



# Survey of Cold Water Lines in Protoplanetary Disks: Indications of Systematic Volatile Depletion

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Received 2016 October 7; revised 2017 April 27; accepted 2017 May 1; published 2017 June 19

## Abstract

We performed very deep searches for 2 ground-state water transitions in 13 protoplanetary disks with the *HIFI* instrument on board the *Herschel Space Observatory*, with integration times up to 12 hr per line. We also searched for, with shallower integrations, two other water transitions that sample warmer gas. The detection rate is low, and the upper limits provided by the observations are generally much lower than predictions of thermo-chemical models with canonical inputs. One ground-state transition is newly detected in the stacked spectrum of AA Tau, DM Tau, LkCa 15, and MWC 480. We run a grid of models to show that the abundance of gas-phase oxygen needs to be reduced by a factor of at least  $\sim 100$  to be consistent with the observational upper limits (and positive detections) if a dust-to-gas mass ratio of 0.01 were to be assumed. As a continuation of previous ideas, we propose that the underlying reason for the depletion of oxygen (hence the low detection rate) is the freeze-out of volatiles such as water and CO onto dust grains followed by grain growth and settling/migration, which permanently removes these gas-phase molecules from the emissive upper layers of the outer disk. Such depletion of volatiles is likely ubiquitous among different disks, though not necessarily to the same degree. The volatiles might be returned back to the gas phase in the inner disk ( $\lesssim 15$  au), which is consistent with current constraints. Comparison with studies on disk dispersal due to photoevaporation indicates that the timescale for volatile depletion is shorter than that of photoevaporation.

**Key words:** astrochemistry – circumstellar matter – molecular processes – planet–disk interactions – planetary systems – planets and satellites: atmospheres

## 1. Introduction

Dust evolution in protoplanetary disks is inevitably coupled with gas evolution and gas-phase chemistry. The dust distribution determines the UV field of the disk, which strongly affects the gas temperature (Glassgold et al. 2004; Woitke et al. 2009) and photo-reaction (photodissociation and photo-desorption) rates (Bergin et al. 2003; van Dishoeck et al. 2006; Bruderer et al. 2009; Öberg et al. 2009). Dust grains also act as a sink of gas-phase molecules, because molecules can freeze out onto the dust grains. The freeze-out process changes the composition of dust particles, and can potentially alter the sticking coefficient of dust coagulation (Machida & Abe 2010; Sato et al. 2016). Among all of the gas-phase species, water is of great interest, not just because of its importance for the origin of water on planets and the possibility for life elsewhere in the universe (see review by van Dishoeck et al. 2014), but also because (1) it is the major carrier of the third most abundant element, oxygen, (2) it is an important coolant (Karska et al. 2013; Nisini et al. 2010), and (3) it may shield other molecules from Ly $\alpha$  photons in some parts of the disk (Bethell & Bergin 2011; Ádámkóvics et al. 2014; Du & Bergin 2014).

We have surveyed 4 water lines in 13 protoplanetary disks with the *HIFI* instrument of the *Herschel Space Telescope*<sup>12</sup> (Table 1). Two of these lines (the ground-state lines) have very deep integrations, and two higher-lying lines have moderately deep integrations. All of the spectra are resolved in velocity. The disks are heterogeneous in nature, with a range of disk masses (in dust) and stellar types. This survey is mostly sensitive to cold ( $T \lesssim 20$  K) water vapor from the outer part of the disk (for a quantitative view, see Section 4.2, where we show that the inner few astronomical units contribute less than 10% to the transitions studied in this survey). In contrast, starting with Carr et al. (2004), many papers have probed the warm-hot water reservoir in the inner few au of disks via infrared lines (e.g., Carr & Najita 2008, 2011; Salyk et al. 2008, 2011, 2015; Pontoppidan et al. 2010a, 2010b; Banzatti et al. 2012, 2015; and Blevins et al. 2016).

<sup>12</sup> *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator Consortia and with important participation from NASA.

**Table 1**  
Overview of the Water Observations

Line	Frequency (GHz)	Source	Date	OBS ID	$t_{\text{obs}}$ (s)
$1_{11}-0_{00}$	1113.342964	AA Tau	2012 Sep 04	1342250602	40542.4
			2013 Feb 26	1342266479	20196.4
		DM Tau	2010 Mar 04	1342191652	43235.3
			2012 Aug 30	1342250453	36576.4
			2012 Aug 31	1342250454	36340.4
$1_{10}-1_{01}$	556.936002	HD 163296	2012 Oct 17	1342253594	19031.4
			2012 Oct 18	1342253595	40285.4
		AA Tau	2012 Mar 27	1342242495	30270.0
			2012 Mar 27	1342242496	29286.5
			2010 Mar 20	1342192365	23903.9
		DM Tau	2012 Aug 29	1342250427	17863.9
			2012 Sep 06	1342250687	19244.9
			2010 Mar 21	1342192516	1914.4
		LkCa 15	2010 Aug 31	1342204003	24044.9
		MWC 480	2010 Sep 01	1342204004	23888.9
		AS 209	2010 Mar 21	1342192518	2087.4
		BP Tau	2010 Mar 21	1342192523	2421.4
		GG Tau	2010 Aug 19	1342203193	1914.4
		GM Aur	2010 Aug 19	1342203209	1981.4
		IM Lup	2011 Feb 15	1342214336	2510.4
		MWC 758	2010 Apr 11	1342194502	2119.4
		T Cha	2010 Apr 12	1342194535	2849.4
		AA Tau	2012 Aug 15	1342249596	5296.5
			2010 Aug 20	1342203259	2263.3
		DM Tau	2012 Aug 15	1342249597	2923.7
$3_{12}-2_{21}$	1153.126822	LkCa 15	2010 Aug 20	1342203257	2263.3
		MWC 480	2011 Apr 01	1342217734	2452.4
		TW Hya	2010 Dec 02	1342210733	3179.4
		HD 100546	2011 Dec 30	1342235779	5358.5
		DM Tau	2010 Sep 02	1342203941	14911.7
			2010 Sep 02	1342203939	14968.7
		MWC 480	2010 Sep 02	1342203936	15104.7
		TW Hya	2010 Jun 09	1342197986	15121.7
$3_{12}-3_{03}$	1097.364791				

The major finding is that while a few sources show positive detections, most of them have no signal at the current noise level, even with very deep integrations, consistent with our earlier *Herschel*-HIFI results (Bergin et al. 2010; Hogerheijde et al. 2011). We model these water lines with a thermochemical code described below, and find that the model predictions tend to be much higher than the observed upper limits, with reasonable and canonical parameters for the sources. This phenomenologically resembles other studies on carbon-bearing species, including CO and atomic carbon in HD 100546, TW Hya, and DM Tau (Bruderer et al. 2012; Favre et al. 2013; Cleeves et al. 2015; Bergin et al. 2016; Kama et al. 2016a; Schwarz et al. 2016). Similar to previous conclusions (Du et al. 2015; Bergin et al. 2016; Kama et al. 2016b), a natural explanation for the disparity between the models and the observations is that volatile elements such as oxygen freeze out onto dust grains and never return back to the gas phase due to dust growth (possibly into multi-kilometer-sized bodies) and settling/migration.

This paper is organized as follows. Section 2 describes details of the water line survey, Section 3 presents a grid of models proposed as an effort to match the observations, and in Section 4 we compare the model results with observed upper limits and detections. In Section 5 we discuss the implications

of the comparison between the models and observations, and finally in Section 6 we summarize the main findings.

## 2. The Water Line Survey

The observations presented in this paper were obtained with the Heterodyne Instrument for the Far-Infrared (HIFI; de Graauw et al. 2010; Roelfsema et al. 2012) on board the *Herschel Space Observatory* (Pilbratt et al. 2010) as part of the Guaranteed Time Key Project “Water in Star-forming Regions with *Herschel*” (WISH; van Dishoeck et al. 2011) and two open-time programs (PI: M. Hogerheijde). With its FWHM beam of  $18''$ – $38''$  at the observing frequencies, *Herschel* covers the entire disk of all sources. Table 1 gives an overview of the observed sources, lines, dates, OBS ID identifiers, and observing times,  $t_{\text{obs}}$ . On-source integration times range between 35% and 45% of  $t_{\text{obs}}$ , with a larger fraction spent on-source for larger  $t_{\text{obs}}$ ; the remainder of  $t_{\text{obs}}$  was spent on the off positions and telescope overheads. Three frequency settings cover more than one line: the setting at 556.9 GHz contains the  $\text{NH}_3$   $1_0-0_0$  line at 572.49817 GHz, the setting at 1113.3 GHz contains the  $^{13}\text{CO}$   $10-9$  line at 1101.3496594 GHz, and the 1153.1 GHz setting covers the  $^{12}\text{CO}$   $10-9$  line at 1151.985452 GHz. Detections of  $\text{H}_2\text{O}$   $1_{10}-1_{01}$  and  $1_{11}-0_{00}$  and

**Table 2**  
Upper Limits of the Water  $1_{10}-1_{01}$ ,  $1_{11}-0_{00}$ ,  $3_{12}-2_{21}$ , and  $3_{12}-3_{03}$  Lines, Together with Other Basic Parameters of Each Source

Source	Line	Upper Limit (mK km s <sup>-1</sup> )	FWHM (km s <sup>-1</sup> )	$M_{\text{star}}$ ( $M_{\odot}$ )	$T_{\text{eff}}$ (K)	$L_{\star}$ ( $L_{\odot}$ )	SpT	$M_{\text{disk}}^a$ $M_{\odot}$	$d$ (pc)	$r_{\text{out}}$ (au)	References
TW Hya	$1_{11}-0_{00}$	<b><math>54.5 \pm 3.7^b</math></b>	1.3	0.8	4100	0.28	K7	0.05	51	215	(4, 5)
	$1_{10}-1_{01}$	<b><math>32.5 \pm 1.4^b</math></b>	1.3								
	$3_{12}-2_{21}$	116.0	1.0								
	$3_{12}-3_{03}$	13.4	1.0								
HD 100546	$1_{11}-0_{00}$	<b><math>247.0 \pm 4.1^b</math></b>	7.3	2.4	10471	32.4	B9Vne	0.005	103	500	(6, 17, 28)
	$1_{10}-1_{01}$	<b><math>163.0 \pm 3.0^b</math></b>	6.6								
	$3_{12}-2_{21}$	895.0	6.5								
AA Tau	$1_{11}-0_{00}$	70.5	4.0	0.76	4060	0.8	K7	0.02	140	160	(12, 27)
	$1_{10}-1_{01}$	19.5	4.0								
	$3_{12}-2_{21}$	583.0	4.0								
DM Tau	$1_{11}-0_{00}$	20.5	1.5	0.65	3705	0.25	M1	0.025	140	750	(3, 9, 13, 23, 29)
	$1_{10}-1_{01}$	7.2	1.5								
	$3_{12}-2_{21}$	336.0	1.5								
	$3_{12}-3_{03}$	46.6	1.5								
HD 163296	$1_{11}-0_{00}$	158.0	9.0	2.3	9333	30.2	A1Ve	0.07	122	450	(6, 19, 30)
	$1_{10}-1_{01}$	236.0	9.0								
LkCa 15	$1_{10}-1_{01}$	20.0	3.0	1.05	4375	0.74	K5	0.03	145	900	(3, 9, 14, 26, 31)
	$3_{12}-2_{21}$	675.0	3.0								
	$3_{12}-3_{03}$	89.0	3.0								
MWC 480	$1_{10}-1_{01}$	34.5	5.0	2.2	8710	32.4	A3ep+sh	0.04	131	170	(7, 21)
	$3_{12}-2_{21}$	1125.0	5.0								
	$3_{12}-3_{03}$	140.0	5.0								
AS 209	$1_{10}-1_{01}$	75.3	3.0	0.9	4250	1.5	K5	0.028	125	120	(1, 2, 15, 32)
BP Tau	$1_{10}-1_{01}$	52.1	2.0	0.77	4055	0.83	K7	0.0012	56	120	(3, 10, 13, 18, 33)
GG Tau	$1_{10}-1_{01}$	86.0	3.0	0.12	3055	0.065	M5.5	0.01	140	500	(3, 16, 22, 34)
GM Aur	$1_{10}-1_{01}$	75.0	3.0	1.22	4750	1.01	K3	0.04	140	300	(1, 3, 9, 24, 35)
MWC 758	$1_{10}-1_{01}$	74.6	3.0	1.8	7600	11	A8Ve	0.01	200	250	(8, 12, 25)
T Cha	$1_{10}-1_{01}$	85.6	4.0	1.1	5888	1.35	G2:e	0.001	66	230	(7, 20)

**Notes.** The quoted upper limits are based on the WBS measurements. The values in the upper limit column with an error bar (in boldface) are positive detections.

<sup>a</sup> Calculated from  $M_{\text{dust}}$  assuming a dust-to-gas mass ratio of 0.01.

<sup>b</sup> These are positive detections, not upper limits.

**References.** 1. Herbig & Bell (1988), 2. Andrews et al. (2009), 3. White & Ghez (2001), 4. Andrews et al. (2012), 5. Bergin et al. (2013), 6. van den Ancker et al. (1997), 7. van den Ancker et al. (1998), 8. Beskrovnaya et al. (1999), 9. Furlan et al. (2009), 10. Johns-Krull et al. (1999), 11. Briceño et al. (2002), 12. Chapillon et al. (2008), 13. Simon et al. (2000), 14. Kraus & Ireland (2012), 15. Andrews et al. (2010), 16. Kenyon et al. (1994), 17. Mulders et al. (2013), 18. Dutrey et al. (2007), 19. Tilling et al. (2012), 20. Huélamo et al. (2015), 21. Hamidouche et al. (2006), 22. Dutrey et al. (1997), 23. Panic (2009), 24. Schneider et al. (2003), 25. Isella et al. (2010), 26. Piétu et al. (2006), 27. Cox et al. (2013), 28. Leinert et al. (2004), 29. Guilloteau & Dutrey (1994), 30. Grady et al. (2000), 31. Isella et al. (2012), 32. Huang et al. (2016), 33. Dutrey et al. (2003), 34. Kawabe et al. (1993), 35. Hughes et al. (2009).

<sup>12</sup>CO 10–9 toward TW Hya and HD 100546, and NH<sub>3</sub> 1<sub>0</sub>–0<sub>0</sub> toward TW Hya only, are presented elsewhere (Hogerheijde et al. 2011; Fedele et al. 2013b, 2016; Salinas et al. 2016; M. Hogerheijde et al. 2017, in preparation) (the  $1_{10}-1_{01}$  line of HD 100546 can be seen in Figure 3 of van Dishoeck et al. 2014). An earlier report on DM Tau containing only a fraction of the data presented here can be found in Bergin et al. (2010). In Appendix B (Figures 10–17) we show the observed spectra of all of the sources and lines that have been surveyed (the CO data for HD 100546 have been published before in Fedele et al. 2013a). Here we focus on the non-detections (upper limits) of the full data set, with the exception that we also report a new detection of the  $1_{10}-1_{01}$  line in the stacked spectrum of AA Tau, DM Tau, LkCa 15, and MWC 480 (Section 4.3).

We performed very deep observations for the  $1_{10}-1_{01}$  and  $1_{11}-0_{00}$  transitions in four sources (AA Tau, DM Tau, LkCa 15, MWC 480). The integration times were motivated by the TW Hya detection. Thus, scaled for distance, if other sources were as strong as TW Hya, we should be able to detect the two lines. To account for the possibility that the ground-state lines might not be well matched to the excitation state of the disk gas, we also observed higher transitions (with less integration times).

For all observations we used dual beam switch mode with a 3' throw. The spectra were recorded with the wide-band spectrometer (WBS) and high-resolution spectrometer (HRS) with respective velocity resolutions of 0.59 and 0.13 km s<sup>-1</sup> around 550 GHz, and 0.3 and 0.067 km s<sup>-1</sup> around 1100 GHz. The data are processed with various HIPE (Herschel Interactive Processing Environment) versions

**Table 3**  
Parameters for the Grid of Models

Stellar type	B, A, F, G, K, M
Disk dust mass	$(0.25, 0.5, 1.0, 2.0) \times 10^{-4} M_{\odot}$
Dust-to-gas mass ratio	0.01, 0.1, 1.0
Oxygen depletion	$10^{-6}, 10^{-4}, 0.01, 0.1, 1.0$

(4.0–12.1.0), which all give consistent results, and are further analyzed with the CLASS software package.<sup>13</sup> HIFI measures the vertical and horizontal polarizations separately. We averaged the two polarization signals together, after verifying their consistency, and only report the upper limits based on the WBS data, because of their lower noise. Intensities on the main-beam antenna temperature scale follow from the in-orbit calibrated  $T_A^*$  antenna temperature scale using main-beam efficiencies  $\eta_{mb} = 0.64$  around 550 GHz and 0.63 around 1100 GHz.<sup>14</sup> Finally, linear spectral baselines are subtracted in a  $\sim 40 \text{ km s}^{-1}$  range around the line frequencies, and rms noise levels are extracted (Table 2). The rms of the integrated intensities (when not detected) are calculated from the FWHM of the low- $J$  CO lines and the per-channel noise. Reported upper limits are  $3\sigma$  where  $\sigma = 1.2 \times \text{rms}$ , with the extra factor 1.2 taking into account an estimated 20% flux calibration uncertainty.

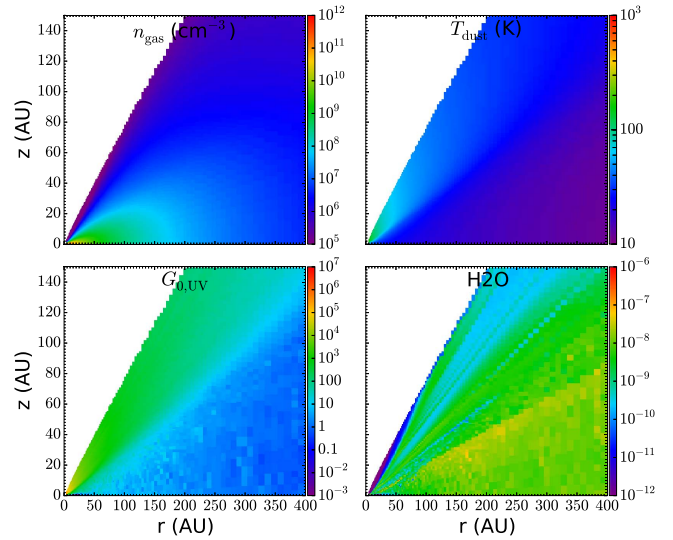
### 3. A Grid of Models

We aim to gain insights into the disk chemistry by a quantitative comparison between the observed upper limits of the water lines with predictions from chemical models. The code for this work is the same as that used in Du & Bergin (2014) and Du et al. (2015). The disk surface density profile is modeled with an analytical prescription (see, e.g., Andrews et al. 2009)

$$\Sigma \propto \left(\frac{r}{r_c}\right)^{-\gamma} \exp\left[-\left(\frac{r}{r_c}\right)^{2-\gamma}\right],$$

where  $\gamma$  is fixed to 1.5, and  $r_c$  is fixed to 400 au (hence essentially a power-law profile). This profile is fixed to limit the number of models in the grid. The power-law index  $\gamma$  in the above formula does not affect the predicted line intensities significantly (when taking values in the usual range  $\sim 1$ –2). The vertical structure is calculated based on hydrostatic equilibrium, iteratively determined by calculating dust temperature with Monte Carlo radiative transfer (Dullemond & Dominik 2004). The gas temperature is calculated based on heating-cooling balance. The chemical calculation is based on the UMIST 2006 network, extended with adsorption, desorption, and dust-surface chemistry. Figure 1 shows the distribution of gas density, dust temperature, UV intensity, and water vapor abundance in an example model.

We run a grid of models for a range of values for four key parameters of a protoplanetary disk (Table 3). We assume that for each disk, its dust mass is well-determined, but its gas mass is not. For a fixed dust mass of the disk, a lower dust-to-gas mass ratio means a higher gas mass. To simulate the effect of loss of oxygen due to ice settlement and migration, we



**Figure 1.** Gas density, dust temperature, UV intensity, and water vapor abundance in an example model. The underlying disk has a dust-to-gas mass ratio of  $10^{-2}$ , dust mass of  $10^{-4} M_{\odot}$ , a stellar spectral type of G, and no oxygen and carbon depletion.

introduce an oxygen depletion factor, which is the oxygen abundance in the model relative to the ISM value. The gas mass and the degree of oxygen depletion are partially degenerate in determining the water emission intensity, but not completely due to their different effect on the temperature calculation. The disk inner radius is fixed to 4 au, and the outer radius is fixed to 400 au. Test runs show that the exact value of the inner radius does not significantly affect the water emission under consideration of this work. The effect of the disk outer radius will be discussed in later sections.

## 4. Results

### 4.1. Observed Upper Limits versus the Models

The correspondence between a specific model in the grid and each of the observed sources is based on matching between the stellar types and the measured disk dust masses. The observed intensities or upper limits of the water lines for each source are scaled to a distance of 100 pc for comparison. We further scaled the values for the  $l_{10}$ – $l_{01}$  and  $l_{11}$ – $0_{00}$  lines with a disk outer radius of 400 au, assuming the line emission is uniformly distributed over the whole disk; namely, for each source, the line intensity (upper limit) to be compared with the models is calculated from the observed value by

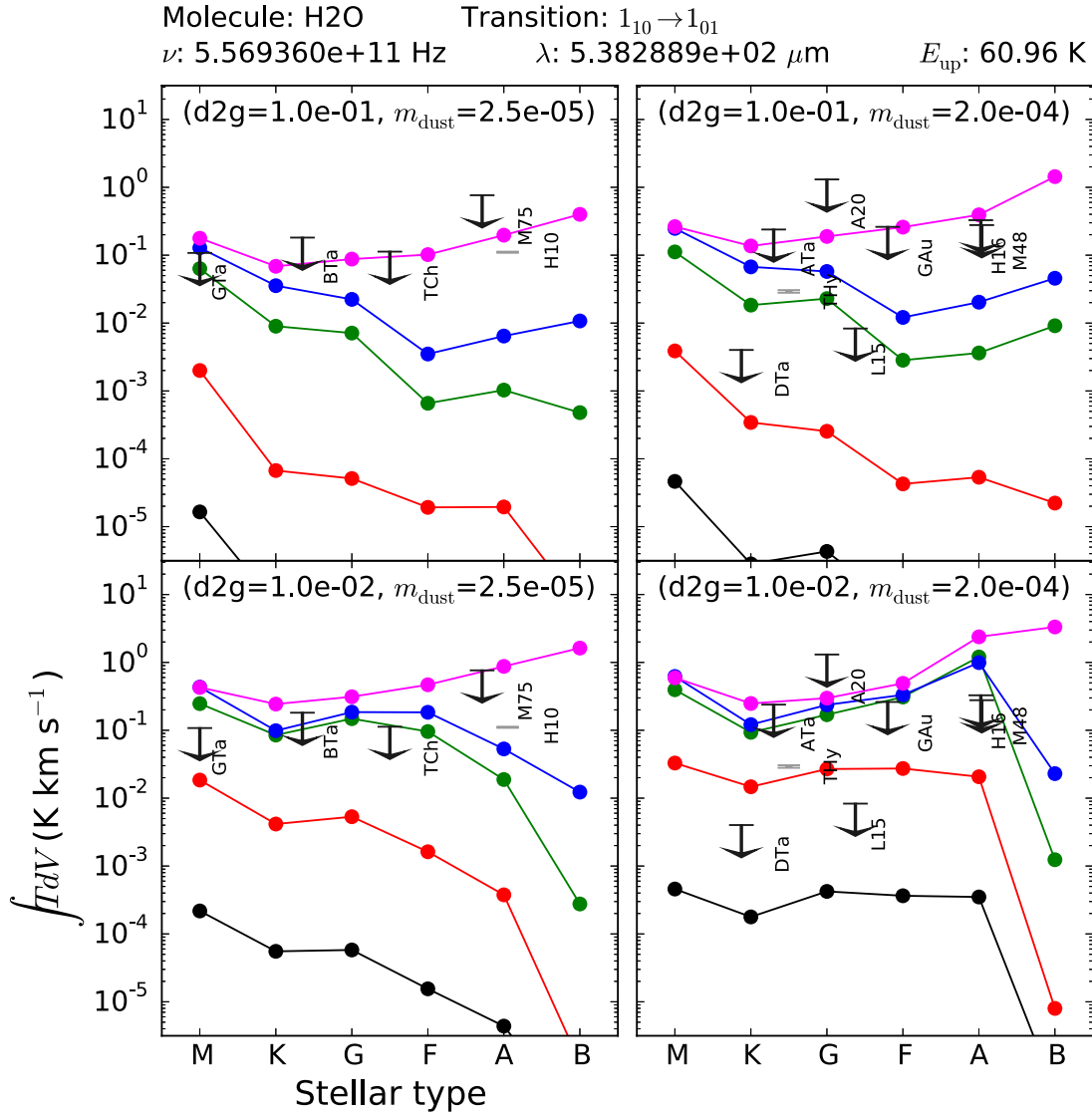
$$I_{\text{model}} = I_{\text{obs}} \left(\frac{400 \text{ au}}{R_{\text{out}}}\right)^2 \left(\frac{d}{100 \text{ pc}}\right)^2.$$

We did not scale the intensities of  $3_{12}$ – $2_{21}$  and  $3_{12}$ – $3_{03}$  with disk size (but they are still scaled with distance), because they mostly originate from the inner disk (see below). For a subset of the parameter space, Figures 2 and 3 show the placement of the observed upper limits (black arrows) for the  $l_{10}$ – $l_{01}$  and  $3_{12}$ – $2_{21}$  transitions together with some detections relative to the models. For more complete data, see Figures 6–9 (in Appendix A). In these figures, each panel corresponds to a specific dust-to-gas mass ratio (d2g) and disk dust mass ( $m_{\text{dust}}$ ). Each panel shows the modeled line intensity as a function of stellar type with different oxygen depletion factors.

<sup>13</sup> See <http://www.iram.fr/IRAMFR/GILDAS>.

<sup>14</sup> HIFI-ICC-RP-2014-001 at <http://herschel.esac.esa.int/twiki/bin/view/Public/HifiCalibrationWeb>.





**Figure 2.** Modeled water  $1_{10}-1_{01}$  line intensities (round dots), together with the observed upper limits (black arrows; scaled to a distance of 100 pc and a disk outer radius of 400 au) and detections (gray error bars). Each panel corresponds to a combination of dust-to-gas mass ratio (varying in the vertical direction) and dust mass (varying in the horizontal direction). The abbreviated source names are shown for each data point (upper limit or error bar); e.g., HD 100546 is shown as H10, and GG Tau as GTa (see Table 2). The upper limits are three times the rms noise plus 20% of systematic uncertainty (the head of each arrow is located at one third of each upper limit). Different colors of the models mean different degree of oxygen depletion. Magenta: no oxygen depletion; blue: 0.1; green: 0.01; red:  $10^{-4}$ ; black:  $10^{-6}$ .

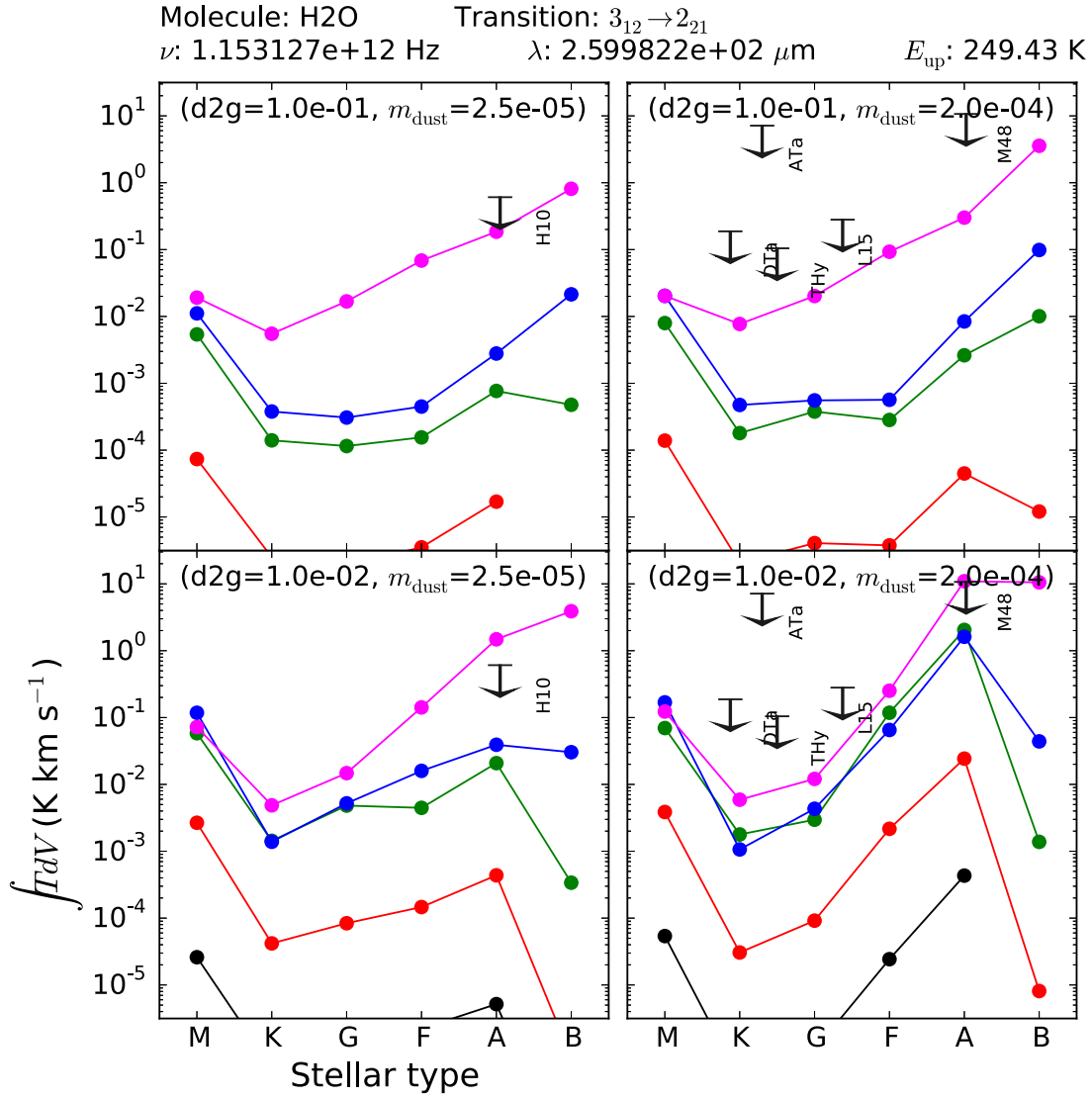
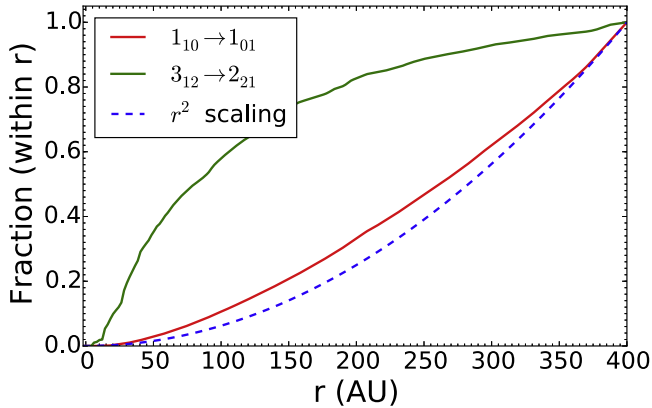
The  $1_{10}-1_{01}$  and  $1_{11}-0_{00}$  lines have upper energy levels of 50–60 K (Figures 2 and 7). With a normal dust-to-gas mass ratio (0.01; bottom panels in the figures), they require a high degree of oxygen depletion (by a factor  $\sim 10^{-2}$  to  $< 10^{-4}$ ) to be consistent with the observed upper limits. Even in the extreme case of dust-to-gas mass ratio being one (i.e., very low gas mass), the models still tend to over-predict the two lines for most sources by at least a factor of a few, and models with oxygen depletion agree better with the data.

The observational upper limits of the  $3_{12}-2_{21}$  and  $3_{12}-3_{03}$  lines are not as constraining as the other two lines, due to their shallower integration times. They are consistent with (but do not infer) a lower degree of depletion for oxygen or no depletion at all. It is possible that future observations may provide more stringent limits on their fluxes, which will require the depletion of oxygen to a degree similar to that of

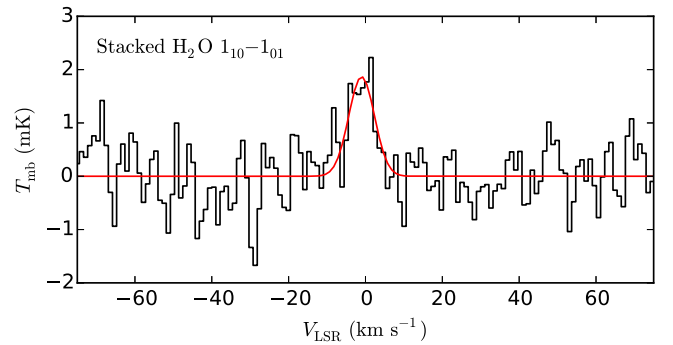
the other two lines. On the other hand, the upper-state energies of  $3_{12}-2_{21}$  and  $3_{12}-3_{03}$  are  $\sim 250$  K, which means that they originate mostly from the inner warm part of the disk. This can be seen in Figure 4, which shows the accumulative distribution of the  $1_{10}-1_{01}$  and  $3_{12}-2_{21}$  lines as a function of radius. A low level of oxygen depletion in the inner disk is consistent with (or even needed for) a scenario found in Du et al. (2015; see also Bergin et al. 2016), in which the elemental abundance of oxygen in the inner disk is not as depleted as in the outer disk, possibly due to inward migration and the subsequent evaporation of icy dust particles.

#### 4.2. Effect of the Disk Size

In our grid of models the disk outer radius is fixed to 400 au, and for comparison we scaled the observational intensities, or upper limits, for  $1_{10}-1_{01}$  and  $1_{11}-0_{00}$  to this disk

Figure 3. Same as Figure 2 except that it is for the  $3_{12}-2_{21}$  line.Figure 4. Cumulative distribution of emission as a function of radius (i.e., the fractional amount of emission within  $r$ ) for the  $1_{10}-1_{01}$  and  $3_{12}-2_{21}$  lines. The underlying disk model is the same as in Figure 1. The dashed line shows a  $r^2$ -scaling relation, which is used for scaling the  $1_{10}-1_{01}$  and  $1_{11}-0_{00}$  transitions.

size, using disk sizes found in the literature. Such a scaling is reasonable, since these two lines are roughly uniformly distributed in the outer disk (see Figure 4). One issue with this

Figure 5. Detection of the water  $1_{10}-1_{01}$  line (557 GHz) in the stacked spectra of AA Tau, DM Tau, MWC 480, and LkCa 15. The integrated intensity (weighted average) is  $15 \pm 3$  mK km s<sup>-1</sup>.

procedure is that for many disks their sizes are not well-known, or not well-defined. For example, the disk outer radius of LkCa 15 inferred from dust is 150 au, while  $^{12}\text{CO}$  gives a value of 900 au (Isella et al. 2012). For the calculation here we always adopt the size of the gas disk as seen in CO when

available, otherwise we use the size inferred from scattered light. Salinas et al. (2016) and M. Hogerheijde et al. (2017, in preparation) also address the radial location of the detected low-excitation water emission lines in TW Hya and HD 100546. It is important to get reliable estimates of  $r_{\text{in}}$  and  $r_{\text{out}}$ .

The disk size does not play a significant role for the  $3_{12}-2_{21}$  and  $3_{12}-3_{03}$  lines, as they mostly originate from the inner warm disk; therefore, we did not rescale them for the disk size.

One may say that water vapor does not necessarily coexist with gas tracers such as CO, or, in other words, the sizes of the water vapor disks are likely to be much smaller than that of the CO disks. Actually, this is exactly our point: in the outer disk, the abundance of gas-phase oxygen (hence water vapor) must be much lower than model predictions from canonical elemental abundances to match the data, which is equivalent to saying that the oxygen (and water vapor) distribution is radially much more compact than other species (such as  $\text{H}_2$ ). One limitation of the current grid of models is that we assume (to limit the number of variables) that the elemental abundances are uniform over the whole disk; in more detailed models for TW Hya and DM Tau, as described in Du et al. (2015) and Bergin et al. (2016), we found that nonuniform elemental distributions (in which oxygen and carbon become more abundant toward the inner disk) are needed to match well with richer data sets (more lines from water and from other species), which is essentially saying that the disk size as seen in volatile oxygen (and carbon) is small compared to the overall gas disk.

#### 4.3. Detection of the $1_{10}-1_{01}$ Line in Stacked Spectra of AA Tau, DM Tau, LkCa 15, and MWC 480

The  $1_{10}-1_{01}$  line is not detected in the individual spectrum of AA Tau, DM Tau, LkCa 15, and MWC 480 (the deepest integrations in our survey), but when their spectra are stacked together after correcting for their different velocities, a feature with an integrated intensity of  $\sim 5\sigma$  emerges (Figure 5). Weighted stacking including all of the sources gives a similar result. Assuming that this line has roughly the same intensity in these four disks, its intensity in each of them would be  $15 \pm 3 \text{ mK km s}^{-1}$ . Comparing this value with Figure 2 shows that, in the case of dust-to-gas mass ratio of 0.01, oxygen has to be depleted relative to the ISM value by a factor of  $\sim 10^{-4}$  (at least in the upper emissive layers) to match the detected intensity.

### 5. Discussions and Implications

We have surveyed 4 water lines (2 ground-state transitions and 2 at higher levels, with the former 2 conducted with very deep integration and the latter 2 with shallower integration) in 13 protoplanetary disks. With the exception of TW Hya, HD 100546, and the stacked data of AA Tau, DM Tau, LkCa 15, and MWC 480, the lines are not detected at the present noise level, while a higher detection rate for the ground-state lines is expected from canonical models.

Previously it has been observationally found that the low-energy emission of water, O I, and CO in TW Hya tend to be weaker than values expected from thermo-chemical models. The current work shows that this is true in a larger sample, with a typical degree of depletion for oxygen of the order of

$10^{-2}$  to  $10^{-4}$ . In our view, the most likely underlying mechanism for this is the coupled evolution of dust and gas chemistry (Bergin et al. 2016), in which the dust particles act as a sink of the volatiles and a vehicle to transport them to the midplane and the inner disk. An analytical study based on similar ideas can be found in Kama et al. (2016b), and a more detailed Monte Carlo simulation is given by Krijt et al. (2016). The low water line emission intensity in the sample indicates that this is likely a ubiquitous phenomenon. Recently Antonellini et al. (2016) proposed that the high noise level caused by the continuum flux was the most likely explanation for the low detection rate of mid-IR water lines in disks around Herbig stars; in our case, the continuum flux is much weaker, and the discrepancy between the upper limits from the data and the canonical models provide useful information about the chemical and physical processes in the disks, and also for Herbig stars.

The depletion of volatiles may not be uniform throughout the disk or be of the same degree for different sources (see, e.g., Ciesla & Cuzzi 2006). The water emission lines in this work originate from cold or lukewarm water vapor (with upper-state energies 53 and 249 K), as opposed to the hot water vapor emission lines detected by Salyk et al. (2008) and Pontoppidan et al. (2010b). Water vapor would exist throughout the disk, and in the outer disk, below its freezing temperature, it is released from the dust grains by photodesorption (Walsh et al. 2010). The current work, together with previous related studies, shows that cold water vapor is depleted (i.e., lower than expected from canonical models).

For the inner disk, a number of studies have found very high column densities of hot water vapor, from  $10^{17}$  to  $10^{21} \text{ cm}^{-2}$ , with values depending on the assumed emitting area (e.g., Salyk et al. 2008 and Doppmann et al. 2011). Abundance ratios of water relative to CO of 1–10 generally indicate high water abundances of order  $10^{-4}$ – $10^{-5}$ , suggesting that the disk surfaces are not “dry” (e.g., Salyk et al. 2011; Mandell et al. 2012), although some classes of disks appear to have less water in their innermost regions (e.g., Najita et al. 2013; Zhang et al. 2013; Banzatti et al. 2017). Carr et al. (2004) found a factor of 10 depletion for the hot ( $\sim 1500 \text{ K}$ ) water vapor within 0.3 au of the young stellar object SVS 13. This value is consistent with Krijt et al. (2016), but is still much less than the typical values found in the present survey. Blevins et al. (2016) demonstrate a quantitative drop of at least 5 orders of magnitude in water abundance from inner to outer disk for their sample of disks with deep VLT, *Spitzer*, and *Herschel* data, similar to what is found here.

The prominent difference between the cold and hot water vapor indicates that the outer disk and inner disk are subject to different processes. While dust grains are growing and settling down to the midplane in the outer disk, in the inner disk they might be stirred up by certain mechanisms and return volatiles back to the gas phase (even large bodies may evaporate interior to the snowline). Due to the differential nature of dust sedimentation, icy particles of a small size can continue to exist in the outer disk for a long time, giving rise to water ice features (Chiang et al. 2001).

A low gas-to-dust mass ratio (maybe close to or even lower than one) could also explain the non-detections. Disks lose gas and dust through accretion and photoevaporation

(Hartmann et al. 1998; Adams et al. 2004; Alexander et al. 2006; Owen et al. 2012; Bae et al. 2013; Gorti et al. 2015), and possibly through other mechanisms (Hollenbach et al. 2000; Alexander et al. 2014). The mass loss rate due to photoevaporation typically lies in the range  $10^{-10}$ – $10^{-7} M_{\odot}$  (Owen et al. 2011). In photoevaporating flows, small dust particles are entrained by gas, while large dust particles are left behind (Hutchison et al. 2016). Gorti & Hollenbach (2009) found that FUV photoevaporation can deplete most of the mass of a  $0.03 M_{\odot}$  disk with timescales  $\sim 1$  Myr, and is most effective in the outer disk. Gorti et al. (2015) found that  $\sim 3 \times 10^{-4} M_{\odot}$  of mass in solids remain after gas disk dispersal. At face value this gives a low gas-to-dust mass ratio.

However, the low value definitely does not apply to sources with gas mass determined directly (Bergin et al. 2013; McClure et al. 2016). We also note that the outer gas disks detected in CO or scattered light for some sources in our sample are not completely gone, and extend to a few hundred au. The observational detection of  $N_2H^+$  and  $HCO^+$  (Thi et al. 2004; Piétu et al. 2007; Qi et al. 2013) in the outer disk also requires the very existence of hydrogen gas (see Aikawa et al. 2015 for detailed calculations), and the CO emission in the outer disk also means some amount of gas still exist there. Furthermore, some disks (e.g., DM Tau, AS 209, and MWC 480) in our sample are still actively accreting. For an accretion rate of  $\sim 10^{-8} M_{\odot} \text{ yr}^{-1}$  (Hartmann et al. 1998; Johns-Krull et al. 2000; Grady et al. 2010), if the gas mass is indeed of the order of  $10^{-4} M_{\odot}$ , then the disk would be gone within  $\sim 10^4$  year; in other words, the probability of seeing the disk in its current state would be  $\lesssim 0.01$ . In reality, it is likely that chemical depletion coupled with dust evolution as we describe here and elsewhere (Du et al. 2015; Bergin et al. 2016) occurs with a timescale shorter than that of photoevaporation (see, e.g., Dullemond & Dominik 2005), perhaps even in the deeply embedded phases (Anderl et al. 2016).

As discussed extensively in Bergin et al. (2016), the depletion of oxygen can have a large effect on the abundances of other species, especially the hydrocarbons (Du et al. 2015). When oxygen is at its canonical ISM abundance ( $\sim 3 \times 10^{-4}$ ), most of the carbon atoms end up in CO. But when oxygen is depleted relative to carbon, the abundances of hydrocarbons will be significantly enhanced. Hence, it would be interesting to survey hydrocarbon emission in these sources. The creation of hydrocarbons is also tied with dust evolution, in that in a segregated disk with larger-sized grains mostly being in the inner region and smaller-sized grains

more diffusively distributed, the UV photons will be able to penetrate deeper into the outer disk, creating large amounts of hydrocarbons. This process is also an evolutionary effect, in the sense that disks with different ages will show different degrees of volatile depletion. Efforts are ongoing to search for hydrocarbon emission in (but not limited to) these sources to test this prediction.

## 6. Summary

In this paper we present a survey of 4 water lines (2 of them with very deep integration) in 13 protoplanetary disks, and compare the observed results with a grid of models. The main findings are as follows.

1. The detection rate is low: only the very-deeply integrated line(s) are detected in TW Hya, HD 100546 (not presented in this paper), and in the stacked spectrum of AA Tau, DM Tau, LkCa 15, and MWC 480.
2. To be consistent with the observational detections and upper limits, it is very likely that oxygen is depleted in the emissive layers of the disk (especially in the outer disk) by a factor of  $\sim 100$ – $10^4$ .
3. Oxygen distribution in the inner disk is less constrained; a lower depletion of oxygen in the inner disk than in the outer disk is consistent with current upper limits.

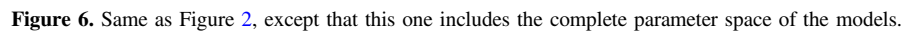
HIFI has been designed and built by a consortium of institutes and university departments from across Europe, Canada, and the United States (NASA) under the leadership of SRON, Netherlands Institute for Space Research, Groningen, The Netherlands, and with major contributions from Germany, France, and the United States. Support for this work was provided by NASA through an award issued by JPL/Caltech. E.A.B. acknowledges support from NASA XRP grant NNX16AB48G. M.H. and E.v.D. acknowledge support from the Netherlands Research School for Astronomy (NOVA) and European Union A-ERC grant 291141 CHEMPLAN. D.F. acknowledges support from the Italian Ministry of Education, Universities and Research project SIR (RBSI14ZRHR).

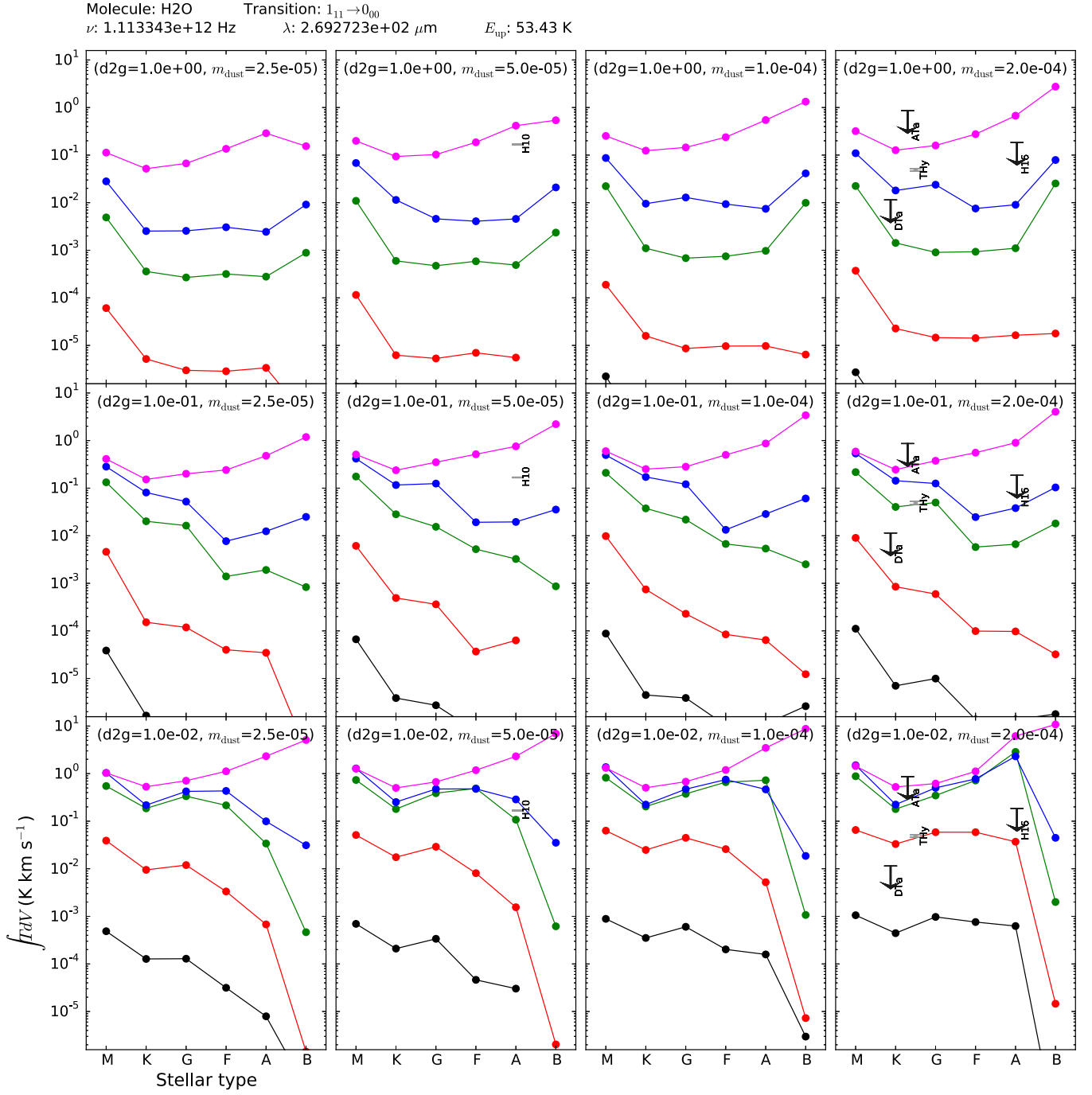
## Appendix A

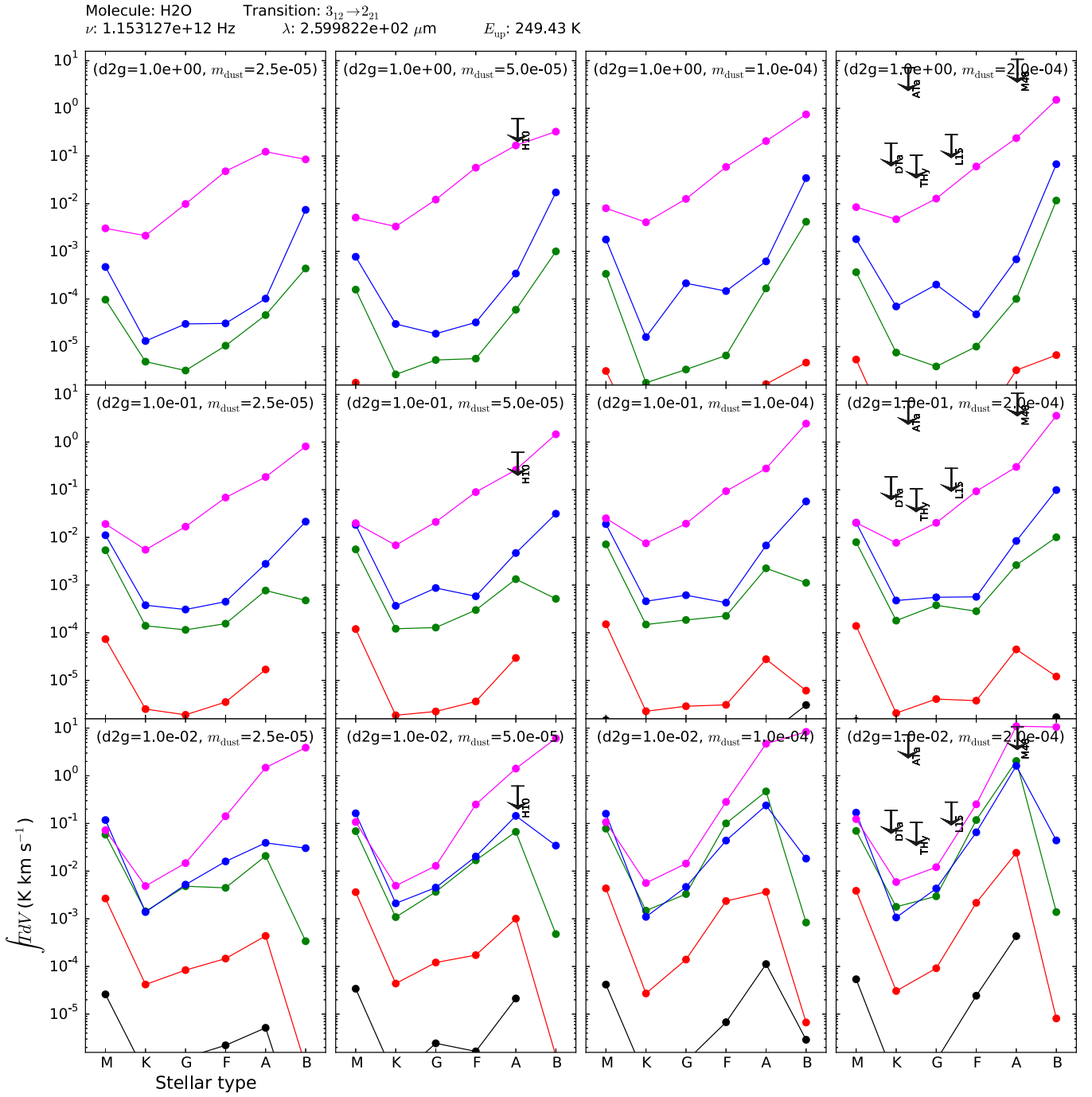
### Modeled Intensities of the Lines Versus Observations

In this appendix we show the complete grid of models (Figures 6–9).

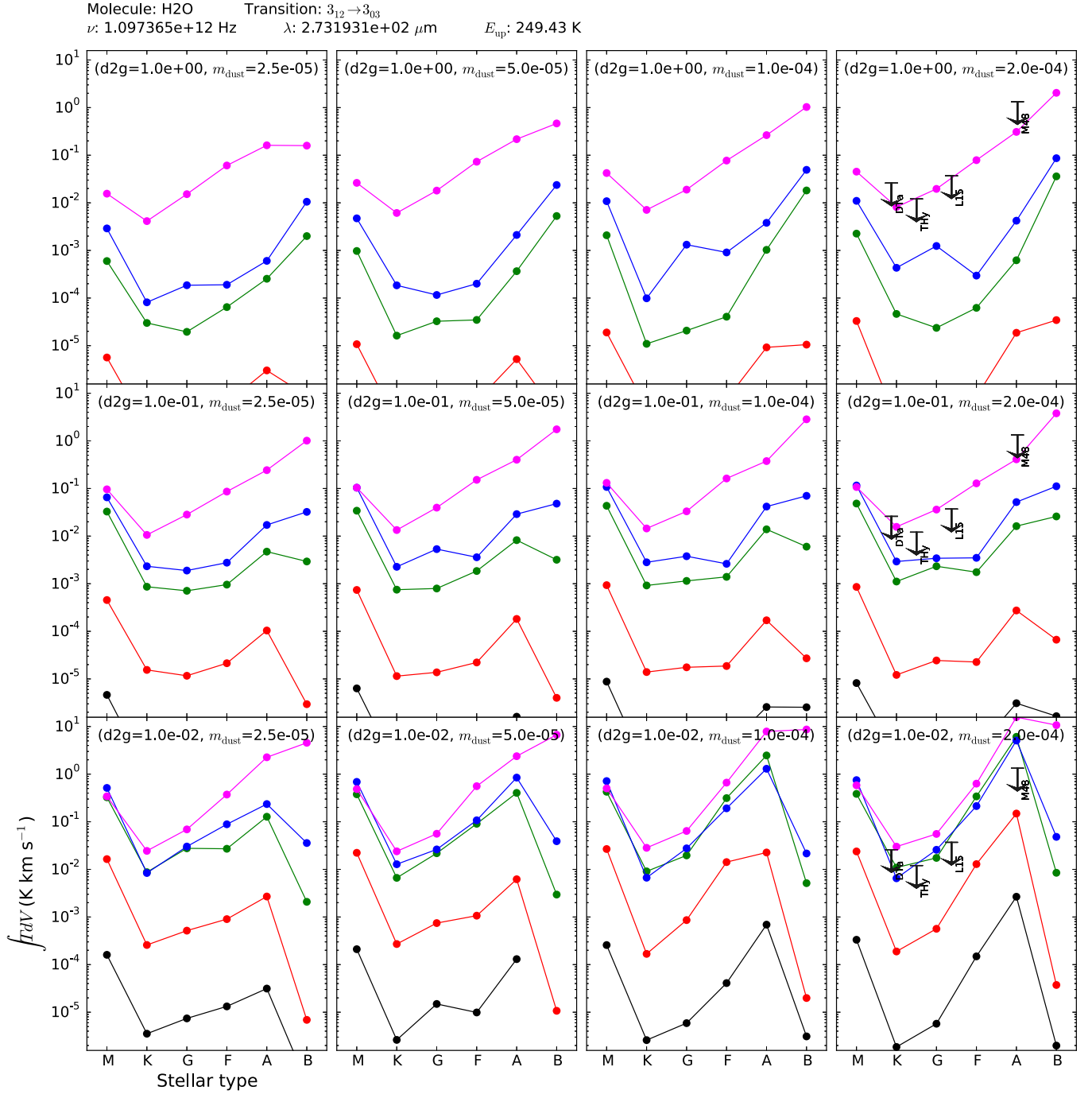




Figure 7. Same as Figure 6, except that it is for the  $1_{11}-0_{00}$  line.



**Figure 8.** Same as Figure 6, except that it is for the  $3_{12} \rightarrow 2_{21}$  line; the difference is that the observed upper limits are *not* rescaled with the disk size.

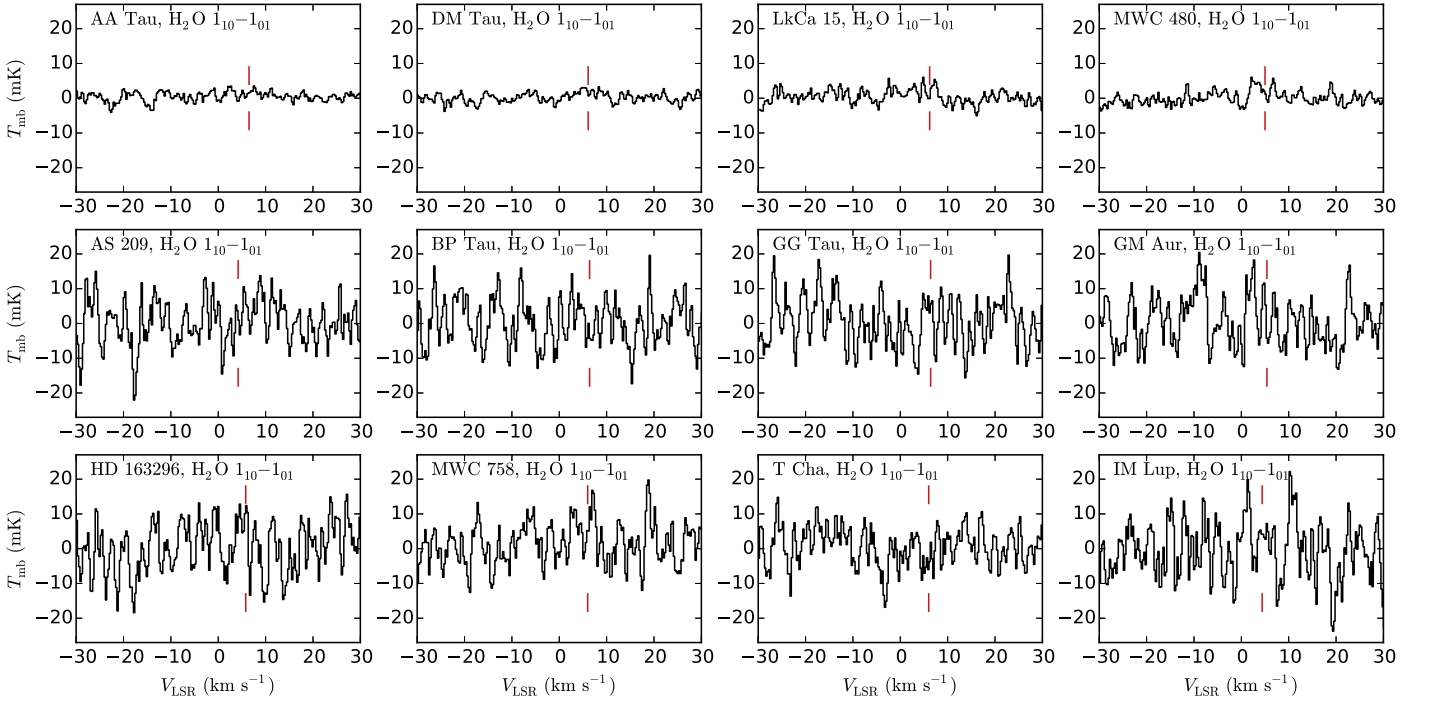
Figure 9. Same as Figure 8, except that it is for the  $3_{12} \rightarrow 3_{03}$  line.

## Appendix B

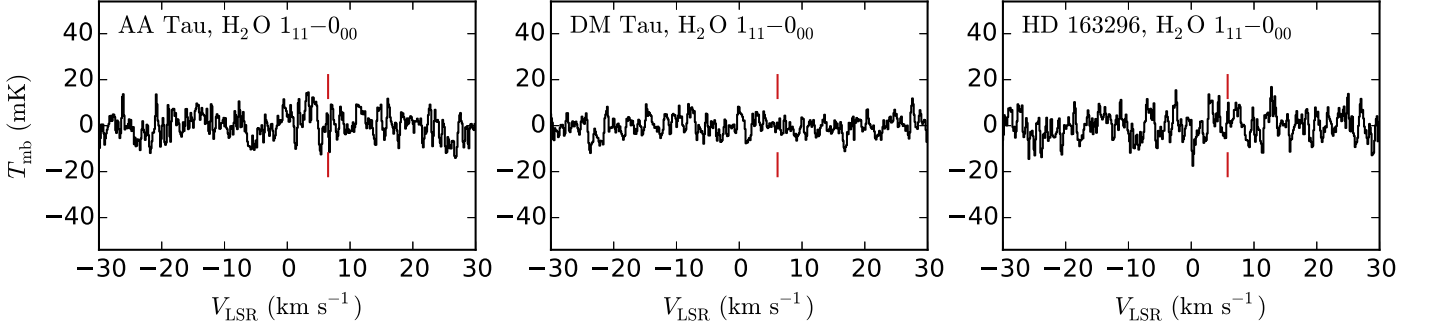
### Observed Spectra for all Sources

In this appendix we show the observed spectra of all of the sources and lines that have been surveyed in our study (Figures 10–17).

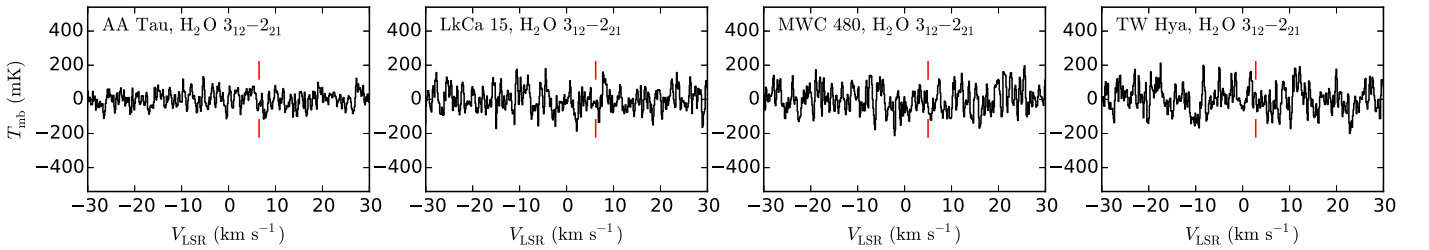




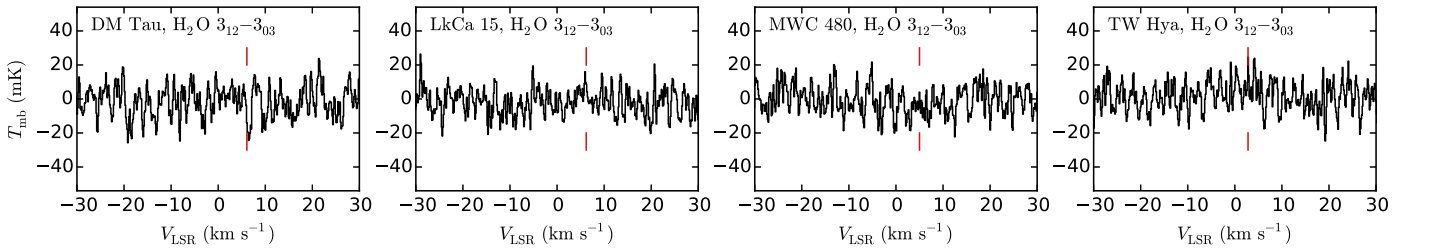
**Figure 10.** Water  $1_{10}-1_{01}$  spectra. The red line marks the  $V_{\text{LSR}}$  of each source.



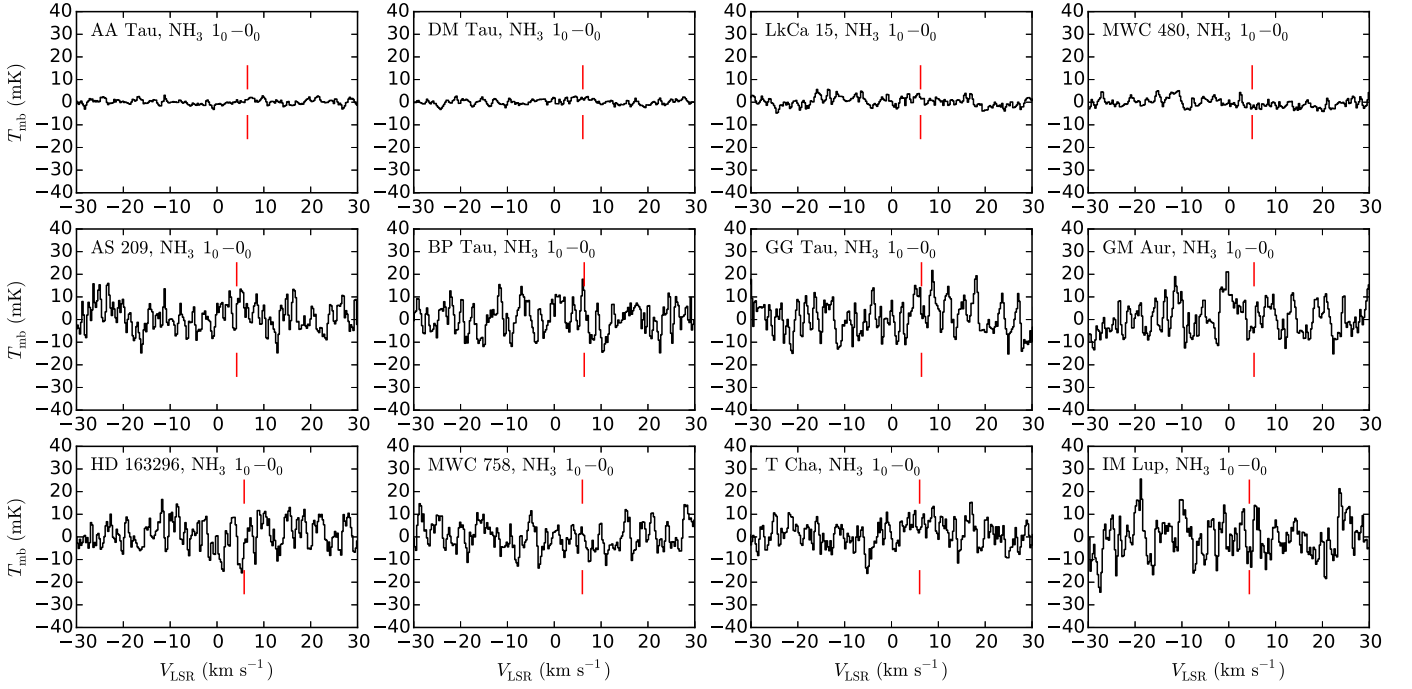
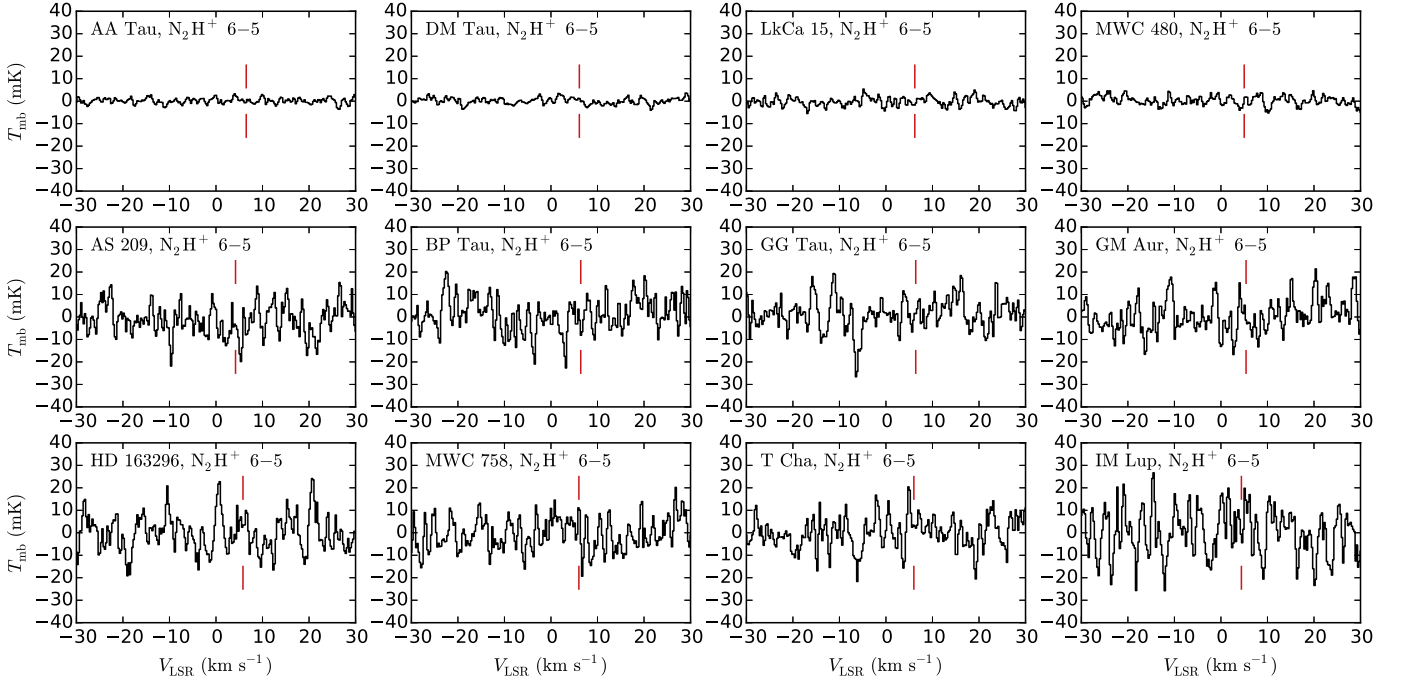
**Figure 11.** Water  $1_{11}-0_{00}$  spectra.



**Figure 12.** Water  $3_{12}-2_{21}$  spectra.



**Figure 13.** Water  $3_{12}-3_{03}$  spectra.

Figure 14.  $\text{NH}_3$  ( $1_0-0_0$ ) spectra.Figure 15.  $\text{N}_2\text{H}^+$  ( $6-5$ ) spectra.

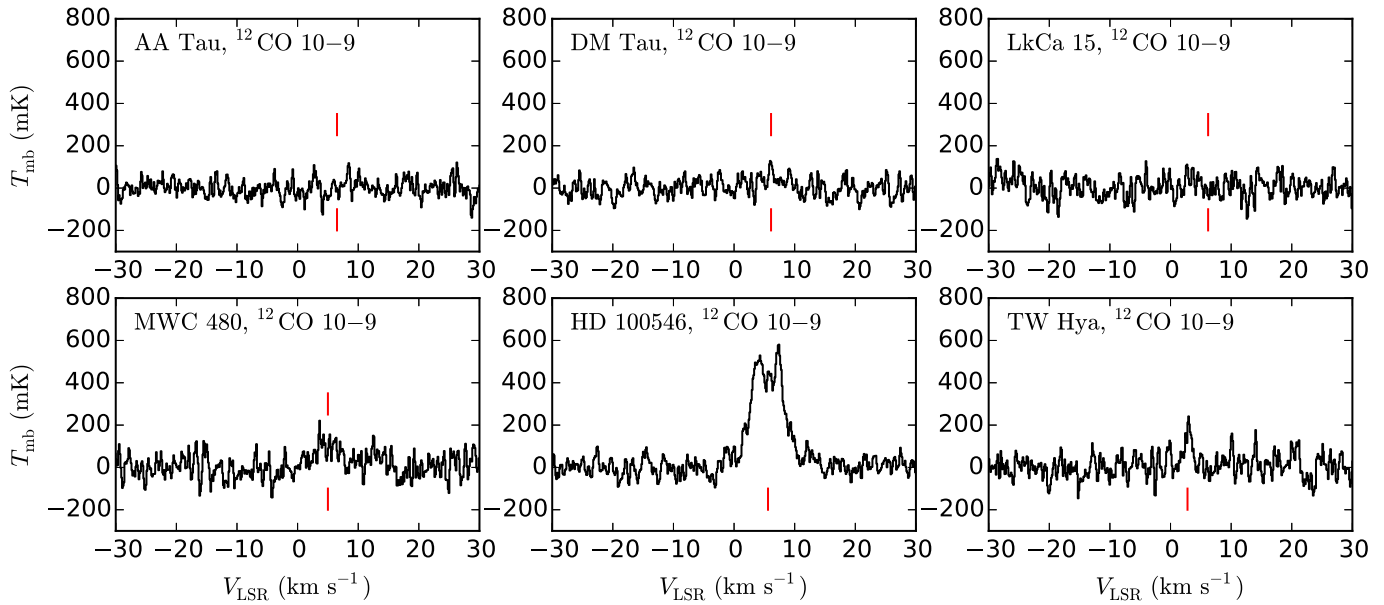
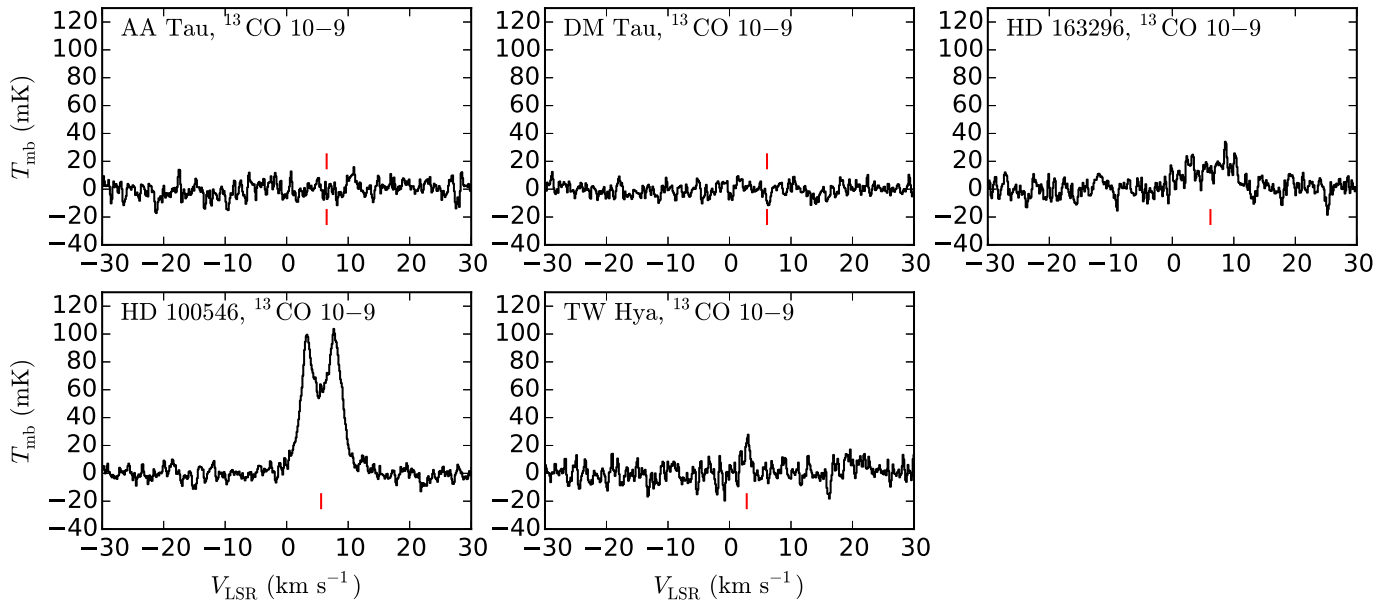


Figure 16. CO (10–9) spectra.

Figure 17.  $^{13}\text{CO}$  (10–9) spectra.

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