USING CO ISOTOPES TO PROBE THE ISM

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1. Introduction

Observations of CO and its most abundant isotopomers ^{13}CO, C^{18}O and C^{17}O have been extensively used over the past 25 years to infer the excitation conditions and to study the physical characteristics of the interstellar medium. These measurements have allowed studies of

- Molecular abundances – forming the foundation of ISM chemistry
- Masses of galaxies – probing the star formation history and 'X-factor'
- Cooling of molecular clouds – tracing the ISM thermodynamics
- Energetics of molecular outflows
- Masses of molecular clouds
- Star Formation histories.

The usual method for estimating the gas properties has at its heart the following chain of inferences connecting observational quantities to H$_2$ column densities

$$\int T_a^* dv \stackrel{\rm LTE}{\longrightarrow} N_{\rm col}(^{13}{\rm CO}) \stackrel{X(^{13}{\rm CO/CO})}{\longrightarrow} N({\rm CO}) \stackrel{X({\rm CO/H_2})}{\longrightarrow} N({\rm H_2}).$$

There are several assumptions involved in this estimate; that the Local Thermodynamic Equilibrium (LTE) approximation can be used to estimate the total ^{13}CO column density; that we can estimate the excitation temperatures and opacity; and that we have good knowledge of the inter-isotopomeric abundance ratios of the ^{13}CO/CO and CO/H$_2$ and the four dimensional (x, y, z, and velocity) structure of a molecular cloud—which has often been assumed homogeneous and spherical with systematic velocity gradients. In fact, looking back over much of the past 25 years of the history of molecular line astronomy, it is remarkable how few reliable determinations of these important conversion factors have been made, particularly since they have had a profound and wide ranging influence on almost all aspects of the field. Recent observational and theoretical models show that neither these conversion factors nor the excitation conditions remain constant within individual clouds, and that many of the 'authoritative' column densities, cloud masses, and molecular abundances that are spread throughout the literature have systematic inaccuracies.

2. Observational Methodology

The column density of a diatomic molecule may be estimated using the emission from a line (such as the $(J+1) \rightarrow J$ transition) of an optically thin(ner, than CO) isotopomer; for the example of the $J = 2$–1 transition;

$$N_{col} = \frac{3.34 \times 10^{14}}{\left[\frac{\nu}{\mathrm{GHz}}\right] \left[\frac{\mu}{\mathrm{Debye}}\right]^2 \left(1 - e^{-\frac{h\nu}{kT_{\mathrm{ex}}}}\right) \left(e^{-\frac{Jh\nu}{2kT_{\mathrm{ex}}}}\right)} \frac{\tau}{1 - e^{-\tau}} \int T_r^* dV \quad \mathrm{cm}^{-2}$$

where $\mathrm{T_{ex}}$ is estimated from the peak CO antenna temperature, $\int T_r{}^* \, dV$ is the integral of the isotopomer's antenna temperature over the line, J is the lower rotational quantum number (1 for the CO J= 2–1 transition), ν is the line frequency, μ is the dipole moment and the opacity, τ, is estimated using the peak intensity of the CO and ^{13}CO lines, remembering that measured antenna temperatures are related to kinetic temperature through the relationship

$$T_{\mathrm{peak}} \cong \frac{h\nu}{k} \frac{(1 - \exp(-\tau))}{\left(\exp\left(\frac{h\nu}{kT_{\mathrm{kin}}}\right) - 1\right)}.$$

The equation for column density assumes that the Planck corrected CO peak temperature is the same as the kinetic temperature (which is then assumed to be equal to the excitation temperature and constant for all the CO rotational levels), that the isotopomer is in LTE, and that the escape probability $\beta = \tau \,/\, (1\text{–}\mathrm{e}^{-\tau})$ accurately accounts for all optical depth effects. It appears from multi-isotopomeric maps we have made of several sources, that LTE column density estimates are unreliable, and systematically lead to under-estimates of true column densities. Indeed, Monte Carlo calculations of several dark clouds (Avery *et al.* 1987) have already shown that the J= 2–1 and 3–2 CO transitions are sub-thermally excited, and that the cloud cores are often hidden by a surrounding lower density envelope. This means that although the most optically thin lines (such as $C^{17}O$) trace emission from the denser regions at the core, the column densities derived using LTE techniques for the more abundant isotopomers are unreliable.

Another LTE technique has been developed to calculate the absorption of a background source by a foreground cloud (Phillips *et al.* 1988; Greaves *et al.* 1995). This models the depth of the self-absorption feature with increasing J-transition, allowing the excitation temperature, T_{ex}, of a linear molecule to be estimated from observations of two adjacent rotational transitions (1 and 2)

$$\frac{\int T_{r_1} dv}{\int T_{r_2} dv} = \frac{\nu_1}{\nu_2} \frac{J}{J+1} \frac{\left(e^{h\upsilon_1 kT_{\rm ex}} - 1\right)}{(1 - e^{-h\upsilon_2 kT_{\rm ex}})} \frac{T_{\rm back_1}}{T_{\rm back_2}},$$

where $\int T_{r1}\ dv$ and $\int T_{r2}\ dv$ are the integrated absorption line intensities for adjacent transitions denoted by (1) ($J \rightarrow J-1$) and (2) ($J+1 \rightarrow J$), at frequencies ν_1 and ν_2, against a background source of temperature T_{back}, assuming both transitions have the same T_{ex}.

3. The Physical Situation

A further example of the difficulties faced by the data modeller is variability of the CO/^{13}CO/C^{18}O ratio—in some dark clouds the ^{13}CO column density is enhanced by selective photodissociation and ion-molecule exchange reactions (van Dishoeck & Black 1988). The photodissociation rates for some other isotopic species are larger than for ^{13}CO owing to smaller self-shielding of the less abundant isotopes. As ^{13}CO is more abundant than C^{18}O, it benefits from greater self-shielding. Since the isotopic lines are shifted in frequency from those of ^{12}CO, mutual shielding will not be significant – detailed modelling of isotopomeric ratios has been presented by several authors including most recently Gierens *et al.* (1992); Köster *et al.* (1994); and Jansen (1995). Further, the ^{13}CO abundance in cool material may also be enhanced due to the ion molecule exchange reaction

$$^{13}\mathrm{C}^{+} + {}^{12}\mathrm{CO} \Leftrightarrow {}^{12}\mathrm{C}^{+} + {}^{13}\mathrm{CO} \quad (+36\ \mathrm{K}),$$

since the reaction from left to right is exothermic, the right-to-left sequence is not efficient in the low temperature gas that forms the bulk of material in molecular clouds—leading to a ^{13}CO overabundance.

4. Recent Observational Data

Recent advances in on-the-fly mapping observing techniques and in low-noise millimetre and submillimetre receiver technology now allow the routine acquisition of maps containing tens of thousands of independent data points, contrasting with the situation just a few years ago, when 'typical' maps contained only a few tens of data points. These modern data sets allow statistical techniques to be applied to search for trends which relate the behaviour of the different isotopomers. The few sources which have

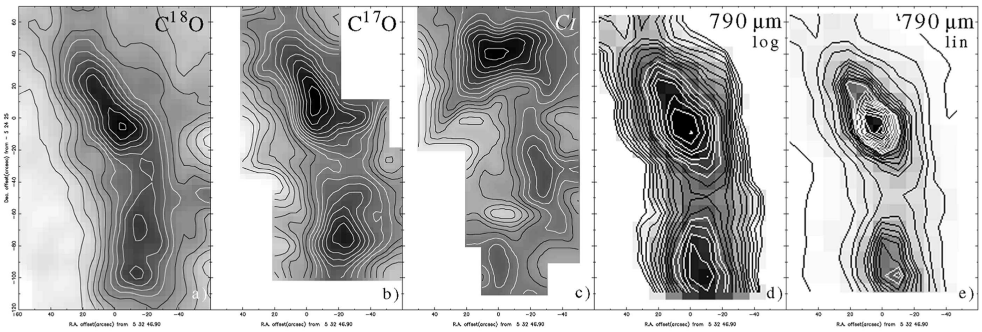

Figure 1. CO and isotopes in the core of the Orion Molecular Cloud

been studied in this way show a complexity far beyond that which simple homogeneous models are able to explain.

In a recent study of gas at the centre of the Orion Nebula, White and Sandell (1995) mapped the CO J=2–1, 3–2 and 4–3 transitions of CO, and various isotopomers including ^{13}CO, C^{18}O, C^{17}O, and 790 μm continuum emission towards the central region of the Orion molecular cloud (OMC-1 cloud), as shown in Figure 1.

Analysing the data in a consistent way, the inter-isotopomeric abundance ratios were estimated over a wide range of column densities as seen in Figure 2. Under favourable geometries, column densities can be related to line-of-sight extinction values. Although this technique may not always trace the extinction between ultraviolet sources which ionise the molecular cloud, this scenario may hold reasonably well for the Orion molecular cloud, since the dominant ionisation sources for the region—the Trapezium Cluster—lie between the earth and the OMC-1 core. The ^{13}CO lines towards Orion are optically thick with the ^{13}CO abundance enhanced in lower column density material because of strong isotopic fractionation. No isotope selective enhancement of the other CO isotopomers was seen; C^{18}O may in fact show a slight depletion in more exposed material. The C^{18}O and C^{17}O lines are optically thin, and correlated with the 790 μm dust continuum emission. Observations of one of the photoionised products of CO, atomic carbon CI, showed that its emission comes from hot, optically thin gas; the abundance ratios of [CI]/[CO] are typically 0.05–0.3, with the larger ratios towards the northern section of the Orion ridge. The CI abundance ratios are also high along the edge of the Bright Bar which is adjacent to the HII region (and the Trapezium cluster which excites it), but decrease in the dense shielded material behind the Bar.

Several studies have suggested that the ratio of ^{13}CO to C^{18}O can

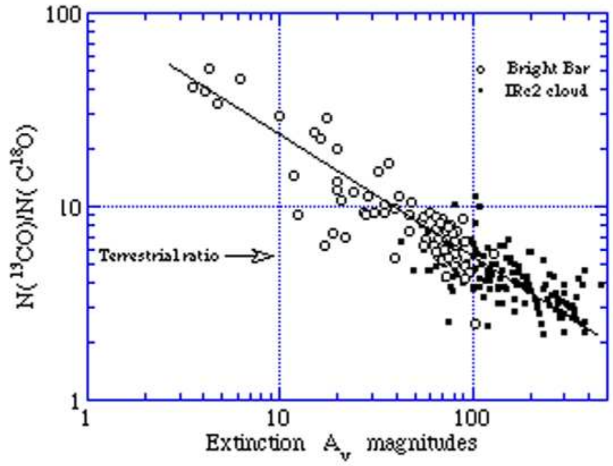

Figure 2. Graphs of $N(^{13}\mathrm{CO})/N(\mathrm{C}^{18}\mathrm{O})$ against extinction as estimated from the $\mathrm{C}^{18}\mathrm{O}$ data. In a) the merged data from the OMC1 cloud and the Bright Bar are shown together. The best fit power law shown is for the relationship $N(^{13}\mathrm{CO})/N(\mathrm{C}^{18}\mathrm{O}) = 80A_{\nu}^{-0.6}$ with a correlation coefficient of 0.91. The regions where the fractionation is high are dominated by emission close to the Bright Bar ionisation front, where the extinction to the Trapezium stars is low, providing strong evidence for $^{13}\mathrm{CO}$ fractionation, whilst the case for a $^{13}\mathrm{CO}$ overabundance in the OMC1 core is less convincing. The bottom axis is given in units of extinction, where this is assumed to be proportional to the $\mathrm{C}^{18}\mathrm{O}$ column density as shown by Lada *et al.* (1994). This assumption may be realistic for Orion, where we are viewing molecular material face on illuminated by the Trapezium stars, which lie between the Earth and Orion, but questionable for other clouds.

exceed the terrestrial ratio (5.5) because of $\mathrm{C}^{18}\mathrm{O}$ photodissociation, and chemical fractionation of $^{13}\mathrm{CO}$ (van Dishoeck & Black 1988; Turner *et al.* 1992; Turner 1993; Fuente *et al.* 1993; Köster *et al.* 1994). The ratio $\mathrm{N}(^{13}\mathrm{CO})/\mathrm{N}(\mathrm{C}^{18}\mathrm{O})$ has been shown to exceed the terrestrial value close to the surfaces of several dark clouds (Frerking *et al.* 1982; Bachiller & Cernicharo 1986; and Lada *et al.* 1994).

Similar trends in inter-isotopomeric intensities have been observed towards about another half dozen sources including S140 (Minchin, Ward-Thompson, & White 1995 a); NGC1977 (Minchin, White, & Ward-Thompson 1995 b); IC1848, B35, Cepheus B (all in preparation); NGC253 (Israel, White, & Baas 1995); and the Serpens Nebula (which is shown below) (White, Casali, & Eiroa 1995). Data towards the Serpens Nebula are shown in Figure 3. A similar analysis was applied to the Serpens data and is illustrated in Figure 4.

Although the $^{13}\mathrm{CO}$ emission from most sources appears to be optically thick (which invalidates the use of $^{13}\mathrm{CO}$ emission in the column density equation—unless the opacity is carefully corrected for), there are just a few sources where $^{13}\mathrm{CO}$ has been shown to be optically thin; including the SE

Figure 3. CO and continuum data for the Serpens Nebula obtained with the JCMT

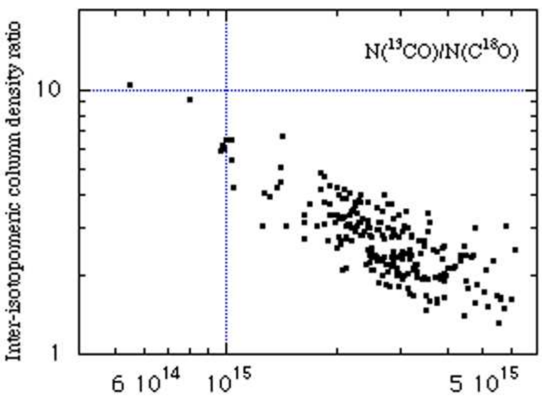

Figure 4. Isotopomeric ratios observed towards the Serpens Nebula

Figure 5. Comparison of $C^{18}O$ J= 1–0, 2–1, and 3–2 column densities derived using LVG and LTE techniques. The LTE estimates are consistently lower, by factors of 4–70, of those from LVG analysis.

lobe of the archetypal molecular outflow source L1551 (Phillips *et al.* 1988; Fridlund & White 1989; Fridlund *et al.* 1996) and in some of the molecular clouds at the edge of the blast wave of the IC443 supernova remnant (White 1994).

5. Modelling the Problem

To examine the uncertainties which might result from use of the LTE analysis, a series of calculations have been made for simple slab geometries, comparing the column densities which would be derived from a set of data analysed separately with an LTE and LVG analysis. The objective of these models is to demonstrate how the choice of model technique can bias the estimate of a column density for different rotational transitions. LVG calculations were performed for clouds with kinetic temperatures of 10 K and 20 K, to determine the column density that would be estimated for various antenna temperatures (for discussion of the technique see Israel, White, & Baas 1995). The H_2 particle density, $n(H_2)$ was set to values of 10^3 and 10^4 cm^{-3}, and column densities calculated for the $C^{18}O$ antenna temperature range observed towards Serpens ($\sim 0.5 - 5$ K). Column density estimates for the J= 1–0, 2–1, and 3–2 transitions were then compared with values derived using the relationships in the LTE equations and are shown in Figure 5.

The LVG column densities estimated from the J= 2–1 lines are $\sim$ 4–8 times, and $\sim$ 12–70 times greater than the LTE estimates, for kinetic temperatures of 20 and 10 K respectively. The difference between LVG and LTE estimates is greatest at the higher $J-$ transitions and in cooler material. Despite the problems highlighted above, it has been a widespread practice amongst many molecular line astronomers to use the LTE approximation and to unjustifiably assume that the ^{13}CO emission is optically thin. It is likely that many of the LTE-based estimates of cloud masses, using the higher rotational transitions of $C^{18}O$ lines to estimate column densities, have under-estimated the true masses. Mass estimates using the ^{13}CO lines to estimate column densities are even more unreliable, due to the finite opacity in this isotopomer. However, in the warm (~ 20 K) moderate density ($\sim 10^4$ cm^{-3}) gas in the central region of the Serpens Nebula, the LTE and LVG estimates agree more closely.

These calculations show that column densities estimated by the LTE model differ by perhaps one order of magnitude compared to those inferred using an LVG model for the cases of low-density, cool gas (see also discussion by Stenholm 1985; Richardson *et al.* 1985). In all cases, the column densities are lower than those in the LVG calculation. This result is consistent with the sub-thermal excitation of the CO isotopomers suggested by Monte Carlo modelling (Avery *et al.* 1987), towards dark clouds observed in the $J=$ 2–1 and 3–2 transitions. This modelling suggested that the cores are often surrounded by lower density envelopes, which can modify the line shapes and temperatures due to material in the core. Schilke *et al.* (1994) have subsequently arrived at similar conclusions towards the Taurus dark cloud core TMC-1. The discrepancies between LTE and LVG estimates are more pronounced at the lower densities and temperatures found in dark clouds, than towards warmer clouds (where most of the published $C^{18}O$ observations to date have been made). This is consistent with the suggestion of Richardson (1994) that the LTE method is only effective at estimating column densities (at the centre of a line) down to an optical depth of $\sim$ unity.

These simple calculations have shown the uncertainties which can occur from use of the LTE technique. Undoubtedly, the problem is more complex—we know that sources are inhomogeneous, clumpy, UV-permeated, have temperature and density gradients, are shocked or turbulent, and exist in chemically evolving regions. There have been many attempts to provide a framework for a more rigorous treatment of the radiative transfer through more realistic complex regions; for example, recent papers by Castets *et al.* (1990); Gierens *et al.* (1992); Köster *et al.* (1994); and references cited within these papers. Discussion of these is beyond the intent of this paper. There remains an urgent need to develop further radiative transfer code which can correctly account for the complex processes we are now beginning to recognise as being present. The best candidate for these would seem to be based around a Monte Carlo approach.

6. Summary

- H_2 and CO column densities based on ^{13}CO data are very uncertain, despite having occupied a central role in the development of molecular line astrophysics
- Many of the estimates of column densities and abundances made in the past are subject to systematic uncertainties as a consequence of the use of the LTE analysis
- The excitation temperatures of the various CO isotopes are often poorly determined, and incorrectly assumed
- ^{13}CO fractionation is common in molecular clouds, and its abundance varies within clouds—this has not been adequately taken account of in estimating cloud masses
- The LTE approximation often inaccurately estimates column density
- Further work on robust Monte Carlo-based radiative transfer models are needed to compliment an explosion of new data on this topic

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