SESSION 4

Laboratory Astrophysics: from Observations to Interpretation
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Laboratory investigations aimed at building a database for the interpretation of JWST spectra

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Abstract. The James Webb Space Telescope (JWST) is expected to be launched in 2021. The JWST's science instruments will provide high quality spectra acquired in the line of sight to young stellar objects whose interpretation will require a robust database of laboratory data. With this in mind, an experimental work is in progress in the Laboratory for Experimental Astrophysics in Catania to study the profile (shape, width, and peak position) of the main infrared bands of molecular species expected to be present in icy grain mantles. Our study also takes into account the modifications induced on icy samples by low-energy cosmic ray bombardment and by thermal processing. Here we present some recent results on deuterium hydrogen monoxide (HDO), N-bearing species, and carbon dioxide (CO_2).

Keywords. Astrochemistry, methods: laboratory, techniques: spectroscopic, molecular processes, ISM: molecules, ISM: lines and bands, infrared: ISM

1. Experimental methods

The experimental results here presented were obtained at INAF - Osservatorio Astrofisico di Catania. The experiments were performed in an ultrahigh vacuum (UHV) chamber ($P \leqslant 10^{-9}$ mbar) in which a KBr substrate is placed in thermal contact with the cold finger of a closed-cycle helium cryocooler (CTI) for which temperature can be varied between 15 and 300 K. The vacuum chamber is placed in the sample compartment of a FTIR spectrometer (Bruker Vertex 70) and transmission spectra of the sample are acquired in the range 7800–400 cm^{-1} (1.28–25 μm) at a resolution of 1 cm^{-1}. The substrate forms an angle of 45° with respect to the IR beam. Pure gas or mixtures are admitted through a needle valve and accrete on the cold substrate. The gas inlet is not faced to the substrate, allowing the background deposition of mixtures which results in the formation of an uniform ice surface on the front side of the substrate, while the ice deposition on the backside of the substrate is prevented by a 20 mm long narrow tube aligned along the path of the IR beam. A rotatable polarizer is placed in the path of

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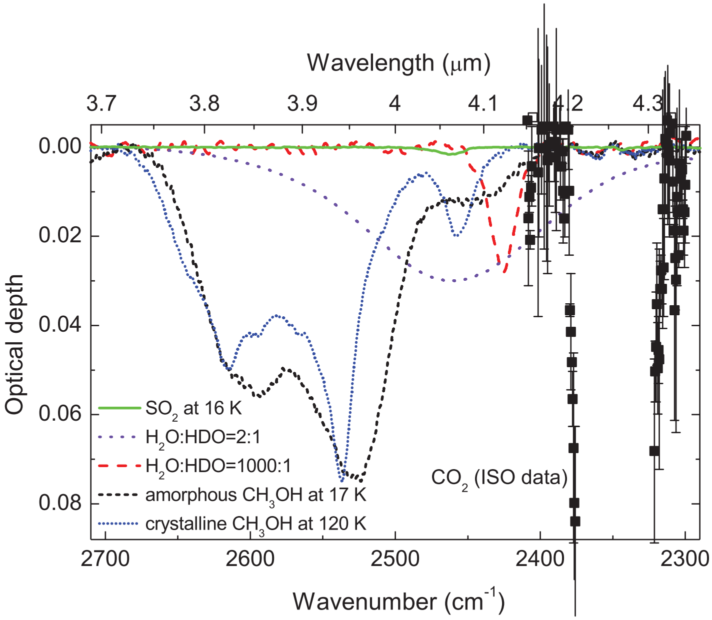

Figure 1. Expected contribution of different ice components in the line of sight to W33A in the 4 μm region. The observed feature attributed to solid CO_2 is also reported.

the IR beam, which enables us to subsequently record spectra in P mode, in which the electric vector is parallel to the plane of incidence, and S mode, in which the electric vector is perpendicular to the plane of incidence. The UHV chamber is connected to a 200 kV ion implanter by Danfysik. An electrostatical sweeping of the ion beam ensures the uniform coverage of the target, and the ion current density <1 μA cm^{-2} prevents its macroscopic heating. More details on the experimental setup and procedure can be found in Urso *et al.* (2016) and Scirè *et al.* (2019). Infrared spectra here presented will be available at Catania database (http://www.oact.inaf.it/weboac/labsp/dbindex.html).

2. Results and Discussion

Solid HDO is expected to be present in icy grain mantles in star forming regions however its detection is highly debated (e.g., Teixeira *et al.* 1999; Dartois *et al.* 2003; Aikawa *et al.* 2012). Furthermore its observation from ground-space telescope is not straightforward since its main feature at about 2450 cm^{-1} (4.1 μm) partially overlaps with telluric CO_2. Recently, Urso *et al.* (2018) have studied the profile (shape, width and peak position) of HDO in various H_2O:HDO mixtures. The effects of ion bombardment and thermal annealing have also been investigated. They have shown that the profile of the O-D stretching mode feature depends on the temperature of the sample, on the structure of the ice matrix (amorphous or crystalline) and on the ice mixture. The O-D stretching mode band partially overlaps with CO_2 asymmetric stretching mode, CH_3OH (methanol) combination mode, and SO_2 (sulfur dioxide) combination mode. As an example, Fig. 1 shows the expected contribution of the different ice components in the line of sight to the high-mass young stellar objects W33A. Laboratory spectra of pure amorphous and crystalline CH_3OH and SO_2 have been scaled on the basis of observed abundances of these species as reported by Allamandola *et al.* (1992) and Boogert *et al.* (1997), respectively. Laboratory spectra relative to H_2O:HDO mixtures have been scaled according to the tentative detection reported by Teixeira *et al.* (1999). The feature attributed to the

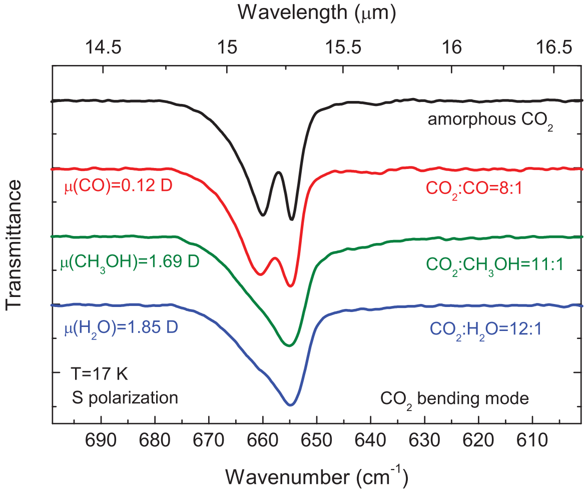

Figure 2. Transmittance spectra, in the 700-600 cm^{-1} region, of pure amorphous solid CO_2 and its mixture with CO, CH_3OH and H_2O. The dipole moment (μ) of these latter species is also reported.

stretching mode of solid CO_2 observed by the Infrared Space Observatory (ISO) is also plotted (Gerakines *et al.* 1999). On the basis of these results HDO is expected to be detected by the JWST.

As concerns N-bearing species, laboratory experiments have shown that HNCO, OCN^-, HCN, and N_2O are formed after ion bombardment of relevant interstellar ice analogue mixtures (such as CH_3OH:N_2, H_2O:CH_4:N_2, and H_2O:CH_4:NH_3; e.g., Palumbo *et al.* 2004; Baratta *et al.* 2015; Fedoseev *et al.* 2018), in addition nitrogen oxides, namely NO, NO_2 and N_2O, are formed after ion bombardment of CO:N_2 mixtures (e.g., Sicilia *et al.* 2012). Molecules containing nitrogen and oxygen with the N−O bond (such as NO, N_2O, and HNO) are considered potential precursors of prebiotic molecules therefore understanding their chemical evolution in space is matter of great interest. Fulvio *et al.* (2019) have estimated that NO should be present on CO-rich icy grain mantles and its band at 1870 cm^{-1} (5.35 μm) should be detectable by the JWST. On the other hand, chemical models and low-temperature laboratory experiments have shown that solid NO could be efficiently "consumed" by addition of H atoms to produce hydrogenated species (Charnley *et al.* 2001; Congiu *et al.* 2012) or by addition of $O/O_2/O_3$ or N atoms to produce NO_2 (Minissale *et al.* 2014). Thus, the detection of N−O bearing species on icy grain mantles and the estimation of their abundances would help us to better understand the chemical evolution of molecules with the N−O bond in space.

Observations carried out with ISO and the Spitzer Space Telescope have shown that CO_2 is ubiquitous in icy grain mantles and is among the most abundant detected species (e.g., Boogert *et al.* 2015). Since its first detection by the Infrared Astronomical Satellite (IRAS) several laboratories have been involved in the experimental study of the CO_2 bands profile in astrophysical relevant mixtures (e.g., Sandford & Allamandola 1990; Baratta & Palumbo 1998; Isokoski *et al.* 2013; Cooke *et al.* 2016; Gerakines & Hudson 2015; Baratta & Palumbo 2017). The mid-infrared spectrum of a thin CO_2 film at low temperature (10-20 K) shows five absorption bands, namely the $^{12}CO_2$ asymmetric stretching mode (ν_3) at about 2343 cm^{-1}, $^{13}CO_2$ asymmetric stretching mode at about 2283 cm^{-1}, $^{12}CO_2$ bending mode (ν_2) with a structured feature peaked at 660 and 655 cm^{-1}, and combination modes $\nu_1+\nu_3$ and $2\nu_2+\nu_3$ at 3707 cm^{-1} and 3600 cm^{-1}, respectively. One of the main debated question about the mid-IR spectrum of solid CO_2

is the profile of the bending mode band. In fact, the two bending modes (in-plane and out-of-plane) have the same energy and differ only in the direction of the bending motion (i.e., degenerate modes). In these circumstances a single absorption band should be observed in the spectrum. Baratta & Palumbo (2017) suggested that during vapor deposition of pure CO_2 samples the formation of dimers takes place (Gómez Castaño *et al.* (2008) and references therein) which give rise to the double peak in the bending mode band profile (Fig. 2), while when a small amount of a polar species (such as H_2O and CH_3OH) is co-deposited with CO_2 the formation of dimers is inhibited and the double peak structure is not observed (Fig. 2).

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