SCIENTIFIC DRIVERS FOR FUTURE HIGH-RESOLUTION FAR-INFRARED SPECTROSCOPY IN SPACE

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ABSTRACT

The principal scientific drivers for high resolution spectroscopy in space at submillimeter and far–infrared wavelengths are briefly reviewed. The main focus is on the physics and chemistry of the various phases of the stellar–interstellar lifecycle, ranging from diffuse interstellar gas to dense star–forming regions, circumstellar envelopes of late–type stars, supernova remnants and comets. The importance of space observations of the H_2O, O_2 and HD molecules will be illustrated in the context of recent ground–based, airborne and ISO results. Desired instrumental features will be addressed.

Keywords: ISM: clouds; ISM: molecules; ISM: abundances; Stars: AGB; Comets

1. INTRODUCTION

It is well known that the far–infrared and submillimeter part of the spectrum contains key information concerning the birth and death of stars and the evolution of galaxies. These are among the most fundamental problems in astrophysics, and worthy of the best available instrumentation. Interstellar and circumstellar atoms and molecules emit hundreds of (unique) lines in this wavelength region, whereas thermal emission from cool dust (T=10–100 K) is the dominant contributor to the continuum emission. In the submillimeter region, one can probe deep into the cocoons of gas and dust surrounding stars in the earliest as well as the last phases of their life, into the dusty tori surrounding active galactic nuclei, and into high redshift galaxies undergoing their first burst of star formation. Because the Earth's atmosphere blocks observations from ground–based telescopes at wavelengths shorter than 350 μm, airborne and space–based observatories are essential to address these scientific questions directly.

The principle scientific drivers for high–spectral resolution spectroscopy lie in our quest for understanding the stellar/interstellar lifecycle in our own Galaxy (see Figure 1). Stars are formed by fragmentation and collapse of interstellar clouds. They interact with their surroundings by emitting ultraviolet photons which ionize, dissociate and heat the nearby interstellar gas. Many low– and intermediate–mass young stellar objects are known to be surrounded by dense circumstellar matter from which planetary systems like our own may form. At the end of their life, stars return a significant fraction of their material to the interstellar medium, either explosively through supernovae or more gradually through stellar winds. Thus, the interstellar medium is continuously enriched with heavy elements synthesized by nuclear reactions during the stars' main–sequence lifetimes, and with silicate cores and carbon–rich compounds formed in the dense envelopes surrounding AGB stars. With high–resolution far–infrared spectroscopy, nearly all phases and virtually all major components of this lifecycle can be probed. A thorough knowlegde of these processes in our own Galaxy is a prerequisite for understanding galaxy– and star–formation at high redshifts.

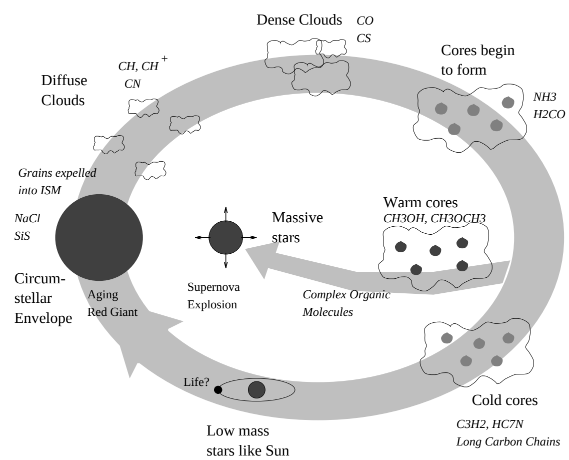

Figure 1: *Schematic illustration how molecules and dust grains cycle from circumstellar envelopes of dying stars through various phases of interstellar matter to the formation of new stars. High–resolution spectroscopic observations with space–based platforms will be able to provide new information on virtually all phases of this cycle (based on Verschuur 1992).*

There have been many excellent recent summaries of the scientific questions to be addressed with far–infrared spectroscopy (see, for example, the 1990 Liège Symposium 'From Ground–Based to Space–Borne Sub-mm Astronomy (ESA SP–314), and the FIRST Report (1993, ESA SCI(93)6) and references cited). This brief review will focus on a few scientific highlights in Galactic research and will summarize some recent observational developments in these areas. The extragalactic scientific drivers have been discussed by Puget at this conference.

2. COMPLETE SPECTRAL LINE SURVEYS

An important advantage of a space mission such as FIRST over ground–based or even airborne observatories is its complete spectral coverage over a wide wavelength range, unhindered by the atmosphere. Complete spectral surveys in the 100-500 μm range should allow an unbiased census of the principal atoms and molecules in the diffuse interstellar gas, dense molecular clouds, photon–dominated regions, hot cores, AGB envelopes, planetary nebulae and supernova remnants. The advantages of complete spectral surveys compared wuth more limited spectral coverage include: (i) direct information on the abundances and distribution of all the principal carbon– (C^+, C, CO) and oxygen– (O, O_2 H_2O) containing species, as well as atomic nitrogen; (ii) constraints on the physical parameters of the region, such as the temperature and density structure, from the observed excitation of the atoms and molecules; (iii) accurate abundance determinations because usually multiple lines for each species and its isotopes are covered and because more accurate relative calibration can be achieved; (iv) direct measurement of the contribution of the lines to the broad–band continuum, which can affect the determination of the dust parameters; (v) information on the total cooling rate of the gas; (vi) more detailed probes of the dynamical processes such as shocks and turbulence by comparing the lineshapes of species with different excitation and chemistry; and (vii) opportunities for unexpected discoveries of new species.

Several line surveys have been performed from the ground in the last 15 years in the 100, 230 and 345 atmospheric windows, and most recently in the 650 GHz window (Harris et al. 1995, Schilke et al. 1997). Most of them have focussed on chemically-rich objects such as the massive star–forming regions Orion/KL (e.g., Blake et al. 1987, Sutton et al. 1995, Schilke et al. 1996) and SgrB2 (e.g., Turner 1991, Sutton et al. 1991), and the carbon–rich AGB star IRC 10216 (e.g., Groesbeck et al. 1994). Together they form a great testimony to the enormous technical advances in the sensitivity of high–frequency submillimeter SIS receivers and the improvements of the quality of submillimeter telescopes in the last few years.

What has been learned from these surveys? First, it is found that for spectroscopically rich objects such as Orion/KL, the lines can contribute up to 50% of

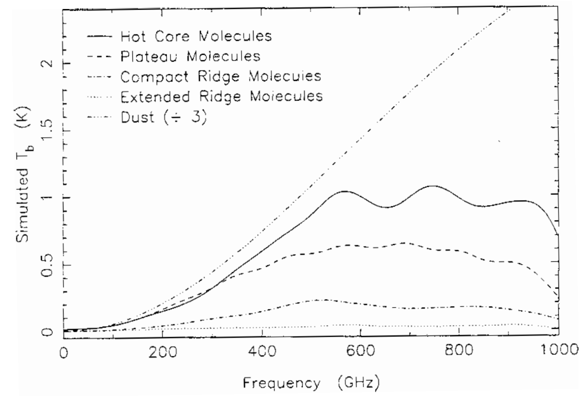

Figure 2: *Simulated line spectra for the different components of Orion–KL smoothed to 100 GHz resolution together with a model dust spectrum assuming an emissivity index of 2.0, a temperature of 200 K, and an optical depth of unity at 350 μm. The dust spectrum has been divided by 3. In the 300–700 GHz range, the summed line emission can contribute up to 50% of the continuum emission (Groesbeck 1994).*

the broadband continuum at 350–650 GHz (Groesbeck 1994). Figure 2 illustrates the line fraction as a function of frequency. However, not all objects show spectra as complex as those of Orion/KL and Sgr B2. In Figure 3, the results of a recent 335–365 GHz survey of three massive star–forming objects in the giant molecular cloud W 3 are presented (Helmich & van Dishoeck 1997). It is clear that large physical and chemical differences occur between the three objects, which can be attributed to different stages in their evolution. During the cold collapse phase, most molecules condense on the surfaces of the grains present in the cloud, where surface reactions modify their composition. When the gas and dust are heated by the radiation from the newly–born star, the molecules start to evaporate back into the gas–phase, probably in a sequence according to their sublimation temperatures. These released molecules drive a rapid, complex organic chemistry, resulting in the "hot core" phase, named after the prototypical Orion/KL hot core region. Shocks associated with the outflow can also return icy grain mantles, as well as destroy some of the refractory material resulting in enhanced emission from sulfur– and silicon–bearing molecules. Finally, after $\sim 10^5$ yr, the chemistry returns to the more quiescent ion–molecule reactions, resulting in a simple spectrum. Thus the chemical composition depends on a delicate interplay between the gas and the grains. Such data also illustrate that most of the diagnostic information lies in the weak lines: surveys need to be sufficiently sensitive to be useful.

The surveys show that often several physical compo-

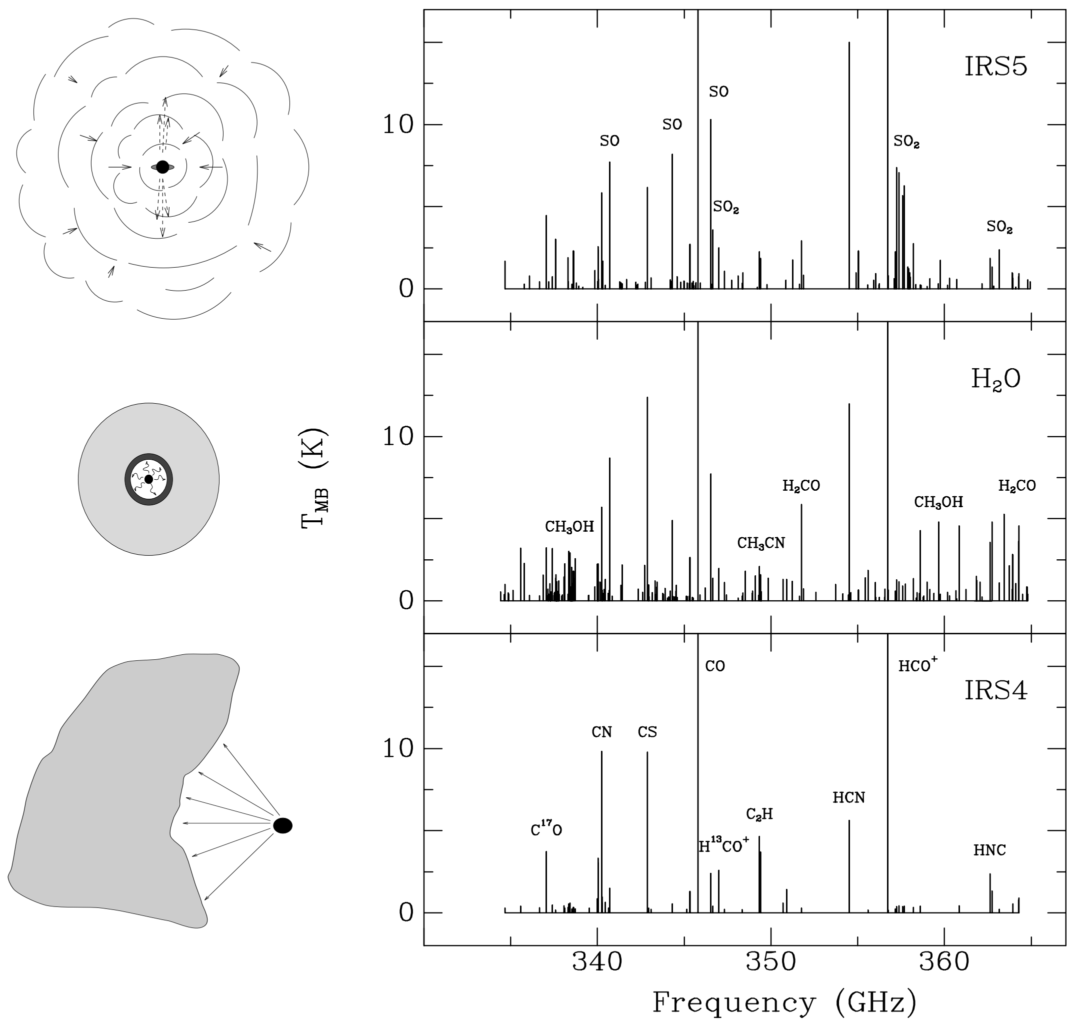

Figure 3: *Summary of the JCMT 335–365 GHz line survey of three massive star–forming regions in the W 3 molecular cloud. The spectra were constructed from the observed line intensities obtained in double–side band mode. About about 90% of this frequency range was covered; the missing 10% was filled in through model excitation calculations, mostly for* SO_2 *and* CH_3OH*. Strong lines in common in the three spectra are labelled in the W 3 IRS4 spectrum only. Large physical and chemical differences are found between the three regions, which are attributed to different evolutionary stages. A possible evolutionary scenario is illustrated by the cartoons: W 3 IRS5 is the youngest object, W 3(*H_2O*) is in the "hot core" phase, and W 3 IRS4 is the oldest object with a well–developed H II region which has broken free of the molecular cloud (based on Helmich & van Dishoeck 1997).*

nents (e.g., hot core, outflow, surrounding cloud) are present in a typical 15–20″ beam. These different physical regimes can sometimes be separated on the basis of line profiles and excitation (Orion/KL: Blake et al. 1987). Recent subarcsec interferometer maps reveal that most of the emission in Orion/KL is concentrated in a 1″ (∼500 AU) region and originates from warm, very dense clumps which are heated and ablated by the nearby massive young star (Blake et al. 1997). A drawback of space–based far-infared observatories is that they will not be able to spatially resolve such structures, even in the nearest star–forming clouds. Wide frequency coverage and high spectral resolution are therefore essential to recover some of this small–scale information indirectly. Finally, the line surveys have stimulated the development of software, which together with line catalogs and a physical model can be used to predict model spectra in frequency ranges which are currently unobservable. Such models need to be tested against higher frequency data and extended to include a full treatment of the radiative transfer and excitation to obtain deeper physical insight.

While ground–based telescopes can probe the spectral characteristics down to 350 μm and airborne platforms such as SOFIA can give an initial impression of the complexity of spectra at shorter wavelengths, only space–based observatories such as FIRST with long, uninterrupted integration times can properly survey the 100–300 μm region. A program covering at least two dozen sources ranging from diffuse gas to old stars should be a major goal of a satellite mission.

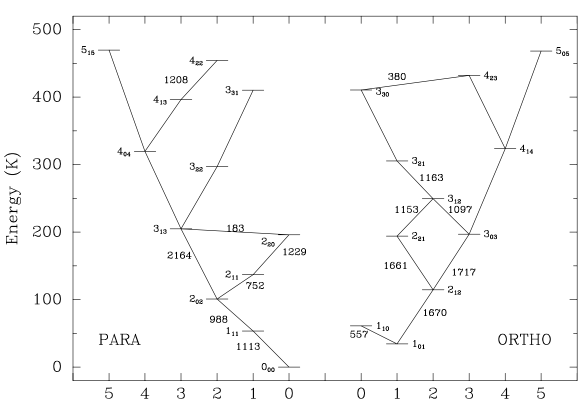

Figure 4: *Energy level diagram of the H_2O molecule. Transition frequencies in GHz are indicated.*

3. H_2O AS A PHYSICAL AND CHEMICAL PROBE

The H_2O molecule plays a very important role in the physics and chemistry of interstellar clouds, oxygen–rich circumstellar shells and solar–system objects such as comets. Because of its complex energy level structure (see Figure 4), it has a large number of lines in the submillimeter and far–infrared wavelength region. The populations of these levels are very sensitive to the physical parameters in the cloud, such as kinetic temperature and density. Moreover, the molecule can be effectively excited by far–infrared radiation due to thermal emission from dust. Thus, the relative strengths of the far–infrared lines should allow detailed information on the physical structure of the region to be extracted. H_2O can also contribute substantially to the cooling of dense, warm molecular gas such as found in shocks and star–forming regions.

On the chemical side, H_2O is thought to form one of the major reservoirs of gas–phase oxygen, together with O_2 and O. Chemical models differ on the relative importance of these species: in some models molecular oxygen O_2 is dominant, in other cases atomic O is most abundant, especially when ultraviolet photons are present, whereas in a third class of high–temperature models most of the oxygen is driven into H_2O. Since none of these species can be observed directly from Earth except under unusual circumstances (masers, rare isotopes, ...), space–based instruments will provide a major advance in this area. Note that because of the high abundances of H_2O and O_2 in the atmosphere, their low–lying lines cannot even be observed from airplane altitudes.

3.1. Recent models

Many models of the abundance and excitation of H_2O in a variety of regions have been developed in the last 20 years at different levels of sophistication (e.g., de Jong 1973, Draine, Roberge & Dalgarno 1983; Neufeld & Melnick 1987, Neufeld 1991). The most recent models for shocks in dense clouds have been developed by Kaufman & Neufeld (1996). Figure 5 shows the predicted spectra of H_2, CO, H_2O and OH for a 40 km s^{-1} C–type shock running into a cloud with a pre–shock density of $\sim 10^5$ cm^{-3}. It is clear that many of the strongest CO and H_2O lines lie in the wavelength region covered by FIRST. The rapid formation of H_2O in warm gas in dense photon–dominated regions (PDRs) close to hot stars such as the Orion Bar has been illustrated, e.g., by Sternberg & Dalgarno (1995). High spectral resolution observations will be important to distinguish the contribution from PDRs and shocks.

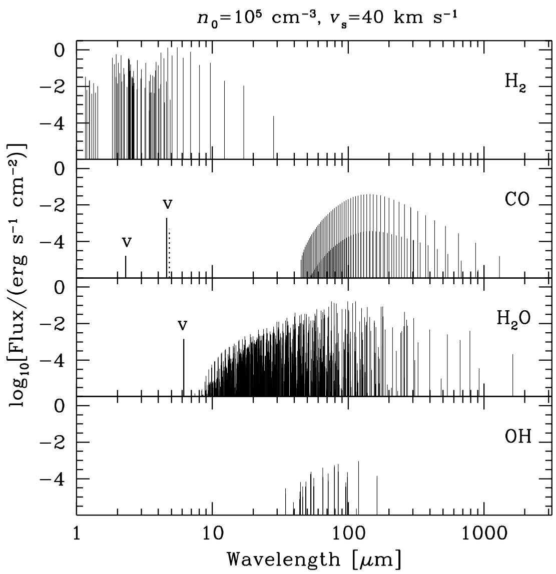

Figure 5: *Line emission from a 40 km* s^{-1} *MHD shock wave propagating in gas with a preshock density of* 10^5 cm^{-3} *(Kaufman & Neufeld 1996).*

Neufeld & Kaufman (1993) and Neufeld et al. (1995) have also assessed the importance of H_2O as a coolant of molecular clouds, and find that it can be dominant at high densities ($> 10^6$ cm^{-3}) and temperatures ($>$ 100 K), if most of the oxygen is in H_2O. Since observations (see below) seem to indicate that on large scales, at most 10–20% of the oxygen is in gas–phase water, its importance as a coolant is diminished. In addition, H_2O can act as a heating agent of the gas, through collisional de–excitation of levels populated by absorption of far–infrared radiation from dust. Until this excitation is better understood, the significance of H_2O as a coolant remains to be determined.

An important class of models for the collapsing envelopes of low mass young stellar objects has recently been developed by Ceccarelli et al. (1996). Early in the evolution (less than 10^5 yr after the onset of collapse), the model temperatures of the gas and dust in the inner ∼500 AU of the envelopes are higher than 100 K, the evaporation temperature of water ice. The release of icy grain mantles increases the gas–phase H_2O abundances by more than two orders of magnitude, resulting in the prediction of strong H_2O far–infrared lines superposed on the continuum (see Figure 6). Whether such lines appear in absorption or emission depends on the detailed geometry of the region.

Finally, updated models of the H_2O emission from circumstellar envelopes have been presented, e.g., by Chen & Neufeld (1995). For all of these models, high spatial and spectral resolution, as well as broad wavelength coverage are essential to properly test them.

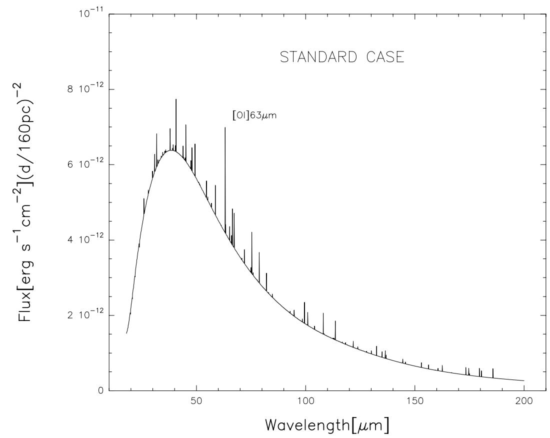

Figure 6: *Line plus continuum spectrum between 20 and 200* μm *of a 1* $M_\odot$ *protostar accreting at* 10^{-5} $M_\odot$ yr^{-1} *at* 10^5 *yr from the start of the collapse, obtained with a resolving power of* 10^4*. Besides the [O I] 63* μm *and some (weak) high level CO transitions, all lines are due to* H_2O *(Ceccarelli et al. 1996).*

3.2. Recent observations

In spite of the difficulties to observe H_2O from the ground or airplane, there have been some important recent observational results which provide the first glimpse of the significance of the H_2O observations. Zmuidzinas et al. (1994, 1996) have detected the $H_2{}^{18}O$ $1_{10} - 1_{01}$ ground–state transition at 547 GHz using an SIS receiver on board the KAO. The line is seen in absorption against the strong dust continuum of SgrB2, and arises in the cooler envelope gas rather than in the hot molecular cores. It implies a relatively low H_2O abundance of only a few $\times 10^{-7}$ relative to H_2. The ground–state line of ortho–H_2O itself at 557 GHz has tentatively been detected in absorption toward Orion by Tauber et al. (1996) using a heterodyne Schottky–diode mixer on a balloon–borne platform. The inferred abundance is again low, of order 10^{-8}. In contrast, higher excitation lines of $H_2^{18}O$ at 203 GHz ($3_{11} - 2_{20}$) and 391 GHz ($4_{14} - 3_{21}$) observed by, e.g., Jacq et al. (1988), Gensheimer et al. (1996) and Zmuidzinas et al. (1996) indicate large H_2O abundances of $\sim 10^{-5}$ in hot core regions with temperatures > 100 K and densities $\geq 10^7$ cm^{-3}, such as present in SgrB2 and Orion/KL. The lack of broad, centrally peaked 557 GHz emission in Orion is consistent with a high abundance and optically thick emission arising from a small region. Cernicharo et al. (1994, 1996) have detected the 183 GHz $3_{13} - 2_{20}$ line from the ground with the IRAM 30m telescope in a number of massive star–forming regions and shocks, but interpretation of the data remains complicated because the line is (at least partly) masing. The same problem affects the submillimeter maser lines seen by Menten et al. (1990, 1995).

The *Infrared Space Observatory* (ISO) is starting to provide useful data on H_2O in a variety of regions, although the resolving power of the spectrometers is limited. Figure 7 shows the spectrum in the 50–200 μm range toward the shock in the Herbig–Haro 54 object obtained by Liseau et al. (1996) with the *Long Wavelength Spectrometer* (LWS). Even at the low resolving power of ~ 200, many strong lines due to CO, H_2O, OH, O and C^+ are seen, illustrating the rich spectral nature of this wavelength region, especially between 150 and 200 μm. The CO lines have been used to constrain the physical characteristics ($T_{\rm kin} \approx 330$ K, $n(H_2) \approx 2 \times 10^5$ cm^{-3}) of the shocked molecular gas. For these parameters, the inferred H_2O abundance is $\sim 10^{-5}$, and the H_2O emission amounts to $\sim 20\%$ of the cooling provided by CO.

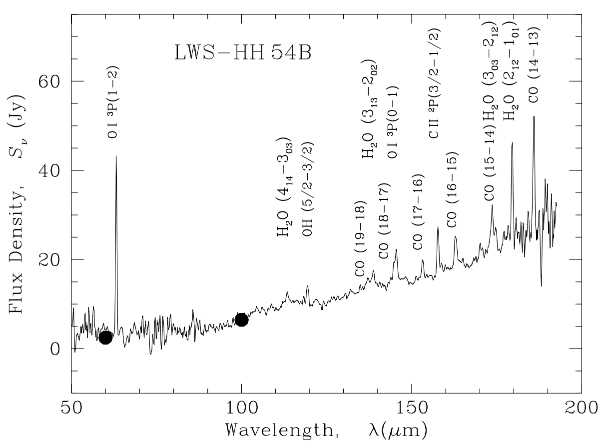

Figure 7: *ISO–LWS far–infrared spectrum toward HH54 showing strong H_2O and CO emission lines from the molecular shock (Liseau et al. 1996).*

H_2O has also been detected in absorption toward embedded infrared sources through its ν_2 bending vibration–rotation lines at 6 μm using the *Short Wavelength Spectrometer* on board ISO (Helmich et al. 1996; van Dishoeck & Helmich 1996). Figure 8 shows the normalized spectra toward four massive young stars obtained with the grating at a resolving power of $\sim$1350. Many lines due to abundant, hot water with excitation temperatures of more than 200 K and abundances of a few $\times 10^{-5}$ are seen for three lines of sight, but not in the colder NGC 7538 IRS9 region. The H_2O abundance appears to correlate with the amount and temperature of warm gas along the line of sight.

The SWS and LWS spectrometers have also detected a veritable forest of H_2O lines in the circumstellar shells of oxygen–rich stars such as W Hya (Neufeld et al. 1996, Barlow et al. 1996), and H_2O has even been identified in the molecular envelope around the planetary nebula NGC 7027 (Liu et al. 1996).

Finally, water is the dominant component of cometary icy mixtures. Because cometary nuclei are thought to have formed in the outer solar system and to have remained at low temperatures during the solar system evolution, they contain the most pristine matter remaining from the collapsing molecular cloud that formed our Sun. Near–infrared vibration–rotation lines of water have been seen in comets Halley and Wilson by Mumma et al. (1987) from the KAO and by Crovisier et al. (1996) in comet Hale-Bopp with ISO. With sufficiently high spectral resolution and S/N, the ortho–para ratio can be derived, which, in turn, provides information on the dust temperature at which the nuclear spins were equilibrated.

In summary, a variety of recent observations of H_2O suggest that the H_2O abundance is low, a few $\times 10^{-7}$ in quiescent clouds, consistent with standard ion–molecule chemistry. In "hot core" and shocked regions, the inferred H_2O abundance is significantly higher, $\sim (1-5) \times 10^{-5}$. Such large H_2O abundances can either be produced by evaporation of icy grain mantles and/or by high–temperature gas–phase reactions. The H_2O is highly excited in these regions and should produce many strong lines in the 100–300 μm region. Limited ground–based mapping of high–excitation H_2O lines (Cernicharo et al. 1994, 1996) or of tracers such as H_3O^+ (Phillips et al. 1992) indicate that the strong thermal H_2O emission arises from very compact regions, $\sim 10''$ or less in Orion.

All of the above mentioned observational techniques suffer from strong limitations. The most important are (i) poor sensitivity, so that the observed lines are often (very) optically thick; (ii) poor spatial resolution: e.g., the ISO–LWS beam is $\sim 80''$; (ii) poor spectral resolution: the highest possible resolution with the LWS is ~ 30 km s^{-1}, so that the line profiles are unresolved. In many cases, the lines are expected to be self–reversed (Betz & Boreiko 1989) so that the integrated intensities are not a good measure of the excitation; (iv) lack of data on the lower excitation lines. As a result, the densest, warmest regions of the interstellar medium with the higher

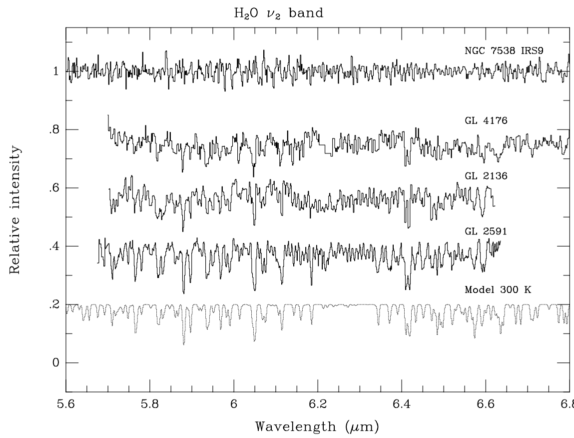

Figure 8: *ISO–SWS normalized spectra of four massive protostellar sources, showing absorption by hot, abundant H_2O. A model H_2O spectrum for a column density of* 2×10^{18} *cm^{-2}, $T_{\rm ex}$=300 K and Doppler parameter b=5 km s^{-1} is shown for comparison (van Dishoeck & Helmich 1996).*

water abundances will mostly be probed by these instruments, but they represent only the "tip of the iceberg". SWAS, ODIN and balloon–borne projects will provide valuable information on the lowest line(s) of H_2O in some regions. However, only FIRST with its high spectral resolution, high sensitivity and broad wavelength coverage will allow the H_2O molecule to be fully developed as a physical and chemical probe of the interstellar, circumstellar and cometary gas.

4. O_2 AND THE GAS-PHASE OXYGEN BUDGET

In contrast with H_2O, the O_2 molecule can be excited at low to moderate densities of $\sim 10^3 - 10^4$ cm^{-3} in interstellar clouds. Most models of the chemistry of quiescent dense clouds predict that O_2 is the major oxygen–bearing species in the gas, together with O. Ground–based searches for O_2 are limited to the $^{16}O^{18}O$ isotopic variety, for which the $2_1 - 0_1$ line at 234 GHz can be observed through the atmosphere. Pagani et al. (1993) have presented a tentative detection of the line in the dark cloud L183, but these observations have not yet been confirmed. The corresponding upper limit is $O_2/H_2 < 10^{-5}$ or O_2/CO<0.07. More sensitive limits of O_2/CO<0.012 have been obtained for external galaxies with sufficiently high velocities to shift the 118 GHz line out of the atmospheric line, but these limits refer to 10 kpc scales (Combes et al. 1991, Liszt 1992).

An independent, elegant method to search for interstellar O_2 is provided by absorption line observations toward bright background quasars. A dense molecular cloud at z=0.69 has been found toward B0218+357 which shows strong $C^{18}O$ absorption. However, a deep search for several O_2 lines has resulted only in upper limits, corresponding to an abundance O_2/CO<0.01 (Combes & Wiklind 1995).

Abundances of O_2 relative to H_2 as low as 10^{-6} form a serious challenge for chemical models, not only with respect to the oxygen chemistry but also regarding that of other carbon– and nitrogen–bearing species since O and O_2 directly affect their abundances.

5. HD AND DEUTERIUM FRACTIONATION

Observations of the HD molecule at 112 μm (2674 GHz) are of cosmological importance to constrain the original amount of deuterium created in the Big Bang and its subsequent destruction in stars. Since HD is expected to contain most of the deuterium in molecular clouds, searches for HD provide one of the most promising methods to determine whether there is a possible deuterium gradient with radius in our Galaxy and in other nearby galaxies. Unfortunately, the molecule is difficult to detect above the dust background because of its small dipole moment. Although ISO may be able to see the line in a few regions, it lacks the spectral resolution to resolve the line. Figure 9 shows the atmospheric transmission at an altitude of 13.7 km in the region around 112 μm, illustrating that the HD line can be sensitively searched for in Galactic regions from airborne platforms such as SOFIA. However, because of many nearby weak atmospheric lines, observations in a wider variety of objects, especially in other galaxies, requires a space observatory such as FIRST.

Figure 9: *Atmospheric transmission in the region around the HD J=1→0 112 μm line at an altitude of 13.7 km (Melnick, private communication).*

Some deuterium will also present as atomic D, and a still unknown fraction may be tied up in other molecules. The large abundances of deuterated molecules such as DCN and DCO^+ have long fascinated astrochemists. Most of the fractionation is thought to derive from reactions at low temperatures with the ions H_2D^+ and CH_2D^+, both of which have their fundamental transitions at submillimeter wavelengths. Thus, these molecules can provide not only information on the deuterium abundance, but also on the temperature history of the cloud. The ground–state line of H_2D^+ at 1374 GHz has possibly been seen in absorption toward Orion IRc2 by Boreiko & Betz (1993) using the KAO. The lowest transitions of a variety of other deuterated hydrides, such as HDO, NH_2D and CH_3D also lie at submillimeter wavelengths. HDO may be particularly interesting, when combined with H_2O observations. The higher excitation $2_{11}-2_{12}$ and $3_{12}-2_{21}$ lines at 241 and 225 GHz have been surveyed from the ground by Jacq et al. (1988, 1990) and Gensheimer et al. (1996). The ground state $1_{01}-0_{00}$ line at 464 GHz lies in a region of good atmospheric transmission and has been detected in Orion (Schulz et al. 1991) and W 3 (Helmich, van Dishoeck & Jansen 1996). Together with the $H_2^{18}O$ observations of Gensheimer et al. (1996), the HDO/H_2O abundance ratio is found to be typically 2×10^{-4} in these "hot core" regions. This is higher than the cosmic abundance ratio [D]/[H]$\approx 1.6\times10^{-5}$, but significantly lower than that of other species such as DCN/HCN.

6. MOLECULAR COMPLEXITY AND SOLID STATE FEATURES

The discovery of small carbonaceous grains and large molecules such as polycyclic aromatic hydrocarbons (PAHs) in interstellar clouds and circumstellar shells has created considerable excitement in recent years (e.g., Tielens 1993). These species typically contain 50 carbon atoms, have large abundances (up to 10^{-6}) and emit characteristic broad vibrational lines at infrared wavelengths. The initial ISO data show that these features are ubiquitous, and the ISO mission will provide important new information on the distribution and variation in composition of these species in different regions (e.g., Verstraete et al. 1996). However, the infrared range is not very specific for characterizing the molecules. The low–lying vibrational modes associated with the bending modes of aromatic rings lie at far–infrared wavelengths and are much more suitable for identification purposes (Zhang et al. 1996). For large PAH's, these modes will blend into a continuum, dust–like opacity, but for smaller PAH's the features are expected to be much narrower and could be picked up against the continuum with high–resolution instrumentation.

The far–infarred spectral region is also very characteristic for lattice vibrations of solids. Very little research has been done on the absorption characteristics of astrophysically relevant mixtures. The peak frequencies and widths of the features are expected to be sensitive to the molecular composition and structure of the mixtures. Even infrared–inactive molecules such as solid N_2 could potentially be observed in this way, thereby providing important information on the nitrogen inventory. Because the features are weak and relatively broad (several cm^{-1}), broad wavelength coverage and good continuum definition are important. This favors a space mission like FIRST over instruments on ground–based telescopes and SOFIA.

7. INSTRUMENTAL RECOMMENDATIONS

Based on the scientific drivers discussed above, the following recommendations for high–resolution instrumentation on space–based observatories such as FIRST can be made.

- The frequency range for the heterodyne instruments should be extended to >1000 GHz to provide good coverage of the multitude of H_2O lines. Useful diagnostic lines of other species such as CO (and isotopes) also lie in this region. A cluster of important H_2O lines is found in the 1000–1250 GHz range, with additional low–lying lines up to 2000 GHz.

- The frequency coverage should be continuous over a large range to conduct line surveys at high frequencies. At ν >1000 GHz, space observations are unique and the spatial resolution is best. Complete spectral coverage also allows the study of H_2O, O_2 and CO lines as functions of redshift.

- Coverage of the low–lying H_2O lines at 557, 752 and 988 GHz and the low–lying O_2 lines at 487 and 773 GHz remains important. A high–resolution channel near the HD 112 μm (2674 GHz) line should be considered.

- High spectral resolution ($\sim$0.5 km s^{-1} or better) is essential to determine the (often complex) line profiles and extract information on the physical and dynamical state of the region.

- Stable and accurate calibration (preferably better than 10%) is required to extract the physical and chemical information from molecular excitation and line surveys.

- Accurate pointing ($\sim$few$''$) is warranted for sideband deconvolution.

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