Astron. Astrophys. 358, 723–727 (2000)

ASTRONOMY
AND
ASTROPHYSICS

On the isotopomeric CO line brightnesses in clumpy photon dominated regions: apparent fractionation of $^{13}CO/C^{18}O$

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Received 23 December 1999 / Accepted 18 February 2000

Abstract. Observations of photon dominated regions (PDRs) show that variations of the $^{13}CO/C^{18}O$ integrated line intensities are closely correlated to the total $C^{18}O$ brightness along the line of sight (l.o.s.). From these intensity variations a change of the $N(^{13}CO)/N(C^{18}O)$ column density ratio from values of about 5 to 40 or larger was deduced in the past. We argue that this is naturally explained by a model of a *clumpy* cloud: low ratios are observed at positions of high l.o.s. column density, where the line emission is dominated by a few large clumps, while high ratios originate at positions covered by many small clumps, having low l.o.s. column density. Quantitative agreement of our models with observations of the S140 and the Orion Bar PDR is achieved without any additional assumptions about the source geometry, thus avoiding the problems of previous models with *plane parallel* geometry, which required an ad hoc correlation between the l.o.s. column density and the attenuation toward the exciting sources. We conclude, that at least for high radiation field environments the $C^{18}O$ integrated line intensity is not a valid column density tracer.

Key words: ISM: clouds – ISM: structure

1. Introduction

Photon dominated regions occur wherever far-ultraviolet (FUV) radiation, e.g. originating in newly formed massive stars, illuminates the surface of molecular clouds and controls the physical and chemical properties of the gas. The attenuation of the FUV intensity with increasing depths into the cloud results in a large temperature gradient and a stratification of the chemical structure on the cloud surface. Most PDR models calculate the cloud structure based on a plane parallel, semi infinite cloud model (Tielens & Hollenbach 1985; Sternberg & Dalgarno 1989). The distance from the ionisation front is parameterized by the visual extinction A_v which is proportional to the column density towards the exciting source. For the dissociation and formation of CO self-shielding plays a crucial role, as the CO dissociation rate is mainly limited by the saturation of the UV-absorption into pre-dissociation levels or coinciding H_2 lines due to increasing column density of the molecules (van Dishoeck & Black 1988). According to its more efficient self-shielding ^{13}CO is enriched in comparison to $C^{18}O$ at low A_v, where the radiation field is strong. Hence the $^{13}CO/C^{18}O$ abundance ratio changes from high values in the range of 30-40 near the ionisation front to values of about 5-7 deep inside the cloud which represent the natural isotopomeric abundance.

Observations of Minchin & White (1995); Minchin et al. (1995), and White & Sandell (1995) show that the $^{13}CO/C^{18}O$ column density ratios, derived from the low-J line brightnesses, vary systematically with the total line-of-sight (l.o.s.) column density which is derived from the $C^{18}O$ brightness alone. Both the absolute value of the abundance ratio and the systematic decrease with increasing column density are at first sight consistent with the fractionation effects predicted by PDR models as discussed above, and these observations are thus commonly referred to as observational confirmation of the PDR scenario. A second thought, however, shows that this interpretation is inconsistent, as is explained in Sect. 2.

On the other hand, molecular clouds are known to be clumpy with a distribution of clump masses and sizes following simple power laws (cf. Stutzki et al. 1998). In this paper we present an explanation of the observed isotopomeric CO abundance variation in a clumpy PDR model. Beyond a statistical distribution of clumps with a specific clump mass/size spectrum over a certain range of sizes no additional assumptions are made about the global structure of the PDR in question. The addition of a nearly homogeneous interclump medium, modeled by an excess of very low mass clumps, can improve the agreement with the observational data.

The $^{13}CO/C^{18}O$ line ratio of the emission of a single cloud fragment (clump) depends on its size: while for large clumps the isotopomeric intensity ratio mainly reflects the different excitation conditions at the positions in the cloud where the lines originate, in the case of smaller clumps the lower self-shielding factor of the rare $C^{18}O$ isotopomer becomes more important and leads to nearly complete destruction of this isotopomer, which results in high values for $^{13}CO/C^{18}O$ (see Störzer et al. 2000). Due to the intrinsic clump size distribution and its statistical spatial distribution the systematic variation of isotopomeric CO line brightness with clump size translates into a variation with total l.o.s. column density. This is due to the fact that positions

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with high total column density are dominated by a few large clumps along the l.o.s., whereas the total column density is low, if only small clumps are present along the l.o.s..

In Sect. 2 we review the observational results on ^{13}CO/C^{18}O fractionation and critically discuss the standard interpretation from the viewpoint of plane parallel models. In Sect. 3 we present our model of the line emission of an inhomogeneous medium with given clump mass spectrum. In Sect. 4 we apply our model to observations of the S140 and Orion Bar region, and we summarize our results in Sect. 5.

2. Discussion of the observed N(^{13}CO)/N(C^{18}O) - A_v relation

Minchin & White (1995), Minchin et al. (1995) and White & Sandell (1995) have published isotopomeric CO low-J observations of various edge on PDRs (Orion Bar, S140 and NGC 1977), which all were analysed in the following way: in a first step the isotopomeric column densities are derived at each position from the corresponding ^{13}CO- and C^{18}O-line integrated intensities, including optical depth correction, if necessary, for the ^{13}CO line. In a second step, using the empirical relation

$$\mathrm{N(C^{18}O)/A_v} = 2.29 \times 10^{14}\ \mathrm{cm^{-2}\ mag^{-1}} \tag{1}$$

(Lada et al. 1994) the visual extinction A_v along the line of sight is deduced from the C^{18}O column density. High N(^{13}CO)/N(C^{18}O) ratios are found to be correlated with low A_v values: N(^{13}CO)/N(C^{18}O) $\propto A_v^{-\beta}$, with β = 0.35 for S140 and β = 0.6 for Orion Bar. The correlation holds over a range of A_v from a few mag to about 100 mag.

These results are interpreted by the authors as observational confirmation for the variation of the ^{13}CO/C^{18}O fractionation with extinction from the exciting UV-source in the context of plane parallel PDR models (e.g. Köster et al. 1994). This argument does not hold, however, because the derived extinction values are measured *along the line-of-sight*, while contrary to that the parameter usually denoted as A_v in the plane parallel models specifies the depth *towards the direction of the incident radiation field*. In the case of edge on PDRs the line of sight and the direction of the incident radiation field are oriented perpendicular and hence the extinction towards the direction of the FUV-field is not observable directly. A correlation between the l.o.s. column density and the extinction towards the exciting source, as assumed by Minchin et al. (1995), appears to be rather ad hoc and is not justified considering the structure of the PDR being stratified along the direction of the incident UV radiation and perpendicular to the l.o.s. direction. Otherwise in a pure face on geometry the l.o.s. sight column density would also be approximately constant over the whole cloud area and the l.o.s. averaged isotopomeric abundance ratio would thus be constant at whatever value corresponds to the abundance ratio averaged over the PDR-transition zone.

We conclude, that in none of these cases or any simple geometrical configuration in between a correlation like the one observed would occur within a *homogeneous* cloud.

3. Calculation of the isotopomeric CO emission from an ensemble of clumps in a PDR

Measurements with increasing spatial resolution have shown molecular clouds to be clumpy with structure being present always down to the smallest scales observationally resolved. In the following, we assume the molecular cloud to be composed of an ensemble of spherical clumps with a given mass (or size) distribution. We calculate the isotopomeric CO line brightness of a clump of given size using the model for spherically symmetric clumps in an isotropic UV field as described by Störzer et al. (1996). The density of each clump follows a power law: $n(r) = n_0(r/R)^{-3/2}$, where n_0 is the density at the surface and R is the total radius of the clump. The photo dissociation factors of CO isotopomeres are those listed by van Dishoeck & Black (1988); the reaction rates for CO and HCO$^+$ fractionation reactions were taken from Langer et al. (1983). The surface integrated intensity of the CO line emission is calculated from the resulting density- and temperature stratification using the ONION radiation transport code for spherically symmetric clouds (Gierens et al. 1992).

An analysis of the theoretically calculated single clump emission shows, that neither a change of the clump averaged density nor a modification of the incident FUV radiation field strength alone, while keeping the other model parameters fixed, results in a large variation of the ^{13}CO/C^{18}O intensities or column densities (Störzer et al. 2000). On the other hand systematic changes in the ^{13}CO/C^{18}O brightness ratio are obtained by changing the clump size: as CO forms in PDRs by self-shielding, the dissociation rate increases with decreasing column density of the CO molecule. While the clump size becomes smaller this effect grows more rapidly for the rarer C^{18}O isotopomer than for ^{13}CO, implying that in small clumps C^{18}O is almost completely dissociated. Projected on the plane-of-the-sky the C^{18}O emitting region of the cloud therefore has a much smaller extent than the ^{13}CO emitting part, resulting in a lower area filling factor. Besides that, the inner region of the cloud, where the C^{18}O line radiation originates, is cooler than the outer, ^{13}CO line forming zones are. Both effects together result in larger ^{13}CO/C^{18}O line ratios for smaller clumps and finally very high brightness ratios arise.

In the case of large clumps the different dissociation factors only affect the CO formation in a thin surface layer of the cloud, while the main part of the emission originates in the interior regions. Hence the geometrical projection effect mentioned above is negligible and the line ratio only reflects the different excitation conditions of the surface layer, from which the ^{13}CO radiation originates, in comparison to the inner clump region, which emits the C^{18}O line. Applying the standard methods of column density determination to the calculated intensities one formally derives column density ratios of about 3-7. The close correspondence to the intrinsic ^{13}C/^{18}O isotopomeric abundance ratio is rather accidental.

In order to estimate the emission from the clumpy cloud as a whole along any particular line of sight we assume the clumps to have a *mass* spectrum of the form

$$\frac{d\mathcal{N}}{dM} = AM^{-\alpha}. \tag{2}$$

Observations show that α is in the range $1.5...2$ (Kramer et al. 1998). The total mass of the clumps is given by

$$\begin{aligned} M_{tot} &= \int_{M_{min}}^{M_{max}} M \frac{d\mathcal{N}}{dM} dM = \int_{M_{min}}^{M_{max}} AM^{1-\alpha} dM \\ &= \frac{A \cdot M_{max}^{2-\alpha}}{2-\alpha} \left[1 - \left(\frac{M_{min}}{M_{max}} \right)^{2-\alpha} \right]. \end{aligned} \tag{3}$$

Because $M_{min}/M_{max} \ll 1$ and $\alpha < 2$ this leads to

$$A \approx \frac{(2-\alpha) \cdot M_{tot}}{M_{max}^{2-\alpha}}, \tag{4}$$

which for observational data is fully determined by the results of the clump decomposition algorithm (cf. Kramer et al. 1998).

To convert Eq. (2) into a clump *size* spectrum using

$$\frac{d\mathcal{N}}{dL} = \frac{d\mathcal{N}}{dM} \frac{dM}{dL}. \tag{5}$$

we assume a clump mass/size relation of the form

$$M = cL^{\gamma} \qquad \Rightarrow \qquad \frac{dM}{dL} = \gamma c L^{\gamma-1} \tag{6}$$

with L the linear extension (diameter) of a clump. We use $\gamma = 3$ and accordingly $c = \frac{4}{3}\pi \langle n \rangle$. This is the simplest choice and describes mass/size relation of a homogeneous spherical clump with mean density $\langle n \rangle$. We should caution that in the context of fractal media other mass/size relations are conceivable, e.g. where the clump column density, rather than the volume density, is fixed on average leading to $\gamma = 2$ (Stutzki et al. 1998). Observations of some clouds seem to suggest values in between, like γ=2.3 (cf. Heithausen et al. 1998).

Inserting Eqs. (2) and (6) in Eq. (5) we can write

$$\frac{d\mathcal{N}}{dL} = A\gamma c M^{-\alpha} \cdot L^{\gamma-1} = A\gamma c^{1-\alpha} L^{-(\alpha-1)\gamma-1}. \tag{7}$$

Our model cloud consists of a large number (≈20 000) of clumps with a size spectrum given by Eq. (7), which are distributed at randomly chosen positions in a cube. The total projected area of the ensemble towards one side of the cube (the direction to the “observer”) corresponds to the cloud size. The clumps have Gaussian distributed velocity components along the observer’s l.o.s.. A background consisting of many very small clumps (with radii typically 1/100 of the telescope beam radius) is added to this distribution. Because these clumps are far below the resolution limit and there are a lot of them at each observational position, their contribution to the total intensity can be interpreted as that of a nearly homogeneous interclump medium which is an usual assumption in more sophisticated PDR models (eg. Meixner & Tielens 1993; Köster et al. 2000). The consideration of this interclump medium gives a slightly better fit to the observational data without changing the result of our model qualitatively. The side of the cube oriented toward the observer is now divided into segments, each of which represents the telescope beam while observing at this specified position. The total beam averaged brightness for each such position is obtained by solving the radiative transfer equation along this l.o.s. through the clump distribution, where the single clump intensities are taken from the PDR model calculations. As long as the clumps are smaller than the beam the filling factor of a single spherical clump scales $\propto (r_{clump}/r_{beam})^2$. For clumps larger than the beam the area filling factor is unity. Fig. (1) shows typical results of our simulation. From the calculated brightness temperatures the ‘formal’ column densities are derived using Eqs. 1 and 2 from White & Sandell (1995). After this ‘N($C^{18}O$)’ is formally converted to ‘$A_{\rm v}$’ and for each l.o.s. the resulting ratio ‘N(^{13}CO)/N($C^{18}O$)’ is plotted against this ‘$A_{\rm v}$’-value.

The reproduction of the observational trend of an apparent $^{13}CO/C^{18}O$ fractionation at low $C^{18}O$ brightnesses by this pro-

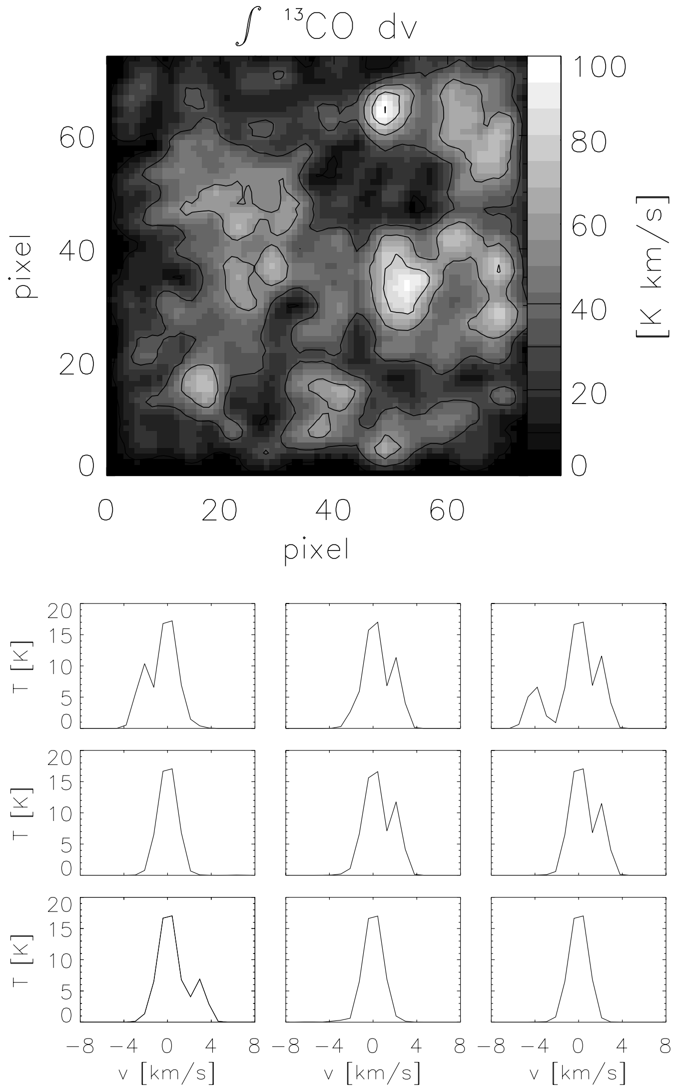

Fig. 1. Typical results of the clumpy cloud model. The upper panel shows a 75×75 pixel map of integrated ^{13}CO J=2-1 line intensity. The ground panel gives an impression of the calculated line profiles at a position located near (60,50).

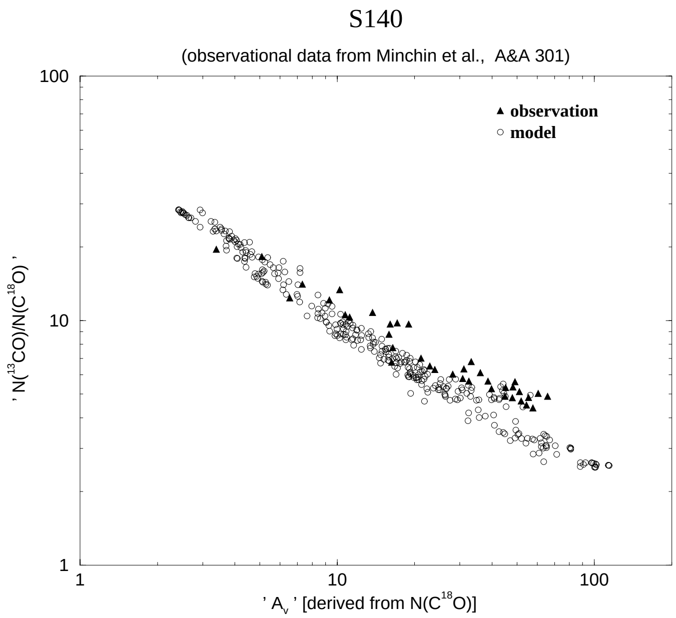

Fig. 2. Comparison of the results derived from the isotopomeric brightness temperatures of a clumpy PDR model with power law clump mass spectrum and the observational data of S140 published by Minchin et al. (1995).

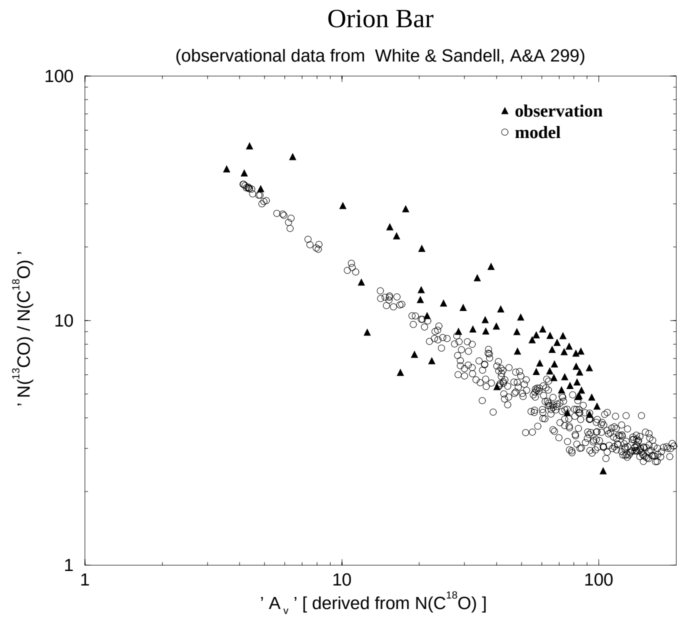

Fig. 3. Same as Fig. 1, but for the Orion Bar data published by White & Sandell (1995).

cedure is due to the fact, that towards some lines of sight the total emission is dominated by a few of the biggest clumps, while at other positions only smaller clumps with smaller filling factors fall into the beam.

If the beam contains only small clumps, this leads to high ‘N(^{13}CO)/N(C^{18}O)’ *values, coinciding with low column density* ‘N(C^{18}O)’ *(and formally derived* ‘A_v’*). In contrast, the* ‘N(^{13}CO)/N(C^{18}O)’ *ratio is small, if the beam is filled also by a few large clumps, from which formally high* ‘A_v’ *values are achieved.* In this model the geometrical configuration of the source, may it be edge on or face on, does not change the resulting correlation between the isotopomeric column density ratio and the resulting ‘A_v’-value.

4. Comparison with observations

For our modelling of the S140 PDR we assume the clumps to have a mean hydrogen particle density of $\langle n \rangle = 10^5$ cm^{-3}. The model FUV field is set to $\chi = 150$ times the mean interstellar radiation field. The parameters needed to calculate the clump size spectrum are $M_{tot} = 840\ M_\odot$, $M_{max} = 160\ M_\odot$ and $\alpha = 1.65$ (Kramer et al. 1998). The clump ensemble covers an area of 1.2 pc^2 and the telescope beam is taken as 10^{-3} pc^2, which corresponds to a resolution of 15$''$(the JCMT beam at 345 GHz) and a source distance of 910 pc. Fig. 2 shows the result for the S140 PDR. The fractionation effect at low ‘A_v’, that means low N(C^{18}O), values is obvious and very similar to the observed one. Like the model results shown the trend of the observational data is also continued to higher ‘A_v’ values, if the data of the outflow region are taken into account (cf. Fig. 5 of Minchin et al. 1995).

In Fig. 3 the corresponding result for the Orion Bar PDR is presented. The radiation field used in this model is stronger ($\chi = 10^5$) and the clump density is higher ($\langle n \rangle = 10^6$ cm^{-3}) than in the case of the S140 model. Because there is no empirical estimation of the clump mass spectrum exponent in the Orion Bar, we use the value $\alpha = 1.72$ deduced by Kramer et al. (1998) for typical massive star forming regions, e.g. Orion B. The best fit to the observations is obtained by choosing the l.o.s. extension of the Bar to be 1.2 pc, which is twice as deep as in the geometrical model of Hogerheijde et al. (1995). From this value, the visible extension of the Bar and a mean gas density of $\langle n \rangle = 10^5$ cm^{-3} a total mass of 250 $M_\odot$ is obtained. We mention that by the clumpy model not only the general trend, but also the statistics of the observational data (many positions with low ratios, only few with high ratios) is reproduced. As in the case of the S140 simulation, the observational data would cover a larger ‘A_v’ range, if also the results of the adjacent OMC1 cloud were shown (cf. Fig. 7a of White & Sandell 1995).

5. Summary and conclusion

We summarize our results as follows:

1. The interpretation of the N(^{13}CO)/N(C^{18}O) correlation with the l.o.s. column density in terms of plane parallel PDR model results, i.e. the variation of the isotopomeric brightness temperatures with increasing distance from the UV-source, is inconsistent with the geometric configuration of the observed edge on PDRs.

2. Due to the depth dependent fractionation and the temperature gradient in spherical PDRs the observed trend of ^{13}CO/C^{18}O brightnesses can be reproduced by an ensemble of different sized clumps with a power law clump mass spectrum (2) and a power law clump size relation (6). A low ^{13}CO/C^{18}O

ratio is obtained towards lines of sight including a few large clumps; lines of sight with small total column densities, i.e. only many small clumps, show a large ratio.

3. Comparison with the observational data for the Orion Bar PDR and the S140 region demonstrates, that a clumpy PDR model can reproduce the observations in a quantitative manner.

4. By the fact that the $^{13}CO/C^{18}O$ intensity ratio in PDRs can change by nearly an order of magnitude we conclude, that in high radiation field environments $C^{18}O$ is not a reliable column density tracer at least for low column density l.o.s. positions.

Acknowledgements. This research was supported by the Deutsche Forschungsgemeinschaft through grant SFB 301 C.

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