.2: The resulting joint posterior distributions for temperature and density as produced for the lower resolution (\(\sim 100\) pc scale data) for the 6 regions which have enough ratios to fit, at this lower resolution.
Fig. A.3: The 16th to 84th percentile range of the MCMC chain for the column density of HCN as found from fitting the observed ratios to those produced by RADEX models.

Fig. A.4: The 16th to 84th percentile range of the MCMC chain for the column density of HCO$^+$ as found from fitting the observed ratios to those produced by RADEX models.
Fig. A.5: The 16th to 84th percentile range of the MCMC chain for the column density of CS as found from fitting the observed ratios to those produced by RADEX models.
Fig. A.6: The produced relative fractional abundances of HCN, HCO$^+$ and CS across the various regions in NGC 1068 at both 40 pc and 100 pc scale.
Appendix B: Additional moment 0 maps

Appendix B.1: HCN(4-3)

Fig. B.1: HCN J(4-3) velocity-integrated moment map. Beam size shown by orange ellipse. The lowest contour displayed is 3σ, where σ = 6.8 K km s⁻¹, with the following contours corresponding to 5σ, 10σ, 20σ, 30σ, 45σ, 70σ, 100σ, 150σ.

Appendix B.2: HCO⁺ (4-3)

Fig. B.2: HCO⁺ J(4-3) velocity-integrated moment map. Beam size shown by orange ellipse. The lowest contour displayed is 3σ, where σ = 6.4 K km s⁻¹, with the following contours corresponding to 5σ, 10σ, 20σ, 30σ, 45σ, 70σ, 100σ, 150σ.