

SPECTROSCOPY OF KEY MOLECULAR SPECIES IN THE FAR-INFRARED

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ABSTRACT

In this paper we briefly analyze the type of molecular transitions and the contribution of polyatomic molecules to the Far-Infrared spectrum of interstellar and circumstellar clouds. For that aim, we present our recent work on **molecular first Far-IR detections**. All the results presented here were taken in the direction of Sgr B2, close to the Galactic Center. Our study is based on Fabry-Perot observations carried out with the Infrared Space Observatory (ISO) Long Wavelength Spectrometer (LWS). In addition, we report our last Far-IR and millimeter observations of water vapour. This incorporates several thermal ortho/para-H₂O transitions and ground-based observations of the 3₁₃-2₂₀ maser transition at 183.31 GHz. Our first Far-IR identifications include molecules such as NH, NH₂, C₃, H₃O⁺. They mainly represent the whole types of molecular transitions likely to occur in molecular clouds Far-IR spectra. In addition to trace the dense gas with never observed before molecular transitions, this work represents a preparatory study for the spectroscopy programs that could be done with *FIRST* in the Far-IR.

Key words: infrared: ISM: lines and bands-ISM: individual (Sagittarius B2) -ISM: molecules-line: identification -molecular data

1. INTRODUCTION

Instruments on-board *FIRST* will provide high spectral resolution observations of the Far-Infrared and Submillimeter spectrum of dense molecular clouds. Not only physical, chemical and kinematic environments will be scrutinized. Detection of new polyatomic molecules and the use of known molecules in a broader range of transitions will offer unique tools for the understanding of dense star forming regions such as Sagittarius B2 molecular cloud. However, determination of the dominant carriers of emission/absorption features in new spectral bands requires an exhaustive knowledge of molecular spectroscopy and some experience with ‘old’ instruments and related wavelengths. Thus, our preparation with *ISO* and other space-based infrared facilities will be of extreme importance for the future.

2. FAR-IR SPECTRUM OF A DENSE MOLECULAR CLOUD

All the results presented here were taken in the direction of Sgr B2 cloud. Due to its high column density is a very opaque source at optical but with high luminosities in Far-IR, millimeter and radio wavelengths. Because of its physical and chemical complexity (clumped structure, envelope, hot cores, ultracompact HII regions, etc) is a unique object for spectroscopy studies and for the searching of new molecules. Here we determine what kind of features do we expect in the Far-IR spectrum of a dense molecular cloud such as Sagittarius B2.

•‘Dust emission’: Emission from dust can only be observed at wavelengths longer than 50 μm due to the low temperatures of the dust grains. UV and visible photons coming from O and B newly born stars heat the grains and are re-emitted as IR-continuum. In the case of Sgr B2, the maximum emission peaks at $\sim 80\mu\text{m}$ and the shape resembles a Planck distribution. A gray-body fitting to the grating observations suggest that dust is relatively cold ($T_d \sim 30\text{ K}$) and that Far-IR continuum is optically thick even at 180 μm (see also Cernicharo et al. 1997).

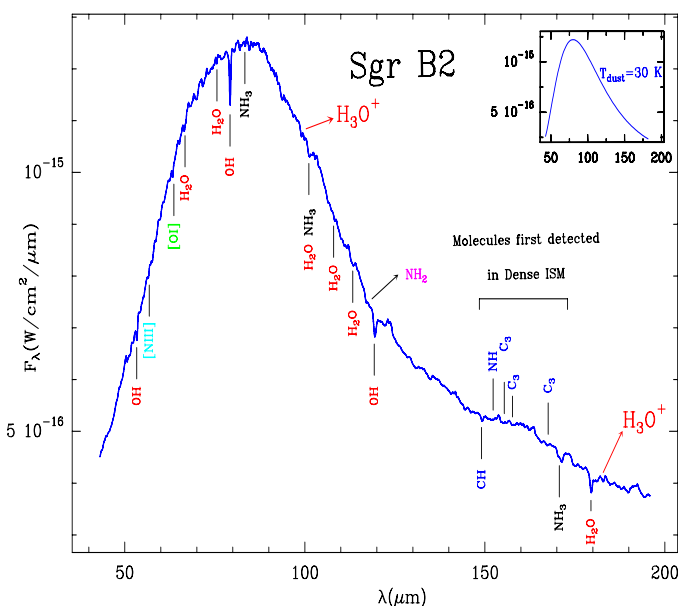


Figure 1. The ISO LWS grating spectrum of Sgr B2 central position between 43 and 196 μm . Main features are labelled. Upper panel: gray-body fit to the continuum dust emission.

•**‘Fine structure/forbidden atomic lines’:** When a Photodissociation region is developed, [OI] 63.18, 145.52 μm and [CII] 157.74 μm lines become the main coolants. In the ultracompact HII regions surrounding hot stars, [OIII] 51.81, 88.35 μm will be also important.

•**‘Molecular transitions’:** The different nuclear degrees of freedom define several types of molecular transitions observable at these wavelengths. Spectrometers on board *FIRST* will enlarge the Far-IR spectral band covered by *ISO* with better resolving powers.

3. POLYATOMIC MOLECULES IN THE FAR-IR SPECTRUM

Rotational transitions of light molecules with permanent electric dipole moment: The number of abundant species with significant dipole moment producing emission or absorption in the Far-IR due to rotational movements is rather reduced (CO, HCN, NH₃, H₂O, NH₂, NH, CH, OH, CH⁺, ...). Here we present the first detection of NH in dense molecular clouds and the first observation of interstellar ortho-NH₂. One could expect a feature-free far-infrared spectrum in interstellar and circumstellar clouds compared with the richness of the mm and submm spectrum of these objects.

Very low- energy vibrational bending modes: Polyatomic molecules like C₃, C₄, C₅, C_n, C₃H, C₄H, C_nH, C₄H₂, C₆H₂, ... however, have low energy vibrational bending modes. The rovibrational transitions between these levels, as in the case of C₃ (see Cernicharo, Goicoechea, Caux 2000), will contribute to the Far-IR spectra of molecular clouds. The detection of the C₃ bending mode opens new possibilities for identifying symmetrical species without permanent dipole moment! Although these species can also be observed in the mid and near-infrared through their stretching vibrational transitions, not all molecular clouds are strong emitters at these wavelengths.

Transitions of slightly asymmetrical molecules:

Other possible molecular features are the b-type transitions of slightly asymmetrical polyatomic species, examples are HOCO⁺, HCO, HNO, HNCO, etc.

Inversion transitions of molecules having a small potential barrier:

Here we present the first Far-IR detection of hydronium ion (Goicoechea & Cernicharo 2001). H₃O⁺ is an oblate symmetric molecule, isoelectronic to NH₃ with the same physical structure, i.e., pyramidal geometry. Like ammonia it has a double minimum vibrational potential so that the oxygen can tunnel through the plane of the hydrogen atoms. In such a kind of molecules (also AsH₃ and PH₃), this leads to a inversion splitting of the rotational levels that can be observed from radio to infrared wavelengths depending on the potential barrier height. Surprisingly, the inversion splitting of H₃O⁺

is very large, $\simeq 55 \text{ cm}^{-1}$, and its fundamental transitions of the ν_2 (umbrella) mode, lay at much higher frequencies than those of the NH₃ splitting ($\simeq 1 \text{ cm}^{-1}$).

4. IMPORTANCE OF EACH MOLECULE

New detected molecular Far-IR features in Sgr B2 are all seen in absorption against the continuum emission of the dust. This means that these transitions come from regions where excitation temperatures are lower than dust temperature ($T_{exc} \leq T_d$). However, determination of excitation mechanisms (collisions, radiation or both) and the role of dust emission is still difficult for molecules having transitions in the infrared domain. Our ISO/LWS observations of Sgr B2 are only sensitive to those regions in front of the infrared continuum sources. Then, the C₃, NH, NH₂ and H₃O⁺ we detect must come from the moderate density and extended envelope of Sgr B2 where collisions are less important and can be neglected as a first approximation.

4.1. H₂O

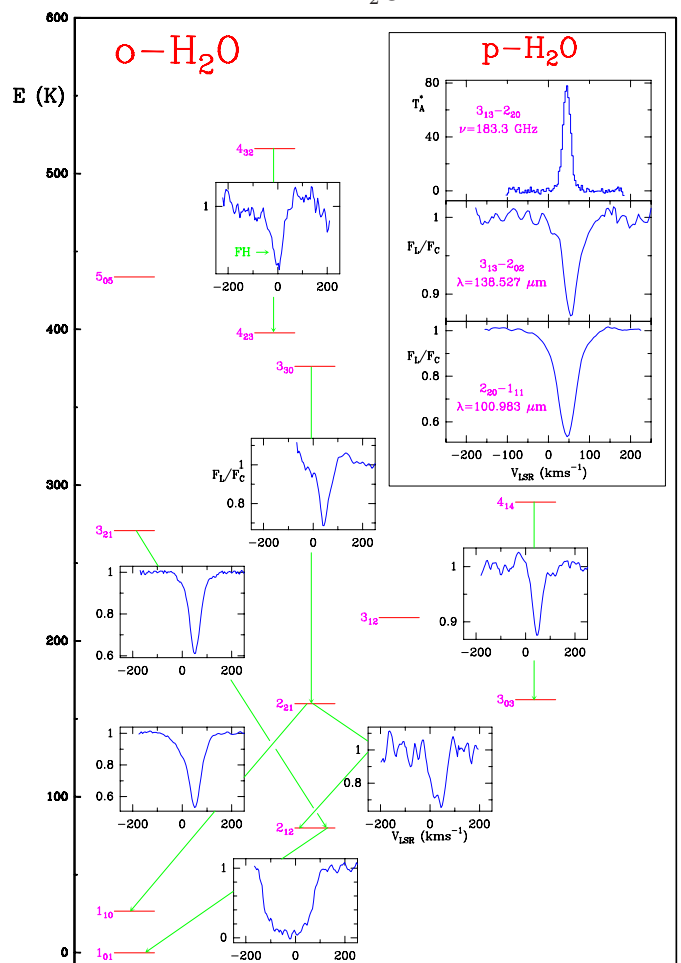


Figure 2. LWS F-P observations of water vapour in Sgr B2. All Far-IR H₂O lines are observed in absorption. The emission feature comes from the 3₁₃-2₂₀ maser transition of para-H₂O.

Water itself is one of the most important and abundant molecules in the ISM. It plays a critical role in the radiative cooling of dense molecular gas: star forming regions, envelopes of evolved stars (from Asymptotic Giant Branch stars to Planetary Nebula), etc. Hence, the determination of its abundance, distribution and formation is decisive for our understanding of chemical and physical process taking place in a great variety of astronomical environments. Here we report on the detection of several thermal transitions of water vapour taken by ISO and proving its ubiquitous presence in the cloud. Moreover, we present the 183.31 GHz $3_{13}-2_{20}$ maser transition of para- H_2O . Data were taken using the 30-m IRAM telescope during 1999.

4.2. H_3O^+

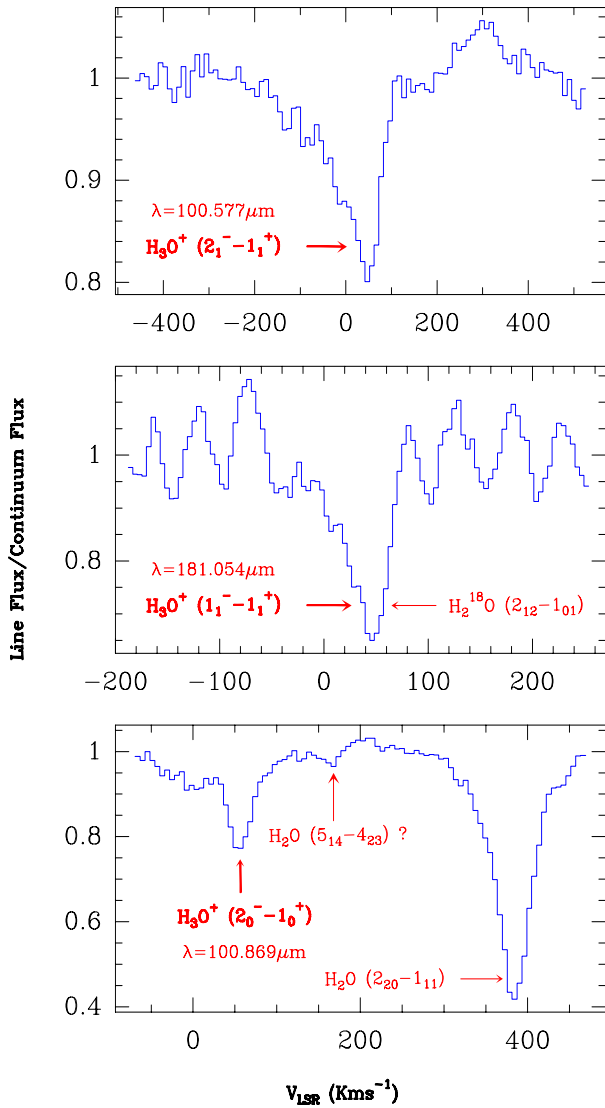


Figure 3. LWS F-P observations of H_3O^+ in Sgr B2. The upper box contains the broad R(1,1) absorption line. Middle, Q(1,1) transition is blended with $2_{12}-1_{01}$ transition of H_2^{18}O . Bottom, spectrum including the R(1,0) and two water vapour features.

H_3O^+ is thought to be formed in the first stages of interstellar oxygen based chemistry and plays a very important role in gas-phase reactions prevailing in dense molecular clouds. Its dissociative recombination leads to the formation of important molecules OH and H_2O with an imprecise branching ratio for each channel of the dissociation. However, this ratio is a crucial parameter for the interstellar chemistry and for the modelling of molecular clouds. We have detected three lines arising from the ν_2 ground-state inversion mode ($0^+ \rightarrow 0^-$) at 55.3 cm^{-1} . Our detections favour a scenario in which water ice may be also formed by surface reactions on dust grains and then released back into the gas by young stars radiation or sputtering. This may explain the high abundance of water in Sgr B2. The derived abundance is $\simeq (1-5) \cdot 10^{-9}$ in agreement with submm observations (Phillips et al. 1992).

4.3. C_3

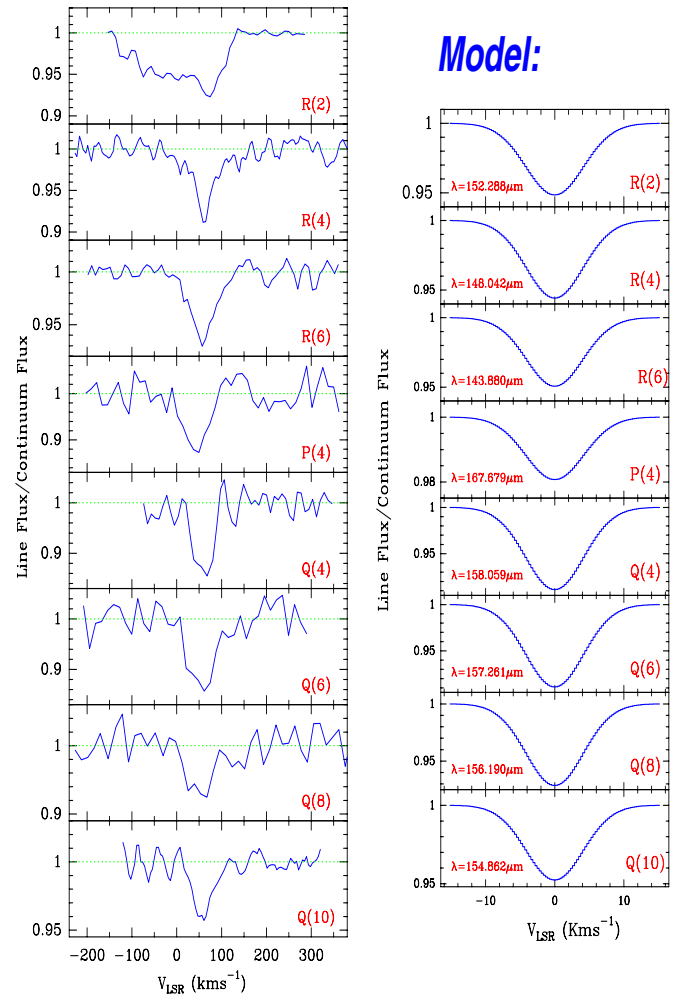


Figure 4. LWS F-P observations of C_3 in Sgr B2. The Q(10) spectrum could also contain the $J=5/2-3/2$ transitions of SH at 154.864 and $154.915 \mu\text{m}$. Right caption: triatomic carbon predicted absorptions in Sgr B2. Lines have not been convolved with the ISO/LWS Fabry-Perot instrumental profile.

Among the carbon chain radicals, triatomic carbon plays an important role in the growth of carbon chains and clusters. A determination of its abundance could improve our understanding of the interstellar chemistry, especially the synthesis of complex hydrocarbons. We have model the C_3 absorption (see Figure 4) following the model and physical parameters adopted by Cernicharo et al. 1997 for water vapour including radiative pumping by dust. The abundance of C_3 in the direction of Sgr B2 is $\simeq 3 \cdot 10^{-8}$ and $\simeq 10^{-9}$ in the molecular gas intersecting the line of sight. This kind of modelization is a first step for further work on carbon chains, C_n , and a preparatory study for the programs that could be carried out with *FIRST*.

4.4. NH & NH₂

Nitrogen based chemistry in dense clouds has been difficult to model due to the trials in detecting simple nitrogen hydrides. Imidogen, NH, and amidogen, NH₂, radicals are especially involved in the production of the abundant ammonia molecule. Here we present the NH 2_3-1_2 transition. NH has been reported in the diffuse ISM through electronic absorption bands (Meyer & Roth 1991) but never in dense molecular clouds. We derive a fractional abundance of a few times $\simeq 10^{-9}$, which is a factor 10 lower than the NH₂ abundance in the Sgr B2 envelope.

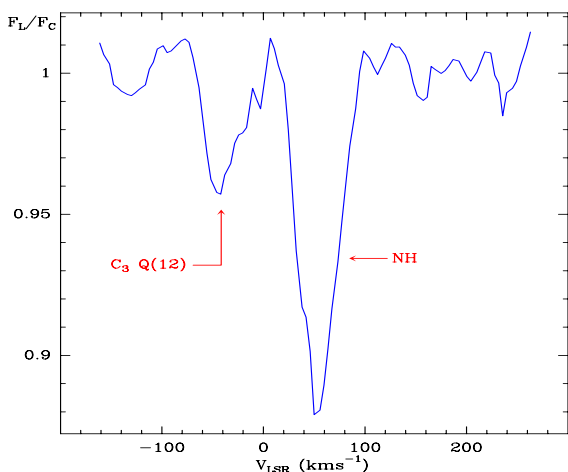


Figure 5. The 2_3-1_2 line of NH in Sgr B2. In the same spectrum the C_3 Q(12) absorption is also detected at 3σ level.

In addition, we present for the first time two features of ortho-NH₂. Absorption lines come from the $2_{20}-1_{11}$ rotational transition. The $1_{10}-1_{01}$ transition of para-NH₂ was observed by van Dishoeck et al. 1993 in the submillimeter domain. They derived a NH₂ abundance of $(1-3) \times 10^{-8}$ relative to H₂. Both molecules have nonvanishing electronic spin which interacts with rotation angular momentum leading to the splitting of each rotational level. Further hyperfine splitting occur due to the nuclear spin of the nitrogen atom. With the present space telescopes spectral resolution is impossible to resolve the hyperfine

structure. However, at the FIRST/HIFI resolving power and if lines are not too broad, we will be able to detect lines coming from different F quantum numbers. This will provide very useful information about individual line opacity.

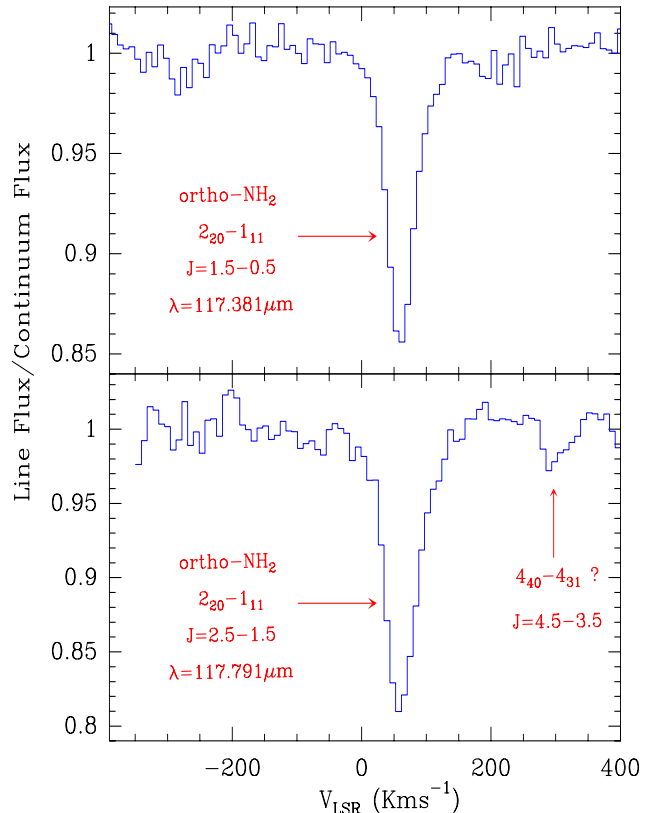


Figure 6. LWS F-P observations of NH₂ in Sgr B2. The intensity scale corresponds to the continuum normalized flux. The wavelength of each transition is indicated at the bottom left corner of each panel. The bottom panel probably contains the $4_{40}-4_{31}$ transition of ortho-NH₂ at 478 K.

5. CONCLUSION

In this contribution we have briefly summarized the different types of molecular transitions occurring in the Far-IR spectrum. Future work on *ISO* data base will prepare us for the future heterodyne space telescopes such as *FIRST*.

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