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Infrared spectra of complex organic molecules in astronomically relevant ice matrices

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Abstract. The identification of complex organic molecules, COMs, in inter- and circumstellar gas phase environments is steadily increasing. The formation of such COMs takes largely place on the icy dust grains, as has been shown in recent laboratory studies. Until now solid state features of smaller molecular species have been directly identified in these environments. The presented work on acetaldehyde (CH_3CHO), ethanol (CH_3CH_2OH), and dimethyl ether (CH_3OCH_3) in different astronomically relevant ice environments and for temperatures in the range 15 to 160 Kelvin, provides the necessary tools to guide or interpret astronomical observations, specifically for upcoming James Webb Space Telescope observations.

Keywords. astrochemistry, methods: laboratory, techniques: spectroscopic, molecular processes

1. Introduction

The first molecule detected in the solid state in the interstellar medium was water (Gillett & Forrest 1973). Over time more than 10 other molecules have been detected in the solid state (i.e. CO, CH_4, CO_2, NH_3, and CH_3OH). The formation of these small molecules and also more complex organic molecules has been linked to icy surfaces on dust grains. With the combined effort of space based telescopes, the Infrared Space Observatory (ISO) and *Spitzer* Space Telescope, laboratory studies, and astrochemical modelling the understanding of the structure and composition of these icy dust grains has been greatly improved (e.g. see reviews by Herbst & van Dishoeck 2009, Boogert *et al.* 2015, and Linnartz *et al.* 2015). With the launch of the *James Webb* Space Telescope (JWST) in the near future and availability of the state-of-the-art instruments, MIRI and NIRSpec, the community will be able to measure spectra with higher spectral and spatial resolution and sensitivity. This improvement allows to search for COMs beyond methanol and to aim to a new level of complexity in interstellar ices. In order to unambiguously identify these COMs, with similar functional groups and thus similar spectral features, we provide in this work the tools to distinguish acetaldehyde (CH_3CHO), ethanol (CH_3CH_2OH), and dimethyl ether (CH_3OCH_3). The matrix in which these COMs reside influences the spectral features, i.e. peak position, FWHM change, and band strengths, and are thus also investigated in this work.

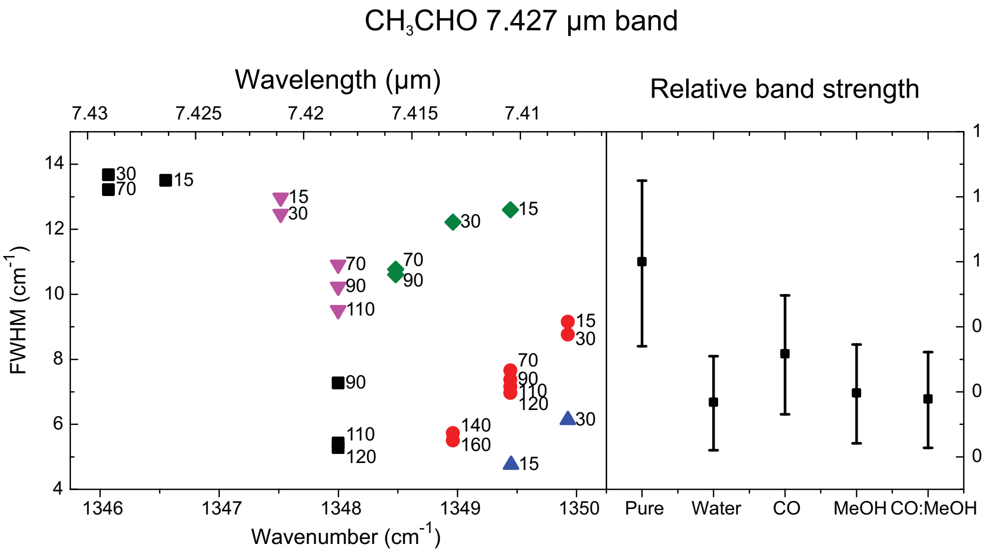

Figure 1. *Left:* peak position vs. FWHM, pure in squares (black), water in circles (red), CO in triangles (blue), methanol in upside down triangles (purple), and CO:CH_3OH in diamonds (green) at various temperatures. *Right:* the relative band strength for the 7.427 μm band at 15 K in the different matrices.

2. Results

The spectra of the selected molecules have been recorded under high vacuum conditions in transmission mode with a FTIRS (Varian 670-IR) in the range 4000-500 cm^{-1} (2.5-20 μm) and a spectral resolution of 1.0 cm^{-1}. These COMs have been measured in pure form but also diluted, 1:20, in the different matrices: water (H_2O), carbon-monoxide (CO), methanol (CH_3OH), and a 1:1 mixture of CO:CH_3OH. The ratio between COM and matrix's is set to 1:20 as an estimate for the dilution of COMs in interstellar ices. For each molecule several transitions have been selected that do not have significant overlaps with the other COMs in this work and are thus good candidates for identification in space. These transitions have been analysed and their FWHM, peak position, and relative band strengths recorded. An example of this can be seen in Fig. 1 were we show the results for the 7.4 μm band of acetaldehyde. It is evident from the left part of the figure that the FWHM and position of the absorption band depend on the matrix in which acetaldehyde resides, but also the temperature of the ice. The right part of the figure indicates that the intensity of this transition decreases when acetaldehyde is diluted in astronomically relevant molecules. The FWHM, peak position, and integrated absorbance ratios of all these transitions will allow astronomers to interpret and identify these COMs in interstellar ices. For more details please see Terwisscha van Scheltinga *et al.* 2018 or visit the Leiden Database for Ice (http://icedb.strw.leidenuniv.nl).

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