DISTRIBUTION OF WATER VAPOR IN MOLECULAR CLOUDS

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ABSTRACT

We report the results of a large-area study of water vapor along the Orion Molecular Cloud ridge, the purpose of which was to determine the depth-dependent distribution of gas-phase water in dense molecular clouds. We find that the water vapor measured toward 77 spatial positions along the face-on Orion ridge, excluding positions surrounding the outflow associated with BN/KL and IRc2, display integrated intensities that correlate strongly with known cloud surface tracers such as CN, C2H, 13CO J = 5–4, and HCN, and less well with the volume tracer N2H+. Moreover, at total column densities corresponding to nH2O < 15 mag, the ratio of H2O to C18O integrated intensities shows a clear rise approaching the cloud surface. We show that this behavior cannot be accounted for by either optical depth or excitation effects, but suggests that gas-phase water abundances fall at large Aν. These results are important as they affect measures of the true water-vapor abundance in molecular clouds by highlighting the limitations of comparing measured water-vapor column densities with such traditional cloud tracers as 12CO or C18O. These results also support cloud models that incorporate freeze out of molecules as a critical component in determining the depth-dependent abundance of water vapor.

Key words: astrochemistry – ISM: abundances – ISM: clouds – ISM: molecules – radio lines: ISM

1. INTRODUCTION

Interstellar water is of continuing interest because of the role water plays in the oxygen chemistry within dense molecular clouds as well as the efforts to trace its abundance and distribution in all phases of cloud evolution through to planet formation. Thanks to a number of space-based observatories operated during the past 15 years, good progress has been made detecting and mapping the distribution of water toward molecular clouds. The highest water abundances, and the strongest water emission, are observed toward warm (i.e., T > 300 K) gas regions, most frequently associated with shock-heated gas generated by high-velocity outflows from young stellar objects and supernovae remnants. This finding is in agreement both with predictions that neutral–neutral reactions (i.e., H2 + O → OH + H and H2 + OH → H2O + H) dominate at these temperatures and are relatively efficient at producing water (cf. Elitzur & de Jong 2000a; Neufeld et al. 2000a; Nisini et al. 2000; Benedettini et al. 2002; Franklin et al. 2008).

However, within most dense (n(H2) > 103 cm−3) molecular cloud complexes, the bulk of the water—vapor plus ice—lies within the cooler (T ≤ 40 K) and more massive quiescent gas component. Knowledge of the depth-dependent abundance of water vapor and water ice in molecular clouds is important for at least two reasons. First, the depth-dependent abundance of water vapor and water ice reflects a competition among a number of important processes, such as photodissociation, photodesorption, gas-phase reactions, gas-grain reactions, and grain-surface reactions, most of which depend upon the gas density and far-ultraviolet (FUV) flux (6 eV < hν < 13.6 eV). A better understanding of these processes and their relative importance thus reduces the uncertainty in virtually all models of the chemical composition of molecular clouds. Second, because oxygen is the most abundant element after hydrogen and helium, the processes that control the amount of oxygen locked in water vapor and, in particular, water ice determine the amount of residual oxygen free to react with other species. In this way, the predicted abundance of a host of species that depend on the gas-phase oxygen-to-carbon or oxygen-to-nitrogen ratio, for example, hinges on knowledge of the main reservoirs of oxygen, such as gas-phase water and water-ice.

Models incorporating the formation and destruction processes mentioned above have been constructed and detailed predictions exist for the water-vapor and water-ice abundance profiles as functions of cloud density and external FUV flux (cf. Hollenbach et al. 2009). Measures of the strength of solid-state H2O absorption features along numerous lines of sight provide good column density distributions for water ice (e.g., Whittet et al. 1998; Sonnenstrucker et al. 2008). Unfortunately, complementary studies of the distribution of gas-phase H2O within quiescent molecular gas have suffered either from a lack of access to the ground-state ortho- and para-water transitions, which probe most of the water column at T < 40 K, or from sparse spatial sampling of most clouds. In this paper we report the results from a large-area, fully sampled study of ground-state water vapor emission toward the Orion Molecular Cloud ridge using the Submillimeter Wave Astronomy Satellite (SWAS).

The SWAS mission was primarily dedicated to the study of (1) the oxygen chemistry in dense (n(H2) ≥ 103 cm−3) molecular clouds throughout our Galaxy, (2) the abundance, distribution, and cooling power of H2O and O2 within these clouds, and (3) the structure and physical conditions in molecular clouds. To achieve these goals, SWAS was designed to detect emission
from five key gas-phase atoms and molecules—water (H$_{16}$O), isotopic water (H$_{18}$O), molecular oxygen (O$_2$), atomic carbon (CI), and isotopic carbon monoxide (13CO). Since the emphasis was on studying the bulk of the colder (T < 40 K) molecular material, SWAS measured those frequencies coinciding with either the ground-state or a low-lying transition in each of these species. The one exception was 13CO, for which the mid-level (E$_{up}/k$ = 79 K) J = 5–4 transition was observed. Table 1 presents a summary of the species and transitions observed by SWAS. A detailed description of the SWAS mission can be found in Melnick et al. (2000b) and Tolls et al. (2004).

The Orion Molecular Cloud ridge is an approximately 10–15 arcmin wide region of warm (T ~ 20–40 K), dense (n(H$_2$) ~ 10$^4$–10$^5$ cm$^{-3}$) gas (cf. Bally et al. 1987; Dutrey et al. 1991; Tatematsu et al. 1993; Bergin et al. 1994, 1996; Ungerechts et al. 1997; Johnstone & Bally 1999) stretching ~ 30 arcmin north and more than 60 arcmin south of BN/KL. As such, the Orion ridge represents the contiguous region with the largest angular size observed in water vapor by SWAS and provided the opportunity to obtain 86 independent spatial samples with SWAS’s 3.3 × 4.5 arcmin beam (at 557 GHz). Equally useful, as illustrated in Figure 1, the Orion ridge presents a face-on geometry viewed from earth with its UV-illuminated surface on the near, earth-facing side. Thus, every line of sight probes a column of gas from its UV-illuminated surface to A$_V$’s in excess of 30 mag in some cases. Those species whose abundance peaks near the cloud surface would be expected to exhibit relatively little variation in the integrated intensity of their optically thin emission between lines of sight whose depth extends beyond the surface layers. Conversely, any optically thin emission from species whose abundance rises to a near-constant value through-out the cloud would be expected to scale with the line-of-sight column density. Thus, by measuring the correlation between the observed H$_2$O integrated intensities and the optically thin integrated intensities of both near-surface and volume-tracing species, it is possible to constrain the depth dependence of the water-vapor emission.

In Section 2 we review the SWAS and Five College Radio Astronomy Observatory (FCRAO) observations used in this study, and in Section 3 we present the results. In Section 4, we describe the role of line optical depth effects and depletion along with two approaches used to analyze the data. In Section 5, we discuss the results and implications for our understanding of the water distribution in dense molecular clouds.

### Table 1

| Species        | Transition | Energy Above Ground State (E$_{up}/k$) | Frequency (GHz) | Critical Density (cm$^{-3}$) |
|----------------|------------|----------------------------------------|-----------------|------------------------------|
| O$_2$          | 3,3–1,2    | 26 K                                   | 487.249         | 10$^5$                       |
| CI             | $^3P_1$–$^3P_0$ | 24 K                                  | 492.161         | 10$^5$                       |
| H$_{13}$O      | $^1_{10}$–$^3_{0}$ | 26 K                                   | 547.676         | 8 × 10$^7$                   |
| 13CO           | $^J = 5$–$^4$ | 79 K                                   | 550.926         | 2 × 10$^5$                   |
| H$_{13}$O      | $^1_{10}$–$^3_{0}$ | 27 K                                   | 556.936         | 8 × 10$^7$                   |

**Notes.**

a Ground-state transition.

b Assuming collisions with ortho- and para-$\text{H}_2$ in the ratio of 0.03, the LTE value at 30 K. The critical density for H$_{13}$O will likely be less than this value due to significant radiation trapping in this line. The critical density for H$_{13}$O could be reduced due to the same effect (see the text).

c Rest frequency of the strongest hyperfine component.

d Henceforth, the most abundant isotopologue of water, H$_2$O, will be denoted simply as H$_2$O.
Strip scans of Jupiter ± 10′ across the beam minor axes and ± 12′ across the beam major axes confirmed (1) that the beams were symmetrical, with no evidence for vignetting or other distortions, (2) that the beam centers were spatially co-aligned to within 5′ or about 1/40th of the FWHM of the minor axis of the 553 GHz beam, and (3) the results of pre-launch instrument testing which showed that the highest sidelobe was suppressed by ∼−17 dB with all other sidelobes below −30 dB out to 15′ from the beam centers (the limit of these measurements).

The SWAS maps cover a grid of regular spacing of 3.2 arcmin, corresponding approximately to the angular diameter of the minor axis of the SWAS beam at 557 GHz, the frequency of the ortho-H$_2$O ground-state transition. All of the SWAS observations reported here were conducted by nodding the entire observatory. Because there was no change in the optical path between on-source and off-source reference observations, the spectral baselines were generally very flat, requiring no more than a first-order fit to the baseline to produce good-quality continuum-subtracted spectra. Spacecraft nodding also ensured that good reference positions were always used; spatial positions up to 3 deg in any direction from the on-source position for each source were selectable and were chosen to coincide with the closest position exhibiting no detectable $^{12}$CO $J$ = 1–0 emission. On-orbit tests indicated that the receiver-AOS system was radiometrically very stable; measurements demonstrated that on-source integration times of ∼ 200 hr continued to exhibit radiometric performance—i.e., spectral noise ∝ $1/\sqrt{\text{time}}$—in both receivers. In addition, SWAS H$_2$O spectra of Orion BN/KL obtained 182 days apart were reproducible within the noise. The SWAS H$_2$O map of Orion was obtained during several periods of source availability between 1998 December 20 and 2003 October 8.

Between 1999 February and May, the FCRAO 16-element SEQUOIA array receiver was used to obtain maps of the $^{12}$CO and $^{13}$CO emission (cf. Plume et al. 2000). Between 2004 January and June, the FCRAO 32 pixel SEQUOIA array receiver (Erickson et al. 1999) was used to obtain maps of the emission from C$_2$H, HCN, N$_2$H$^+$, CH$_3$OH, C$^{18}$O, and CN. In 2005 April, further observations were obtained in C$_2$H and N$_2$H$^+$ repeating regions in Orion where the emission was weak. The spectral lines observed by the FCRAO are summarized in Table 1. The region mapped in Orion covered the full spatial extent of the SWAS H$_2$O observations. For all observations, the data were obtained using an On-The-Fly observing technique. SEQUOIA has the capability of observing two frequencies simultaneously with a bandwidth of 50 MHz and 1024 spectral channels per pixel and is not included in the analysis. All offsets are relative to $\alpha = 05^h35^m14^s5$, $\delta = -05^o22'37''$ (J2000).

The results of our mapping efforts are shown in Figures 2–6. Figure 2 shows a portion of the central ridge of the Orion Molecular Ridge made in the $^{13}$CO $J$ = 1–0 110.2 GHz transition using the FCRAO (see Table 1). The beam size was 47′′. The larger gray-outlined region encompasses the region mapped in the H$_2$O 1$\rightarrow$0, 556.9 GHz transition by SWAS. The inner region, denoted by the gray square, includes gas also subject to strong outflow shocks and is not included in the analysis. All offsets are relative to $\alpha = 05^h35^m14^s5$, $\delta = -05^o22'37''$ (J2000).

Figure 2. Integrated intensity map of the Orion Molecular Ridge made in the $^{13}$CO $J$ = 1–0 110.2 GHz transition using the FCRAO (see Table 1). The beam size was 47′′. The larger gray-outlined region encompasses the region mapped in the H$_2$O 1$\rightarrow$0, 556.9 GHz transition by SWAS. The inner region, denoted by the gray square, includes gas also subject to strong outflow shocks and is not included in the analysis. All offsets are relative to $\alpha = 05^h35^m14^s5$, $\delta = -05^o22'37''$ (J2000).

3. RESULTS

The line profiles vary for different tracers and different sources. For example, in the center of Orion, there is a prominent outflow component that contributes significantly to the total intensity. There are also tracers with multiple hyperfine components, such as CN, C$_2$H, HCN, and N$_2$H$^+$. To better recover the intensity of the relatively quiescent gas of interest here, one or more Gaussian components have been fitted to each spectrum. When multiple hyperfine components were present, the fitting was restricted by fixing (1) the relative spacing between peaks to correspond to the known spectral separation between hyperfine components and (2) the common line widths of each component. For example, to fit the HCN emission, we allowed the LSR velocity of the main component to be a free parameter, $v_0$, and required that the other two components be centered at $v_0 - 7.064$ km s$^{-1}$ and $v_0 + 4.842$ km s$^{-1}$, respectively, and that all components have the same line width. In this way, the hyperfine components were treated as correlated Gaussian peaks to best recover the total line flux.
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Figure 3. Maps of the Orion Molecular Ridge obtained with 46″–60″ spatial resolution using the FCRAO (see Table 1). The peak integrated intensities (∫T_A dν), in K km s⁻¹, are 47.39 (¹³CO), 6.896 (C¹⁸O), 14.16 (N₂H⁺), 29.85 (CN), 325.3 (HCN), 6.556 (C₂H). Contours superposed on the ¹³CO and C¹⁸O maps are in units of 0.10 of the peak value, with the peak contour shown being 0.9. Contours superposed on the N₂H⁺, CN, HCN, and C₂H maps are in units of 0.15 of the peak value. The larger outlined region encompasses the region mapped in the H₂¹⁸O 1₁₀–1₁₁, 556.9 GHz transition by SWAS. The inner region, denoted by the square, includes gas also subject to strong outflow shocks and is not included in the analysis. All offsets are relative to α = 0₅₅₃₅₃₉₅, δ = −₀₂₂₂₃₇ (J2000).

Molecular Cloud traced by the 110.2 GHz ¹³CO 1–0 transition. The irregularly shaped area outlined in gray encompasses the region mapped in the 556.9 GHz 1₁₀–1₁₁, 556.9 GHz transition by SWAS. The smaller gray square centered on (Δα, Δδ) = (0, 0) shows the area affected by the strong outflows from BN/KL and IRc2. Because the gas associated with the outflow shocks possesses temperatures, densities, and chemical abundances distinct from the surrounding quiescent material (cf. Blake et al. 1987), data from within this area are excluded from the following analysis. Figure 3 shows the central region of the ridge mapped with 46″–60″ spatial resolution in six of the seven species observed using FCRAO (the 115.3 GHz ¹³CO 1–0 map is not shown since its emission is optically thick within most of the area mapped by SWAS). As in Figure 2, both the region mapped in H₂O by SWAS and the excluded shock-affected area are outlined.

Figure 4 shows the SWAS 556.9 GHz 1₁₀–1₁₁, 556.9 GHz integrated intensity map of the ridge along with the spectra upon which the map is based. Figures 5 and 6 show the 492.2 GHz C¹³N₁ −¹³N₀ and 550.9 GHz ¹³CO 5–4 integrated intensity maps of the ridge, respectively, also obtained using SWAS, as well as an expanded view of the area mapped deeply in H₂O.

A total of 86 spatial positions along the ridge were observed by SWAS with sufficient total integration times to either obtain convincing detections of H₂O emission or set meaningful upper limits to this emission. A considerably larger number of ridge positions were observed using SWAS for which the total...
integration times were less, but nonetheless sufficient to obtain good signal-to-noise spectra of the stronger CI and $^{13}$CO $J = 5–4$ emission (Plume et al. 2000). These shorter-integration-time measurements were used to construct the extended (beyond the water-map) CI and $^{13}$CO maps shown in Figures 5 and 6. Thus, with the exclusion of the nine shock-affected lines of sight surrounding position (0, 0), there remain 77 spatial positions for which integrated intensities were obtained for all species and which form the basis of the analysis of the quiescent gas. As noted in Section 2, the spatial grid of beam positions and the beam size—synthesized in the case of the higher spatial resolution FCRAO maps—are the same for all species.

4. ANALYSIS

4.1. Line Optical Depth Effects

$H_2O$. Optical depth effects can lead to an underestimate of the total water column density along a given line of sight, creating the appearance that water is a surface tracer when it is not. Such can be the case for water under certain restricted conditions (cf. Poelman et al. 2007). Is this the case here? The $1_{10}–1_{01}$ transition of $H_2^{16}O$ has a high critical density, $\sim 8 \times 10^7$ cm$^{-3}$ at 30 K, and is expected to have a high optical depth for even a relatively low ortho-$H_2O$ column density. Thus, line trapping plays an important role in the excitation of this transition. For large optical depths, the “effective critical density” is $A_{\text{sc}} / (C_{\text{sc}} \tau_{L})$, where $A_{\text{sc}}$ is the spontaneous emission rate, $C_{\text{sc}}$ is the collisional de-excitation rate, and $\tau_{L}$ is the line-center optical depth. For densities less than the effective critical density, line photons may scatter multiple times but will eventually escape the cloud. In this limit, the line radiation is “effectively optically thin.”

We examine the question of whether the observed $H_2O$ lines toward the Orion ridge are effectively thin in two ways. First, we compute the emergent $H_2O$ $1_{10}–1_{01}$ line flux for a set of densities and water abundances representative of the Orion ridge. These results are shown in Figure 7. The line fluxes were computed under the large velocity gradient (LVG) approximation (see Neufeld & Melnick 1987, 1991); the collisional rate coefficients with $o-H_2$ and $p-H_2$ for the lowest 45 $H_2O$ rotational energy levels, corresponding to a maximum upper-level temperature of $\sim 2000$ K, are those reported by Faure et al. (2007), the first five levels of which at 20 K are those reported by Dubernet et al. (2006). In order to bound the range of likely $H_2$ ortho-to-para ratios (OPR), which is presently unknown, results are given for the LTE OPR value at 30 K as well as an OPR value of 3. Among the 77 spatial positions considered here, the average measured $H_2O$ line width is 3.9 km s$^{-1}$; we assume a line width of 3.5 km s$^{-1}$ in our calculations. Finally, we adopt a slab geometry which, because it yields the lowest escape probability for a given line-center optical depth, is the most conservative assumption; a polynomial fit to the exact expression for the photon escape probability from a plane-parallel emitting region (Hummer & Rybicki 1982) is used.
The maximum H$_2$O integrated antenna temperature, $\int T_A d\nu$, among the 77 positions considered is 3.26 K km s$^{-1}$. As can be seen in Figure 7, for integrated intensities below the maximum observed, the line flux increases with column density very nearly linearly, as expected for optically thin emission; the deviation from linear behavior is less than 20% in all cases. Finally, similar analyses for gas temperatures of 20 K and 50 K (not shown) support the conclusion that the H$_2$O 1$_{10}$–1$_{10}$ emission is effectively thin.

This result is consistent with that of Linke et al. (1977), who showed that if the main-beam antenna temperature, $T_{mb}$, satisfies $T_{mb} \ll (h\nu/4k) \exp(-h\nu/kT)$, then collisional excitation of the upper 1$_{10}$ level always results in a photon that escapes the cloud. At a kinetic temperature, $T$, of 30 K, the H$_2$O 556.9 GHz line is effectively thin if $T_{mb} < 2.7$ K, or the antenna temperature is less than 2.5 K (for $\eta_{mb} = 0.9$). The peak observed antenna temperature for the H$_2$O emission from the Orion ridge is $\sim$0.4 K, after correction for the SWAS main-beam efficiency. Thus, unless the beam filling factor for the H$_2$O emission is much less than 0.16, which appears unlikely given the distribution of gas shown in Figures 2–6, the H$_2$O emission is effectively optically thin. Future H$_2$O 556.9 GHz mapping observations toward the Orion ridge using the Herschel Space Observatory should be able to further test this assumption.

13CO. We are also interested in knowing whether the observed 13CO emission provides a good measure of total cloud depth. To assess this, we compute the 13CO column density required to achieve a line optical depth of 1 in the $J = 1$–0 transition using the RADEX LVG code (Van der Tak et al. 2007), the Einstein A-coefficients and collision cross sections from the Leiden Atomic and Molecular Database (Schöier et al. 2005) for the lowest 40 rotational energy levels, and the assumption of no CO
Figure 6. Left: SWAS integrated intensity map of the Orion Molecular Ridge in the $^{13}$CO $J = 5–4$ 550.9 GHz transition (see Table 1). Right: subset of the extended SWAS $^{13}$CO $J = 5–4$ map obtained with the longer integration times used to measure the H$_2^{16}$O $1_{0(10)}$–$1_{0(11)}$ 556.9 GHz emission. The peak $^{13}$CO $J = 5–4$ integrated intensity is 69.1 K km s$^{-1}$ and the contours are in increments of 7 K km s$^{-1}$ from an integrated intensity of 3 K km s$^{-1}$. All offsets are relative to $\alpha = 05^h35^m14^s5$, $\delta = -05^o22'37''$ (J2000).

freeze out. Line widths of 1.5 and 3 km s$^{-1}$ are assumed; the average observed $^{13}$CO $J = 1–0$ line FWHM is 2.8 km s$^{-1}$. As shown in Figure 8, for a gas temperature of 30 K, the $^{13}$CO $J = 1–0$ transition should be optically thin in most cases of interest here. However, because a few lines of sight have a $^{13}$CO line width less than 1.5 km s$^{-1}$, or may have a temperature less than 30 K, we choose to reference our measurements against the C$^{18}$O $J = 1–0$ transition to ensure a measure of the total cloud column density without concern for optical depth effects.

HCN, CN, C$_2$H, and N$_2$H$^+$. Several of the molecules observed have distinct hyperfine structure that can be used to estimate the optical depth of these lines. In the $J = 1–0$ transition of HCN, we observe the $F = 1–1$, $F = 2–1$, and $F = 0–1$ hyperfine lines; in the $J = 1–0$ transition of N$_2$H$^+$, we observe the $F_1 = 1–1$, $F_1 = 2–1$, and $F_1 = 0–0$ hyperfine lines; in the $N = 1–0$, $J = 1/2–1/2$ transition of C$_2$H, we observe the $F = 1–1$ and $F = 0–1$ hyperfine lines; and, in the $N = 1–0$, $J = 3/2–1/2$ transition of CN, we observe the $F = 3/2–3/2$, $F = 1/2–1/2$, $F = 5/2–3/2$, and $F = 3/2–1/2$ hyperfine lines. If we assume that the hyperfine lines are populated according to LTE, we can use the observed hyperfine ratios to determine the optical depth in the strongest hyperfine component. The greatest leverage on the optical depth comes from the ratio of the strongest to the weakest hyperfine line; for spectra with good signal-to-noise ratios, relatively accurate optical depths can then be derived. For those HCN, CN, C$_2$H, and N$_2$H$^+$ spectra with good measures of all hyperfine components, we find that more than 90% of these spectra are consistent with line-center optical depths of less than 1 and, in no instance, was a line-center optical depth greater than 1.5.
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\[ X(\text{H}_2\text{O}) = 1 \times 10^{-7} \]
\[ X(\text{H}_2\text{O}) = 5 \times 10^{-7} \]
\[ X(\text{H}_2\text{O}) = 5 \times 10^{-8} \]
\[ n(\text{H}_2) = 3 \times 10^4 \text{ cm}^{-3} \]
\[ n(\text{H}_2) = 3 \times 10^5 \text{ cm}^{-3} \]
\[ n(\text{H}_2) = 3 \times 10^6 \text{ cm}^{-3} \]

**Figure 7.** Plots of computed \( \text{H}_2\text{O} \) integrated antenna temperature for a Gaussian line, \( 1.064 \times \int T_A dv \), versus \( \text{H}_2 \) column density. The calculations assume a slab geometry, a gas temperature of 30 K, and a line width of 3.5 km s\(^{-1}\). The horizontal dashed line in each plot denotes the maximum integrated antenna temperature measured among the 77 spatial positions sampled, 3.26 K km s\(^{-1}\). Thus, the \( \text{H}_2\text{O} \) integrated intensities from all observed positions can be reproduced by conditions below the dashed line. Upper left: curves of \( \int T_A dv \) vs. \( N(\text{H}_2) \) for \( X(\text{H}_2\text{O}) = 10^{-7} \), an \( \text{H}_2 \text{O PR} = 0.03 \), the LTE value at \( T = 30 \) K, an \( \text{H}_2\text{O OPR} = 3 \), and \( \text{H}_2 \) densities of \( 3 \times 10^4, 10^5, \) and \( 3 \times 10^5 \) cm\(^{-3}\). Upper right: same as the upper left plot, except the \( \text{H}_2 \text{O OPR} \) is assumed to be 3. Lower left: curves of \( \int T_A dv \) vs. \( N(\text{H}_2) \) for \( n(\text{H}_2) = 10^5 \), an \( \text{H}_2 \text{O PR} = 0.03 \), an \( \text{H}_2\text{O OPR} = 3 \), and assumed total (ortho+para) \( \text{H}_2\text{O} \) abundances of \( 5 \times 10^{-8}, 10^{-7}, \) and \( 5 \times 10^{-7} \). Lower right: same as the lower left plot, except the \( \text{H}_2 \) OPR is assumed to be 3. The depth into the cloud, measured in magnitudes of visual extinction, assumes \( N(\text{H}_2) = 9.5 \times 10^{20} \text{ A}_V \text{ cm}^{-2} \).

**4.2. CO Depletion**

The \( \text{C}^{18}\text{O} \) integrated intensity can be used as a reliable measure of cloud depth only if CO remains undepleted throughout the column of gas observed. The gas-phase CO abundance is depleted mainly in two ways.

First, it is assumed that all CO that strike dust grains when the grain temperatures are \( T_{gr} \lesssim 20 \) K will stick to the surface and be removed from the gas phase. The timescale for this process is \( \sim 6 \times 10^4 \frac{[5 \times 10^3 \text{ cm}^3/n(\text{H}_2)\] (30 K / T_{gr})^{1/2}}{\text{yr}} \) (cf. Hollenbach et al. 2009), thus leading to the rapid freeze out of CO unless subsequently desorbed.

Second, in regions where grain temperatures are above the sublimation temperature of CO-ice, but below that of \( \text{H}_2\text{O} \)-ice, i.e., \( 20 \text{ K} < T_{gr} < 90 \text{ K} \), CO can still be depleted through reactions with \( \text{He}^+ \) and the continuous removal of elemental O from the gas-phase. Specifically, \( \text{He}^+ \) created by cosmic rays can react with CO to produce \( \text{C}^+, \text{O}, \) and \( \text{He} \). The O thus produced can react to reform CO in the gas-phase or form \( \text{H}_2\text{O} \) in the gas-phase or on grain surfaces. Whether formed in the gas-phase or on grains, most of the \( \text{H}_2\text{O} \) will eventually end up on grain surfaces, where it will remain unless desorbed. In the absence of significant FUV photodesorption or cosmic-ray desorption, this process results in a steady decrease in the gas-phase elemental oxygen abundance and the significant depletion of CO in about \( 10^6 \) years.

It is well established that CO suffers strong depletion in the central parts of dense low-mass cloud cores, such as B68 (Bergin et al. 2006), L1544 (Caselli et al. 1999), L1498 (Willacy et al. 1998), IC 5146 (Kramer et al. 1999), and the Taurus molecular cloud (Pineda et al. 2010). Given the low dust temperatures measured toward the cores of these regions, it is assumed that direct CO freeze out onto grains is primarily responsible for the observed depletion.
Is CO depletion significant within the Orion ridge? There are three reasons to believe that it is not a factor here. First, infrared and submillimeter observations toward the Orion ridge are best fit by dust temperatures between about 20 K and 30 K (e.g., Johnstone & Bally 1999; Mookerjea et al. 2000), making it unlikely that direct freeze out of CO onto dust grains is occurring. Second, unlike in cold cores, Zinchenko et al. (2009) find no evidence for CO depletion within other regions of high-mass star formation studied—i.e., W3, DR21, S140, S187, and S255. Third, the ratio of N$_2$H$^+$ to C$^{18}$O integrated intensities toward the Orion ridge varies only by about a factor of two over the full range of observed C$^{18}$O integrated intensities. Since negligible N$_2$H$^+$ depletion is observed toward colder regions of comparable density (see Tafalla et al. 2004 and references therein), particularly for depths into the cloud corresponding to the visual extinction range of greatest interest here, i.e., $A_V < 20$ (e.g., Bergin et al. 2002), the N$_2$H$^+$-to-C$^{18}$O ratio would be expected to increase by several orders of magnitude if CO depletion were significant. The absence of any substantial CO depletion may suggest that the age of the Orion ridge is less than the timescale for CO depletion by He$^+$ destruction. Thus, throughout the remainder of this paper, we assume that CO is undepleted within the portion of the ridge observed in H$_2$O by SWAS.

4.3. Abundance Profiles

Because of the face-on appearance of the Orion ridge and its relatively strong extended emission, which permits many independent spatial samples, this source offers a particularly good opportunity to study observationally the distribution of water vapor in dense molecular clouds. To do so, we seek to examine correlations between gas-phase H$_2$O and a number of other species whose distribution with depth is believed to be well understood. With a face-on appearance, one method for investigating the line-of-sight distribution of a species is to plot its integrated intensity versus that of C$^{18}$O (for the same spatial positions), where the optically thin C$^{18}$O $J = 1$–0 emission serves as a proxy for the total column thickness of a given line of sight. Relating the C$^{18}$O $J = 1$–0 integrated intensity to the total C$^{18}$O column density, $N$(C$^{18}$O), can be approached in two ways.

First, by assuming the C$^{18}$O emission is optically thin and the background radiation terms can be ignored, it is possible to derive a simple analytical relation between the column density in the upper $J = 1$ state of the transition and the integrated intensity of the line (in K km s$^{-1}$), corrected by main-beam efficiency ($\sim 0.5$ for FCRAO at the C$^{18}$O line frequency):

$$N(J = 1) = 3.8 \times 10^{14} \times \int T_R(C^{18}O) \, dv \, \text{cm}^{-2},$$

where $T_R$ is the radiation temperature ($= T_A^*$/main-beam efficiency).

Using a standard partition function, this gives the following expression for the total C$^{18}$O column density:

$$N(C^{18}O) = 4.8 \times 10^{13} T^{0.65} \times \int T_R(C^{18}O) \, dv \, \text{cm}^{-2},$$

where $T$ is the gas temperature.

Second, using the LVG approximation, assuming an H$_2$ density of $10^5$ cm$^{-3}$, and including all of the background radiation terms, we compute the C$^{18}$O integrated intensity for a range of column densities and temperatures. Fitting these data, we obtain the relation:

$$N(C^{18}O) = 1.9 \times 10^{14} T^{0.65} \times \int T_R(C^{18}O) \, dv \, \text{cm}^{-2}.$$ 

This expression is accurate for temperatures between 15 and 100 K and column densities where the emission is optically thin. As shown in Figure 9, the two expressions are in good agreement, particularly over the range of temperatures most applicable to the Orion ridge—i.e., 20–40 K (cf. Ungerechts et al. 1997). At $T = 30$ K, the optically thin criterion is satisfied if the maximum column density divided by line width (in km s$^{-1}$) is $N(C^{18}O)/\Delta v < 3 \times 10^{16}$ s km$^{-1}$ cm$^{-2}$. Since the measured C$^{18}$O $J = 1$–0 integrated intensities are all less than $4$ K km s$^{-1}$, implying $N(C^{18}O) < 7 \times 10^{15}$ cm$^{-2}$, and the C$^{18}$O line widths are all greater than 0.95 km s$^{-1}$, the optically thin assumption is justified for the lines of sight considered here.

The relation between the C$^{18}$O and H$_2$ column densities is best established in dark clouds and is based on extinction determinations from the Two Micron All Sky Survey (2MASS) data. For example, Kainulainen et al. (2006) examine the ratio of $N$(C$^{18}$O) and $A_V$ in Chamaeleon I and III-B using 2MASS and SEST data. Expressed in terms of the total visual extinction, $A_V$, averaging the two clouds presented in their paper yields approximately

$$A_V = 5 \times 10^{-15} N(C^{18}O) + 2.3$$

$$= 0.95 T^{0.65} \int T_R(C^{18}O) \, dv + 2.3 \, \text{mag}.$$ 

The offset is due to extinction of the surface layers where the gas-phase carbon is C$^+$ or CI, and not CO, and is uncertain and appears to vary from cloud to cloud (see summary by Harjupää et al. 2004). Ignoring the offset, this relation leads to an abundance ratio of $N$(C$^{18}$O)/$N$(H$_2$) $\sim 2 \times 10^{-7}$. The depth into the cloud, $A_V$, measured in visual magnitudes of extinction, as a function of C$^{18}$O integrated intensity for a range of assumed
temperatures is shown in Figure 10. These results are in good agreement with the previous study of Lada et al. (1994).

Figures 11 and 12 show plots of the ratio of the H$_2$O, C$_2$H, HCN, CN, C$_1$8O, J = 1–0, and N$_2$H$^+$ integrated intensities to those of C$_1$8O J = 1–0 as a function of the C$_1$8O J = 1–0 integrated intensity. The corresponding depth into the cloud, in visual magnitudes, is shown along the top axis of each plot. For these values, Equation (4) is used assuming $T = 30$ K. For the near-surface depths of particular interest here, corresponding to C$_1$8O integrated intensities less than about 1.5 K km s$^{-1}$, the AV derived from the C$_1$8O intensity is relatively insensitive to the assumed temperature.

Because the emission from most species toward BN/KL is strongly affected by the outflow, the data corresponding to the (Δα, Δδ) = (0, 0) and surrounding eight positions are not included in these plots. To better reveal any trends (by reducing the scatter in the 77 data points), the ratio values have been co-averaged in bins of C$_1$8O J = 1–0 integrated intensity of width 0.2 K km s$^{-1}$ in the x-axis. The plotted y-value within each bin is the weighted mean, $\mu = \Sigma(y_{i}/\sigma_{i}^{2})/\Sigma(1/\sigma_{i}^{2})$, of the i data points lying within that bin, where $y_{i}$ is the ratio of the integrated intensity, I, of species a to species b for point i, i.e., $y_{i} = I_{a,i}/I_{b,i}$, and $\sigma_{i} = \sqrt{(y_{i}^{2}(\sigma_{a,i}^{2}/I_{a,i}^{2} + \sigma_{b,i}^{2}/I_{b,i}^{2}))^{1/2}}$, where $\sigma_{a,i}$ and $\sigma_{b,i}$ are the 1σ uncertainties associated with the ith integrated intensity for species a and b, respectively. The 1σ y-value error bars represent the uncertainty of the mean, $\sigma_{a} = [1/\Sigma(1/\sigma_{i}^{2})]^{1/2}$. Though barely visible in these plots, the 1σ error bars representing the x-value dispersion within each bin are also shown.

The results fall broadly into two categories—i.e., those species that exhibit an increase in their integrated intensities relative to C$_1$8O toward lower AV’s and one that shows an increase in this ratio with depth. Specifically, C$_2$H, CN, HCN, and CI all show a steady rise in the observed intensity ratio toward the cloud surface, with the possible indication that the CN and HCN profiles subsequently decrease at AV < 5. Conversely, the ratio of N$_2$H$^+$ to C$_1$8O integrated intensities appears to increase with depth.

One measure of whether these plots convey an accurate picture of the abundance profiles is provided by the observed profile of C$^{13}$O/C$^{18}$O integrated intensities, shown in Figure 12. Assuming the observed C$^{13}$O J = 1–0 line is optically thin and depletion of CO is not significant along the ridge, the C$^{13}$O/C$^{18}$O intensity ratio deep in the cloud is expected to reflect the isotopic ratio of $^{16}$O/$^{18}$O of 500 and $^{12}$C/$^{13}$C of between 43 (Hawkins & Jura 1987; Stacey et al. 1993; Savage et al. 2002) and 65 (Langer & Penzias 1990), i.e., C$^{13}$O/C$^{18}$O $\simeq$ 8–12. The observed C$^{13}$O/C$^{18}$O intensity ratio deep in the cloud is in good agreement with these values and, thus, provides reason to believe the inferred profiles are descriptive of the actual profiles.

Figure 11 clearly shows an increase in the H$_2$O/C$^{18}$O intensity ratio at AV $< 15$, with a steady rise toward the cloud surface. Because the increase is evident between AV $\sim 5$ and 15, where the C$^{18}$O abundance is predicted to be approximately constant, the inferred increase in the H$_2$O emission toward the cloud surface appears to be real.

### 4.4. Principal Component Analysis

A second method for studying the correlations between species involves use of multivariate analysis referred to as principal component analysis (PCA). PCA’s goal is to find, among linear combinations of the data variables, a sequence of orthogonal, or completely uncorrelated, factors that most efficiently explain the differences in the data. Details of this method are provided elsewhere (cf. Ungerechts et al. 1997 for applications to astronomical mapping data) and will not be repeated here, except to note that the PCA approach provides a useful and compact means for quantifying the commonality between maps made in different transitions.

In PCA, we attempt to explain the total variability of p correlated variables through the use of p orthogonal principal components (PCs). The components themselves are merely weighted linear combinations of the original variables such that PC 1 accounts for the maximum variance in the data of any possible linear combination, PC 2 accounts for the maximum
Figure 11. Plots of the ratio of the H$_2$O, C$_2$H, HCN, and CN integrated intensities to the C$^{18}$O $J = 1$–0 integrated intensity versus the C$^{18}$O $J = 1$–0 integrated intensity. Using Equation (4) and assuming a gas temperature of 30 K, the ratios are also presented as a function of visual magnitude, A$_V$. The 77 spatial positions observed have been binned according to their C$^{18}$O integrated intensities and co-averaged in 20 equal x-axis bins of 0.2 K km s$^{-1}$ to reduce the dispersion in each plot. The x–y error bars for each point represent the error-weighted mean and 1σ uncertainty in the mean for the co-averaged points in each bin. The high point at a C$^{18}$O integrated intensity of 3.3 K km s$^{-1}$ represents one spatial sample corresponding to position $\Delta\alpha, \Delta\delta = 6.4, 0$. The proximity of this one sight line to BN/KL is likely responsible for the elevated ratio values seen in these plots.

amount of variance not explained by PC 1 and that is orthogonal to PC 1, and so on. Even though use of all p PCs permits the full reconstruction of the original data, in many cases the first few PCs are sufficient to capture most of the variance in the data. Thus, we can express each observed map (to within the noise) as a different linear combination of just two or three maps (i.e., two or three PCs).

To ensure that the analysis gives equal weighting to each line—versus allowing the brightest lines to dominate the analysis—the integrated intensities for each spectral line have been mean subtracted and divided by the standard deviation. In addition, to reduce the variance due to excitation and varying line emissivity, only those transitions with a critical density greater than 10$^4$ cm$^{-3}$ (see Table 1) are included in the PCA. The results are shown in Figure 13.

The interpretation of these results is straightforward. The top panel in Figure 13 plots the fraction of the total variance in the data captured by each PC. For the data considered here, 90% of the total variance between species is accounted for with PCs 1 and 2, and 96% of the total variance is accounted for with the addition of PC 3.

The lower two panels in Figure 13 plot the coefficients for the first and second, and second and third PCs, respectively. Because almost all of the variation in the data is in PCs 1 and 2, the bottom left panel is most relevant. There are two key elements in the plot to note: (1) the degree to which each vector approaches the unit circle and (2) the clustering of vectors. Because the PCs are normalized such that the quadrature sum of the coefficients for each species is unity, the proximity of the points to the circle of unit radius is a measure of the degree to which any two PCs
Figure 12. Same as Figure 11, except for the ratio of the CI, $^{13}$CO, and N$_2$H$^+$ integrated intensities to the C$^{18}$O $J = 1$–0 integrated intensity and the H$_2$O to N$_2$H$^+$ integrated intensities to the C$^{18}$O $J = 1$–0 integrated intensity. Note that one point at the lowest C$^{18}$O integrated intensity is excluded from the bottom two panels due to the absence of detectable N$_2$H$^+$ emission from these positions.

The vectors representing H$_2$O and N$_2$H$^+$ in this plot show the greatest separation, suggesting no particular correlation exists between the lines of sight where the H$_2$O and N$_2$H$^+$ integrated intensities are strong.

The bottom right panel in Figure 13, i.e., PC 2 versus PC 3, shows the distribution of residual variance between the species. The short vectors (from the 0,0 point) illustrate quantitatively the relative unimportance of additional sources of variance between species beyond those captured in the first two PCs.

5. DISCUSSION

The distribution of water vapor within a molecular cloud depends upon both the gas-phase chemistry that forms H$_2$O and a number of important micro-physics processes. These processes include the rate at which oxygen atoms strike dust grains and combine with hydrogen on their surfaces to form OH and H$_2$O, the rate at which such H$_2$O is removed from...
Figure 13. Results of PCA analysis for high (i.e., $>10^4$ cm$^{-3}$) critical density species. Top: fraction of the total variance accounted for by each PC, along with the cumulative fraction for the first $n$ PCs as a function of $n$. Bottom left: coefficients for the first and second PCs needed to approximate the maps of each transition. Bottom right: coefficients for the second and third PCs.

grain surfaces by incident UV photons (i.e., photodesorption) and cosmic rays, and the rate at which gas-phase H$_2$O is destroyed by UV photons (i.e., photodissociation). Because these processes are operative in all quiescent molecular clouds to varying degrees, testing models that incorporate the necessary chemistry and physics is important. Water is a particularly good diagnostic since its gas-phase abundance is sensitive to all of the above processes. In addition, water is a molecule of great (and growing) inherent interest.

The need to refine our understanding of water vapor in molecular clouds, and the motivation for this study, results from two main SWAS findings. First, it became clear early in the SWAS mission that more than just gas-phase chemical models are needed to explain the inferred H$_2$O abundances toward quiescent clouds. In particular, in cold ($T \lesssim 30$ K), dense ($n$(H$_2$) $\gtrsim 10^5$ cm$^{-3}$) clouds, the inferred abundance of gaseous H$_2$O is $\sim$ 100 to 1000 times less than the predictions of ion–neutral gas-phase chemical models and the O$_2$ abundance is at least 100 times less than predictions (cf. Neufeld et al. 1995, 2000b, 2003; Snell et al. 2000a, 2000b, 2000c; Goldsmith et al. 2000; Bergin et al. 2000; Melnick 2004).

A post-flight review of the SWAS data revealed a second important clue. As shown in Figure 14, the peak antenna temperatures observed toward 83 giant and dark cloud cores display a relatively small spread in values; almost 70% of the sources observed have a peak antenna temperature within a factor of two of 100 mK. To understand why this is significant, it is useful to consider how the line emission scales with the physical conditions. For effectively thin emission, the $1_{01}-1_{00}$ 556.9 GHz integrated intensity can be expressed as

$$\int T_A d\nu = \eta_{\text{mb}} C_{\text{f}} \left( \frac{h\nu}{4\pi} \right) \left( \frac{c^3}{2\nu^3} \right) x(o-H_2O)$$

$$\times N(H_2) n(H_2) e^{-h\nu/kT_k} \text{ K km s}^{-1}, \quad (5)$$

where $\nu$ is the line frequency, $x(o-H_2O)$ is the ortho-H$_2$O abundance (relative to H$_2$), $N(H_2)$ is the H$_2$ column density, and $n(H_2)$ is the H$_2$ volume density. Consequently, in the optically thin limit, the integrated intensity increases linearly with increasing H$_2$ column and volume densities, even if the line center optical depth is large. Since the measured velocity-resolved line widths (FWHM) toward quiescent giant and dark clouds are all within a factor of two of 5 km s$^{-1}$, the peak antenna temperatures should reflect the spread in $x(o-H_2O)$, $N(H_2)$, and $n(H_2)$ among the sources.

The relatively small variation in the peak H$_2$O line intensity between sources with more than order-of-magnitude differences in H$_2$ column densities (inferred from both $^{13}$CO and C$^{18}$O measurements), and H$_2$ volume densities (inferred from a variety of molecular species) suggests that the ortho-water column density, i.e., $x(o-H_2O) N(H_2)$, and H$_2$ density within the water-emitting region are not particularly sensitive to the total depth and peak density of the target clouds. Such could only be the case if the water-vapor emission originates predominantly from a zone within the cloud whose density, column density, and H$_2$O
and find that the value of \( \mu \)ii, measured toward 83 dark and giant cloud cores by SWAS. Almost 70% of the sources were observed to have peak \( T_A^* \)'s within a factor of two of 100 mK, while more than 80% of the sources exhibit peak \( T_A^* \)'s between 50 and 300 mK (gray area). This distribution is much narrower than would be expected based on the spread of column densities and volume densities of the sources in the sample (see the text).

abundance are tightly coupled, with little variation from cloud to cloud.

Ideally, it would be desirable to directly measure the depth dependence of the water emission. Regrettably, this is impossible with the face-on appearance of the Orion ridge and attempts to do so indirectly—for example, by modeling the emission from each of the 77 lines of sight considered here—are complicated by often unknown variations in the physical conditions along the ridge, including the varying incident FUV flux. Instead, we seek to extract the desired information from the ensemble of data, such as whether the water-vapor emission correlates better with surface tracers (i.e., species whose depth of peak abundance is relatively small and located near the cloud surface), or volume tracers (i.e., species whose abundance increases and attains a near-constant maximum with depth into the cloud).

Models of photodissociation regions (PDRs) provide the detailed predictions necessary to identify the surface and volume tracers. Unfortunately, the depth-dependent abundance profiles are affected by the strength of the incident FUV field, which varies along the Orion ridge. Stacey et al. (1993) have modeled the FUV-sensitive 157.74 \( \mu \)m [C ii] emission from OMC-1 and find that the value of \( G_0 \), the factor by which the FUV field exceeds the local interstellar value, at \( d \) parsecs projected distance, or \( \theta_{arc} \) arcmin angular separation, between the Trapezium cluster and a given point along the ridge is given by

\[
G_0 = \frac{8.6 \times 10^3}{(d^2 + d_c^2)^{1/3}} = \frac{8.6 \times 10^3}{(480 \tan(\theta_{arc}/60))^2 + 0.152)^{1/3}},
\]

where \( d_c \) is the distance, in parsecs, along the line of sight between the foreground Trapezium cluster and the molecular cloud, assumed to be 0.39 pc (see Figure 1). Thus, for the ridge positions considered here, \( G_0 \) is expected to vary between \( \sim 2 \times 10^4 \) and \( \sim 100 \) from about 5–30 arcmin from BN/KL, respectively. The presence of a large number of B-stars in the Orion molecular cloud complex, in addition to the OB stars in the Trapezium cluster, suggests that the strength of the FUV field predicted by Equation (6) far from BN/KL is likely to be a lower limit.

Figure 15 shows the predicted depth-dependent gas-phase abundance profiles for the observed species for \( 100 \leq G_0 \leq 2 \times 10^3 \), while Figure 16 shows the predicted profiles for \( 10^4 \leq G_0 \leq 2 \times 10^5 \). It is important to note that these models assume that H2O remains in the gas phase throughout the cloud and does not freeze out. As discussed earlier, the freeze out of H2O locks elemental oxygen in ice, reducing the gas-phase oxygen abundance and altering the gas-phase chemistry. If this is the case, as the current data suggest, then the abundance profiles in Figures 15 and 16 no longer reflect the actual abundance profiles at depths greater than \( A_v \sim 6–8 \) where H2O begins to freeze out for the densities and \( G_0 \)'s relevant to the Orion ridge (see Hollenbach et al. 2009). Nevertheless, the H2O freeze-out point lies beyond the depth where all but two of the species observed here—i.e., CO and \( N_2H^+ \)—peak and, thus, these figures provide some guidance. (As discussed in Section 4.2, it is assumed that CO and \( N_2H^+ \) are undepleted within the region of interest here.)

Over the broad range of FUV field strengths relevant here, species such as C, CN, C2H, and HCN are predicted to reach their peak abundance within 8 visual magnitudes of the cloud surface and subsequently decrease in abundance. Though observations of CI provide some evidence for emission in molecular cloud interiors (e.g., Keene et al. 1985), its creation via CO photodissociation clearly establishes this species as a surface tracer. C2H and CN have been found to trace the edges of clouds exposed to UV radiation (Jansen et al. 1995a; Rodríguez-Franco et al. 1998). In general, these simple carbon-based radicals can form rapidly via reactions between C and \( C^+ \) with other simple molecules (e.g., Sternberg & Dalgarno 1995). This will lead CN and C2H to trace regions where CI and \( C^+ \) are abundant (e.g., the cloud surface). The formation of HCN is more complex, with several contributing pathways, but in general this species can form in abundance in regions where CI/CO \( \sim 1 \), and thus it too can appear in abundance at low to moderate extinctions where CI is present.

Alternately, species such as \( ^{12}C^{16}O \), \( ^{13}C^{16}O \), \( ^{18}C^{16}O \), and \( N_2H^+ \) rise in abundance between 2 and 8 visual magnitudes of the surface.
and maintain near-constant values with increasing depth. In the case of N$_2$H$^+$, this molecule requires the a priori formation of N$_2$, which itself forms in a staged process through N + OH → NO + H and NO + N → N$_2$ + O. These neutral–neutral reactions are not fast enough to compensate for photodissociation, leading N$_2$H$^+$ to preferentially appear in abundance only at greater depths.

For CI, CN, HCN, C$_2$H, $^{13}$CO, and N$_2$H$^+$, the trends indicated in the models are reflected in the observed profiles shown in Figures 11 and 12. Because the C$_{18}$O abundance is predicted to decrease sharply for $A_V < 5$ (due to FUV photodestruction of the molecule), it is useful to restrict our consideration to $A_V \gtrsim 5$ where the C$_{18}$O abundance is predicted to be relatively constant. Specifically, C$_2$H, CN, and CI, all of which have their predicted peak abundance at $A_V < 4$ over the full range of $G_o$, show a steady rise in the observed intensity ratio toward the cloud surface. Likewise, HCN, which is predicted to peak in its abundance at $A_V \simeq 6\sim 7$, shows an increase in the measured HCN/C$_{18}$O intensity ratio toward these $A_V$’s, with perhaps an indication that the HCN abundance may yet be higher than predicted at $A_V \sim 5$. Conversely, N$_2$H$^+$, which is predicted to achieve a near-constant abundance at $A_V \gtrsim 9$, if anything shows a slightly increasing N$_2$H$^+$/C$_{18}$O intensity ratio beyond an $A_V$ of $\sim 25$. Within a number of other high-mass clouds, the N$_2$H$^+$ abundance is observed to increase in regions of lower fractional ionization due to decreased rates of dissociative recombination (Zinchenko et al. 2009). This may also explain the rise in the N$_2$H$^+$/C$_{18}$O intensity ratio toward higher $A_V$’s observed in Orion.

However, the observed H$_2$O profile is in conspicuous disagreement with the predictions of the PDR models summarized in Figures 15 and 16. These models, which neglect H$_2$O freeze out, predict a steady increase in the gas-phase water abundance between an $A_V \sim 2$ and 10, reaching a steady-state abundance of $\sim 2 \times 10^{-5}$. In addition to predicting a gas-phase H$_2$O abundance more than two orders of magnitude greater than observed, the predicted H$_2$O abundance profile would lead to a tighter correlation with N$_2$H$^+$, and a reduced correlation with $^{13}$CO ($J = 5\rightarrow 4$, CN, HCN, and C$_2$H, than indicated by the PCA.

It is worth asking whether the correlation between the H$_2$O emission and the other surface tracers reflects little more than the preferential excitation of water vapor in the warmer surface layers? To examine this possibility we consider three cases shown in Figure 17. First, we compute the depth-dependent H$_2$O emission resulting from the PDR models of Sternberg & Dalgarno (1995), who considered the chemistry within dense ($n$(H$_2$) = $5 \times 10^5$ cm$^{-3}$) gas subject to strong ($G_o = 2 \times 10^5$) external FUV irradiation, but no H$_2$O freeze out. In their model, H$_2$O is produced at $A_V = 0.6$ and $T = 800$ K by the neutral–neutral reactions, O + H$_2$ → OH + H and OH + H$_2$ → H$_2$O + H. However, the abundance of H$_2$O in this hot gas layer is suppressed by the high FUV field which rapidly photodissociates the water. Deeper into the cloud, i.e., at $A_V > 5$, where the FUV is attenuated and the gas temperature has dropped to $\sim 22$ K in their model, a series of gas-phase ion–neutral reactions produces a relatively high abundance of H$_2$O ($x$(o–H$_2$O) $\sim 3 \times 10^{-5}$) which survives photodestruction. For the sample case considered, this model would result in more than 90% of the water vapor emission arising between $A_V = 5$ and 20, and this fraction would be expected to increase further with increasing cloud depth. Even for a line of sight with a total depth equivalent to $A_V = 10$, approximately 80% of the water-vapor emission is calculated to arise at $A_V > 5$. Thus, a PDR model which considers water formed only in the gas phase, and which remains in the gas phase through the depth of the cloud, does not fit the Orion data.

To assess the case of constant water vapor abundance throughout the cloud volume, we apply the Sternberg and Dalgarno model above, except the ortho-H$_2$O abundance is assumed to be $5 \times 10^{-7}$ (relative to H$_2$) and constant with depth. This value is at the high end of, but nonetheless consistent with, the range of water abundances inferred from SWAS observations of quiescent clouds, assuming the depths of the H$_2$O and H$_2$ regions are the same (e.g., Snell et al. 2000c). As shown in the middle panel of Figure 17, most of the water-vapor emission originates throughout the volume of the cloud. Nonetheless, for clouds of total depth less than an $A_V$ of about 12, more than half of the total water emission would originate in the warm surface layers (i.e., $A_V \lesssim 3$). In practice, however, the presence of a $G_o \gtrsim 100$ FUV field would destroy almost all of the water near the cloud surface, as is evident from the H$_2$O abundance profiles in Figures 15 and 16, and more recently confirmed by Hollenbach et al. (2009). Thus, for the case of a constant water abundance throughout the cloud, the water emission would again be expected to increase with cloud depth, which it does not.

Third, we consider a temperature and H$_2$O abundance profile based on the model of Hollenbach et al. (2009), except for $n$(H$_2$) = $5 \times 10^4$ cm$^{-3}$ and $G_o = 10^5$. In this model, the temperature and chemical structure of a cloud are determined not only by the gas-phase chemistry, but also by the freezing of species onto grains, simple grain surface chemistry, and desorption (including FUV photodesorption) of ices. The resulting gas-phase H$_2$O abundance is found to peak in a region between the cloud surface, where H$_2$O is photo-destroyed by FUV photons, and the deeper interior, where the FUV field is highly attenuated and gas-phase H$_2$O depletes rapidly onto grains as frozen water-ice (see Figure 18). Because the sublimation temperature of water-ice is high (i.e., $\gtrsim 90$ K), it remains on the grains until sputtered off by the passage of a nondissociative shock, heated by an embedded source, photodesorbed by FUV radiation, or removed by cosmic rays. Specifically, this
Figure 17. Calculated fraction of the total H$_2$O emission arising from various depths into a dense cloud between $A_V = 0$ to 20. Left panel: profiles of temperature and H$_2$O abundance obtained from Sternberg & Dalgarno (1995) for a PDR with $n$(H$_2$) = $5 \times 10^5$ cm$^{-3}$ and $G_0 = 2 \times 10^5$. The profiles in their paper cover the range $0 < A_V < 10$; our calculations were extended to an $A_V$ of 20 by assuming that both the temperature and H$_2$O abundance at $A_V = 10$ have reached equilibrium values that apply between $A_V = 10$ and 20. Middle panel: for the case of a constant water abundance, we use the Sternberg & Dalgarno PDR density and temperature profile, but assume a constant H$_2$O abundance of $5 \times 10^{-7}$, consistent with maximum H$_2$O abundance predicted by Hollenbach et al. (2009). Right panel: profiles of temperature and H$_2$O abundance from Hollenbach et al. (2009) model. In all cases, the collisional rates of Faure et al. (2007) were used and ortho-to-para H$_2$ and H$_2$O ratios of 3:1 and total line width of 3 km s$^{-1}$ were assumed.

Figure 18. Left: schematic depiction of water-vapor zone within molecular clouds, including the main processes affecting the gas-phase water abundance. Center: H$_2$O and H$_2$O-ice abundances for a cloud with $n = 10^4$ cm$^{-3}$ but with a variety of FUV field strengths incident on the cloud surface (after Hollenbach et al. 2009). Right: effect of changing the gas density for the FUV field strength $G_0 = 10^2$ where, following the convention used in Hollenbach et al. (2009), $n$ is the gas-phase hydrogen nucleus number density [$\sim n$(H) + 2$n$(H$_2$) + $n$(H$^+$)]. The Hollenbach et al. (2009) results depict steady state abundance profiles, including CO depletion due to reactions with He$^+$. Prior to the depletion of CO, the gas-phase H$_2$O abundances at high $A_V$ will be greater than shown here, though the peak of water abundance at intermediate $A_V$ is likely retained (see the text).
model predicts that the gas-phase H₂O and O₂ lies predominantly between an AV of approximately 3 and 8 for Gₐ = 1–10⁵, with the peak abundance occurring at a depth proportional to \( \ln (G_\text{av}/n_H) \), where \( n_H \) is the gas-phase hydrogen nucleus number density. As shown in the right panel of Figure 17, for this scenario (\( G_\text{av} = 10^4 \)) all of the water-vapor emission is predicted to arise from within a narrow range of depths around AV \( \sim 10 \) corresponding to the peak in the gas-phase H₂O abundance. For lower values of \( G_\text{av} \), but approximately equivalent densities, the peak gas-phase H₂O abundance shifts to lower AV’s, as shown in the center and right panels of Figure 18. However, unlike the assumptions underlying our analysis of the Orion ridge observations, the Hollenbach et al. models shown in Figure 18 depict steady-state abundance profiles, which include the effects of CO destruction due to He⁺. Without CO depletion, these models underestimate the gas-phase H₂O and CO abundances at high AV. However, the peak of water abundance at intermediate AV is likely preserved, consistent with the observations.

Finally, we note that the observed C₂H and N₂H⁺ transitions have similar excitation energies and critical densities (see Table 1), yet show strikingly different depth profiles (e.g., Figures 11 and 12). Thus, the variations in their depth-dependent integrated intensity profiles are not the result of excitation conditions.

Limits to the assumption of a simple homogeneous slab geometry, illuminated from one side, are also seen in the data. Specifically the intensity ratios for species such as CI, CN, HCN, and C₂H exhibit values at high AV’s (e.g., \( \gtrsim 15 \) mag) that exceed those expected on the basis of their low deep-cloud abundances as shown in Figures 15 and 16. This is most likely the result of the Orion ridge being somewhat clumpy (cf. Stacey et al. 1993 and references therein), permitting partial penetration of FUV photons deep into the cloud interior. In addition, B stars embedded within the molecular cloud may provide additional FUV flux. Thus, emission characteristic of predominately surface tracers can still be generated, albeit at a lower intensity, well within the cloud interior. In addition, if the effects of H₂O freeze out are added to the models shown in Figures 15 and 16, the deep-cloud abundance of CI, CN, HCN, and C₂H may be altered. This effect notwithstanding, the derived emission profiles for these species follow the trends predicted from PDR models, at least up to the depth where H₂O freezes out.

The conclusion that ground-state water-vapor emission is observed to arise primarily near molecular cloud surfaces is in accord with models, like Hollenbach et al. (2009), in which the gas-phase water abundance peaks where rates of photodestruction, photodesorption, and freeze-out balance. In this model, the distance from the cloud surface to the peak water-vapor abundance scales as \( \ln (G_\text{av}/n_H) \) and the range of depths over which the water vapor is relatively abundant is self regulating and remains approximately constant. Consequently, the water-vapor column density remains approximately constant over a broad range of FUV fluxes and densities, thus explaining the relatively narrow distribution of observed H₂O 1\( 10^{	ext{a}+1} \) peak antenna temperatures.

This picture is also consistent with the low observed upper limits to the O₂ abundance (Goldsmith et al. 2000). Since the ion–neutral reactions leading to the formation of O₂ depend upon the abundance of gas-phase O (via the reaction O + OH \( \rightarrow \) O₂+ H), reducing the atomic oxygen abundance by locking it in water ice suppresses O₂ production where water ice becomes abundant—i.e., beyond an AV of \( \sim 2 \) to 10. Thus, like water vapor, gas-phase O₂ is restricted to a relatively narrow zone between where it is photodestroyed near the cloud surface and where its formation is suppressed by a diminishing supply of atomic oxygen. Detailed calculations (e.g., Hollenbach et al. 2009) indicate that the resulting O₂ column densities are typically between \( 10^{15} \) and \( 10^{16} \text{ cm}^{-2} \), consistent with current observed limits.

Finally, evidence supporting an increasing column density of water-ice with depth is provided by observations of the water-ice band at 3 \( \mu \text{m} \) toward Taurus (Whittet et al. 2001) and Rho Ophiuchus (Tanaka et al. 1990), and the water-ice band at 6 \( \mu \text{m} \) toward Cepheus A East (Sonntentrucker et al. 2008). The onset for water-ice formation toward Taurus, Rho Ophiuchus, and Cepheus A East is determined to occur at AV’s of \( \sim 3.2, \sim 10 \), and 2.3 visual magnitudes, respectively, with the variation due primarily to the different FUV radiation environments for each cloud. These observations also confirm the presence of significant amounts of water-ice (\( \chi (\text{H₂O}_{\text{ice}}) > 5 \times 10^{-5} \)) in the deep interior of dense clouds (e.g., Nummelin et al. 2001; Boogert et al. 2004; Sonntentrucker et al. 2008). The detection of CO₂ ice with an abundance of \( \sim 2 \times 10^{-5} \) (Boogert et al. 2004; Sonntentrucker et al. 2008) further attests to the importance of ices as a repository of oxygen that would otherwise be available to form gas-phase H₂O and O₂.

In summary, the results of the observational study presented here show that most of the water vapor detected toward the Orion Molecular Cloud ridge originates near the cloud surface, between an AV of about 2 and 10. This finding is in general agreement with PDR models that consider the effects of photodissociation, grain-surface chemistry, photodesorption, and freeze out in addition to gas-phase chemistry. Future observations with the Herschel Space Observatory will allow more detailed follow-up studies of the water-vapor distribution in molecular clouds in several ways. First, Herschel’s smaller beam size at 557 GHz—40′′ versus \( \sim 230′′ \) for SWAS—will permit many more spatial samples than obtained here, improving the statistics for the type of analysis applied here. Second, access to additional ortho- and para-H₂O transitions will enable a more direct determination of the physical conditions in the water-vapor emitting region. Combined, these capabilities will allow increasingly stringent tests of our models of water in molecular clouds.

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