ICE Observations with SPICA

Helen Fraser

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Why ice?


MATTHEW McCONAUGHEY
ANNE HATHAWAY
JESSICA CHASTAIN
AND MICHAEL CAINE
THE END OF EARTH WILL NOT BE THE END OF US.
FROM THE DIRECTOR OF THE DARK KNIGHT TRILOGY AND INCEPTION
INTERSTELLAR
COMING SOON


A FILM BY CHRISTOPHER NOLAN
INTERSTELLAR
IN CINEMAS NOVEMBER 7

The "Universal" Water Cycle

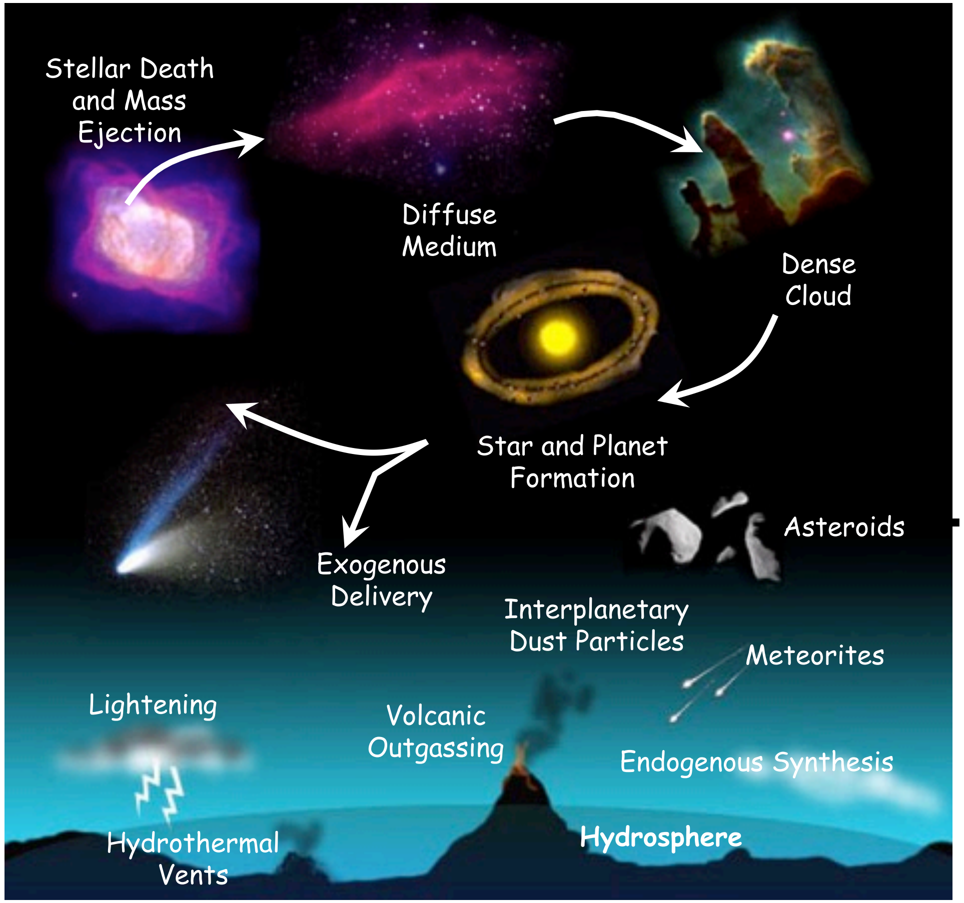


Image adapted from Stars 'R' Us material

Water in ISM =
SOLID / GAS Ø ONLY

Planetary systems =
Water can vitally ALSO exist in liquid Ø which provides the environment for biological, geological & atmospheric evolution.

ICE = largest molecular reservoir in Universe (excluding (H_2))

In SFR SOLID H_2O = more abundant than gas-phase CO!!!!!!!

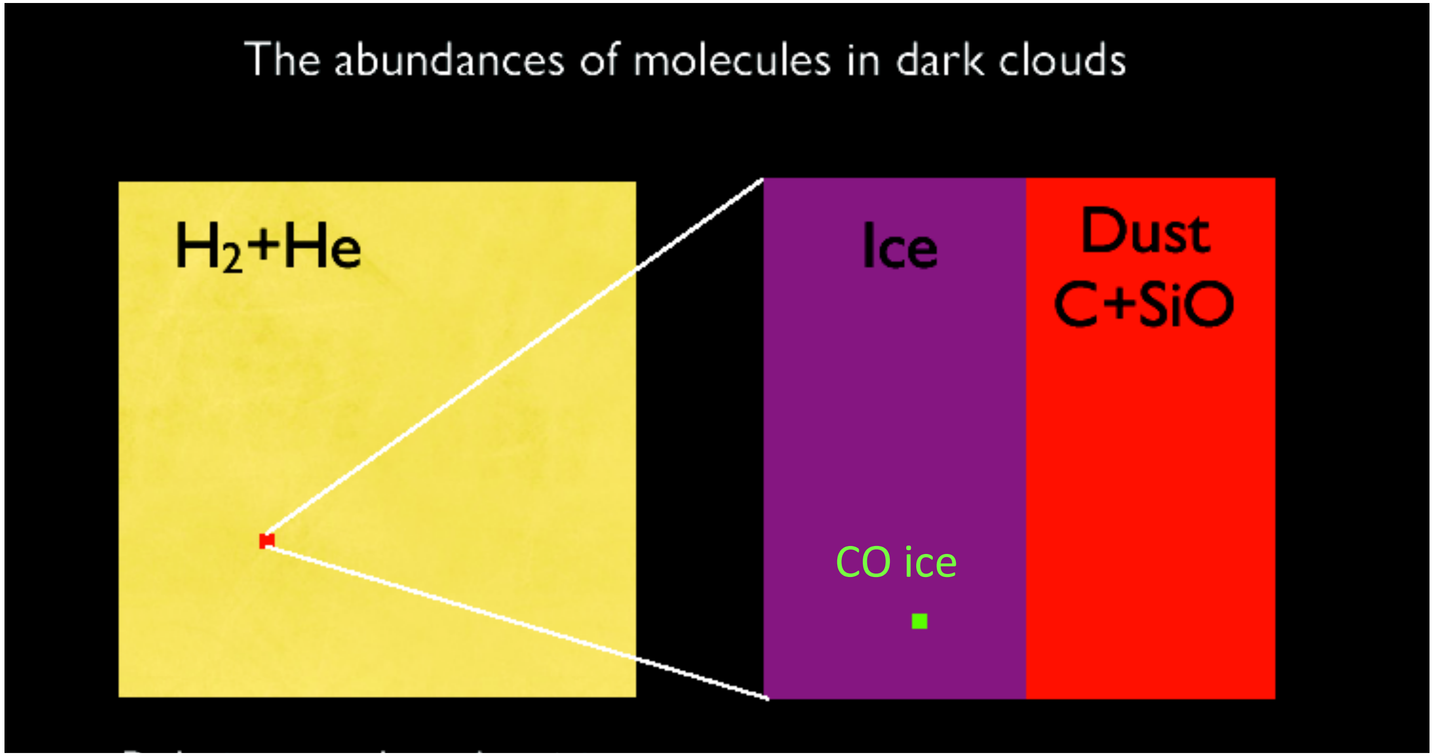


Image courtesy of K Pontoppidan

Affects gas-solid synergy (molecular reservoir (trapping))

→ Affects grain sticking (ice porosity = “glue”)

Affects reactivity (binding sites and surface area) / H_2 formation

Affects mobility (deuteration exchange & outgassing)

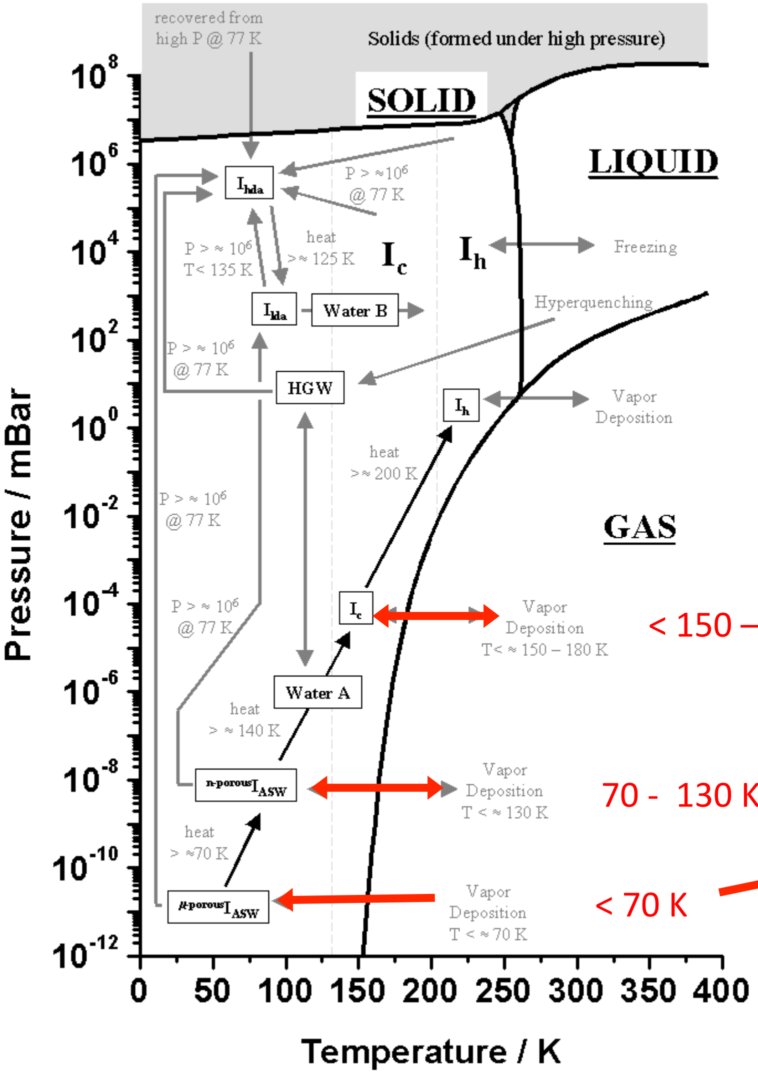
SPICA

- unique access to 12 – 210 μm
  - strongest gas cooling lines (of H_2O & isotopes) – rotational low J transitions (cold water)…higher J (warm gas / shocked gas / desorbed gas)
  - Ice esp. water at 44 and 63 μm
  - large grains
  - COMS & chemical link to ice

KILLER BENEFIT = concurrent view of the gas, dust, and ice involved in planet formation processes i.e. connecting the inner and outer disc (hot vs cold)

KILLER WINS = differentiate PHASE of ice
= potential ice scattering spectra
= "see" ice inside disks
= potential for ice linked to COMS – chemical links

The low P : low T Phase Diagram of H_2O

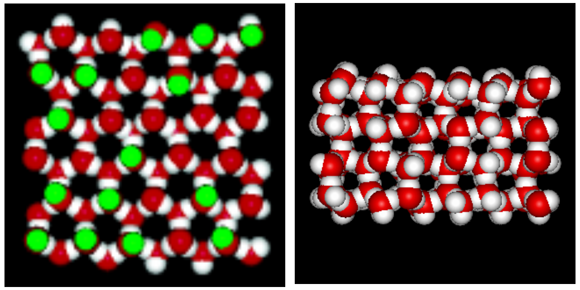


Ehrenfreund, Fraser, et. al. P&SS, 51, 473 (2003)

< 150 –180 K

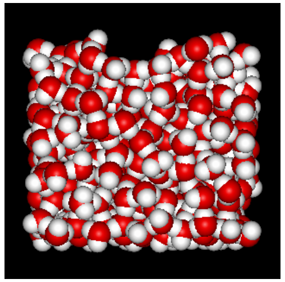
70 - 130 K

< 70 K

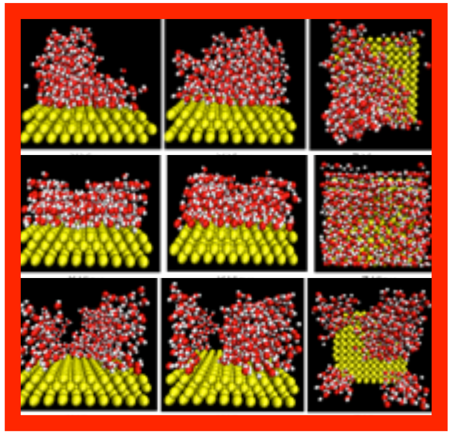


cubic crystalline ice I_c

compact ASW



porous ASW



Al Halabi et. al. JCP 120, 3358 (2004)

Al Halabi, Fraser et. al. A&A, 422, 777 (2004)

Essmann & Geiger
JCP 123, 234505 (1995)
[SPC/E: 1 trajectory
60 K surf, 150 K H_2O]

Miller et al JCP (2015)
in prep

Elkind & Fraser JCP (2015)
in prep

Ice 44 / 63 micron - SPICA

Molecular ices as temperature indicators for interstellar dust: the 44- and 62-μm lattice features of H_2O ice

R. G. Smith, G. Robinson, A. R. Hyland and G. L. Carpenter

ABSTRACT

Smith et al (2004) MNRAS
62/44 ratio can be growth dependent – can constrain ice deposition / growth mechanism

Measurements of the 44-μm band of H_2O ice deposited on amorphous carbon and amorphous silicate substrates

Marco M. Maldoni,[1*] Garry Robinson,[1*] R. G. Smith,[1*] W. W. Duley[2*] and A. Scott[2]

ABSTRACT

We present 20–110 μm absorbance spectra of H_2O ice, deposited on amorphous-carbon and silicate substrates, obtained over the 10–140 K temperature range. The measurements have been carried out in a manner that simulates the deposition, warming and cooling of H_2O ice mantles on interstellar and circumstellar grains. For H_2O ice films deposited on these substrates we find (i) similar 44-μm-band peak wavelength temperature dependences, (ii) no bandshape differences in the respective spectra, and (iii) a structural phase transition occurring between 120 and 130 K. In comparison with published data obtained using a polyethylene substrate, the 52-μm feature (the longitudinal optical mode) observed in our

Maldoni et al MNRAS (1999)
44 micron band SUBSTRATE dependent
Temperature dependency
Wing beyond 62 micron – reflects substrate

The Astrophysical Journal, 401:353–360, 1992 December 10

FAR-INFRARED SPECTRAL STUDIES OF PHASE CHANGES IN WATER ICE INDUCED BY PROTON IRRADIATION

Marla H. Moore

Astrochemistry Branch, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, MD 20771

AND

Reggie L. Hudson

Department of Chemistry, Eckerd College, St. Petersburg, FL 33733

ABSTRACT

Far-infrared spectra from 20 μm (500 cm^{-1}) to 100 μm (100 cm^{-1}) of water ice have been measured over the temperature range of 13–155 K. Amorphous and crystalline water ice are easily identified in far-infrared spectra since amorphous ice has one broad absorption peak near 45 μm (220 cm^{-1}) and crystalline has absorptions near 44 μm (229 cm^{-1}) and 62 μm (162 cm^{-1}).

We have observed radiation-induced phase changes in both amorphous and crystalline ice. Crystalline ice converts to an amorphous phase when irradiated at temperatures between 77 and 13 K. The conversion rate increases as the temperature is decreased and the converted fraction is dose dependent. No radiation-induced changes are detected in amorphous ice between 125 and 36 K. However, far-infrared spectra of proton-irradiated ices near 13 K show interconversion between the amorphous and crystalline ice phases beginning at doses near 2 eV $molecule^{-1}$ and continuing cyclically with increased dose. A quadrupole mass spectrometer

Moore & Hudson ApJ (1992)
Effects of proton irradiation (energetic processing on 44 / 63 mciron bands)

Bertie et al (1969)
44 micron = TO mode (closer 45 in amorph 43 in cryst)
63 micron = LA mode (usually weaker)
52 Micron = LO mode
LO / TO can be thickness & porosity dependent
LA / TO related to amorph / crystalline
Likely require GOOD lab data (opticcal const)
Peak intensity ratio uusally similar 44/62 therefore if 62 present 44 strong

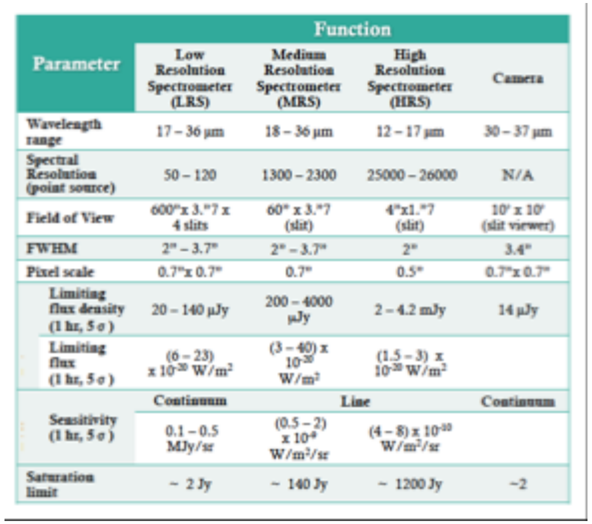
Curtis et al (2005) Applied Optics
Full set H2O optical const 15-200 micron
Temperature dependent

Measurement of the temperature-dependent optical constants of water ice in the 15–200 μm range

Daniel B. Curtis, Bhavani Rajaram, Owen B. Toon, and Margaret A. Tolbert

Need to considerspectroscopic effects
NEED TO CONSIDER EARLY LAB LIMITS: NOT ASW!!!

SMI

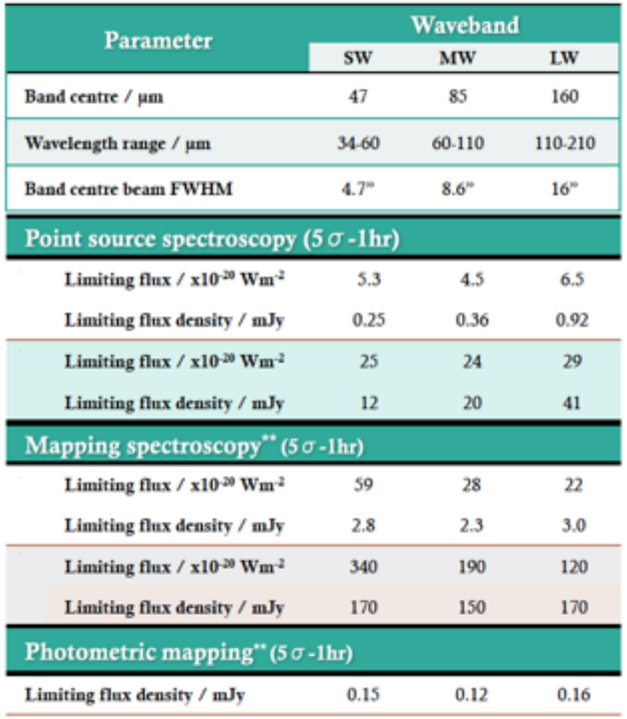


Parameter	Function			
	Low Resolution Spectrometer (LRS)	Medium Resolution Spectrometer (MRS)	High Resolution Spectrometer (HRS)	Camera
Wavelength range	17 – 36 μm	18 – 36 μm	12 – 17 μm	30 – 37 μm
Spectral Resolution (point source)	50 – 120	1300 – 2300	25000 – 26000	N/A
Field of View	600"x 3."7 x 4 slits	60" x 3."7 (slit)	4"x1."7 (slit)	10' x 10' (slit viewer)
FWHM	2" – 3.7"	2" – 3.7"	2"	3.4"
Pixel scale	0.7"x 0.7"	0.7"	0.5"	0.7"x 0.7"
Limiting flux density (1 hr, 5 σ)	20 – 140 μJy	200 – 4000 μJy	2 – 4.2 mJy	14 μJy
Limiting flux (1 hr, 5 σ)	(6 – 23) x 10^{-20} W/m^2	(3 – 40) x 10^{-20} W/m^2	(1.5 – 3) x 10^{-20} W/m^2	
	Continuum	Line		Continuum
Sensitivity (1 hr, 5 σ)	0.1 – 0.5 MJy/sr	(0.5 – 2) x 10^{-9} W/m^2/sr	(4 – 8) x 10^{-10} W/m^2/sr	
Saturation limit	~ 2 Jy	~ 140 Jy	~ 1200 Jy	~2

Ice spectra ??
MR & HR
(different sources)
Mostly HR CO2 / NH3 ices

Sensitivity etc means we COULD look @ BG stars & Pre-stellar cores…??

SAFARI



Parameter	Waveband		
	SW	MW	LW
Band centre / μm	47	85	160
Wavelength range / μm	34-60	60-110	110-210
Band centre beam FWHM	4.7"	8.6"	16"
Point source spectroscopy (5 σ -1hr)			
Limiting flux / x10^{-20} Wm^{-2}	5.3	4.5	6.5
Limiting flux density / mJy	0.25	0.36	0.92
Limiting flux / x10^{-20} Wm^{-2}	25	24	29
Limiting flux density / mJy	12	20	41
Mapping spectroscopy (5 σ -1hr)**			
Limiting flux / x10^{-20} Wm^{-2}	59	28	22
Limiting flux density / mJy	2.8	2.3	3.0
Limiting flux / x10^{-20} Wm^{-2}	340	190	120
Limiting flux density / mJy	170	150	170
Photometric mapping (5 σ -1hr)**			
Limiting flux density / mJy	0.15	0.12	0.16

Ice mapping SW & MW
Gas phase line survey
– linked to dust
Ice scattering emission?
Dust / ice synergy:
- continuum SED

MAIN INSTRUMENT FIR & ICE

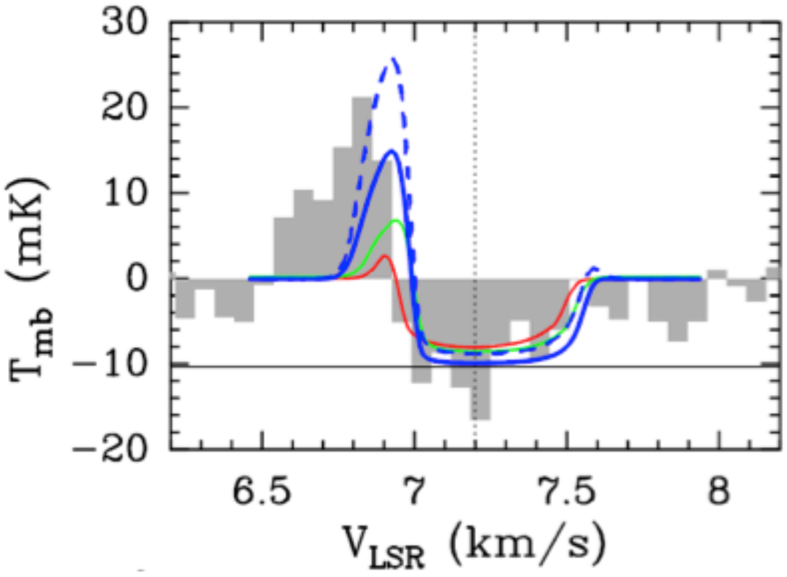
So how does SPICA fit with existing “Rolls Royce” facilitites…

Herschel picture

PRESTELLAR ISM:

Hershel HIFI data – shows gas Ø water lines x100 weaker than predicted = All water (essentially) in pre-stellar cores frozen out as ice

H_2O (g) in a COLD PRE-STELLAR CORE



Caselli et al (2012) ApJ

DISKS:

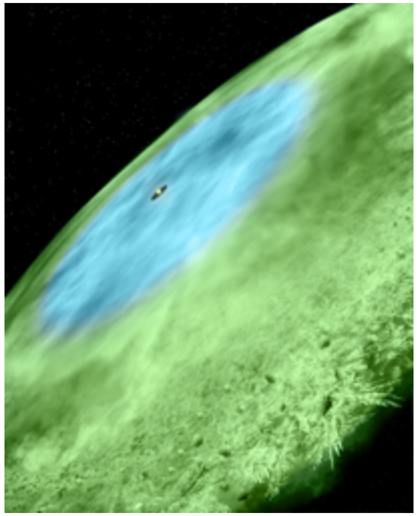
Tentative ice detections ONLY no real advance on ISO! & 63 μm ONLY

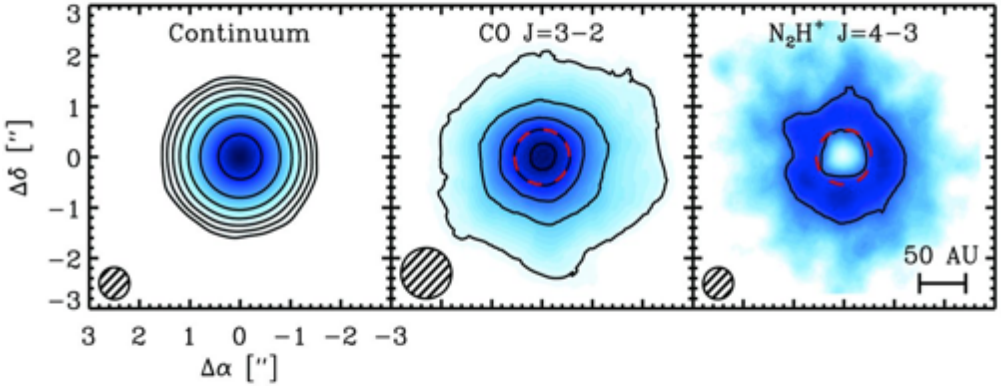
(Malfait et al. 1999; McClure et al. 2012).

Water detections in disks (tracing cold gas and higher J – warmed / desorbed gas) & shocked gas

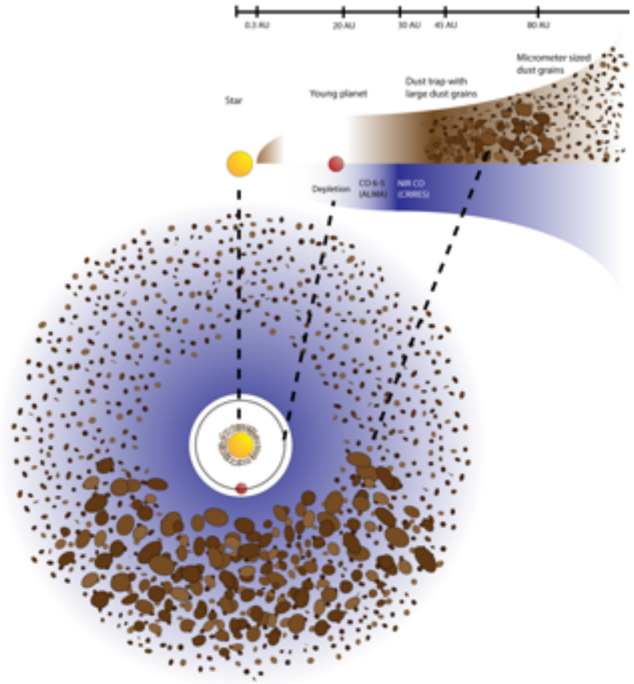
(e.g., Hogerheijde et al. 2011, Fedele et al. 2013 Kristensen et al 2014)

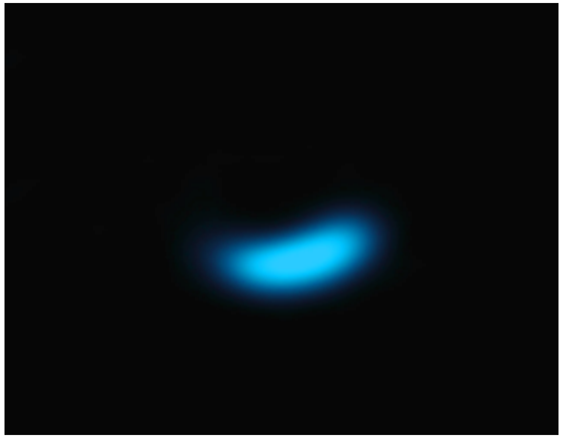
ALMA – COLD GAS





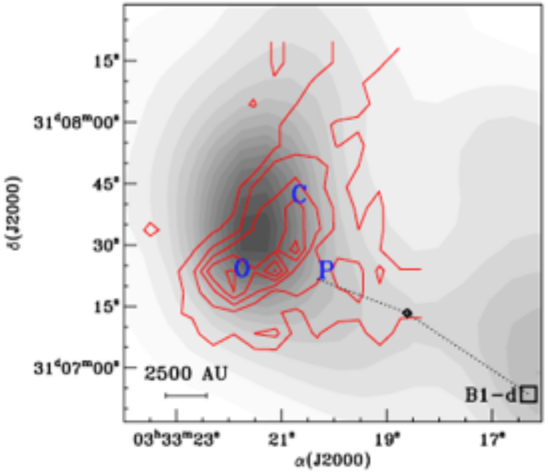
Qi et al Science (2013)

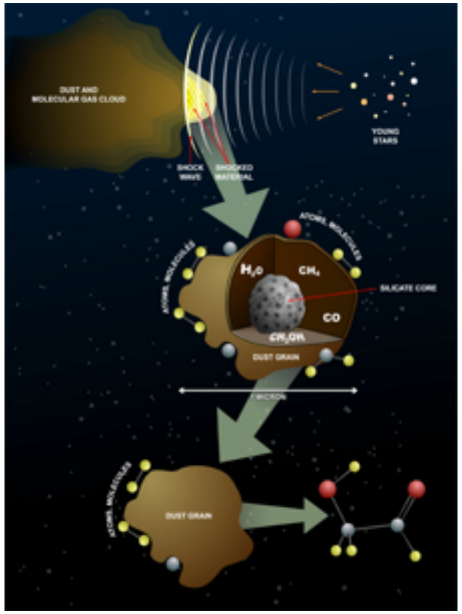


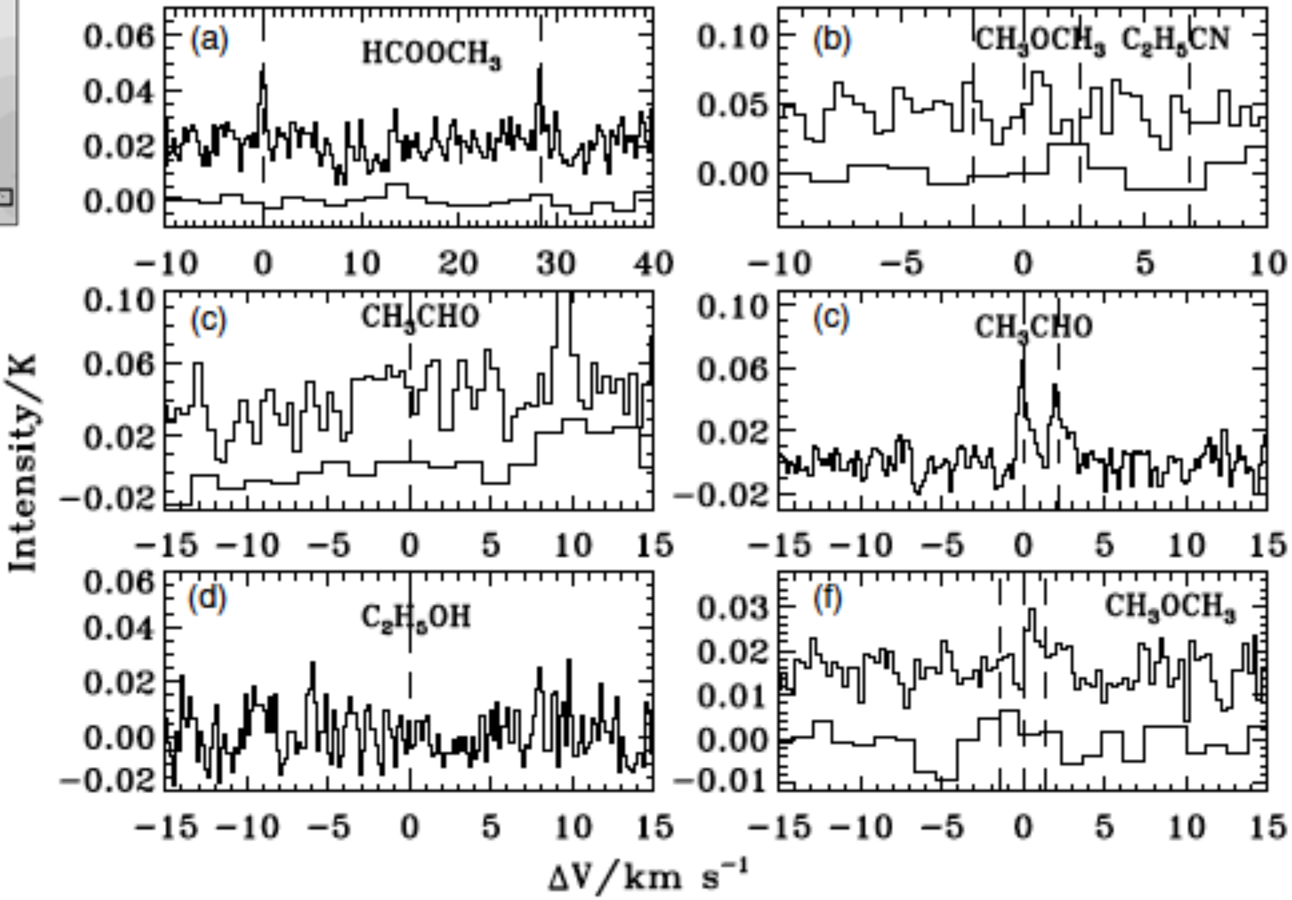


ALMA (ESO/NAOJNRAO) / Nienke van der Marel et al Science (2013)

Inferring Ice from Gas Detections

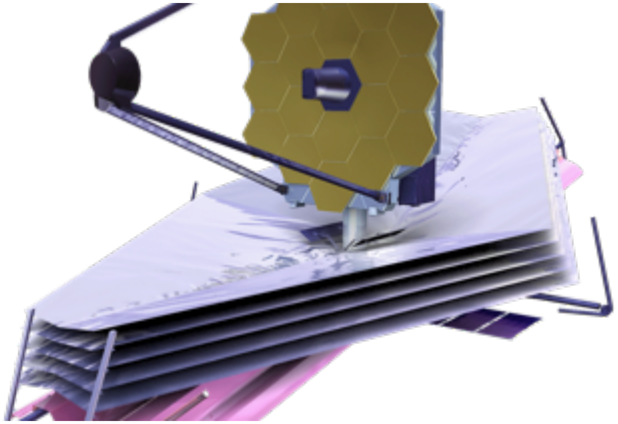




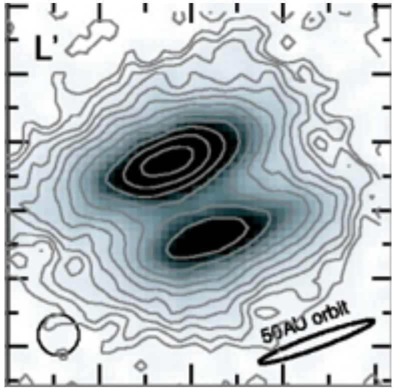


e.g. Oberg et al A&A (2010)

JWST / ALMA
“Snow Lines” & “Soot Lines”
IMAGING & detailed SPECTRA



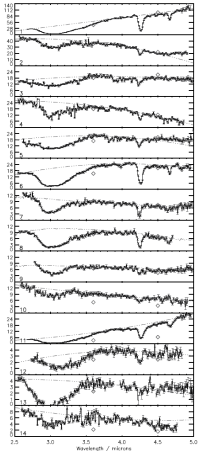
imaging



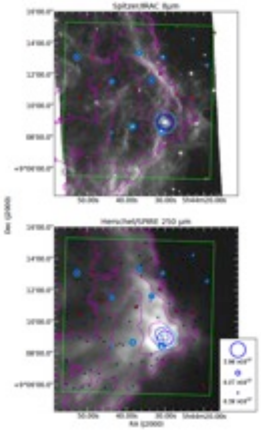
HV Tau C
Terada et al. (2007, 2012)
1X1'' FOV@0.12” FWHM
3 mcirons

mapping

spectra

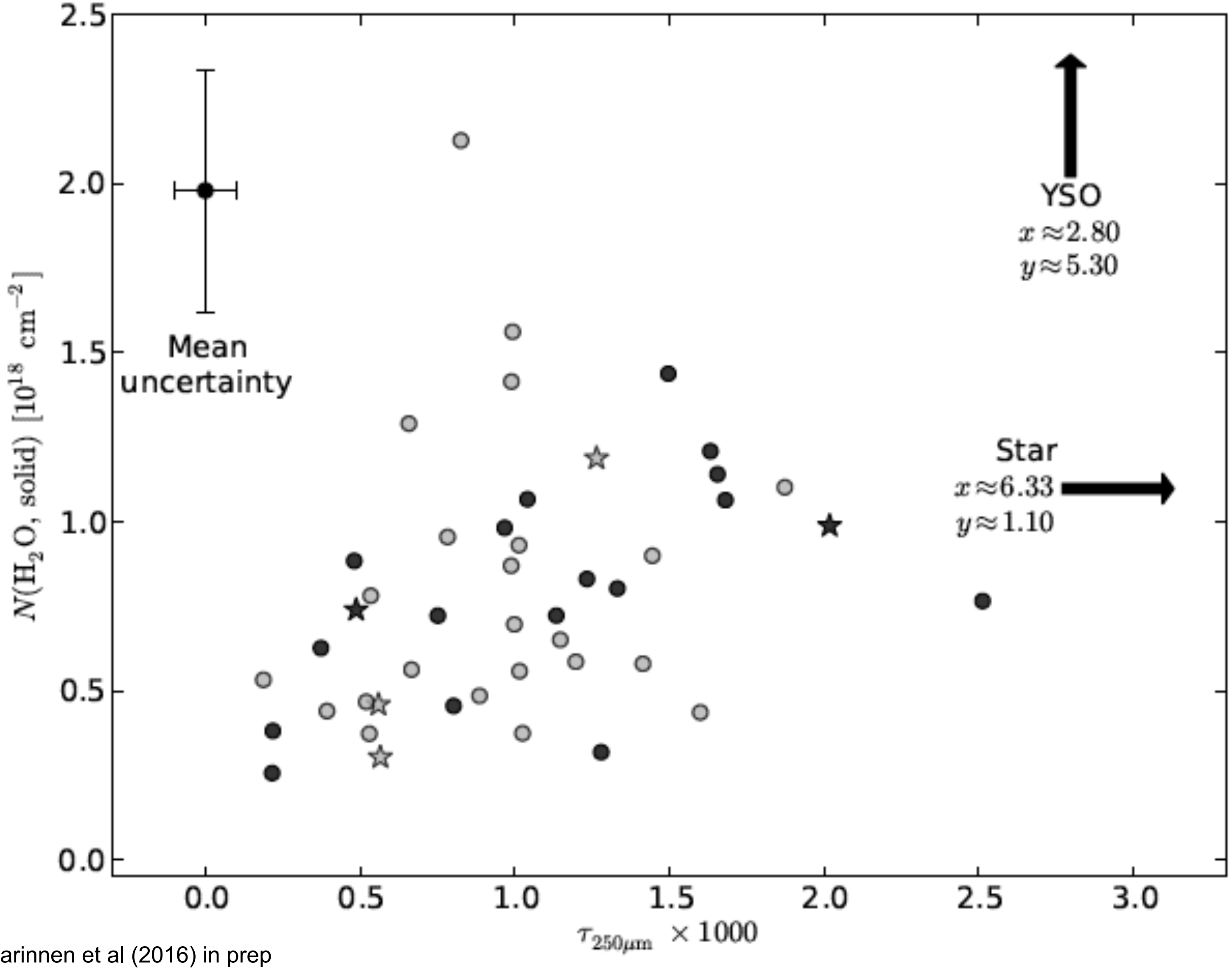


e.g. Noble et al (2013)
ApJ
Boogert et al (2015)
ARAA



Suutarinnen et al (2016)
in prep
AKARI Ice mapping
2-5 microns

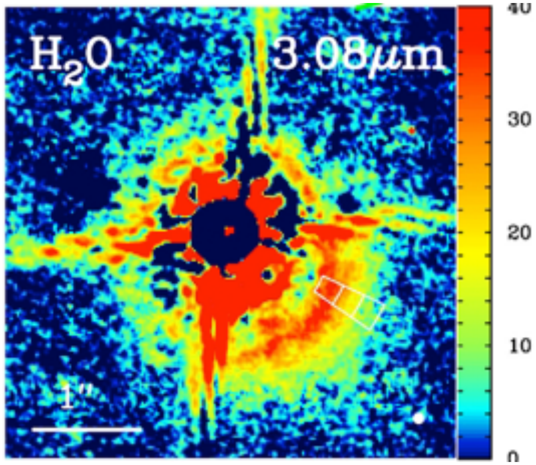
What else is related to ice? DUST!!



Suutarinnen et al (2016) in prep

METIS – E-ELT [L & M NO N]

Coronagraphic spectrophotometry (+adaptive optics)
Herbig Ae star HD 142527
3 μm ‘image of disk ice band in scattered light.
(Honda et al (2009)



METIS NIR SPECTROMETER IMAGING + FILTER

NIRCam / JWST with coronograph
Scattered light probes older more tenuous disks cf absorption = larger evolutionary range

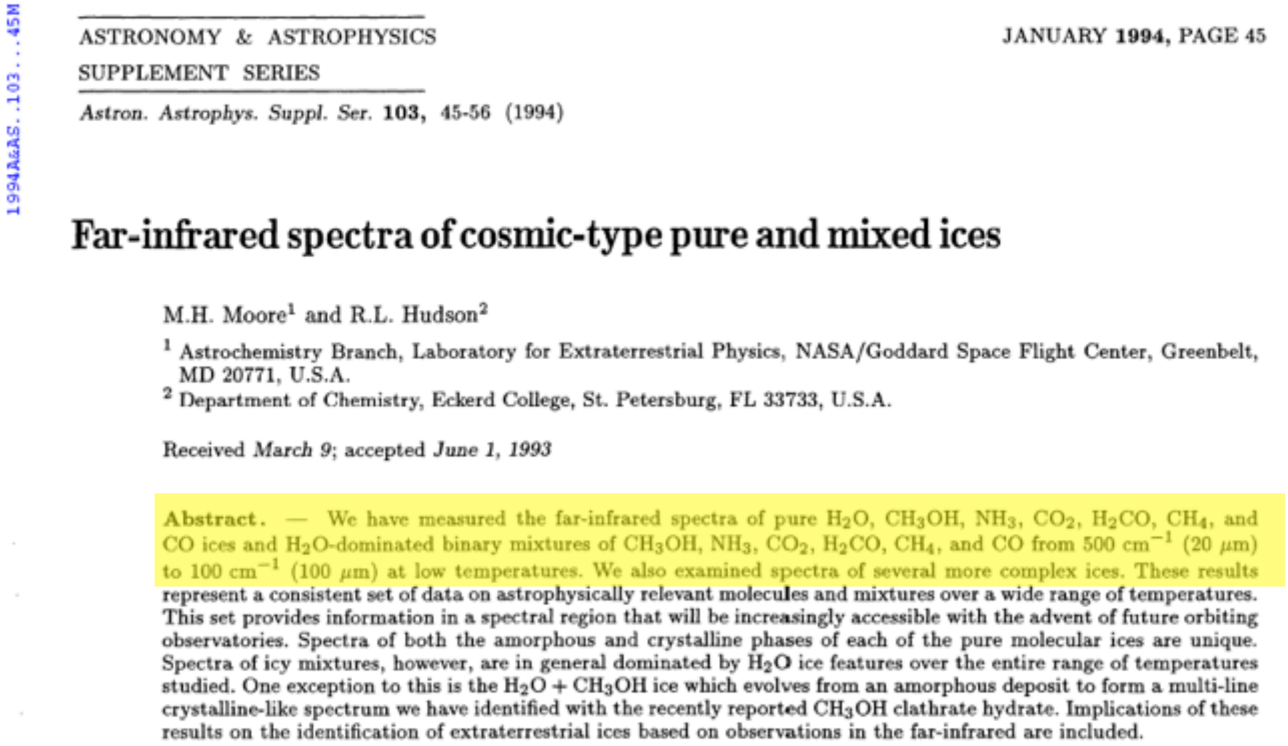
SPICA – has potential to observe FIR scattering from ices

NOT really emission – in FIR
Ices still exhibit absorption spectra

ALSO – VERY HIGH RESOLUTION
WARM GAS PHASE LINES
(AKIN TO e.g. VLT-CRIRES)

Ice Mapping - SPICA

Need to consider other ices:



1994A&AS..103...45M

ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

JANUARY **1994**, PAGE 45

Astron. Astrophys. Suppl. Ser. **103**, 45-56 (1994)

Far-infrared spectra of cosmic-type pure and mixed ices

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[1] Astrochemistry Branch, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, U.S.A.
[2] Department of Chemistry, Eckerd College, St. Petersburg, FL 33733, U.S.A.

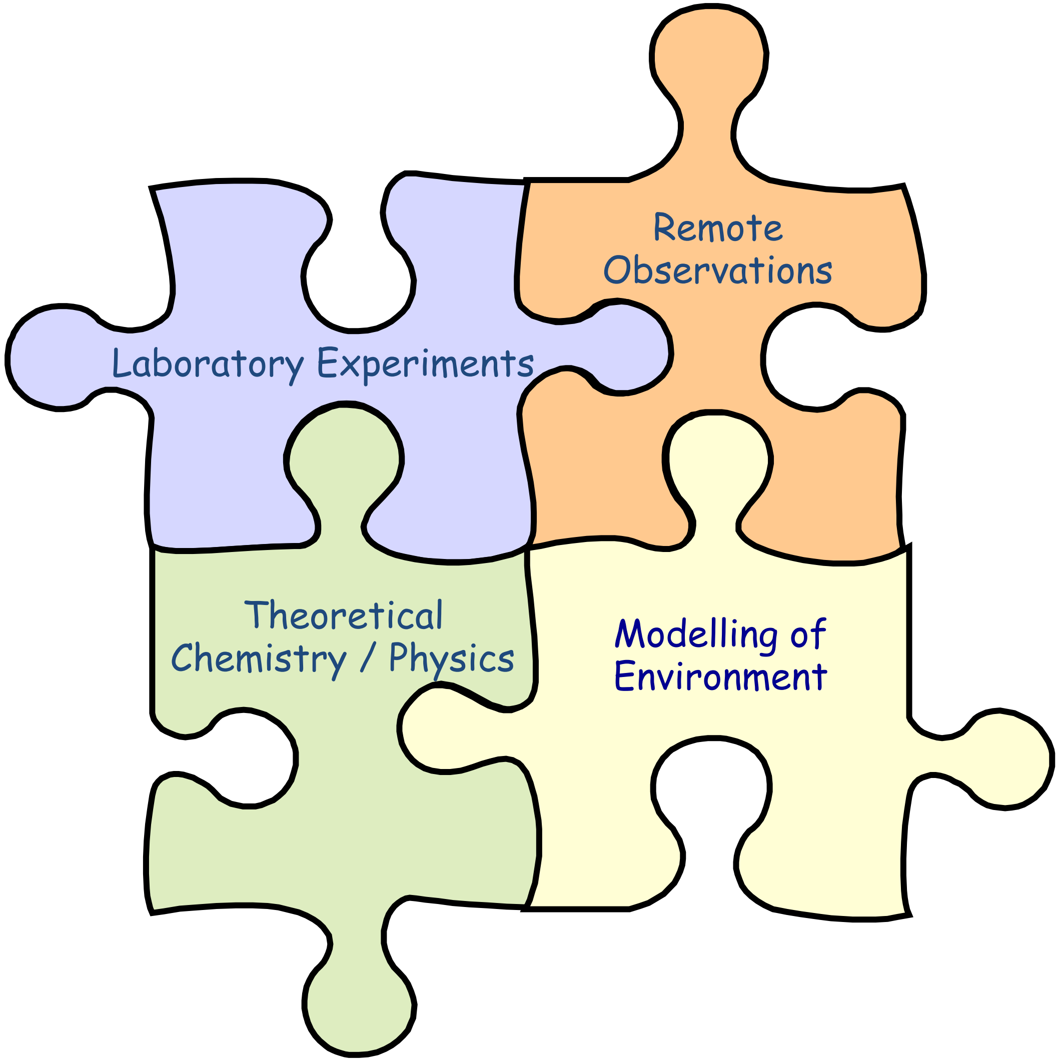
Received *March 9*; accepted *June 1, 1993*

Abstract. — We have measured the far-infrared spectra of pure H_2O, CH_3OH, NH_3, CO_2, H_2CO, CH_4, and CO ices and H_2O-dominated binary mixtures of CH_3OH, NH_3, CO_2, H_2CO, CH_4, and CO from 500 cm^{-1} (20 μm) to 100 cm^{-1} (100 μm) at low temperatures. We also examined spectra of several more complex ices. These results represent a consistent set of data on astrophysically relevant molecules and mixtures over a wide range of temperatures. This set provides information in a spectral region that will be increasingly accessible with the advent of future orbiting observatories. Spectra of both the amorphous and crystalline phases of each of the pure molecular ices are unique. Spectra of icy mixtures, however, are in general dominated by H_2O ice features over the entire range of temperatures studied. One exception to this is the $H_2O + CH_3OH$ ice which evolves from an amorphous deposit to form a multi-line crystalline-like spectrum we have identified with the recently reported CH_3OH clathrate hydrate. Implications of these results on the identification of extraterrestrial ices based on observations in the far-infrared are included.

Pure & H_20+
H_2O
CH_3OH
NH_3
CO_2
H_2CO
CH_4
CO

20-100 micron

How do we build understanding?



It's still a
HUGE
issue where support data comes from
and how it is accessed

Where is the lab data in gas / solid
(ice / minerology) phases to support
data interpretation and
understanding?

Terahertz Desorption Emission Spectroscopy (THz-DES)

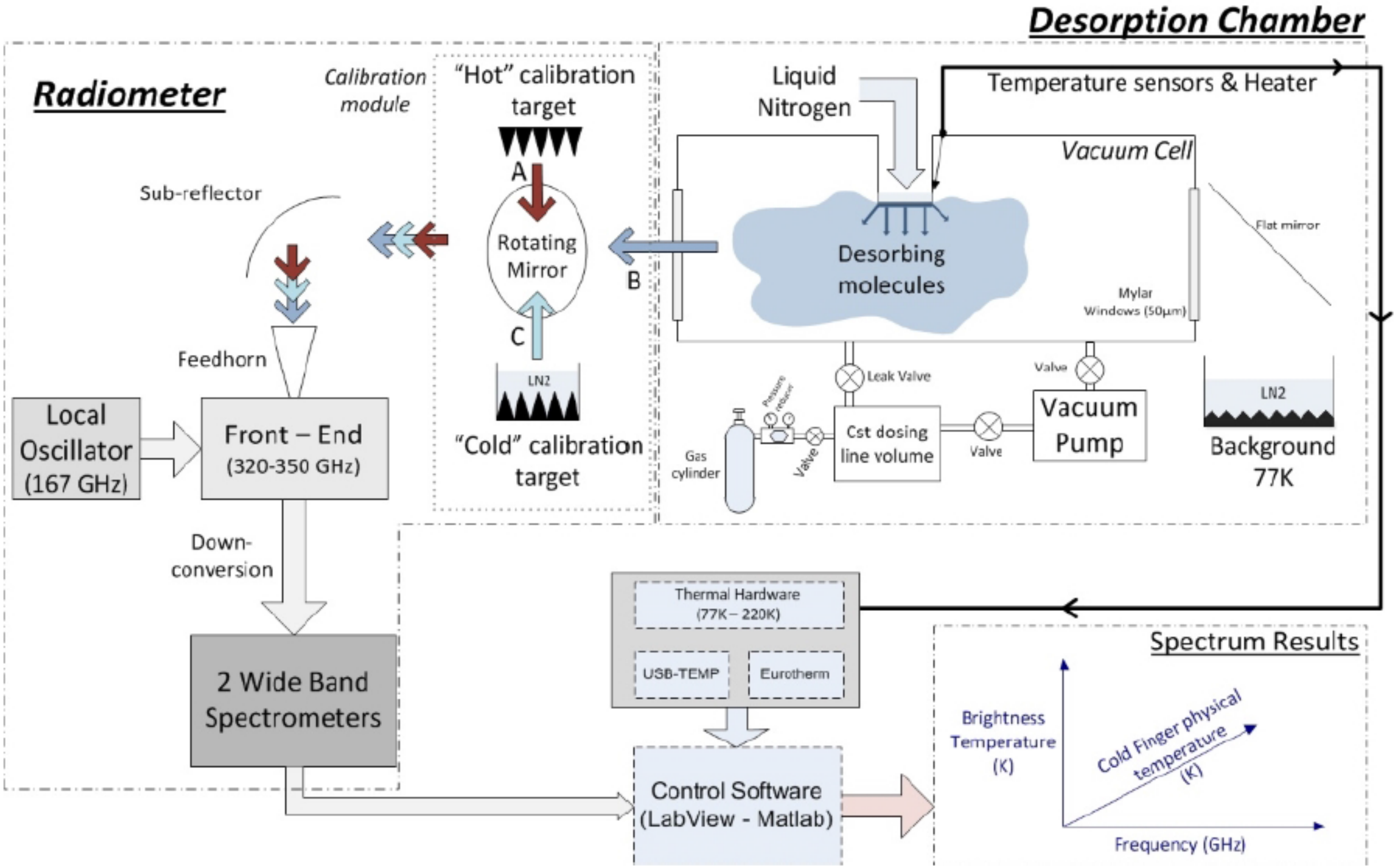
(with Brian Ellison (RAL Space)
& Geoff Blake (Caltech) & S Ioppolo (OU) RSURF)

1. **Are COMS produced in gas / solid phase?**
2. **Do radicals / ions desorb from surfaces?**
3. **Are A/E o/p ratios affected by surface desorption?**

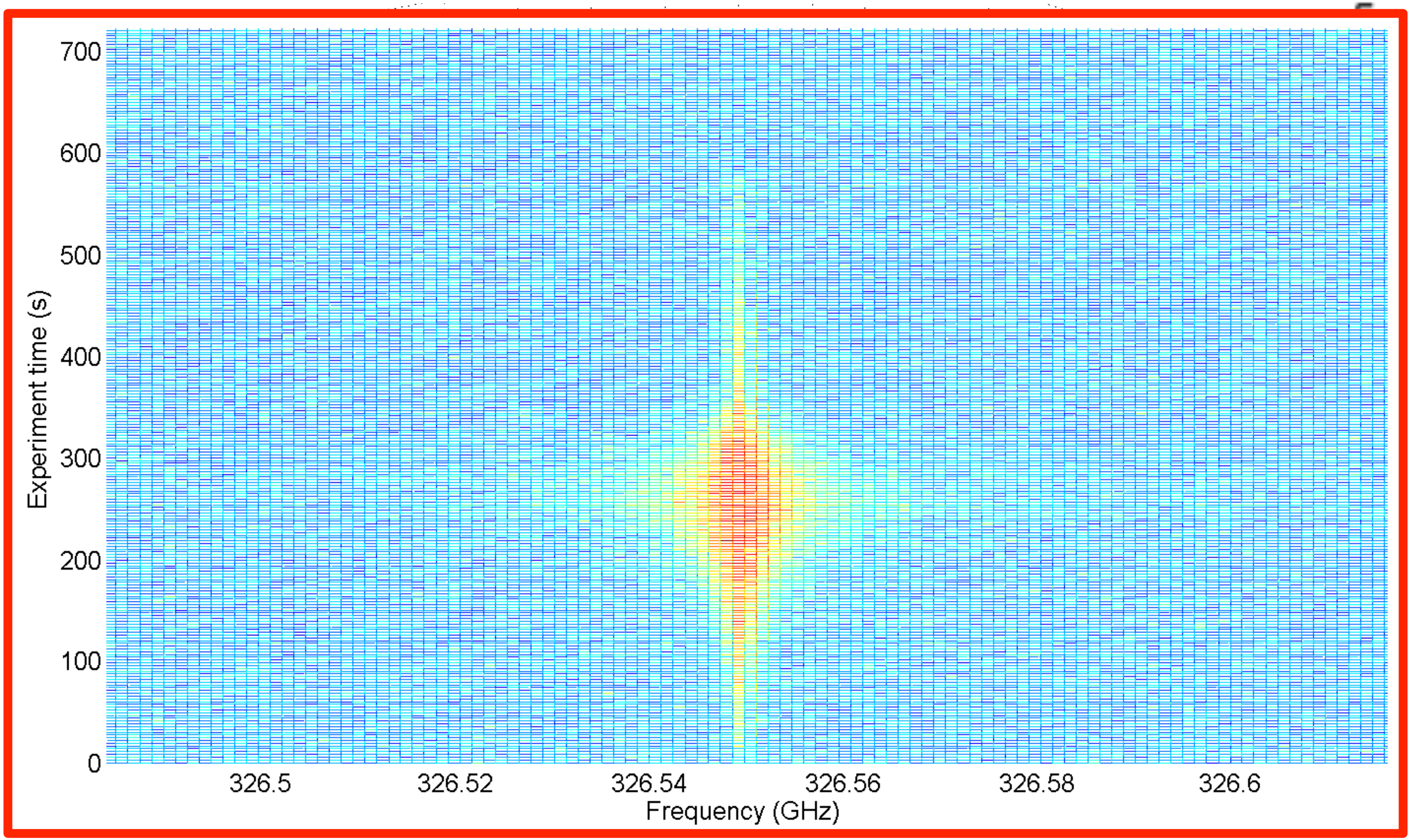
Auiriacombe et al (2015) Rev Sci Inst in prep

Proof of Concept:“ALMA” in the lab

The Open University



H_2O and N_2O desorption



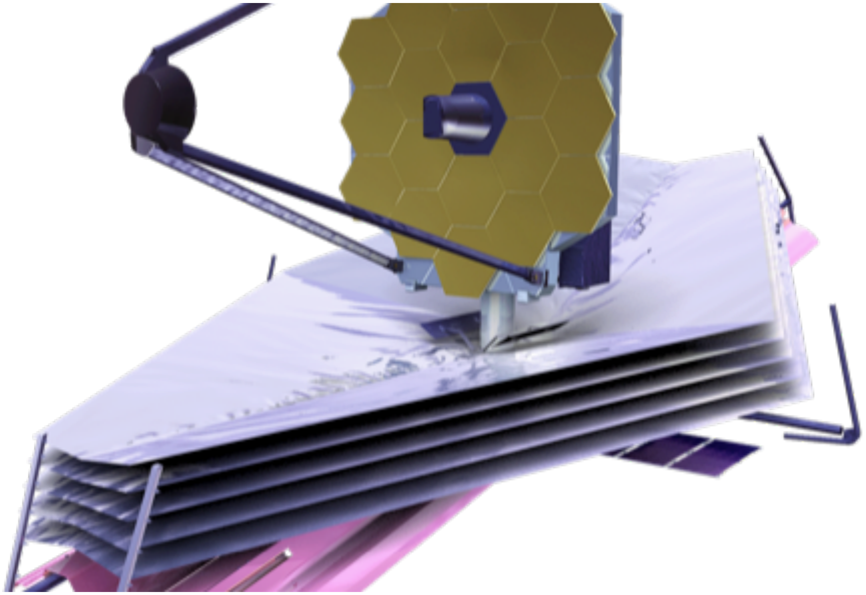
Auiriacombe et al (2016) Rev Sci Inst in prep

SPICA GALACTIC SCIENCE

- *How is water delivered to the planets?* ✓
- *How do solids evolve from pristine dust to differentiated bodies, and what is the link with our own Solar System?* ✓
- *When does the gas supply exhaust during the planet forming phase?* ✓
- *How does gas dissipation and photo-evaporation set the clock for planet formation?* ✓

Currently disk heavy – gap for UK niche & expertise in pre-stellar regions

JWST – huge advantages “our ice machine” / warm gas



Parallel observing

Spectral Coverage

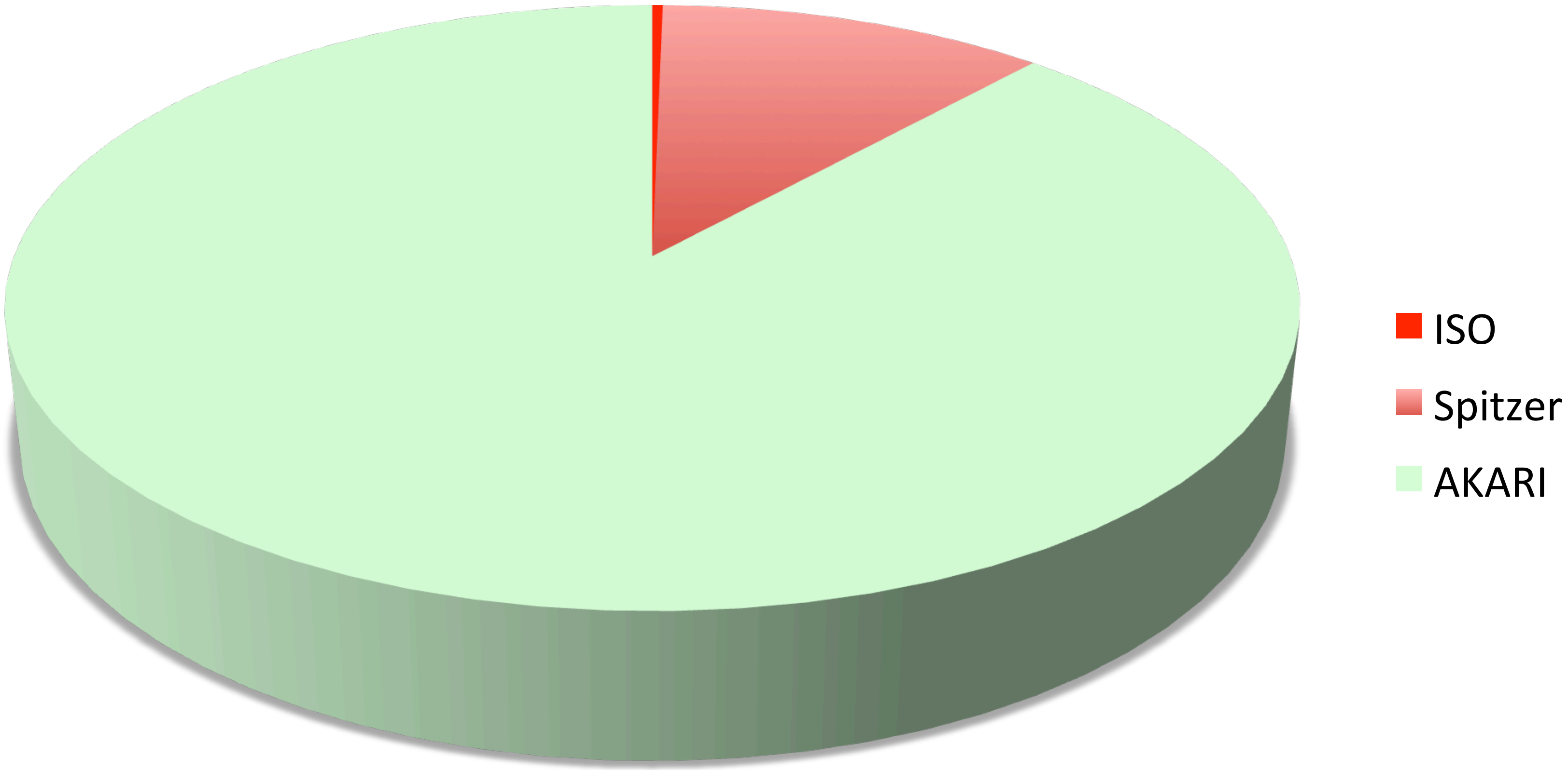
Resolution

Sensitivity

NIRSpec: (masked) spectroscopy 1-5 μm at R=100-3000 **PLUS**
MIRI: imaging (+ coronagraphy) and spectroscopy 5-28 μm at R=100-3000
NIRCam: 1-5 μm narrow and broad band imaging (including coronagraph) (slitless spectroscopy)

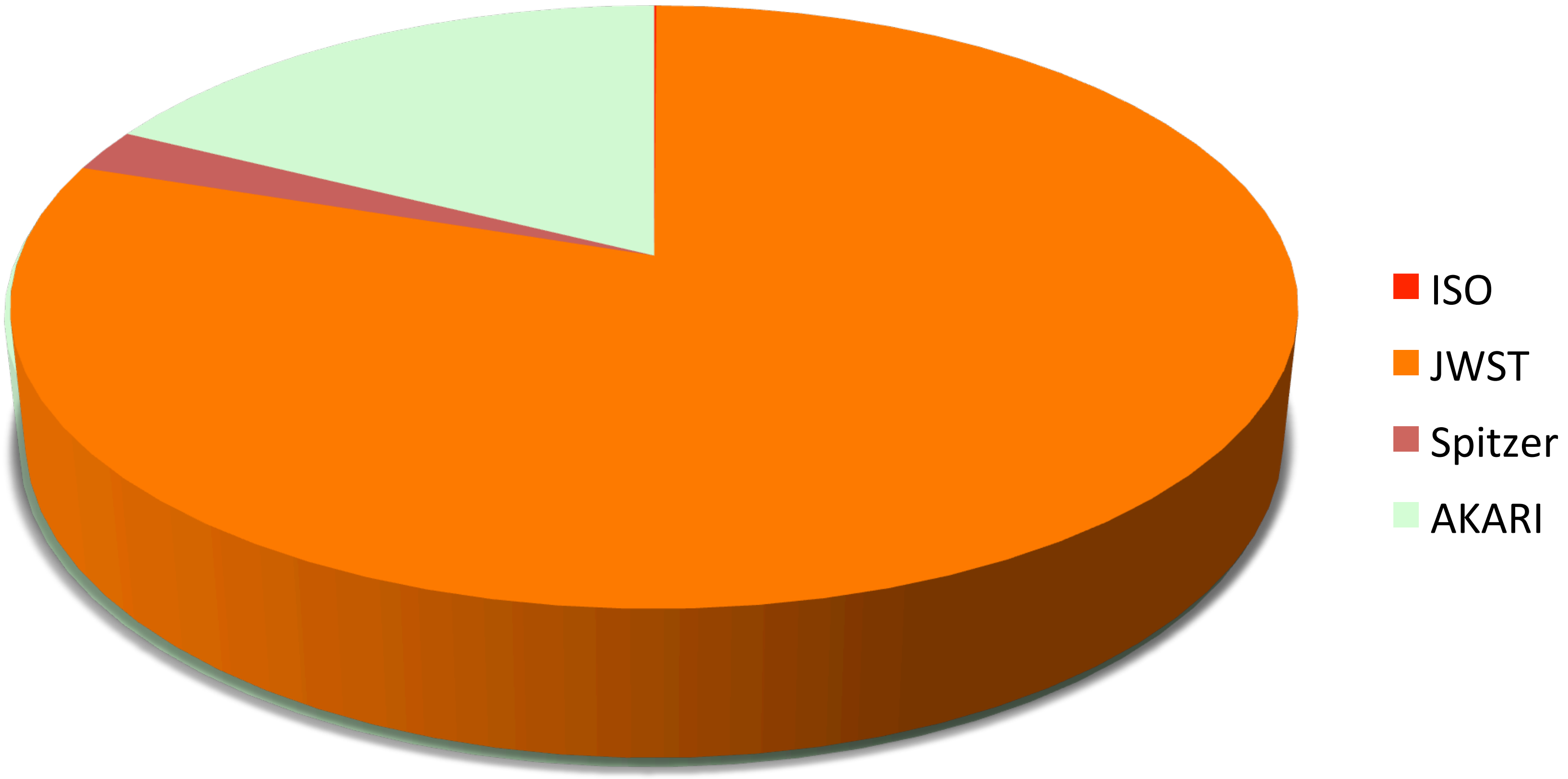
Spatial resolution 3-28 μm: 0.12-1.1 arcsec (21-190 AU for cloud at 150 pc distance)

No. of Observed Background Stars with Ice



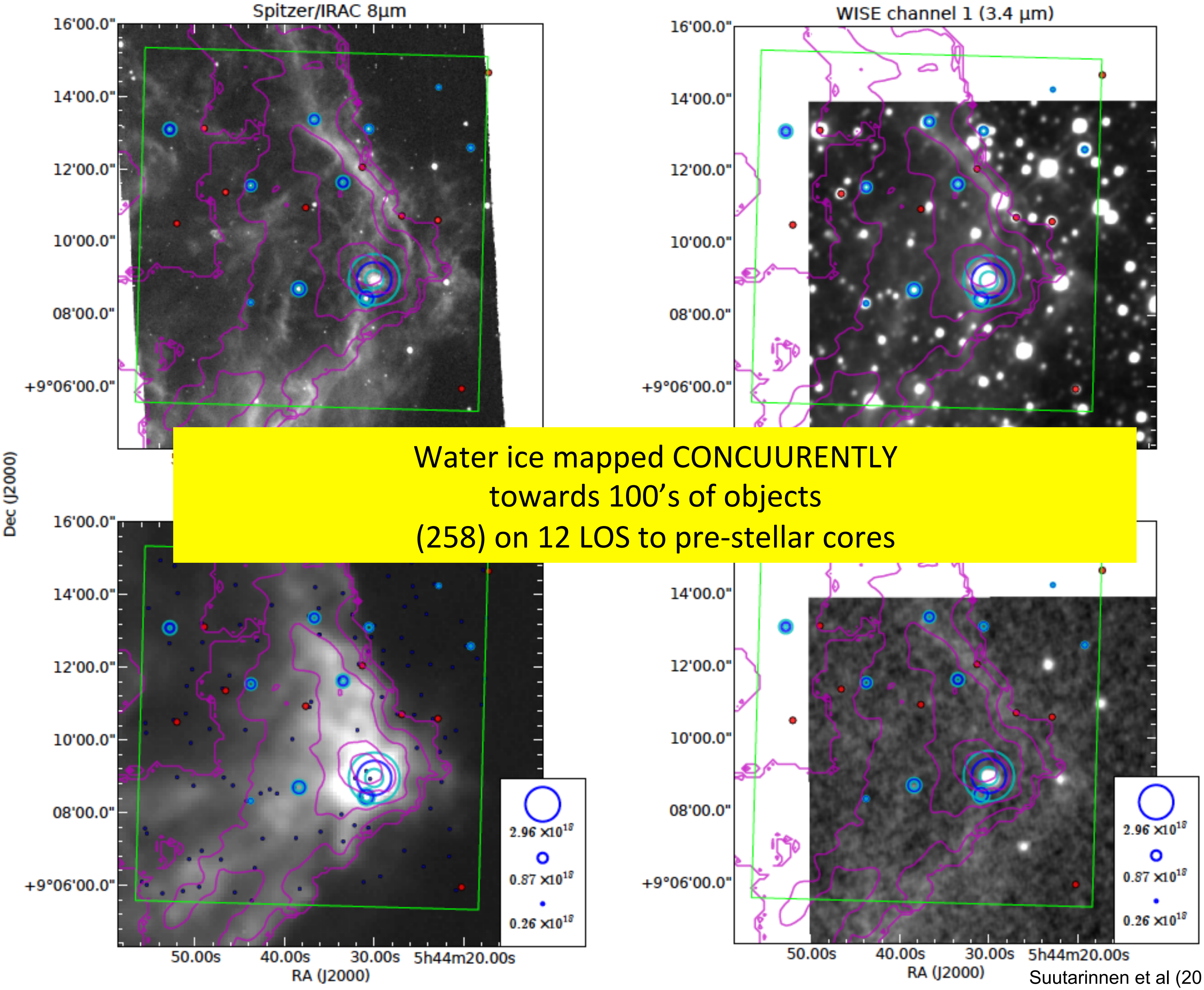
CAVEAT:- Current background star ice observations trace ices well before collapse.

No. of Observed Background Stars with Ice



CAVEAT:- Current background star ice observations trace ices well before collapse.
JWST will ALSO have the sensitivity to study HIGHLY EXTINCTED LoS CLOSE to collapse
cf. A_V~90 background stars requires S/N=100 for ~1 mJy continuum at 3-5 μm

Ice Mapping



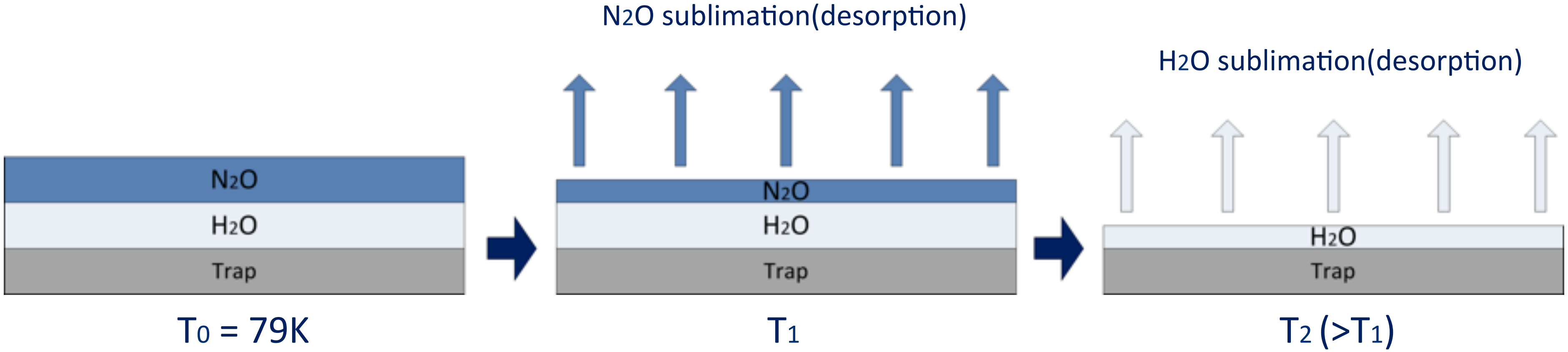
Water ice mapped CONCUURENTLY
towards 100's of objects
(258) on 12 LOS to pre-stellar cores

Suutarinnen et al (2015) in prep

Proof of Concept: "ALMA" in the lab

The Open University

observe spectra
of desorbing gas Φ
molecules
IN EMISSION



N_2O sublimation(desorption)

H_2O sublimation(desorption)

N_2O

H_2O

Trap

N_2O

H_2O

Trap

H_2O

Trap

T_0 = 79K

T_1

T_2 (>T_1)

Auiriacombe et al (2015) Rev Sci Inst in prep

Extra-Galactic Ice Observations, key e.g.

- 1st Observations : Spoon et al A&A (2003) A&A

CO & OCN ice towards galactic centre of starburst/AGN galaxy NGC4945

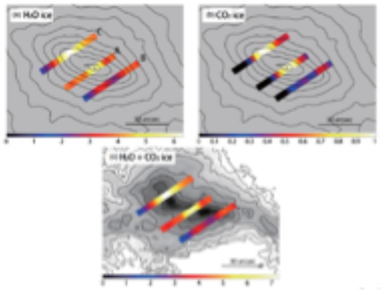
- Many studies of LMC / SMC suggesting ice abundance is linked to metalicity – higher CO_2 in LMC, lower H_2O; higher CO and CH_3OH

e.g. IRAS 05328-6827 (LMC) van Loon et al (2005)

Shimonishi et al Ap J (2008), A&A (2010), ApJ (2013)

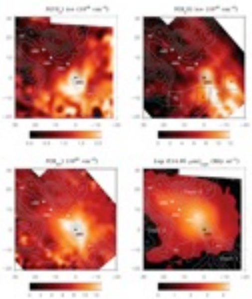
Seale et al (2011) ApJ

Olivera et al (2011) (2013) MNRAS

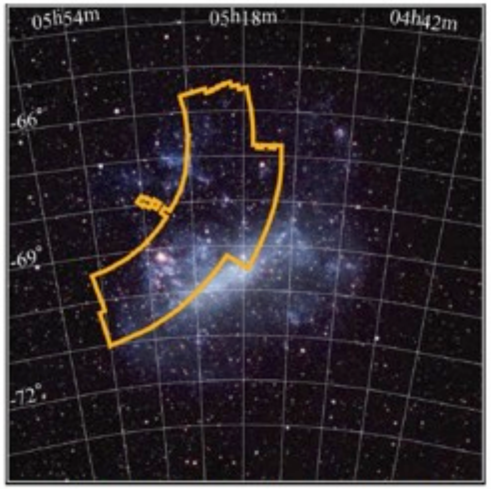


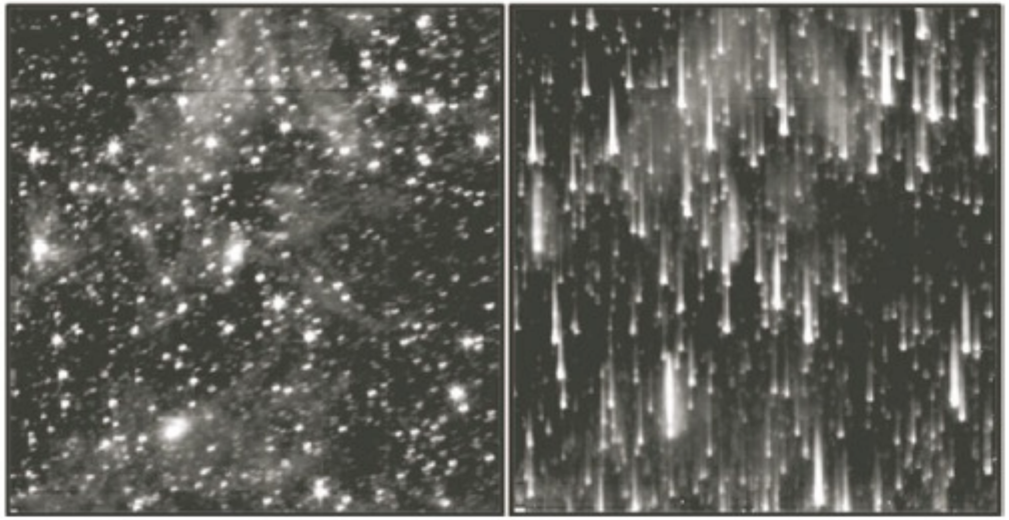
- Ice in edge on starburst galaxy NGC253 (Yamaguishi et al (2011))
- Ice in M82 (Yamaguishi et al (2013))

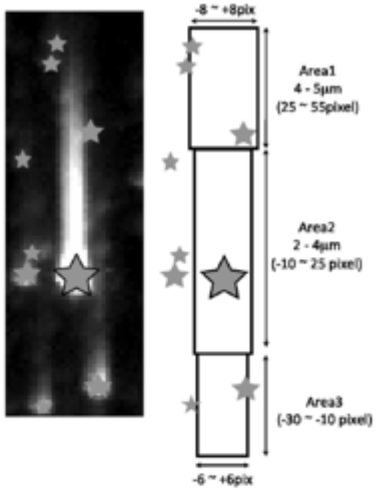
- Against H II regions (Sonnentrucker (2008)

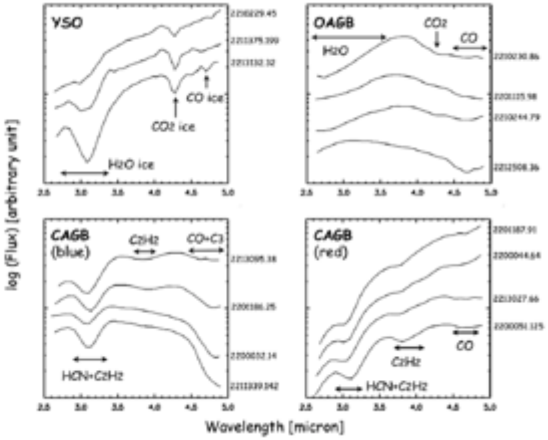


LMC / SMC “Local Galaxies”
Resolving YSOs



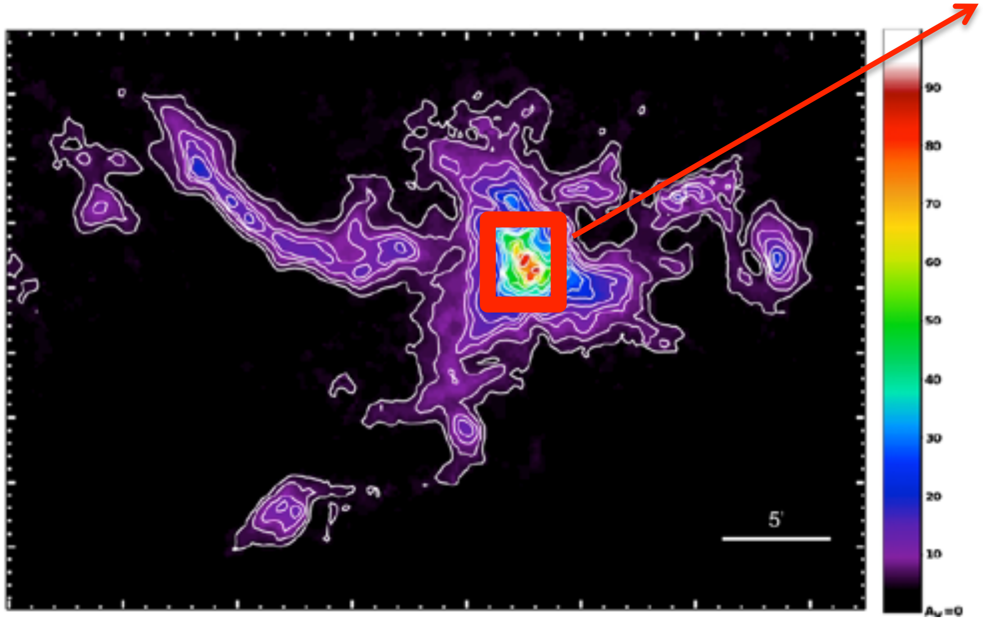






e.g. Shimonishi et al ApJ (2013)

What could JWST do?



B 59 star-forming core. A_V contours 5-90 mag
derived from background stars [Roman-Zuniga et al. 2010]

JWST/NIRSpec Micro Shutter Array (MSA):

- 1-5 μm, R~3000
- >100 targets simultaneously
- 3’x3’field of view > AKARI (no confusion)

JWST/NIR CAM Slitless Spectroscopy mode:

- 2-5 μm, R <<< (100 is enough)
- all targets at once
- 0. 2 mJy sources

(2 oom > Spitzer 1 oom > AKARI)

CHALLEGE = DATA REDUCTION

JWST/MIRI cluster mode:

- 5-28.3 um, R~3000
- 1 target at a time
- 0. 2 mJy sources (2 oom > Spitzer 1 oom > AKARI)

Ice Mapping - SPICA

To get good mapping data (abs[background source??] vs. emission);

- Calibration is VITAL – really good wavelength data across SW & MW / HW
- Linked intrinsically to good SEDs (ideal maps – need long lambda – cf ice & dust)
- Multi-lambda mapping = huge difference
- To fully map line profile say something about chemistry = need R=3000 (300 not enough)
- Zodical light - could be limited by sky itself