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# GAS-PHASE $H_2O$ AND $CO_2$ TOWARD MASSIVE PROTOSTARS

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## ABSTRACT

We present a study of gas-phase $H_2O$ and $CO_2$ toward a sample of 14 massive protostars with the ISO-SWS. Modeling of the $H_2O$ spectra using a homogeneous model with a constant excitation temperature $T_{\rm ex}$ shows that the $H_2O$ abundances increase with temperature, up to a few times $10^{-5}$ with respect to $H_2$ for the hottest sources ($T_{\rm ex} \sim 500$ K). This is still a factor of 10 lower than the $H_2O$ ice abundances observed toward cold sources in which evaporation is not significant (Keane et al. 2001). Gas-phase $CO_2$ is not abundant in our sources. The abundances are nearly constant for $T_{\rm ex} \gtrsim 100$ K at a value of a few times $10^{-7}$, much lower than the solid-state abundances of $\sim$1–3$\times 10^{-6}$ (Gerakines et al. 1999). For both $H_2O$ and $CO_2$ the gas/solid ratio increases with temperature, but the increase is much stronger for $H_2O$ than for $CO_2$, suggesting a different type of chemistry. In addition to the homogeneous models, a power law model has been developed for one of our sources, based on the physical structure of this region as determined from submillimeter data by van der Tak et al. (1999). The resulting $H_2O$ model spectrum gives a good fit to the data.

Key words: Star-formation – gas-phase molecules – abundances

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## 1. INTRODUCTION

The Infrared Space Observatory (ISO) has provided us with a wealth of new data in the infrared from regions of massive star formation. This includes unique information on molecules such as $H_2O$ and $CO_2$, which are difficult to observe from the ground due to the Earth's atmosphere. $H_2O$ and $CO_2$ are among the most abundant species in the envelopes of massive protostars and play a key role in the chemistry in these regions. $H_2O$ is a particularly powerful molecule to study the interaction of the protostar with its environment. In warm regions and shocks all gas-phase oxygen not locked up in CO is thought to be driven into $H_2O$, predicting greatly enhanced gas-phase $H_2O$ abundances. Also, its level populations are influenced by mid- and far-infrared radiation from warm dust, in addition to collisions. Observations of the well-studied star-forming region Orion-KL indeed show strong gas-phase $H_2O$ lines, corresponding to abundances up to $10^{-4}$ (van Dishoeck et al. 1998, Gonzalez-Alfonso et al. 1998, Harwit et al. 1998, Wright et al. 2000). High resolution Fabry-Pérot observations of pure rotational $H_2O$ lines suggest that this gas is associated with warm and shocked regions (Wright et al. 2000). The $CO_2$ molecule on the other hand cannot be observed through rotational transitions, because it does not have a permanent dipole moment. The excitation temperature of these types of molecules can be a useful indicator of the kinetic temperature of the region.

We have studied gas-phase $H_2O$ and $CO_2$ toward a sample of 14 massive young stellar objects including GL 2136, GL 2591, W 3 IRS5, NGC 7538 IRS9, MonR2 IRS3 and GL 490 (see Table 1). The luminosities of these objects are $\sim 10^4$–$10^5$ $L_\odot$, the masses of the envelopes are $\sim$100 $M_\odot$ and their distances are $\sim$1-4 kpc. Most of these objects show a multitude of gas-phase $H_2O$ absorption lines around 6 $\mu$m in the SWS spectra, originating in the $\nu_2$ ro-vibrational band. The ro-vibrational band at 15 $\mu$m of gas-phase $CO_2$ has also been detected in many sources. The LWS spectra, however, do not show strong lines of gas-phase $H_2O$ (Wright et al. 1997). A subset of these sources has been studied previously by van Dishoeck & Helmich (1996) and van Dishoeck (1998).

Both molecules have also been detected in the solid phase toward many massive protostars (e.g. Gerakines et al. 1999, Keane et al. 2001). This allows us to determine gas/solid ratios. In addition, most of these sources show a rich submillimeter emission spectrum, allowing the derivation of temperature and density profiles (van der Tak et al. 2000).

## 2. OBSERVATIONS AND REDUCTION

The $\nu_2$ ro-vibrational bands of gas-phase $H_2O$ and $CO_2$ around 6 $\mu$m and 15 $\mu$m, respectively, have been observed with the Short Wavelength Spectrometer (SWS) in the AOT6 grating mode. All spectra have been reduced using the standard pipeline reduction routines starting from SPD level. In addition, the instrumental fringes have been removed by fitting a cosine to the data (Lahuis & van Dishoeck 2000). The 6 $\mu$m spectra have been rebinned to a spectral resolution of $\Delta\lambda$=0.0020 $\mu$m and the 15 $\mu$m

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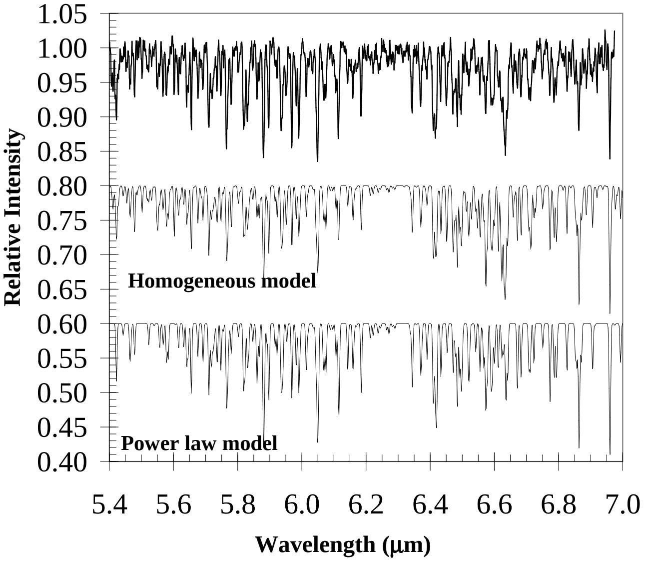

*Figure 1. $H_2O$ spectra toward the massive protostar GL 2591. The top panel shows the data, the middle and bottom panel the homogeneous and power law model, respectively.*

spectra to $\Delta\lambda$=0.0035 $\mu$m. The $S/N$ ratio on the continuum is typically 50-100 in the final spectra.

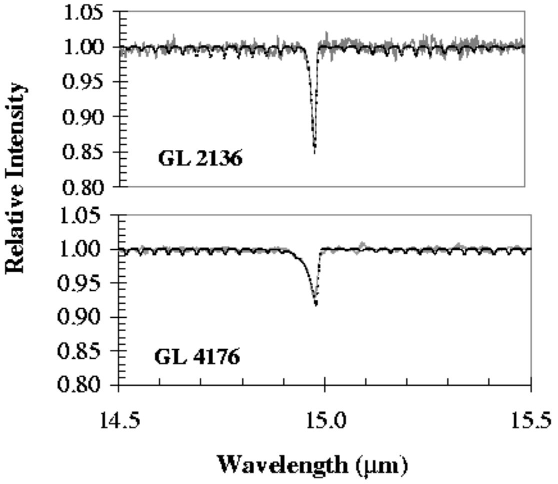

*Figure 2. $CO_2$ spectra toward the massive protostars GL 2136 and GL 4176. The grey solid lines are the data, the black dashed lines the models. The solid $CO_2$ feature has been divided out.*

## 3. MODELING

The modeling of the spectra has been performed using synthetic spectra from Helmich (1996), assuming a homogeneous source with a single temperature $T_{\rm ex}$ and column density $N$. Since the $H_2O$ models are sensitive to different Doppler $b$-values, a range of values between 1.5 and 10 km s$^{-1}$ has been used. For $CO_2$ the models are not sensitive to the linewidth, so a mean value of $b$=3 km s$^{-1}$ is adopted here. This is in agreement with observations of other ro-vibrational absorption lines in the same wavelength region toward these sources. The best fit to the data has then been determined using the reduced $\chi^2_\nu$-method. Some good fitting models are shown in Fig. 1 and 2 for $H_2O$ and $CO_2$ respectively. An example of $\chi^2_\nu$ contours is shown in Fig. 3 for the source GL 2136. This figure illustrates that for low $b$-values (i.e. $b$ <2.5 km s$^{-1}$) the temperature and column density of the gas-phase $H_2O$ is not well constrained. In the following analysis $b$=5 km s$^{-1}$ is adopted for $H_2O$. This corresponds to the mean value of the $^{13}$CO $v$=1-0 absorption line widths found by Mitchell et al. (1990).

*Table 1. Preliminary results from modeling of the $H_2O$ and $CO_2$ spectra using constant $T_{\rm ex}$.*

| Source | $T_{\rm ex}(H_2O)$ K | $N(H_2O)^e$ $10^{18}$cm$^{-2}$ | $T_{\rm ex}(CO_2)$ K | $N(CO_2)$ $10^{16}$cm$^{-2}$ |
|---|---|---|---|---|
| GL2136 | 500 | 1.5 | 175 | 2.7 |
| GL2591 | 450 | 3.5 | 500 | 2.5 |
| GL4176 | 400 | 1.5 | 500 | 2.5 |
| GL2059 | 500 | 1.0 | 500 | <0.3 |
| MonR2 IRS3 | 300 | 0.6 | 300 | 2.0 |
| GL490 | 107$^a$ | <0.3 | 107 | <0.2 |
| NGC3576 | 500 | 1.5 | 500 | <0.7 |
| NGC7538 IRS1 | 176$^b$ | <0.2 | 400 | 0.8 |
| NGC7538 IRS9 | 180$^b$ | <0.2 | 150 | 0.8 |
| NGC2024 IRS2 | 44$^c$ | <0.09 | 44 | <0.2 |
| S140 IRS1 | 390$^b$ | <0.2 | 390 | <0.6 |
| W33A | 120$^b$ | <0.2 | 300 | 2.3 |
| W3 IRS4 | 55$^d$ | <0.3 | 80 | <0.3 |
| W3 IRS5 | 400 | 0.4 | 350 | 0.7 |

[a] $T_{\rm ex}$(CO) from Mitchell et al. (1995)
[b] $T_{\rm ex}(^{13}$CO) from Mitchell et al. (1990)
[c] $T_{\rm ex}(^{13}$CO) from Black & Willner (1984)
[d] $T_{\rm kin}$ from Helmich (1996)
[e] Assuming $b$=5 km s$^{-1}$

## 4. ANALYSIS

### 4.1. $H_2O$

### 4.1.1. Homogeneous models

The results of the homogeneous model analysis for $H_2O$ are presented in Fig. 4 and Table 1. It is seen that sources with higher excitation temperatures have higher column densities, although the increase is not very strong. The column densities have been converted into abundances with respect to the hot $H_2$ gas, since the spectra show primarily the warmer $H_2O$ gas. The $H_2$ column densities have been

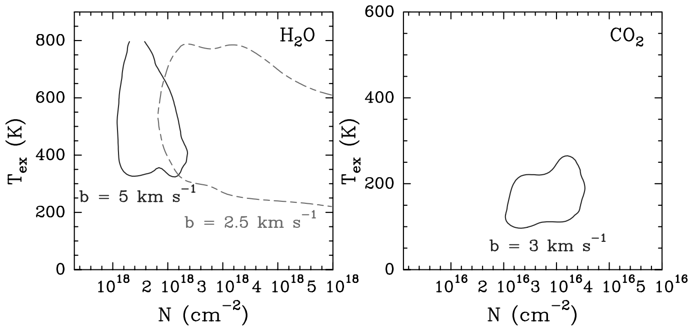

*Figure 3.* $\chi^2_\nu$*-contours of good fitting homogeneous models for* $H_2O$ *and* $CO_2$ *toward the massive protostar GL 2136.*

derived from infrared observations of $^{13}$CO assuming a $^{12}$CO/$^{13}$CO ratio of 60 and a $^{12}$CO/H$_2$ ratio of $2{\times}10^{-4}$ (e.g. Mitchell et al. 1990, Lacy et al. 1994). The resulting abundances increase with temperature, up to a few times $10^{-5}$ for the hottest sources ($T_{\rm ex} \sim 500$ K) (Fig.4). The presence of strong $C_2H_2$ absorption toward the same sources (Lahuis & van Dishoeck 2000) and the absence of this molecule in the well-known shocked regions Peak 1 and Peak 2 in Orion (Boonman et al. 2001) suggest that shocks do not play a dominant role. Hot core models by Charnley (1997) indicate $H_2O$ abundances of $\sim 10^{-5}$ for $T$=300 K, consistent with our values. However, he assumes that the initial solid-state abundance of $H_2O$ is $\sim$$10^{-5}$, a factor of 10 lower than observed toward cold sources in which evaporation is not significant (Keane et al. 2001). This discrepancy suggests that part of the evaporated $H_2O$ is probably destroyed through rapid gas-phase reactions leading to atomic oxygen.

### 4.1.2. Power law model

Although the homogeneous models provide a good fit to the data, they probably do not reflect the true excitation mechanism of the $H_2O$ molecule. Since the level populations of $H_2O$ are influenced by radiation from warm dust, pumping has to be included in the models. Also submillimeter observations show that both a temperature and density gradient is present in these objects (van der Tak et al. 2000), and therefore an abundance gradient. Therefore we have set up a power law model for one of our sources GL 2591, using the models by Doty & Neufeld (1997). In this model a density gradient $\propto$ r$^{-1.25}$ (van der Tak et al. 1999) is used. The temperature and abundance profiles are shown in Fig. 5. Only gas-phase chemistry is included at this point. Although Doty & Neufeld report no significant changes in their models if gas-grain chemistry is included, further investigations have to confirm this. Similar models will be set up for all other sources in our sample. The resulting model spectrum for GL 2591 (Fig. 1) gives a good fit to the data.

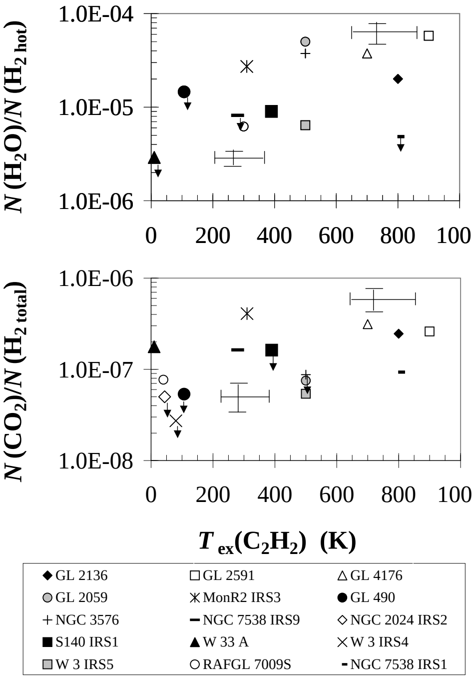

*Figure 4. Top panel:* $H_2O$ *abundances with respect to hot* $H_2$ *gas. Bottom panel:* $CO_2$ *abundances with respect to total* $H_2$ *gas. The excitation temperature of* $C_2H_2$ *is used as a tracer of the warm gas (see Lahuis & van Dishoeck 2000). Typical errorbars are indicated in the figure. The intermediate mass protostar AFGL 7009S (Dartois et al. 1998) is added for comparison.*

Because of the high $H_2O$ abundance derived from the rovibrational lines, some pure rotational $H_2O$ lines are expected in the LWS spectra. However, reduction of these spectra for GL 2591 only shows a hint of one line in absorption (Wright et al. 1997). A first quick look at the LWS spectra of the other sources shows only a few pure rotational lines of $H_2O$. Since the LWS beam is so large ($\sim$80″ diameter) compared to the angular size of the infrared sources, this suggests that the hot water fills only a small fraction of the LWS beam (< few arcseconds) close to the protostar, consistent with Fig. 5.

### 4.2. CO$_2$

The homogeneous model analysis for gas-phase $CO_2$ shows that this molecule is not very abundant in our sources. The column densities show only a weak increase with temperature, whereas the abundances are roughly constant for $T_{\rm ex} \gtrsim 100$ K at a value of a few $\times 10^{-7}$. Since both warm and cold $CO_2$ is detected, the abundances are given with respect to the total $H_2$ column density (Fig. 4). These abundances are much lower than the solid-state abundances of $\sim$1–$3{\times}10^{-6}$ (Gerakines et al. 1999). This suggests that $CO_2$ is also being rapidly destroyed in the gas-phase after evaporation from the grains. Shock chemistry has been suggested by Charnley & Kaufman (2000),

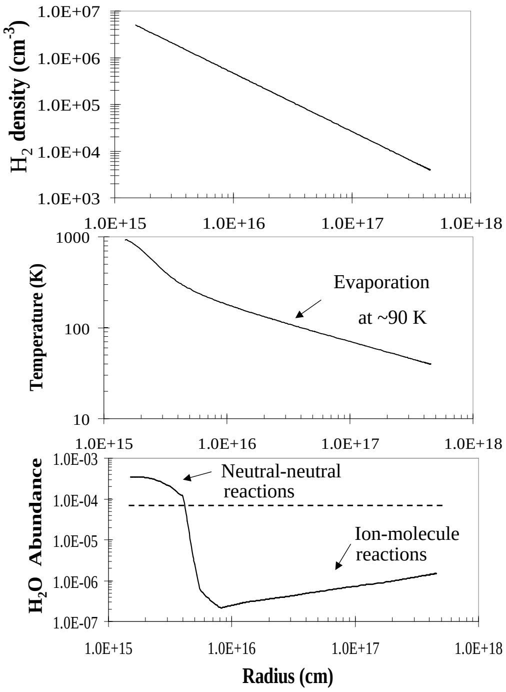

*Figure 5. Power law models for $H_2O$ based on the model by Doty & Neufeld (1997) for GL 2591. The dashed line denotes the $H_2O$ abundance found from the homogeneous models.*

but more detailed models including evaporation have to be developed to determine the nature of these reactions.

### 4.3. Gas/solid ratios

From the column densities derived from the homogeneous models for $H_2O$ and $CO_2$, gas/solid ratios can been determined, using the solid-state features of $H_2O$ (Keane et al. 2001) and $CO_2$ (Gerakines et al. 1999) as observed with ISO-SWS toward the same objects. For both species this ratio increases with temperature, consistent with the location of both species in the warm inner part of the envelope. However the increase is much stronger for $H_2O$ than for $CO_2$, although $CO_2$ is more volatile than $H_2O$. The higher ratios for the warmer sources indicate that they are in a later evolutionary stage than the sources with low gas/solid ratios (van der Tak et al. 2000, van Dishoeck & van der Tak 2000).

## 5. Conclusions

Gas-phase $H_2O$ and $CO_2$ are detected towards a large number of massive protostars with ISO-SWS. Modeling of the spectra shows that $H_2O$ is hot and abundant. The abundances of gas-phase $CO_2$ are however not very high. Chemical models will be developed in the near future to attempt to explain the differences between these molecules and to investigate the possible destruction of these species through gas-phase reactions. A power law physical-chemical model for one source shows good agreement with the data. The LWS data for the same sources show mostly a lack of pure rotational $H_2O$ lines, indicating that the warm gas probed by the ro-vibrational lines is located close to the protostar.

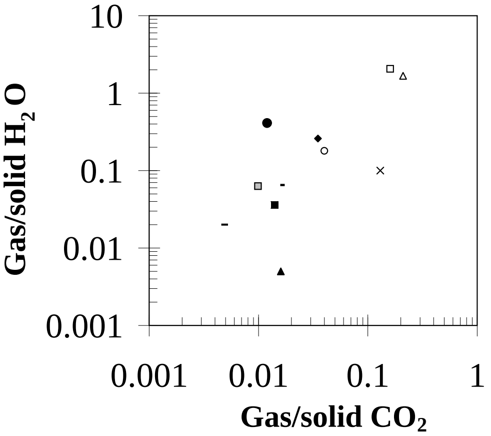

*Figure 6. Gas/solid ratios for $H_2O$ and $CO_2$. The symbols are the same as in Fig. 4.*

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