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Laboratory data in support of JWST observations of interstellar ices

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Abstract. Experimental and theoretical studies have shown that Complex Organic Molecules (COMs) can be formed on icy dusty grains in molecular clouds and protoplanetary disks. The number of astronomical detections of solid COMs, however, is very limited. With the upcoming launch of the James Webb Space Telescope (JWST) this should change, but in order to identify solid state features of COMs, accurate laboratory data are needed. Here we present high resolution (0.5 cm^{-1}) infrared ice spectra of acetone (C_3H_6O) and methyl formate ($HCOOCH_3$), two molecules already identified in astronomical gas phase surveys, whose interstellar synthesis is expected to follow solid state pathways.

Keywords. Infrared spectroscopy, Ice analogs, Methyl formate, Acetone, Interstellar molecules.

1. Introduction

The importance of interstellar ice as formation site for complex molecules contrasts the fact that less than 5% of the species identified in the inter and circumstellar medium were detected in the solid state (Linnartz *et al.* 2015; Boogert *et al.* 2015; McGuire 2018). The main reason for this is that it is much harder to unambiguously identify species in the solid state. As the molecules cannot freely rotate in ices, microwave and submillimiter spectroscopy cannot be applied. The vibrational modes are very sensitive to the chemical environment, temperature, and moreover, similar functional groups of different molecules can absorb at overlapping wavelengths. For these reasons, astronomically relevant ice spectra are required to interpret observational data.

With the upcoming launch of JWST, IR spectra of ices in star forming regions will become available with a spatial and spectroscopical resolution not available so far. In order to interpret these data and to assign the spectral features, laboratory work is needed. This work presents accurate IR ice spectra, recorded for a set of varying parameters (temperature and mixing ratios) of two COMs already identified in the gas phase: acetone (C_3H_6O) and methyl formate ($HCOOCH_3$). This work is a complement to recent studies of acetaldehyde, ethanol and dimethylether (Terwisscha van Scheltinga et al. 2018).

2. Experimental

The measurements are taken in a high-vacuum setup. The samples are prepared from pure or premixed gases in a 2 L balloon with a total pressure of 20 mbar and are admitted in the HV chamber (base pressure of $\sim 2 \times 10^{-7}$ Torr) through a calibrated needle valve. The mixtures are background deposited onto a ZnSe substrate pre-cooled to 15 K.

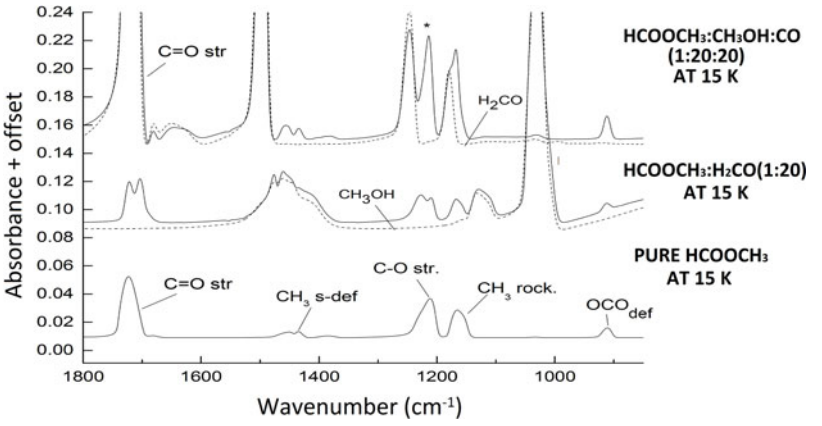

Figure 1. IR spectra of $HCOOCH_3$ mixtures. All spectra are offset for better visualization.

The ices are grown up to a thickness of approximately 4000 ML. Thick ices guarantee that water deposition from the background gas can be neglected. The analyzed ices are mixtures of C_3H_6O embedded in H_2O, CO_2, CH_4, CO and CH_3OH in a proportion of 1:5 and 1:20 for the two component mixtures and 1:2.5:2.5 and 1:10:10 for the three component mixtures. For $HCOOCH_3$ containing ices the matrix components are H_2CO, CO_2, CO and CH_3OH in a proportion of 1:20 for the two component mixtures and 1:20:20 for the three component mixtures. The spectra are collected in transmission mode, from 500 - 4000 cm^{-1} (20 - 2.5 μm) at resolution 0.5 cm^{-1} using a Varian 670 FTIR spectrometer. Spectra are recorded for different temperatures, typically covering the range from 15 - 250 K during a temperature increase of about 25 K h^{-1}. For more details about the experimental methodology see Ligterink *et al.* (2018).

3. Results and Discussion

The infrared spectra of acetone and methyl formate have several prominent bands. However, when embedded in ice matrices, most of these bands are hard to see due to overlap with bands of the matrix molecules. The CH_3 stretch modes of both acetone and methyl formate (in the 2900 cm^{-1}–3100 cm^{-1} region) overlap with CH_3 modes of methanol and CH_2 modes of formaldehyde. The strong C=O stretching mode of methyl formate also overlaps with the C=O stretching mode of H_2CO.

Analyzing the acquired spectra however, we can identify bands that would enable JWST detection of these molecules. For acetone these bands are the C=O stretch mode around 1710 cm^{-1}, the CH_3 symmetrical deformation band around 1363 cm^{-1} and the CCC asymmetrical deformation band around 1228 cm^{-1}. For $HCOOCH_3$, the bands are the C-O stretch around 1210 cm^{-1}, CH_3 rocking around 1165 cm^{-1} and the OCO deformation mode around 911 cm^{-1} (see Fig. 1). A detailed discussion of the spectra is being prepared for publication (Rachid et al. 2020, *in prep*); all the recorded spectra will be available on the Leiden Ice Database (http://icedb.strw.leidenuniv.nl/).

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