Laboratory Spectroscopy of Ices of Astrophysical Interest

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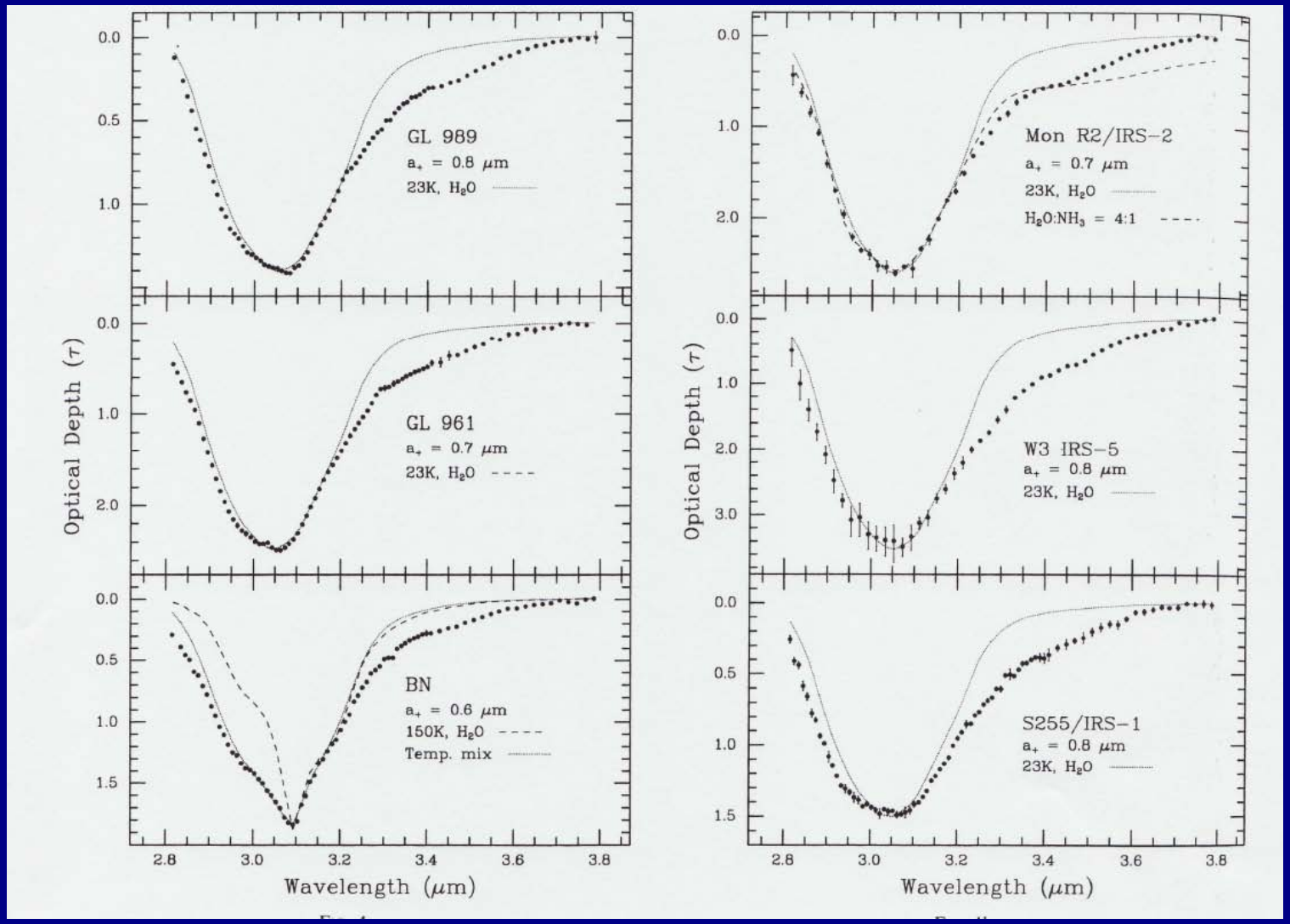
Some Icy Space Environments

Identified Interstellar Ices

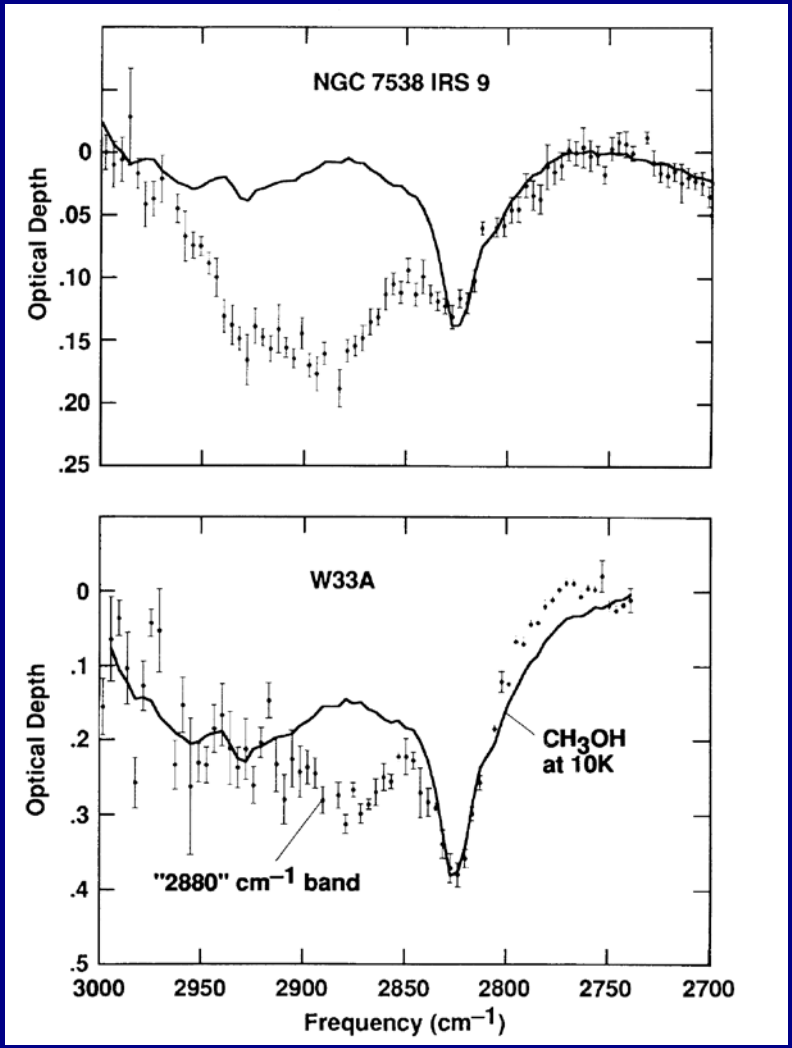
Wavelength (μm)	Molecule	Vibrational mode	Reference
3.05	**H_2O**	O-H str	Gillett & Forrest 1973 ; Gillett et al. 1975 ; Merrill et al. 1976
3.53	**CH_3OH**	CH_3- str	Allamandola et al. 1992
4.27	**CO_2**	Antisym. Str	de Graauw et al. 1996
4.38	**$^{13}CO_2$**	CO str	de Graauw et al. 1996
4.62	**OCN^-**	C=N str	Grim and Greenberg 1987; Demyk et al. 1998
4.67	**CO**	CO str	Lacy et al. 1985; Larson et al. 1985; Whittet et al. 1985; Geballe et al. 1986
4.90	**OCS**	CO str	Palumbo et al. 1995
7.7	**CH_4**	CH def	Lacy et al. 1991
15.2	**CO_2**	CO_2 bending	de Graauw et al. 1996
44	**H_2O**	t opt & long acou	Papoular et al. 1978; Erickson et al. 1981; Omont et al. 1990; Dartois et al. 1998

Example # 1: H_2O at 3.05 μm (3279 cm^{-1})



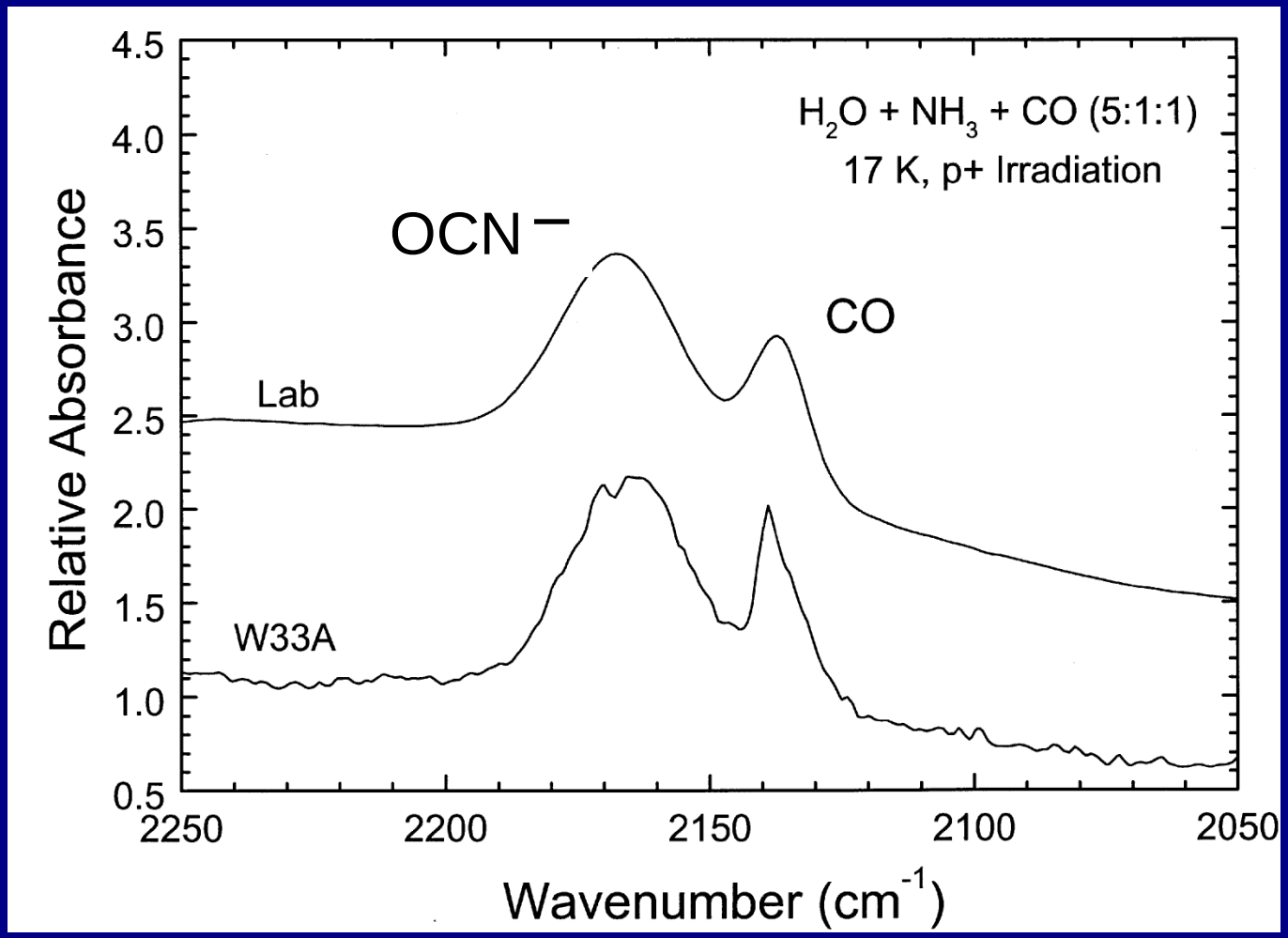
Smith et al. 1989

Example # 2: CH_3OH at 3.53 μm (2885 cm^{-1})



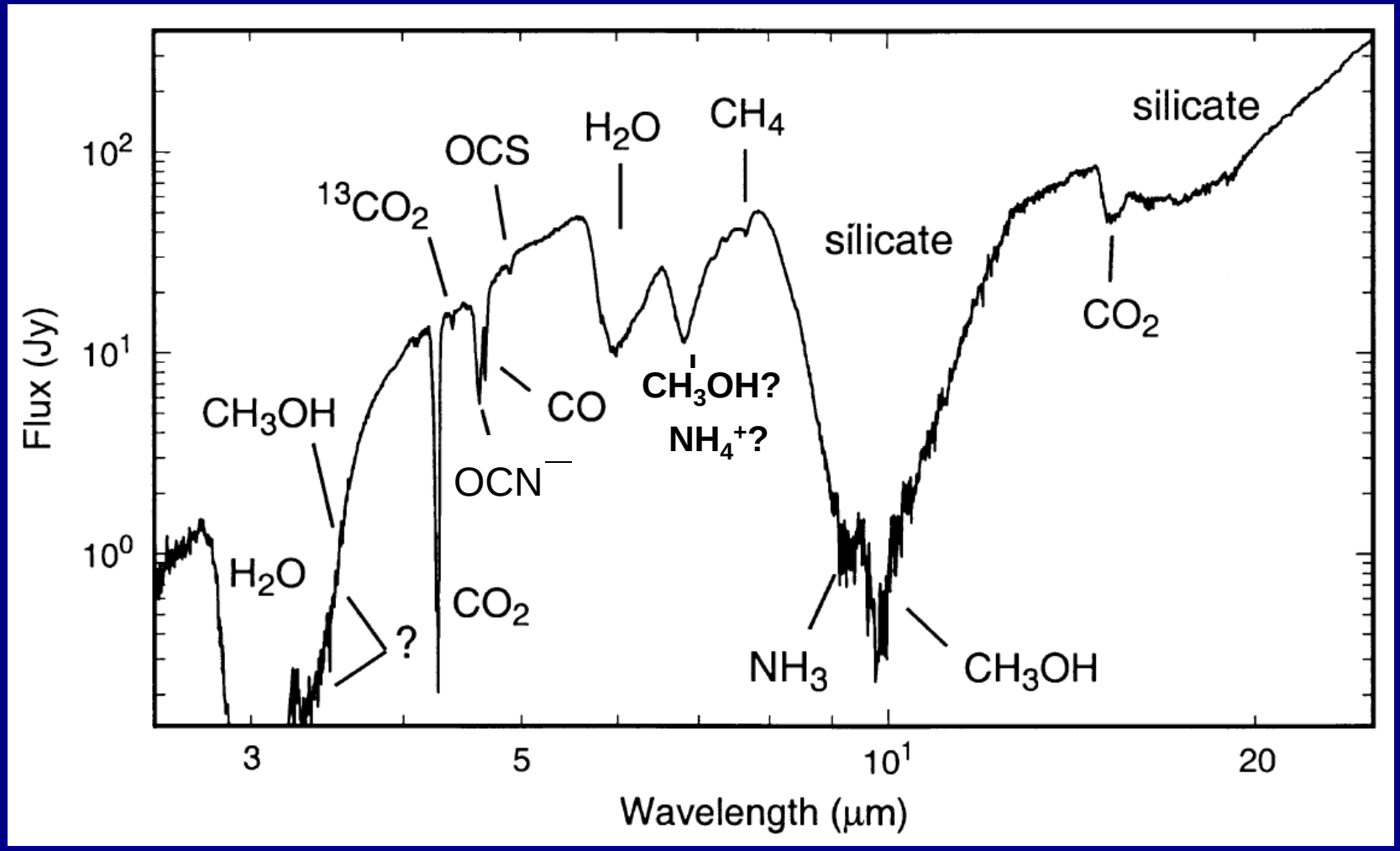
Allamandola et al. 1992

Example # 3: OCN^- at 4.62 μm (2165 cm^{-1})

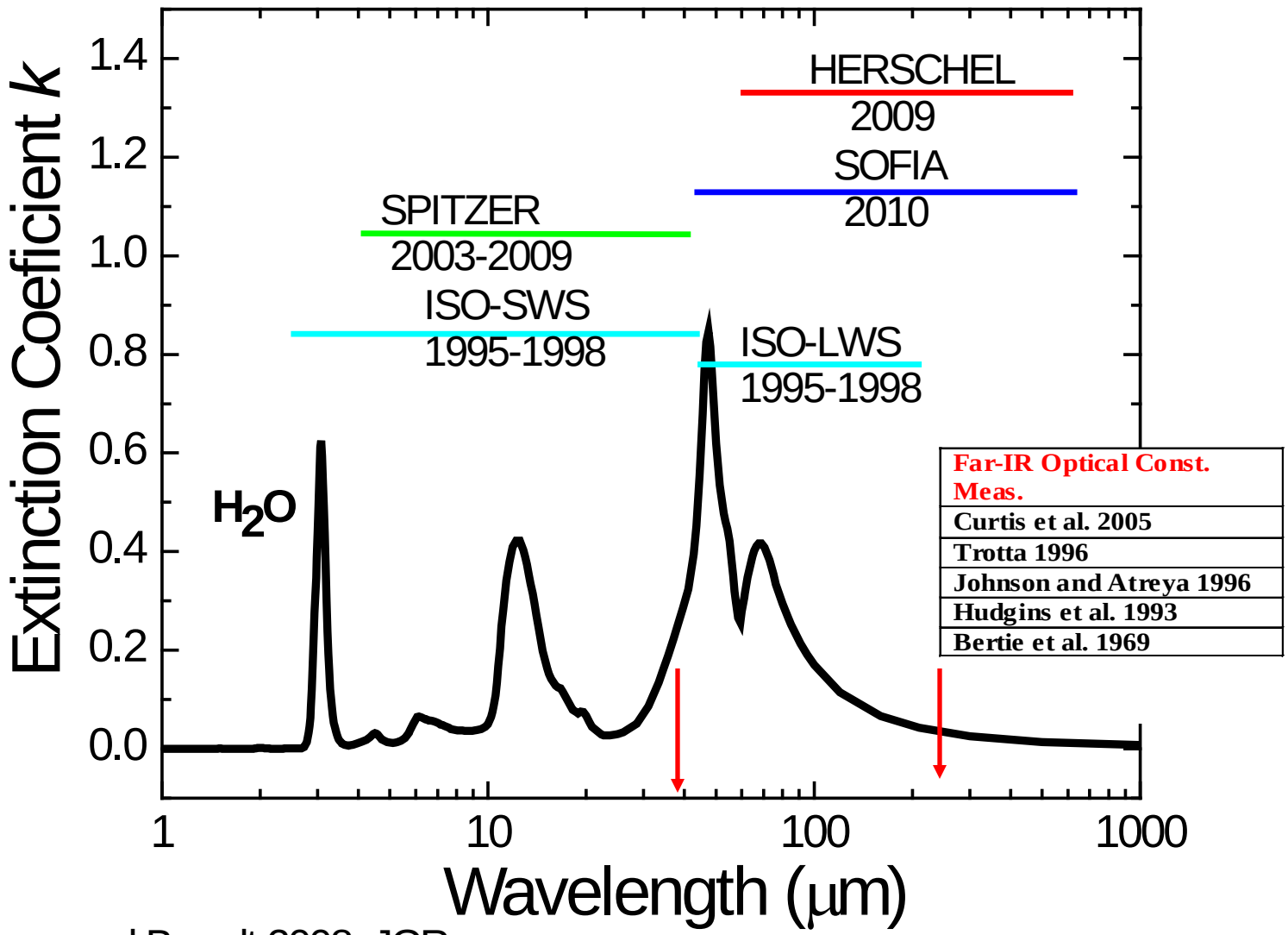


Hudson et al. 2001 and references therein

Complete ISO 2.4 – 25 µm SWS flux spectrum of W33A



Gibb et al. 2000



Warren and Brandt 2008, JGR

Factors affecting general characteristics
of IR absorption features such as
precise peak position, band shape, and FWHM

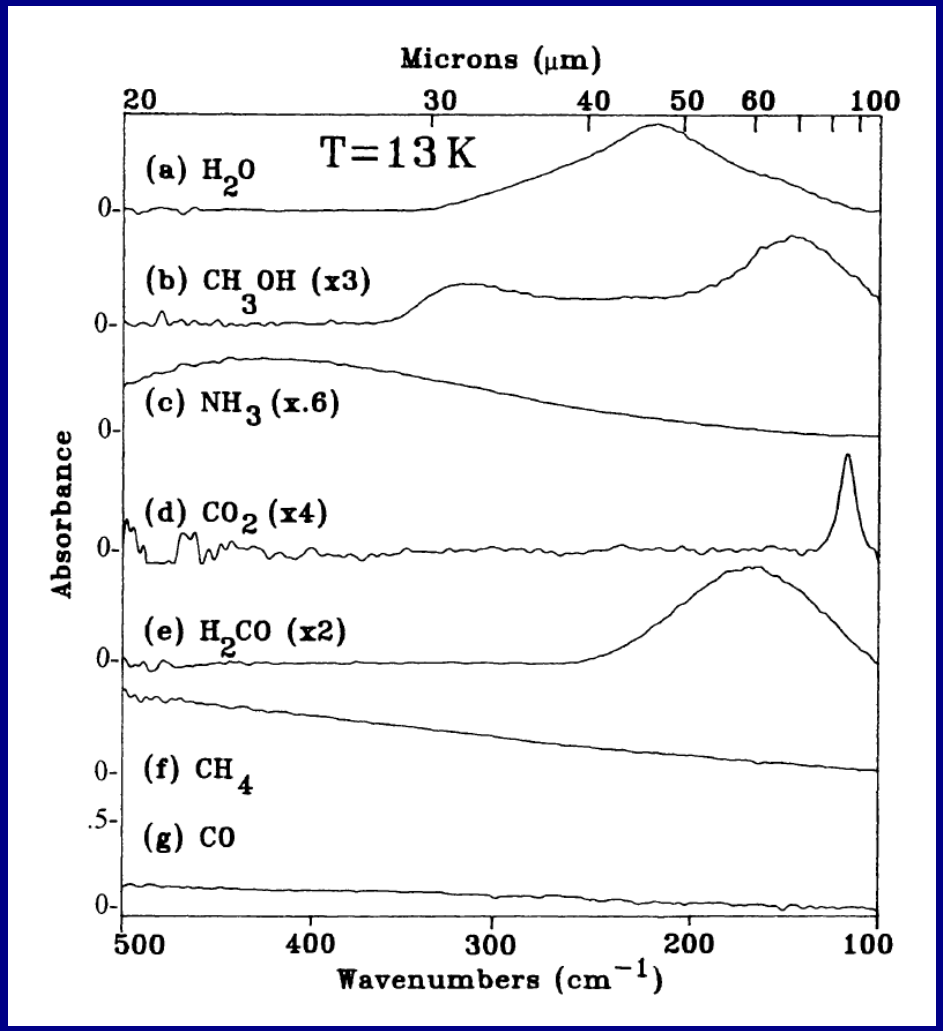
Pure Ices

(1) Phase - Amorphous and Crystalline
(2) Temperature
(3) Crystalline quality

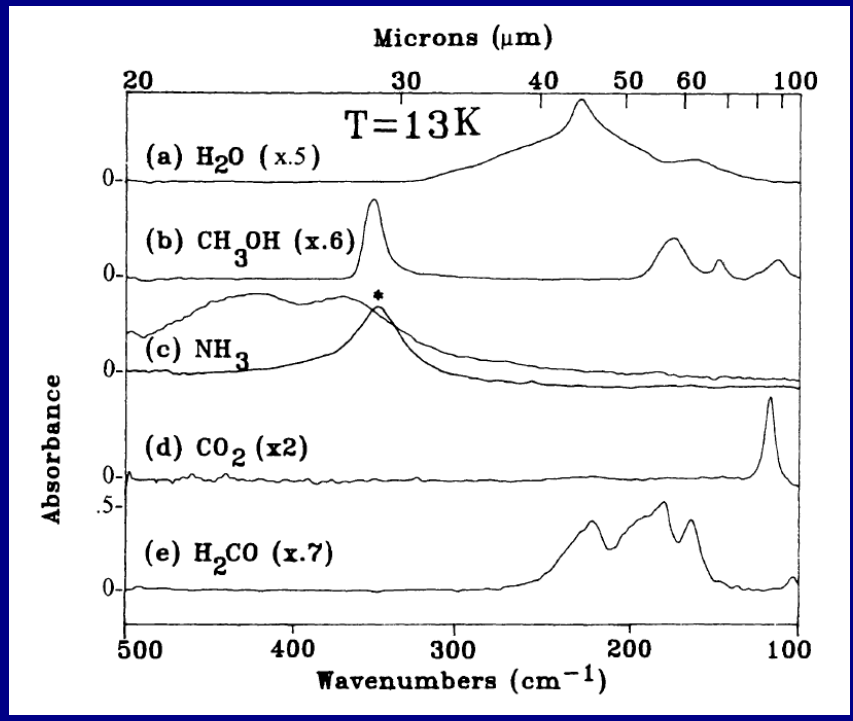
(1) Peak position, band shape, and FWHM depend on:

Phase (Example # 1)

Amorphous



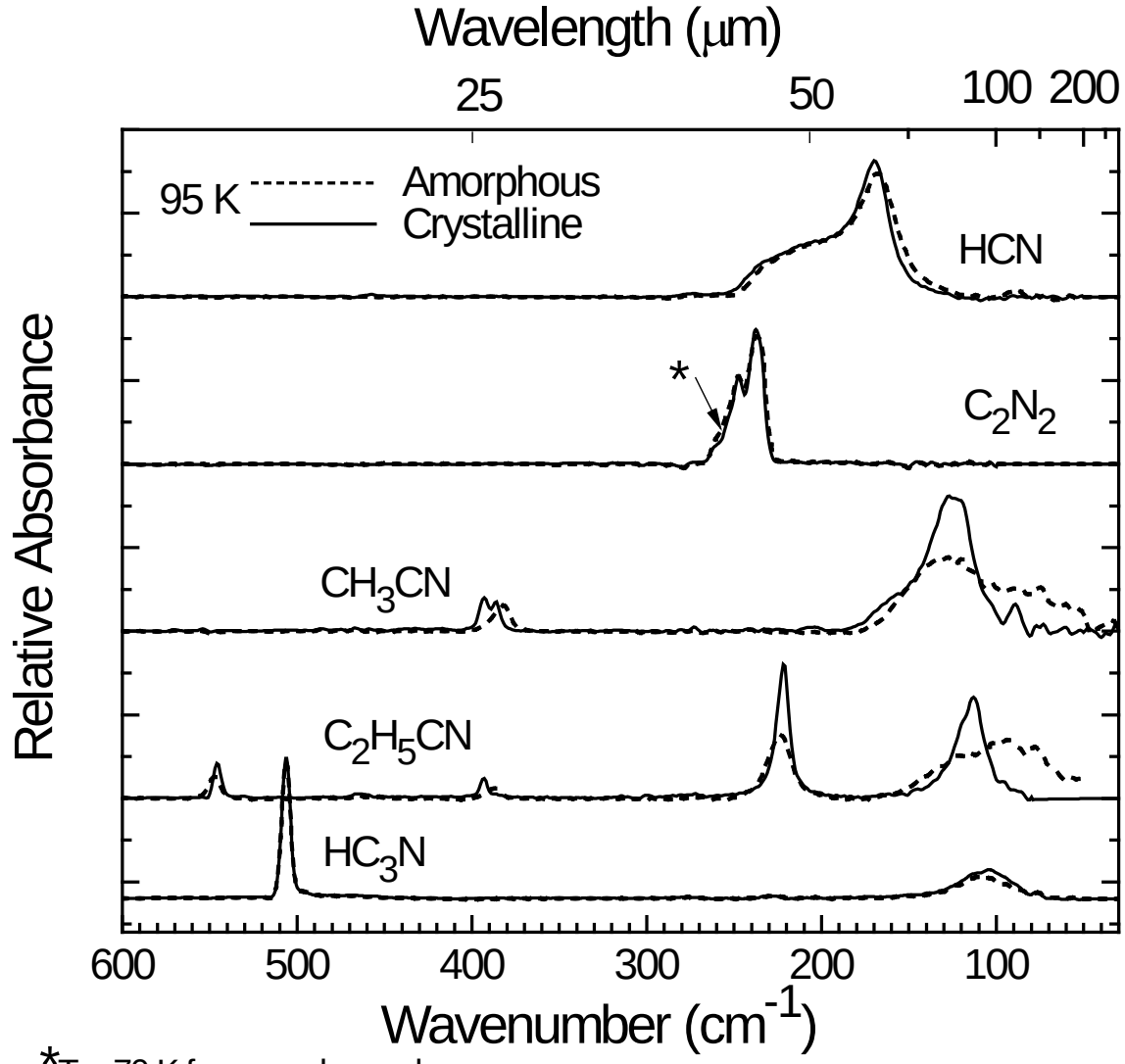
Crystalline



Moore et al. 1995

Peak position, band shape, and FWHM depend on:

Phase (Example # 2)



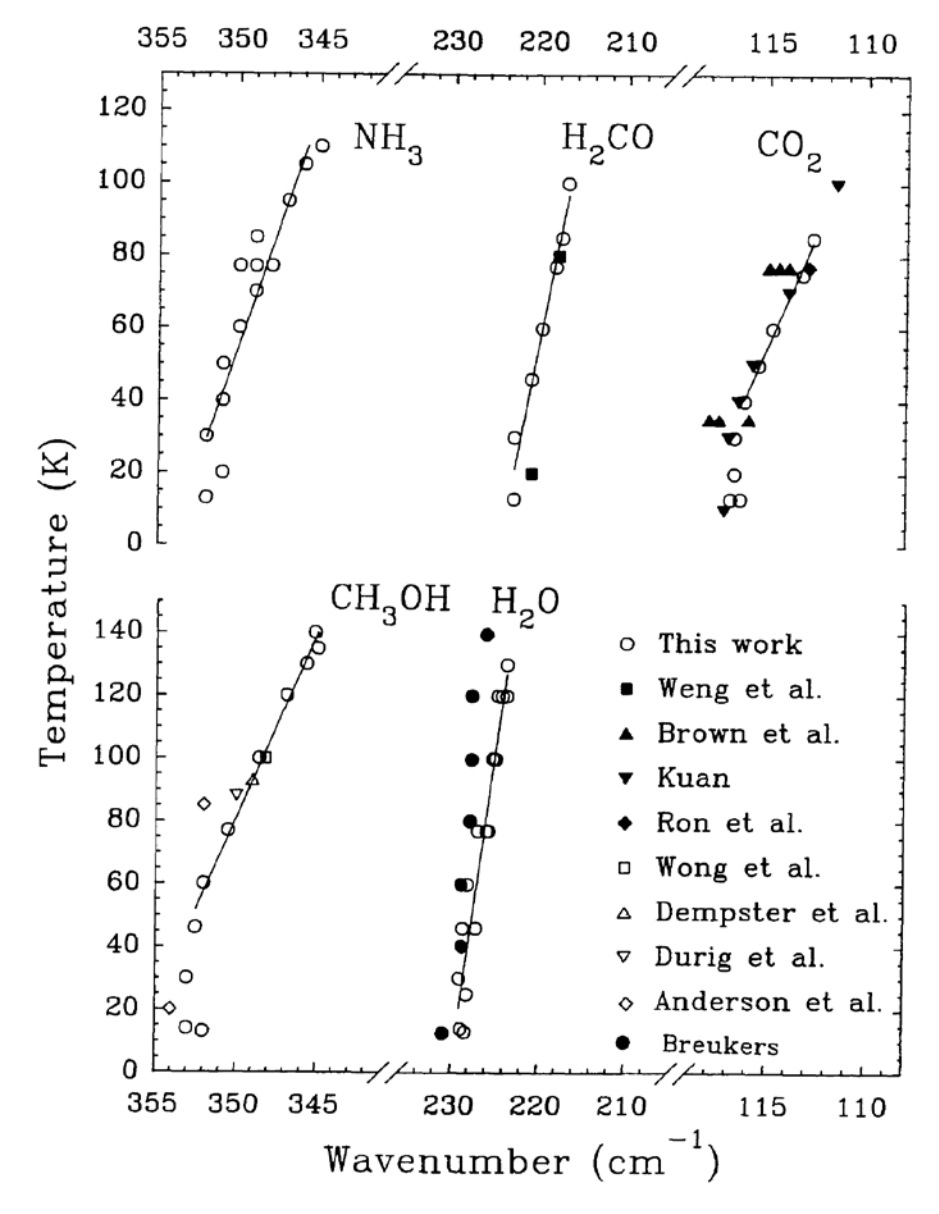
*T = 70 K for amorphous-phase

Moore et al. 2010

(2) Peak position of crystalline-phase ices depends on:

Temperature

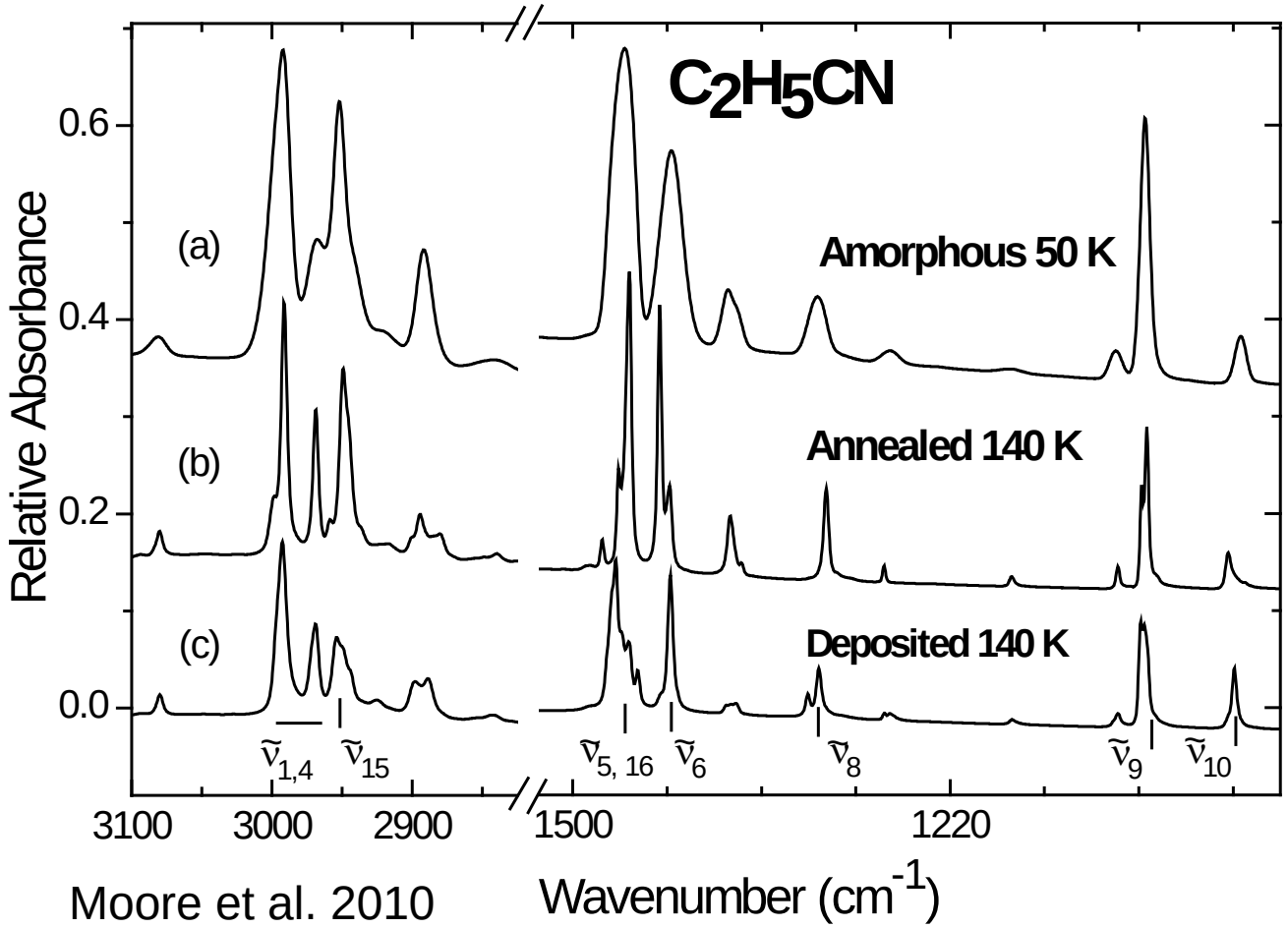
Changes are reversible



Moore and Hudson 1994

(3) Peak position, b**and shape, band splitting, and FWHM depend on:**

Crystalline Quality



Moore et al. 2010

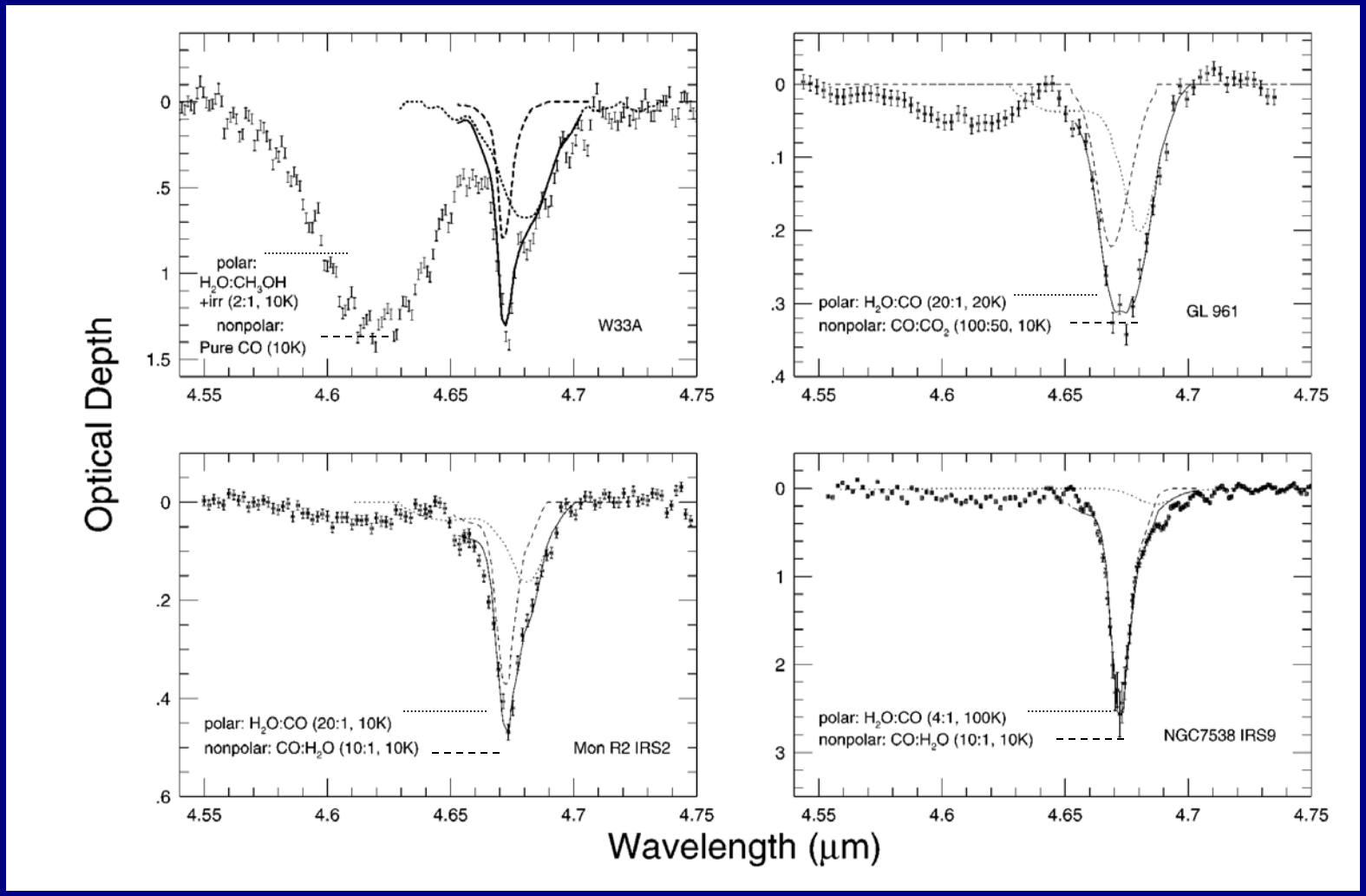
Factors affecting general characteristics of IR absorption features such as peak position, band shape, and FWHM

Icy Mixtures

(1) Matrix material, e.g. polar or non-polar
(2) Concentration
(3) Temperature
(4) Phase
(5) Crystalline quality

(1) Peak position, band shape, and FWHM depend on:

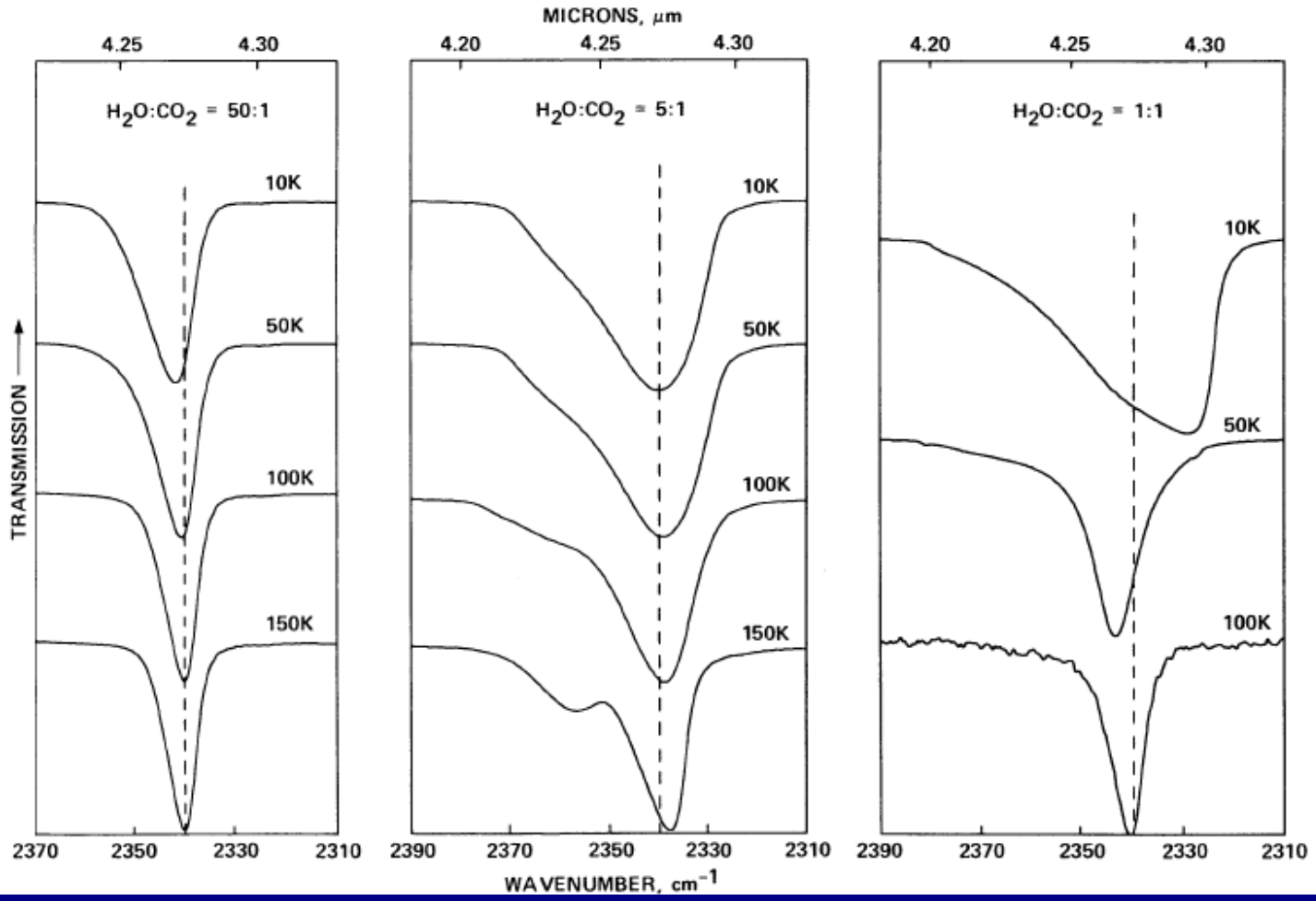
Matrix



Chiar et al. 1995

Peak position, band shape, and FWHM depend on:

(2) Concentration and (3) Temperature



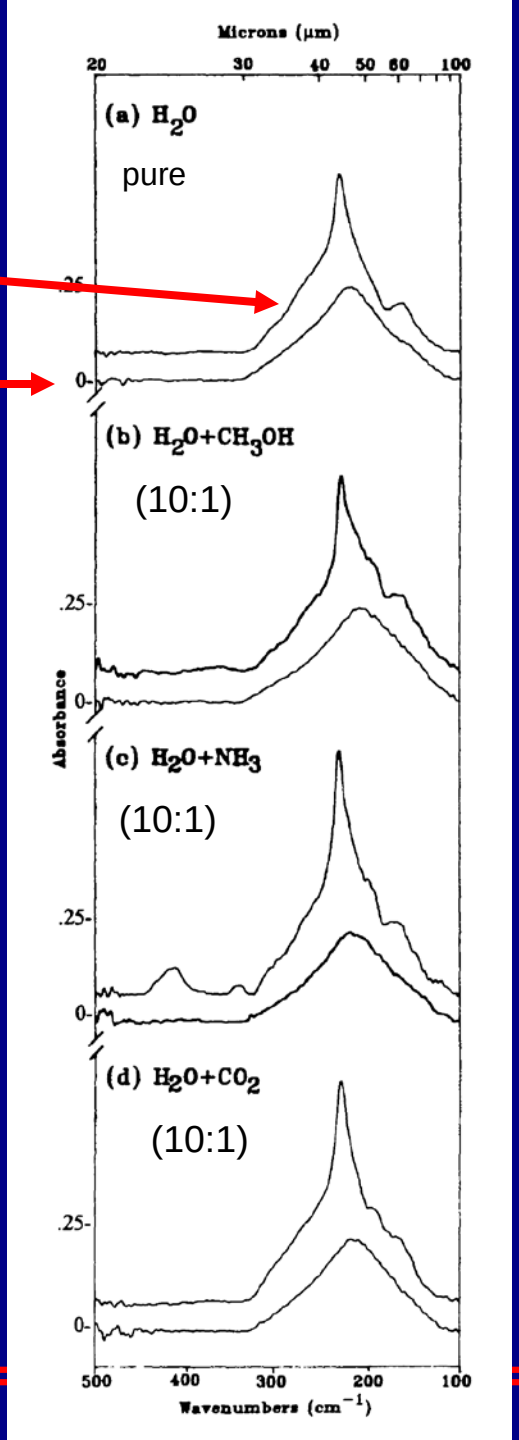
Sandford and Allamandola 1990

(3) Peak position, band shape, and FWHM depend on:

crystalline

Phase

amorphous



Far-IR spectra comparing amorphous and crystalline-phase pure H_2O with H_2O-dominate mixtures

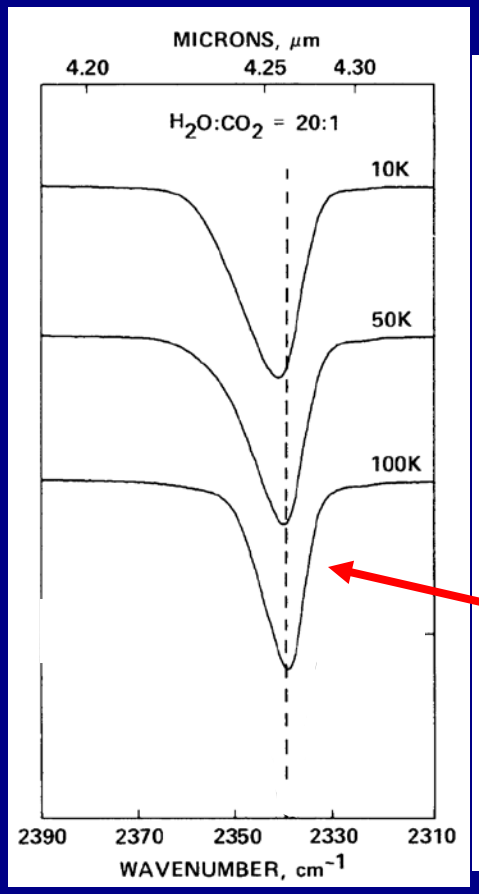
Moore and Hudson 1995

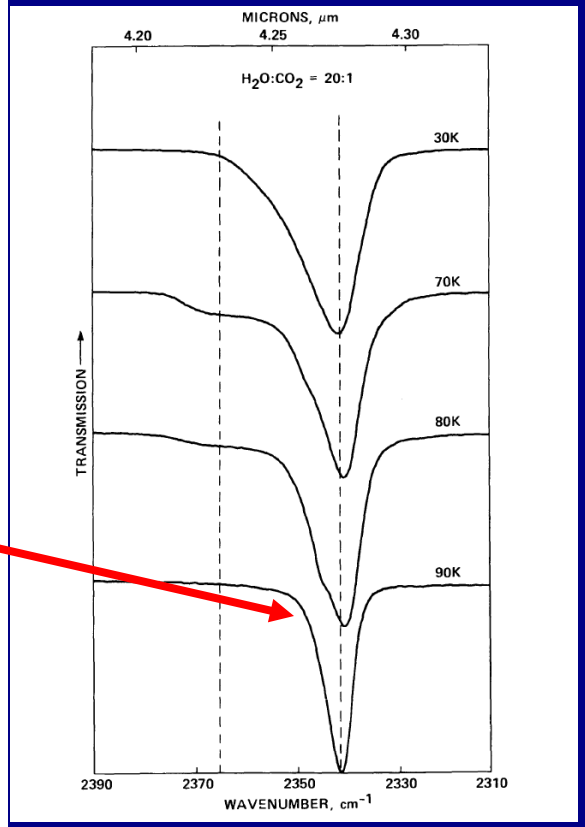
(5) FWHM depends on:

Crystalline Quality

$^{12}CO_2$ band in $H_2O:CO_2$ ice

as a function of warming





as a function of deposition temperature

Sandford and Allamandola 1990
also see discussion in Schmitt et al. 1998, and Smith et al. 1984

Calculated parameters from laboratory data of value for astronomers

1. Intrinsic band strength (*A*-value)

2. Absorption coefficient (α)

3. Optical constants (real (*n*) and imaginary (*k*) parts of the complex refractive index)

(1) Intrinsic band strength, *A*-value (cm/molec) – knowing the A-value and the area of the absorption feature means you can calculate the column density of that material in the observed line of site.

Potentially unsafe laboratory assumptions:

Density

Thickness

(2) Absorption coefficient, α, (cm^{-1}) – knowing α one can estimate the extinction coefficient (k) using

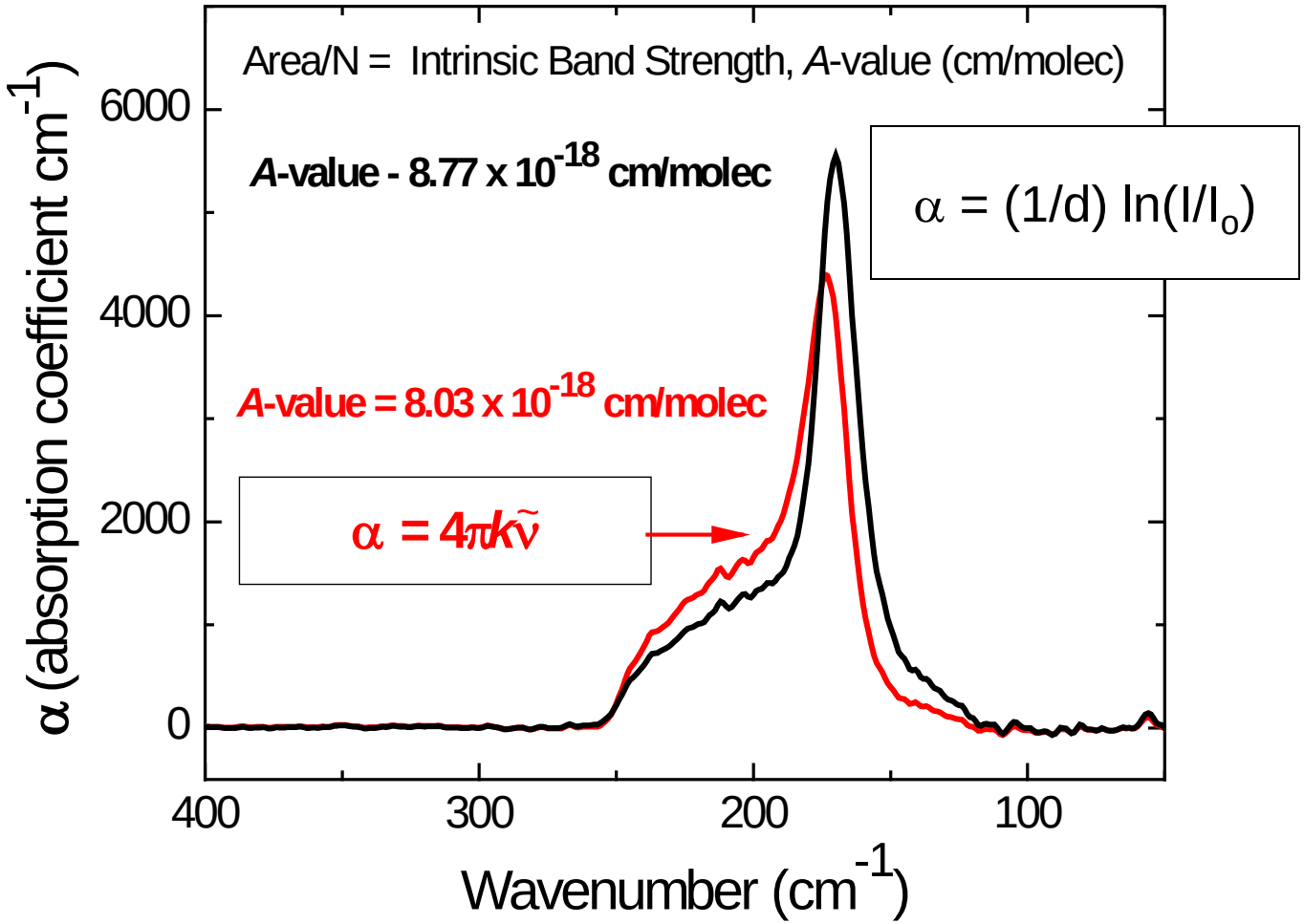
$$k = \alpha / 4\pi\tilde{\nu}.$$

Potentially unsafe laboratory assumptions:

Thickness

Reflection losses are negligible

Example -- error in *A*-value when you don't consider reflection losses



(3) Optical constants (*n* and *k*-values) – knowing these values, observed spectra can be treated quantitatively using a radiative transfer approach. Combined with scattering theory and particle size distributions, one can calculate synthetic spectra for fitting purposes.

Potentially unsafe laboratory assumptions

Thickness

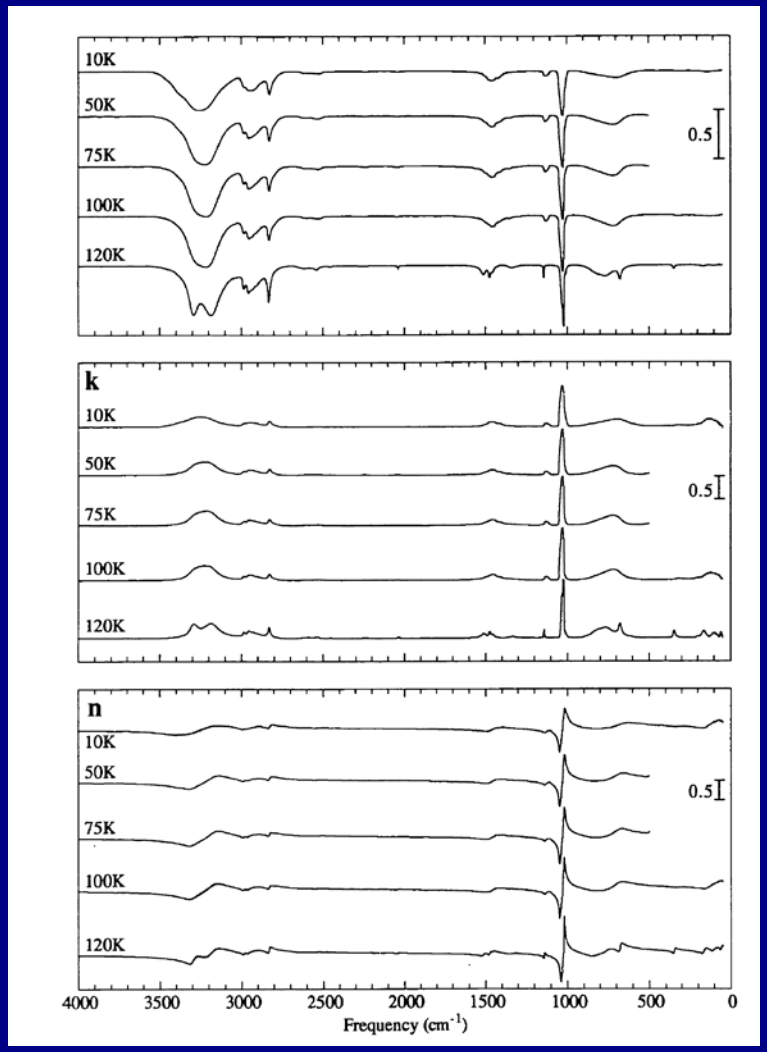
Density

Index of refraction

Summary of Some Current and Future Needs

- Laboratory IR spectroscopy of ices/icy-mixtures (relevant temperature and phase)
- Extraction of optical constants from spectra (mid-IR and far-IR regions)
- Determination of index of refraction
- Measurement of ice density for well determined laboratory conditions

CH_3OH



Hudgins et al. 1993

Existing Optical Constants Example #1

Amorphous- phase ice at different temperatures

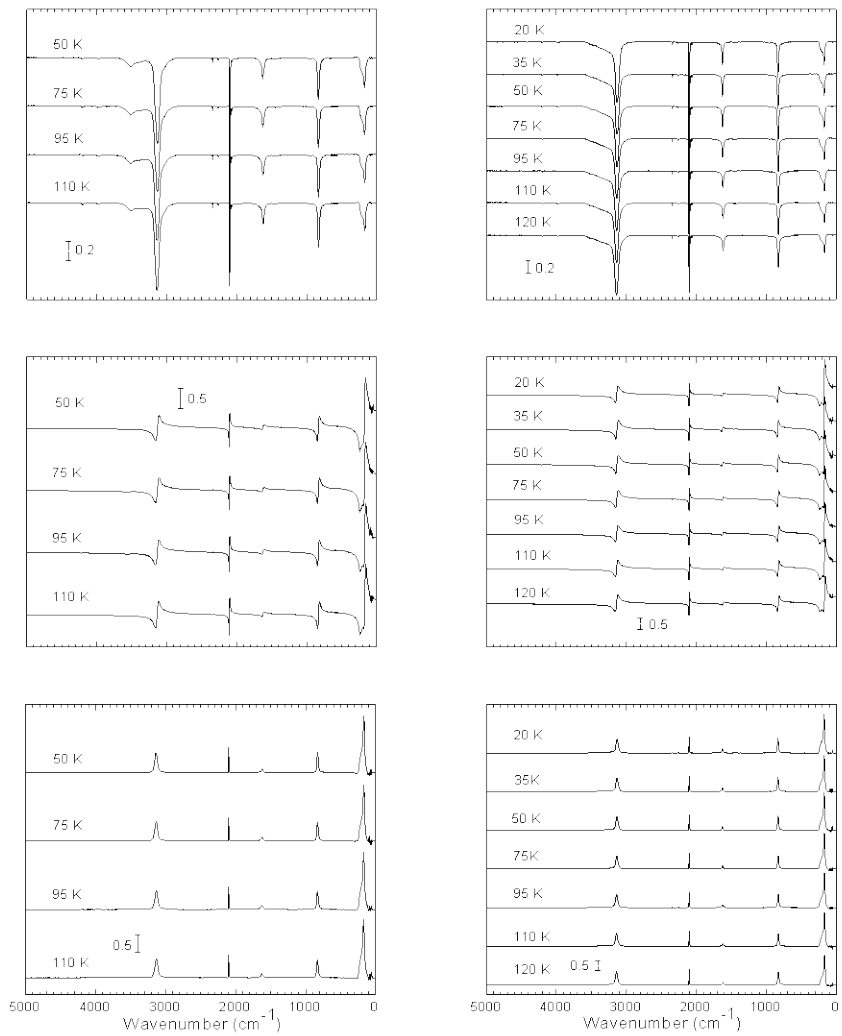
4000 - 500 cm^{-1}

H_2O	**CO**
CO_2	**CH_3OH**
CH_4	**OCS**
Mixtures	

500 – 50 cm^{-1}

H_2O	**CH_3OH**
H2O + CH3OH + NH3 + CO	

HCN



a. amorphous

b. crystalline

Moore et al. 2010

Existing Optical Constants
Example #2 - nitriles
Amorphous- and Crystalline phase ices at different temperatures

5000 - 30 cm^{-1}

HCN	HC_3N
C_2N_2	C_2H_5CN
CH_3CN	

http://science.gsfc.nasa.gov/691/cosmicice/

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The Cosmic Ice Laboratory

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Our research area is laboratory astronomy. We conduct radiation, photochemical, and other experiments related to comets, interstellar matter, and icy satellite surfaces. Since 2003 we have been a member of the Goddard Center for Astrobiology.

The Cosmic Ice Laboratory - What We Do

Our laboratory is part of the Astrochemistry Branch in the Laboratory for Extraterrestrial Physics at NASA's Goddard Space Flight Center. We specialize in studying the spectra, the chemistry, and the physical properties of ices relevant to comets, icy satellites and planets, and the coatings of dust grains in the interstellar medium. Although many cosmic ices are dominated by H_2O, they also contain "prebiotic" molecules such as CO, CO_2, CH_4, NH_3, and CH_3OH. In studying these molecules we are probing the early, ancient chemistry which eventually led to the origin of life.

In our laboratory we prepare ices by using a cryostat to condense gas-phase mixtures to temperatures as low as 10 K. The ices are made in a vacuum system to simulate the low pressure of outer space, and also to avoid undesirable contamination from the Earth's atmosphere. An infrared spectrometer is used to record spectra of an ice during experiments.

Our laboratory set-up is unusual because it is interfaced not only to a Van de Graaff accelerator, that can produce protons at energies up to about 1 million

Acknowledgements

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