DETECTION OF EXTENDED HOT WATER IN THE OUTFLOW FROM NGC 2071

GARY J. MELNICK AND VOLKER TOLLS
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138;
gmelnick@cfa.harvard.edu, vtolls@cfa.harvard.edu

DAVID A. NEUFELD, YUAN YUAN, AND PAULE SONNENTRUCKER
Department of Physics and Astronomy, Johns Hopkins University, 3400 North Charles Street, Baltimore, MD 21218;
neufeld@pha.jhu.edu, yuanyuan@pha.jhu.edu, sonnentr@pha.jhu.edu

DAN M. WATSON
Department of Physics and Astronomy, University of Rochester,
Rochester, NY 14627; dmw@pas.rochester.edu

EDWIN A. BERGIN
Department of Astronomy, University of Michigan, 825 Dennison Building,
Ann Arbor, MI 48109; ebergin@umich.edu

AND

MICHAEL J. KAUFMAN
Department of Physics and Astronomy, San Jose State University, One Washington Square,
San Jose, CA 95192-0106; mkaufman@email.sjsu.edu

Received 2008 March 5; accepted 2008 April 24

ABSTRACT

We report the results of spectroscopic mapping observations carried out toward an ~1′ × 1′ region within the northern lobe of the outflow from NGC 2071 using the Infrared Spectrograph (IRS) of the Spitzer Space Telescope. These observations covered the 5.2–37 μm spectral region and have led to the detection of a number of ionic, atomic, and molecular lines, including fine-structure emission of Si+, Fe+, S++, S++, the S(0)−S(7) pure rotational lines of H2, the R(3) and R(4) transitions of HD, and at least eleven transitions of H2O. In addition, the 6.2, 7.4, 7.6, 7.9, 8.6, and 11.3 μm PAH emission bands were also observed and several transitions of OH were tentatively detected. Most of the detected line transitions were strong enough to map, including, for the first time, three transitions of hot H2O. We find that (1) the water emission is extended; (2) the extended emission is aligned with the outflow; and (3) the spatial distribution of the water emission generally follows that observed for H2. Based on the measured line intensities, we derive an HD abundance relative to H2 of (1.1−1.8) × 10−5 and an H2O number density of 12−29 cm−3. The H2 density in the water-emitting region is not well constrained by our observations, but is likely between 3 × 106 and 106 cm−3, yielding an H2O abundance relative to H2 of between 2 × 10−5 and 6 × 10−5. Finally, we note a possible departure from the H2O ortho-to-para ratio of 3 : 1 expected for water formed in hot postshocked gas, suggesting that a significant fraction of the water vapor we detect may arise from H2O sputtered from cold dust grains.

Subject headings: ISM: abundances — ISM: jets and outflows — ISM: molecules — stars: formation — stars: winds, outflows

1. INTRODUCTION

Outflows from young stellar objects provide a natural laboratory toward which it is possible to test the predictions of chemical models thought to apply to warm (T ∼ 300 K), dense [n(H2) ≥ 104 cm−3] gas. Among these predictions is that water will be formed rapidly in the warm gas via a set of neutral-neutral reactions (Elitzur & de Jong 1978; Elitzur & Watson 1978). Moreover, these reactions can potentially convert all of the oxygen not locked in CO into H2O (Bergin et al. 1998). Indeed, the gas-phase water abundances toward shock-heated gas associated with outflows is found to be higher than that within cold, quiescent molecular clouds (Harwit et al. 1998; Melnick et al. 2000; Neufeld et al. 2000; Nisini et al. 2000; Benedettini et al. 2002), although the inferred abundances rarely approach [H2O]/[H2] ~ 10−4 as would be expected for the full conversion of all oxygen not in CO into H2O. In addition, an unknown fraction of the elevated gas-phase water abundance is likely due to the removal of water ice from grains that pass through nondissociative shocks (Draine et al. 1983). Based on a detailed analysis of ground-state ortho-water spectra obtained by the Submillimeter Wave Astronomy Satellite (SWAS) toward 18 outflow sources, Franklin et al. (2008) propose that the lower than expected water abundances within these sources is due to the small fraction of outflow material that actually passes through strong shocks. This also implies that the beam filling factor of regions with highly abundant water is lower than previously assumed. Unfortunately, these previous observations lacked the spatial resolution to determine the detailed water distribution. Thus, the interpretation was hampered by uncertainties in both the fraction of the beam filled with H2O emission and the physical conditions in the H2O-emitting gas as might be revealed by cospatial emission from H2. With beam sizes that range between 1.8′′ and 5.5′′, depending on wavelength, and high sensitivity, the Infrared Spectrometer (IRS) aboard the Spitzer Space Telescope has enabled the study of H2O, H2, and HD with unprecedented detail. In this paper, we describe observations of the outflow source NGC 2071 and report the first detection of spatially extended, hot H2O vapor with Spitzer IRS. In addition to H2O, we have also mapped the ground-vibrational state distribution of H2, as well as low-lying rotational and fine-structure emission from HD, Si i, Fe ii, and Si ii.
NGC 2071 is a region of active star formation, located inside the northern part of the Orion B (L1630) molecular cloud complex at a distance of 390 pc (Anthony-Twarog 1982). The region of interest in this study lies approximately 4° north of the optical reflection nebula NGC 2071 and is the site of a prominent outflow. The H$_2$ S(1) 2.12 μm emission (Eislöffel 2000), along with the region observed here. Near-infrared continuum imaging and spectroscopy of this area reveal a cluster of infrared sources near the center of this outflow (Walther et al. 1991, 1993). The detection of a bipolar thermal radio jet from source IRS3 oriented in the direction of the NGC 2071 North flow, and of a ring of H$_2$O maser spots perpendicular to the flow axis (Torrelles et al. 1998), suggest that IRS3 is the driving source of the NGC 2071 North flow. The outflow, which extends more than 6′, has been mapped previously in CO (Snell et al. 1984; Moranty-Schiefen et al. 1989), CS (Zhou et al. 1991), SO, SiO, and HCO$^+$ (e.g., Chermin & Masson 1992, 1993), and in H$_2$ S(1) (e.g., Eislöffel 2000, and references therein). The presence of high-velocity gas—as high as 60 km s$^{-1}$—and the enhanced abundance of species such as SO and SiO (e.g., Chermin & Masson 1993) suggest that shock processing of the outflow gas is highly likely.

In this paper, we present the results of Spitzer IRS observations toward the northern lobe of the NGC 2071 outflow and discuss the new understanding revealed through high spatial resolution mapping in the lines of H$_2$ S(0) S(7), HD R(3) and R(4), Si i, Fe ii, S i, and three transitions of H$_2$O: 725–616, 634–505, and 734–625. In addition, we present spectra that include several other H$_2$O features along with several lines that we tentatively ascribe to OH. Section 2 summarizes the observations and § 3 presents the results. Section 4 describes the calculations used to analyze the line data and the conclusions are discussed in § 5.

### 2. OBSERVATIONS AND DATA REDUCTION

NGC 2071 was observed on 2004 October 20 and 21 as part of Spitzer Space Telescope Cycle 1 General Observer (GO) program 3423. The observations utilized the Long-High (LH), Short-High (SH), and Short-Low (SL) modules to achieve the highest possible spectral resolving power and complete spectral coverage available to IRS. The mapped areas were approximately 1′ × 1′ for LH and SH and approximately 1′ × 1.5′ for SL, obtained by stepping in spacings of half-slit width perpendicular to the slit and in ~4/5 of the slit length parallel to the slit. The raw data were processed with the Spitzer Science Center (SSC) pipeline version S12.0.2, which provided basic calibrated data (BCD). Further data reduction utilized a data pipeline developed by our group. This pipeline incorporates procedures for removing bad or “hot” pixels, utilizing the SMART software package (Higdon et al. 2004) for calibration and extraction of spectra at each position along the slit, applies a slit loss correction function (SLCF) to correct the flux calibration performed for point-like sources to extended sources, and automatically fits Gaussian lines and second-order polynomials to a set of predetermined spectral lines at each position. The first three steps of this data processing are described in more detail in Neufeld et al. (2006a). The line fitting was performed iteratively to achieve the best-fit parameters. In some cases, the resulting line maps exhibited noticeable striping attributable to varying pixel sensitivity across the slit and by the aftereffects of correcting for bad pixels. A pixel response correction factor (PRCF) was determined to remove striping in the final maps of all LH and SH observations. We used a statistical approach to determine the relative sensitivity in each pixel while preserving the total flux in all pixels across the slit. Details of this method are provided in Neufeld et al. (2007).

### 3. RESULTS

The observed spectra show emission from molecular, atomic, and ionic species as well as a number of PAH features. In particular, we detect emission from [S i], [S ii], [Fe ii], and [Si ii] transitions, H$_2$ rotational lines from S(0) to S(7), HD R(3) and R(4) transitions, and at least 11 H$_2$O transitions. Most of the line emission was strong enough to detect over extended regions, and these maps are shown in Figures 2–6. All maps have been normalized to the peak line intensities listed in Table 1. For reference, the positions of the three strongest peaks in the H$_2$ S(1) 17 μm emission are marked as P1, P2, and P3 on these maps. As can be seen in Figure 4, the strongest water emission lies close to the peak of the H$_2$ S(1) 17 μm emission (position P1 in Fig. 4). It is also clear that (1) the water emission is extended; (2) this extended emission is generally aligned with the outflow; and (3) the water emission exhibits secondary peaks toward positions of enhanced H$_2$ emission. Figure 7 shows a direct comparison of the spatial distribution of the H$_2$O (725–616) emission versus that due to the ro-vibrational H$_2$ 1–0 S(1) and pure rotational H$_2$ S(1) emission. While the overall distribution of the two species is quite similar, the peaks of the H$_2$O and H$_2$ are sometimes offset with respect to each other. For example, the peaks of the H$_2$O 725–616 and the H$_2$ S(1) emission are offset by 3.8′′, which exceeds the stated IRS sky registration error, and thus is likely real.

The spectra obtained toward the water emission peaks closest to positions P1 and P2 are shown in Figures 8–10. In order to reduce the baseline noise, we averaged the data toward the water peaks using a Gaussian weighting function with a wavelength-dependent HPBW of between 11.0′′ at 27.0 μm and 14.7′′ at 5.5 μm. The final synthetic beams have effective beam widths of 15′′ for all wavelengths of interest (Neufeld et al. 2006a). The spectrum labeled H$_2$O Peak 1 is centered at R.A. 05:47:58.3′′, decl. +00:22:52.16′′ (J2000.0), while the spectrum labeled H$_2$O Peak 2 is centered at R.A. 05:47:6.70′′, decl. +00:22:43.04′′ (J2000.0). For almost all of the H$_2$O and H$_2$ transitions detected,
Fig. 2.—Map of the northern lobe of the outflow from NGC 2071 as traced by H$_2$ S(0) through S(3) emission. Offsets are relative to the measured peak of the H$_2$ 17.035 μm S(1) emission centered at R.A. 05h 47m 08.08s, decl. +00° 22' 50.74" (J2000.0). The peak intensity for each transition is provided in Table 1. Positions P1, P2, and P3 are fiducials that mark the positions of the first, second, and third strongest peaks in the H$_2$ S(1) emission. The positions of other known sources in the field are also shown (cf. Walther et al. 1993).
Fig. 3.—Same as Fig. 2, except for H$_2$ S(4) through S(7) emission.
Fig. 4.—Same as Fig. 2, except for $\text{H}_2\text{O} \, 7_{25} - 6_{16} \, 29.837 \, \mu \text{m}, \, 6_{34} - 5_{05} \, 30.899 \, \mu \text{m} \, (\text{blended with} \, \text{H}_2\text{O} \, 8_{34} - 7_{43} \, 30.871 \, \mu \text{m}), \, \text{and} \, 7_{34} - 6_{25} \, 34.549 \, \mu \text{m} \, \text{emission. The H}_2\text{O} \, 7_{34} - 6_{25} \, \text{map is truncated because} \, \text{Spitzer IRS} \, \text{was exposed to a strong source while slewing to the NGC 2071 field. This caused latent signal levels at the long-wavelength end of LH and, thus, we conservatively omitted these less-reliable observations.}$
the 15″ synthetic beam is sufficiently large to encompass the water emission as well as the bulk of the H$_2$ emission toward each peak. The measured line fluxes for the water features associated with H$_2$O Peak 1 are provided in Table 2. Unfortunately, at the spectral resolving power of the Spitzer IRS many of the H$_2$O features are blends of two or more H$_2$O transitions. The extinction-corrected line fluxes for the other key species in this spectrum are given in Table 3. We also note the tentative detection of emission from a number of OH rotational transitions (see Figs. 8 and 9) whose upper levels lie as much as $\sim$3500 K above the ground.

Direct measures of the extinction toward the NGC 2071 outflow are not available. Instead, we inferred the required extinction corrections as a function of wavelength in the Spitzer bandpass by fitting the wings of the silicate absorption feature at 9.7 μm, hence minimizing the effects of line saturation when present. Our silicate fitting model uses the renormalized synthetic Galactic extinction curve per unit hydrogen column density calculated for $RV = 3.1$ or for $RV = 5.5$ (Draine 2003a, 2003b) in linear combination with a first-degree polynomial and four Gaussians with fixed widths and fixed centers to account for emission from interfering lines. Since the gas clumps probed by our data have dust properties most probably intermediate between diffuse and dense molecular clouds, the extinction corrections we adopted represent the mean of the extinction corrections we obtained for $RV = 3.1$ and those we obtained for $RV = 5.5$.

4. WATER CALCULATIONS

To assess how the H$_2$O line strengths measured here constrain the water abundance, the equilibrium level populations of all ortho and para rotational levels of the ground H$_2$O vibrational state with energies $E/k$ up to 7700 K have been calculated using an escape probability method described by Neufeld & Melnick (1991). In modeling the excitation of water vapor, we are limited by the availability of molecular data. Thus far, at the high temperatures of relevance here, a complete set of rate coefficients has only been computed for collisional excitation of H$_2$O by He (Green et al. 1993). A new and accurate nine-dimensional potential energy surface has recently been computed for H$_2$O-H$_2$ (Faure et al. 2005), and quantal calculations are currently underway (M.-L. Dubernet 2007, private communication), to obtain rate coefficients for the collisional excitation of H$_2$O by H$_2$. However, quantal results for transitions involving the high-lying rotational states observed by Spitzer have not yet been completed. Nevertheless, for the subset of those transitions that show the largest rate coefficients, Faure et al. (2007) have recently performed quasi-classical trajectory (QCT) calculations to estimate the collisional rates, and have kindly made the results available to us prior to publication. Unfortunately, transitions with small rate coefficients still play a significant role in the excitation of the spectral lines that we have observed with Spitzer; for those transitions, we have had to use the Green et al. (1993) results, scaled by a factor 1.348 to account for the difference between the H$_2$O-He and H$_2$O-H$_2$ reduced masses. Finally, a polynomial fit to the exact expression for the photon escape probability from a plane-parallel emitting region (Hummer & Rybicki 1982) is used.

We assume that the physical conditions within H$_2$O Peak 1 are those required to reproduce the measured H$_2$ S(0)–S(7) flux from the same region. Table 4 summarizes these physical conditions. The model H$_2$ column densities are assumed to be those consistent with a simple shock model in which

$$N(H_2) = 6.45 \times 10^{20} \left( \frac{n(H_2)}{10^5} \right)^{0.3} \left( \frac{T_{gas}}{1000} \right)^{-0.555} \text{cm}^{-2},$$

(1)

where $n(H_2)$ is the density in the postshock gas (Neufeld et al. 2006a). We assume that the fraction of the beam filled by the warm and hot H$_2$O is given by the ratio of the measured values of $N(H_2)$ given in Table 4 to those derived above. To estimate the physical parameters from the eight H$_2$ rotational lines, we have performed calculations in which the emitting region is approximated by a two-component model for two different cases: (1) clouds with homogenous density; and (2) clouds with homogenous pressure.
Fig. 6.—Same as Fig. 2, except for Si $^3P_1-^3P_2$ 25.249 \( \mu \)m, Fe $^2D_{7/2}-^2D_{9/2}$ 25.988 \( \mu \)m, and Si $^2P_{3/2}^2-^2P_{1/2}$ 34.815 \( \mu \)m emission.
The six best-fit parameters (temperature, column density, and H$_2$ ortho-to-para ratio for the two components) are determined by minimizing the rms of ln (measured C$_{\text{ux}}$/computed C$_{\text{ux}}$) for the H$_2$ S(0)–S(7) lines. Results were obtained for a series of H$_2$ number densities ranging from 10$^4$ to 10$^7$ cm$^{-3}$, and pressures ($\frac{p}{k}$) ranging from 10$^7$ to 10$^{10}$ cm$^{-3}$ K. The greatest differences between the two models—homogenous density or pressure—appear at low densities (or low pressures), where the pressure-balanced assumption requires a relatively higher temperature for the hot component. The results of the two models converge as LTE is approached for the higher-lying transitions, i.e., for number densities greater than 10$^5$ cm$^{-3}$ (or pressures/$k$ greater than 10$^8$ cm$^{-3}$ K). In this case, the best-fit temperature for the warm component is around 300–360 K while that for the hot component is around 1000–1500 K.

Using the physical conditions that best fit the H$_2$ observations, the abundances of H$_2$O and HD toward H$_2$O Peak 1 were then derived. For H$_2$O, the total (ortho+para) abundance at each assumed density was varied to produce the best overall fit to the features listed in Table 2. We choose these features to fit because they are the strongest observed transitions between 5 and 36.5 $\mu$m toward H$_2$O Peak 1; both the observed and predicted line fluxes for H$_2$O transitions lying at $\lambda < 29 \mu$m are less than 5 MJy sr$^{-1}$, and most typically less than about 3 MJy sr$^{-1}$, rendering their unambiguous identification above the noise difficult. As discussed further below, the H$_2$O ortho-to-para ratio was treated as a free parameter. Similarly, the abundance of HD was determined by fitting the measured R(3) and R(4) line fluxes, although the best-fit HD abundance is not a sensitive function of number density due to the moderately low critical densities of the R(3) and R(4) transitions of $\sim$10$^5$–10$^6$ cm$^{-3}$. Finally, it would be useful to also fit the measured OH rotational lines. Unfortunately, the lack of reliable collisional rate coefficients for these high-lying transitions makes the results of such a calculation uncertain at this time.

As shown in Figure 11, fits to the H$_2$ and HD emission lines alone favor gas with higher densities or pressures. The best-fit HD abundance relative to H$_2$ is between 1.1 $\times$ 10$^{-2}$ and 1.8 $\times$ 10$^{-5}$, with only a weak dependence on density as noted above. This abundance is very similar to those derived previously from observations of HD R(3) and R(4) in other shocked regions that we have observed with Spitzer (Neufeld et al. 2006b). Fits to the

### Table 1: Peak Intensity for Each Mapped Transition

| Species | Transition | Rest Wavelength ($\mu$m) | Peak Intensity ($10^{-6}$ erg cm$^{-2}$ s$^{-1}$ sr$^{-1}$) |
|---------|------------|-------------------------|----------------------------------------------------------|
| H$_2$O  | 7$_{25}$–6$_{16}$ | 29.837 | 4.39 |
|         | 6$_{14}$–5$_{15}$ | 30.899 | 7.08 |
|         | 8$_{15}$–7$_{15}$ | 30.871 | ... |
| H$_2$   | S(0)       | 28.221 | 21.10 |
|         | S(1)       | 17.035 | 189.31 |
|         | S(2)       | 12.727 | 1721 |
|         | S(3)       | 9.665 | 1421 |
|         | S(4)       | 8.025 | 1200 |
|         | S(5)       | 6.909 | 3300 |
|         | S(6)       | 6.109 | 1746 |
|         | S(7)       | 5.511 | 1800 |
| HD      | R(3)       | 28.502 | 3.37 |
|         | R(4)       | 23.034 | 6.20 |
| S       | $^3P_1$–$^3P_2$ | 25.249 | 201.70 |
| Fe ii   | $^3P_{1/2}$–$^3P_{3/2}$ | 25.988 | 40.84 |
| Si ii   | $^2P_{3/2}$–$^2P_{1/2}$ | 34.815 | 55.41 |

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![Fig. 7.—Top: Contours of H$_2$O 7$_{25}$–6$_{16}$ 29.837 $\mu$m emission superposed on the Eisloeffel (2000) H$_2$ 1–0 S(1) 2.12 $\mu$m map. Middle: Contours of H$_2$ S(1) emission superposed on the map of HD 7$_{25}$–6$_{16}$ 29.837 $\mu$m emission. Bottom: Contours of HD R(3) emission superposed on the map of HD R(3) 28.502 $\mu$m emission.](EXTENDED HOT WATER IN NGC 2071 883)
Fig. 8.—Portion of the Spitzer IRS spectra obtained in a 15" synthesized beam toward H$_2$O Peaks 1 and 2 (see text). The H$_2^{16}$O transition(s) associated with each detected feature are shown. In the absence of higher spectral resolving power, we are not able to observationally determine the extent to which each transition contributes to the total flux measured for each blended feature. In addition to Si $\text{II}$ and S $\text{III}$ lines in the band, we also note the tentative detection of OH $^4\text{II} \rightarrow 17/2 \rightarrow 15/2 \approx 30.277 \mu$m, $^2\text{II} 19/2 \rightarrow 17/2 \approx 30.346 \mu$m, $^2\text{II} 17/2 \rightarrow 15/2 \approx 30.657 \mu$m. Unidentified lines are denoted with a U.
Fig. 9.—Portion of the Spitzer IRS spectra obtained in a 15′ synthesized beam toward H2O Peaks 1 and 2 (see text). Of particular note is the ground rotational transition of para-H2 at 28.219 μm, two HD rotational transitions, R(3) and R(4), at 28.502 and 23.034 μm, respectively, and the tentative detection of OH $^{2}\Pi_{1/2} 19/2+^{2}/2$ $^{2}\Pi_{3/2} 23/2^{+2} 21/2+27.393$ μm, $^{2}\Pi_{1/2} 21/2^{+} 19/2^{+} 27.454$ μm, $^{2}\Pi_{1/2} 19/2^{+} 17/2^{+} 27.652$ μm, $^{2}\Pi_{1/2} 19/2^{+} 17/2^{+} 27.697$ μm, $^{2}\Pi_{1/2} 23/2^{+} 21/2^{+} 25.035$ μm, and $^{2}\Pi_{1/2} 23/2^{+} 21/2^{+} 25.090$ μm. Unidentified lines are denoted with a U.
Fig. 10.—Portion of the Spitzer IRS spectra obtained in a 15″ synthesized beam toward H$_2$O Peaks 1 and 2 (see text). Of note are the prominent lines of H$_2$S(1) through (7). Both spectra also show broad PAH emission features with peak wavelengths of 6.22, 7.41, 7.59, 7.85, 8.61, and 11.3 μm.
### TABLE 2
**Beam-Averaged Line Fluxes for the H$_2$O Features Toward H$_2$O Peak 1**

| H$_2$O Feature ($\mu$m) | Ortho (o) / Para (p) | Transition | Rest Wavelength ($\mu$m) | Extinction-Corrected Line Flux $\times 10^{-21}$ into 15'' Beam* |
|------------------------|----------------------|------------|--------------------------|---------------------------------------------------------------|
| 36.21                  | p                    | $\nu_{24} - \nu_{15}$ | 36.21                    | 1.57                                                          |
| 35.92                  | o                    | $\nu_{22} - \nu_{11}$ | 35.93                    | 0.70                                                          |
| 35.67                  | p                    | $\nu_{21} - \nu_{10}$ | 35.90                    | ...                                                          |
| 35.45                  | o                    | $\nu_{20} - \nu_{10}$ | 35.47                    | 2.43                                                          |
| 34.55                  | o                    | $\nu_{19} - \nu_{10}$ | 35.49                    | 2.02                                                          |
| 33.13                  | p                    | $\nu_{18} - \nu_{10}$ | 33.12                    | 0.64                                                          |
| 32.99                  | o                    | $\nu_{17} - \nu_{10}$ | 33.05                    | 1.42                                                          |
| 31.75                  | o                    | $\nu_{16} - \nu_{10}$ | 31.77                    | 0.70                                                          |
| 30.89                  | o                    | $\nu_{15} - \nu_{10}$ | 30.87                    | 1.82                                                          |
| 30.53                  | p                    | $\nu_{14} - \nu_{10}$ | 30.51                    | 0.63                                                          |
| 29.84                  | o                    | $\nu_{13} - \nu_{10}$ | 29.82                    | 1.27                                                          |

* At the spectral resolving power of Spitzer IRS, some H$_2$O features may be blends of two or more H$_2$O transitions. The line fluxes listed here represent the total flux for each H$_2$O feature.

### TABLE 3
**Beam-Averaged Line Fluxes for Key Species Toward H$_2$O Peak 1**

| Species | Transition | Rest Wavelength ($\mu$m) | Extinction-Corrected Line Flux $\times 10^{-21}$ into 15'' Beam* |
|---------|------------|--------------------------|---------------------------------------------------------------|
| H$_2$   | S(7)       | 5.5112                   | 275.2                                                         |
| H$_2$   | S(6)       | 6.1086                   | 110.9                                                        |
| H$_2$   | S(5)       | 6.9095                   | 513.0                                                        |
| H$_2$   | S(4)       | 8.0251                   | 207.0                                                        |
| H$_2$   | S(3)       | 9.6649                   | 474.4                                                        |
| H$_2$   | S(2)       | 12.2786                  | 138.1                                                        |
| H$_2$   | S(1)       | 17.0348                  | 68.3                                                         |
| HD      | R(4)       | 23.0338                  | 2.2                                                          |
| OH      | $^2\Pi_{3/2}$ $23/2^+ - 21/2^-$ | 25.0351                    | 0.41                                                         |
| OH      | $^2\Pi_{3/2}$ $23/2^+ - 21/2^-$ | 25.0899                    | 0.48                                                         |
| [S i]   | $^3P_1 - ^3P_2$ | 25.2940                   | 78.8                                                         |
| [Fe ii] | $^4D_{7/2} - ^4D_{5/2}$ | 25.9883                   | 7.6                                                          |
| OH      | $^2\Pi_{3/2}$ $21/2^+ - 19/2^-$ | 27.3935                   | 0.13                                                         |
| OH      | $^2\Pi_{3/2}$ $21/2^+ - 19/2^-$ | 27.4546                   | 0.58                                                         |
| OH      | $^2\Pi_{1/2}$ $19/2^- - 17/2^-$ | 27.6516                   | 0.31                                                         |
| OH      | $^2\Pi_{1/2}$ $19/2^- - 17/2^-$ | 27.6967                   | 0.25                                                         |
| H$_2$   | S(0)       | 28.2188                  | 9.1                                                          |
| HD      | R(3)       | 28.5020                  | 2.3                                                          |
| OH      | $^2\Pi_{3/2}$ $19/2^- - 17/2^-$ | 30.2772                   | 0.25                                                         |
| OH      | $^2\Pi_{3/2}$ $19/2^- - 17/2^-$ | 30.3459                   | 0.60                                                         |
| OH      | $^2\Pi_{1/2}$ $17/2^- - 15/2^-$ | 30.6573                   | 0.33                                                         |
| OH      | $^2\Pi_{1/2}$ $17/2^- - 15/2^-$ | 30.7063                   | 0.37                                                         |
| [S iii] | $^3P_1 - ^3P_0$ | 33.4800                   | 1.5                                                          |
| [Si ii] | $^2P_{5/2} - ^2P_{3/2}$ | 34.8152                   | 18.7                                                         |
H$_2$O features were computed in two ways. First, fits to 10 of the 11 H$_2$O features in Table 2 were calculated assuming an H$_2$O ortho-to-para ratio of 3:1 as well as an ortho-to-para ratio that was allowed to vary in order to achieve the best overall fit at each density between $10^4$ and $10^7$ cm$^{-3}$. The strong feature at 34.55 $\mu$m was not included. The conditions needed to reproduce the flux in this line resulted in fluxes in the other H$_2$O transitions that are in significant disagreement with the observations. Thus, we conclude that either this line is blended with an unknown feature or uncertainties in the collision rates may be resulting in lower than actual populations in the upper 7$_{34}$ state. Second, to better isolate the effects of varying the H$_2$O ortho-to-para ratio, we examined the three strongest features in which the only contribution to the line flux was an ortho-H$_2$O transition, at 33.13 and 36.21 $\mu$m, or a para-H$_2$O transition, at 33.13 and 36.21 $\mu$m. These results are also shown in Figure 11. Based on fits to the water data alone, H$_2$ densities in the water-emitting region of between about $3 \times 10^4$ and $3 \times 10^5$ cm$^{-3}$ appear favored. The best fits to the isolated ortho and para features are achieved for H$_2$ densities between $3 \times 10^4$ and $10^5$ cm$^{-3}$ and an assumed H$_2$O ortho-to-para ratio of between 1.5 and 1.6.

The best-fit water abundances are shown in Figure 12. To a good approximation, the best fits to the H$_2$O line fluxes are proportional

![Figure 11](image1)

**Figure 11.** Root mean square goodness of fit of the computed fluxes at each density for H$_2$ S(0)–S(7) (filled squares); HD R(3) and R(4) (filled circles); H$_2$O Case 1: the H$_2$O features listed in Table 2, with the exception of the 34.55 $\mu$m feature, and assuming an ortho-to-para ratio of 3:1 (open squares); H$_2$O Case 2: the pure ortho- or para-H$_2$O lines at 29.84, 33.13, and 36.21 $\mu$m and assuming an ortho-to-para ratio of 3:1 (filled diamonds); H$_2$O Case 3: the H$_2$O features listed in Table 2, with the exception of the 34.55 $\mu$m feature, and assuming an ortho-to-para ratio that has been allowed to vary to produce the best fit to the data at each density (open circles); H$_2$O Case 4: the pure ortho- or para-H$_2$O lines at 29.84, 33.13, and 36.21 $\mu$m and assuming an ortho-to-para ratio that has been allowed to vary to produce the best fit to the data at each density (filled triangles).

![Figure 12](image2)

**Figure 12.** Total (ortho+para) water abundance, at each assumed density, that produces the best overall fit to (1) the H$_2$O features listed in Table 2, with the exception of the 34.55 $\mu$m feature, and assuming an ortho-to-para ratio of 3:1 (solid line); (2) the H$_2$O features listed in Table 2, with the exception of the 34.55 $\mu$m feature, and assuming an ortho-to-para ratio that has been allowed to vary to produce the best fit to the data at each density (dot-dashed line); (3) the 29.84, 33.13, and 36.21 $\mu$m features and assuming an ortho-to-para ratio of 3:1 (dashed line); and (4) the 29.84, 33.13, and 36.21 $\mu$m features and assuming an ortho-to-para ratio that has been allowed to vary to produce the best fit to the data at each density (dotted line).
to the H₂ density × the water abundance, resulting in a derived number density of H₂O molecules of 12–29 cm⁻³, independent of H₂ density. This is a consequence of the fact that the observed transitions have critical densities >10⁹ cm⁻³ and are optically thin under the conditions considered here. In this limit, the flux in an ortho-H₂O (or para-H₂O) line is

\[
F = \frac{A_{ul} \nu_{ul} n \ell}{4\pi} = \frac{A_{ul} \nu_{ul} [n(H₂) \chi(H₂O) f_u \xi_{op}]}{4\pi} \Omega,
\]

where \(A_{ul}\) is the transition spontaneous emission rate, \(\nu_{ul}\) is the transition frequency, \(n(H₂)\) is the H₂ density, \(\ell\) is the depth of the emitting region, \(\chi(H₂O)\) is the water abundance relative to H₂, \(f_u\) is the fractional population in the upper state of the emitting transition, \(\xi_{op}\) is the fraction of all H₂O molecules in the ortho (or para) state, and \(\Omega\) is the solid angle of the water emitting region.

Figure 13 shows the resulting 29–36.5 μm water spectrum computed for an H₂ density of 10⁵ cm⁻³ and H₂O ortho-to-para ratios of 3:1 and 1.55:1, the latter being the best-fit ortho-to-para ratio at a density of 10⁵ cm⁻³. The computed spectra were convolved with a Gaussian profile whose width was selected to match the IRS LH resolving power, \(\lambda/\Delta\lambda\), of 600 (FWHM). As can be seen in Figure 13, the differences between the spectrum computed assuming an H₂O ortho-to-para ratio of 3:1 and 1.55:1 are small. Nevertheless, assuming an ortho-to-para ratio less than 3:1 results in a slightly better overall fit to the H₂O data and suggests a possible departure from the usual assumption that water in post-shocked gas is always present in the LTE ortho-to-para ratio of 3:1. This tentative finding is discussed further in the next section.

Taking into account the H₂, HD, and H₂O spectra, the overall best fits to these data favor an H₂ density in the range 3×10⁴–10⁵ cm⁻³, and 2×10⁻⁵ ≤ \(\chi(H₂O)\) ≤ 6×10⁻⁴. Unfortunately, the present data do not allow us to better constrain the H₂ density, and thus the water abundance, within the emitting region. However, as we discuss in the next section, future observations planned for the Herschel Space Observatory may permit more direct measures of the H₂ density.

5. DISCUSSION

The capabilities of the Spitzer IRS instrument has enabled the study of outflow regions in ways that were not possible previously. In particular, the ability to map the distribution and intensity of
key species, such as H$_2$, HD, Fe$^+$, Si$^+$, S, and, of course, H$_2$O, with a spatial resolution of a few arcseconds permits more stringent tests of our understanding of the structure and composition of outflows. Earlier space missions, such as the Infrared Space Observatory (ISO), SWAS, and Odin have established the correlation between outflows from young stellar objects and strong water emission (e.g., Harwit et al. 1998; Melnick et al. 2000; Neufeld et al. 2000; Nisini et al. 2000; Giannini et al. 2001; Benedettini et al. 2002). Unfortunately, these observations were conducted with large beams relative to Spitzer IRS or, in the case of the ISO Short-Wavelength Spectrometer with its 10$''$ beam, lower sensitivity than Spitzer IRS. As a result, the filling factor of H$_2$O within the beam was not always directly known or key species helpful in the interpretation of the water data, such as H$_2$ and HD, were not detected. The observations reported here remedy most, but not all, of these previous shortcomings.

The primary goal of this study is the further understanding of water in outflows. Unlike the production of water in quiescent molecular clouds, which proceeds via a set of relatively slow ion-neutral reactions in the gas phase (e.g., Herbst & Klemperer 1973), or through the photodesorption of water formed on the surface of dust grains (e.g., Hollenbach et al. 2008), the material in outflows often passes through a shock which both compresses and heats the gas. In the postshocked region of nondissociative, or C-type, shocks (Draine 1980), with shock velocities, $v_S$, $\geq$10 km s$^{-1}$, temperatures exceed 300 K, enabling a pair of neutral-neutral reactions (H$_2$ + O $\rightarrow$ OH + H and H$_2$ + OH $\rightarrow$ H$_2$O + H) that can rapidly convert all gas-phase oxygen not bound in CO into H$_2$O (Elitzur & de Jong 1978). For $v_S$ $\geq$ 50 km s$^{-1}$, most C-type shocks break down, giving rise to dissociative, or J-type, shocks. Molecules are completely dissociated, either by either the precursor UV field generated by the hot gas near the shock front or by collisions in the shock, and then reform on grain surfaces in the cooler ($\sim$400 K) CO downstream gas (Hollenbach & McKee 1989). Because C-type shocks have very low ionic abundances, strong Si $\pi$ (34.8 $\mu$m) and Fe $\pi$ (26.0 $\mu$m) emission is considered a tracer of J-type shocks.

The Spitzer IRS data suggest that both J- and C-type shocks are present in the portion of the outflow observed here. The strong Si $\pi$ and Fe $\pi$ emission evident in Figure 6 follows the outflow, peaking close to H$_2$ positions P3 and P2, and lies closer to the source of the outflow than the most prominent H$_2$ position, P1. This may indicate the presence of fast-moving gas along the center of the outflow which has been slowed as it approaches position P1. This picture is supported by previous CO $J = 3$–2 observations (Chernin & Masson 1992), which revealed well-collimated, high-velocity (30–60 km s$^{-1}$) gas in a symmetric bipolar outflow only within 1.5$''$ of the source, presumed close to IRS3. Moreover, the CO data show velocity peaks appearing at $\pm$1$''$ from the source. Further support is provided by the pronounced peak in the S $\iota$ (25.2 $\mu$m) emission (see Fig. 6) near position P1. In the J-type shock models of Hollenbach & McKee (1989) for densities between 10$^4$ and 10$^6$ cm$^{-3}$, the strongest S $\iota$ emission arises at the lowest velocities (i.e., $v_S$ $\sim$ 30 km s$^{-1}$), whereas both the Si $\pi$ and Fe $\pi$ emission increase with shock velocity. In addition, previous Spitzer IRS observations of supernovae remnants (Neufeld et al. 2007) show a strong correlation between the S $\iota$ and H$_2$ S(1)–S(7) spatial distribution, suggesting that most of the S $\iota$ emission arises in the slower, nondissociative shocks. This could account for the difference in the spatial distribution of Si $\pi$, Fe $\pi$, and S $\iota$.

That the H$_2$ S(1) peak emission appears to be located closer to the source of the outflow (near IRS3) than all of the higher-lying H$_2$ transitions, i.e., S(2)–S(7), as well as that of the H$_2$O may also be explained by this scenario. In the multiple-shock picture, the H$_2$ S(1) emission could arise primarily in the $\sim$400 K gas behind a moderate J-type shock, the postshock region in which it is predicted that H$_2$ is reformed (Hollenbach & McKee 1989). Meanwhile, the higher-lying H$_2$ and H$_2$O lines would arise from behind the C-type shock slightly farther from the outflow source in which gas temperatures can heat molecules to more than 2000 K.

The good fit to the H$_2$ and HD data (see Fig. 11) obtained with conditions characteristic of a C-type shock provide the best evidence for the coexistence of a nondissociative shock. Based on the morphology of the Si $\pi$, Fe $\pi$, and H$_2$ emission, it is tempting to suggest that the C-type shock emission arises in the entrained slower-moving shocked material surrounding the high-velocity J-type shock gas, which itself slows and transitions to a C-type shock near position P1.

That the water emission follows closely the H$_2$ emission is in accord with the predictions of C-type shock models. Unfortunately, our inability to unambiguously determine the H$_2$ density in the water-emitting region from the Spitzer IRS data prevents us from fully testing the other key prediction of the C-type shock models, namely that the water abundance will be high [i.e., $\chi$(H$_2$O) $\geq$ 10$^{-4}$] in the postshocked gas. Other observations provide general support for the density range preferred here. Zhou et al. (1991) have observed the NGC 2071 outflow in the CS $J = 2$–1, 5–4, 6–5, and 7–6 transitions. Their best fit to the CS emission yield densities of (1–4) $\times$ 10$^3$ cm$^{-3}$. Unfortunately, the varying beam sizes with which these observations were conducted, ranging between 11$''$ and 24$''$, along with uncertainties in the gas temperature and the surface filling factors for the different transitions, contribute to the overall uncertainty in the density determination. Nonetheless, if this range of densities applies to H$_2$O Peak 1 region, then the best-fit water abundance would lie between approximately 5 $\times$ 10$^{-5}$ and 2 $\times$ 10$^{-4}$ relative to H$_2$, which still represents a significant abundance enhancement above that found in quiescent molecular clouds (e.g., Snell et al. 2000) and is consistent with the predictions of C-type shock models.

Future observations of far-IR high-J CO lines—planned for the Photodetector Array Camera and Spectrometer (PACS) instrument aboard the Herschel Space Observatory—promise to yield a valuable means of estimating the H$_2$ density in NGC 2071. Given the gas temperatures and column densities derived from our Spitzer observations of the H$_2$ S(0)–S(7) rotational transitions, we have computed the CO line intensities expected for a CO abundance of 10$^{-4}$ relative to H$_2$. The sample results shown in Figure 14 were obtained by means of a statistical equilibrium calculation in which we adopted the molecular data described in Neufeld & Kaufman (1993). Figure 14 indicates that far-IR transitions of CO should be readily detectable with Herschel and that their strengths will provide a key probe of the gas density over exactly the desired range: 4 $\leq$ log (H$_2$/cm$^{-3}$) $\leq$ 6.5. Here, the dashed line corresponds to the Herschel PACS spectral line sensitivity of $\sim$2 $\times$ 10$^{-6}$ erg cm$^{-2}$ s$^{-1}$ sr$^{-1}$ (5 $\sigma$ in 1 hr, corresponding to a flux of 5 $\times$ 10$^{-18}$ W m$^{-2}$ into a 9.7$''$ pixel). Because the CO lines are optically thin, the predicted line intensities are proportional to the assumed CO abundance. However, the far-IR line ratios (Fig. 15) are independent of the assumed CO abundances and would provide a good estimate of densities in the range 5 $\leq$ log (H$_2$/cm$^{-3}$) $\leq$ 6.5 without any required knowledge of the CO abundance.

The question of the distribution and abundance of the gas-phase water is important not just because the answers test the...
validity of long-standing chemical predictions; many models of the larger ambient clouds take as a starting point certain molecular enrichment due to the passage of nearby shocks. A recent analysis of 18 molecular outflows by Franklin et al. (2008) based on observations of the ground-state ortho-H$_2$O transition from SWAS and the $J=1-0$ transition of $^{12}$CO and $^{13}$CO obtained with the Five College Radio Astronomy Observatory shows that the ortho-H$_2$O abundance (relative to H$_2$) in most outflows is between $10^{-7}$ and $10^{-6}$, assuming the H$_2$O and CO emission arises in the same gas. However, an examination of the water abundance as a function of outflow velocity reveals a strong dependence; the water abundance rises with outflow velocity, reaching abundances of $\sim 10^{-3}$ at the highest velocities. However, the mass associated with the highest velocity emission is found to be small compared with the total outflow mass, leading to the conclusion that only a small fraction of the outflowing molecular gas has passed through shocks strong enough to fully convert the gas-phase oxygen to water. Using the measurements obtained here, combined with the data soon to be available from Herschel, it will be possible to independently test this conclusion.

Finally, our potential detection of an H$_2$O ortho-to-para ratio that is not in equilibrium at the gas temperature may hint at the origin of the water vapor emission we detect. The lowest energy level of para-H$_2$O is $\sim 34$ K below that of ortho-H$_2$O and, as such, the ratio of the ortho and para populations in LTE is temperature dependent. When water forms in the gas phase via exothermic reactions the energy released is much greater than this energy difference and the ortho-to-para ratio will reflect the 3:1 ratio of statistical weights between these species. When water forms on the surfaces of cold dust grains, it is believed that the energy generated by the chemical reaction is shared with the grain and the water molecules should equilibrate to an ortho-to-para ratio that reflects the grain temperature (e.g., Limbach et al. 2006). If the grain temperature is below $\sim 50$ K, then the ortho-to-para ratio will lie below 3:1. In this regard, it has been known for many years that water in numerous cometary comae exhibits an ortho-to-para ratio below 3:1, which has been attributed to formation at temperatures of $\sim 25$–$30$ K (e.g., Mumma et al. 1987; Bonev et al. 2007).

Our measurements, while uncertain, potentially limit the ortho-to-para ratio to between 1.5 and 2.5, or equivalent temperatures of $\sim 20$ and 30 K. If the water is produced entirely in shocks via the well-known sequence of neutral-neutral reactions, the ortho-to-para ratio should be 3:1. However, if the water enters the gas phase via sputtering from cold grain surfaces, then the ratio would reflect equilibrium at the grain temperature. A mixture of both sputtering and gas-phase formation cannot be ruled out, and thus this measurement represents an upper limit to the ortho-to-para ratio of water ice. If our measurement is confirmed, this would therefore suggest that a significant amount of the H$_2$O emission we detect has its source in water vapor produced from grain sputtering and not via gas-phase reactions.

G. J. M. gratefully acknowledges the financial support of NASA grant NNG06GB30G from the Long Term Space Astrophysics (LTSA) Research Program and through an award issued by JPL/Caltech (Support Agreement 1265773). The work of D. A. N. was partially supported by grant NAG5-13114 from NASA’s Long Term Space Astrophysics (LTSA) Research Program. This work is based on observations made with the Spitzer Space Telescope, which is operated by JPL/Caltech under NASA contract 1407.
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