SOFIA/EXES OBSERVATIONS OF WATER ABSORPTION IN THE PROTOSTAR AFGL 2591 AT HIGH SPECTRAL RESOLUTION

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ABSTRACT

We present high spectral resolution (∼3 km s⁻¹) observations of the ν2 ro-vibrational band of H₂O in the 6.086–6.135 μm range toward the massive protostar AFGL 2591 using the Echelon-Cross-Echelle Spectrograph (EXES) on the Stratospheric Observatory for Infrared Astronomy (SOFIA). Ten absorption features are detected in total, with seven caused by transitions in the ν2 band of H₂O, two by transitions in the first vibrationally excited ν2 band of H₂O, and one by a transition in the ν2 band of H₂¹⁸O. Among the detected transitions is the ν2 1₁→0₁₀ line that probes the lowest-lying rotational level of para-H₂O. The stronger transitions appear to be optically thick, but reach maximum absorption at a depth of about 25%, suggesting that the background source is only partially covered by the absorbing gas or that the absorption arises within the 6 μm emitting photosphere. Assuming a covering fraction of 25%, the H₂O column density and rotational temperature that best fit the observed absorption lines are \( N(\text{H}_2\text{O}) = (1.3 ± 0.3) \times 10^{19} \text{ cm}^{-2} \) and \( T = 640 ± 80 \text{ K} \).

Key words: stars: protostars

1. INTRODUCTION

Water, despite being one of the most abundant species in the molecular interstellar medium (ISM), is difficult to observe in astrophysical objects due to its prevalence in the Earth’s atmosphere (see van Dishoeck et al. 2013 for a comprehensive review of astronomical water observations). Ground-based observations of H₂O have primarily targeted maser emission, most frequently the \( J_{K_a K_c} = 0_{1,0}→5_{2,3} \) transition near 22 GHz that was utilized in the initial detection of interstellar water (Cheung et al. 1969), although some have also focused on rotational and ro-vibrational transitions out of high-lying rotational levels in the mid-IR (Pontoppidan et al. 2010) and near-IR (Najita et al. 2000, p. 457; Carr et al. 2004; Salyk et al. 2008; Indriolo et al. 2013), respectively. These latter observations are possible because many high-lying rotational levels are not significantly populated in the Earth’s atmosphere, but their scope is limited to astrophysical sources with warm \( (T > 300 \text{ K}) \), dense gas.

Observations of the lowest-lying rotational levels of water—those able to probe cold gas—have required space-based observatories. The Infrared Space Observatory-Short Wavelength Spectrometer (ISO-SWS; de Graauw et al. 1996; Kessler et al. 1996) covered the ν2 ro-vibrational band (symmetric bending mode) of H₂O centered near 6 μm, and absorption out of the lowest-lying levels of the ortho and para nuclear spin modifications (1₁₁₀ and 0₁₁₀, respectively) was detected toward several massive protostars (Boonman & van Dishoeck 2003). Due to the low spectral resolution of the observing configuration \( (\lambda/\Delta\lambda \sim 1400) \) using SWS in AO16 grating mode, these lines were significantly blended with absorption from other nearby H₂O lines, making the determination of level-specific column densities impossible. Instead, the entire ν2 band was fit simultaneously assuming a single temperature to determine the total water column density, \( N(\text{H}_2\text{O}) \). The Submillimeter Wave Astronomy Satellite (SWAS; Melnick et al. 2000b) provided much higher spectral resolution (∼1 km s⁻¹) and covered the 1₁₀→1₀₁ pure rotational transition of H₂O at 557 GHz. This line was observed in both emission and absorption in multiple sources (e.g., Melnick et al. 2000a; Snell et al. 2000), demonstrating the ability to probe cold water. More recently, the study of low-lying rotational levels at high spectral resolution (∼0.5 km s⁻¹) has been facilitated by the Heterodyne Instrument for the Far-Infrared (HIFI; de Graauw et al. 2010) on board the Herschel Space Observatory (Pilbratt et al. 2010). Water has been detected in both emission and absorption out of levels with \( E \lesssim 200 \text{ K} \) in several protostars (e.g., van Dishoeck et al. 2011; van der Tak et al. 2013), and in absorption out of the 0₁₀₀ and 1₁₀₁ levels in the molecular ISM (e.g., Sonnentrucker et al. 2010; Flagey et al. 2013). Observations that resolve the velocity structure of absorption lines are vital to both determining level-specific column densities and understanding the dynamics of the absorbing/emitting regions. This is especially important for protostars as such objects contain multiple dynamical components (e.g., disk, envelope, jets, outflows, shocks).

AFGL 2591 is a region of ongoing high-mass star formation. The radio continuum source VLA 3 (for a description of sources, see Torrelles et al. 2014 and references therein) is the brightest mid-IR source in the region and drives a bipolar outflow. It was previously observed at 5–7 μm as part of the aforementioned ISO-SWS study, from which Boonman & van...
Dishoeck (2003) reported a best-fit water column density of $N(\text{H}_2\text{O}) = (3.5 \pm 1.5) \times 10^{18}$ cm$^{-2}$ at $T = 450 \pm 150$ K, assuming a Doppler line width of 5 km s$^{-1}$. Known kinematic components associated with AFGL 2591 include (1) the protostellar envelope with systemic velocity $-5.5$ km s$^{-1}$ in the local standard of rest (LSR) frame (van der Tak et al. 1999); (2) a blueshifted outflow at $-25$ km s$^{-1} < v_{\text{LSR}} < -6$ km s$^{-1}$ (Emprechtinger et al. 2012; van der Tak et al. 2013); (3) a redshifted outflow at $3$ km s$^{-1} < v_{\text{LSR}} < 15$ km s$^{-1}$ (Lada et al. 1984); (4) material entrained in a jet or wind, indicated by absorption in the $v = 1-0$ band of $^{12}\text{CO}$ that extends to $-196$ km s$^{-1}$ in the form of an asymmetric blue wing (van der Tak et al. 1999). There is also evidence of a rotating disk around VLA 3, although gas velocities in the disk match those of the envelope (van der Tak et al. 2006; Wang et al. 2012). The interested reader is referred to cartoon pictures (van der Tak et al. 1999, 2006; van der Wiel et al. 2011; Sanna et al. 2012; Wang et al. 2012) and multi-wavelength images (Johnston et al. 2013) of AFGL 2591 to gain a better understanding of the region. Because of the low spectral resolution of the ISO-SWS observations, it has been impossible to say with certainty which component gives rise to the H$_2$O absorption. To do so—and to better constrain the water column density and rotational temperature—we have targeted multiple transitions in the $\nu_2$ band of H$_2$O using the Echelon-Cross-Echelle Spectrograph (EXES; Richter et al. 2010) on board the Stratospheric Observatory for Infrared Astronomy (SOFIA; Young et al. 2012).

SOFIA operates at altitudes above 39,000 ft (11,887 m), where the precipitable water vapor burden is routinely less than 0.02 mm. Under these conditions the 6 $\mu$m region of the Earth’s atmosphere is no longer opaque, as it is from the ground. EXES provides high spectral resolution ($\approx$3 km s$^{-1}$) capabilities in the 4.5–28.3 $\mu$m range, making it well-suited for velocity-resolved observations of individual ro-vibrational transitions of the $\nu_2$ band of H$_2$O in astrophysical sources. We present here the first spectrally resolved detections of 10 absorption lines from transitions in the $\nu_2$ bands of H$_2$O and H$_2^{18}$O, including a detection probing the ground para level, $0_0(1)$. This highlights the opportunity to further probe water in cold molecular clouds without the need for a space-based observatory by utilizing EXES on SOFIA.

2. OBSERVATIONS AND DATA REDUCTION

AFGL 2591 VLA 3 was observed using EXES on board SOFIA at an altitude of 43,000 ft (13,106 m) on 2014 April 10 (UT) as part of instrument commissioning observations. Spectra were acquired in cross-dispersed high-resolution mode with a central wavelength of 6.1125 $\mu$m, using a slit length of 9″9, and a slit width of 1″9 to provide a resolving power (resolution) of 86,000 (3.5 km s$^{-1}$), with the resolution element sampled by 8 pixels. The telescope was nodded after every 27 s of integration, enabling subtraction of telluric emission lines, and the total exposure time for AFGL 2591 was 1134 s. Prior to observing the target, a calibration sequence was taken using the same wavelength setting and slit width. This sequence consisted of observations of the internal blackbody unit set to 260 ± 0.1 K and of blank sky (Lacy et al. 2002). These calibration frames were used to correct for blaze efficiency, pixel-to-pixel sensitivity variations, and also to provide a first order flux calibration using the expected photon counts from the blackbody unit. The bright star Vega was observed during a flight leg 2 hr before the science observations at the same altitude and air mass as AFGL 2591 for use as a telluric standard star. The observing sequence was similar to that employed for AFGL 2591.

Data were processed using the Redux pipeline (Clarke et al. 2015) with the fspextool software package—a modification of the Spextool package (Cushing et al. 2004) —which performs source profile construction, extraction and background aperture definition, optimal extraction, and wavelength calibration for EXES data. The preliminary wavelength scale output from the pipeline was refined by shifting the
shows the spectra for each transition shifted into the LSR frame following conversion from wavelength to line-of-sight velocity.

3. ANALYSIS

Absorption lines in Figure 2 were fit using a function of the form

\[ I = I_0 \left( 1 - f_e \left[ 1 - \exp \left( -\tau_0 \exp \left( \frac{(v - v_{\text{LSR}})}{2\sigma_v^2} \right) \right) \right] \right) \]  

(1)

where \( I_0 \) is the continuum level, \( f_e \) is the fraction of the background source covered by absorbing material, and the optical depth is assumed to have a Gaussian profile with optical depth at line center \( \tau_0 \), LSR velocity at line center \( v_{\text{LSR}} \), and velocity dispersion \( \sigma_v \). The \( \nu_2 \) \( 3_{1,2} \rightarrow 2_{2,1} \) and \( \nu_2 \) \( 4_{2,2} \rightarrow 3_{3,1} \) transitions were fit simultaneously (second and fourth panels from the bottom in Figure 2) using a version of this function modified for multiple lines. The \( \nu_2 \) \( 5_{3,3} \rightarrow 4_{4,0} \) and \( \nu_2 \) \( 3_{2,1} \rightarrow 3_{1,2} \) transitions (third from top and top panels) were fit separately despite their proximity to each other as there is no significant blending of the features. Due to interfering features near the \( \nu_2 \) \( 1_{1,0} \) transitions and \( \nu_2 \) \( 3_{1,1} \) transitions (bottom and third from bottom panels; see figure caption for explanation of features) only data at \( v_{\text{LSR}} = -23 \) km s\(^{-1}\) were used to constrain fits of these transitions. As the absorption features are broad with respect to the instrumental spectral resolution, we expect the lines to be resolved and convert the optical depth profile fit to a column density profile via

\[ \frac{dN}{dv} = \tau(v) \frac{g_i}{g_u} \frac{8\pi}{\mu A\lambda^2} \]  

(2)

under the assumption that the absorption is unsaturated, where \( g_i \) and \( g_u \) are statistical weights in the lower and upper states, respectively, \( \mu \) is the spontaneous emission coefficient, and \( A \) is the transition wavelength. We then integrate over the absorption feature in velocity space to determine the column density in the lower state of the observed transition.

Initial fits were made assuming that the absorbing gas completely covers the background source (\( f_e = 1 \)) and are shown as red curves in Figure 2. Resulting parameters for each transition are reported in Table 1. Inferred column densities are converted to \( \ln(f/N/g_i) \) and plotted versus lower state energy as red squares in Figure 3. The black dashed line shows the relationship expected for \( N(\text{H}_2\text{O}) = 3.5 \times 10^{18} \) cm\(^{-2}\) in local thermodynamic equilibrium (LTE) at \( T = 450 \) K (Boonman & van Dishoeck 2003). Column densities in the \( 3_{3,1}, 4_{3,1}, 4_{4,1}, \) and \( 4_{4,0} \) states are in agreement with predictions based on these values, but the states with \( E/k_B < 300 \) K are below predicted values, while vibrationally excited states are above predicted values. No single temperature provides a good fit to all nine points, but if we exclude levels with \( E/k_B < 300 \) K then we find \( N(\text{H}_2\text{O}) = (3.7 \pm 0.8) \times 10^{18} \) cm\(^{-2}\) in LTE at \( T = 590 \pm 50 \) K (marked by the red dotted line in Figure 3).

Assuming \( T \) and \( N(\text{H}_2\text{O}) \) from Boonman & van Dishoeck (2003), the \( \nu_2 \) \( 3_{1,2} \rightarrow 3_{0,3} \) transition should be saturated at line center, which is not the case. If the background source is partially covered by absorbing material or if the water absorption arises within the 6 \( \mu \)m emitting photosphere, then it is possible for optically thick, saturated lines to cause only a
| Transition\(^a\) | Wavelength (\(\mu m\)) | \(E_i/k_b\) (K) | \(g_i\) | \(A\) (s\(^{-1}\)) | \(v_{LSR}\) (km s\(^{-1}\)) | \(\sigma_i\) (km s\(^{-1}\)) | \(\theta\) | \(\ln (f_r N_i/N_b)\) |
|----------------|-----------------|-----------------|-------|-----------------|-----------------|-----------------|-------|-----------------|
| 1–0 5\(31,2\)-4,1,1 | 6.0887005 | 702.3 | 27 | 0.35 | –11.4 | 6.0 | 0.13 ± 0.03 | 35.2 ± 0.3 |
| 1–0 5\(31,2\)-4,3,1 | 6.0964081 | 552.3 | 9 | 0.73 | –11.7 | 5.5 | 0.13 ± 0.03 | 35.5 ± 0.3 |
| 2–1 2\(31,2\)-2,1,2 | 6.1009690 | 2412.9 | 15 | 5.92 | –9.7 | 5.5 | 0.09 ± 0.03 | 32.7 ± 0.4 |
| \(^{1}\)\(H_2\)\(^1\)\(O\) | 1–0 3\(31,2\)-3,1,2 | 6.1034870 | 248.7 | 21 | 6.40 | –10.4 | 4.7 | 0.06 ± 0.03 | 31.8 ± 0.5 |
| 1–0 3\(31,2\)-3,4,0 | 6.1039868 | 702.3 | 9 | 0.34 | –9.6 | 5.5 | 0.06 ± 0.03 | 35.4 ± 0.6 |
| 1–0 4\(31,2\)-3,3,1 | 6.1061925 | 410.4 | 7 | 0.53 | –10.5 | 7.3 | 0.12 ± 0.03 | 36.2 ± 0.3 |
| 1–0 3\(31,2\)-2,2,1 | 6.1068262 | 194.1 | 15 | 1.12 | –14.2 | 8.5 | 0.20 ± 0.04 | 35.2 ± 0.2 |
| 2–1 4\(31,2\)-3,1,3 | 6.1131638 | 2502.7 | 7 | 15.8 | –8.4 | 4.4 | 0.12 ± 0.03 | 32.2 ± 0.3 |
| 1–0 3\(31,2\)-3,0,3 | 6.1137707 | 196.8 | 21 | 6.24 | –16.9 | 8.5 | 0.34 ± 0.04 | 34.0 ± 0.1 |
| 1–0 1\(11,1\)-0,0,0 | 6.1163311 | 0 | 1 | 7.46 | –15.7 | 8.7 | 0.30 ± 0.04 | 35.7 ± 0.1 |

Notes. Columns 2–5 give the transition wavelength, \(\lambda\), lower state energy, \(E_i/k_b\), lower-state statistical weight, \(g_i\), and the spontaneous emission coefficient, \(A\), respectively. Columns 6–8 give the best-fit parameters from Equation (1), with covering fractions of 100% and 25% assumed in the top and bottom halves of the table, respectively. Uncertainties in \(v_{LSR}\) and \(\sigma_i\) are estimated to be 0.3 km s\(^{-1}\) at the 1\(\sigma\) level. Uncertainties in \(\theta\) assume that the uncertainty in the absorption depth at line center is equal to the root mean square noise level of 0.03 in the continuum of the ratioed spectrum prior to the removal of baseline fluctuations. The Doppler parameter, \(b\), and line FWHM are related to \(\sigma_i\) via the equations \(b = \sigma_i \sqrt{2}\) and FWHM = \(\sigma_i \sqrt{2 \ln(2)}\).

\(^a\) Transition labels are given as \(v_1-v_3\) \(I_{KJ_{K^*-K}}\), where a single prime denotes the upper state and double prime denotes the lower state, and both the \(v_1\) and \(v_3\) vibrational quantum numbers are omitted as they are 0 in all cases.

**Figure 3.** Rotation diagram for the nine detected \(H_2O\) transitions. The black dashed line is for \(N(\text{H}_2\text{O}) = 3.5 \times 10^{18} \text{ cm}^{-2}\) and LTE at 450 K as reported by Boonman & van Dishoeck (2003). Red squares and open blue diamonds denote covering fractions of 1 and 0.25, respectively. Lower limits are indicated by upward-pointing arrows. Note that the \(y\)-axis shows \(\ln (\frac{N(\text{H}_2\text{O})}{\beta_{K^*}})\), (i.e., it is scaled to the average column density in front of the entire background source). For optically thin absorption lines the value does not change significantly with covering fraction, but for optically thick lines (e.g., \(v_2 1, 1\)-0,0,0) the value increases substantially as \(f_r\) approaches the absorption depth. The red dotted line marks \(T = 590\) K and \(N(\text{H}_2\text{O}) = 3.7 \times 10^{18} \text{ cm}^{-2}\) for \(f_r = 1\), and is the best fit to levels with \(E_i/k_b > 300\) K. The blue dash–dot line marks \(T = 640\) K and \(N(\text{H}_2\text{O}) = 1.3 \times 10^{19} \text{ cm}^{-2}\) for \(f_r = 0.25\), and is the best fit to the seven unsaturated transitions.
fractional decrease in the continuum level. The minimum possible fractional coverage is equal to the depth of the strongest absorption line under consideration, in our case the $\nu_2 \, 3_{1,2}-3_{0,3}$ transition. However, the perceived astrophysical absorption from this transition is greatly affected by its telluric counterpart, and the line depth is highly dependent on the atmospheric division procedure. The same is true for the strongest line, the $\nu_2 \, 1_{1,1}-0_{0,0}$ transition. We use both lines in estimating the minimum covering fraction, choosing $f_c = 0.25$, but caution that this is highly uncertain. Fits using $f_c = 0.25$ are shown as blue curves in Figure 2, and resulting parameters are again in Table 1. Inferred column densities are plotted as open blue diamonds in Figure 3. Scaling by the covering fraction demonstrates that column densities inferred from optically thick transitions increase much more than those inferred from optically thin transitions as $f_c$ decreases, but at $f_c = 0.25$ the saturated $\nu_2 \, 3_{1,2}-3_{0,3}$ and $\nu_2 \, 1_{1,1}-0_{0,0}$ transitions only provide lower limits on column densities. A fit to the seven unsaturated transitions is shown by the blue dash-dot line in Figure 3 and corresponds to $N$ (H$_2$O) = (1.3 ± 0.3) × 10$^{19}$ cm$^{-2}$ in LTE at $T = 640 \pm 80$ K.

4. DISCUSSION

The pure rotational $1_{1,1}-0_{0,0}$ transition of H$_2$O at 1113.343 GHz (269.3 $\mu$m) is seen in both emission and absorption toward AFGL 2591 (van der Tak et al. 2013; Kâźmierczak-Barthel et al. 2014; Choi et al. 2015). The emission component arises in the protostellar envelope, and the absorption components in the blueshifted outflow and foreground gas. This absorption probes the same quantum state as the $\nu_2 \, 1_{1,1}-0_{0,0}$ transition, but a direct comparison is hindered by several effects. The emitting regions at 6 $\mu$m and 1.1 THz ($\sim$270 $\mu$m) are likely different, so that gas probed by one transition may not necessarily be probed by the other. Our EXES observations used a 9.9 by 1.0$''$ slit centered on VLA 3, while HIFI observations at 1113 GHz have a roughly circular beam with FWHM $\sim$19$''$, again meaning that different regions are being probed. Finally, emission from the $(\nu_1 \nu_2 \nu_3) J_K_K, J_{K,K} = (000)\,1_{1,1}$ state (53.4 K above ground) is extremely strong and interferes with the absorption features at 1113 GHz, whereas emission from the $(010)\,1_{1,1}$ state (2352 K above ground) is not observed, leaving the 6.1163311 $\mu$m line unobsured. All of these effects must be considered when comparing any results from HIFI and EXES.

As described in Section 1, different components of AFGL 2591 are distinguished by line of sight velocities, line profiles, and observed molecules. The H$_2$O absorption lines are centered at roughly $-16$ km s$^{-1}$ with FWHM $\sim$20 km s$^{-1}$ for the three lowest-lying levels and shift to $-11$ km s$^{-1}$ with FWHM $\sim$13 km s$^{-1}$ for the higher-lying levels, best matching the blueshifted outflow. These line profiles are most similar to absorption seen in HCN and C$_2$H$_2$ (Knez 2006, observed at 13 $\mu$m) as well as specific absorption components of $^{13}$CO and vibrationally excited $^{12}$CO (Mitchell et al. 1989; van der Tak et al. 1999, observed at 4.7 $\mu$m), all of which are thought to arise in hot, dense gas close to the central protostar. Several 22 GHz H$_2$O masers are observed throughout the region, with many concentrated in the walls of the blueshifted outflow associated with VLA 3 (Trinidad et al. 2003; Sanna et al. 2012; Torrelles et al. 2014). Although maser velocities are primarily at $V_{LSR} \lesssim -18$ km s$^{-1}$, absorption by gas in small, shocked clumps could explain the small covering fraction required by our analysis. Given the above, we posit that the H$_2$O absorption observed with EXES arises in hot, dense gas at the base of the blueshifted outflow.

Water emission attributed to the outflow component is observed with HIFI in multiple transitions as a broad feature (van der Tak et al. 2013; Kâźmierczak-Barthel et al. 2014; Choi et al. 2015), but is centered closer to the systemic velocity of the envelope than the absorption we see. Analysis of the H$_2$O outflow emission by Choi et al. (2015) indicates a temperature of $T \sim 70-90$ K and column density of $N$ (H$_2$O) $\sim 4 \times 10^{13}$ cm$^{-2}$, similar to results found by Karska et al. (2014) who analyzed unresolved H$_2$O absorption observed with PACS on Herschel, finding $T = 160 \pm 130$ K and $N$ (H$_2$O) $\sim 10^{14}$ cm$^{-2}$. These values are significantly below what we find, suggesting that EXES and HIFI/PACS observations trace different components. Between the broad and narrow water emission observed with HIFI, the broad absorption observed with EXES, and the abundant maser spots, it is evident that the water-containing gas in AFGL 2591 is both spatially and kinematically complex. Interpreting the various observations of H$_2$O in AFGL 2591 in unison will require utilizing a physical model that includes radiative transfer accounting for absorption, stimulated and spontaneous emission, and collisional (de-)excitation, as well as kinematic and geometric effects.

5. SUMMARY

We have detected ten absorption features arising from warm gas in AFGL 2591 caused by ro-vibrational transitions of water, including seven from the $\nu_2$ band of H$_2$O, two from the vibrationally excited $\nu_2$ band of H$_2$O, and one from the $\nu_2$ band of H$_2$O. Among the detected absorption lines is the $\nu_2 \, 1_{1,1}-0_{0,0}$ transition at 6.1163311 $\mu$m, which probes the ground state of para-H$_2$O. Relative strengths of absorption features are suggestive of a covering fraction less than 1 (or absorption arising within the 6 $\mu$m emitting photosphere), with a limit of $f_c \geq 0.25$ set by the depth of the strongest absorption features. Analysis of the level populations assuming $f_c = 0.25$ results in $N$ (H$_2$O) = (1.3 ± 0.3) × 10$^{19}$ cm$^{-2}$ for LTE at $T = 640 \pm 80$ K. Line profiles best match the blueshifted outflow component, and we ascribe the absorption to hot, dense gas at the base of the outflow. The temperature and column density inferred by our analysis are much larger than those reported by Choi et al. (2015) for the outflow component observed in H$_2$O emission by HIFI. Uncertainty in whether the EXES and HIFI observations are probing the same gas makes the combined interpretation of both datasets difficult, and a physical model of AFGL 2591 that includes radiative transfer will be necessary for such an analysis. Clearly though, observations of the $\nu_2$ ro-vibrational band of H$_2$O at high spectral resolution—observations uniquely achievable with EXES on SOFIA—add important information for interpreting this region and others.

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