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An ISO SWS view of interstellar ices – First results*

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Abstract. The availability of SWS data from the Infrared Space Observatory is a landmark in the study of interstellar ices. This paper presents a brief review of what was known prior to the launch of ISO, and attempts a synthesis of what has been learned from the ISO observations available to date. Key areas of uncertainty are identified to provide a basis for future research.

Key words: ISM: molecules – dust, extinction – Infrared: interstellar: lines – Stars: pre-main sequence

1. Background

The existence of interstellar ices was first proposed many years ago by Lindblad (1935), but observational confirmation had to await the availability of infrared spectrometers on ground-based and airborne telescopes some four decades later. Earliest observations, of the strong vibrational resonance of H_2O at a wavelength of $3\,\mu$m, showed that water-ice is not in fact a major constituent of dust in *diffuse* regions of the interstellar medium (Knacke et al. 1969; Gillett et al. 1975), where grains appear to be composed of more robust materials such as silicates and refractory carbon. H_2O and other molecular ices naturally require a shielded environment in which to accumulate and survive, presumably as mantles on refractory cores. The ubiquity of ices in molecular clouds was subsequently confirmed by a wealth of ground-based observations over the past 20 years (e.g. Merrill et al. 1976; Willner et al. 1982; Whittet et al. 1983; Lacy et al. 1984; see Schutte 1996 and Whittet 1993, 1996 for reviews and further references).

Of particular interest to astrochemistry is the presence of carbon-bearing species in the ices. Those detected to date include CO, CH_3OH and CH_4. Being much more volatile than H_2O, CO, in particular, probes ice properties in more shielded regions of molecular clouds. The sensitivity of CO to its molecular environment within the ice mantles provides an important diagnostic of the nature and evolution of grain mantles in the densest regions. Studies of the CO feature at $4.67\,\mu$m support the existence of distinct polar (H_2O-rich) and non-polar (H_2O-poor) layers in the mantles (Tielens et al. 1991; Chiar et al. 1995), thought to form under different physical conditions distinguished by the presence or absence of atomic hydrogen in the gas. Other spectral signatures have potential for study of grain processing in regions of active star formation. When a simple ice mixture containing molecules such as H_2O, NH_3 and CO becomes irradiated, radicals are produced which may recombine to form more complex species. Examples of likely photoproducts include CO_2, H_2CO and CN-bearing compounds (Lacy et al. 1984; d'Hendecourt et al. 1986; Sandford et al. 1988). The $4.62\,\mu$m feature detected in several embedded sources is attributed to C≡N bonds in a nitrile or isonitrile ('XCN') formed by photoprocessing of nitrogenous ices. However, several other potentially abundant primary or product molecules are not available to ground-based observation.

The availability of a grating-resolution instrument in space represents an advance in our spectroscopic capability at least as significant as that which occurred when such instruments were first used on ground-based telescopes more than two decades ago. The short wavelength spectrometer (SWS) of the Infrared Space Observatory (ISO; Kessler et al. 1996) is already providing a wealth of important new results and detections. In the following sections we attempt to give a synthesis of these first results.

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* Based on observations with ISO, an ESA project with instruments funded by ESA Member States (especially the PI countries France, Germany, the Netherlands and the United Kingdom) and with the participation of ISAS and NASA.

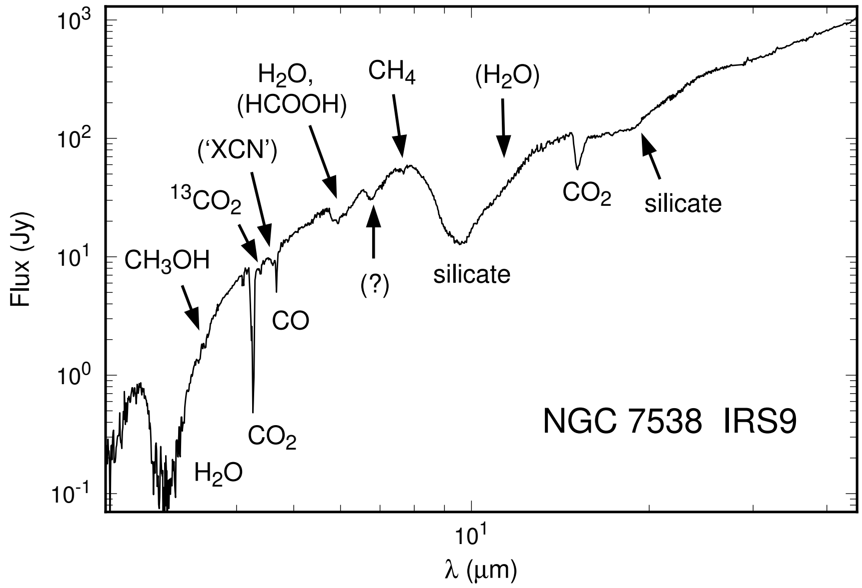

Fig. 1. SWS spectrum of NGC 7538 IRS9, covering the full SWS spectral range from 2.4 to 45 μm at a resolving power of $\sim$ 500. Various solid state absorption features discussed in the text are labelled. Unless otherwise noted, these are reliable detections (uncertain or ambiguous assignations are in brackets).

2. An inventory of ices towards NGC 7538 IRS9

NGC 7538 IRS9 has the richest solid state infrared spectrum of all sources with extensive ISO SWS data available at the time of writing. The spectrum illustrated in Fig. 1 covers the full spectral range available with the SWS (2.4–45 μm). This was obtained in template mode AOT01 (speed 2) at a resolving power of $\lambda/\Delta\lambda \sim 250$. The instrument and reduction techniques are described by de Graauw et al. (1996a). Solid state features of silicates and various molecular ices are labelled in Fig. 1. Note that, although good for qualitative overview of the entire spectrum, the AOT01 observations are of insufficient resolution and reliability for detailed quantitative analysis of the absorption profiles in this spectrum. At present, the effects of detector hysteresis at the rapid scanning speed of this SWS observing mode on the observed spectrum are not well known. More reliable and higher resolution observations of NGC 7538 IRS9 (SWS mode AOT06) for selected spectral regions are reported elsewhere in this volume (Boogert et al. 1996; de Graauw et al. 1996b; Schutte et al. 1996; van Dishoeck et al. 1996). Where available, we prefer to make use of AOT06 observations for detailed quantitative work.

The most striking aspect of the spectrum in Fig. 1 is its apparent simplicity. Besides the strong 9.7 μm silicate feature, it is dominated by the 3.0 μm H_2O stretching mode. The absence of other strong features suggests that H_2O is the dominant component of interstellar ices. Table 1 presents a compilation of column densities and relative abundances for various species detected towards NGC 7538 IRS9 (in some cases making use of ground-based as well as ISO data). The most important trace species detected are CO_2 (15%) and CO (12%). Note that profile fitting procedures allow separate determination of CO and CO_2 column densities in polar and nonpolar components of the ices. CO and CO_2 are more abundant in nonpolar and polar ices, respectively. CH_3OH, CH_4, 'XCN' and (tentatively) HCOOH also appear to be present at levels of a few percent relative to H_2O.

Potentially important molecules missing from Table 1 include NH_3, O_2 and N_2. Low flux levels preclude a search for the 2.96 μm N–H stretching mode of NH_3 in NGC 7538 IRS9; non-detections in several other sources suggest that its abundance is typically no more than a few percent (Smith et al. 1989; Whittet et al. 1996). O_2 and N_2 have only weakly allowed infrared absorption features (Ehrenfreund et al. 1992), both of which fall in difficult regions of the spectrum for detection due to blending with much stronger features. The presence of these important molecules can therefore be inferred only indirectly, as matrix constituents influencing the profiles of the CO and CO_2 bands, or via detection of their photolysis products.

Another important species that cannot be included in our inventory is the unknown carrier of the 6.8 μm feature (Fig. 1). In view of its strength (comparable with the H_2O bending mode), this species seems likely to be reasonably abundant. The most straightforward interpretation, in terms of the $-CH_3$ deformation mode of CH_3OH (Tielens et al. 1984), is untenable in view of the weakness of other methanol features (Grim et al. 1991). Presently,

Table 1. Column densities and relative abundances of species detected in ices towards NGC 7538 IRS9.

Species	Feature (μm)	N ($10^{17}\,cm^{-2}$)	Abundance (% H_2O)	Notes
H_2O	3.0, 6.0	80	100	1, 2
CH_3OH	3.53	3–9	4–12	3
CH_4	7.67	1.3	2	4
CO polar	4.67	3.2	4	5
CO apolar	4.67	6.4	8	5
CO_2 polar	15.3	7.3	9	6
CO_2 apolar	15.3	4.6	6	6
XCN	4.62	(1.5)	2	7
HCOOH	5.83	(2.4)	3	2, 8

Notes: [1] Willner et al. (1982). [2] Schutte et al. (1996). [3] Uncertainties due to assumed continuum and matrix composition; Allamandola et al. (1992); Chiar et al. (1996). [4] Boogert et al. (1996). [5] Tielens et al. (1991). [6] de Graauw et al. (1996b). [7] Lacy et al. (1984); Tegler et al. (1995); assumed band strength.
[8] Tentative identification.

Table 2. Relative abundances of ices in the ISM, compared with typical cometary values (Mumma et al. 1993, 1996). Data for Elias 16 are from Chiar et al. (1995, 1996). The XCN result for GL 2136 is based on data from Geballe (1986); all other data for NGC 7538 IRS9, GL 2136 and W33A are from references listed in Table 1. The H_2O abundance for W33A was estimated from the 6.0 μm feature only as the 3.0 μm feature is saturated.

Species	Elias 16	N7538	GL2136	W33A	Comet
H_2O	100	100	100	100	100
CH_3OH	<3	4–12	4	5–9	0.3–5
CH_4	—	2	—	0.4	0.2–1.2
CO polar	3	4	3	0.7	—
CO apolar	22	8	—	0.3	—
CO total	25	12	3	1	5–7
CO_2 polar	—	9	7	—	—
CO_2 apolar	—	6	5	—	—
CO_2 total	—	15	12	—	3
XCN	<2	2	<1	2	—

no other satisfactory candidate has been suggested (see Schutte et al. 1996 for further discussion).

3. Comparison with other lines of sight

Table 2 compares abundances in NGC 7538 IRS9, two other dust-embedded young stellar objects (GL 2136 and W33A), and a background field star (Elias 16) sampling material in the Taurus dark cloud. Data for these 'interstellar' lines of sight are compared with typical values measured in comets, all results being expressed as percentage by number relative to H_2O.

Considering first the interstellar sources, it is striking that the abundance of nonpolar CO is much less stable than that of other species, as expected in view of its volatility. Sources are listed in sequence of decreasing CO abundance, which seems likely to represent a sequence of increasing thermal processing of the ices (see Smith et al. 1989). The ices towards Elias 16 are assumed to be remote from any embedded source, whereas a large fraction of those towards GL 2136 and W33A may reside in relatively warm gas close to the sources themselves (see Mitchell et al. 1990). NGC 7538 IRS9 appears to represent an intermediate case between these extremes, with both pristine and thermally processed ices existing somewhere in the line of sight.

In contrast to CO, the abundance of solid CO_2 in the ISM appears to be relatively stable. Five objects discussed by de Graauw et al. (1996b) have CO_2/H_2O ratios in the range 12–16%. An important issue is whether CO_2 forms primarily by grain surface reactions or by energetic processing of ices containing CO (Grim & d'Hendecourt 1986). If energetic processing is the primary source, we have to assume similar degrees of irradiation in diverse lines of sight. If surface reactions dominate, then CO_2 may be ubiquitous. An observational test would be to investigate whether CO_2 can be detected in shielded regions deep within dark clouds. No ISO data yet exist for Elias 16 which might enable us to answer this question directly. Indirect observational evidence for an *absence* of CO_2 is provided by fits to the 4.67 μm CO profile: whereas good matches are found with laboratory CO:CO_2 mixtures in some embedded objects, Elias 16 and other field star studied to date are best fit with mixtures lacking CO_2 (Chiar et al. 1995 and in preparation). On the other hand, the presence of CO_2 absorption in clouds obscuring the Galactic Center (de Graauw et al. 1996b) and in the field star Elias 43 behind the ρ Oph dark cloud (Boogert et al., in preparation) are suggestive that CO_2 is a widespread component of molecular clouds, not limited to the environs of embedded stars. We note, however, that physical conditions in the molecular clouds obscuring the Galactic Center are not well constrained, and that the ρ Oph cloud is subject to a relatively high local radiation field due to the close proximity of an OB association.

The results in Table 2 show that cometary and interstellar abundances are comparable for CH_3OH and CH_4, whilst the cometary CO abundance is within the range of interstellar values. A surprise is the rather low apparent abundance of CO_2 in comets. If comets are composed primarily of ices from the parent molecular cloud, subject to some modest degree of processing in the solar nebula (e.g. Greenberg & Hage 1990), one would expect the CO_2 abundance in comets to be at least as high as in the ISM.

4. Future research

The SWS on ISO promises to advance observational studies of interstellar ices to a much greater degree than was previously possible using ground-based and airborne facilities alone. Within two years, we can expect to have ~ 25 complete 2–45 μm spectra of embedded protostars and background field stars, and an even larger number of spectra covering selected features such as those of CO_2. This will allow us to address some of the most fundamental questions of astrochemistry. Of foremost importance is a census of the volatile inventory of interstellar ices, in particular of the carbon bearing molecules. Given the possible interrelationship of interstellar and cometary ices, this has direct bearing on the volatile and organic inventory of the planets, including the Earth. Such a sample of spectra will allow us probe the formation and evolution of interstellar ices in great detail. Striking among these early results is the presence of various carbon-bearing molecules at different stages of oxidation (i.e., CO, CO_2, CH_3OH, CH_4) at comparable abundances. This strongly suggests the presence of oxidizing and hydrogenating agents in the accreting gas (i.e., atomic H and O). A key question is how the composition of the ices is influenced by low and high mass star formation. Future progress will lead to a much better understanding of the relative roles of grain surface chemistry, thermal sublimation and UV photolysis. Finally, although present studies are concerned primarily with the strongest features, deeper searches for absorption signatures of minor components will also be valuable. Among the "missing" species is the major reservoir of nitrogen. Careful analysis of CO and CO_2 band profiles might reveal the presence of N_2 in the ices. Other species we might reasonably expect to discover in the near future are HCN, C_2H_2, H_2O_2, O_3, HOCN, HNCO, H_2CO_3 and N_2H_4, all of which have absorption features accessible to ISO.

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