

Infrared spectra of complex organic molecules in astronomically relevant ice matrices I

Acetaldehyde, ethanol, and dimethyl ether

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ABSTRACT

Context. The number of identified complex organic molecules (COMs) in inter- and circumstellar gas-phase environments is steadily increasing. Recent laboratory studies show that many such species form on icy dust grains. At present only smaller molecular species have been directly identified in space in the solid state. Accurate spectroscopic laboratory data of frozen COMs, embedded in ice matrices containing ingredients related to their formation scheme, are still largely lacking.

Aims. This work provides infrared reference spectra of acetaldehyde (CH_3CHO), ethanol ($\text{CH}_3\text{CH}_2\text{OH}$), and dimethyl ether (CH_3OCH_3) recorded in a variety of ice environments and for astronomically relevant temperatures, as needed to guide or interpret astronomical observations, specifically for upcoming James Webb Space Telescope observations.

Methods. Fourier transform transmission spectroscopy ($500\text{--}4000\text{ cm}^{-1}$ / $20\text{--}2.5\text{ }\mu\text{m}$, 1.0 cm^{-1} resolution) was used to investigate solid acetaldehyde, ethanol and dimethyl ether, pure or mixed with water, CO, methanol, or CO:methanol. These species were deposited on a cryogenically cooled infrared transmissive window at 15 K. A heating ramp was applied, during which IR spectra were recorded until all ice constituents were thermally desorbed.

Results. We present a large number of reference spectra that can be compared with astronomical data. Accurate band positions and band widths are provided for the studied ice mixtures and temperatures. Special efforts have been put into those bands of each molecule that are best suited for identification. For acetaldehyde the 7.427 and $5.803\text{ }\mu\text{m}$ bands are recommended, for ethanol the 11.36 and $7.240\text{ }\mu\text{m}$ bands are good candidates, and for dimethyl ether bands at 9.141 and $8.011\text{ }\mu\text{m}$ can be used. All spectra are publicly available in the Leiden Database for Ice.

Key words. astrochemistry - methods: laboratory: molecular - techniques:spectroscopic - molecular processes

1. Introduction

Water was the first molecule to be detected in the solid state in the interstellar medium (Gillett & Forrest 1973). Since then more than 10 other molecules have been identified in icy form (i.e. CO, CO_2 , CH_4 , NH_3 and CH_3OH) and it has become clear that icy dust grains play a key role in the formation of both these small molecules and more complex organic molecules (COMs), such as glycolaldehyde (HOCH_2CHO) and ethylene glycol ($\text{HOCH}_2\text{CH}_2\text{OH}$). The combined outcome of

astronomical observations, specifically space based missions such as the *Infrared Space Observatory* (ISO) and *Spitzer Space Telescope* (Kessler et al. 1996; Werner et al. 2004), laboratory, and astrochemical modelling studies have resulted in a detailed picture of the composition and structure of ice mantles on interstellar dust grains and the chemical processes taking place (see reviews by Gibb et al. 2000; Herbst & van Dishoeck 2009; Öberg et al. 2011; Caselli & Ceccarelli 2012; Tielens 2013; Boogert et al. 2015; Linnartz et al. 2015; Öberg 2016). It is generally accepted that interstellar ices form on the surface of dust grains in cold

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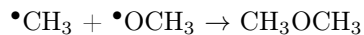
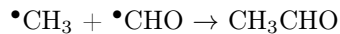
dark clouds through accretion in two distinct layers: a polar H₂O-rich and an apolar CO-rich layer. Water, together with NH₃, CO₂, and CH₄, forms through atom addition reactions in lower density environments (Hiraoka et al. 1995; Miyauchi et al. 2008; Oba et al. 2009; Dulieu et al. 2010; Hidaka et al. 2011; Linnartz et al. 2011; Oba et al. 2012; Lamberts et al. 2013, 2014; Fedoseev et al. 2015). At later stages, when densities increase and temperatures decrease along with the ongoing cloud collapse, CO freeze-out from the gas phase occurs, forming a CO coating on top of the water rich layer (Tielens et al. 1991; Pontoppidan 2006). Subsequent hydrogenation processes transform CO to H₂CO and H₂CO to CH₃OH (Watanabe & Kouchi 2002; Fuchs et al. 2009), resulting in CO ice intimately mixed with methanol (Cuppen et al. 2011; Penteado et al. 2015). Radical recombination processes in various starting mixtures, triggered by energetic (i.e. UV photons or cosmic rays) or non-energetic (i.e. atom additions) were shown to provide pathways towards the formation of more complex molecules (see reviews of Linnartz et al. 2015; Öberg 2016).

The molecules H₂O, CO, CO₂, CH₄, NH₃, and CH₃OH make up the bulk of interstellar ice (Ehrenfreund & Charnley 2000; Öberg et al. 2011), but less abundant species have been observed as well. These include species such as OCS and OCN⁻ (Palumbo et al. 1995; van Broekhuizen et al. 2004). A number of COMs, such as formic acid (HCOOH), acetaldehyde (CH₃CHO), and ethanol (CH₃CH₂OH), have been tentatively detected based on spectroscopic features at 7.2 and 7.4 μm (Schutte et al. 1999; Öberg et al. 2011). Several other spectroscopic features, such as the 6.0 and 6.8 μm bands, remain only partly identified (Schutte et al. 1996; Boudin et al. 1998; Gibb & Whittet 2002; Boogert et al. 2008). Limited astronomical detection sensitivity combined with a lack of high resolution laboratory data have thus far prohibited secure solid state identifications of COMs other than methanol, but their presence in interstellar ices is generally accepted and also further supported by the recent detection of a number of COMs on comet 67P/Churyumov-Gerasimenko and in its coma (Goesmann et al. 2015; Altwegg et al. 2017).

With the upcoming launch of the *James Webb Space Telescope* (JWST) in 2019, new instruments such as MIRI (Mid InfraRed Instrument; Wright et al. 2015) and NIRSpec (Near InfraRed Spectrograph; Posselt et al. 2004) will become available to record telluric free spectra of interstellar ices at higher spectral and spatial resolution and with higher sensitivity than possible so far. This opens up new possibilities to search for and study the level of molecular complexity in interstellar ices. To aid in the search for larger molecules in the solid state, high resolution IR laboratory spectra are required. The ice matrix environment and its temperature have to be taken into account since these influence the spectral appearance of vibrational bands.

In this work we present the infrared spectra of acetaldehyde, ethanol, and dimethyl ether, respectively, CH₃CHO, CH₃CH₂OH, and CH₃OCH₃. The choice for these three species, an aldehyde, an alcohol, and an ether, is motivated by previous tentative identifications (Boudin et al. 1998; Schutte et al. 1999; Öberg et al. 2011), their astronomical gas-phase identification and high abundance (e.g. Turner 1991; Gibb et al. 2000; Cazaux et al. 2003; Bisschop et al. 2007b; Taquet et al. 2015; Müller et al. 2016), and

their common formation scheme upon UV irradiation of methanol ice (Öberg et al. 2009). Formation of these molecules is seen in energetic processing experiments of methanol ice (Gerakines et al. 1996; Bennett et al. 2007; Öberg et al. 2009; Boamah et al. 2014) and starts with cleavage of the CH₃OH bonds. This results in a reservoir of radicals that can be used for their formation as follows:



Formation of dimethyl ether and ethanol has also been studied by radical recombination reactions starting from CH₄:H₂O mixtures (Bergantini et al. 2017). Besides energetic radical recombination reactions, other formation pathways and links between the three molecules exist as well. For example, acetaldehyde has been proposed as a solid state precursor of ethanol. A hydrogen atom addition experiment showed that acetaldehyde can at least partially (>20%) be transformed into ethanol (Bisschop et al. 2007a).

Acetaldehyde itself has been proposed to form as a spin-off in the well-studied CO+H → HCO → H₂CO → H₃CO → CH₃OH chain (Charnley 2004); HCO may directly interact with a C-atom, to form HCCO that upon hydrogenation yields CH₃CHO (Charnley & Rodgers 2005).

This work presents a detailed study of the IR spectral characteristics of CH₃CHO, CH₃CH₂OH, and CH₃OCH₃ in pure form and mixed in the interstellar relevant ice matrices H₂O, CO, CH₃OH, and CO:CH₃OH. Section 2 contains the experimental details and measurement protocols. The results of the measurements are presented and discussed in section 3. In section 4 the astronomical relevance of the new data is illustrated. The conclusions are summarized in Sect. 5. A complete overview with all data obtained in this study is available from the Appendices.

2. Experimental

2.1. Set-up

The ice spectra are recorded in a high-vacuum (HV) set-up, which is described in detail by Bossa et al. (2015). A central stainless steel chamber is evacuated by a 300 ls⁻¹ turbomolecular pump, backed by a double stage rotary vane pump (8 m³ hr⁻¹). This allows a base pressure of ~10⁻⁷ mbar at room temperature. The pressure is monitored by an Agilent FRG-720 full range gauge. Ices are grown on an infrared transmissive ZnSe window that is cryogenically cooled to a lowest temperature of 12 K by a closed cycle helium cryostat. The temperature of the window is monitored by a LakeShore 330 temperature controller, which regulates a feedback loop between a resistive heating wire and a silicon diode temperature sensor. An absolute temperature accuracy of ±2 K and a relative accuracy of ±1 K is acquired with this diode. The IR beam of a Fourier Transform InfraRed Spectrometer (FTIRS; Varian 670-IR) is aligned through the window to obtain IR spectra of the samples. The spectrometer covers a range of 4000 to 500 cm⁻¹ (2.5–20 μm) at spectral resolutions as high as 0.1 cm⁻¹. Sam-

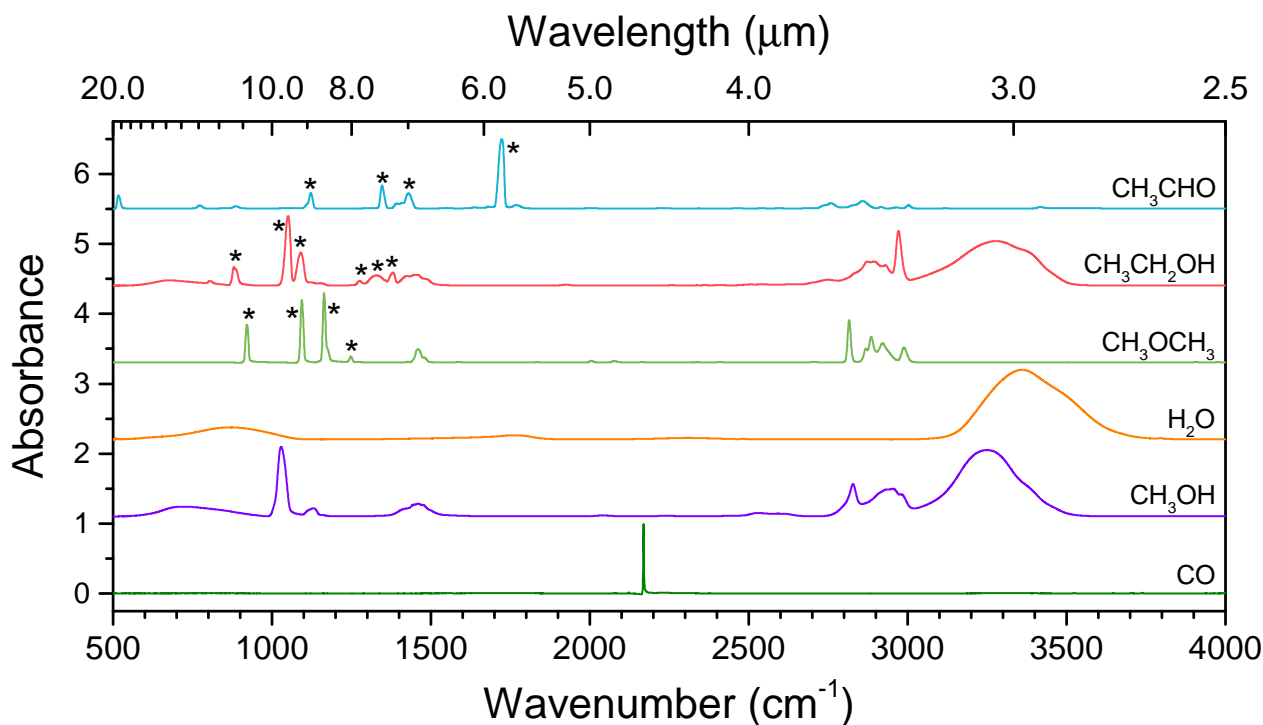


Fig. 1: Spectra of pure acetaldehyde (blue), ethanol (red), dimethyl ether (green), water (orange) methanol (purple), and CO (dark green) normalized to one in the range of 2.5 to 20.0 μm . The bands investigated in this work are indicated with an asterisk (*).

ples are externally prepared in a 2L glass bulb using a separate multi-line gas mixing system. The gas mixing line is turbomolecularly pumped to pressures $< 1 \times 10^{-4}$ mbar. Gas mixtures are made by sequential addition of its components. Two gas independent gauges, covering various pressure ranges ensure that accurate mixing ratios are obtained with a maximum error of $< 10\%$. The liquids and gases used in these experiments are acetaldehyde (Sigma-Aldrich, 99.5%), ethanol (Biosolve, 99.9%), dimethyl ether (Sigma-Aldrich, 99.9%), water (Milli-Q, Type I), carbon monoxide (Linde gas, 99.997%), and methanol (Sigma-Aldrich, 99.9%). Liquid samples are purified with freeze-pump-thaw cycles before use.

2.2. Measurement protocol

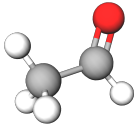
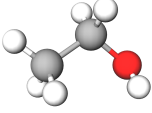
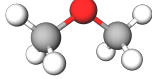
Pure or premixed gases are background deposited onto the 15 K cold sample via an inlet valve. A standard pressure of 20 mbar in the glass bulb is used to prevent a decreasing inlet pressure gradient during deposition. Bi-mixed gases are prepared in a 1:20 ratio and tri-mixed gases in a 1:20:20 ratio, where the smallest fraction is the COM under investigation. These dilution factors ensure that the COM mainly interacts with the surrounding matrix, resulting in matrix shifted IR vibrational bands. Ices are grown at 15 K to a column density of ~ 4500 ML (1 monolayer is 1×10^{15} molecules cm^{-2}) on the window. This coverage ensures that any influence of background contamination, mainly water depositing at a rate of less than 30 ML hr^{-1} , can be neglected. During deposition, IR spectra are recorded at 1 cm^{-1} resolution (0.5 cm^{-1} step size) and averaged over 61 scans (equals 2 minutes) to trace the ice growth and deter-

mine when the ice is ~ 4500 ML thick. From the integration of the IR band absorption, the column density of the species N_{species} is determined according to

$$N_{\text{species}} = \ln(10) \frac{\int_{\text{band}} \log_{10} \left(\frac{I_0(\tilde{\nu})}{I(\tilde{\nu})} \right) d\tilde{\nu}}{A'}, \quad (1)$$

where $\int_{\text{band}} \log_{10} \left(\frac{I_0(\tilde{\nu})}{I(\tilde{\nu})} \right) d\tilde{\nu}$ is the integrated absorbance of the band and $I_0(\tilde{\nu})$ and $I(\tilde{\nu})$ are the flux received and transmitted by the sample, respectively, and A' is the apparent band strength in cm molecule^{-1} . It is important to realize that strongly absorbing bands may get saturated at high coverages, resulting in unreliable column density measurements. In the experiments conducted, the CO band at 2135 cm^{-1} reaches saturation at high coverage, as do certain bands of pure acetaldehyde and dimethyl ether. For these species, bands with a lower band strength or isotopologues can be used. The measured column densities give an indication whether the mixed ice composition still matches the gas-phase mixing ratio and whether the COMs are sufficiently diluted in the matrix. Small variations in the composition of the gas mixture and matrix interactions complicate accurate ice mixing ratio determinations. The apparent band strengths are listed in Table 1 and taken from literature for acetaldehyde and ethanol. For the dimethyl ether bands at 923 , 1095 , and 1164 cm^{-1} the band strength value is approximated from a methane:dimethyl ether mixture, prepared at a one to one ratio in the gas phase. Assuming this ratio is maintained in the ice and matrix interactions are negligible, the apparent band strength is determined from a comparison with the methane 1302

Table 1: Selected bands of acetaldehyde, ethanol, and dimethyl ether

Species	Formula	Mode	Peak position*		A'		
			cm^{-1}	μm	cm molec.^{-1}		
	Acetaldehyde	CH ₃ CHO	CH ₃ rock. + CC stretch.	1122.3	8.909	$1.3 \times 10^{-17,a}$	
			+ CCO bend.				
			CH ₃ s-deform. + CH wag.	1346.2	7.427		
			CH ₃ deform.	1429.4	6.995		
			CO stretch.	1723.0	5.803		
	Ethanol	CH ₃ CH ₂ OH	CC stretch.	879.8	11.36	$3.24 \times 10^{-18,b}$	
			CO stretch.	1051.0	9.514	$1.41 \times 10^{-17,b}$	
			CH ₃ rock.	1090.5	9.170	$7.35 \times 10^{-18,b}$	
			CH ₂ tors.	1275.2	7.842		
			OH deform.	1330.2	7.518		
			CH ₃ s-deform.	1381.3	7.240		
	Dimethyl ether	CH ₃ OCH ₃	COC stretch.	921.3	10.85	$5.0 \times 10^{-18,c}$	
			COC stretch. + CH ₃ rock.	1093.9	9.141	$9.2 \times 10^{-18,c}$	
			COC stretch. + CH ₃ rock.	1163.8	8.592	$9.8 \times 10^{-18,c}$	
			CH ₃ rock.	1248.2	8.011		

Notes. *Peak position of the pure molecule at 15 K. ^aSchutte et al. (1999), ^bHudson (2017), ^cThis work. Note that throughout literature there seems to be disagreement in the assignment of certain modes, particularly for ethanol.

cm^{-1} band area and its known apparent band strength of $8.0 \times 10^{-18} \text{ cm molec.}^{-1}$ (Bouilloud et al. 2015).

After deposition the sample is linearly heated at a rate of 25 K hr^{-1} , until it is fully desorbed from the window. The low temperature ramp ensures that the ice has sufficient time to undergo structural changes, particularly from the amorphous to the crystalline phase. During heating IR spectra are continuously recorded and averaged over 256 scans to trace spectral changes versus temperature.

2.3. Analysis protocol

Owing to the very large amount of spectra that are recorded during the experiments, we only present samples of representative IR spectra for temperatures at which significant spectral changes occur. These spectra are baseline subtracted and the peak position and band width at full width at half maximum (FWHM) are determined for selected spectral features. When the band of a COM overlaps with a spectral feature of a matrix molecule, also the matrix feature is subtracted where possible. In the case of band splitting, the least intense component is only taken into account when its peak position is clearly distinguishable. In a few cases splitted peaks rival in intensity and are heavily overlapping and it is not possible to fit a FWHM for the individual components. Here the FWHM of the combined peaks is determined. Peaks are selected for analysis mainly based on their intensity and potential as an ice tracer, i.e. selecting wavelengths for which no strong overlap with known interstellar features exist.

Identification of vibrational modes of the three species studied here is realized by comparison with available spectra from liquid and solid state literature (Plyler 1952; Evans

& Bernstein 1956; Barnes & Hallam 1970; Allan et al. 1971; Hollenstein & Günthard 1971; Mikawa et al. 1971; Cousan & Bouteiller 1998). Optical effects such as longitudinal optical - transverse optical (LO-TO) splitting and particle shape effects are not explicitly taken into account. Since spectra are recorded at normal incidence with unpolarized light, only the TO modes are recorded. However, certain combinations of polarized light and angles of incidence can result in the LO phonon mode showing up (Baratta et al. 2000; Palumbo et al. 2006). Also particle shape effects can shift transition bands with respect to recorded laboratory spectra (Baratta & Palumbo 1998). Such effects affect only the spectra of more abundant species, such as CO or CO₂, and are not considered to be relevant for COMs.

3. Results and discussion

In this section selected results of the acetaldehyde, ethanol, and dimethyl ether experiments are presented. These are representative for the much larger data set given in the Appendix. All the selected spectra used in this work are publicly available from the Leiden Database for Ice (<http://icedb.strw.leidenuniv.nl>), spectra recorded for other temperatures are available on request. Figure 1 shows the IR spectra of pure acetaldehyde, ethanol, and dimethyl ether ice at 15 K; the bands that are fully analysed are indicated with an asterisk (*) and spectra of pure water, CO, and methanol ice. Figures of the spectra of COMs mixed in water, CO, methanol, and CO:methanol at 15 K are shown in Appendix A. In Table 1, these selected bands are listed together with their peak positions and, if available, apparent band strength in pure ices at 15 K. Appendix B presents the results of the analysis of the selected bands,

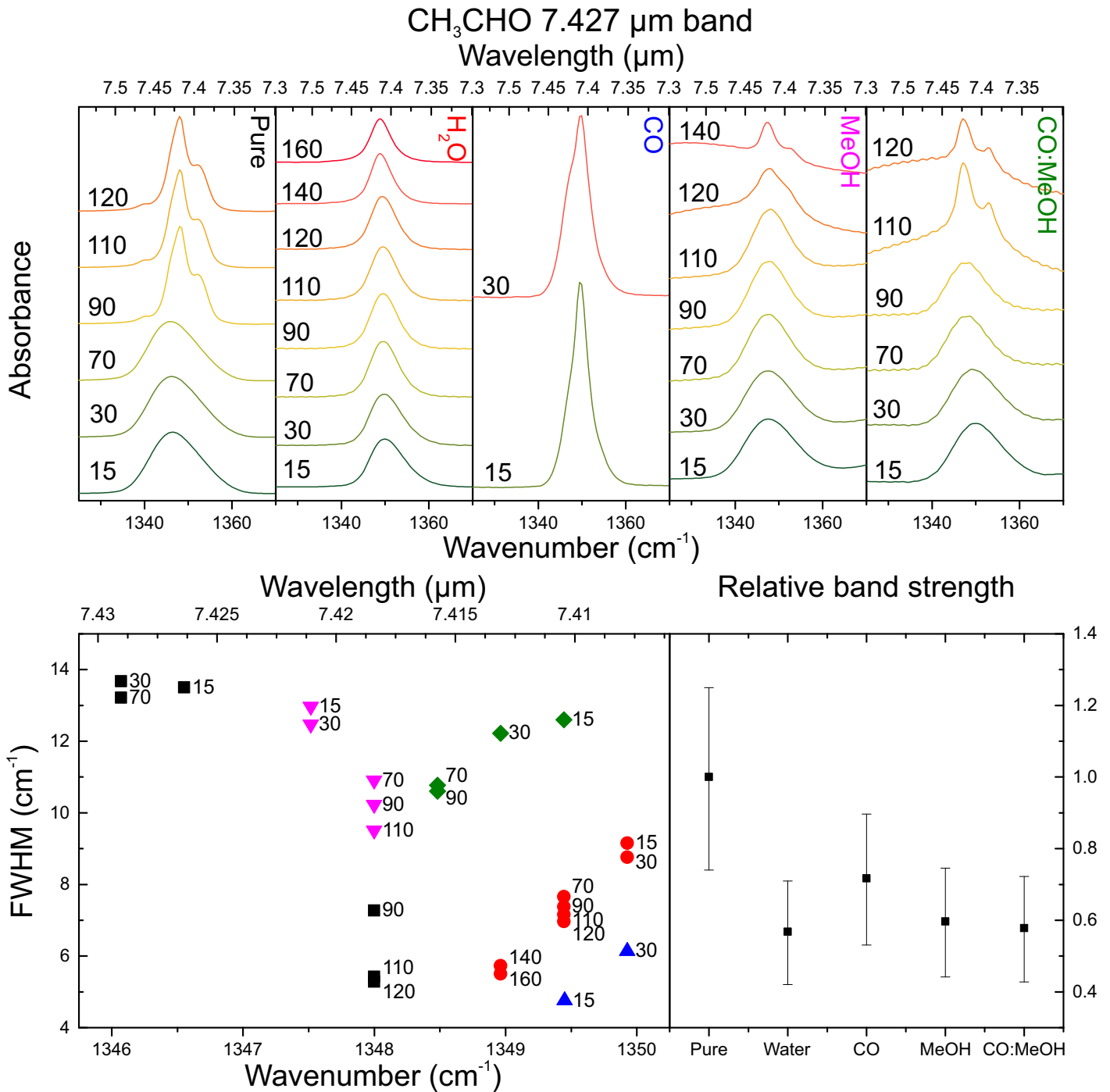


Fig. 2: Top: from left to right the acetaldehyde 7.427 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 7.427 μ m band at 15 K in various matrices.

listing peak positions, FWHMs, and integrated absorbance ratios at various temperatures and for different ice matrices. A representative example of the tables listed in the Appendix is shown in Table 2 for the acetaldehyde CH₃s-deformation + CH wagging mode at 1346.6 cm^{-1} at 15 K.

For easier interpretation the results are represented in a number of plots; see Figs. 2, 3, and 4 for examples. Each plot covers the data of one band. In all plots, the top panels show spectroscopic changes of the band under thermal processing in pure and mixed ices. The bottom left panels

plot peak position versus FWHM, showing trends in the band. The bottom right panels give an indication of how the band strengths change relative to each other in various matrices. Assuming that the ice column density is roughly the same for each experiment and that the gas mixing ratio is close to the ice mixing ratio, the mixed ices are corrected for their dilution factor. Owing to various uncertainties in this method, this results in relatively large error bars for the band strengths. This is unfortunate as this would allow us to interpret the spectroscopic identifications - the primary goal of this work - also in terms of accurate column densi-

Table 2: Peak position and FWHM of the acetaldehyde CH₃ s-deformation + CH wagging mode at 15 K in various matrices.

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
CH ₃ CHO	15	1346.6	7.4264	–	–	13.5	0.0744*
CH ₃ CHO :H ₂ O		1349.9	7.4078	1349.9	7.4078	9.2	0.0502
CH ₃ CHO :CO		1349.4	7.4104	–	–	4.8	0.0262
CH ₃ CHO :CH ₃ OH		1347.5	7.4211	–	–	13.0	0.0714
CH ₃ CHO :CO:CH ₃ OH		1349.4	7.4105	–	–	12.6	0.0691

Notes. Excerpt from Table B.1. *FWHM result of two or more blended peaks.

ties. The remaining figures of other bands can be found in Appendix C.

A few general statements can be made. Most peaks display peak narrowing under thermal processing, which is due to the ice changing to a crystalline phase with increasing temperature. Mixed ice in CO and CO:CH₃OH are exceptions due to the volatility of CO and its removal from the ice at relatively low temperatures. Above 30 K, the desorption temperature of CO (Öberg et al. 2005), these ices are often seen to display peak broadening.

Peak splitting, especially at high temperatures is another effect that is generally seen. This can be caused by two or more modes contributing to a single feature at low temperatures and becoming visible as the peaks begin to narrow at higher temperatures. Alternatively, the matrix can play a role and a peak is split owing to different interactions of a functional group with its surroundings. For example, an ice can segregate under thermal processing and have part of the COM still intimately mixed with the matrix molecule, while another part is forming COM clusters. Segregation is an effect most clearly seen in the COM:CO ice mixtures.

Integrated absorbance ratios are given for the bands under investigation in each ice mixture. These ratios can provide a tool to estimate the likelihood of observing other bands upon detection of a specific transition. They can also be used as conversion factors to determine band strengths from known band strengths. The bands are normalized on the band with highest integrated absorbance at 15 K, unless this band is suspected to be in saturation or when the data set is incomplete over the investigated temperature range.

3.1. Acetaldehyde

Acetaldehyde hosts four significant features in the 5.5 - 12.5 μm region (see Fig. 1). Some smaller features are also visible, such as the CC stretching + CH₃ rocking mode close to 11 μm , however, its intensity is very small compared to the other bands. Two characteristic vibrational modes of acetaldehyde at 6.995 and 8.909 μm coincide with methanol CH₃ rocking and deformation modes and are likely obscured in interstellar spectra. A solid state identification of acetaldehyde based on these vibrational modes is unlikely. The CO stretching mode is the most prominent band in this spectrum. However, its location at 5.8 μm coincides with the CO stretching mode of many other molecules, such as formaldehyde (H₂CO), formic acid (HCOOH), or formamide (NH₂CHO), which are expected to be present in interstellar ice, making it likely that this band is blended.

The fourth band is the CH₃ s-deformation + CH wagging mode around 7.427 μm , which is found to have no substantial overlap with abundant bulk interstellar ice components and therefore is most suited for a successful solid state identification of this molecule.

Figure 2 shows the results of the analysed data of the CH₃ s-deformation + CH wagging band. Under thermal processing the band widths are generally seen to decrease; this is caused by crystallization in the ice. Peak positions shift as well, with clear blue shifting trends visible for the CO:CH₃OH and water mixtures. In the case of the CO:CH₃OH mixture this is likely because of the loss of CO from the matrix, while for the water mixture the interaction between acetaldehyde and crystalline water is more likely the cause. In some cases, at high temperature CH₃CHO undergoes peak splitting, making identification through FWHM challenging. However, this can also be used as a tool to determine the ice temperature. The comparison of peak position makes it in general easy to distinguish between pure acetaldehyde, acetaldehyde mixed in CH₃OH, and CO:CH₃OH, acetaldehyde mixed in CO, and acetaldehyde mixed in water. The 7.427 μm band shows a substantial decrease in band strength by about 40% when acetaldehyde is surrounded by matrix molecules.

The acetaldehyde CO stretching band underlines the above findings, given it is clearly observed (see Fig. C.3). Especially at low ice temperatures of 15 and 30 K clear peak shifts are visible between the CO:CH₃OH matrix at 5.84 μm , the water matrix at 5.825 μm , and the pure matrix, or in a CH₃OH matrix at around 5.805 μm .

3.2. Ethanol

The spectrum of pure ethanol in Fig. 1 shows a strong CC stretching band at 11.36 μm , CO stretching mode at 9.514 μm , and CH₃ rocking mode at 9.170 μm . A number of weaker modes are seen between 6.5 and 8.5 μm : specifically the CH₂ torsion mode at 7.842 μm , the OH deformation mode at 7.518 μm , and the CH₃ symmetric deformation mode at 7.240 μm . Overlap with spectral features of bulk interstellar ice species such as water and methanol is an issue for the three strongest bands, coinciding with either the water libration mode or CO stretching and CH₃ rocking modes of methanol. Also the prominent broad silicate feature is present at \sim 9.7 μm . Although the other ethanol modes are substantially weaker, they fall within a spectral region that is generally clean of strong transitions.

The ethanol 7.240 μm band is a possible candidate for identification. Figure 3 shows the data of this band. Ethanol

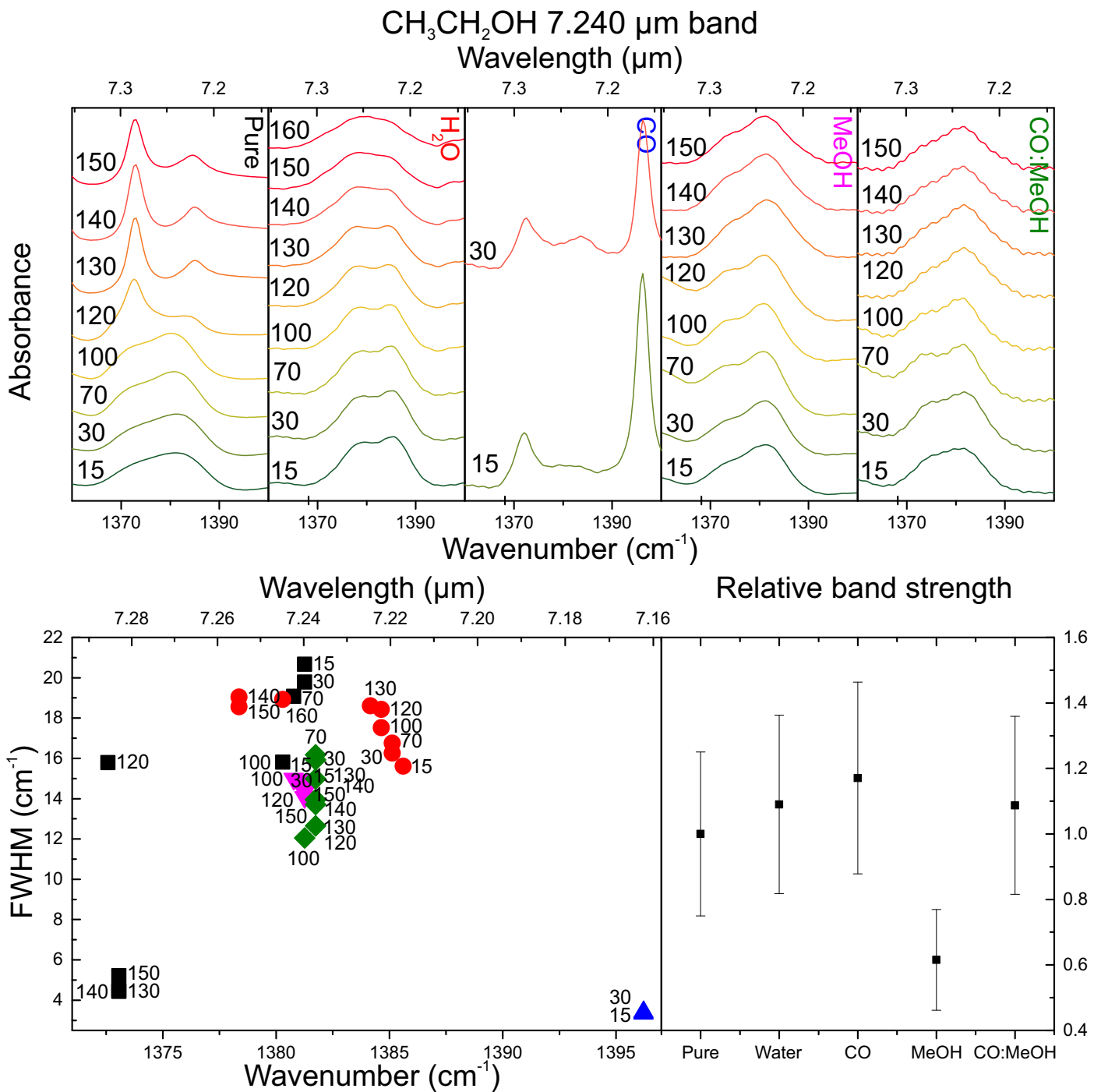


Fig. 3: Top: from left to right the ethanol 7.240 μm band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 7.240 μm band at 15 K in various matrices.

mixed in water can be distinguished from other features by a $\sim 3 \text{ cm}^{-1}$ peak shift from other mixtures. In general it is found that the ethanol:water mixture is relatively easy to distinguish, but the other mixtures display much overlap in peak position and FWHM. The CH₂ torsion, OH deformation mode, and CH₃ symmetric deformation mode are hard to identify in the ethanol:CO mixture owing to the appearance of many more modes. Band areas and relative band strengths of these modes are therefore not considered. The band strength is seen to vary substantially for the various bands, but does not show a clear trend.

3.3. Dimethyl ether

Three strong bands of dimethyl ether are found at 10.85, 9.141, and 8.592 μm for the COC stretching and two COC stretching + CH₃ rocking modes, respectively. A much weaker CH₃ rocking mode is found at 8.011 μm. The first two overlap with known interstellar ice features of methanol, water, and silicates and are therefore less suited for an identification, while the third likely falls in the wing of such features and may still be used. Even though it is a weak mode, the 8.011 μm band falls in a relatively empty

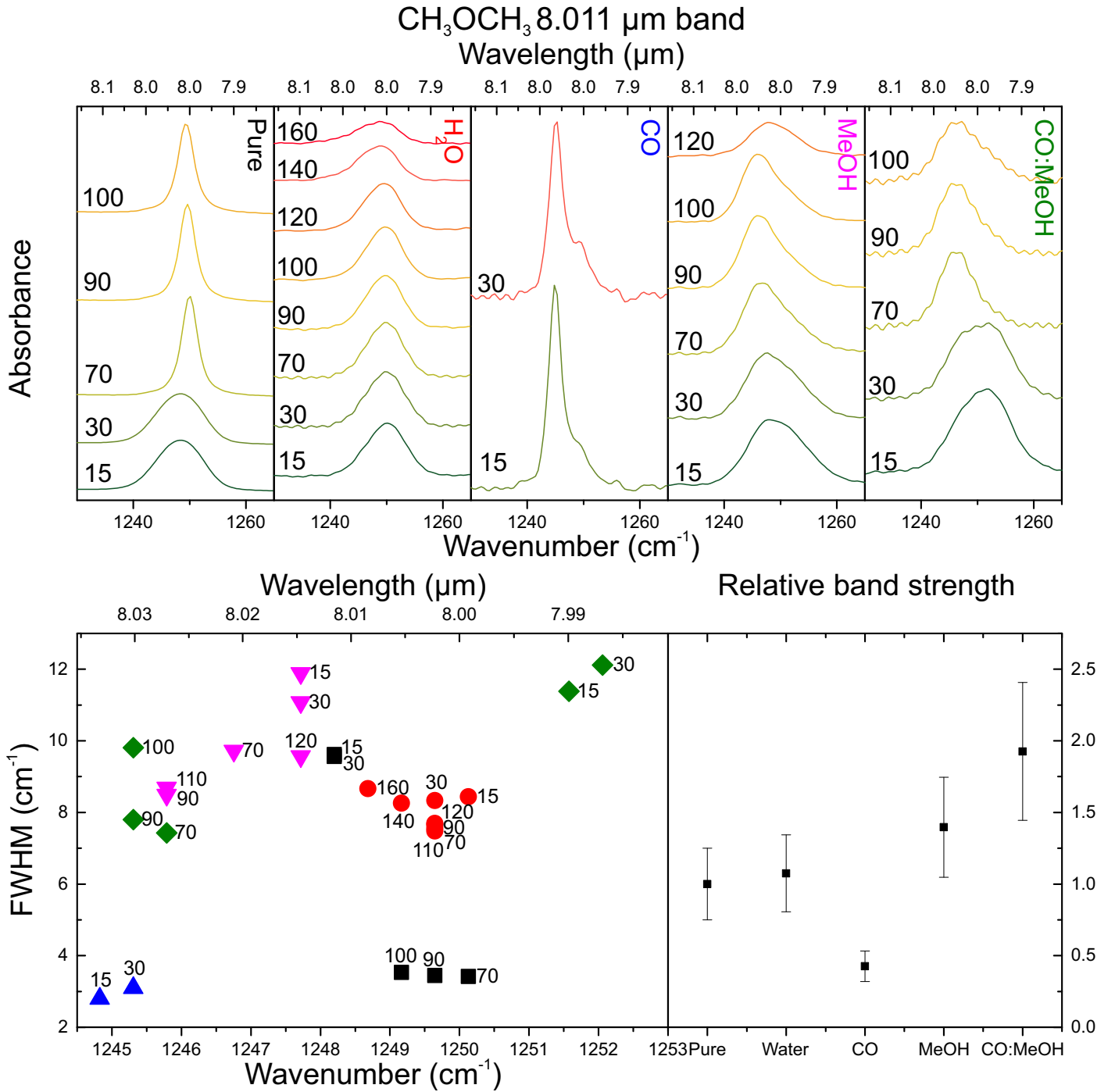


Fig. 4: Top: from left to right the dimethyl ether 8.011 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 8.011 μ m band at 15 K in various matrices.

region of interstellar ice spectra. This feature could therefore be most suited for a dimethyl ether identification; see Fig. 4.

For the 8.011 μ m band clear differences are seen depending on the matrix. The spectra of pure and methanol mixture are distinguishable from those of the water and CO:CH₃OH mixtures by a $\sim 2 \text{ cm}^{-1}$ peak shift of the low temperature spectra at 15 and 30 K. In water this band displays a narrower peak compared to the other ices. The other bands also show many clear differences in peak position and FWHM between the various ice mixtures. A charac-

teristic peak splitting structure at low temperatures is seen for the 10.85 μ m band when mixed in water, methanol, or CO:CH₃OH. Interestingly, the relative band strength shows a substantial increase in the CH₃OH and CO:CH₃OH mixtures for the 8.011 μ m band. Other modes do not show such clear differences. Also it is interesting to note the fact that the COC stretching mode has the largest band area when mixed in water, while in the other mixtures this is always the CH₃ rocking mode at 8.592 μ m (see Appendix B.6).

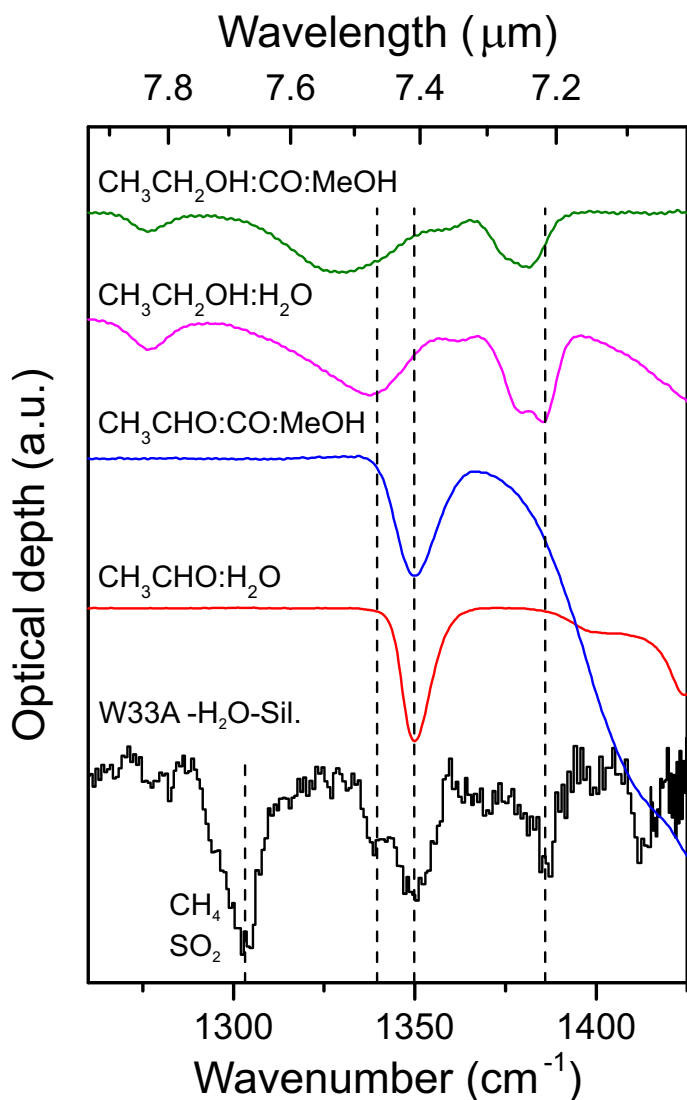


Fig. 5: Continuum and water and silicate subtracted spectrum of W33A plotted together with ice spectra of ethanol and acetaldehyde at 15 K, mixed in CO:CH₃OH and H₂O. Features in the W33A spectrum are indicated with dashed lines at 7.22, 7.40, and 7.47 μm . The large spectral feature at 7.67 μm is due to CH₄ and SO₂.

4. COM ice features in W33A

Our extensive measurements of frozen COMs are needed in the analysis of the many spectra of dense clouds, embedded protostars, and inclined protoplanetary disks that will be obtained with the upcoming *JWST* mission at high sensitivity and medium spectral resolution (R of up to 3,500). Here, we demonstrate their use by a reanalysis of a spectrum of the massive protostar W 33A obtained with the Infrared Space Observatory's Short Wavelength Spectrometer (Astronomical Observation Template 1; $R = 800$). This is one of the few sources for which a high quality mid-IR spectrum is available (Gibb et al. 2000). In the 7 to 8 μm region three prominent features at 7.25, 7.41, and 7.67 μm have been described previously in the literature. The 7.25 μm feature has been attributed to both CH₃CH₂OH and HCOOH (Schutte et al. 1999; Öberg et al. 2011), the 7.41

μm feature has been attributed to HCOO⁻ and CH₃CHO (Schutte et al. 1999), and the 7.67 μm band has been identified as solid methane with potentially contributions of SO₂ (Boogert et al. 1996).

In this work we make use of the water and silicate subtracted spectrum of W33A, shown in Fig. 5 with a straight line local continuum subtraction. The aforementioned features are visible, although the 7.41 μm feature seems to have two contributions at 7.47 and 7.40 μm and the 7.25 μm feature is found at 7.22 μm . The spectra of ethanol and acetaldehyde mixed in CO:CH₃OH and H₂O are plotted in the same figure. The peak position of the 7.40 μm feature can be reproduced well by the acetaldehyde CH₃ s-deformation mode in both mixtures. However, the band in CO:methanol mixture seems to be too broad to justly reproduce the W33A 7.40 μm feature and also this band covers the 7.47 μm feature next to it. The other two features at 7.22 and 7.47 μm could be the result of the CH₃ s-deformation and OH deformation modes of ethanol. Particularly, the CH₃CH₂OH:H₂O mixture coincides with the peak locations of the 7.22 and 7.47 μm features in the W33A spectrum. While the identification of acetaldehyde and ethanol are plausible, detection of additional features would strengthen the assignment. We checked and found that none of the other CH₃CHO and CH₃CH₂OH bands have an anti-coincidence with the W33A spectrum.

Upper limits to the ice column densities of ethanol and acetaldehyde can be given based on the integrated optical depth of their potential features. Schutte et al. (1999) give integrated τ values of 2.0 ± 0.3 and 1.6 ± 0.5 cm⁻¹, respectively. Band strength values of ethanol and acetaldehyde are taken from the literature and used to calculate the column densities of the two features. The ethanol band strength of the CO stretch mode at 9.514 μm has been determined to be 1.41×10^{-17} cm molecule⁻¹ by (Hudson 2017). Using the integrated absorbance ratio CH₃ s-def. / CO str. = 0.20 at 15 K from Table B.16, the band strength of the CH₃ stretch mode is determined to be 2.8×10^{-18} cm molecule⁻¹. The effect of the matrix on the relative band strength is small for both the ethanol CO stretch and CH₃ s-deformation modes, as can be seen from Figs. 3 and C.5, and therefore assumed to be negligible. Assuming the entire 7.22 μm feature is caused by ethanol, this results in a column density of $7.1 \pm 0.2 \times 10^{17}$ cm⁻².

In Schutte et al. (1999), the acetaldehyde band strength is given as 1.3×10^{-17} cm molecule⁻¹ for the CO stretch mode based on data from Wexler (1967). The integrated absorbance ratio of CO stretching / CH₃ s-deforming + CH wagging = 4.32 in pure acetaldehyde at 15 K in laboratory experiments. As the CO stretching mode is likely saturated, the ratio may thus be higher. Using this ratio, the band strength of the CH₃ s-deformation mode is found to be 3.0×10^{-18} cm molecule⁻¹. As can be seen in Fig. 2, the relative band strength of this mode decreases substantially in mixtures by about 40%. The band strength of the CH₃ s-deformation mode in mixed ices is thus 1.8×10^{-18} cm molecule⁻¹. If the entire 7.40 μm feature is attributed to CH₃CHO, the resulting column density is $8.9 \pm 3 \times 10^{17}$ cm⁻².

In all likelihood the 7.22 and 7.40 μm features contain contributions of other molecules, mainly HCOOH and HCOO⁻ and the reported values should therefore be seen as upper limits. Using solid water and methanol column densities of 3.8×10^{19} and 1.7×10^{18} cm⁻², respec-

Table 3: Ice upper limits and gas-phase abundances of ethanol and acetaldehyde towards W33A. Abundances given in %.

Species	Ice		Gas phase ^c
	$/N(\text{H}_2\text{O})^a$	$/N(\text{CH}_3\text{OH})^b$	$/N(\text{CH}_3\text{OH})$
$\text{CH}_3\text{CH}_2\text{OH}$	≤ 1.9	≤ 42	2.4
CH_3CHO	≤ 2.3	≤ 52	≤ 0.2

Notes. ^aKeane et al. (2001); ^bDartois et al. (1999); ^cBisschop et al. (2007b)

tively, towards W33A (Dartois et al. 1999; Keane et al. 2001), the upper limit abundance ratios of ethanol and acetaldehyde can be determined. The abundance ratio $N(\text{COM})/N(\text{H}_2\text{O})$ is found to be $\leq 1.9\%$ and $\leq 2.3\%$, while $N(\text{COM})/N(\text{CH}_3\text{OH})$ is $\leq 42\%$ and $\leq 52\%$ for ethanol and acetaldehyde, respectively. The abundances with respect to water are in good agreement with previously reported values of $\leq 4\%$ and $\leq 3.6\%$ for ethanol and acetaldehyde, respectively (Boudin et al. 1998; Schutte et al. 1999).

The $N(\text{COM})/N(\text{CH}_3\text{OH})$ upper limit ice abundance can be compared with known gas-phase abundances towards W33A. These are given as $N(\text{CH}_3\text{CH}_2\text{OH})/N(\text{CH}_3\text{OH}) = 2.4\%$ and $N(\text{CH}_3\text{CHO})/N(\text{CH}_3\text{OH}) < 0.2\%$ (Bisschop et al. 2007b) and are substantially lower than the ice upper limits. Interferometric observations with the Atacama Large Millimeter/submillimeter Array are needed to spatially resolve these molecules and determine more accurate abundances. Beside being upper limits, this difference may be linked to the process that transfers solid state species into the gas phase, causing molecules to fragment, or to other destruction of species in the gas phase. An overview of the COM abundances in ice and in the gas phase towards W33A is given in Table 3.

The spectroscopic data presented in this paper, combined with the improvements in terms of sensitivity and resolution of JWST, will aid in confirming these detections and distinguish other potential contributors to these features. More observations, particularly towards low-mass sources, will give additional information about the carriers of these features.

5. Conclusions

This paper adds to and extends on data of three important interstellar ice candidates: acetaldehyde, ethanol, and dimethyl ether. A number of selected bands are fully characterized in FWHM and peak positions and show clear changes in various matrices. Our conclusions are summarized as follows:

1. The most promising bands to identify the COMs studied here in interstellar ice spectra are the 7.427 and 5.88 μm bands of acetaldehyde, the 7.240 and 11.36 μm bands of ethanol, and the 8.011 and 8.592 μm bands of dimethyl ether.
2. Matrix characteristic shifts in peak position and FWHM are seen for several bands. The acetaldehyde CH_3 deformation and CO stretching mode can be distinguished in the H_2O , CO, CH_3OH , and $\text{CO}:\text{CH}_3\text{OH}$ matrices.
3. Ethanol shows generally less distinctive shifts and only bands in the water matrix are unique. At low temperatures matrix specific dimethyl ether band shifts can be identified, specifically for the CH_3 rocking mode at 8.011 μm .
4. Given the higher complexity of the involved spectra, unambiguous identifications need to involve different bands that reflect bandwidths and intensity ratios as found in the laboratory studies. The dependence on matrix environment and temperature provides a tool to use these transitions as a remote diagnostic instrument.
5. Analysis of the ISO W33A spectrum in the 7 μm region shows a number of features that can be assigned to the COMs studied in this work. The 7.40 μm feature matches the position of the CH_3 s-deformation mode of acetaldehyde, and the 7.22 μm feature is plausibly caused by the CH_3 s-deformation mode of ethanol. It is likely that 7.22 μm band is specifically caused by ethanol mixed in water. Abundances of both molecules with respect to water ice are determined to be $\leq 2.3\%$ and $\leq 3.4\%$ for acetaldehyde and ethanol, respectively.

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Appendix A: Spectra

The following figures show the spectra of acetaldehyde, ethanol, and dimethylether mixed in water, CO, methanol, and CO:methanol in the range of 2.5 to 20.0 μm . All spectra are taken at 15 K.

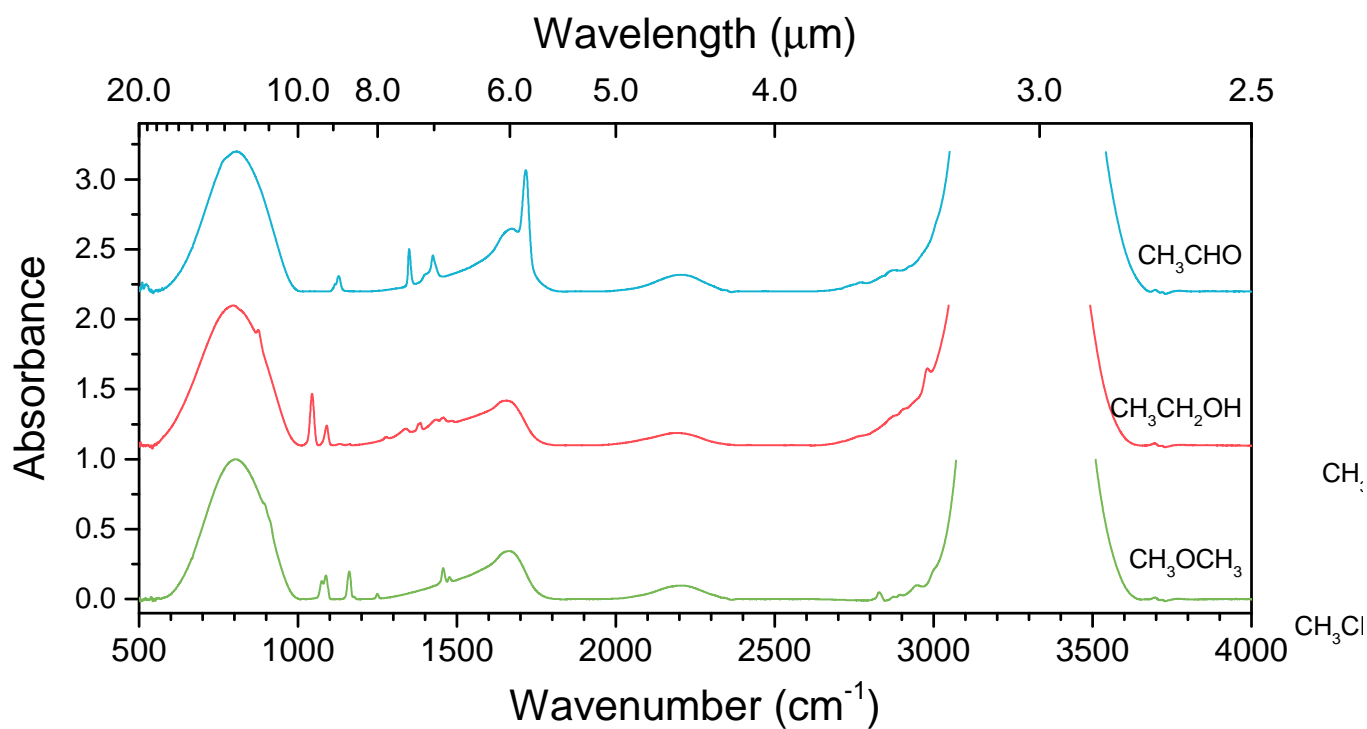


Fig. A.1: Spectra of acetaldehyde (blue), ethanol (red), and dimethyl ether (green) mixed in water at 15 K in the range of 2.5 to 20.0 μm .

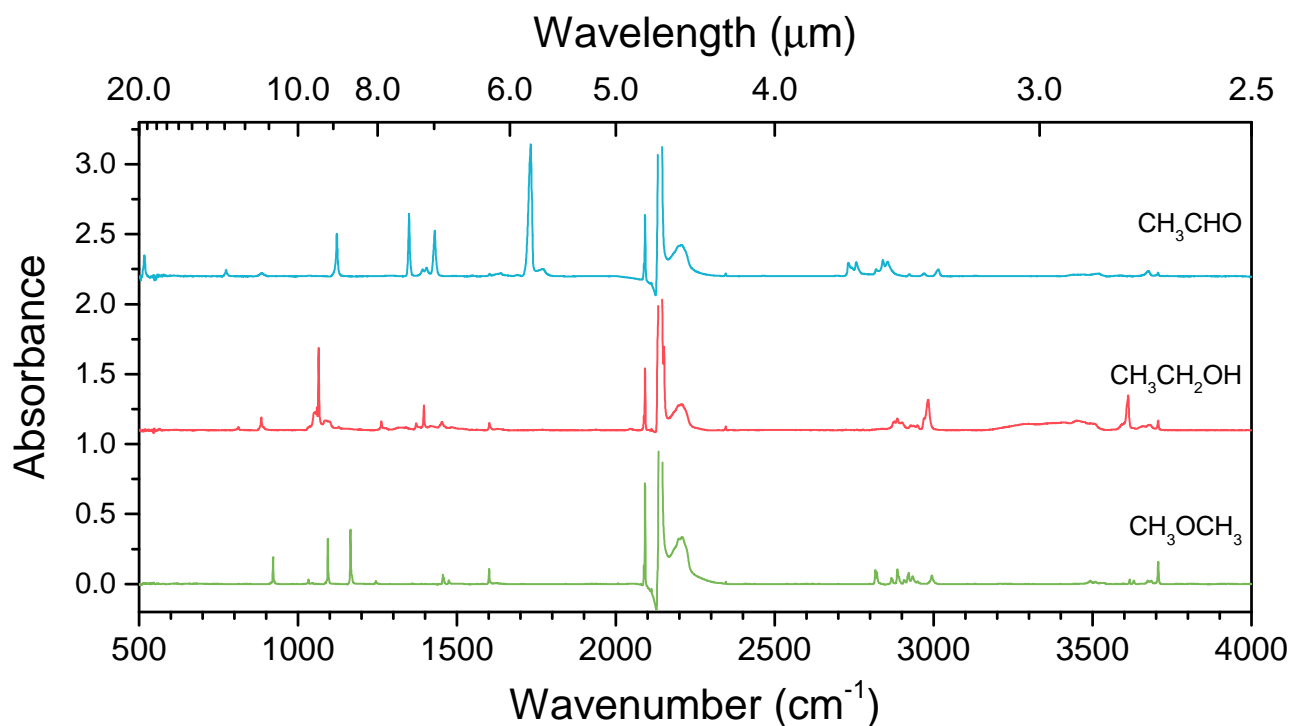


Fig. A.2: Spectra of acetaldehyde (blue), ethanol (red), and dimethyl ether (green) mixed in CO at 15 K in the range of 2.5 to 20.0 μm .

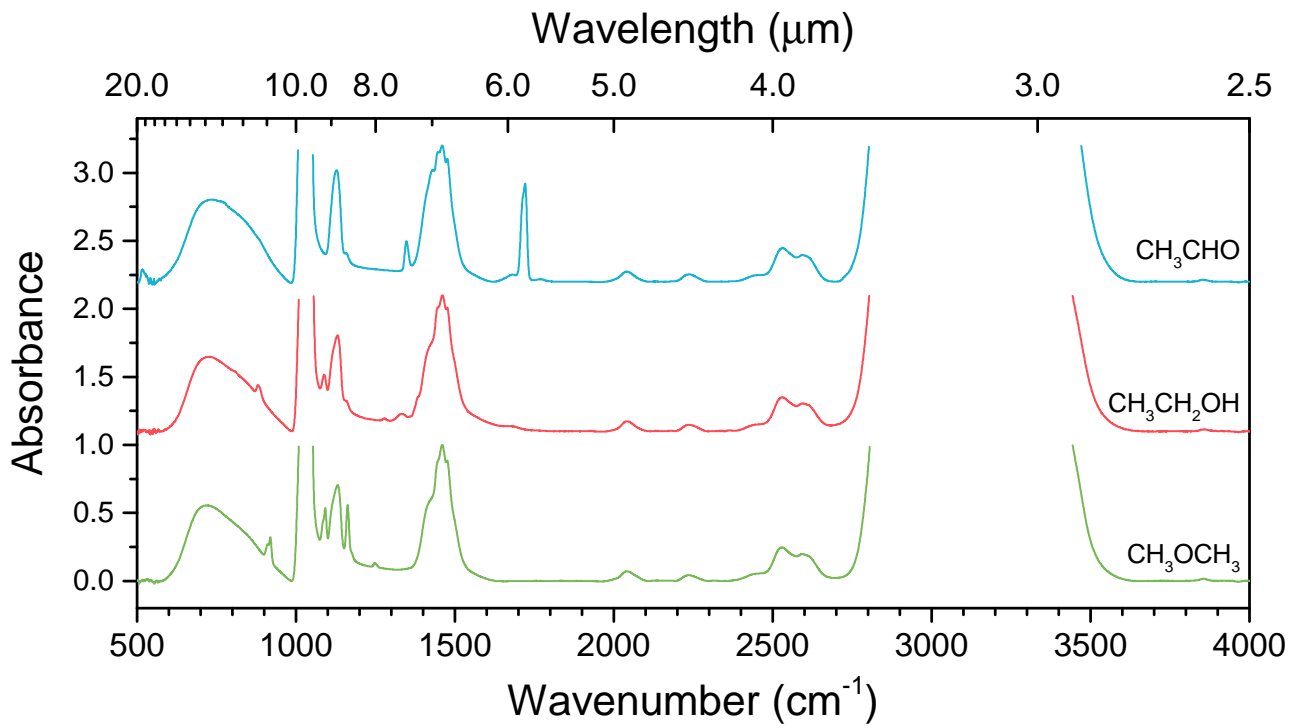


Fig. A.3: Spectra of acetaldehyde (blue), ethanol (red), and dimethyl ether (green) mixed in methanol at 15 K in the range of 2.5 to 20.0 μm .

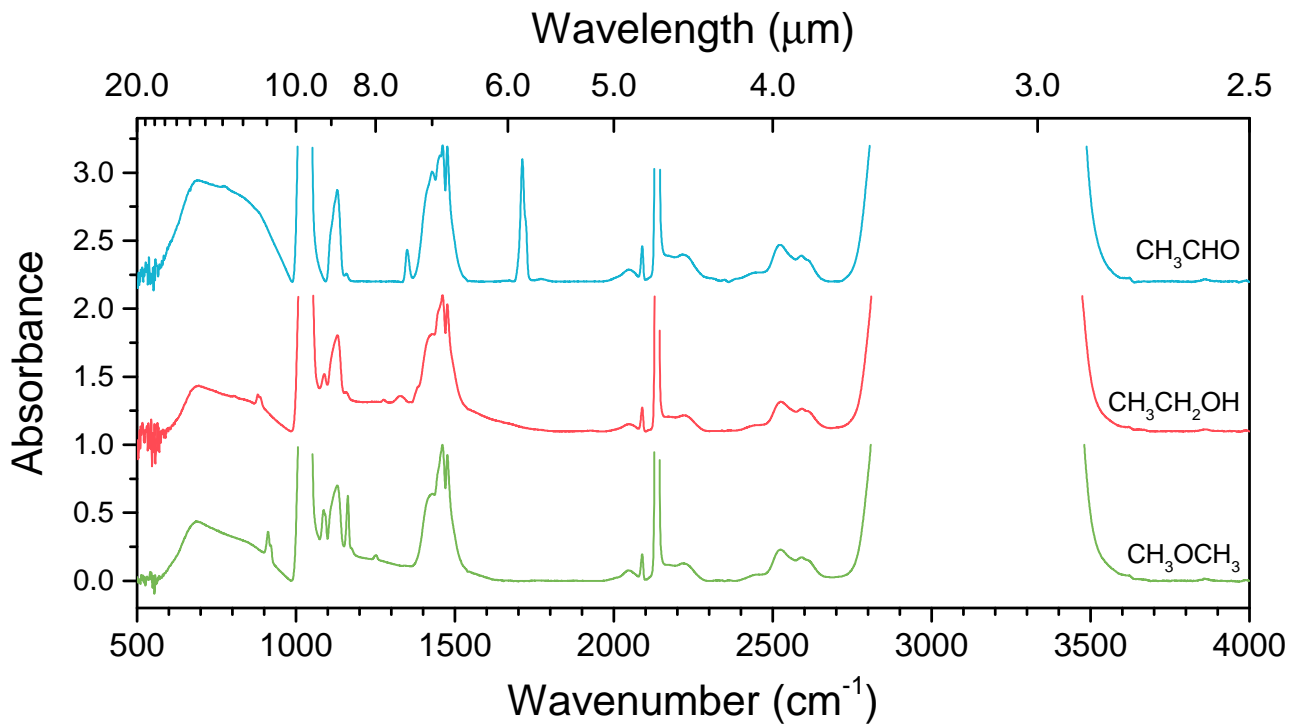


Fig. A.4: Spectra of acetaldehyde (blue), ethanol (red), and dimethyl ether (green) mixed in CO:CH₃OH at 15 K in the range of 2.5 to 20.0 μm .

Appendix B: Overview of peak position, FWHM, and integrated absorbance ratios of selected transitions

In this section tables are presented that list peak positions, FWHMs, and integrated absorbance ratios of selected acetaldehyde, ethanol, and dimethyl ether transitions. Where necessary, peak positions are given of both baseline corrected and matrix subtracted spectra. The peak position and FWHM are given in wavenumber (cm^{-1}) and wavelength (μm). Separate tables list the variation in band intensities over a range of temperatures for each mixture (e.g. Table B.5). Values in these tables are usually normalized to the strongest transition at 15 K, which also remains identifiable over the entire temperature range. Exceptions are made for bands that are potentially in saturation, for example the CO stretching mode in pure acetaldehyde ice.

In the tables various asterisks are used to indicate special circumstances. An asterick indicates that the FWHM is the result of two or more blended peaks. Double astericks indicate multiple peaks, which are often caused by a different matrix or surrounding interactions of the band. Occasionally the matrix cannot be properly subtracted from the feature under investigation, which results in FWHMs with higher uncertainty or in FWHMs that cannot be determined at all. Finally, a triple astericks indicates ice transitions that are thought to be strong enough to saturate the IR spectrometer signal.

Appendix B.1: Acetaldehyde

Table B.1: Peak positions and FWHM of the acetaldehyde CH₃ rocking + CC stretching + CCO bending mode at 8.909 μm.

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
Pure	15	1122.4	8.9097	–	–	13.0	0.1032
CH ₃ CHO :H ₂ O		1116.1	8.9598	1116.1	8.9598	–	–
		1127.7	8.8678	1127.7	8.8678	14.3	0.1121
CH ₃ CHO :CO		1121.9	8.9136	–	–	5.0	0.0394
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	30	1122.4	8.9097	–	–	13.0	0.1031
CH ₃ CHO :H ₂ O		1117.5	8.9482	1117.5	8.9482	–	–
		1126.7	8.8754	1126.7	8.8754	14.3	0.1124
CH ₃ CHO :CO		1121.9	8.9136	–	–	5.5	0.0439
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	70	1122.4	8.9097	–	–	12.5	0.0993
CH ₃ CHO :H ₂ O		1118.0	8.9443	1118.0	8.9443	–	–
		1124.8	8.8906	1124.8	8.8906	16.3	0.1290
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	90	1119.0	8.9366	–	–	6.4	0.0513*
		1120.9	8.9212	–	–	–	–
CH ₃ CHO :H ₂ O		1118.0	8.9443	1118.0	8.9443	–	–
		1124.3	8.8945	1124.3	8.8945	16.0	0.1268*
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	110	1118.5	8.9405	–	–	6.1	0.0485*
		1120.9	8.9212	–	–	–	–
CH ₃ CHO :H ₂ O		1118.0	8.9443	1118.0	8.9443	–	–
		1124.3	8.8945	1124.3	8.8945	16.0	0.1274*
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	120	1118.5	8.9405	–	–	5.9	0.0473
		1120.9	8.9212	–	–	–	–
CH ₃ CHO :H ₂ O		1117.5	8.9482	1117.5	8.9482	16.2	0.1291
		1122.4	8.9097	1122.4	8.9097	–	–
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO	140	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1116.1	8.9598	1116.1	8.9598	10.0	0.0804
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	160	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1116.6	8.9559	1116.6	8.9559	10.1	0.0813
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.2: Peak position and FWHM of the acetaldehyde CH₃ s-deformation + CH wagging mode at 7.427 μm.

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
CH ₃ CHO	15	1346.6	7.4264	–	–	13.5	0.0744*
CH ₃ CHO :H ₂ O		1349.9	7.4078	1349.9	7.4078	9.2	0.0502
CH ₃ CHO :CO		1349.4	7.4104	–	–	4.8	0.0262
CH ₃ CHO :CH ₃ OH		1347.5	7.4211	–	–	13.0	0.0714
CH ₃ CHO :CO:CH ₃ OH		1349.4	7.4105	–	–	12.6	0.0691
CH ₃ CHO	30	1346.1	7.4290	–	–	13.7	0.0754
CH ₃ CHO :H ₂ O		1349.9	7.4078	1349.9	7.4078	8.8	0.0481
CH ₃ CHO :CO		1349.9	7.4078	–	–	6.1	0.0337*
CH ₃ CHO :CH ₃ OH		1347.5	7.4211	–	–	12.5	0.0686
CH ₃ CHO :CO:CH ₃ OH		1349.0	7.4131	–	–	12.2	0.0671
CH ₃ CHO	70	1346.1	7.4290	–	–	13.2	0.0729
CH ₃ CHO :H ₂ O		1349.4	7.4105	1349.4	7.4105	7.7	0.0420
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1348.0	7.4184	–	–	10.9	0.0600
CH ₃ CHO :CO:CH ₃ OH		1348.5	7.4158	–	–	10.8	0.0592
CH ₃ CHO	90	1348.0	7.4184	–	–	7.3	0.0400*
		1351.9	7.3972	–	–	–	–
CH ₃ CHO :H ₂ O		1349.4	7.4105	1349.4	7.4105	7.4	0.0405
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1348.0	7.4184	–	–	10.2	0.0563
CH ₃ CHO :CO:CH ₃ OH	1348.5	7.4158	–	–	10.6	0.0584	
CH ₃ CHO	110	1348.0	7.4184	–	–	5.4	0.0298
		1351.9	7.3972	–	–	–	–
CH ₃ CHO :H ₂ O		1349.4	7.4105	1349.4	7.4105	7.2	0.0393
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1348.0	7.4184	–	–	9.5	0.0524
CH ₃ CHO :CO:CH ₃ OH	1347.0	7.4237	–	–	–	**	
	1352.8	7.3920	–	–	–	**	
CH ₃ CHO	120	1348.0	7.4184	–	–	5.3	0.0291
		1352.3	7.3946	–	–	–	–
CH ₃ CHO :H ₂ O		1349.4	7.4105	1349.4	7.4105	7.0	0.0383
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1348.0	7.4184	–	–	–	**
CH ₃ CHO :CO:CH ₃ OH	1347.0	7.4237	–	–	–	**	
	1352.8	7.3920	–	–	–	**	
CH ₃ CHO	140	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1349.0	7.4131	1349.0	7.4131	5.7	0.0315
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1347.5	7.4211	–	–	–	**
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	160	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1349.0	7.4131	1349.0	7.4131	5.5	0.0302
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.3: Peak position and FWHM of the acetaldehyde CH₃ deformation mode at 6.995 μm.

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
CH ₃ CHO	15	1429.5	6.9956	–	–	22.6	0.1105
CH ₃ CHO :H ₂ O		1424.2	7.0216	1424.2	7.0216	17.0	0.0837
CH ₃ CHO :CO		1430.4	6.9909	–	–	7.7	0.0379
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	30	1429.5	6.9956	–	–	22.8	0.1115
CH ₃ CHO :H ₂ O		1424.7	7.0192	1424.2	7.0216	15.7	0.0772
CH ₃ CHO :CO		1430.4	6.9909	–	–	9.0	0.0438
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	70	1428.5	7.0003	–	–	22.6	0.1106
CH ₃ CHO :H ₂ O		1424.7	7.0192	1424.7	7.0192	14.2	0.0697
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	90	1422.7	7.0288	–	–	–	–
CH ₃ CHO :H ₂ O		1430.4	6.9909	–	–	13.3	0.0655*
CH ₃ CHO :CO		1425.1	7.0169	1425.1	7.0169	13.7	0.0676
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	110	1422.7	7.0288	–	–	–	–
CH ₃ CHO :H ₂ O		1430.4	6.9909	–	–	13.3	0.0653*
CH ₃ CHO :CO		1425.1	7.0169	1425.1	7.0169	13.1	0.0645
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	120	1422.7	7.0288	–	–	–	–
CH ₃ CHO :H ₂ O		1430.4	6.9909	–	–	13.4	0.0656*
CH ₃ CHO :CO		1425.1	7.0169	1425.1	7.0169	12.3	0.0603
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	140	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1425.1	7.0169	1425.1	7.0169	9.9	0.0488
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO	160	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1425.1	7.0169	1424.7	7.0192	9.9	0.0488
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.4: Peak position and FWHM of the acetaldehyde CO stretching mode at 5.803 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm^{-1})	(μm)	(cm^{-1})	(μm)	(cm^{-1})	(μm)
CH ₃ CHO***	15	1723.6	5.8019	–	–	19.5	0.0659
CH ₃ CHO :H ₂ O		1716.8	5.8247	1717.8	5.8215	20.9	0.0709
CH ₃ CHO :CO		1732.2	5.7729	–	–	12.6	0.0419
CH ₃ CHO :CH ₃ OH		1721.2	5.8101	–	–	20.4	0.0690
CH ₃ CHO :CO:CH ₃ OH		1712.5	5.8395	–	–	17.3	0.0589*
CH ₃ CHO***	30	1723.6	5.8019	–	–	20.2	0.0682
CH ₃ CHO :H ₂ O		1716.8	5.8247	1717.8	5.8215	21.2	0.0719
CH ₃ CHO :CO		1732.2	5.7729	–	–	12.9	–
CH ₃ CHO :CH ₃ OH		1721.6	5.8084	–	–	18.6	0.0630
CH ₃ CHO :CO:CH ₃ OH		1712.0	5.8411	–	–	19.3	0.0654*
		1722.6	5.8052	–	–	–	–
CH ₃ CHO***	70	1721.2	5.8101	–	–	21.1	0.0713
CH ₃ CHO :H ₂ O		1719.2	5.8166	1719.2	5.8166	20.2	0.0685
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1722.1	5.8068	–	–	11.9	0.0401
CH ₃ CHO :CO:CH ₃ OH		1723.1	5.8035	–	–	9.2	0.0311
CH ₃ CHO***	90	1717.8	5.8215	–	–	18.9	0.0640*
		1722.6	5.8052	–	–	–	–
CH ₃ CHO :H ₂ O		1719.2	5.8166	1719.7	5.8149	19.8	0.0669
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1722.6	5.8052	–	–	10.6	0.0356
CH ₃ CHO :CO:CH ₃ OH	1723.1	5.8035	–	–	9.5	0.0320	
CH ₃ CHO***	110	1717.8	5.8215	–	–	18.2	0.0615*
		1722.6	5.8052	–	–	–	–
CH ₃ CHO :H ₂ O		1719.7	5.8149	1719.7	5.8149	20.3	0.0684
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1723.1	5.8035	–	–	10.3	0.0347
CH ₃ CHO :CO:CH ₃ OH		1717.8	5.8215	–	–	–	–
		1720.2	5.8133	–	–	–	–
		1725.0	5.7971	–	–	13.2	0.0445*
CH ₃ CHO***	120	1718.3	5.8198	–	–	17.6	0.0595*
		1722.6	5.8052	–	–	–	–
CH ₃ CHO :H ₂ O		1719.7	5.8149	1720.7	5.8117	21.4	0.0722*
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1716.8	5.8247	–	–	18.5	0.0627*
		1722.1	5.8068	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		1717.8	5.8215	–	–	–	–
	1720.2	5.8133	–	–	–	–	
		1725.0	5.7971	–	–	12.3	0.0415*
CH ₃ CHO***	140	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1730.8	5.7777	1730.8	5.7777	17.2	0.0576*
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		1717.8	5.8215	–	9.1495	–	–
		1724.5	5.7987	–	8.5959	12.2	0.0412*
CH ₃ CHO :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CHO***	160	–	–	–	–	–	–
CH ₃ CHO :H ₂ O		1731.8	5.7745	1731.8	5.7745	12.5	0.0417
CH ₃ CHO :CO		–	–	–	–	–	–
CH ₃ CHO :CH ₃ OH		–	–	–	–	–	–
CH ₃ CHO :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Appendix B.2: Acetaldehyde band areas

Table B.5: Integrated absorbance ratios of selected transitions in pure acetaldehyde.

Temperature (K)	CH ₃ rock. + CC stretch. + CCO bend. 8.909 μ m	CH ₃ deform. + CH wag. 7.427 μ m	CH ₃ deform. 6.995 μ m	CO stretch. 5.803 μ m
15	0.72	1.00	1.07	4.32
30	0.73	1.00	1.07	4.36
70	0.70	0.95	0.99	4.27
90	0.59	0.85	0.87	4.16
110	0.58	0.83	0.85	4.09
120	0.57	0.81	0.82	4.01

Notes. Owing to possible saturation of the C=O stretch mode the band intensities are normalized on the CH₃ s-deformation band at 15 K

Table B.6: Integrated absorbance ratios of selected transitions in acetaldehyde:H₂O.

Temperature (K)	CH ₃ rock. + CC stretch. + CCO bend. 8.909 μ m	CH ₃ deform. + CH wag. 7.427 μ m	CH ₃ deform. 6.995 μ m	CO stretch. 5.803 μ m
15	0.15	0.21	0.27	1.00
30	0.16	0.21	0.25	1.02
70	0.15	0.21	0.22	1.00
90	0.15	0.03	0.22	1.01
110	0.15	0.19	0.20	0.94
120	0.15	0.18	0.19	0.83
140	0.12	0.15	0.17	0.61
160	0.11	0.13	0.12	0.57

Table B.7: Integrated absorbance ratios of selected transitions in acetaldehyde:CO.

Temperature (K)	CH ₃ rock. + CC stretch. + CCO bend. 8.909 μ m	CH ₃ deform. + CH wag. 7.427 μ m	CH ₃ deform. 6.995 μ m	CO stretch. 5.803 μ m
15	0.18	0.21	0.25	1.00
30	0.18	0.22	0.24	1.00

Table B.8: Integrated absorbance ratios of selected transitions in acetaldehyde:CH₃OH.

Temperature (K)	CH ₃ rock. + CC stretch. + CCO bend. 8.909 μ m	CH ₃ deform. + CH wag. 7.427 μ m	CH ₃ deform. 6.995 μ m	CO stretch. 5.803 μ m
15	–	0.19	–	1.00
30	–	0.19	–	0.99
70	–	0.18	–	0.95
90	–	0.17	–	0.94
110	–	0.16	–	0.96
120	–	–	–	0.62
140	–	–	–	0.35

Table B.9: Integrated absorbance ratios of selected transitions in acetaldehyde:CO:CH₃OH.

Temperature (K)	CH ₃ rock. + CC stretch. + CCO bend. 8.909 μ m	CH ₃ deform. + CH wag. 7.427 μ m	CH ₃ deform. 6.995 μ m	CO stretch. 5.803 μ m
15	–	0.17	–	1.00
30	–	0.17	–	0.94
70	–	0.15	–	0.76
90	–	0.14	–	0.78
110	–	–	–	0.82
120	–	–	–	0.48

Appendix B.3: Ethanol

Table B.10: Peak position and FWHM of the ethanol CC stretching mode at 11.36 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm^{-1})	(μm)	(cm^{-1})	(μm)	(cm^{-1})	(μm)
CH ₃ CH ₂ OH	15	879.9	11.3654	–	–	18.3	0.2344*
CH ₃ CH ₂ OH :H ₂ O		875.0	11.4280	877.0	11.4029	11.7	0.1526
CH ₃ CH ₂ OH :CO		884.7	11.3035	–	–	3.8	0.0482
CH ₃ CH ₂ OH :CH ₃ OH		880.3	11.3592	882.3	11.3344	16.4	0.2105
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.3	11.3592	880.8	11.3530	16.4	0.2097*
		887.6	11.2666	888.1	11.2605	–	–
CH ₃ CH ₂ OH	30	880.3	11.3592	–	–	17.9	0.2292*
CH ₃ CH ₂ OH :H ₂ O		874.6	11.4343	877.0	11.4029	12.1	0.1574
CH ₃ CH ₂ OH :CO		884.2	11.3096	–	–	4.1	0.0528
CH ₃ CH ₂ OH :CH ₃ OH		880.8	11.3530	882.3	11.3344	16.2	0.2074
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.8	11.3530	880.8	11.3530	16.2	0.2073*
		888.1	11.2605	888.1	11.2605	–	–
CH ₃ CH ₂ OH	70	881.8	11.3406	–	–	17.3	0.2211*
CH ₃ CH ₂ OH :H ₂ O		874.1	11.4406	876.5	11.4092	11.8	0.1540
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		881.3	11.3468	882.8	11.3282	15.5	0.1976
CH ₃ CH ₂ OH :CO:CH ₃ OH		881.3	11.3468	–	–	–	–
		887.6	11.2666	888.1	11.2605	14.3	0.1830*
CH ₃ CH ₂ OH	100	881.8	11.3406	–	–	16.8	0.2144*
CH ₃ CH ₂ OH :H ₂ O		874.1	11.4406	876.5	11.4092	11.0	0.1429
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		881.3	11.3468	883.2	11.3220	14.8	0.1894
CH ₃ CH ₂ OH :CO:CH ₃ OH		883.2	11.3220	887.6	11.2666	14.4	0.1838*
		–	–	–	–	–	–
CH ₃ CH ₂ OH	120	882.3	11.3344	–	–	14.2	0.1805*
		891.0	11.2240	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		873.1	11.4533	876.0	11.4154	11.5	0.1493
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		880.8	11.3530	882.3	11.3344	16.5	0.2107
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.8	11.3530	883.2	11.3220	–	–
	889.5	11.2422	889.5	11.2422	18.5	0.2355*	
CH ₃ CH ₂ OH	130	882.8	11.3282	–	–	5.2	0.0662
		891.4	11.2179	–	–	5.4	0.0678
CH ₃ CH ₂ OH :H ₂ O		873.6	11.4469	876.0	11.4154	11.4	0.1485
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		878.9	11.3779	882.3	11.3344	18.2	0.2319
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.8	11.3530	883.2	11.3220	16.4	0.2098*
CH ₃ CH ₂ OH	140	882.8	11.3282	–	–	5.0	0.0642
		891.4	11.2179	–	–	5.2	0.0659
CH ₃ CH ₂ OH :H ₂ O		872.6	11.4596	876.0	11.4154	11.7	0.1518
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		880.8	11.3530	881.8	11.3406	15.4	0.1964
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.8	11.3530	881.3	11.3468	15.1	0.1934
CH ₃ CH ₂ OH	150	882.8	11.3282	–	–	5.6	0.0713
		891.0	11.2240	–	–	5.5	0.0688
CH ₃ CH ₂ OH :H ₂ O		873.1	11.4533	876.0	11.4154	12.2	0.1582
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		880.8	11.3530	881.3	11.3468	14.0	0.1800
CH ₃ CH ₂ OH :CO:CH ₃ OH		880.8	11.3530	881.3	11.3468	13.6	0.1740
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		872.1	11.4659	876.0	11.4154	12.3	0.1605
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–
		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.11: Peak position and FWHM of the ethanol CO stretching mode at 9.514 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm^{-1})	(μm)	(cm^{-1})	(μm)	(cm^{-1})	(μm)
CH ₃ CH ₂ OH	15	1051.0	9.5146	–	–	19.0	0.1724
CH ₃ CH ₂ OH :H ₂ O		1044.3	9.5761	1044.3	9.5761	14.3	0.1315
CH ₃ CH ₂ OH :CO		1065.0	9.3897	–	–	2.9	0.0253
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH	30	1051.0	9.5146	–	–	17.6	0.1598
CH ₃ CH ₂ OH :H ₂ O		1044.3	9.5761	1044.3	9.5761	14.2	0.1307
CH ₃ CH ₂ OH :CO		1065.0	9.3897	–	–	2.8	0.0243
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH	70	1051.0	9.5146	–	–	16.0	0.1442
CH ₃ CH ₂ OH :H ₂ O		1043.8	9.5805	1043.8	9.5805	14.0	0.1288
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH	100	1051.0	9.5146	–	–	15.0	0.1358
CH ₃ CH ₂ OH :H ₂ O		1043.8	9.5805	1043.8	9.5805	14.0	0.1282
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH	120	1046.2	9.5585	–	–	14.3	0.1296*
		1055.4	9.4755	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1043.8	9.5805	1043.8	9.5805	14.1	0.1294
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CH ₂ OH	130	1045.7	9.5629	–	–	6.8	0.0624
		1056.3	9.4669	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1043.8	9.5805	1043.8	9.5805	14.4	0.1325
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CH ₂ OH	140	1045.7	9.5629	–	–	6.7	0.0611
		1056.3	9.4669	–	–	6.5	0.0586
CH ₃ CH ₂ OH :H ₂ O		1044.3	9.5761	1044.3	9.5761	16.0	0.1469
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CH ₂ OH	150	1045.7	9.5629	–	–	7.6	0.0690
		1055.8	9.4712	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1044.3	9.5761	1044.3	9.5761	17.1	0.1564
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH	–	–	–	–	–	–	
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1044.7	9.5717	1044.7	9.5717	17.9	0.1641
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.12: Peak position and FWHM of the ethanol CH₃ rocking mode at 9.170 μm.

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
CH ₃ CH ₂ OH	15	1090.5	9.1697	–	–	24.4	0.2057
CH ₃ CH ₂ OH :H ₂ O		1090.1	9.1738	1090.1	9.1738	12.9	0.1085
CH ₃ CH ₂ OH :CO		1084.8	9.2186	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1088.6	9.1859	1088.6	9.1859	11.8	0.0996
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1087.7	9.1941	11.8	0.1001
CH ₃ CH ₂ OH	30	1091.0	9.1657	–	–	23.5	0.1978
CH ₃ CH ₂ OH :H ₂ O		1090.1	9.1738	1090.1	9.1738	13.0	0.1097
CH ₃ CH ₂ OH :CO		1097.8	9.1093	–	–	25.3	0.2122
CH ₃ CH ₂ OH :CH ₃ OH		1089.1	9.1819	1089.6	9.1778	11.3	0.0954
CH ₃ CH ₂ OH :CO:CH ₃ OH		1090.1	9.1738	1089.6	9.1778	11.3	0.0955
CH ₃ CH ₂ OH	70	1091.5	9.1616	–	–	21.4	0.1799
CH ₃ CH ₂ OH :H ₂ O		1090.1	9.1738	1090.1	9.1738	12.7	0.1067
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1089.6	9.1778	1090.1	9.1738	11.0	0.0926
CH ₃ CH ₂ OH :CO:CH ₃ OH		1091.5	9.1616	1091.5	9.1616	10.9	0.0915
CH ₃ CH ₂ OH	100	1091.5	9.1616	–	–	20.6	0.1732
CH ₃ CH ₂ OH :H ₂ O		1089.6	9.1778	1089.6	9.1778	12.6	0.1064
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1089.6	9.1778	1090.1	9.1738	10.7	0.0901
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1089.6	9.1778	10.9	0.0921
CH ₃ CH ₂ OH	120	1093.0	9.1495	–	–	20.4	0.1711
CH ₃ CH ₂ OH :H ₂ O		1089.6	9.1778	1089.6	9.1778	12.8	0.1076
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1089.1	9.1819	1089.6	9.1778	10.5	0.0881
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1089.6	9.1778	10.7	0.0903
CH ₃ CH ₂ OH	130	1095.9	9.1253	–	–	17.8	0.1492
CH ₃ CH ₂ OH :H ₂ O		1089.6	9.1778	1089.6	9.1778	12.8	0.1080
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1089.1	9.1819	1089.1	9.1819	10.2	0.0857
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1089.6	9.1778	9.7	0.0815
CH ₃ CH ₂ OH	140	1095.9	9.1253	–	–	16.9	0.1414
CH ₃ CH ₂ OH :H ₂ O		1089.6	9.1778	1089.6	9.1778	13.4	0.1127
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1089.6	9.1778	1090.1	9.1738	12.1	0.1019
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1089.6	9.1778	12.6	0.1063
CH ₃ CH ₂ OH	150	1094.9	9.1334	–	–	17.2	0.1444
CH ₃ CH ₂ OH :H ₂ O		1088.6	9.1859	1088.6	9.1860	14.6	0.1230
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1090.1	9.1738	1090.1	9.1738	12.2	0.1024
CH ₃ CH ₂ OH :CO:CH ₃ OH		1089.6	9.1778	1089.6	9.1778	12.4	0.1043
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1088.6	9.1859	1088.6	9.1859	15.1	0.1275
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.13: Peak position and FWHM of the ethanol CH₂ torsion mode at 7.842 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm^{-1})	(μm)	(cm^{-1})	(μm)	(cm^{-1})	(μm)
CH ₃ CH ₂ OH	15	1275.2	7.8419	–	–	18.5	0.1133
CH ₃ CH ₂ OH :H ₂ O		1278.1	7.8242	1276.2	7.8360	11.9	0.0728
CH ₃ CH ₂ OH :CO		1262.2	7.9228	–	–	3.7	0.0231
		1273.8	7.8508	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1278.6	7.8212	1278.6	7.8212	12.2	0.0746
CH ₃ CH ₂ OH :CO:CH ₃ OH		1276.2	7.8360	1276.2	7.8360	11.5	0.0707
CH ₃ CH ₂ OH	30	1275.7	7.8390	–	–	16.9	0.1035
CH ₃ CH ₂ OH :H ₂ O		1276.2	7.8360	1276.2	7.8360	12.8	0.0784
CH ₃ CH ₂ OH :CO		1262.7	7.9198	–	–	3.1	0.0193
		1276.2	7.8360	–	–	20.6	0.1257
CH ₃ CH ₂ OH :CH ₃ OH		1278.6	7.8212	1278.6	7.8212	11.1	0.0680
CH ₃ CH ₂ OH :CO:CH ₃ OH		1276.2	7.8360	1276.2	7.8360	10.3	0.0630
CH ₃ CH ₂ OH	70	1276.2	7.8360	–	–	14.4	0.0881
CH ₃ CH ₂ OH :H ₂ O		1278.1	7.8242	1276.2	7.8360	12.5	0.0766
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1278.6	7.8212	1278.6	7.8212	12.1	0.0738
CH ₃ CH ₂ OH :CO:CH ₃ OH		1278.6	7.8212	1278.6	7.8212	10.0	0.0612
CH ₃ CH ₂ OH	100	1276.2	7.8360	–	–	13.9	0.0853
CH ₃ CH ₂ OH :H ₂ O		1278.1	7.8242	1278.1	7.8242	13.0	0.0796
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1278.6	7.8212	1278.6	7.8212	11.6	0.0711**
CH ₃ CH ₂ OH :CO:CH ₃ OH		1278.6	7.8212	1278.6	7.8212	12.2	0.0744
CH ₃ CH ₂ OH	120	1277.6	7.8271	–	–	10.5	0.0643
CH ₃ CH ₂ OH :H ₂ O		1278.1	7.8242	1276.2	7.8360	13.4	0.0823
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1279.1	7.8183	1278.6	7.8212	9.1	0.0556**
CH ₃ CH ₂ OH :CO:CH ₃ OH		1280.5	7.8094	1278.6	7.8212	8.2	0.0501
CH ₃ CH ₂ OH	130	1278.1	7.8242	–	–	7.3	0.0448
CH ₃ CH ₂ OH :H ₂ O		1277.6	7.8271	1276.6	7.8330	13.5	0.0829
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1280.5	7.8094	1278.6	7.8212	8.9	0.0547
CH ₃ CH ₂ OH :CO:CH ₃ OH		1278.6	7.8212	1278.6	7.8212	8.1	0.0495
CH ₃ CH ₂ OH	140	1277.6	7.8271	–	–	7.0	0.0427
CH ₃ CH ₂ OH :H ₂ O		1277.6	7.8271	1276.2	7.8360	14.0	0.0862
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1279.1	7.8183	1278.1	7.8242	8.5	0.0519
CH ₃ CH ₂ OH :CO:CH ₃ OH		1280.5	7.8094	1276.2	7.8360	9.8	0.0604
CH ₃ CH ₂ OH	150	1277.6	7.8271	–	–	7.7	0.0471
CH ₃ CH ₂ OH :H ₂ O		1277.6	7.8271	1275.2	7.8419	13.5	0.0827
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1278.1	7.8242	1276.2	7.8360	9.6	0.0590
CH ₃ CH ₂ OH :CO:CH ₃ OH		1278.6	7.8212	1276.2	7.8360	9.9	0.0609
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1277.1	7.8301	1275.2	7.8419	13.5	0.0831
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.14: Peak position and FWHM of the ethanol OH deformation mode at 7.518 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$ (cm^{-1})	(μm)	$\lambda_{\text{peak,-matrix}}$ (cm^{-1})	(μm)	FWHM (cm^{-1}) (μm)	
CH ₃ CH ₂ OH	15	1330.2	7.5179	–	–	50.9	0.2865
CH ₃ CH ₂ OH :H ₂ O		1337.9	7.4745	1337.4	7.4772	30.1	0.1690
CH ₃ CH ₂ OH :CO		1339.3	7.4665	–	–	40.6	0.2306*
CH ₃ CH ₂ OH :CH ₃ OH		1332.6	7.5043	1332.6	7.5043	33.6	0.1894
CH ₃ CH ₂ OH :CO:CH ₃ OH		1328.7	7.5261	1329.2	7.5233	33.7	0.1904
CH ₃ CH ₂ OH	30	1330.2	7.5179	–	–	48.6	0.2726
CH ₃ CH ₂ OH :H ₂ O		1337.9	7.4745	1337.9	7.4745	32.3	0.1816
CH ₃ CH ₂ OH :CO		1326.8	7.5370	–	–	38.4	0.2176*
CH ₃ CH ₂ OH :CH ₃ OH		1335.5	7.4880	1333.1	7.5016	35.0	0.1967
CH ₃ CH ₂ OH :CO:CH ₃ OH		1331.1	7.5125	1331.1	7.5125	30.1	0.1698
CH ₃ CH ₂ OH	70	1329.7	7.5206	–	–	49.4	0.2770
CH ₃ CH ₂ OH :H ₂ O		1339.8	7.4638	1337.9	7.4745	31.3	0.1758
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1335.5	7.4880	1333053.0	7.5016	43.4	0.2426
CH ₃ CH ₂ OH :CO:CH ₃ OH		1335.5	7.4880	1331.1	7.5125	38.8	0.2165
CH ₃ CH ₂ OH	100	1329.7	7.5206	–	–	49.4	0.2770
CH ₃ CH ₂ OH :H ₂ O		1339.8	7.4638	1337.9	7.4745	31.6	0.1771
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1335.5	7.4880	1331.1	7.5125	33.3	0.1875
CH ₃ CH ₂ OH :CO:CH ₃ OH		1335.5	7.4880	1331.1	7.5125	32.1	0.1807
CH ₃ CH ₂ OH	120	1325.3	7.5452	–	–	20.5	0.1166*
CH ₃ CH ₂ OH :H ₂ O		1357.6	7.3657	–	–	–	–
CH ₃ CH ₂ OH :CO		1340.3	7.4611	1337.4	7.4772	32.9	0.1844
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH	130	1324.4	7.5507	–	–	13.6	0.0778
CH ₃ CH ₂ OH :H ₂ O		1357.6	7.3657	–	–	4.9	0.0264
CH ₃ CH ₂ OH :CO		1341.2	7.4557	1337.4	7.4772	32.8	0.1843
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH	140	1324.4	7.5507	–	–	13.7	0.0783
CH ₃ CH ₂ OH :H ₂ O		1357.6	7.3657	–	–	5.2	0.0281
CH ₃ CH ₂ OH :CO		1341.2	7.4557	1337.4	7.4772	34.4	0.1933
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH	150	1324.4	7.5507	–	–	14.3	0.0819
CH ₃ CH ₂ OH :H ₂ O		1357.6	7.3657	–	–	6.7	0.0362
CH ₃ CH ₂ OH :CO		1341.2	7.4557	1338.4	7.4719	32.4	0.1825
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–**
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1341.2	7.4557	1335.0	7.4907	34.8	0.1960
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.15: Peak position and FWHM of the ethanol CH₃ s-deformation mode at 7.240 μm.

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)	(cm ⁻¹)	(μm)
CH ₃ CH ₂ OH	15	1381.3	7.2397	–	–	20.7	0.1088*
CH ₃ CH ₂ OH :H ₂ O		1379.8	7.2473	1379.3	7.2499	–	–
		1385.6	7.2171	1385.6	7.2171	15.6	0.0817
CH ₃ CH ₂ OH :CO		1372.1	7.2881	–	–	5.7	0.0304
		1396.2	7.1622	–	–	3.4	0.0175
CH ₃ CH ₂ OH :CH ₃ OH		1383.7	7.2271	1381.3	7.2397	14.9	0.0782**
CH ₃ CH ₂ OH :CO:CH ₃ OH	1384.2	7.2246	1381.7	7.2372	15.0	0.0788**	
CH ₃ CH ₂ OH	30	1381.3	7.2397	–	–	19.8	0.1042*
CH ₃ CH ₂ OH :H ₂ O		1379.8	7.2473	1379.3	7.2499	–	–
		1385.6	7.2171	1385.1	7.2196	16.3	0.0852*
CH ₃ CH ₂ OH :CO		1372.6	7.2855	–	–	7.5	0.0397
		1383.7	7.2271	–	–	–	–
		1396.2	7.1622	–	–	3.3	0.0171
CH ₃ CH ₂ OH :CH ₃ OH	1384.2	7.2246	1381.3	7.2397	14.9	0.0784**	
CH ₃ CH ₂ OH :CO:CH ₃ OH	1383.7	7.2271	1381.7	7.2372	15.9	0.0838**	
CH ₃ CH ₂ OH	70	1380.8	7.2423	–	–	19.1	0.1005*
CH ₃ CH ₂ OH :H ₂ O		1379.3	7.2499	1379.3	7.2499	–	–
		1385.1	7.2196	1385.1	7.2196	16.7	0.0878
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1383.2	7.2297	1380.8	7.2423	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		1381.7	7.2372	1381.7	7.2372	16.2	0.0853**
CH ₃ CH ₂ OH	100	1380.3	7.2448	–	–	15.8	0.0833*
CH ₃ CH ₂ OH :H ₂ O		1379.3	7.2499	1378.9	7.2524	–	–
		1385.1	7.2196	1384.6	7.2221	17.5	0.0919*
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1382.2	7.2347	1380.8	7.2423	15.0	0.0790**
CH ₃ CH ₂ OH :CO:CH ₃ OH		1381.7	7.2372	1381.3	7.2397	12.1	0.0635**
CH ₃ CH ₂ OH	120	1372.6	7.2855	–	–	15.8	0.0833
		1382.7	7.2322	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1378.9	7.2524	1378.4	7.2549	–	–
		1384.6	7.2221	1384.6	7.2221	18.4	0.0967*
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1381.7	7.2372	1381.3	7.2397	14.1	0.0740**
CH ₃ CH ₂ OH :CO:CH ₃ OH	1381.7	7.2372	1381.7	7.2372	12.6	0.0664**	
CH ₃ CH ₂ OH	130	1373.1	7.2830	–	–	4.4	0.0235
		1385.1	7.2196	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1378.4	7.2549	1378.4	7.2549	–	–
		1384.6	7.2221	1384.2	7.2246	18.6	0.0977*
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1381.3	7.2397	1381.3	7.2397	14.6	0.0767**
CH ₃ CH ₂ OH :CO:CH ₃ OH	1381.7	7.2372	1381.7	7.2372	13.7	0.0721**	
CH ₃ CH ₂ OH	140	1373.1	7.2830	–	–	4.5	0.0239
		1385.1	7.2196	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1380.3	7.2448	1378.4	7.2549	19.0	0.1000*
		1384.2	7.2246	1383.7	7.2271	–	–
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1381.3	7.2397	1381.3	7.2397	14.6	0.0769**
CH ₃ CH ₂ OH :CO:CH ₃ OH	1381.3	7.2397	1381.7	7.2372	13.9	0.0733**	
CH ₃ CH ₂ OH	150	1373.1	7.2830	–	–	5.2	0.0277
		1384.6	7.2221	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1380.3	7.2448	1378.4	7.2549	18.6	0.0975*
		1383.7	7.2271	1383.7	7.2271	–	–
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		1381.7	7.2372	1381.3	7.2397	14.3	0.0752**
CH ₃ CH ₂ OH :CO:CH ₃ OH	1381.7	7.2372	1381.7	7.2372	14.0	0.0734**	
CH ₃ CH ₂ OH	160	–	–	–	–	–	–
CH ₃ CH ₂ OH :H ₂ O		1380.3	7.2448	1380.3	7.2448	18.9	0.0994
CH ₃ CH ₂ OH :CO		–	–	–	–	–	–
CH ₃ CH ₂ OH :CH ₃ OH		–	–	–	–	–	–
CH ₃ CH ₂ OH :CO:CH ₃ OH		–	–	–	–	–	–

Appendix B.4: Ethanol normalized band areas

Table B.16: Integrated absorbance ratios of selected transitions in pure ethanol.

Temperature (K)	CC stretch. $11.36\mu\text{m}$	CO stretch. $9.514\mu\text{m}$	CH ₃ rock. $9.170\mu\text{m}$	CH ₂ tors. $7.842\mu\text{m}$	OH deform. $7.518\mu\text{m}$	CH ₃ s-deform. $7.240\mu\text{m}$
15	0.23	1.00	0.59	0.06	0.35	0.20
30	0.24	1.00	0.63	0.06	0.34	0.20
70	0.24	1.00	0.65	0.06	0.38	0.23
100	0.25	1.03	0.66	0.06	0.42	0.25
120	0.28	1.04	0.64	0.05	0.47	0.23
130	0.29	1.03	0.64	0.04	0.43	0.20
140	0.28	1.02	0.64	0.04	0.44	0.21
150	0.26	0.96	0.59	0.04	0.41	0.20

Table B.17: Integrated absorbance ratios of selected transitions in ethanol:H₂O.

Temperature (K)	CC stretch. $11.36\mu\text{m}$	CO stretch. $9.514\mu\text{m}$	CH ₃ rock. $9.170\mu\text{m}$	CH ₂ tors. $7.842\mu\text{m}$	OH deform. $7.518\mu\text{m}$	CH ₃ s-deform. $7.240\mu\text{m}$
15	0.16	1.00	0.35	0.04	0.24	0.17
30	0.17	1.01	0.35	0.05	0.28	0.19
70	0.16	1.01	0.34	0.05	0.28	0.20
100	0.12	0.97	0.33	0.05	0.30	0.21
120	0.12	0.93	0.33	0.05	0.30	0.21
130	0.12	0.93	0.33	0.04	0.27	0.21
140	0.11	0.88	0.35	0.04	0.26	0.20
150	0.11	0.86	0.36	0.04	0.21	0.16
160	0.09	0.74	0.32	0.03	0.17	0.14

Table B.18: Integrated absorbance ratios of selected transitions in ethanol:CH₃OH.

Temperature (K)	CC stretch. $11.36\mu\text{m}$	CO stretch. $9.514\mu\text{m}$	CH ₃ rock. $9.170\mu\text{m}$	CH ₂ tors. $7.842\mu\text{m}$	OH deform. $7.518\mu\text{m}$	CH ₃ s-deform. $7.240\mu\text{m}$
15	1.00	–	0.99	0.16	1.50	0.57
30	1.00	–	1.09	0.16	1.83	0.62
70	1.01	–	1.38	0.19	3.14	0.81
100	1.00	–	1.36	0.18	2.38	0.66
120	1.05	–	1.12	0.18	–	0.85
130	0.97	–	0.92	0.10	–	0.67
140	0.98	–	1.12	0.09	–	0.66
150	0.90	–	0.99	0.10	–	0.54

Table B.19: Integrated absorbance ratios of selected transitions in ethanol:CO:CH₃OH.

Temperature (K)	CC stretch. $11.36\mu\text{m}$	CO stretch. $9.514\mu\text{m}$	CH ₃ rock. $9.170\mu\text{m}$	CH ₂ tors. $7.842\mu\text{m}$	OH deform. $7.518\mu\text{m}$	CH ₃ s-deform. $7.240\mu\text{m}$
15	1.00	–	0.87	0.19	1.73	0.66
30	1.00	–	1.09	0.19	1.89	0.91
70	0.94	–	1.37	0.19	2.80	0.79
100	0.94	–	1.39	0.23	2.40	0.69
120	0.77	–	1.03	0.11	–	0.61
130	0.87	–	1.20	0.11	–	0.62
140	0.90	–	1.16	0.12	–	0.57
150	0.89	–	1.06	0.12	–	0.54

Appendix B.5: Dimethyl ether

Table B.20: Peak position and FWHM of the dimethyl ether COC stretching mode at 10.85 μm .

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm^{-1})	(μm)	(cm^{-1})	(μm)	(cm^{-1})	(μm)
CH ₃ OCH ₃	15	921.8	10.8483	–	–	10.6	0.1245
CH ₃ OCH ₃ :H ₂ O		898.2	11.1336	898.2	11.1336	–	–
CH ₃ OCH ₃ :CO		913.1	10.9514	913.1	10.9514	27.9	0.3406*
CH ₃ OCH ₃ :CH ₃ OH		921.8	10.8483	–	–	2.1	0.0248
CH ₃ OCH ₃ :CO:CH ₃ OH		911.2	10.9745	911.7	10.9687	–	–
		919.4	10.8767	919.4	10.8767	15.5	0.1846*
		912.2	10.9629	912.6	10.9571	15.9	0.1904*
		920.8	10.8596	921.3	10.8539	–	–
CH ₃ OCH ₃	30	921.3	10.8539	–	–	10.6	0.1243
CH ₃ OCH ₃ :H ₂ O		897.7	11.1396	898.2	11.1336	–	–
CH ₃ OCH ₃ :CO		914.1	10.9398	913.6	10.9456	27.5	0.3358*
CH ₃ OCH ₃ :CH ₃ OH		921.8	10.8483	–	–	2.2	0.0253
CH ₃ OCH ₃ :CO:CH ₃ OH		911.2	10.9745	911.7	10.9687	–	–
		919.4	10.8767	919.9	10871.0000	9.0	0.1062
		912.6	10.9571	912.6	10.9571	16.2	0.1933*
		921.3	10.8539	921.3	10.8539	–	–
CH ₃ OCH ₃	70	914.1	10.9398	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		918.0	10.8938	–	–	4.1	0.0492
CH ₃ OCH ₃ :CO		896.3	11.1575	898.2	11.1336	–	–
CH ₃ OCH ₃ :CH ₃ OH		913.6	10.9456	913.6	10.9456	15.2	0.1834
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
		910.7	10.9803	911.2	10.9745	–	–
		919.9	10.8710	919.9	10.8710	6.9	0.0815
		911.2	10.9745	911.2	10.9745	–	–
		920.4	10.8653	920.4	10.8653	6.1	0.0723
CH ₃ OCH ₃	90	914.1	10.9398	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		918.0	10.8938	–	–	6.3	0.0755*
CH ₃ OCH ₃ :CO		–	–	898.7	11.1276	–	–
CH ₃ OCH ₃ :CH ₃ OH		913.6	10.9456	913.6	10.9456	15.0	0.1807
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
		910.7	10.9803	911.2	10.9745	–	–
		919.9	10.8710	920.4	10.8653	6.4	0.0760
		911.2	10.9745	911.2	10.9745	–	–
		919.9	10.8710	919.9	10.8710	6.4	0.0755
CH ₃ OCH ₃	100	914.6	10.9340	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		918.0	10.8938	–	–	6.3	0.0744
CH ₃ OCH ₃ :CO		–	–	898.2	11.1336	–	–
CH ₃ OCH ₃ :CH ₃ OH		913.1	10.9514	913.6	10.9456	14.0	0.1688
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
		910.7	10.9803	910.7	10.9803	–	–
		920.4	10.8653	920.4	10.8653	6.3	0.0744
		911.2	10.9745	911.2	10.9745	–	–
		920.4	10.8653	920.4	10.8653	6.4	0.0754
CH ₃ OCH ₃	120	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		912.6	10.9571	913.6	10.9456	13.8	0.1656
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		907.3	11.0212	911.7	10.9687	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		918.4	10.8881	919.4	10.8767	19.5	0.2327
		–	–	–	–	–	–
CH ₃ OCH ₃	140	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		912.6	10.9571	914.6	10.9340	13.9	0.1659
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃	160	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		913.1	10.9514	913.1	10.9514	13.2	0.1580
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction.

Table B.21: Peak position and FWHM of the dimethyl ether COC stretching + CH₃ rocking mode at 9.141 μ m.

Mixture	Temperature (K)	$\lambda_{\text{peak, -baseline}}$		$\lambda_{\text{peak, -matrix}}$		FWHM	
		(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)
CH ₃ OCH ₃	15	1094.4	9.1374	–	–	10.9	0.0912
CH ₃ OCH ₃ :H ₂ O		1074.6	9.3055	1074.6	9.3055	–	–
		1087.7	9.1941	1088.1	9.1900	24.7	0.2111*
CH ₃ OCH ₃ :CO		1093.9	9.1414	–	–	2.0	0.0168
CH ₃ OCH ₃ :CH ₃ OH		1092.0	9.1576	1092.0	9.1576	12.5	0.1055*
CH ₃ OCH ₃ :CO:CH ₃ OH		1087.2	9.1982	1087.2	9.1982	13.8	0.1162
CH ₃ OCH ₃	30	1093.9	9.1414	–	–	10.9	0.0909
CH ₃ OCH ₃ :H ₂ O		1074.2	9.3096	1074.2	9.3096	–	–
		1087.7	9.1941	1087.7	9.1941	23.4	0.1994*
CH ₃ OCH ₃ :CO		1094.4	9.1374	–	–	2.2	0.0182
CH ₃ OCH ₃ :CH ₃ OH		1092.5	9.1535	1092.5	9.1535	8.6	0.0723*
CH ₃ OCH ₃ :CO:CH ₃ OH		1086.7	9.2023	1086.7	9.2023	–	–
		1093.0	9.1495	1093.0	9.1495	14.2	0.1195*
CH ₃ OCH ₃ ***	70	1091.5	9.1616	–	–	3.9	0.0326
CH ₃ OCH ₃ :H ₂ O		1074.2	9.3096	1074.2	9.3096	–	–
		1088.1	9.1900	1088.6	9.1860	11.8	0.0997
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.6	0.0554
CH ₃ OCH ₃ :CO:CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.1	0.0508
CH ₃ OCH ₃ ***	90	1091.5	9.1616	–	–	3.6	0.0299
CH ₃ OCH ₃ :H ₂ O		1074.2	9.3096	1074.2	9.3096	–	–
		1088.6	9.1859	1088.6	9.1859	11.3	0.0957
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.2	0.0517
CH ₃ OCH ₃ :CO:CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.2	0.0515
CH ₃ OCH ₃ ***	100	1091.5	9.1616	–	–	3.5	0.0294
CH ₃ OCH ₃ :H ₂ O		1073.7	9.3138	1072.7	9.3222	–	–
		1088.6	9.1859	1088.6	9.1859	11.1	0.0940
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.0	0.0506
CH ₃ OCH ₃ :CO:CH ₃ OH		1093.0	9.1495	1093.0	9.1495	6.2	0.0522
CH ₃ OCH ₃ ***	120	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1073.7	9.3138	1073.2	9.3180	–	–
		1088.6	9.1859	1088.6	9.1859	12.1	0.1016
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1084.8	9.2186	1085.2	9.2145	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		1093.0	9.1495	1093.4	9.1454	15.5	0.1305
CH ₃ OCH ₃ ***	140	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1089.6	9.1778	1089.6	9.1778	–	–
		1095.9	9.1253	1095.9	9.1253	13.3	0.1121
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ ***	160	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1090.5	9.1697	1090.5	9.1697	–	–
		1095.9	9.1253	1095.9	9.1253	10.9	0.0911
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.22: Peak position and FWHM of the dimethyl ether COC stretching and CH₃ rocking mode at 8.592 μ m.

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)
CH ₃ OCH ₃	15	1164.3	8.5888	–	–	9.7	0.0714
CH ₃ OCH ₃ :H ₂ O		1161.4	8.6102	1161.4	8.6102	12.5	0.0924
CH ₃ OCH ₃ :CO		1165.3	8.5817	–	–	2.4	0.0177
CH ₃ OCH ₃ :CH ₃ OH		1162.9	8.5994	1162.9	8.5994	9.6	0.0712
CH ₃ OCH ₃ :CO:CH ₃ OH		1163.3	8.5959	1163.3	8.5959	8.2	0.0608
CH ₃ OCH ₃	30	1163.8	8.5923	–	–	9.7	0.0712
CH ₃ OCH ₃ :H ₂ O		1161.9	8.6066	1161.9	8.6066	12.1	0.0895
CH ₃ OCH ₃ :CO		1165.8	8.5781	–	–	2.7	0.0196
CH ₃ OCH ₃ :CH ₃ OH		1162.9	8.5994	1162.9	8.5994	9.0	0.0668
CH ₃ OCH ₃ :CO:CH ₃ OH		1163.3	8.5959	1163.3	8.5959	7.8	0.0578
CH ₃ OCH ₃ ***	70	1163.8	8.5923	–	–	3.9	0.0291
CH ₃ OCH ₃ :H ₂ O		1162.4	8.6030	1162.4	8.6030	10.2	0.0759
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1162.9	8.5994	1163.3	8.5959	7.8	0.0576
CH ₃ OCH ₃ :CO:CH ₃ OH		1163.8	8.5923	1163.8	8.5923	7.0	0.0514
CH ₃ OCH ₃ ***	90	1163.8	8.5923	–	–	3.6	0.0268
CH ₃ OCH ₃ :H ₂ O		1162.4	8.6030	1162.4	8.6030	9.4	0.0697
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1163.3	8.5959	1163.3	8.5959	7.2	0.0534
CH ₃ OCH ₃ :CO:CH ₃ OH		1163.3	8.5959	1163.3	8.5959	7.2	0.0531
CH ₃ OCH ₃ ***	100	1163.8	8.5923	–	–	3.7	0.0270
CH ₃ OCH ₃ :H ₂ O		1162.4	8.6030	1162.9	8.5994	9.1	0.0673
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1163.3	8.5959	1163.3	8.5959	7.1	0.0522
CH ₃ OCH ₃ :CO:CH ₃ OH		1163.3	8.5959	1163.3	8.5959	7.2	0.0535
CH ₃ OCH ₃	120	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1163.3	8.5959	1163.3	8.5959	8.8	0.0651
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1160.9	8.6137	1161.4	8.6102	10.4	0.0770
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃	140	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1165.8	8.5781	1165.8	8.5781	9.0	0.0661
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃	160	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1167.2	8.5675	1167.2	8.5675	8.8	0.0648
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Table B.23: Peak position and FWHM of the dimethyl ether CH₃ rocking mode at 8.011 μ m.

Mixture	Temperature (K)	$\lambda_{\text{peak,-baseline}}$		$\lambda_{\text{peak,-matrix}}$		FWHM	
		(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)	(cm ⁻¹)	(μ m)
CH ₃ OCH ₃	15	1248.2	8.0115	–	–	9.6	0.0617
CH ₃ OCH ₃ :H ₂ O		1250.1	7.9992	1250.1	7.9992	8.4	0.0540
CH ₃ OCH ₃ :CO		1244.8	8.0333	–	–	2.8	0.0180
CH ₃ OCH ₃ :CH ₃ OH		1247.7	8.0146	1247.7	8.0146	11.9	0.0761
CH ₃ OCH ₃ :CO:CH ₃ OH		1251.6	7.9899	1251.6	7.9899	11.4	0.0728
CH ₃ OCH ₃	30	1248.2	8.0115	–	–	9.6	0.0614
CH ₃ OCH ₃ :H ₂ O		1249.6	8.0023	1249.6	8.0023	8.3	0.0534
CH ₃ OCH ₃ :CO		1245.3	8.0301	–	–	3.1	0.0200
CH ₃ OCH ₃ :CH ₃ OH		1247.7	8.0146	1247.7	8.0146	11.1	0.0710
CH ₃ OCH ₃ :CO:CH ₃ OH		1252.1	7.9869	1252.1	7.9869	12.1	0.0775
CH ₃ OCH ₃	70	1250.1	7.9992	–	–	3.4	0.0219
CH ₃ OCH ₃ :H ₂ O		1249.6	8.0023	1249.6	8.0023	7.6	0.0484
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1246.8	8.0209	1246.8	8.0208	9.7	0.0624
CH ₃ OCH ₃ :CO:CH ₃ OH		1245.8	8.0270	1245.8	8.0270	7.4	0.0478
CH ₃ OCH ₃	90	1249.6	8.0023	–	–	3.4	0.0221
CH ₃ OCH ₃ :H ₂ O		1249.6	8.0023	1249.6	8.0023	7.7	0.0490
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1245.8	8.0270	1245.8	8.0270	8.5	0.0546
CH ₃ OCH ₃ :CO:CH ₃ OH		1245.3	8.0301	1245.3	8.0301	7.8	0.0502
CH ₃ OCH ₃	100	1249.2	8.0054	–	–	3.5	0.0226
CH ₃ OCH ₃ :H ₂ O		1249.6	8.0023	1249.6	8.0023	7.5	0.0479
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1245.8	8.0270	1245.8	8.0270	8.7	0.0559
CH ₃ OCH ₃ :CO:CH ₃ OH		1245.3	8.0301	1245.3	8.0301	9.8	0.0630
CH ₃ OCH ₃	120	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1249.6	8.0023	1249.6	8.0023	7.7	0.0493
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		1248.2	8.0115	1247.7	8.0146	9.6	0.0614
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃	140	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1249.2	8.0054	1249.2	8.0054	8.3	0.0530
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃	160	–	–	–	–	–	–
CH ₃ OCH ₃ :H ₂ O		1248.7	8.0084	1248.7	8.0084	8.7	0.0556
CH ₃ OCH ₃ :CO		–	–	–	–	–	–
CH ₃ OCH ₃ :CH ₃ OH		–	–	–	–	–	–
CH ₃ OCH ₃ :CO:CH ₃ OH		–	–	–	–	–	–

Notes. *FWHM result of two or more blended peaks. **FWHM uncertain/not determined owing to uncertain matrix subtraction. ***Transition likely saturated.

Appendix B.6: Dimethyl ether band areas

Table B.24: Integrated absorbance ratios of selected transitions in pure dimethyl ether.

Temperature (K)	COC stretch. $10.85\mu\text{m}$	COC stretch. + CH_3 rock. $9.141\mu\text{m}$	COC stretch. + CH_3 rock. $8.592\mu\text{m}$	CH_3 rock. $8.011\mu\text{m}$
15	0.49	0.83	1.00	0.06
30	0.49	0.83	0.99	0.07
70	0.48	0.79	0.85	0.06
90	0.48	0.78	0.84	0.06
100	0.46	0.74	0.80	0.06

Table B.25: Integrated absorbance ratios of selected transitions in dimethyl ether: H_2O .

Temperature (K)	COC stretch. $10.85\mu\text{m}$	COC stretch. + CH_3 rock. $9.141\mu\text{m}$	COC stretch. + CH_3 rock. $8.592\mu\text{m}$	CH_3 rock. $8.011\mu\text{m}$
15	0.36	1.00	0.74	0.08
30	0.40	0.99	0.80	0.08
70	0.38	0.94	0.79	0.07
90	0.37	0.91	0.78	0.07
100	0.34	0.89	0.78	0.07
120	0.30	0.84	0.80	0.06
140	0.17	0.71	0.79	0.05
160	0.10	0.61	0.73	0.04

Table B.26: Integrated absorbance ratios of selected transitions in dimethyl ether: CO .

Temperature (K)	COC stretch. $10.85\mu\text{m}$	COC stretch. + CH_3 rock. $9.141\mu\text{m}$	COC stretch. + CH_3 rock. $8.592\mu\text{m}$	CH_3 rock. $8.011\mu\text{m}$
15	0.45	0.66	1.00	0.06
30	0.45	0.70	1.00	0.07

Table B.27: Integrated absorbance ratios of selected transitions in dimethyl ether: CH_3OH .

Temperature (K)	COC stretch. $10.85\mu\text{m}$	COC stretch. + CH_3 rock. $9.141\mu\text{m}$	COC stretch. + CH_3 rock. $8.592\mu\text{m}$	CH_3 rock. $8.011\mu\text{m}$
15	0.71	0.71	1.00	0.10
30	0.69	0.77	1.04	0.09
70	0.65	0.83	1.04	0.09
90	0.63	0.84	1.08	0.08
100	0.60	0.82	1.05	0.08
120	0.29	0.39	0.38	0.04

Table B.28: Integrated absorbance ratios of selected transitions in dimethyl ether: $\text{CO}:\text{CH}_3\text{OH}$.

Temperature (K)	COC stretch. $10.85\mu\text{m}$	COC stretch. + CH_3 rock. $9.141\mu\text{m}$	COC stretch. + CH_3 rock. $8.592\mu\text{m}$	CH_3 rock. $8.011\mu\text{m}$
15	0.81	0.88	1.00	0.13
30	0.83	1.02	1.13	0.12
70	0.63	0.86	1.04	0.08
90	0.63	0.83	1.00	0.08
100	0.51	0.67	0.77	0.07

Appendix C: Spectroscopic data of selected bands

Appendix C.1: Acetaldehyde

Appendix C.2: Ethanol

Appendix C.3: Dimethyl ether

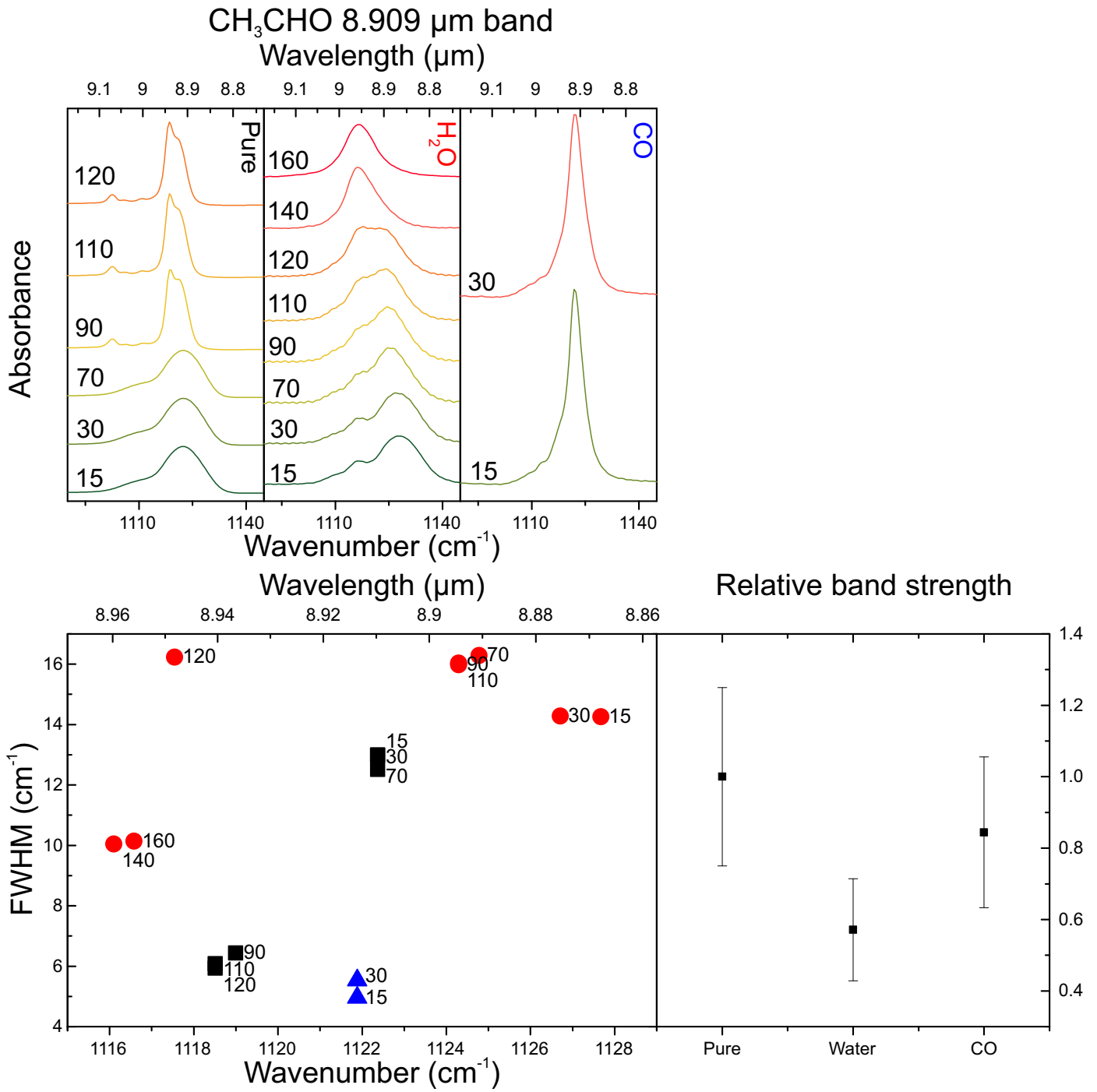


Fig. C.1: Top: from left to right the acetaldehyde 8.909 μm band pure (black) and in water (red) and CO (blue) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 8.909 μm band at 15 K in various matrices.

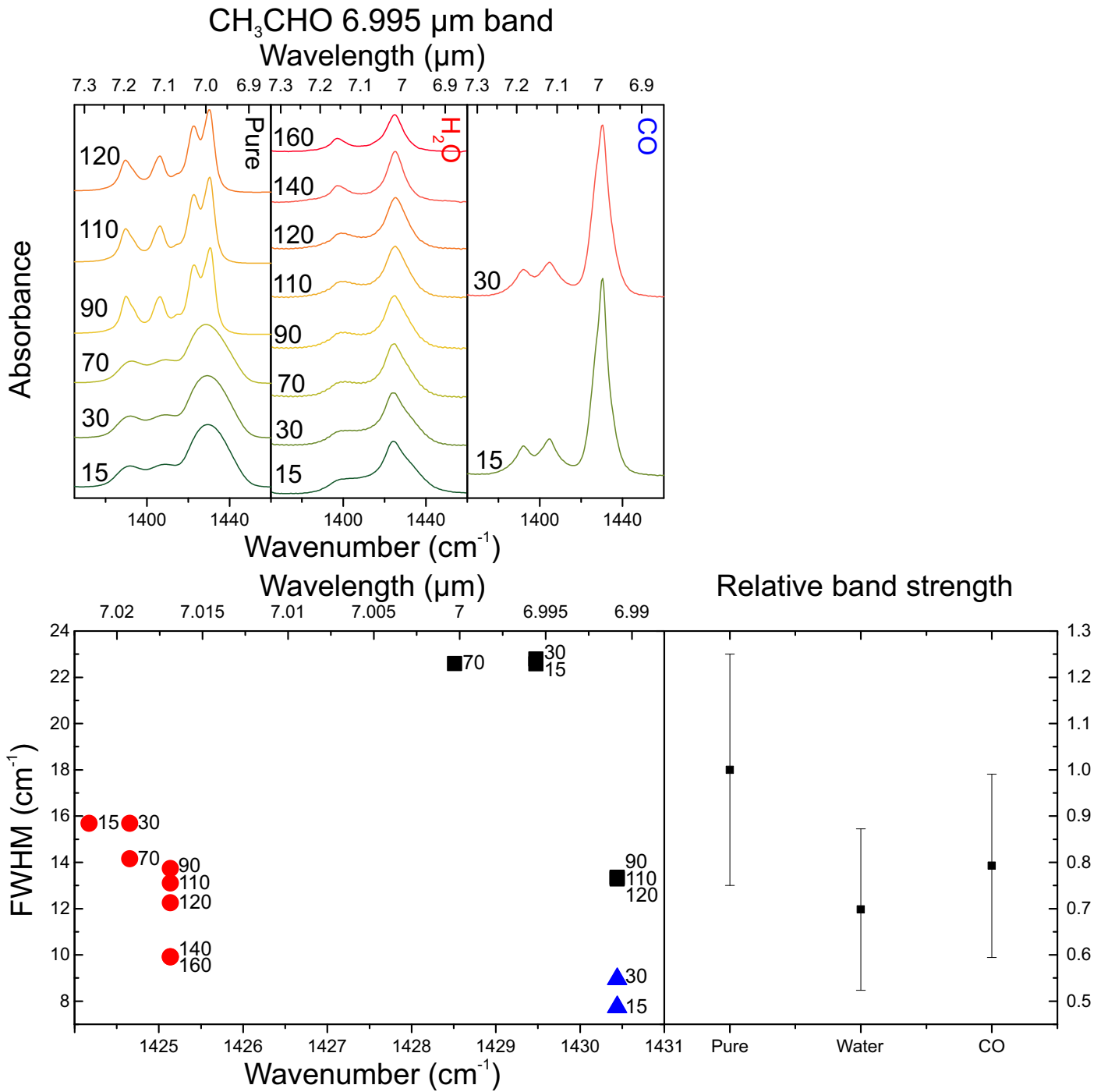


Fig. C.2: Top: from left to right the acetaldehyde 6.995 μ m band pure (black) and in water (red) and CO (blue) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 6.995 μ m band at 15 K in various matrices.

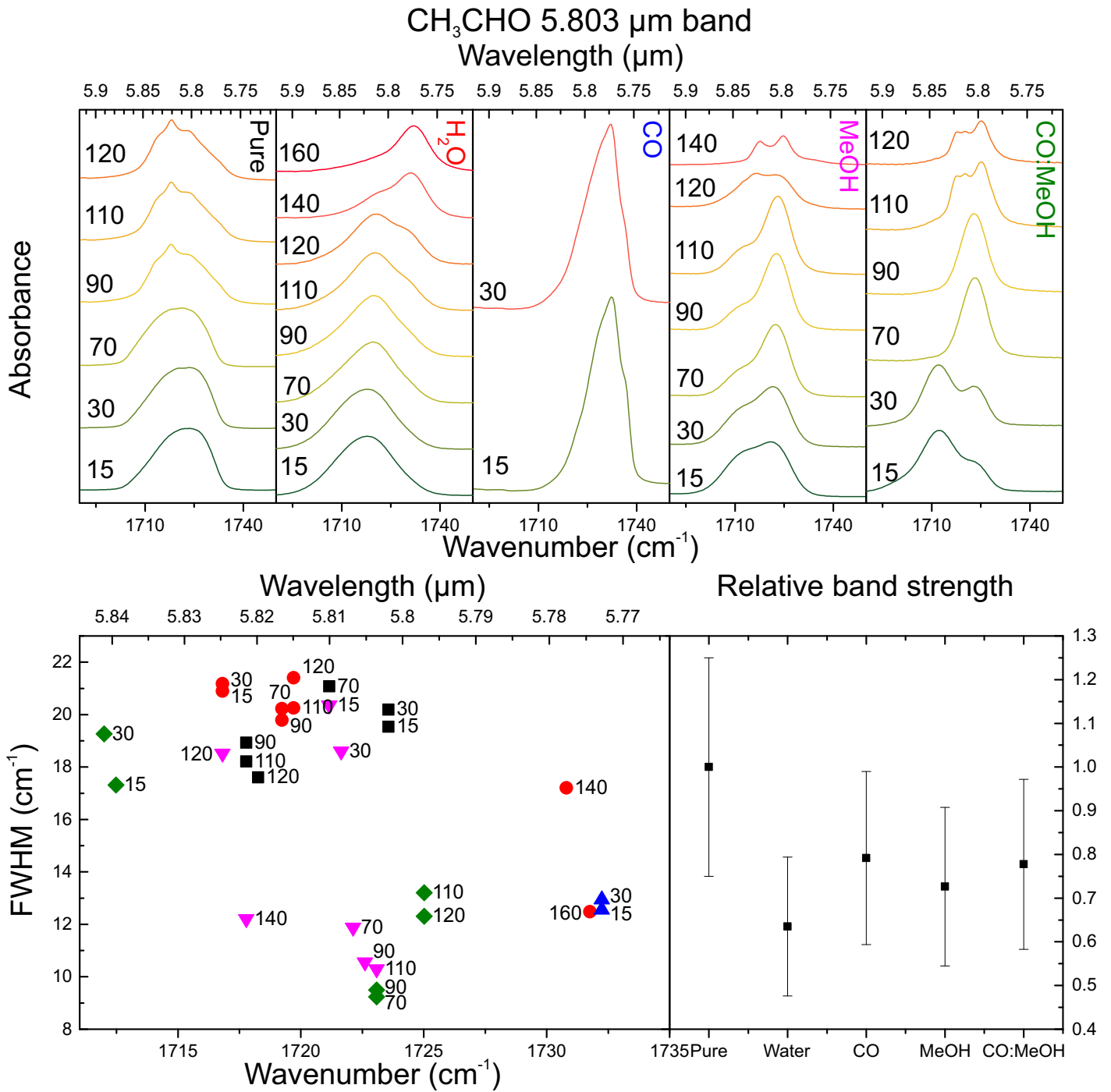


Fig. C.3: Top: from left to right the acetaldehyde 5.803 μm band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 5.803 μm band at 15 K in various matrices.

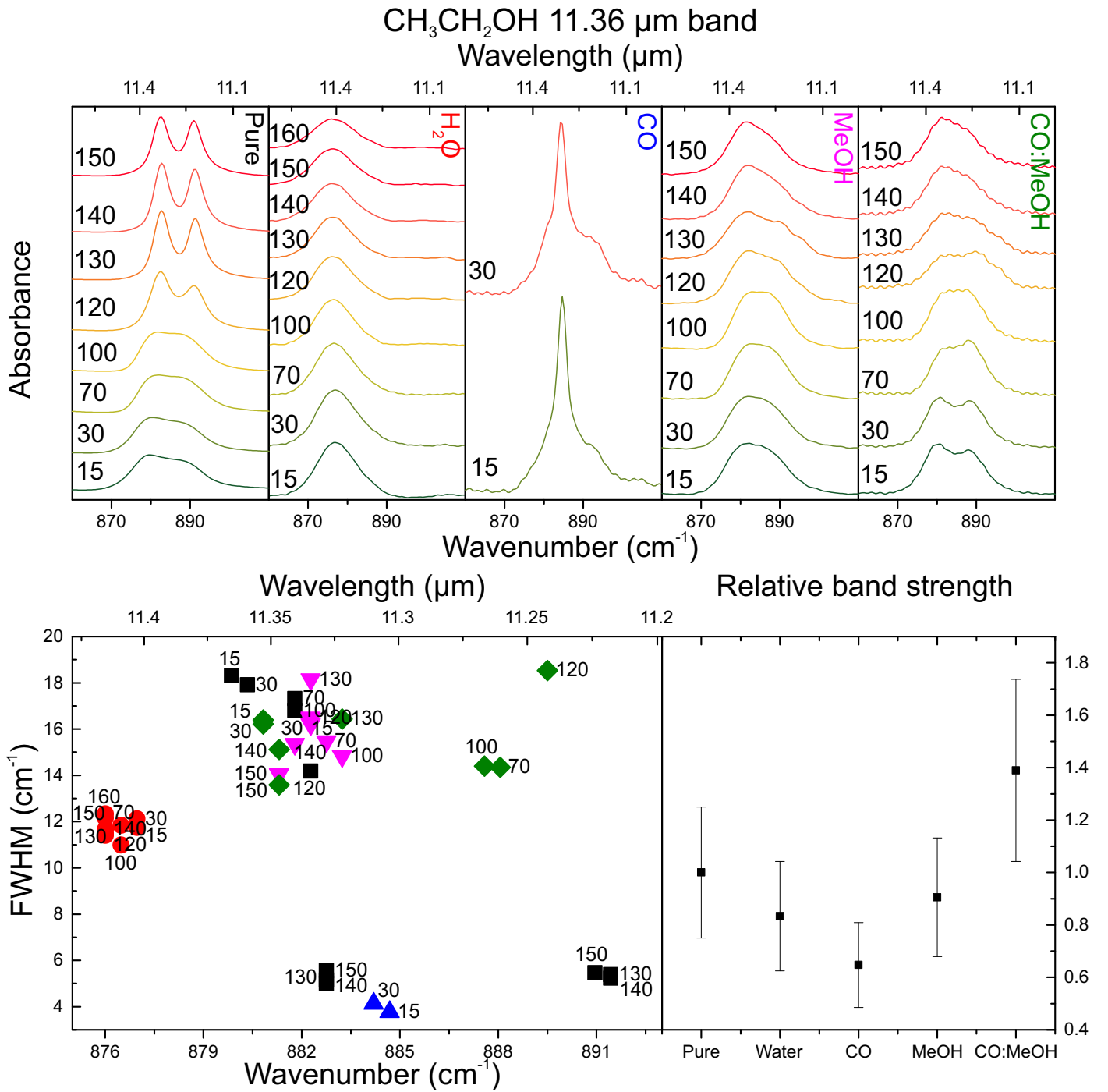


Fig. C.4: Top: from left to right the ethanol 11.36 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 11.36 μ m band at 15 K in various matrices.

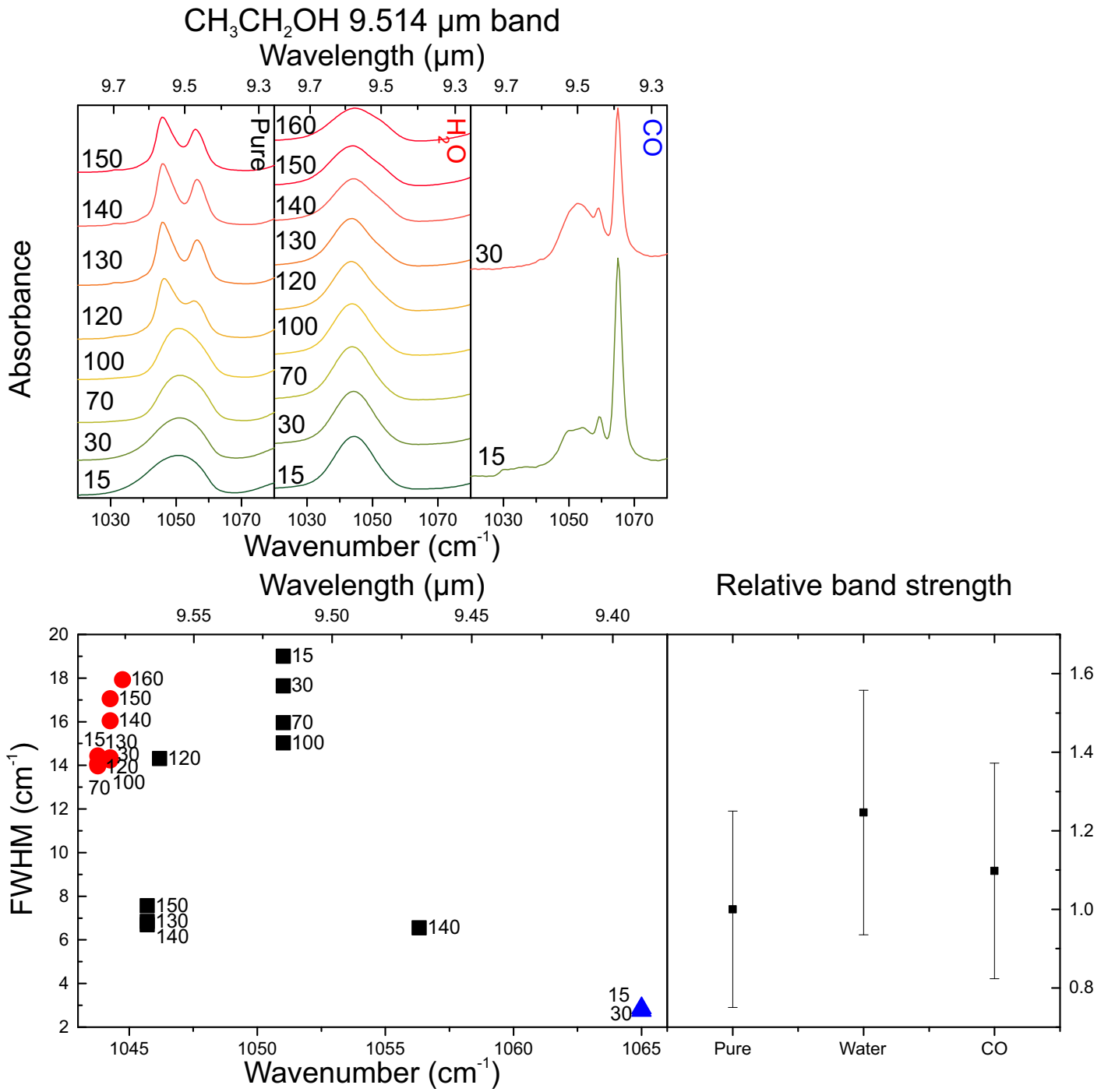


Fig. C.5: Top: from left to right the ethanol 9.514 μm band pure (black) and in water (red) and CO (blue) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 9.514 μm band at 15 K in various matrices.

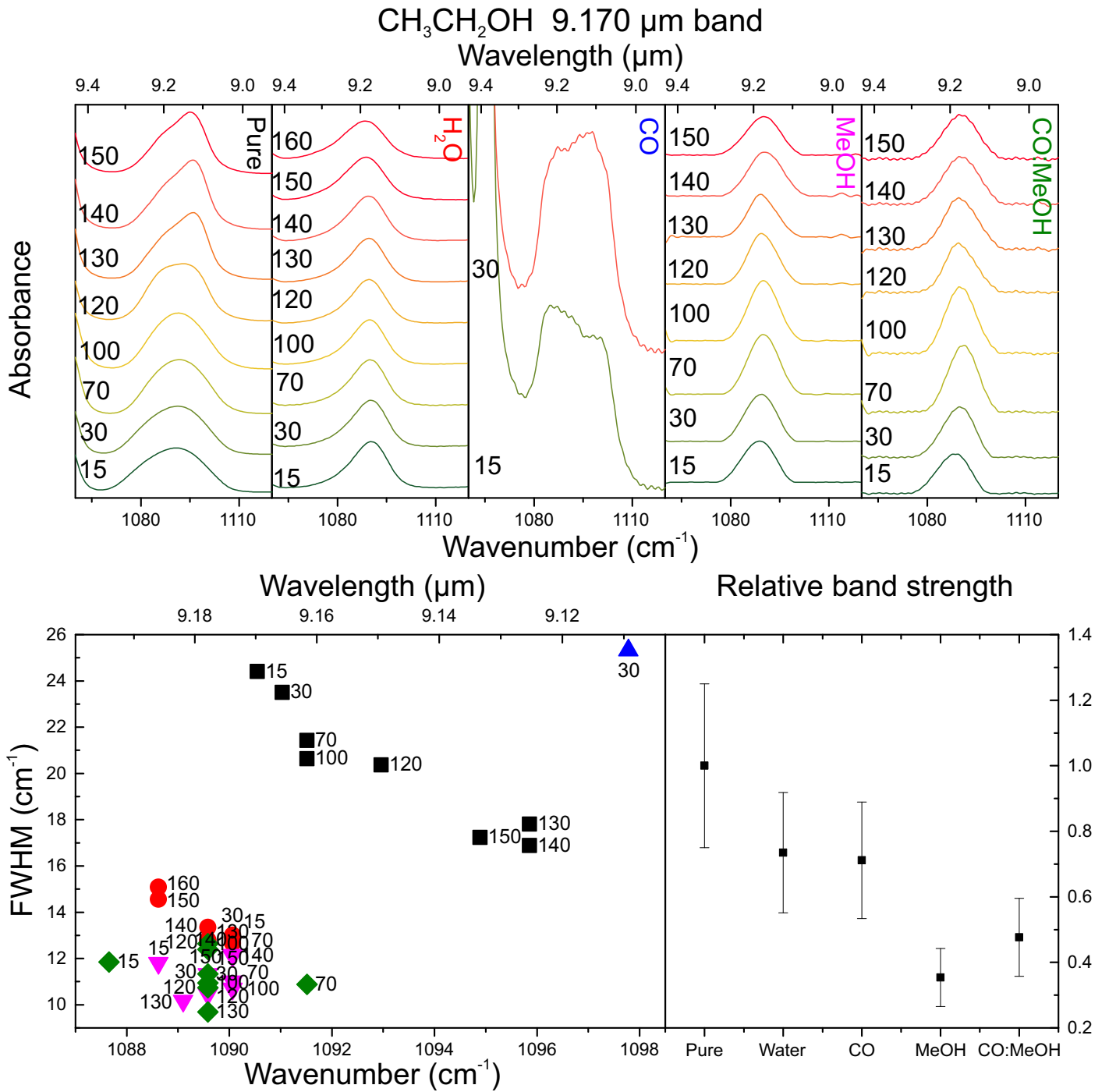


Fig. C.6: Top: from left to right the ethanol 9.170 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 9.170 μ m band at 15 K in various matrices.

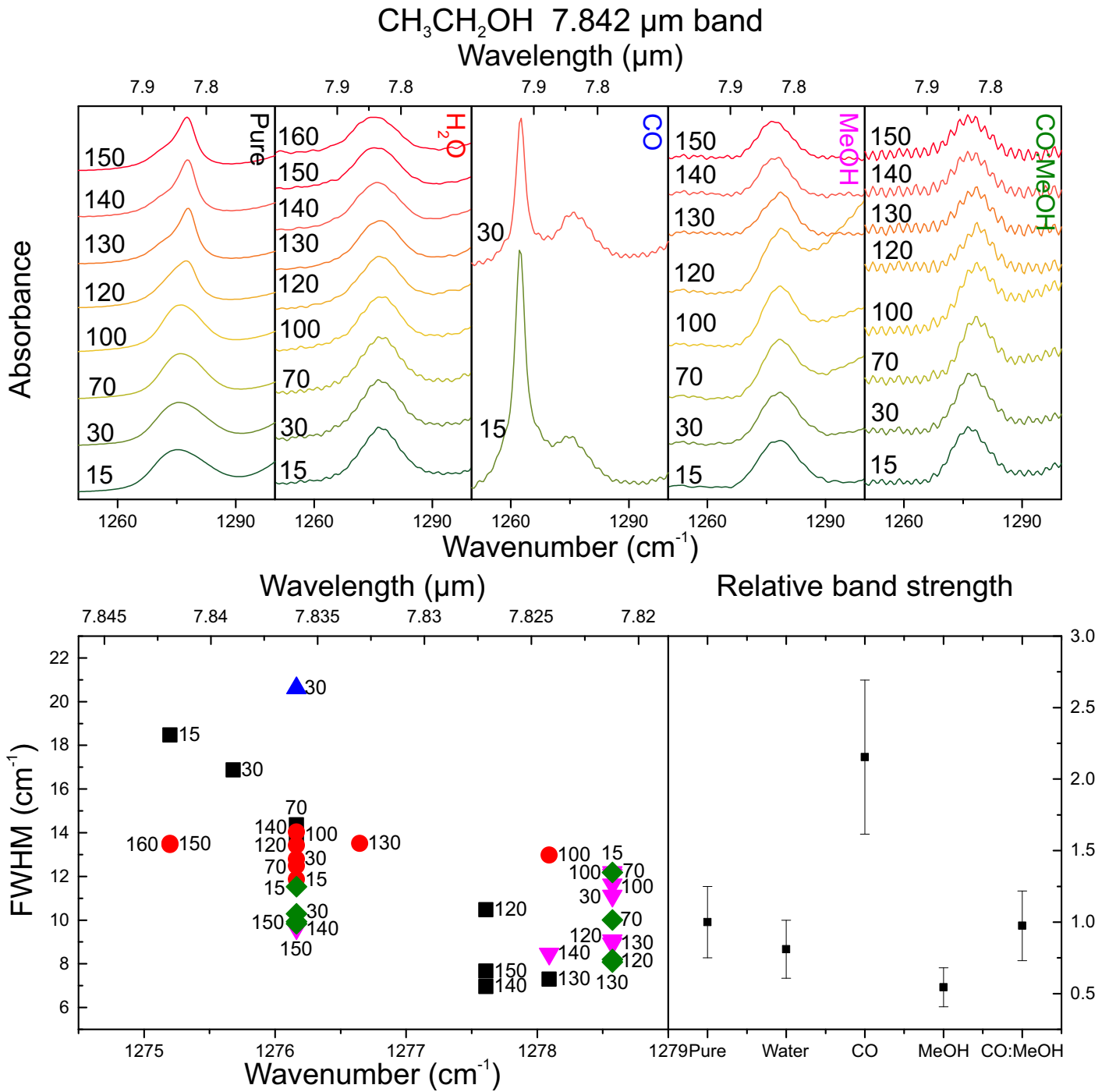


Fig. C.7: Top: from left to right the ethanol 7.842 μm band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 7.842 μm band at 15 K in various matrices.

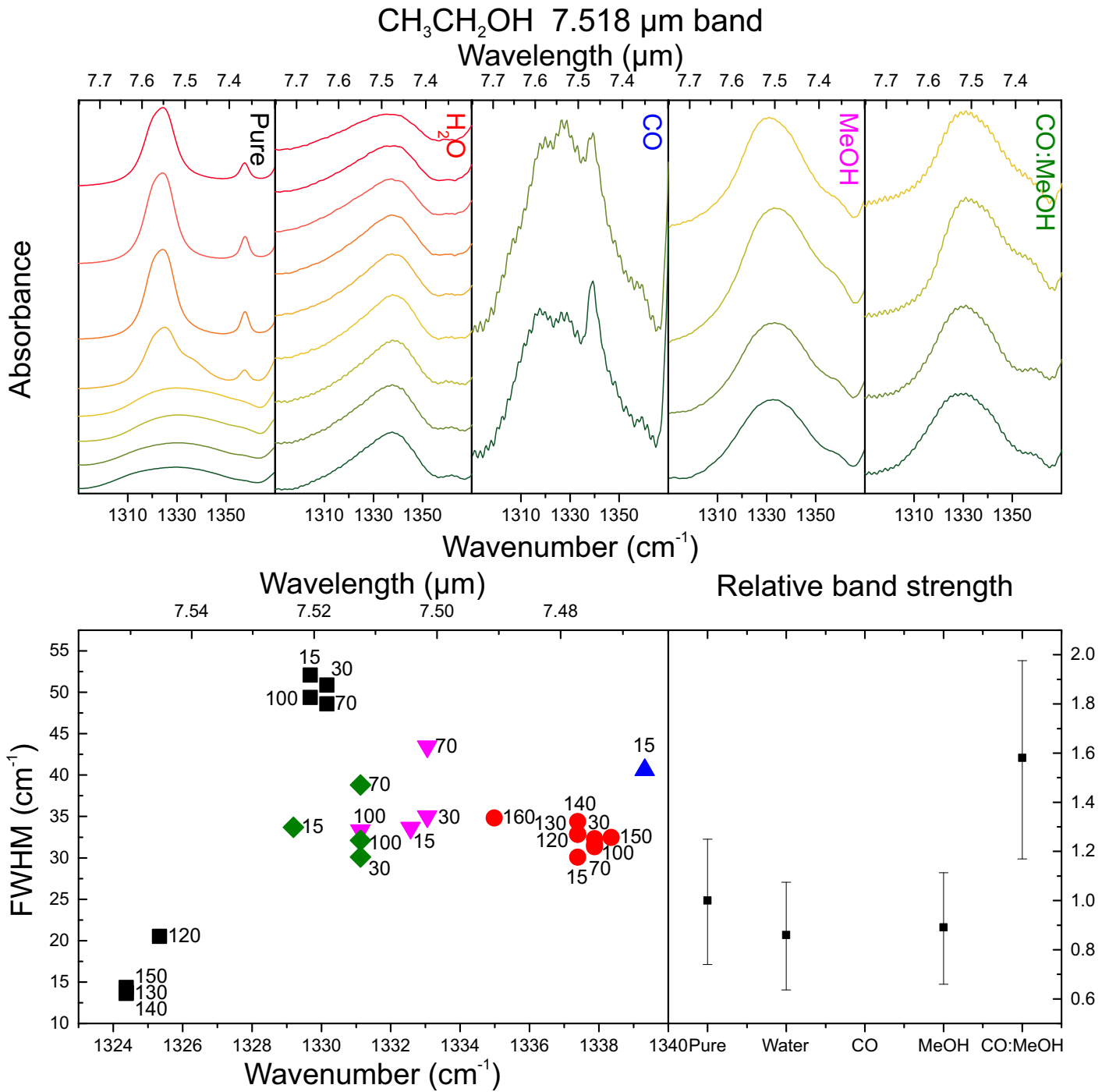


Fig. C.8: Top: from left to right the ethanol 7.518 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 7.518 μ m band at 15 K in various matrices.

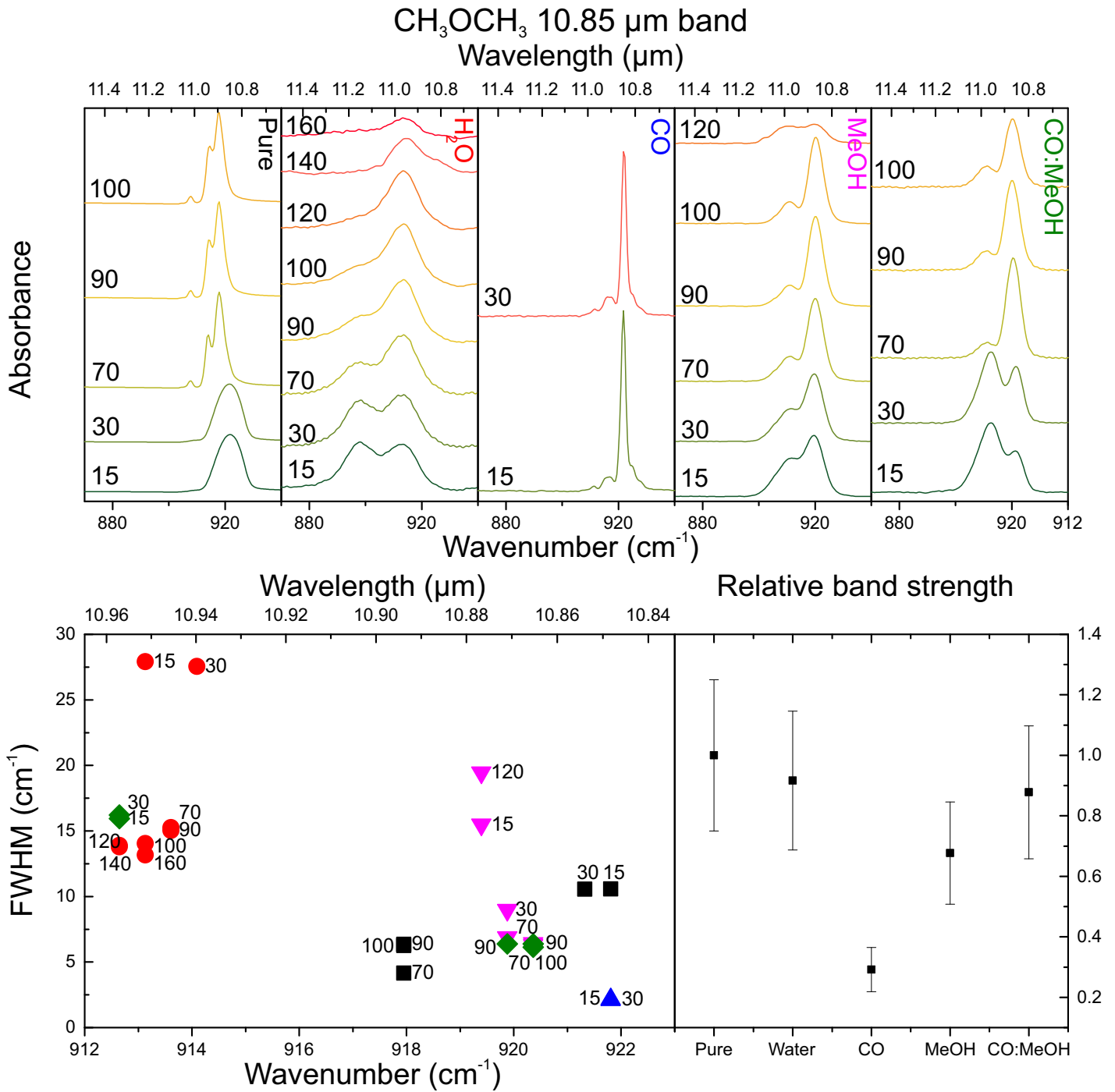


Fig. C.9: Top: from left to right the dimethyl ether 10.85 μm band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 10.85 μm band at 15 K in various matrices.

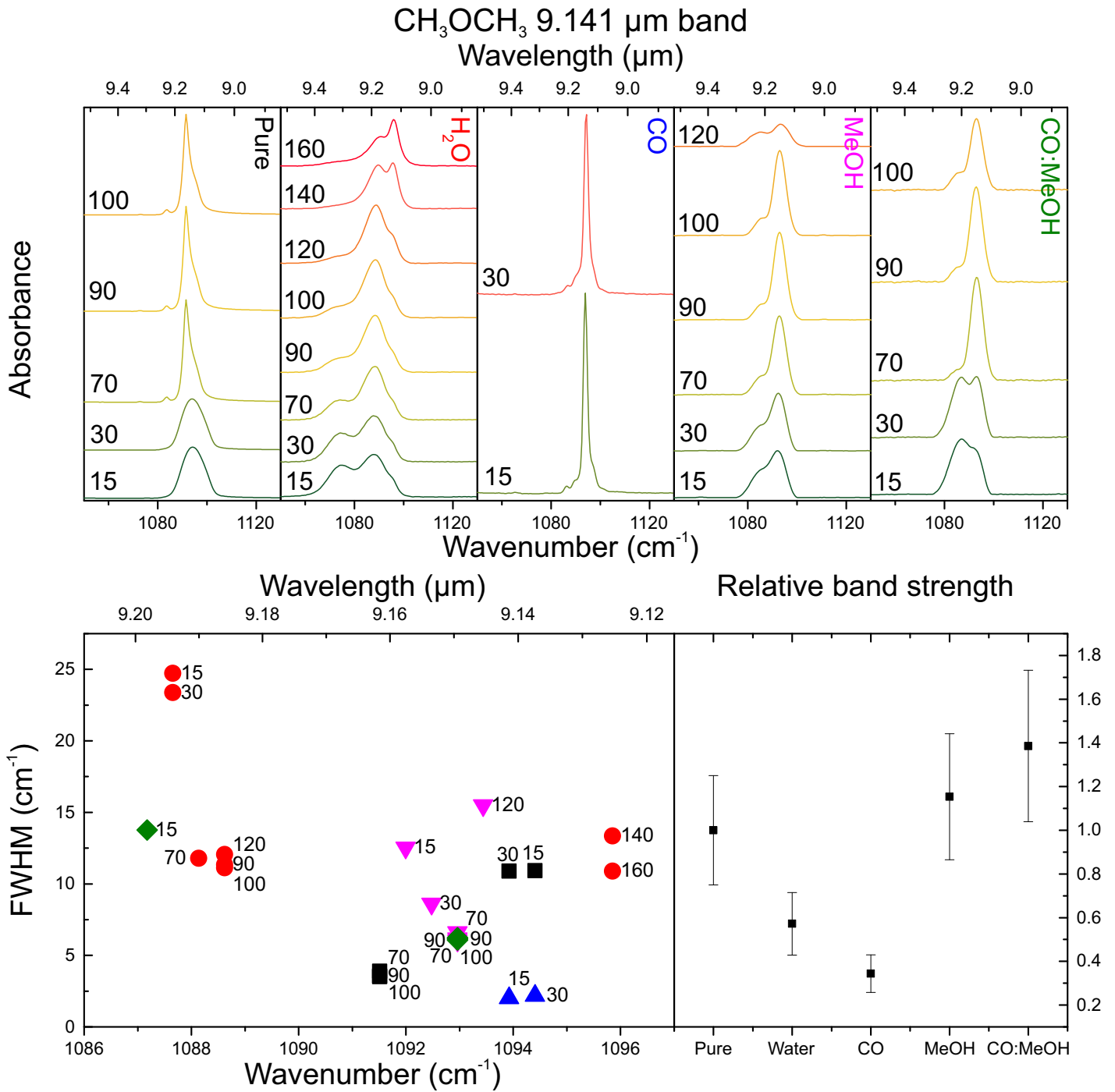


Fig. C.10: Top: from left to right the dimethyl ether 9.141 μ m band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 9.141 μ m band at 15 K in various matrices.

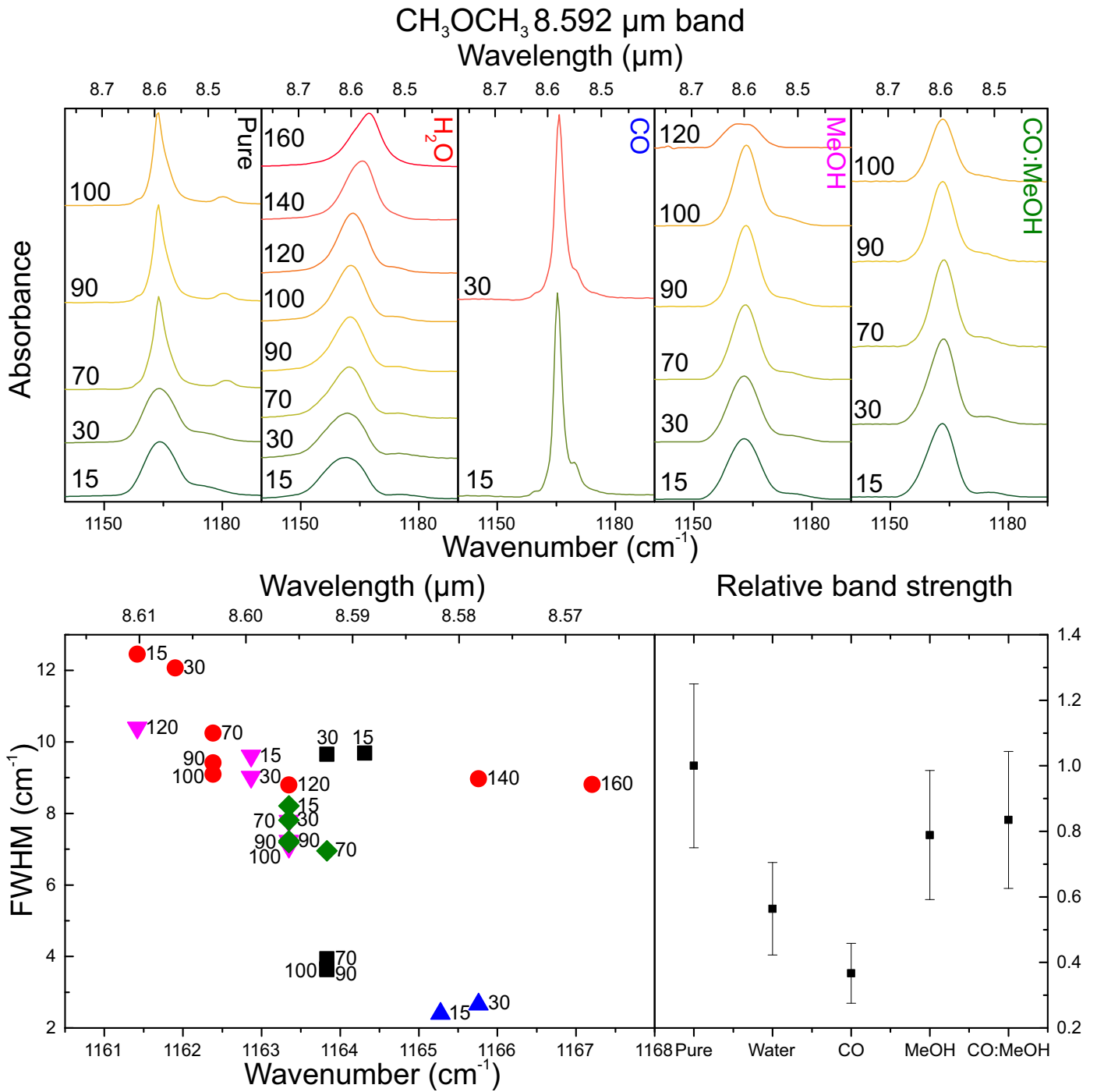


Fig. C.11: Top: from left to right the dimethyl ether 8.592 μm band pure (black) and in water (red), CO (blue), methanol (purple), and CO:CH₃OH (green) at various temperatures. Bottom left: peak position vs. FWHM plot, using the same colour coding. Bottom right: the relative band strength for the 8.592 μm band at 15 K in various matrices.