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Bands of solid CO$_2$ in the 2–3 μm spectrum of S 140:IRS1[⋆]

J. V. Keane[1], A. C. A. Boogert[2], A. G. G. M. Tielens[1,3], P. Ehrenfreund[4], and W. A. Schutte[4]

[1] Kapteyn Astronomical Institute, PO Box 800, 9700 AV Groningen, The Netherlands
[2] California Institute of Technology, Downs Laboratory of Physics 320-47, Pasadena CA 91125, USA
[3] SRON, PO Box 800, 9700 AV Groningen, The Netherlands
[4] Leiden Observatory, PO Box 9513, 2300 RA Leiden, The Netherlands

Abstract. We investigate the 2–3 μm ISO–SWS spectrum of the luminous protostellar object S 140:IRS1. Two narrow absorption features are detected at 2.70 and 2.77 μm, which are well fitted with laboratory spectra of the $\nu_1 + \nu_3$ and the $2\nu_2 + \nu_3$ combination modes of solid CO$_2$. The ice in this line of sight must have been subjected to significant heating, in agreement with previously studied CO$_2$ bands. A combined laboratory fit to all CO$_2$ bands detected toward S 140:IRS1 shows, among others, the need for particle shape calculations for the CO$_2$ stretch mode. Finally, we discuss the absence of features of isolated H$_2$O and dangling OH groups in the spectrum of S 140:IRS1.

Key words. ISM: molecules – ISM: abundances – stars: S 140:IRS1 – infrared: stars

1. Introduction

Ice species toward massive protostars were discovered by their characteristic stretching and bending modes at infrared wavelengths (e.g. Willner et al. 1982; Ehrenfreund & Schutte 2000). From band profile analyses, it is now well established that in specific interstellar environments the most abundant species (H$_2$O, CH$_3$OH and CO$_2$) reside on the grain mantle mixed with highly diluted volatiles (CO, CH$_4$, OCS) (e.g. Tielens et al. 1991; Gibb et al. 2000). A spectral region that received little attention so far is the 2–3 μm region, as wavelengths longer than 2.6 μm are not observable from the ground, a problem remedied by the launch of the Infrared Space Observatory (ISO). Laboratory studies show that this region is awash with a wide variety of combination modes and isolated bands of ices including those of CO$_2$ and H$_2$O (Hagen & Tielens 1981; Sandford & Allamandola 1990, 1993; Ehrenfreund et al. 1996).

The abundant presence of CO$_2$ ice in molecular clouds and star forming regions has been well established (d'Hendecourt & de Muizon 1989; de Graauw et al. 1996; d'Hendecourt et al. 1996; Gürtler et al. 1996; Whittet et al.

1998). Recently, detailed studies of the ^{12}CO$_2$ (Gerakines et al. 1999; Boogert 1999) interstellar absorption bands have revealed that variations in the profile of these bands reflect different degrees of thermal processing of the ice mantles and variation in their chemical composition. The ^{12}CO$_2$ bands are due to strong transitions and hence the detailed profiles and peak positions will depend on the grain shape and shape (Ehrenfreund et al. 1997; Boogert et al. 1999; Baratta et al. 2000). The conclusions based on the ^{12}CO$_2$ bands are confirmed by an analysis of the much weaker ^{13}CO$_2$ band (Boogert et al. 2000), for which grain shape effects are unimportant. The CO$_2$ combination modes, which absorb weakly in the 2–3 μm spectral region, are also not affected by particle shape effects, and provide a new and independent test of the physical and chemical properties of interstellar CO$_2$-ices.

Isolated molecules have been studied extensively in the laboratory in the 2–3 μm spectral (Sandford et al. 1990, 1993; Ehrenfreund et al. 1996). Thermal and energetic processes in the interstellar medium destroy sites in the ice matrix where such pockets could reside and lead to conversion of isolated molecules over relatively short time-scales into polymers. Therefore the detection of features due to isolated molecules requires cold and UV shielded astronomical environments.

In this letter, we identify for the first time the CO$_2$ combination modes along the line of sight toward an embedded object and perform a search for bands of isolated molecules.
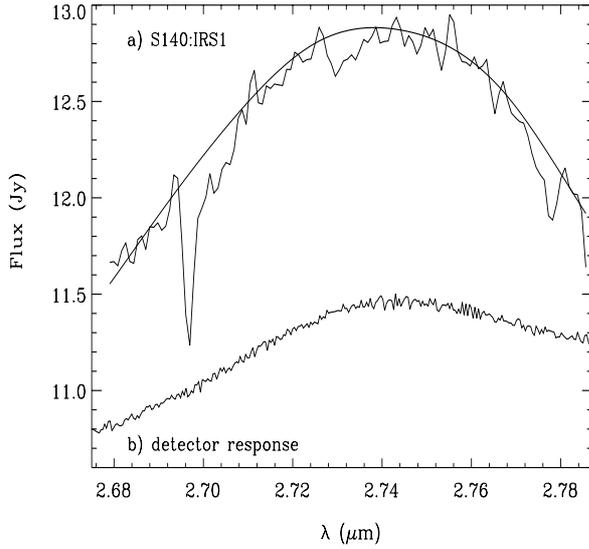
Fig. 1. ISO-SWS AOT 6 spectrum of S 140:IRS1 **a)**. For comparison the detector response, scaled to the brightness of this source, is shown **b)**.

2. Observations

The protostellar object S 140:IRS1 was observed with ISO-SWS in the high resolution "SWS06" mode (de Graauw et al. 1996). The spectrum was reduced with version 9.5 of the SWS pipeline using the latest calibration files. All detector scans were checked for excessive noise levels, deviating continuum slopes, flux levels and dark current jumps. Clipping all points that deviate by 3σ or more ensured that hits due to cosmic rays were also removed. Bad scans were cut out of the data and the remaining scans were averaged and rebinned to two points per resolution element at the maximum resolving power of band 1b ($R \sim 2500$). Figure 1 shows the final reduced spectrum. Also plotted is the detector response curve to check the reliability of the observed spectrum. No obvious residuals of the detector responsivity are apparent in the interstellar spectrum, that might affect our study of narrow absorption features.

3. Results

The spectrum of S 140:IRS1 shows two narrow absorption features near 2.70 μm and 2.78 μm and perhaps a broader absorption feature around 2.73 μm. The independent up and down scans agree well for the 2.70 μm band and this feature is detected at the $>6\sigma$ level. The 2.78 μm band differs in the individual scans and this feature is only detected at the 3σ level. The 2.73 μm feature occurs only at the 2 σ level and will require further confirmation. The spectrum was converted to optical depth scale by adopting the polynomial continuum shown in Fig. 1. The peak positions, widths ($FWHM$) and central optical depths are summarized in Table 1.

Table 1. Spectroscopic properties of the absorption features. Errors are shown in the parenthesis.

λ (μm)	Feature	ν cm^{-1}	$FWHM$ cm^{-1}	τ^{a}
2.70	$\nu_1 + \nu_3$	3707.8 (0.5)	4 (1)	0.076
2.78	$2\nu_2 + \nu_3$	3600.3 (1.15)	5 (1.5)	0.026
2.73		3660.5 (3)	10 (1.5)	0.014

[a] Error on τ is 0.007.

4. Identification of CO_2 combination modes

The 2.70 and 2.78 μm bands seen in the astronomical observations match the $\nu_1 + \nu_3$ and $2\nu_2 + \nu_3$ combination bands of CO_2, measured in the laboratory. These bands have been studied in detail by Sandford & Allamandola (1990) and Ehrenfreund et al. (1997) in various ice mixtures at different temperatures. The $2\nu_2 + \nu_3$ combination mode has a similar behaviour as the $\nu_1 + \nu_3$ mode at 10 K. Astronomical observations indicate the existence of of different types of ices, such as hydrogen-rich (H_2O dominated, polar ices) or hydrogen-poor (apolar ices, as well as thermally processed ices. In pure 10 K CO_2 ice or CO dominant ice mixtures, the peak position of the $\nu_1 + \nu_3$ band is centred at higher frequencies and has a slightly narrower width than the observed interstellar feature. When H_2O is added a large broadening and substantial shift to lower frequencies is observed. A slight narrowing, but an even greater shift to lower frequencies, occurs when CH_3OH is added (Boogert et al. 2000). This difference between polar mixtures (H_2O or CH_3OH dominated) and apolar mixtures (e.g. CO dominated) is similar to that observed by Ehrenfreund et al. (1998) and Boogert et al. (2000) for the fundamental $^{12}CO_2$ and $^{13}CO_2$ bands.

After an initial broadening, the widths of both combination bands narrow dramatically with increasing temperature. The CO_2 is then in a segregated, pure CO_2 state (Ehrenfreund et al. 1999; Boogert et al. 2000). A comparison of the interstellar CO_2 combination bands with laboratory CO_2 profiles in different mixtures reveals that both the positions and the widths of the interstellar features can well matched by various mixtures provided that the laboratory ices are heated (Figs. 2a,b,c,d) in order that "segregated boundary phases of pure CO_2" are formed. Thus, the observed interstellar CO_2 combination bands in S 140:IRS1 reflect a pure segregated CO_2 phase. The broader 3660 cm^{-1} (2.73 μm) interstellar feature is not matched by any of the CO_2 laboratory mixtures.

5. Alternative candidates

5.1. Isolated water

Isolated H_2O, in low temperature matrices, has been extensively studied in the laboratory and displays a set of bands between 2.5 and 2.9 μm, with both position and width sensitive to matrix composition and concentration
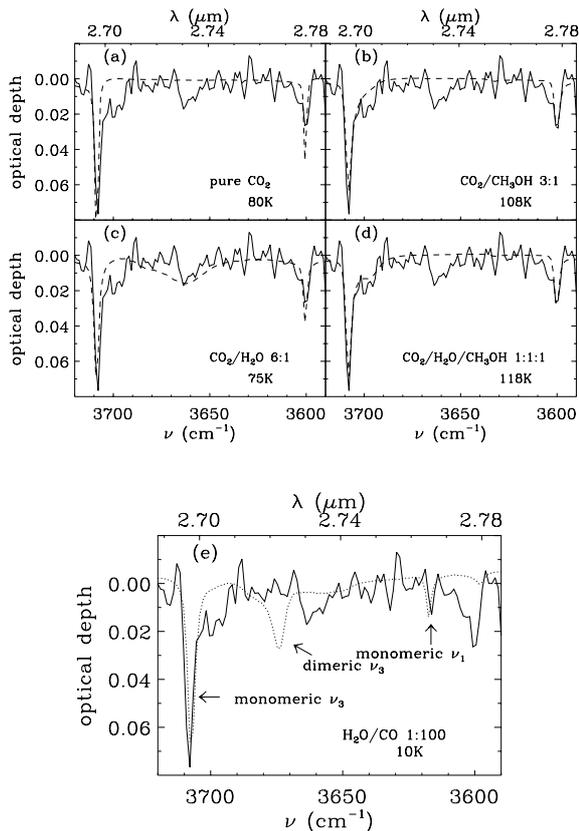
Fig. 2. A comparison of the S 140:IRS1 CO_2 combination modes with various heated laboratory ice spectra **a–d)**. Additionally, isolated H_2O in a CO matrix is compared to the ISO-SWS spectrum **e)**.
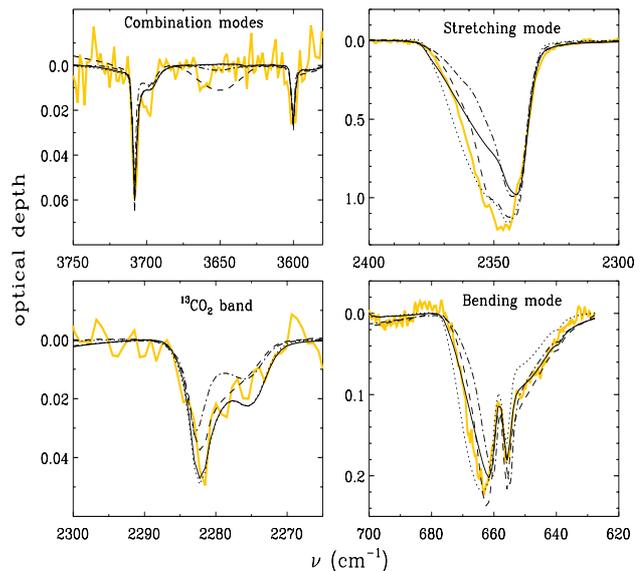

Fig. 3. Simultaneous fits to all the detected solid CO_2 bands toward S 140:IRS1 by different laboratory mixtures. The dot-dashed line denotes a fit based on the observed abundances, the dashed line represents the polar + annealed fit of Gerakines et al. (1999), the solid line denotes the annealed mixture of Boogert et al. (2000), and the dotted line represents the particle shape corrected spectrum of the annealed mixture (see Sect. 6).

(Hagen & Tielens 1981; Ehrenfreund et al. 1996). Monomers and dimers show sharp bands (ν_3 and ν_1) between 3800 cm^{-1} and 3400 cm^{-1}. The position and the width of the interstellar 3700 cm^{-1} feature can be well matched by isolated monomeric H_2O in a CO dominated matrix (Fig. 2e). The ν_1 mode of monomeric H_2O, on the other hand, is at a higher frequency than the interstellar 3600 cm^{-1} feature. An assignment of the 2.70 μm band with monomeric H_2O requires a significant amount of CO (CO/H_2O > 100) but the amount of CO detected along the line sight toward S 140:IRS1 is very small (<1%). Hence, we conclude that the observed interstellar 2.70 μm band is not due to isolated H_2O.

5.2. Dangling OH-groups

Water molecules link to each other in clusters through hydrogen bonds and the last OH group is referred to as a dangling bond. The relative intensity and position of the band depends strongly on the matrix composition (Hagen & Tielens 1981). CO_2 will act as a weak base resulting in a broad, weak OH-stretching band lying between 3700 cm^{-1} and the main OH-stretching band of completely bonded H_2O molecules (Hagen et al. 1983). The terminal OH-band may account for the interstellar "3660 cm^{-1}" feature (if it is real).

6. Discussion

Extensive analyses of the CO_2 bands toward different lines of sight (Gerakines et al. 1999) yield inconclusive results about the exact composition of ice mantles. In the case of S 140:IRS1, the line of sight is dominated by H_2O and the only other major species present is CO_2 which is 20% relative to H_2O. CH_3OH is a very minor constituent of the ice mantle toward S 140:IRS1 (<3% of H_2O; Allamandola et al. 1992). Furthermore, the lack of volatile species, such as CO, indicate that this line of sight is warm. Fitting the interstellar CO_2 bands by a heated laboratory mixture constrained by the observed H_2O, CO_2, and CH_3OH abundances (Fig. 3; dot-dashed line) reveals that the combination modes are the only bands that are reasonably matched. The spectral signatures of the other CO_2 bands are poorly matched by this mixture and in particular the stretching mode is significantly narrower than the interstellar band. Gerakines et al. (1999) have shown that the CO_2 stretching and bending modes can be well matched by a combination of the heated mixture of H_2O:CO_2:CH_3OH = 1:1:1 and an H_2O:CO_2 = 100:14 polar mixture at 10 K (Fig. 3; dashed line). The CO_2 combination bands are well fitted by this model since the heated component produces a segregated boundary pure CO_2 phase required to match these bands (Sect. 4). However, due to the large contribution by the apolar mixture (50%), a broad feature appears around 3650 cm^{-1} that is not apparent in the interstellar spectrum. Alternatively, Boogert et al. (2000) have shown that the heated H_2O:CO_2:CH_3OH = 1:1:1 mixture alone provides an excellent fit to the CO_2 bending mode (Fig. 3;

solid line). The combination modes and the $^{13}CO_2$ band are also well matched. However, the profile of the CO_2 stretching mode is not as successfully reproduced. One possible reason may be that the absorption profile is very sensitive to the shape and size of the grains. Ehrenfreund et al. (1997) showed that particle shape effects are important for strong transitions and that substantial profile changes occur. Assuming a distribution of ellipsoidally shaped particles and adopting the method of grain shape corrections applied by Ehrenfreund et al. (1997), we find that the blue side of the CO_2 stretching mode is now better fitted (Fig. 3; dotted line). However, there is still considerable uncertainty regarding the optical constants (Barrata et al. 2000) and which type of particles should be used. Due to the inherent weakness of the combination bands and the $^{13}CO_2$ band, they are insensitive to grain shape and hence there are no variations in their spectral profiles.

Two crucial results emerge from fitting the various mixtures to all the solid CO_2 bands observed toward S 140:IRS1. Firstly, the combination modes are only fitted if the various mixtures are heated so that a segregated boundary phase of pure CO_2 is formed. Hence, the CO_2 combination bands are not useful in constraining the ice mantle composition. Secondly, a mixture based on the observed interstellar abundances fails to match the observed solid CO_2 bands. The best fitting mixtures of Gerakines et al. (1999) and Boogert et al. (2000) reveal that the CO_2 bands are only successfully matched by laboratory mixtures that contain significant amounts of CH_3OH which contradict the observations that show CH_3OH is a minor constituent of the ice toward S 140:IRS1. The current laboratory database does not contain a sufficiently extensive range of CH_3OH mixtures and therefore the effects of varying CH_3OH intensities in $H_2O{:}CO_2$ mixtures are not readily assessable. Thus, further laboratory studies of CH_3OH in $H_2O{:}CO_2$ matrices are required.

The CO_2 column density can be determined from the central optical depth and *FWHM*, using the band strength of pure solid CO_2 determined by Gerakines et al. (1995). We find that the column densities derived, from both combination bands, agree with the CO_2 stretching and bending mode column densities (4.2×10^{17} cm^{-2}; Gerakines et al. 1999). This agreement also shows that over this wide wavelength range (2.7–16 μm) the same ice column is probed. Hence, in contrast to previous discussions – which centred on the methanol column density derived from the 3.5 μm and 6.8 μm absorption features (Allamandola et al. 1992) –, radiation transfer effects do not mar the column density derivations, at least for S 140:IRS1.

7. Conclusions

We have presented ISO-SWS observations of the 2–3 μm region toward the embedded object S 140:IRS1. The spectrum shows for the first time two narrow absorption features near 2.7 and 2.77 μm attributed to the combination modes ($\nu_1 + \nu_3$ and $2\nu_2 + \nu_3$) of solid CO_2 ice.

The derived column densities agree with previous estimates derived from the CO_2 stretching and bending modes. The main results presented here show that simultaneous fits to the solid CO_2 stretching, bending, combination and $^{13}CO_2$ bands are achieved using an $H_2O{:}CO_2{:}CH_3OH = 1{:}1{:}1$ laboratory mixture. This illustrates that the relative strengths and profiles of the combination bands are in good agreement with the other CO_2 bands. Applying particle shape corrections significantly improved the fit to the peak of the fundamental CO_2 stretching mode. Furthermore, isolated water can be excluded as a cause of these bands, however multimers near 2.7 μm may be present.

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