TRACING PROTOSTELLAR EVOLUTION BY OBSERVATIONS OF ICES

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Abstract

The energetic phenomena associated with protostars alter the physical and chemical state of the material in the clouds, envelopes, and disks that surround them. In particular, the structure and composition of icy mantles on dust grains can potentially be strongly influenced by processes such as thermal heating, ultraviolet irradiation, cosmic rays, and shocks. In this paper we discuss the evidence for these processes by analyzing observations of ice bands in the infrared spectra of high and low mass protostars. ISO observations have shown that thermal processing, i.e. sublimation and crystallization, of ices plays an important role in the envelopes of high mass protostars. In fact, the ice bands may be used as a tracer of the evolution of the protostar. Toward low mass protostars, the unprecedented sensitivity and spectral resolution of the NIRSPEC spectrometer at the Keck II telescope allow a detailed analysis of ice band profiles. The first observations of ices in circumstellar disks around low mass protostars are discussed. We show that the apolar, volatile, CO ices in the upper layers of the slightly inclined edge-on circumstellar disk of L1489 IRS have evaporated. The energetic formation of new molecules, such as CO_2 and 'XCN', does not occur, however. New insights into the nature of apolar ices are evident from the newly detected band of ^{13}CO. In this paper we also present complementary observations obtained with (sub-)millimeter single dish telescopes and interferometers along the same 'icy' lines of sight. These are essential to characterize the line of sight conditions and determine the location of the ices observed in a pencil absorption beam.

Key words: astrochemistry – infrared: ISM – ISM: molecules – planetary systems: protoplanetary disks – stars: formation

1. Introduction

The condensation of atoms and molecules on grains in cold dense clouds leads to the formation of icy mantles. This is a chemically active process in which new molecules are formed. The type of molecules and the composition of the ice mantles being created depends critically on the composition of the accreting gas (Tielens & Hagen 1982). At high atomic hydrogen abundances, H_2 and H_2O are easily formed. While H_2 is released due to its low binding energy on the grains, H_2O creates an icy mantle, likely mixed with hydrogenated forms of C (e.g. CH_4) and CO (e.g., H_2CO and CH_3OH). At later stages, when the accreting gas is primarily molecular, a mantle of different composition is formed, likely CO– and perhaps N_2– or O_2–rich. Thus, it is not unlikely that during the evolution of the molecular cloud, layers of different composition are being formed on the same grain. Also, the ice composition may depend on the location of the grain within the cloud, as the cloud becomes increasingly more atomic from the inner regions to the outskirts. Movement of grains through such a cloud may also lead to the formation of ice layers of different composition. In general, the different types of ices, CO–rich and H_2O–rich are referred to as "apolar" and "polar" ices due to their different dipole moments, which determines the sublimation temperature (typically 18 K for CO–rich ices, and 90 K for H_2O–rich ices on interstellar time scales; Nakagawa 1980).

Once such an icy grain has been formed, it can be subject to a range of processes that destroy or alter the composition and structure of the ice. Heating of the grains by optical or near infrared light can sublimate the ices, and of course the apolar ices evaporate before the polar ices. Heating can also lead to a rearrangement of the molecules in the ice, i.e. crystallize the deposited amorphous ice and segregate the different molecules within (Blake et al. 1991). This is generally referred to as *thermal* processing of the ices. Higher energy photons (ultraviolet, X ray) and cosmic rays can actually break chemical bonds and

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create radicals which will react and form simple (CO_2, CH_3OH) or more complex species (e.g. polycyclic aromatic hydrocarbons or PAHs; hexamethylene tetramine or HMT; OCN^-; Schutte 1999). This is referred to as *energetic* processing of the ices.

It is expected that as a grain with an icy mantle migrates from a dense molecular cloud to a protostellar envelope and circumstellar disk and finally is incorporated in a comet or a planetesimal, it is affected by at least some and perhaps all of these processes. Which processes are most important is still largely unknown and thus the question as to whether the pristine ices of dense molecular clouds are included mostly unaltered or heavily processed before ending up in present day solar system ices is as yet unanswered.

We will discuss the observational signatures of ice processing that have been found toward well studied high mass protostars in §2. In §3 we will present observations of ices in low mass protostars, and in particular address the location of ices along the line of sight. In §4 we focus on observations of ices in disks of low mass protostars and we address the question as to whether the ices in disks show signs of processing. Finally, in §5 we present the discovery of a new molecule in the ices, ^{13}CO, and show that its absorption band significantly constrains the composition of apolar CO ices. Directions for future work are discussed in §6.

2. Ice Processing Massive Protostars

There is a fair amount of observational evidence that massive protostars process the ices in their envelopes. Sharp features were observed in the 3.0 μm H_2O ice band toward several massive protostars, indicating ice crystallization (Smith, Sellgren & Tokunaga 1989). Crystallization was also inferred from the $^{12}CO_2$ bending mode at 15 μm (Gerakines et al. 1999), and the $^{13}CO_2$ stretching mode at 4.38 μm (Boogert et al. 2000a). Based on this, an evolutionary sequence has been proposed in which massive protostars progressively thermally process the ices in their envelopes (Fig. 1). This may well occur on a time scale of a few 10^4 years, the typical hot core life time (Boogert et al. 2000a). Such a heating trend is also seen in several other tracers, such as in an increased gas/solid abundance ratio (van Dishoeck et al. 1998), in an increased dust temperature (Boogert et al. 2000a) and in the temperature and density structure of these envelopes (van der Tak et al. 2000). We thus conclude that thermal processing of ices is readily observed toward high mass protostars and in fact the observations of ice bands seems to be a good *tracer* of the evolution of the envelopes of massive protostars.

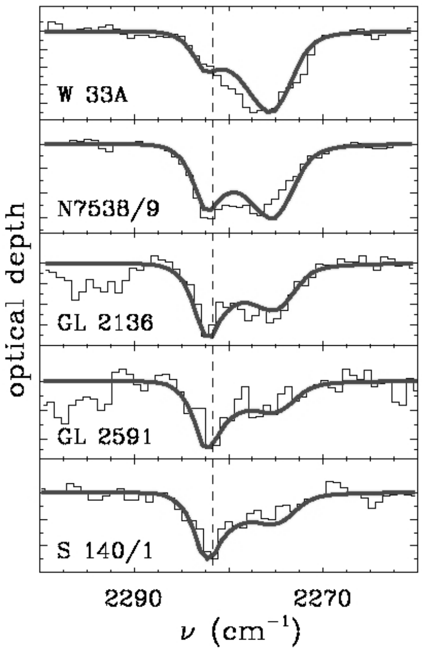

Figure 1. The absorption band of solid $^{13}CO_2$ as a tracer of heating of the envelopes of massive protostars. The thick, smooth lines represent laboratory fits of H_2O, CH_3OH and CO_2 mixed in about equal quantities at temperatures increasing from top to bottom, showing the crystallization effect.

3. Low Mass Protostars: Where are the Ices?

Are the effects of ice processing observed toward high mass protostars important toward low mass protostars as well? Like high mass protostars, the infrared spectra of low mass protostars are often dominated by ice absorption features, as is shown in the ISO/SWS spectrum of Elias 29, a protostar in the ρ Ophiuchi cloud (Fig. 2). The ice bands do not show signs of crystallization and although the solid CO abundance is low, most of the CO is in the apolar phase (Boogert et al. 2000b). Interestingly, abundant warm molecular gas is present in the immediate environment of Elias 29 itself (Boogert et al. 2000b; Ceccarelli et al. 2002). The lack of ice processing can only be properly interpreted if the location of the ices along the pencil absorption line of sight is known. A technique for determining this is illustrated in Fig. 3. Bright $C^{18}O$ 2–1 emission is detection in this line of sight in a 32" single dish beam, at a range of velocities. No emission peak is seen toward Elias 29 however. In contrast, weak

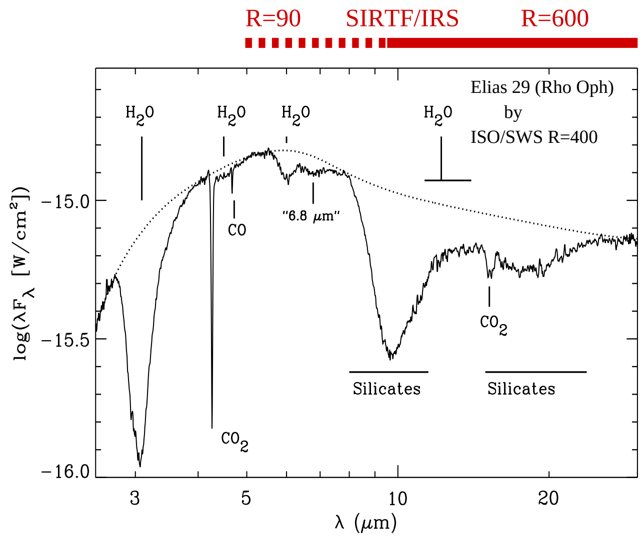

Figure 2. ISO/SWS infrared spectrum of Elias 29, a low mass protostar in the ρ Oph cloud, showing the dominance of ice and dust absorption features. At the top we indicate the wavelength coverage and corresponding resolving power of the IRS spectrometer on board the SIRTF satellite, to be launched in 2003.

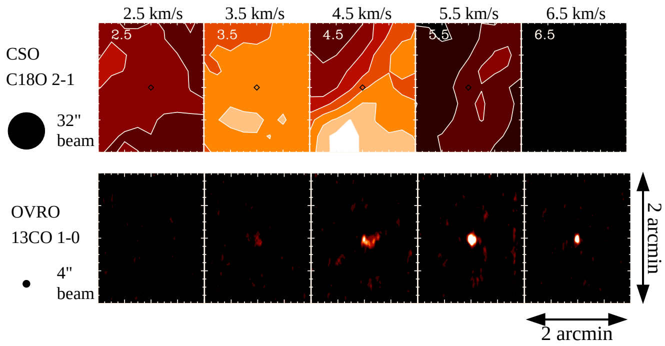

Figure 3. Single dish channel maps of $C^{18}O$ 2-1 emission (top) compared to interferometer ^{13}CO 1-0 emission (bottom) toward Elias 29 in the ρ Oph cloud. Note the larger $v_{\rm LSR}$ velocity of Elias 29 in the interferometer map. Also, corrected for the isotope ratio and beam dilution, the expected signal of Elias 29 in the single dish map is a factor of 60 less than the detected emission of extended foreground clouds.

CO emission is detected on the near infrared position at higher velocities in a 4" interferometer beam. It is concluded that in this particular line of sight, the foreground clouds have a column corresponding to A_V=20 and are responsible for at least 75% of the detected ices (Boogert et al. 2002c). Hence, this line of sight is less suited to study ices in the direct environment of low mass protostars. The situation is however quite different in other lines of sight, as is shown in the next section.

4. Low Mass Protostars: Ices in Disks

A low mass protostar with a well characterized line of sight is L1489 IRS in the Taurus molecular cloud. Millimeter interferometer maps show a large 2000 AU radius flattened structure around this object (Hogerheijde 2001). Detailed models of the velocity structure in combination with continuum maps indicate that this structure is in fact an edge on disk in (almost) Keplerian rotation, but with a noticeable infall component. This is thus a highly interesting target for infrared absorption studies of circumstellar gas and ices. We have obtained high spectral resolution (R=25,000; Δv=12 km s^{-1}) observations in the atmospheric M band of L1489 IRS with the NIRSPEC spectrometer at the Keck II telescope (McLean et al. 1998). The 4.7 μm spectrum shows deep ^{12}CO $v = 1{-}0$ ro-vibrational absorption lines with extensive red shifted wings, up to 100 km s^{-1}, confirming the infalling nature of this edge-on disk. The same 4.7 μm Keck/NIRSPEC spectrum also shows a prominent absorption band of solid CO (Fig. 4a). This is a rare case in which ices in a protostellar disk can be directly seen [1]. Other claims for the detection of ices in edge on disks have been made for Elias 18 (Shuping et al. 2001), RNO 91 (Weintraub et al. 1994), and CRBR 2422.8-3423 (Thi et al. 2002).

4.1. Ice Processing in Disks

The detection of solid CO in the edge-on disk of L1489 IRS allows a direct investigation of the composition and processing history of ices in a protostellar disk. Our approach is a phenomenological one (Boogert et al. 2002a). We compare the CO band profile of L1489 IRS with that observed in a line of sight which is most likely pristine: the massive protostar NGC 7538 : IRS9. This protostar has a cold envelope with unprocessed ices and a modest hot core (Mitchell et al. 1990; van der Tak et al. 2000; Boogert et al. 2000a). In fact, its ice spectrum very much resembles that of background stars tracing quiescent molecular cloud material. Figure 4c shows a comparison of the CO band profiles of L1489 IRS and NGC 7538 : IRS9. Both spectra have a narrow central peak surrounded by blue and red wings. The red wing is the polar ice component (CO mixed with H_2O), the central peak is the apolar component (likely pure CO; see §5), and the newly discovered blue wing may originate in a CO:CO_2 ice. When

[1] Foreground clouds toward L1489 IRS have an extinction of A_V=2 (Hogerheijde 2001) and do not harbor ices.

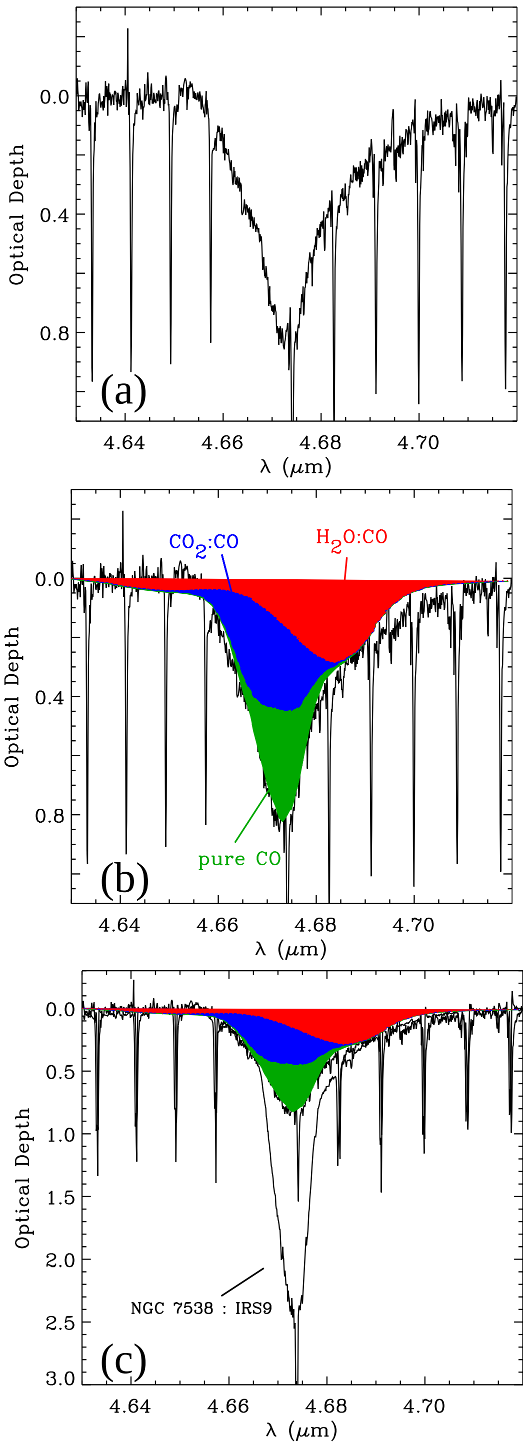

Figure 4. The M band R=25,000 Keck/NIRSPEC spectrum of the low mass protostar L1489 IRS, showing narrow ^{12}*CO absorption lines and a broad multi-component band of solid CO* **(a)**. *Both the gas and ices reside in the edge-on disk of L1489 IRS. The colored surfaces indicate the laboratory fits discussed in the text* **(b)**. *Panel* **(c)** *shows a comparison with the massive protostar NGC 7538 : IRS9.*

both spectra are scaled such that the wings match, it is obvious that the central, apolar peak of L1489 IRS is much less prominent (Fig. 4c). This empirical approach thus leads to the straightforward conclusion that the ices in the L1489 IRS disk are processed in the sense that the most volatile ices have evaporated. At first blush, this is consistent with Hubble Space Telescope images, which indicate a non-negligible disk inclination (0-30° with 0° being edge-on). The pencil absorption beam therefore traces warm upper disk layers where the most volatile ices have evaporated.

Are there, besides evaporation, other processing mechanisms at work in the upper disk layers? If the ices are hit by energetic photons or cosmic rays, it is expected that new molecules such as CO_2 are efficiently formed (e.g. Gerakines, Schutte & Ehrenfreund 1996). This would give rise to a significant broadening of the central absorption band profile. Such broadening is not observed. At high CO_2/CO mixing ratios, a shift to shorter wavelengths is expected. However, the column density of the CO responsible for the blue shoulder, normalized to the H_2O ice column, is the same in both sources (∼3%). Hence, in the upper disk layers traced in the L1489 IRS line of sight no energetic formation of CO_2 has occurred. Similarly, the 'XCN' band at 4.62 μm, often thought to be an indicator of energetic processing, is not detected in this line of sight (Chiar et al. 1998). To conclude, in the upper layers of the disk around L1489 IRS thermal processing (sublimation) of the most volatile, apolar, CO–rich ices has taken place, but energetic processing has not. Perhaps the line of sight traces the upper layers of the *outer* flaring disk and the radiation field is soft.

5. Detection of Solid ^{13}CO

Determining the origin of the ^{12}CO absorption band is complicated by the interaction of light with the interstellar grains. Polarization of the molecular dipoles induces a grain surface charge, which resonates with the dipoles themselves and can lead to large shifts of the peak absorption wavelength and to a broader profile. This effect is largest at large dipole concentrations, i.e. for pure ices. The central feature of the ^{12}CO band may well result from a pure CO ice, and thus grain shape effects lead to an ambiguouity in detailed fits to this band. However, ^{13}CO molecules are always diluted in a ^{12}CO mixture and thus the absorption band of ^{13}CO is not influenced by the particle shape. Therefore, in principle it is a better tracer of the composition of interstellar CO ices.

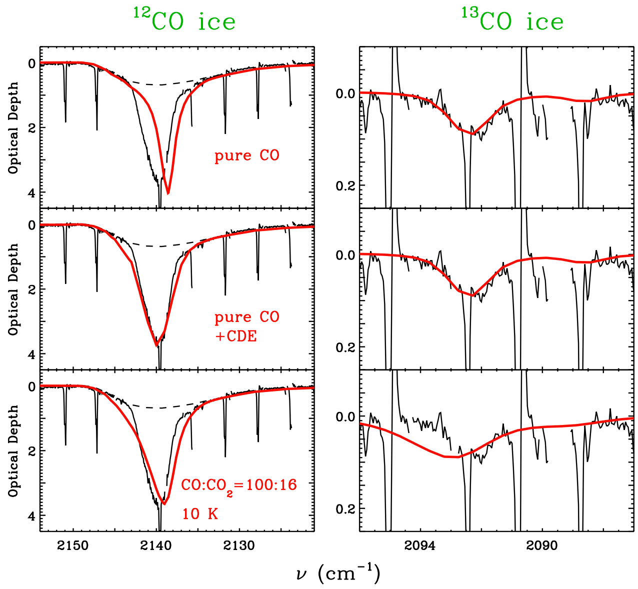

Figure 5. Detection of solid ^{13}CO *toward NGC 7538 : IRS9 (right panels). The left panel shows the* ^{12}CO *band. From top to bottom different laboratory fits are shown: pure CO, pure CO on ellipsoidal grains, and a CO:CO*$_2$ *mixture*

We accordingly observed the ^{13}CO stretching mode at 4.78 μm in the massive protostar NGC 7538 : IRS9 with Keck/NIRSPEC (Boogert et al. 2002a). The discovery of this band is shown in Fig. 5. As can be seen, the high spectral resolution of R=25,000 is crucial in order to separate the ^{13}CO ice band from narrow ^{12}CO and ^{13}CO emission and absorption lines along the line of sight as well as telluric absorption lines.

5.1. New Clues to the Nature of Apolar Ices

We use laboratory simulations to confine the composition of interstellar ices (Fig. 5). The interstellar ^{13}CO band is remarkably narrow (1.50 cm^{-1}). In fact, it is narrower than the ^{13}CO band in most available laboratory mixtures. Best fits are obtained by pure CO ices. Slightly worse, but still reasonable fits are also obtained by mixtures of CO with N_2. CO:O_2 mixtures only give good fits when they are heated, which may not be reasonable given the large apolar ice abundance in this line of sight. Interestingly, small contaminations with CO_2 broaden the ^{13}CO band so much that CO:CO_2 mixtures can be entirely excluded as the carrier of the prominent narrow central peak of the interstellar CO band (Fig. 5, bottom panels). Finally, as mentioned above, simultaneous fits of the ^{12}CO and ^{13}CO bands indicate the importance of grain shape corrections for the ^{12}CO band. While a pure CO ice matches the ^{13}CO band, it completely mismatches the ^{12}CO band (Fig. 5, top panels), unless we assume the ice mantles are on ellipsoidal grains (Fig. 5, middle panels). A model with a continuous distribution of ellipsoidal shapes, simulating irregularly shaped grains, gives the best fit to the ^{12}CO band. Interestingly, the $^{12}CO_2$ bending mode at 15 μm is matched by the same grain shape model!

6. Conclusions and Future Work

We have shown that the shapes of interstellar ice bands are modified by the influence of protostars. For massive protostars, the heating of envelopes is reflected in increased crystallization of the CO_2 bands. For low mass protostars it is crucial to study the line of sight conditions in order to interprete the ice bands. Much work still needs to be done in this area. In some detail we analyze the line of sight of the low mass protostar L1489 IRS. This source is surrounded by a 2000 AU radius edge on disk, through which we see the gas and ices in absorption in high resolution 4.7 μm Keck/NIRSPEC spectra. We empirically determine that the most volatile CO ices (apolar component) in this disk are largely evaporated. This is attributed to the fact that the disk is inclined (by at most 30°) and that the absorption line of sight traces the warm disk upper layers. In contrast, no energetic processing is seen, i.e. no CO_2 or XCN species have been formed. Clearly, the importance of processing and general interpretation of the solid CO band must be tested against a larger sample of protostars. This is now possible with the availability of high resolution M band spectrometers on large telescopes (Pontoppidan, this volume). An independent view on the ice processing history of low mass protostars (and thus on the link between protostellar and solar system ices) will be provided by observations of the sensitive CO_2 bending mode for a complete sample of low mass protostars with the IRS spectrometer on board the SIRTF satellite. Finally, we report the first detection of the absorption band of solid ^{13}CO toward the massive protostar NGC 7538 : IRS9. This offers a new view on the nature of apolar ices. It is concluded that apolar ices are likely purely CO, although CO:N_2 mixtures cannot be excluded, on top of ellipsoidally or irregularly shaped grains. Mixtures of CO with CO_2 can be excluded with a high degree of confidence. As is true above, more lines of sight need to be studied in the sensitive band of ^{13}CO. High spectral resolution spectrometers at large telescopes will allow us to do so.

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