Laboratory investigations on the chemical and optical properties of interstellar ice analogs

Maria Elisabetta Palumbo
Istituto Nazionale di Astrofisica
Osservatorio Astrofisico di Catania
maria.palumbo@inaf.it

THE ASTROPHYSICAL JOURNAL, 449:674–680, 1995 August 20

SOLID CARBONYL SULPHIDE (OCS) IN W33A

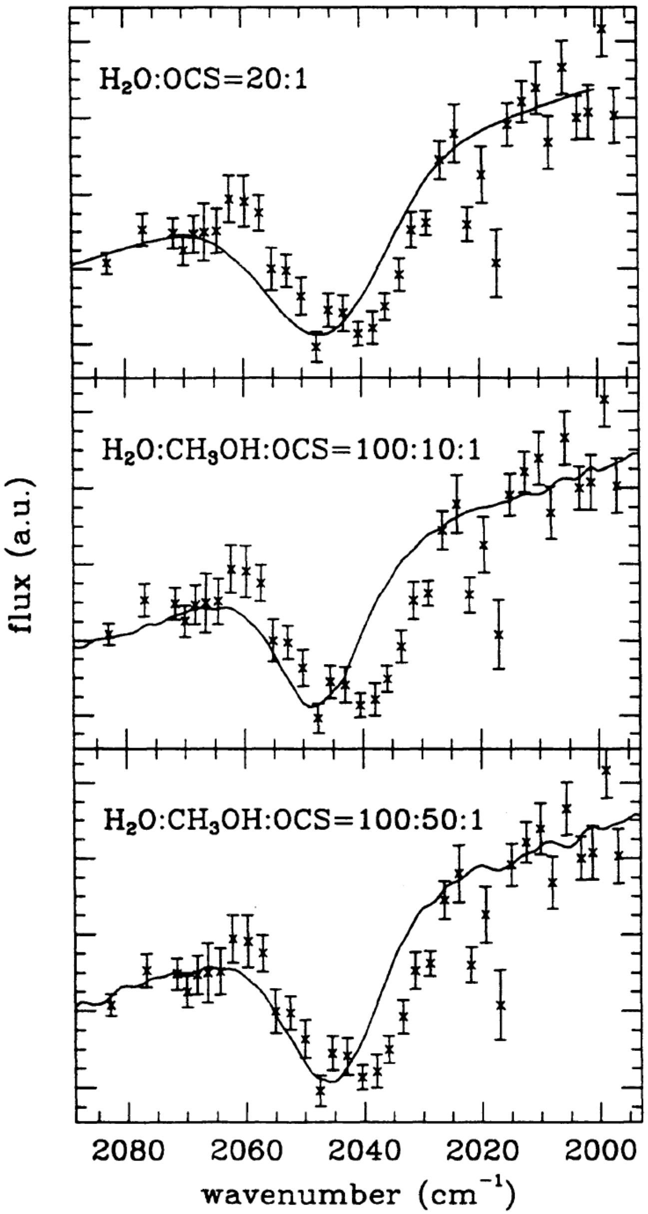
M. E. PALUMBO
Istituto di Astronomia, Università di Catania, Viale A. Doria 6, 95125 Catania, Italy
A. G. G. M. TIELENS
NASA/Ames Research Center, MS 245-3, Moffett Field, CA 94035
AND
A. T. TOKUNAGA
Institute for Astronomy, University of Hawaii, 2680 Woodlawn Drive, Honolulu, HI 96822
Received 1994 November 16; accepted 1995 March 6

THE ASTROPHYSICAL JOURNAL, 479:839–844, 1997 April 20

SOLID CARBONYL SULFIDE (OCS) IN DENSE MOLECULAR CLOUDS

M. E. PALUMBO
Osservatorio Astrofisico di Catania, Viale A. Doria 6, I-95125 Catania, Italy
T. R. GEBALLE
Joint Astronomy Centre, 660 N. A'ohoku Place, Hilo, HI 96720
AND
A. G. G. M. TIELENS
NASA/Ames Research Center, MS 245-3, Moffet Field, CA 94035
Received 1996 May 20; accepted 1996 October 10

Solid OCS in icy grain mantles



Ↄ CARBONYL SULPHIDE (OCS) IN W33A

M. E. Palumbo
ɔnomia, Università di Catania, Viale A. Doria 6, 95125 Catania, Italy
A. G. G. M. Tielens
/Ames Research Center, MS 245-3, Moffett Field, CA 94035
AND
A. T. Tokunaga
ıomy, University of Hawaii, 2680 Woodlawn Dri

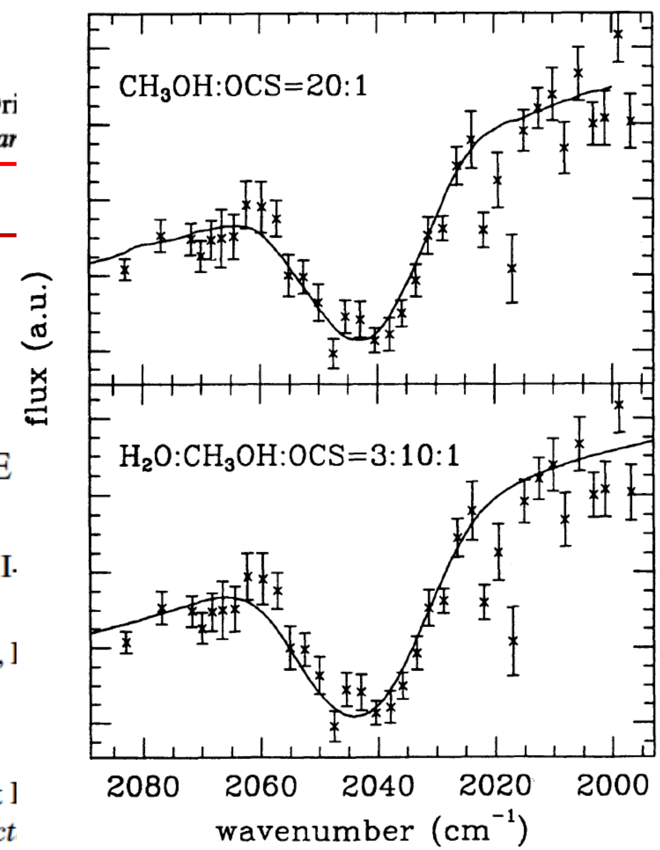
Received 1994 November 16; accepted 1995 Mar

April 20
inted in U.S.A.

⅃L SULFIDE (OCS) IN DENSE

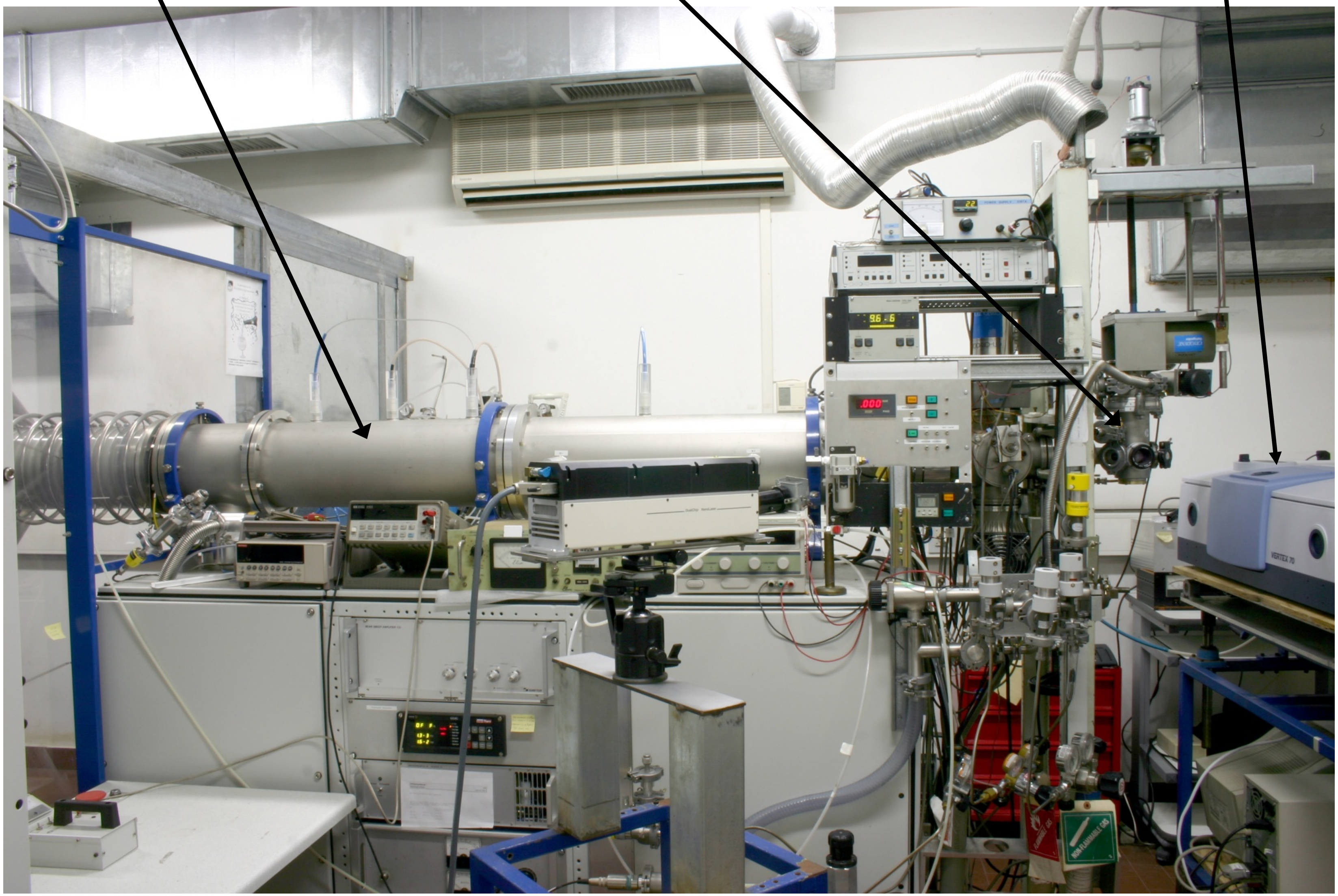
M. E. Palumbo
rio Astrofisico di Catania, Viale A. Doria 6, I-
T. R. Geballe
t Astronomy Centre, 660 N. A'ohoku Place, I
AND
A. G. G. M. Tielens
A/Ames Research Center, MS 245-3, Moffet I

Received 1996 May 20; accepted 1996 Oct

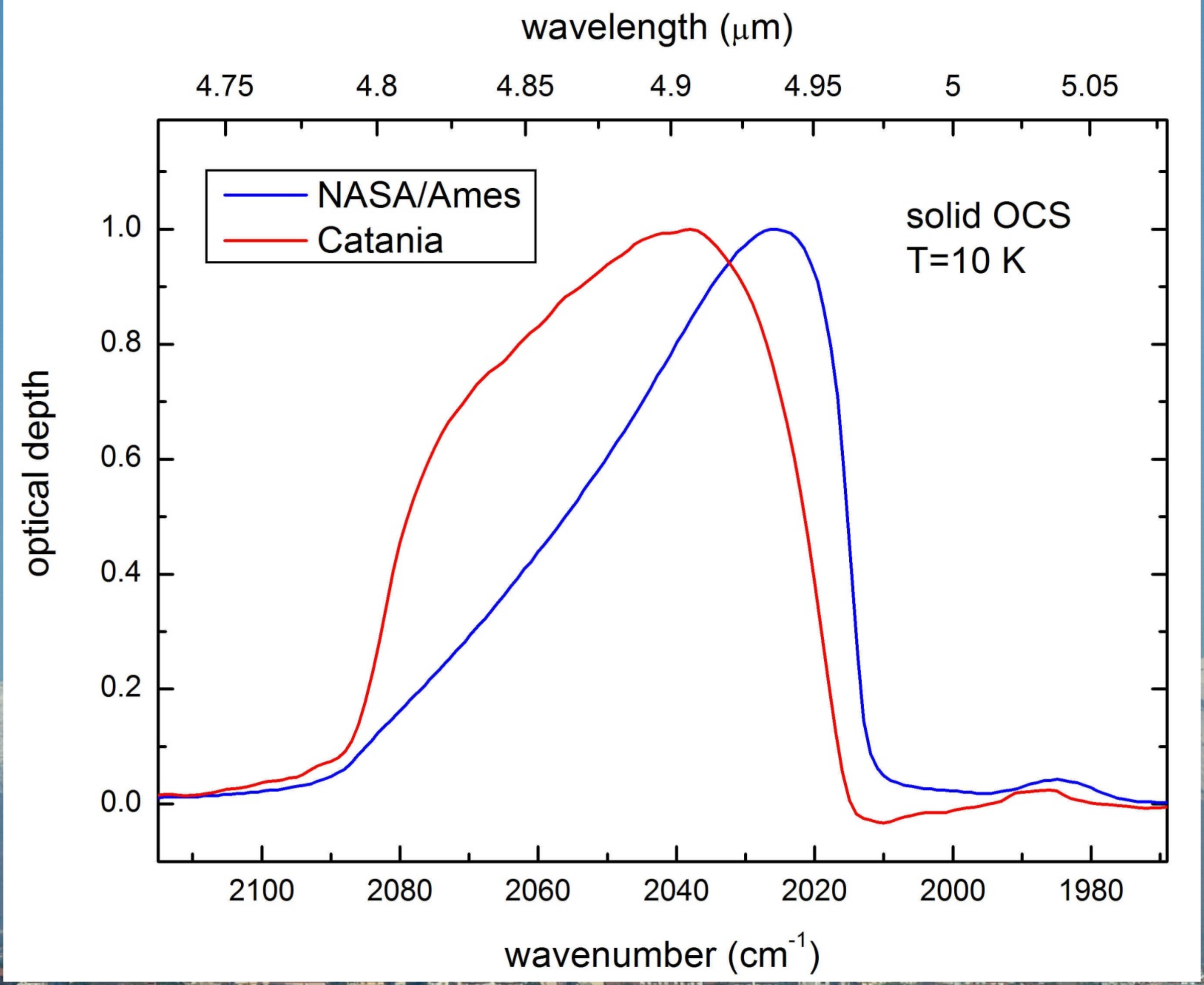


Laboratory for Experimental Astrophysics
Catania

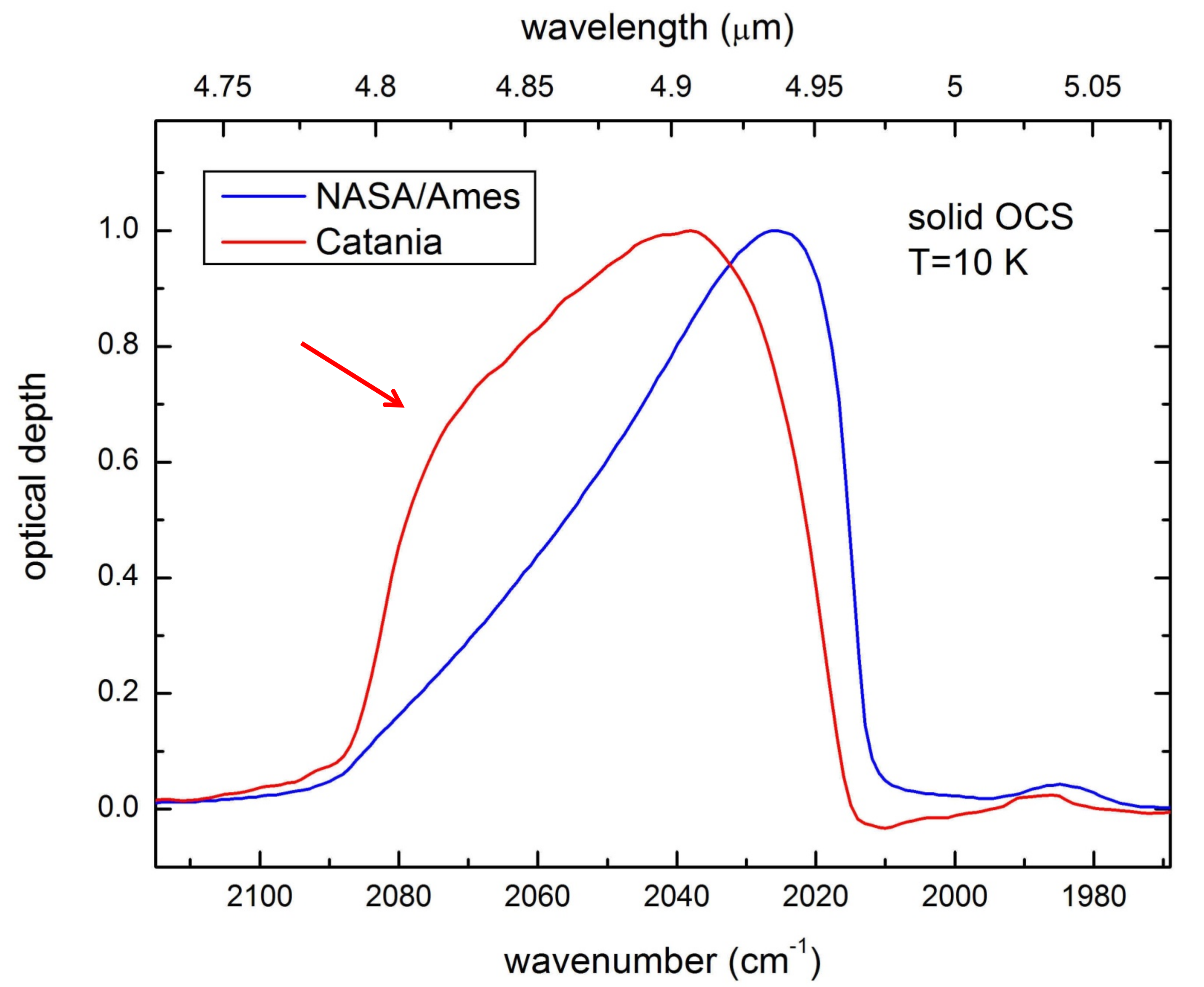
Ion beam **Vacuum chamber** **FTIR spectrometer**



IR spectra of solid OCS

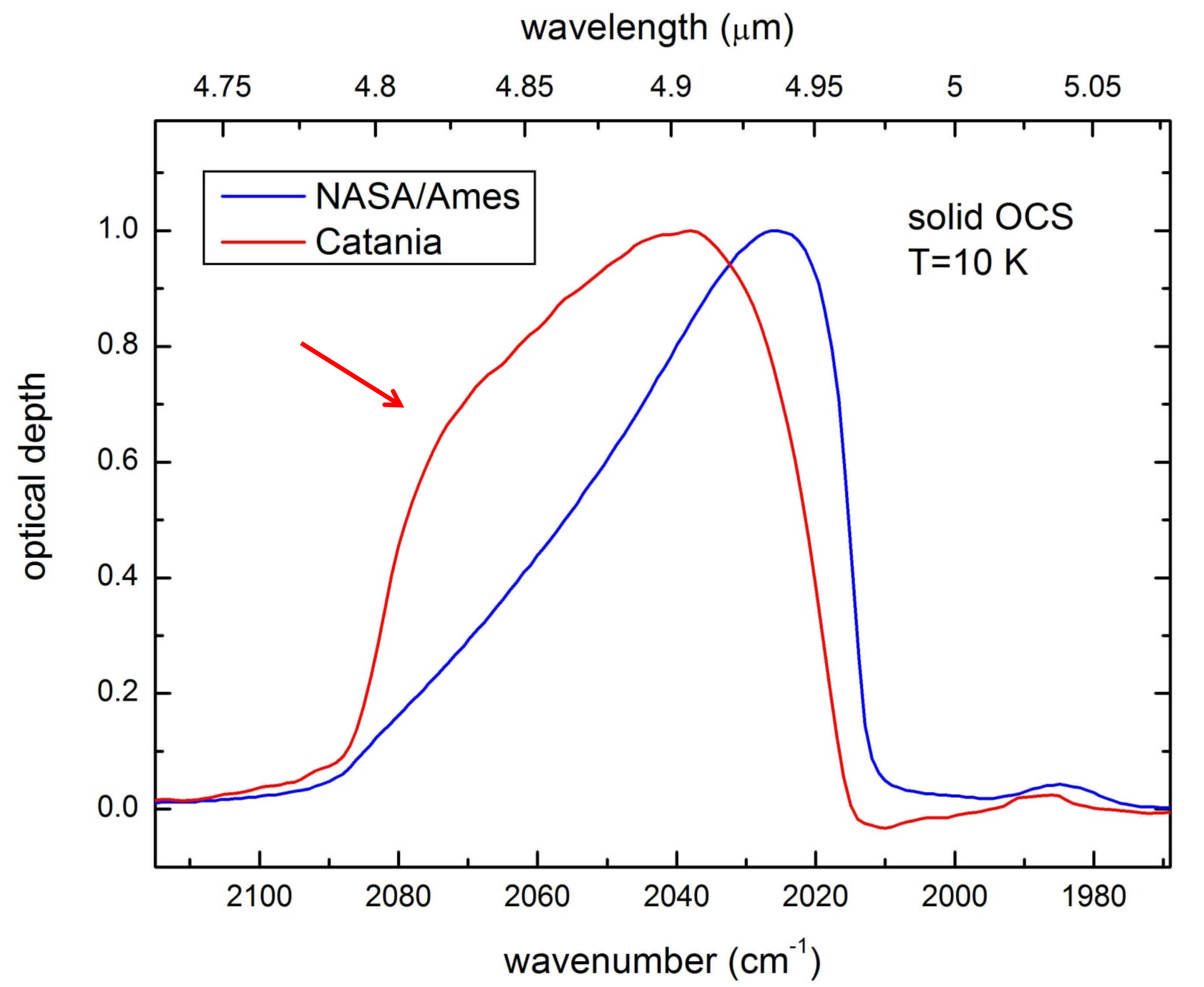


IR spectra of solid OCS



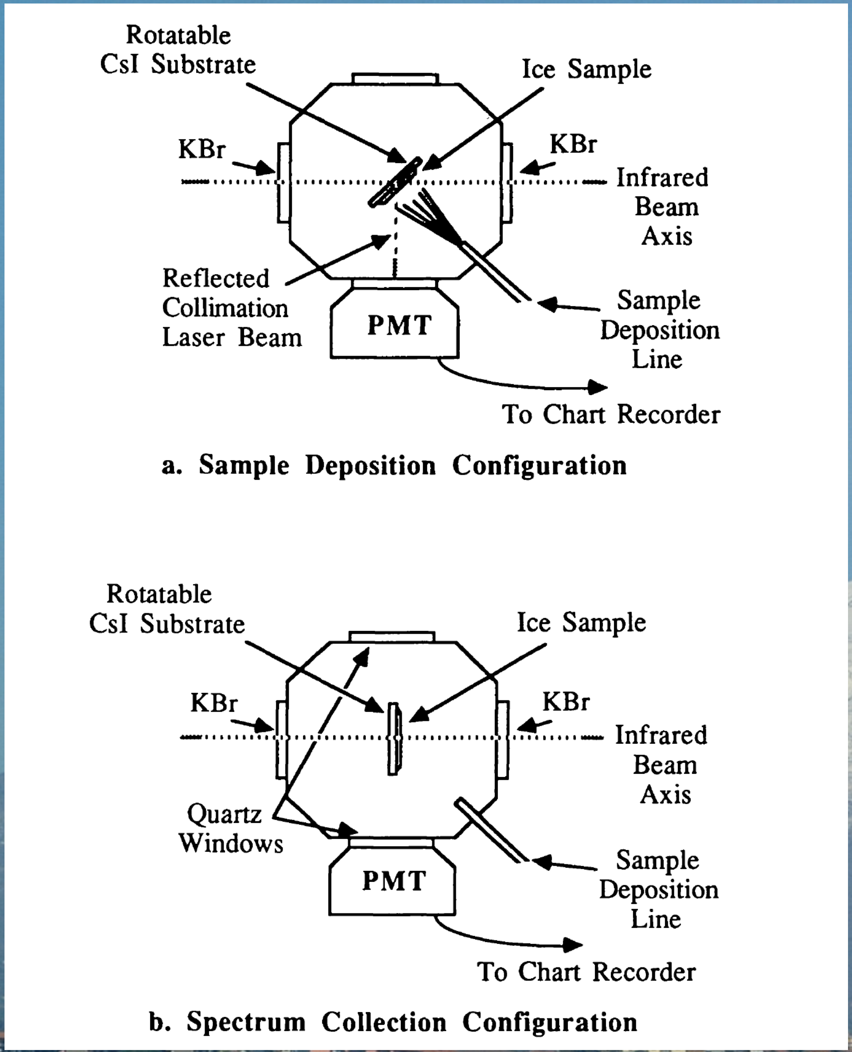
IR spectra of solid OCS

- ➢**Substrate**
- ➢**Temperature**
- ➢**Deposition rate**

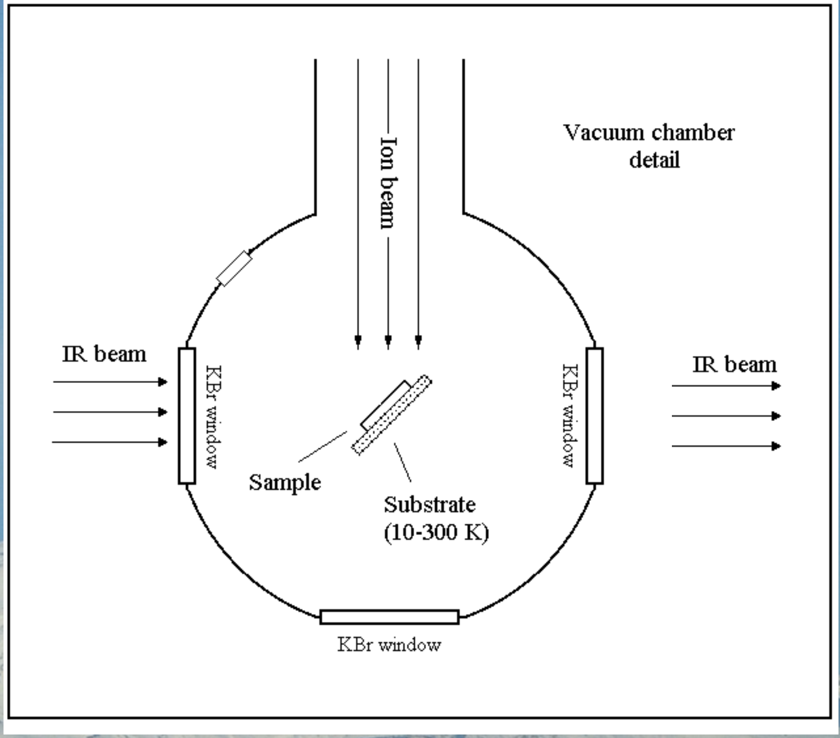


Infrared spectra at normal and oblique incidence

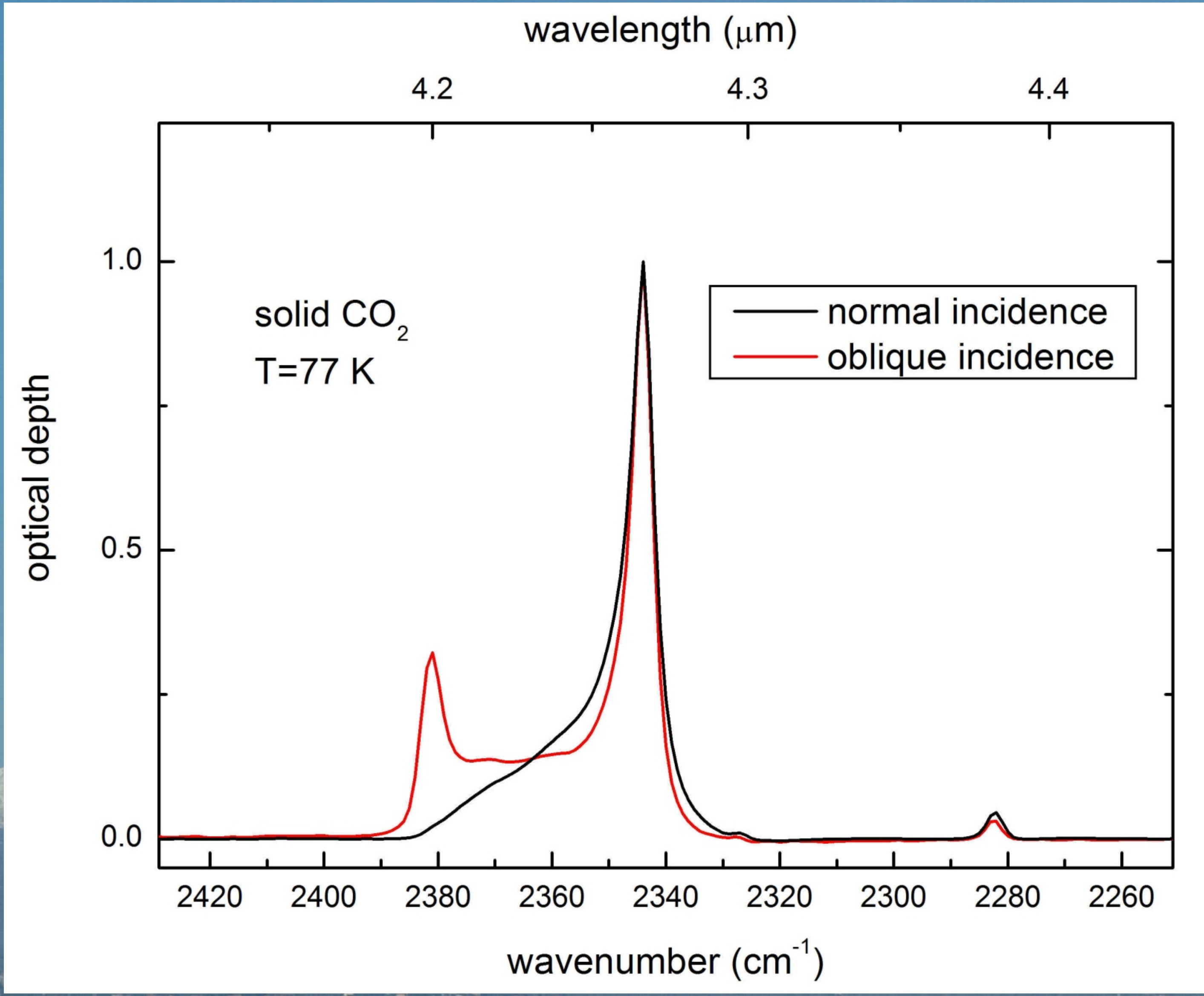
NASA/Ames Research Center
(e.g. Hudgins et al. 1993)



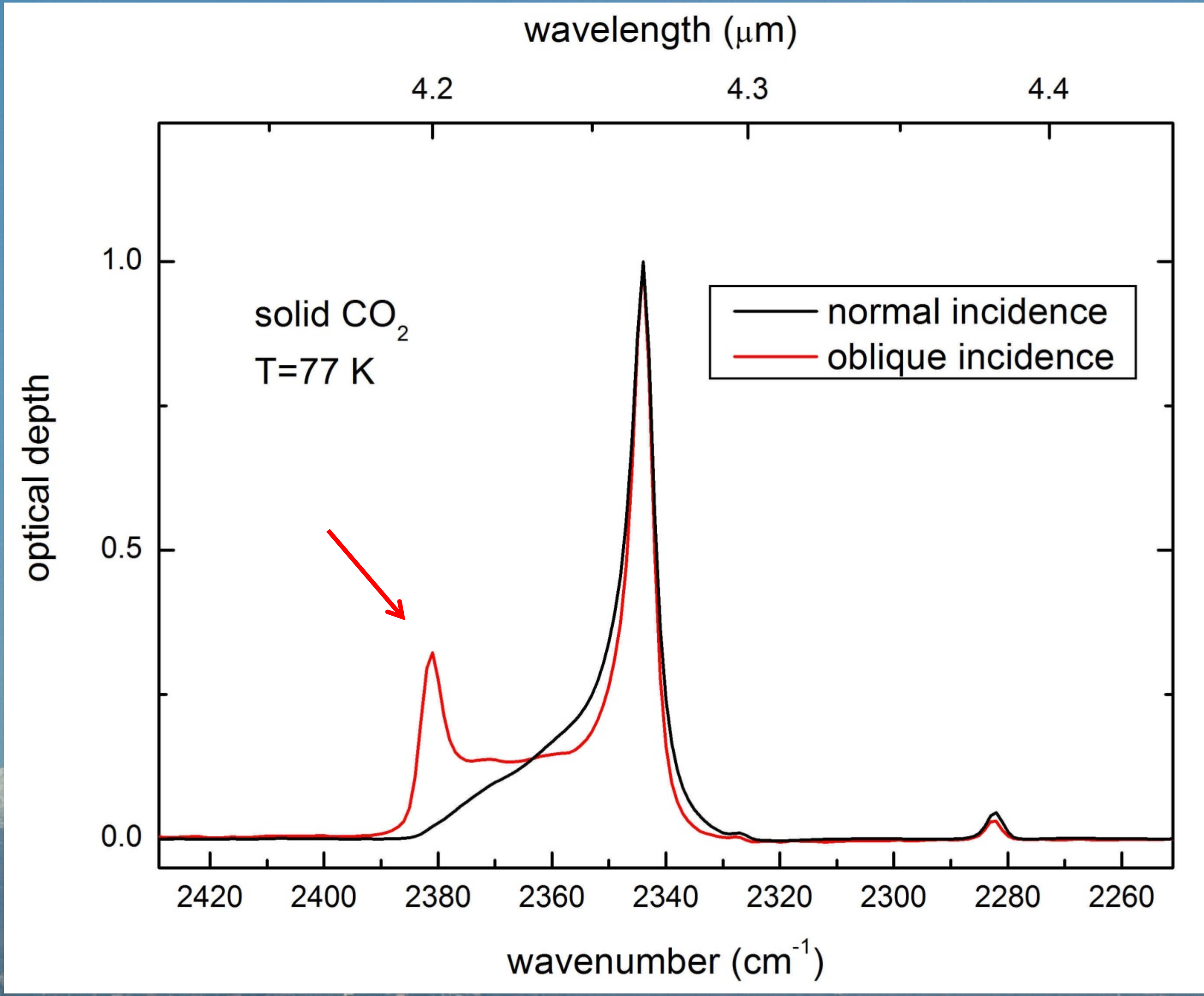
Catania Laboratory
(e.g. Palumbo 1997)



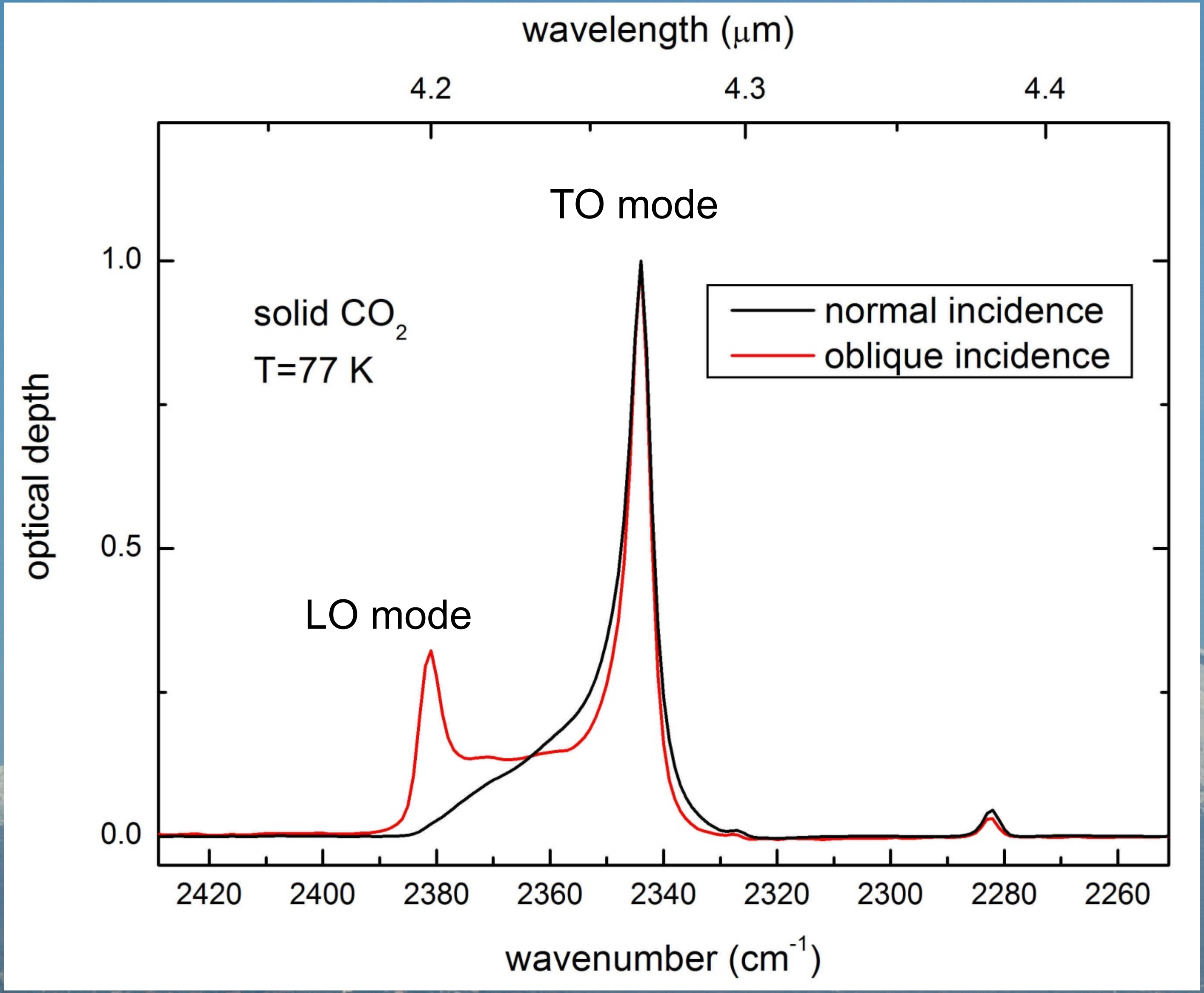
Infrared spectra at normal and oblique incidence



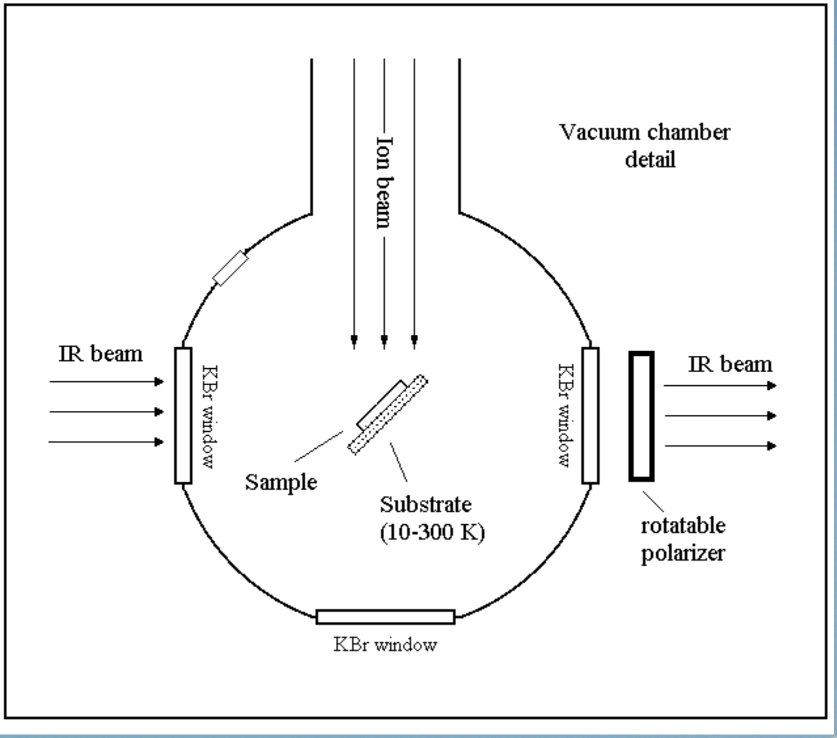
Infrared spectra at normal and oblique incidence



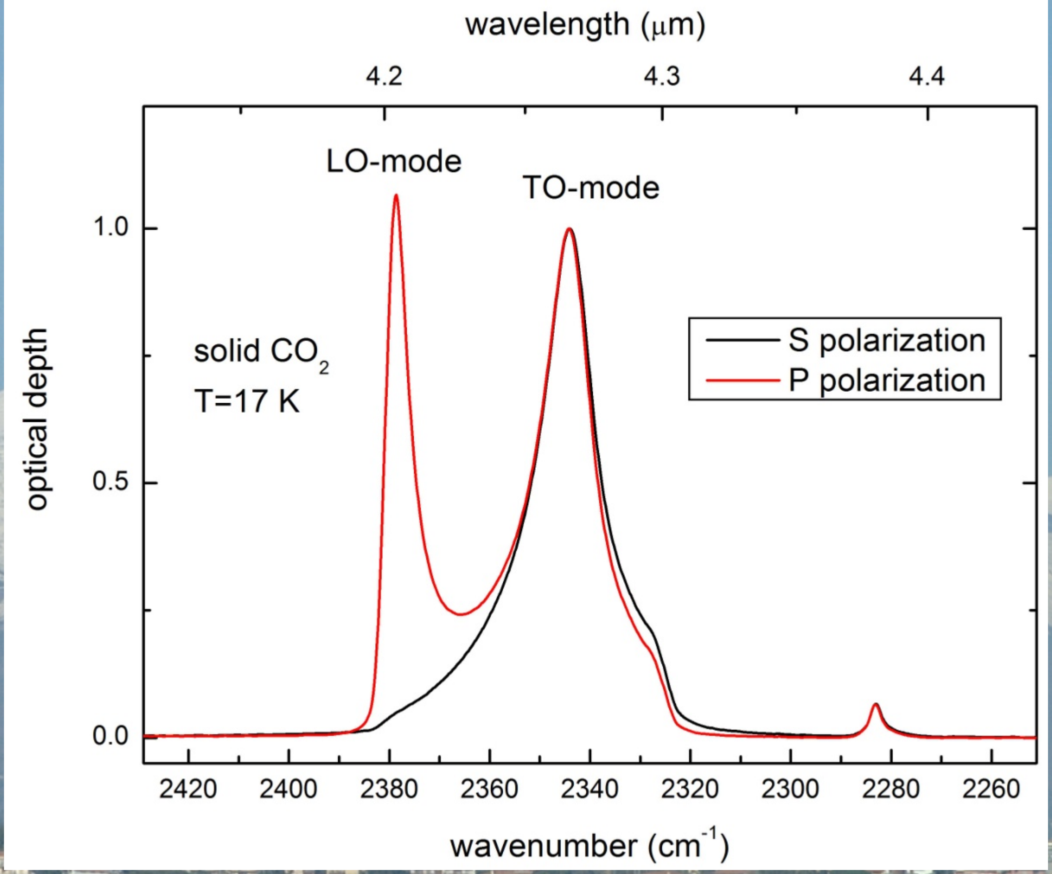
Infrared spectra at normal and oblique incidence



Infrared spectra at oblique incidence

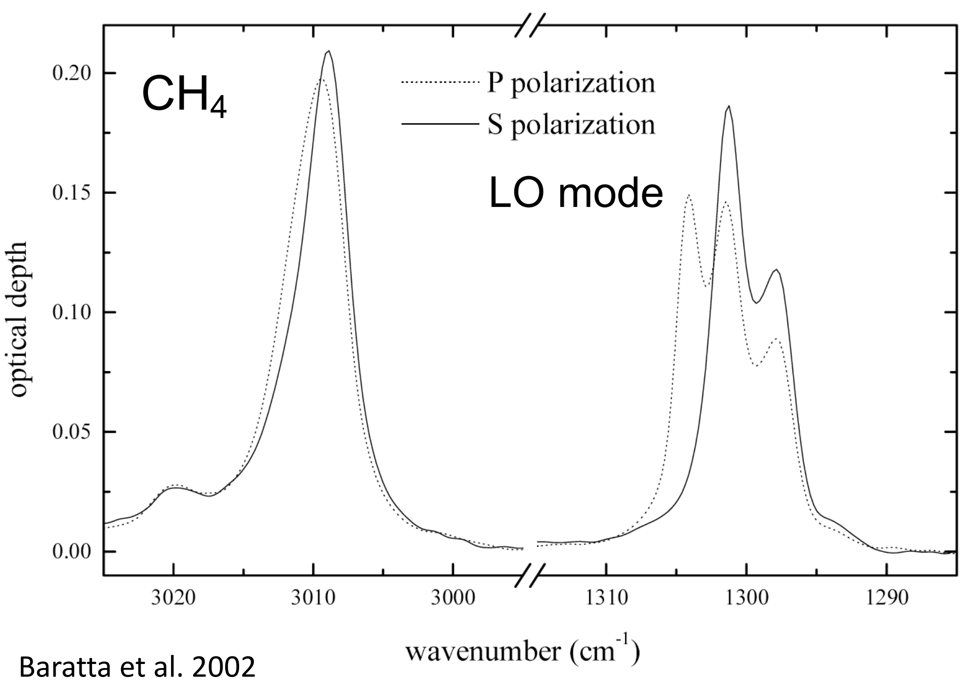


At oblique incidence a band due to the LO mode CANNOT be present in the spectra taken when you select the S component with the polarizer while it can be observed when you select the P component.

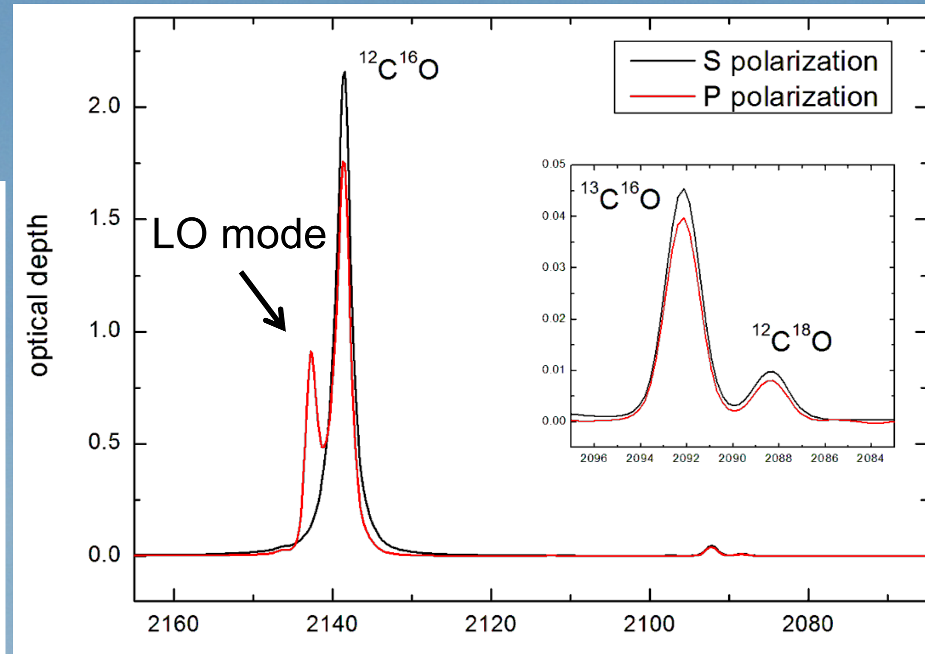


The LO-TO splitting is usually observed in strong bands (i.e. fundamental modes).

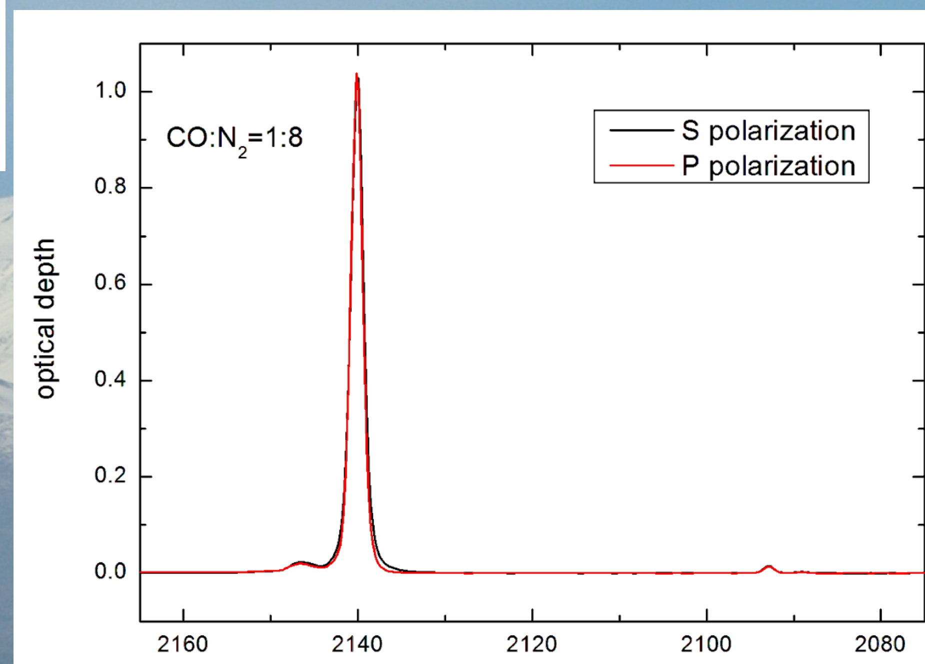
Infrared spectra at oblique incidence



Baratta et al. 2002



Palumbo et al. 2006



Sicilia et al. 2012

The LO-TO splitting is usually observed in strong bands (i.e. fundamental modes).

LO-TO splitting

solid CO

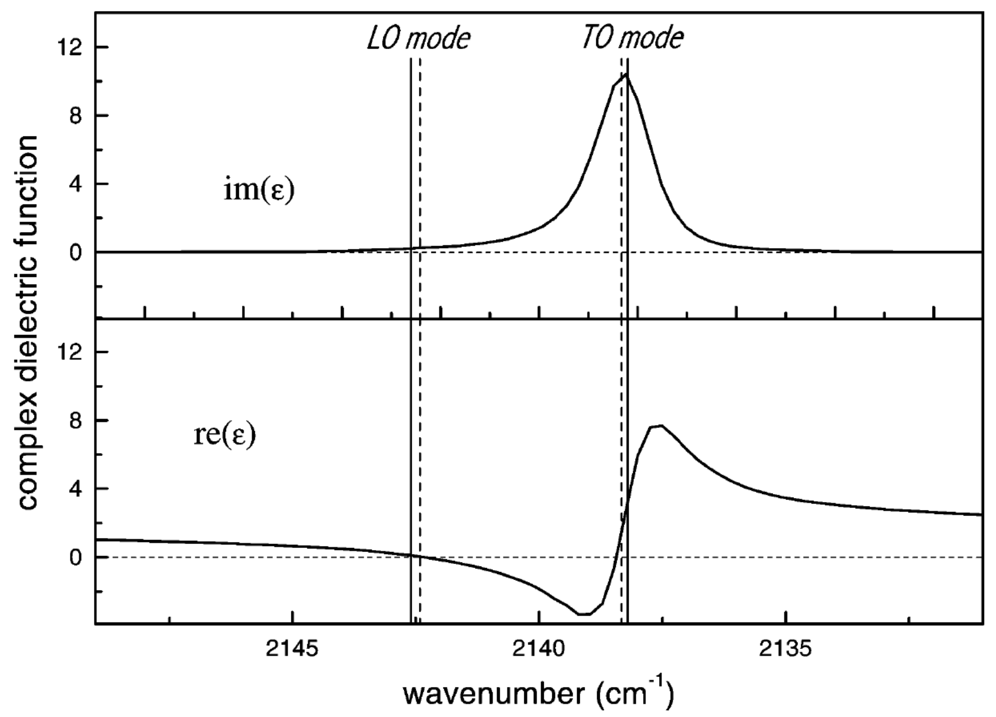
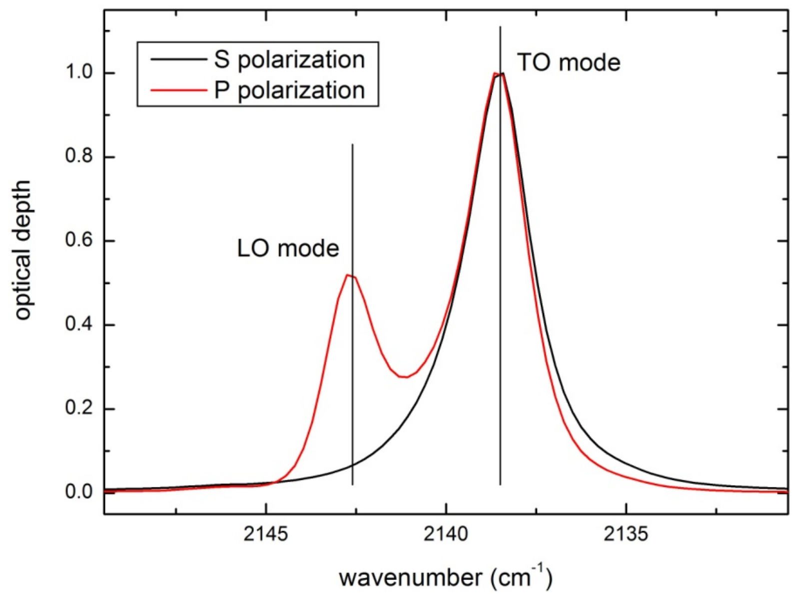


Fig. 3 Complex dielectric function of solid CO at 15 K in the 2150–2130 cm^{-1} range. Vertical solid and dashed lines give the expected positions of the TO mode and LO mode (see text).

Palumbo et al. 2006, PCCP 8, 279



The wave numbers of the LO and TO modes can be approximated either by the minimum and maximum of |ε| respectively (solid lines in Fig. 3), or by the maximum of the energy-loss function given by Im(1/ε) and maximum of ε'' respectively (dashed lines in Fig. 3).

Particle size and shape effects

- ✓In the laboratory we take spectra of thin films
- ✓In space we observe ice grain mantles

Is it possible to compare the profile of absorption bands of thin films (bulk) to the band’s profiles in astronomical spectra?

SOMETIMES!

Particle size and shape effects

Particle size and shape can have very important effects on the profile of absorption features. For strong transitions in small particles, this class of electromagnetic modes is referred to as "surface modes" (van de Hulst 1957; Bohren and Huffman 1983).

- ✓Shift of peak position with respect to laboratory (bulk) spectra
- ✓Sub-peaks appear

Depend on optical constants

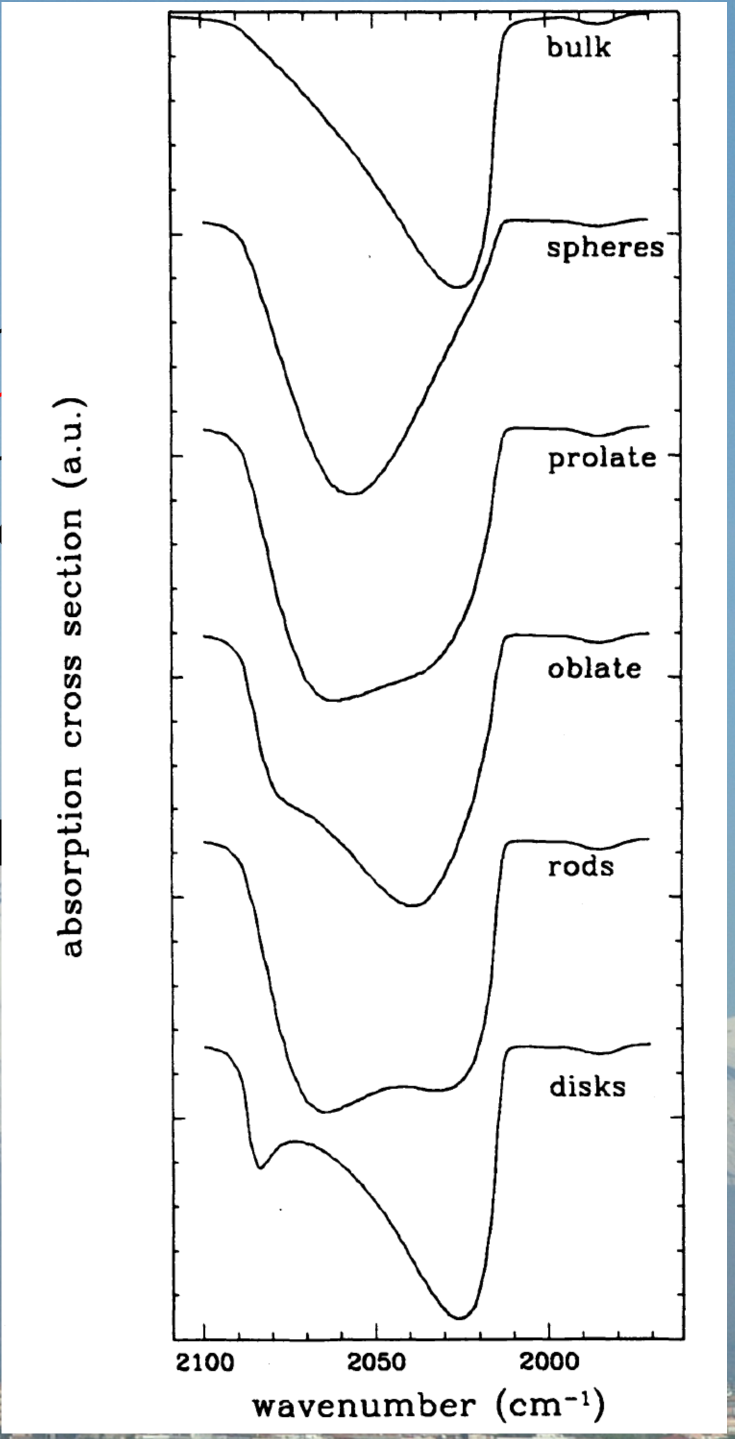
Particle size and sh

Particle size and shape can have very i profile of absorption features. For stro particles, this class of electromagnetic m "surface modes" (van de Hulst 1957; Bohr

✓Shift of peak position with respect to
✓Sub-peaks appear

Depend on optical co

Solid OCS
Palumbo M.E., Tokunaga A., Tielens A.G.G.M., 1995



Comparison between different sets of optical constants

Ehrenfreund et al. 1997

Solid CO

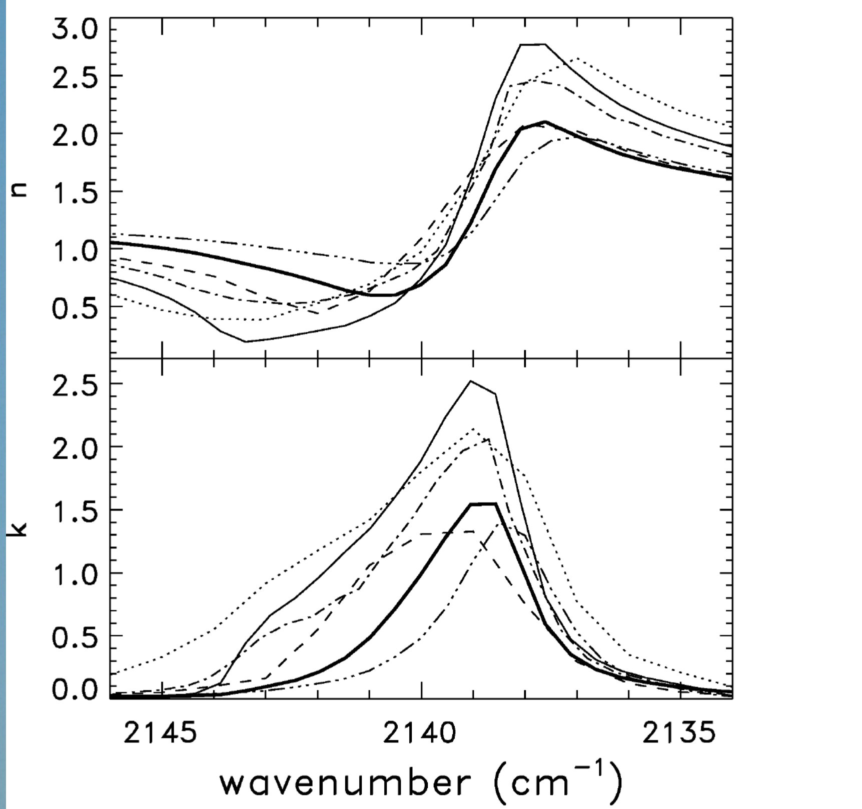


Fig. 17. The optical constants for the fundamental mode of pure CO ice, derived in different studies (see text for abbreviations): this work (thin solid line), B97 (dash), E97 (dash-dot), T96 (dash-triple dots), and T91 (dots). The thick solid line are the constants calculated from our transmission spectrum, assuming a two times larger sample thickness.

Solid CO_2

stretching mode and bending mode

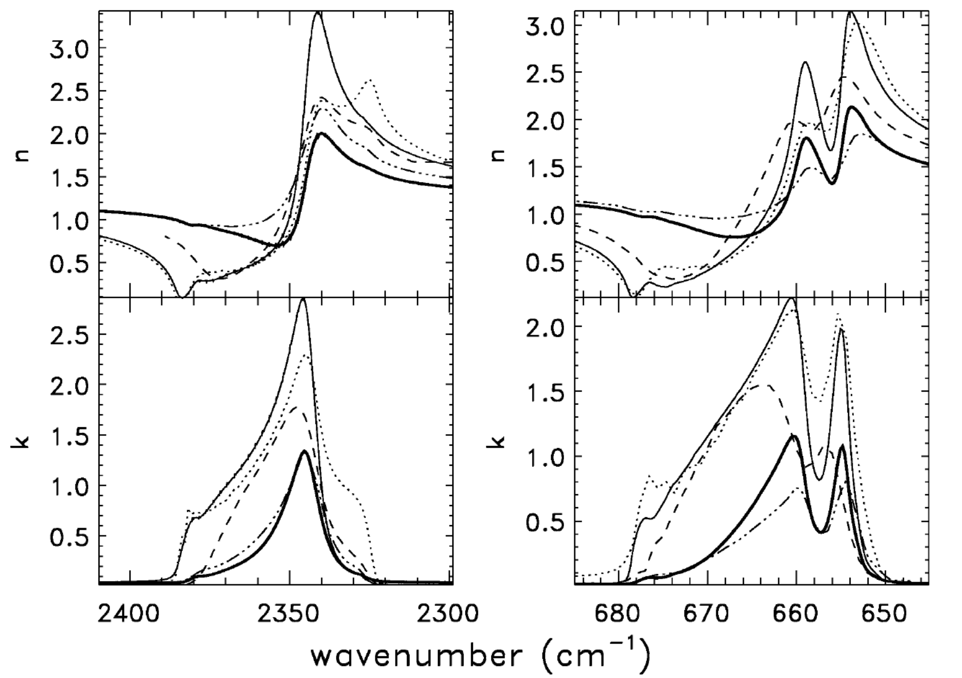


Fig. 19. The optical constants for the stretch (left) and bend (right) of pure CO_2 ice, derived in different studies: this work (thin solid line), B97 (dash), T96 (dash-triple dots), and H93 (dots). The thick solid line are the constants calculated from our transmission spectrum, assuming a 2.7 times larger sample thickness.

Solid CO

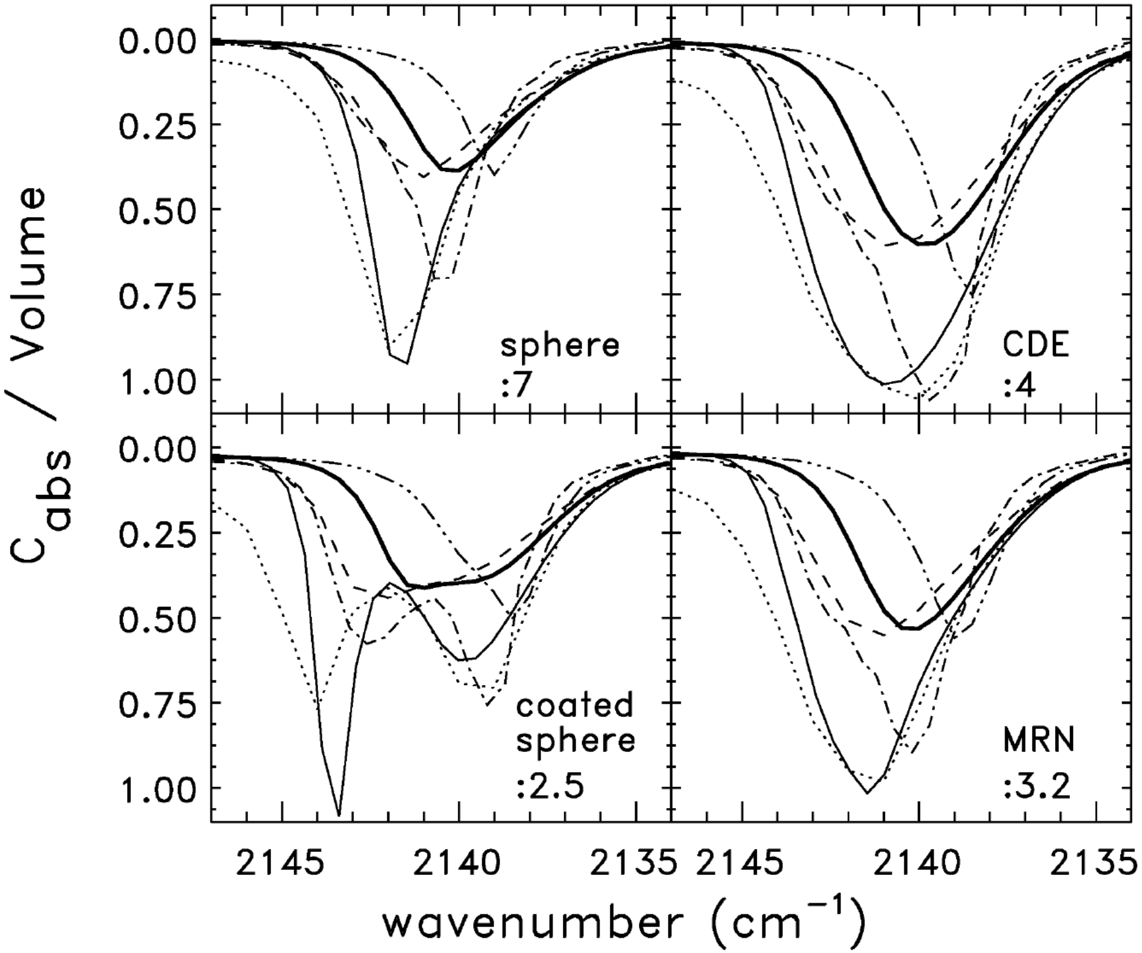
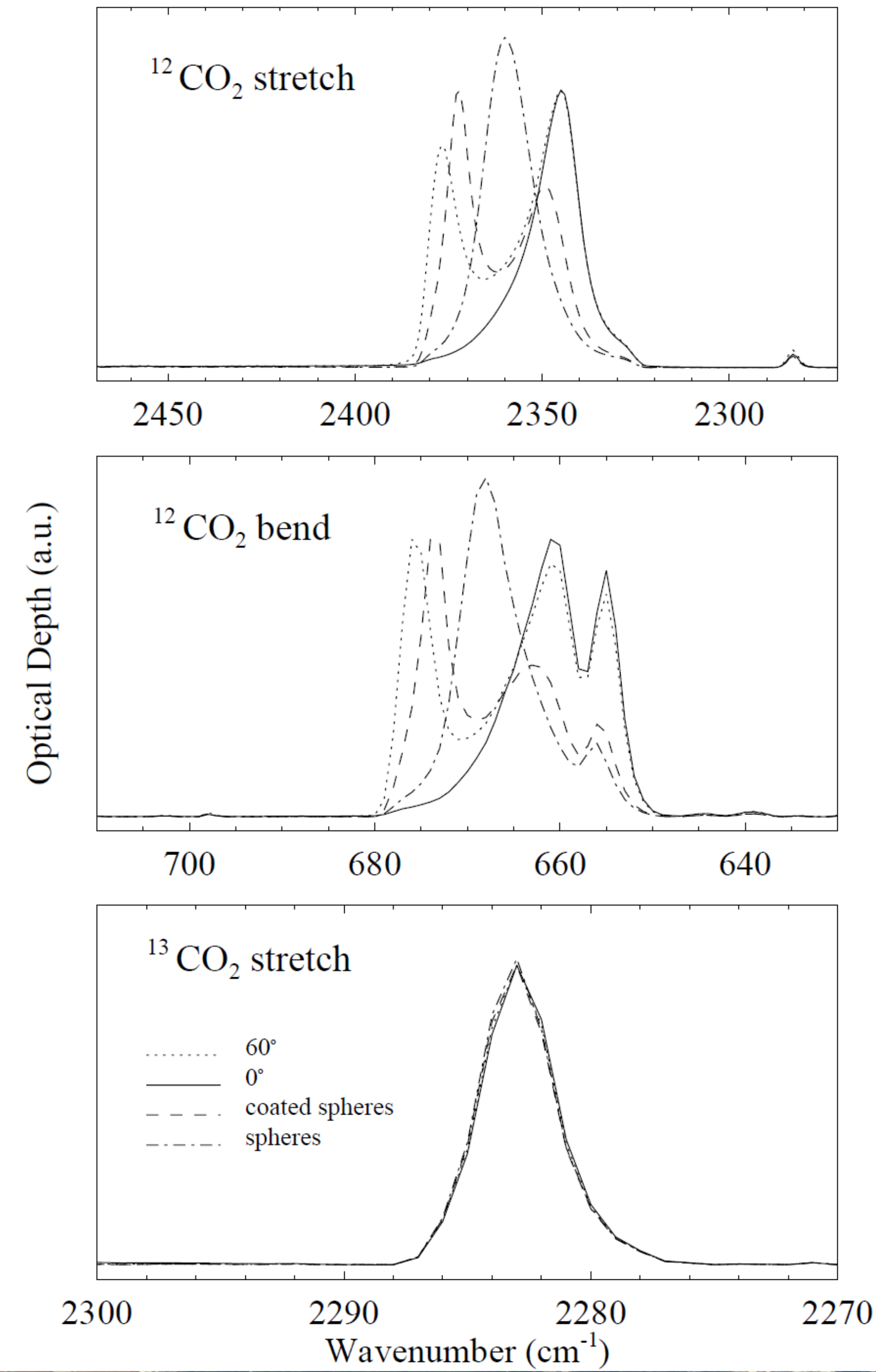


Fig. 18. Absorption cross sections for the pure solid CO fundamental mode for different dust models, using the optical constants shown in Fig. 17. Models in the small particle limit were calculated for pure ice spheres, silicate spheres with an ice mantle of equal volume, a continuous distribution of ellipsoids (CDE) and an MRN size distribution with 0.01 μm thick ice mantles and silicate cores. The cross sections have been scaled by the number given in the right-lower corner of each panel.

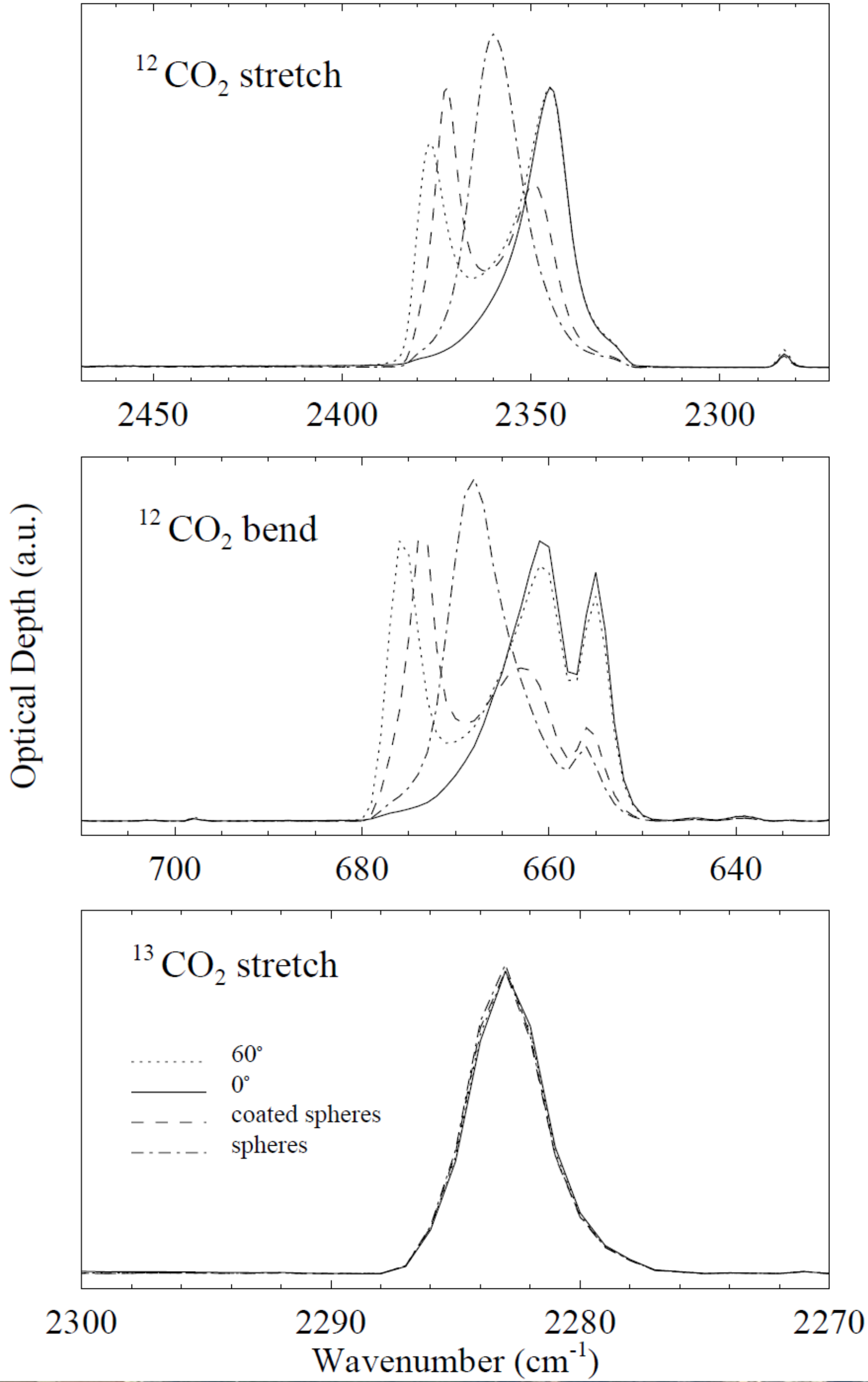
Different band's profiles result from different sets of optical constants

Ehrenfreund et al. 1997



Quoting Bohren & Huffman (1983): "All of this illustrates a general rule, which we can state but not prove: if there is an interesting effect in a thin film, there will be a corresponding effect in small particles".

Baratta et al. 2000
Baratta et al. 2002
Palumbo et al. 2006
Ioppolo et al. 2009
Fulvio et al. 2009
Abdulgalil et al. 2013
Urso et al. 2016
Baratta and Palumbo 2017

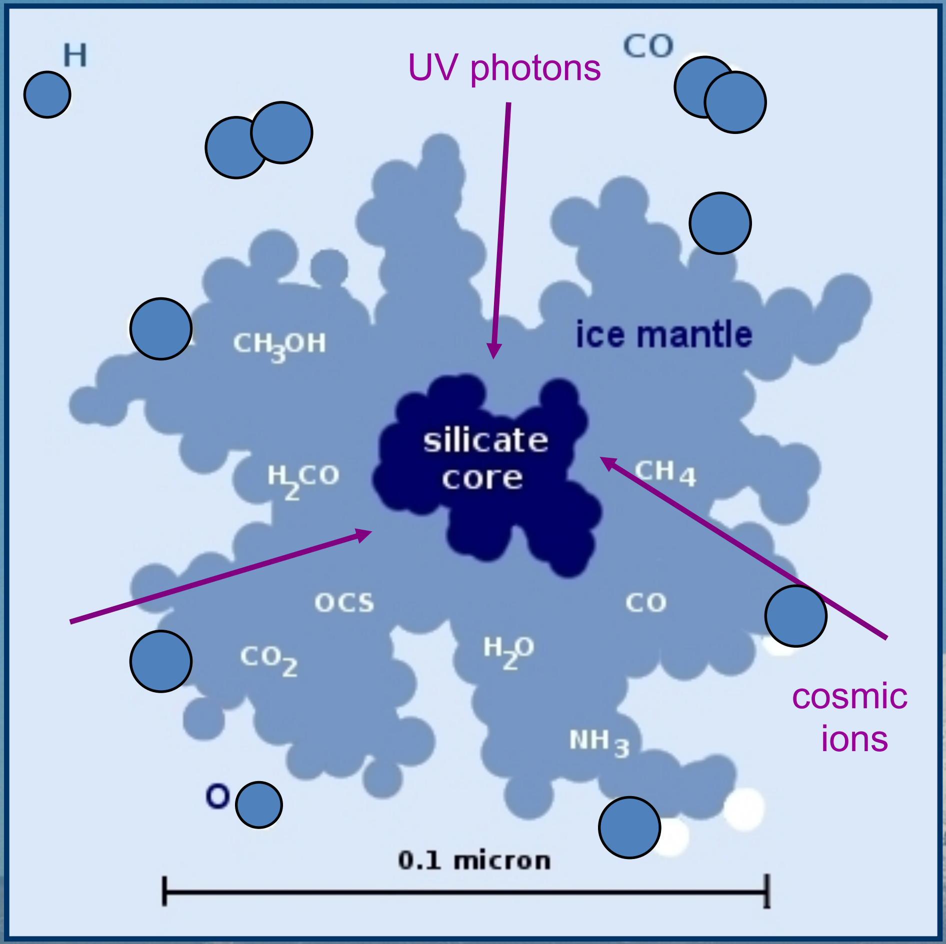


Quoting Bohren & Huffman (1983): “All of this illustrates a general rule, which we can state but not prove: if there is an interesting effect in a thin film, there will be a corresponding effect in small particles”.

If the profile does not depend on the position of the polarizer (P or S) then laboratory spectra of thin films can safely be compared directly to astronomical observations

Baratta et al. 2000
Baratta et al. 2002
Palumbo et al. 2006
Ioppolo et al. 2009
Fulvio et al. 2009
Abdulgalil et al. 2013
Urso et al. 2016
Baratta and Palumbo 2017

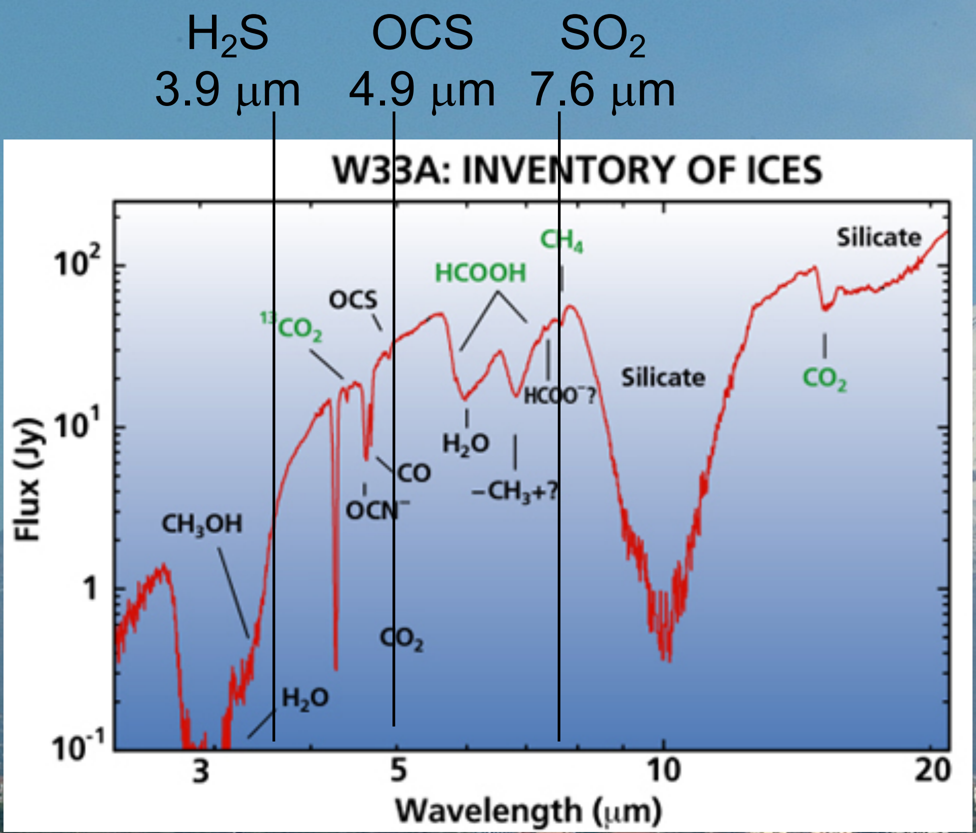
Icy grain mantles



- Freeze out of gas phase species (CO)
- Grain surface reactions (H_2O, CH_3OH, CH_4, H_2S)
- Energetic processing of icy mantles (CO_2 , OCS)

S-bearing species in icy grain mantles

Source	Abundances			
	N(OCS)/N(H_2O)	N(SO_2)/N(H_2O)	N(OCS)/N(H)[a]	N(SO_2)/N(H)[a]
Mon R2 IRS 2	5.5×10^{-4b}		3.2×10^{-8b}	
AFGL 989	1.0×10^{-3b}		2.3×10^{-8b}	
W33A	4.0×10^{-4b}	$(3.1 \pm 1.6) \times 10^{-3c}$	7.0×10^{-8b}	$(6.2 \pm 3.2) \times 10^{-7c}$
NGC 7538 IRS 1	$<5.0 \times 10^{-4d}$	$(8.0 \pm 2.0) \times 10^{-3c}$	$<7.6 \times 10^{-9d}$	$(1.2 \pm 0.3) \times 10^{-7c}$
NGC 7538 IRS 9	5.0×10^{-4e}	$<5.0 \times 10^{-3c}$	3.4×10^{-8e}	$<3.4 \times 10^{-7c}$



S-bearing species towards high-mass YSOs (Palumbo et al. 1995, 1997; Boogert et al. 1997; Gibb et al. 2004)

H_2S upper limits (Smith 1991)

SO_2 upper limits towards low-mass YSOs (Oberg et al. 2008)

Open questions

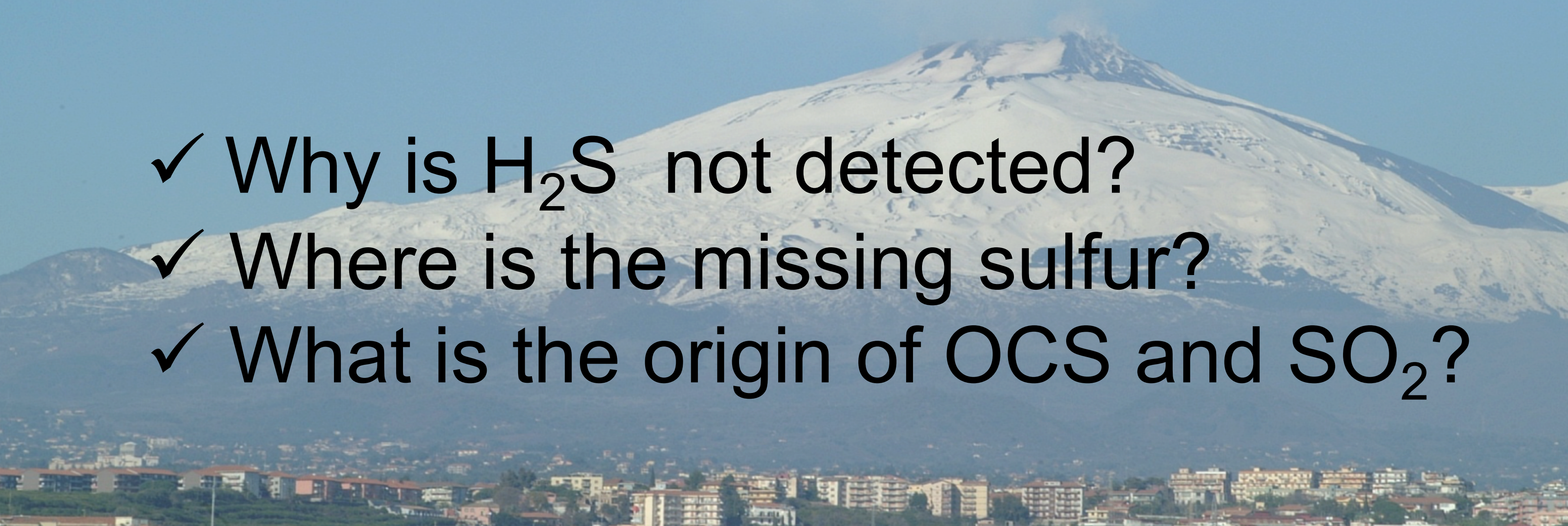
➢ Theoretical gas-phase chemistry models require very low elemental S abundances in order to explain the observations of S-bearing molecules in molecular clouds.

- abundance of S in the diffuse ISM about 10^{-6}-10^{-5} w.r.t. H (van Steenbergen & Shull 1988; Sofia et al. 1994; Lodders 2003)

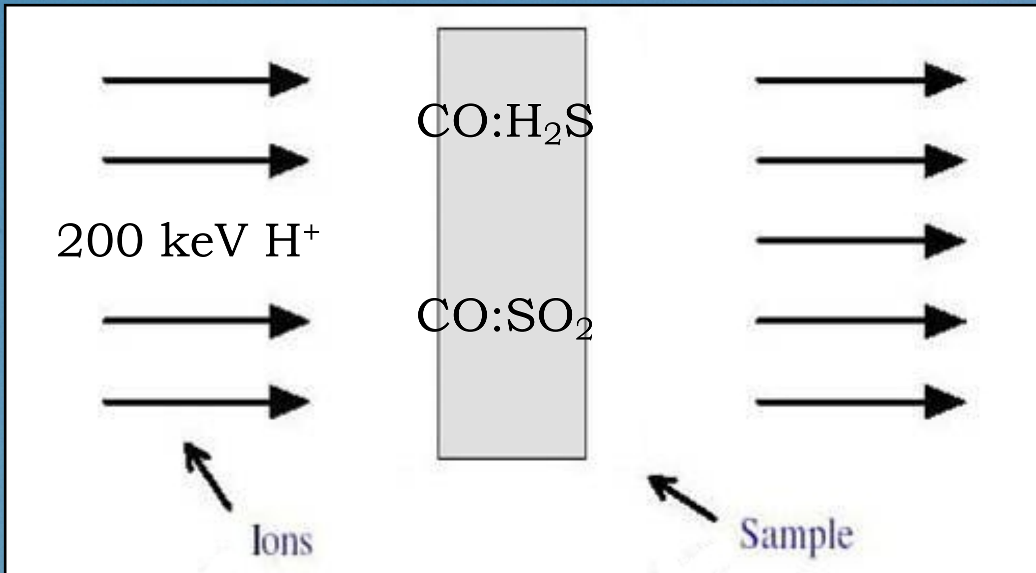
- abundance of S in gas-grain models of dense molecular clouds, 10^{-9}-10^{-8} w.r.t. H (e.g. Doty et al. 2002; Garrod et al. 2007; Aikawa et al. 2008)

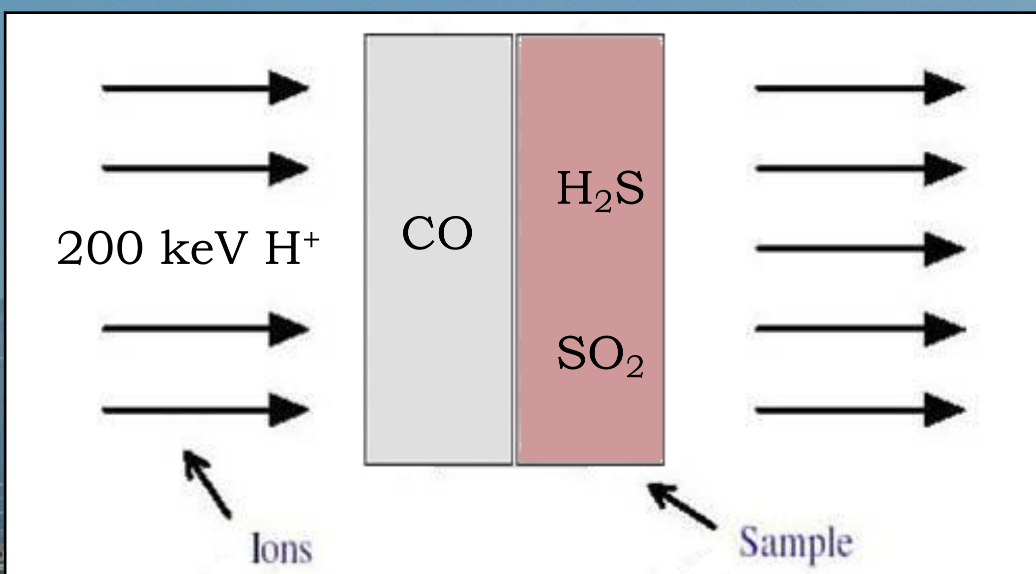
➢ Models predict large quantities of H_2S on grains after hydrogenation of S atoms.

✓ Why is H_2S not detected?
✓ Where is the missing sulfur?
✓ What is the origin of OCS and SO_2?



Mixed and layered samples





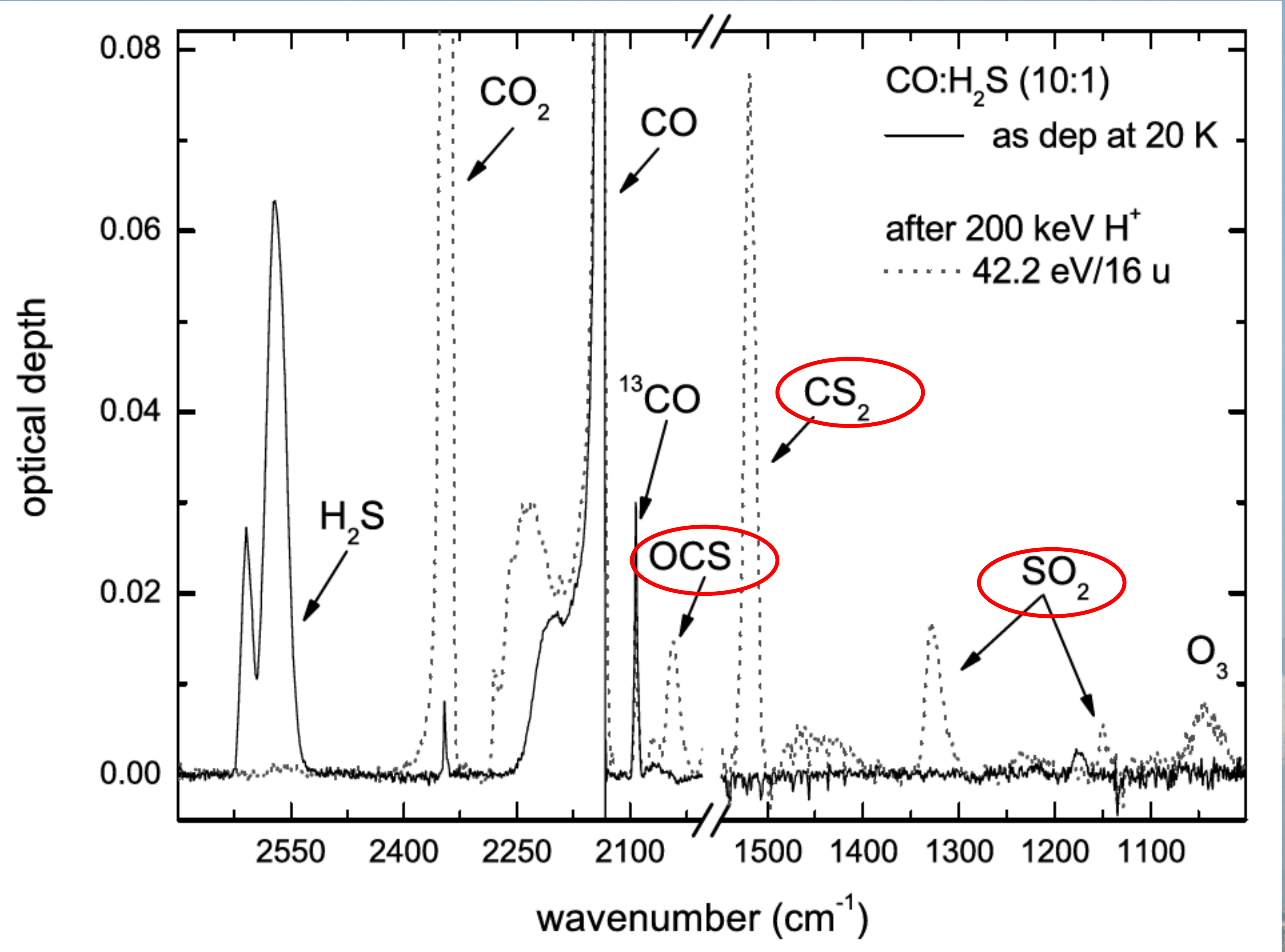
Studied samples (T=16-20 K)

- ✓ pure CO
- ✓ pure H_2S
- ✓ pure SO_2
- ✓ CO/H_2S layer
- ✓ $CO:H_2S$=10:1 (mixture 1)
- ✓ $CO:H_2S$=1:10 (mixture 1)
- ✓ CO/SO_2 layer
- ✓ $CO:SO_2$=5:1

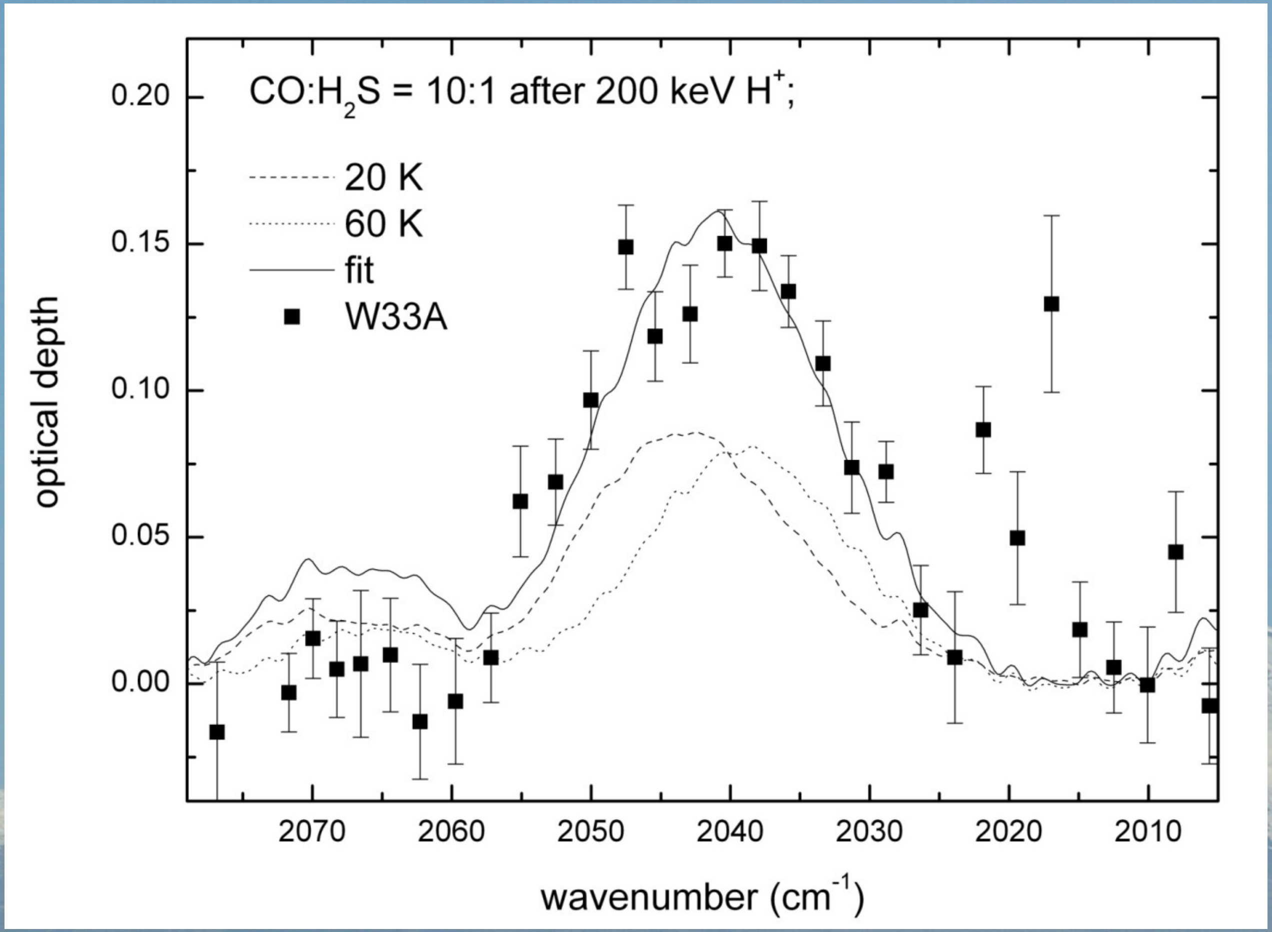
Palumbo et al. 2008, ApJ 685, 1033
Garozzo et al. 2008, Pl. Sp. Sci. 56, 1300
Garozzo et al. 2010, A&A 509, A67

$CO:H_2S$=10:1 +200 keV H^+

Ferrante et al. 2008, ApJ 684, 1210
Garozzo et al. 2010, A&A 509, A67



Comparison with observations

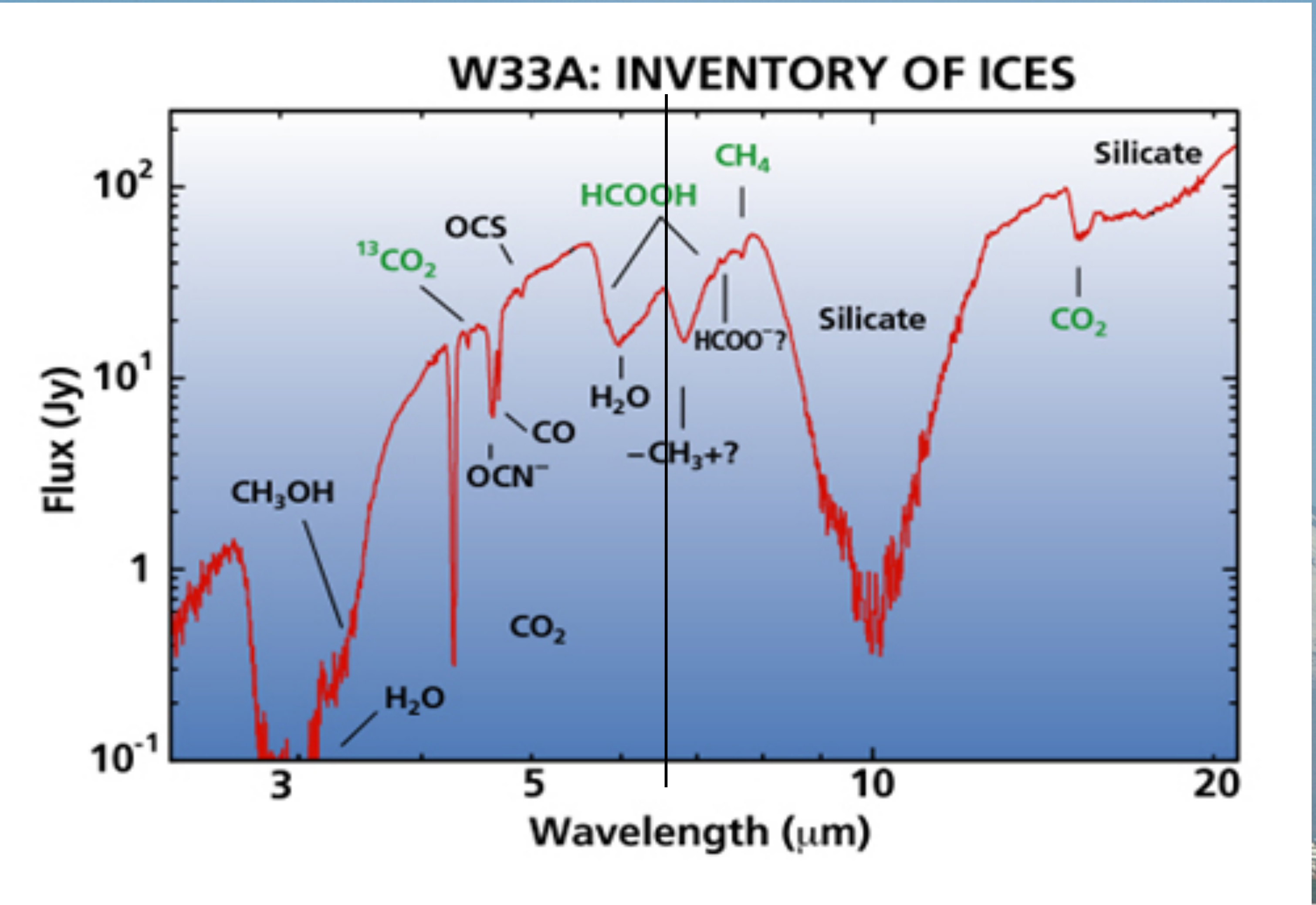


Ferrante et al. 2008, ApJ 684, 1210
Garozzo et al. 2010, A&A 509, A67

Evidence of temperature gradient along the line of sight

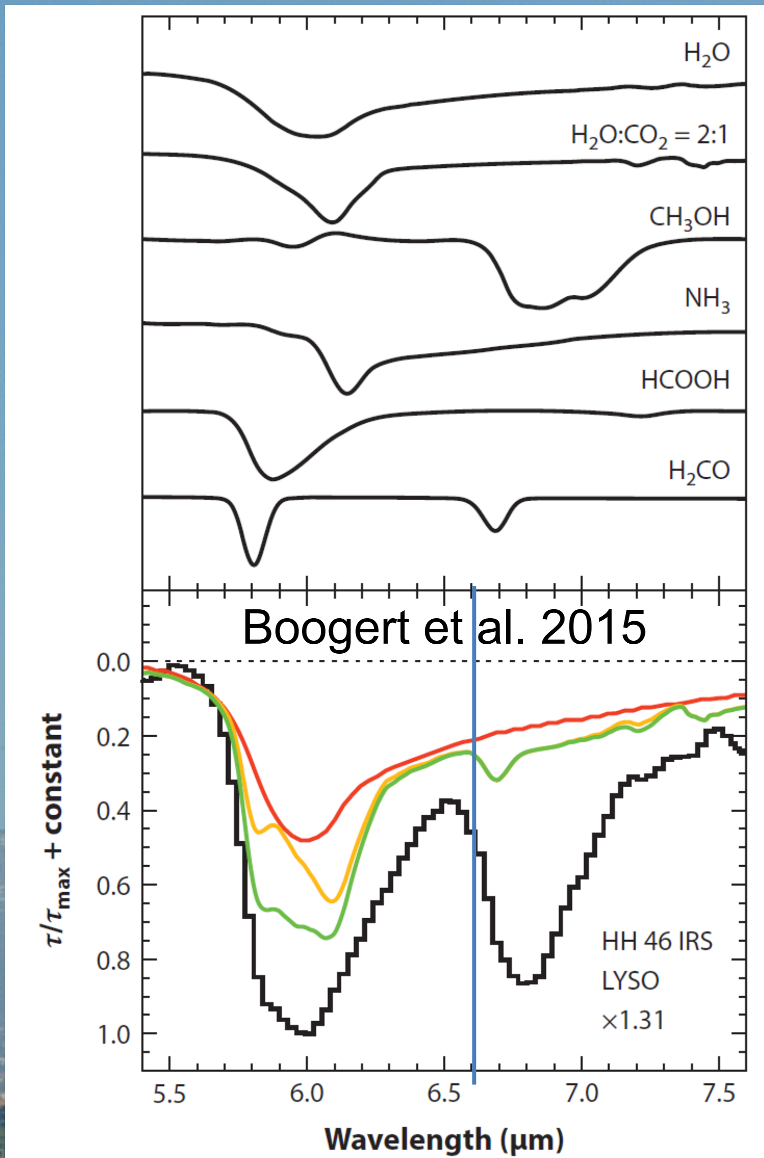
CS_2 in icy grain mantles?

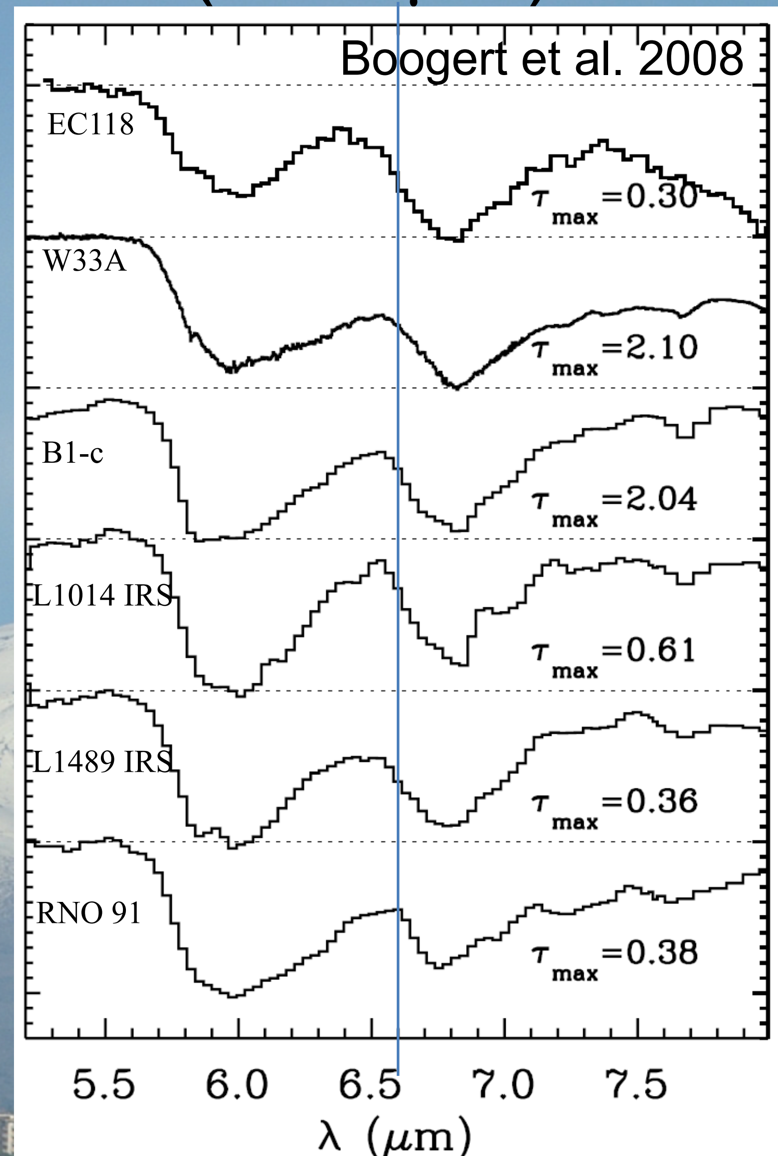
main band at 1515 cm^{-1} (6.60 μm)



CS_2 in icy grain mantles?

main band at 1515 cm^{-1} (6.60 μm)





JWST – ERS

PI: Melissa McClure
co-PI: A.C.A. Boogert and H. Linnartz
Program ID 1309

IceAge: Chemical evolution of ices during star formation

- ✓ Prestellar core
- ✓ Class 0 protostar
- ✓ Class I protostar
- ✓ Protoplanetary disk

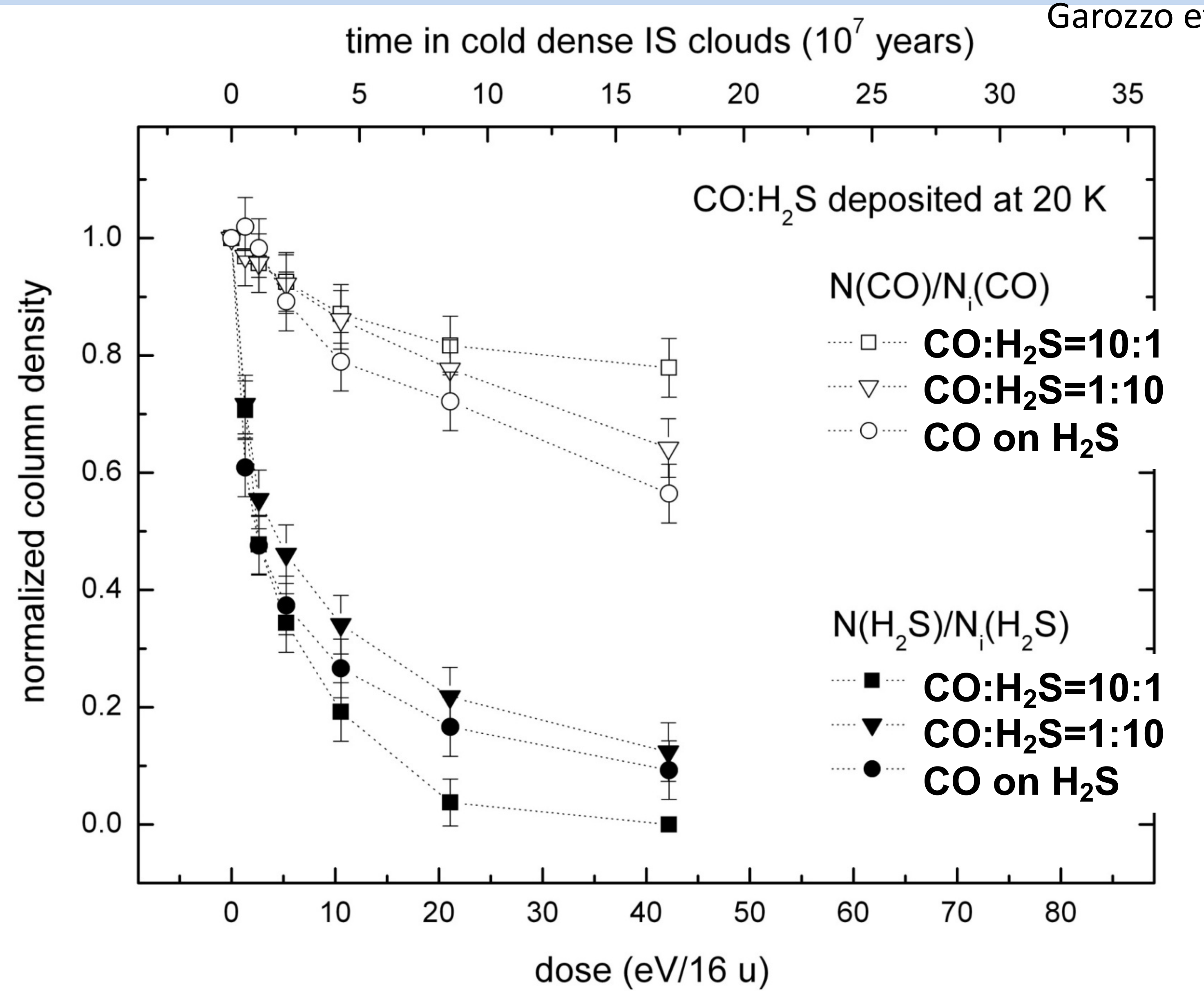
- **NIRSpec and MIRI**
- **R = 1500 – 3000**
- **S/N = 100 – 300**

Acknowledgments

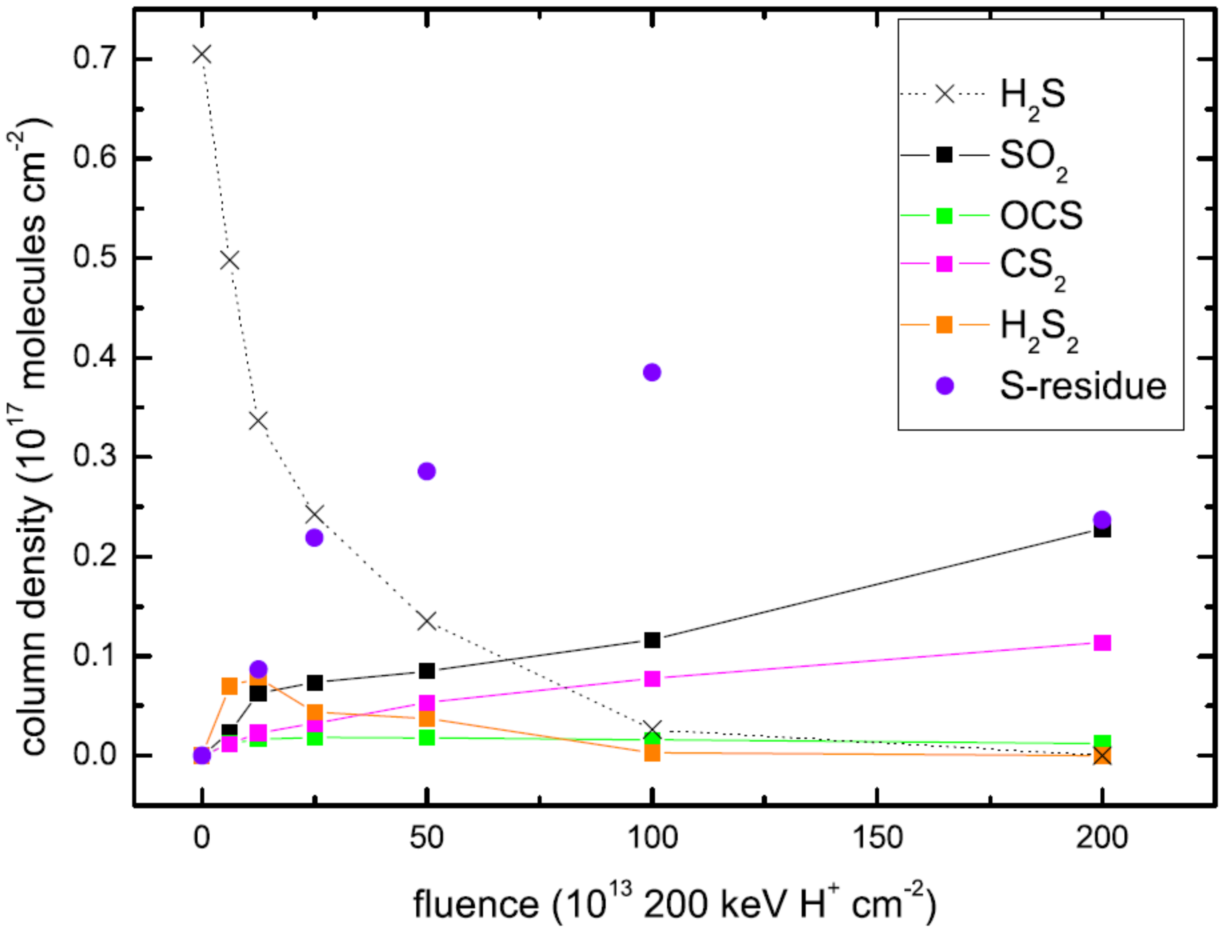
iALMA
Genesis - SKA
REGIONE SICILIA
Osservatorio Astrofisico di Catania
cost
EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY
MIUR PRIN
VAMDC
Virtual Atomic and Molecular Data Centre
asi
LASSIE
Vamos Seguro
INAF

H_2S and CO destruction

Garozzo et al. 2010



S-rich residue



Woods P.M., Occhiogrosso A., Viti S., Kanuchova Z., Palumbo M.E., Price S.D., 2015, MNRAS 450, 1256