University of
St Andrews

St Andrews Centre for Exoplanet Science

Chemical evolution of PPDs employing optical constants of cosmic-ray processed ice into ProDiMo code

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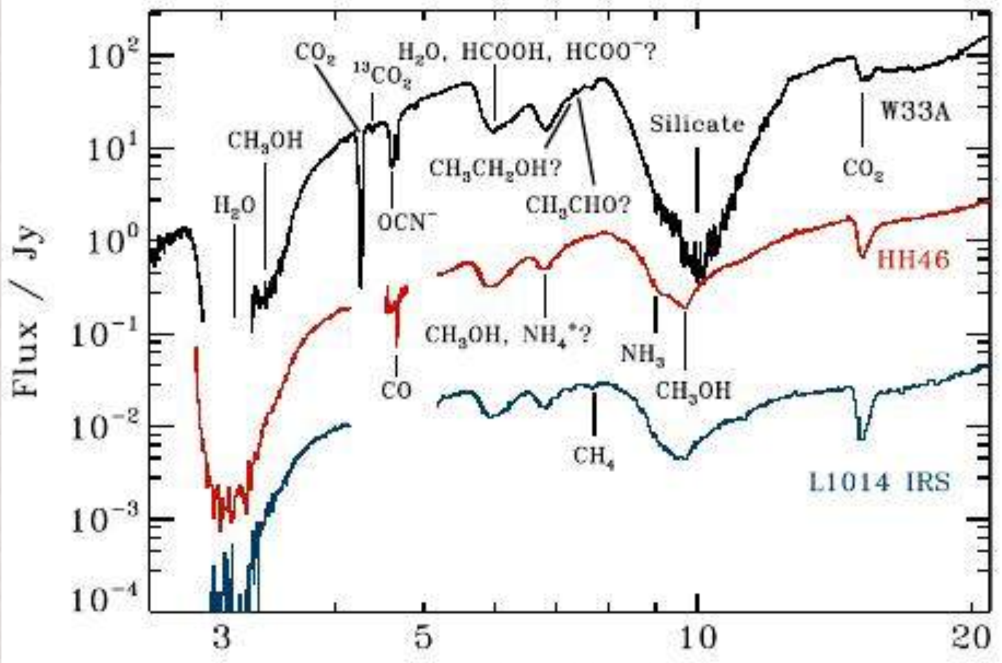
Collaborators: Peter Woitke, Michiel Min, Sergio Pilling, Inga Kamp, Christiane Helling

Cosmic Rays: the salt of the star formation recipe
Florence - Italy

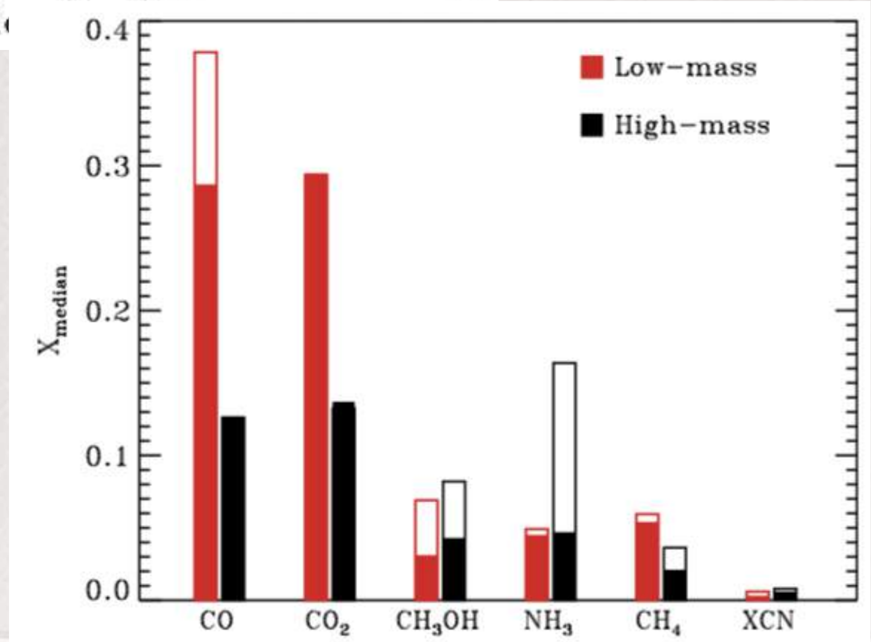
UNIVERSIDADE DO VALE DO PARAÍBA
São José dos Campos - SP

FAPESP
FUNDAÇÃO DE AMPARO À PESQUISA
DO ESTADO DE SÃO PAULO

Ices in Young Stellar Objects



Öberg+2011



- *Infrared spectrum shows a large inventory of ices toward YSOs;*
- *Organics (C-bearing molecules) observed between 5 - 8 microns;*
- *CO is the most abundant molecules in Low-mass YSOs and CH3OH is the most abundant organic.*

Methodologies to address chemical abundance

RATE EQUATIONS

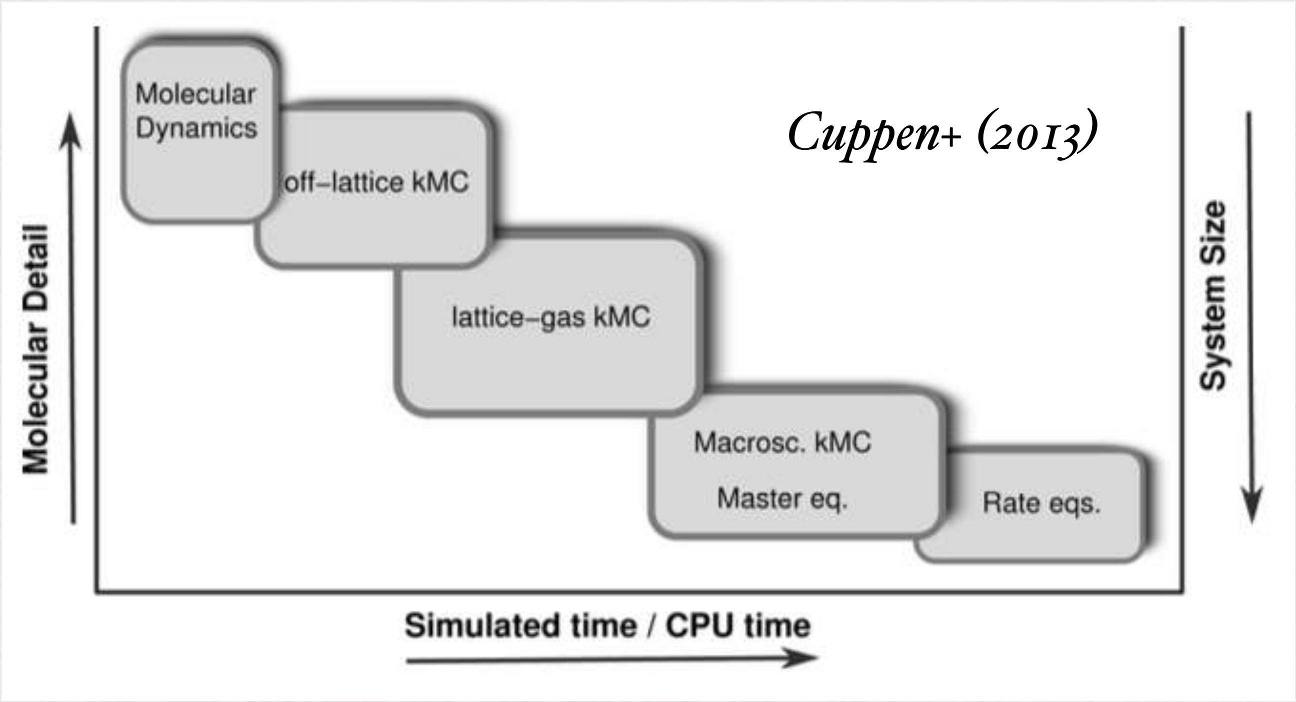
CHEMICAL ABUNDANCE

COMPLEX REFRACTIVE INDEX (CRI)

KINETIC MONTE CARLO

+

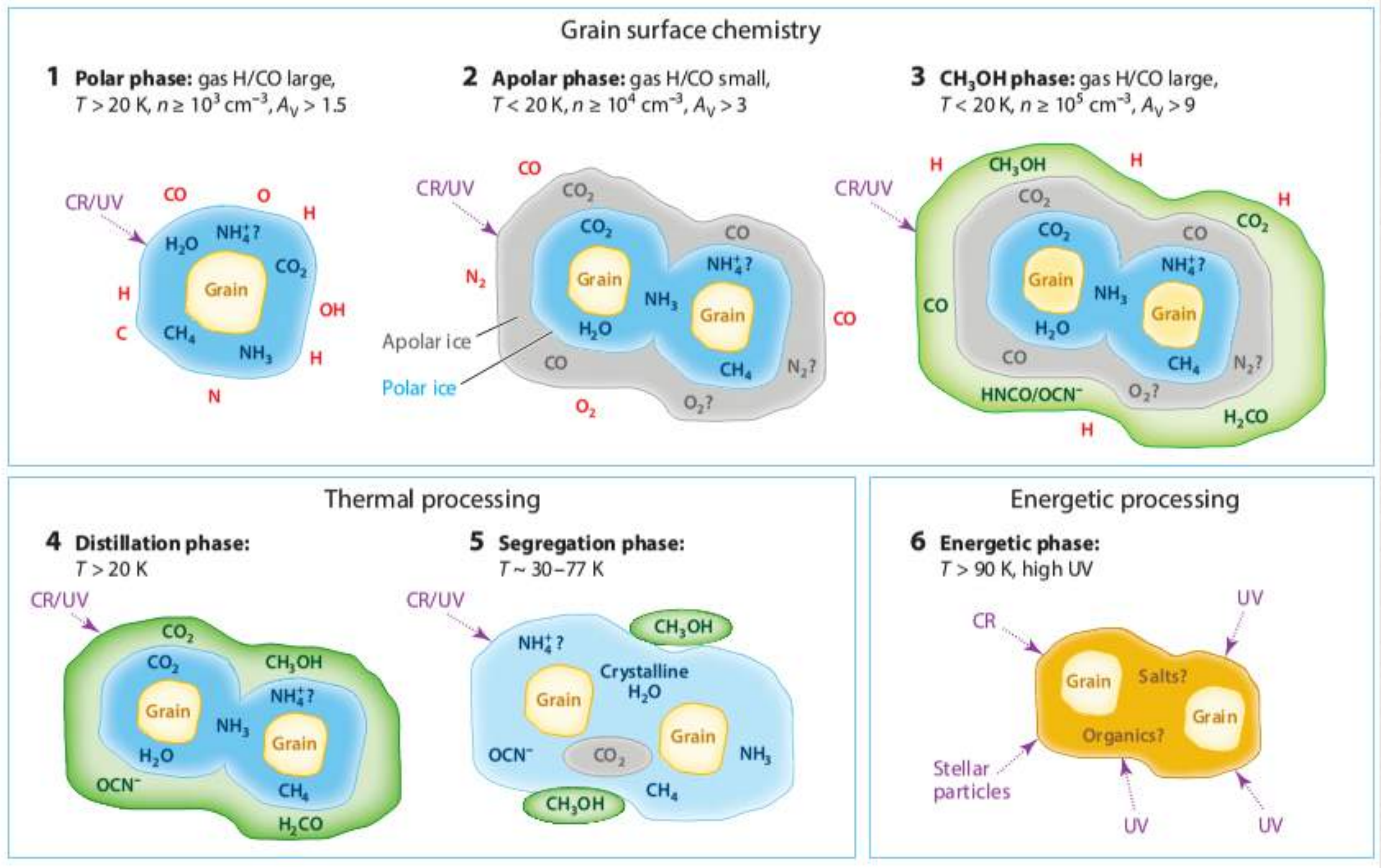
MASTER EQUATION

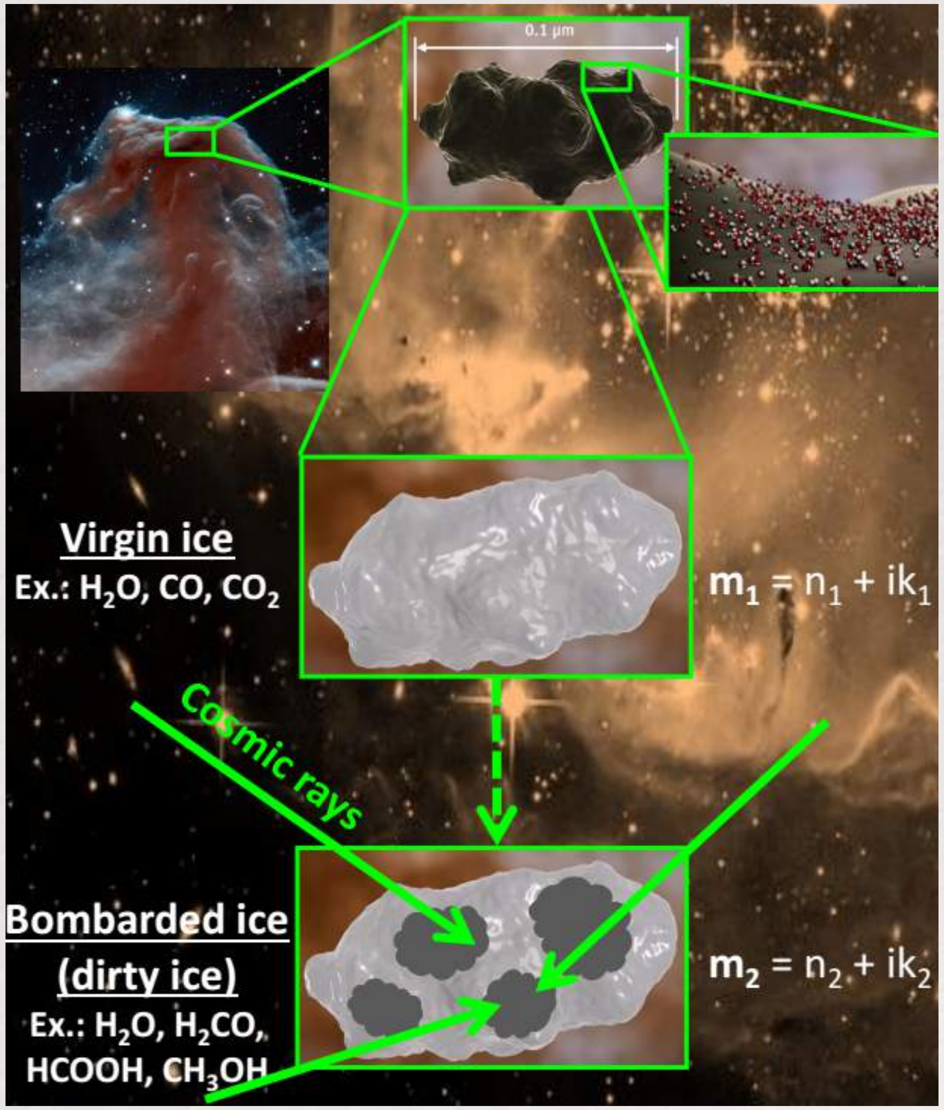


Cuppen+ (2013)

Complex Refractive Index of astrophysical ices

Boogert+ (2015)

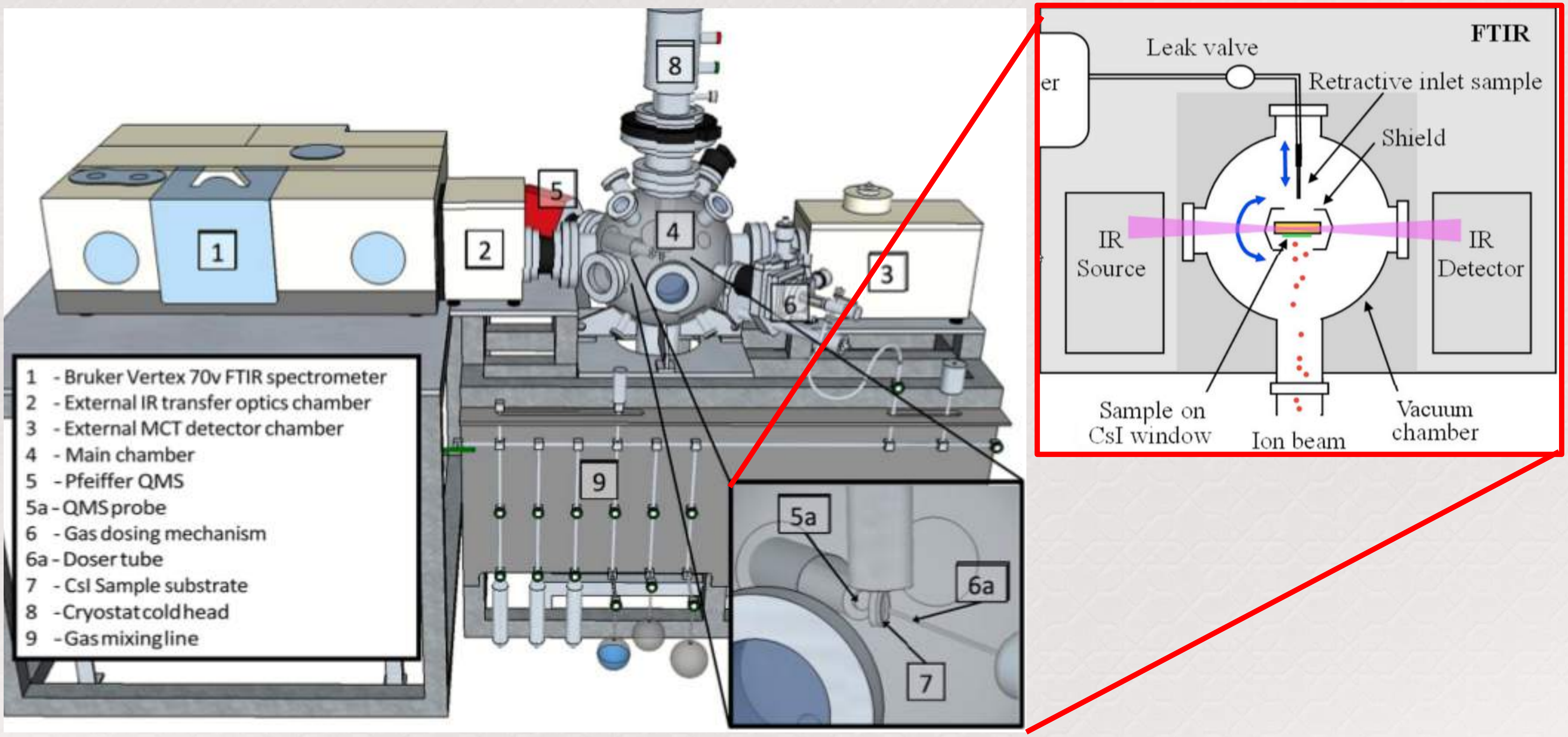




CRI store the chemical information of processed ices

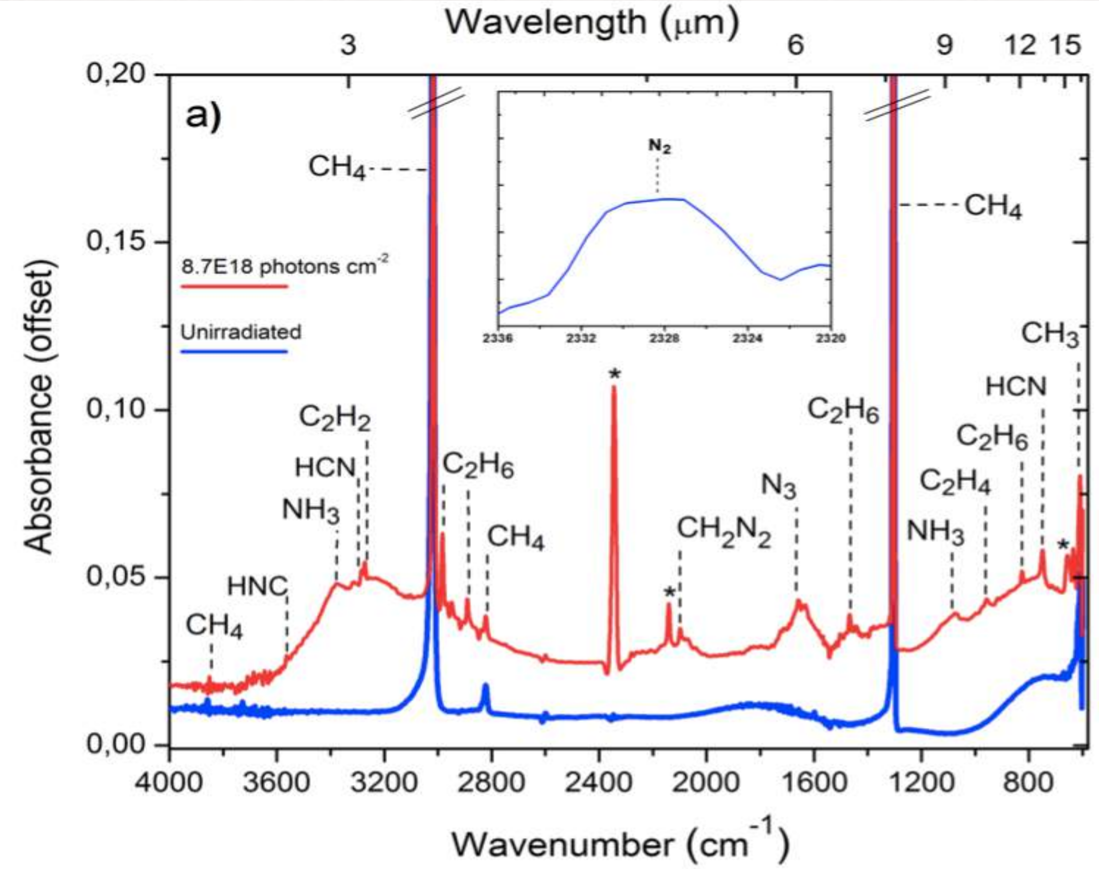
How the CRI are calculated?
Part I

Oberg, 2016

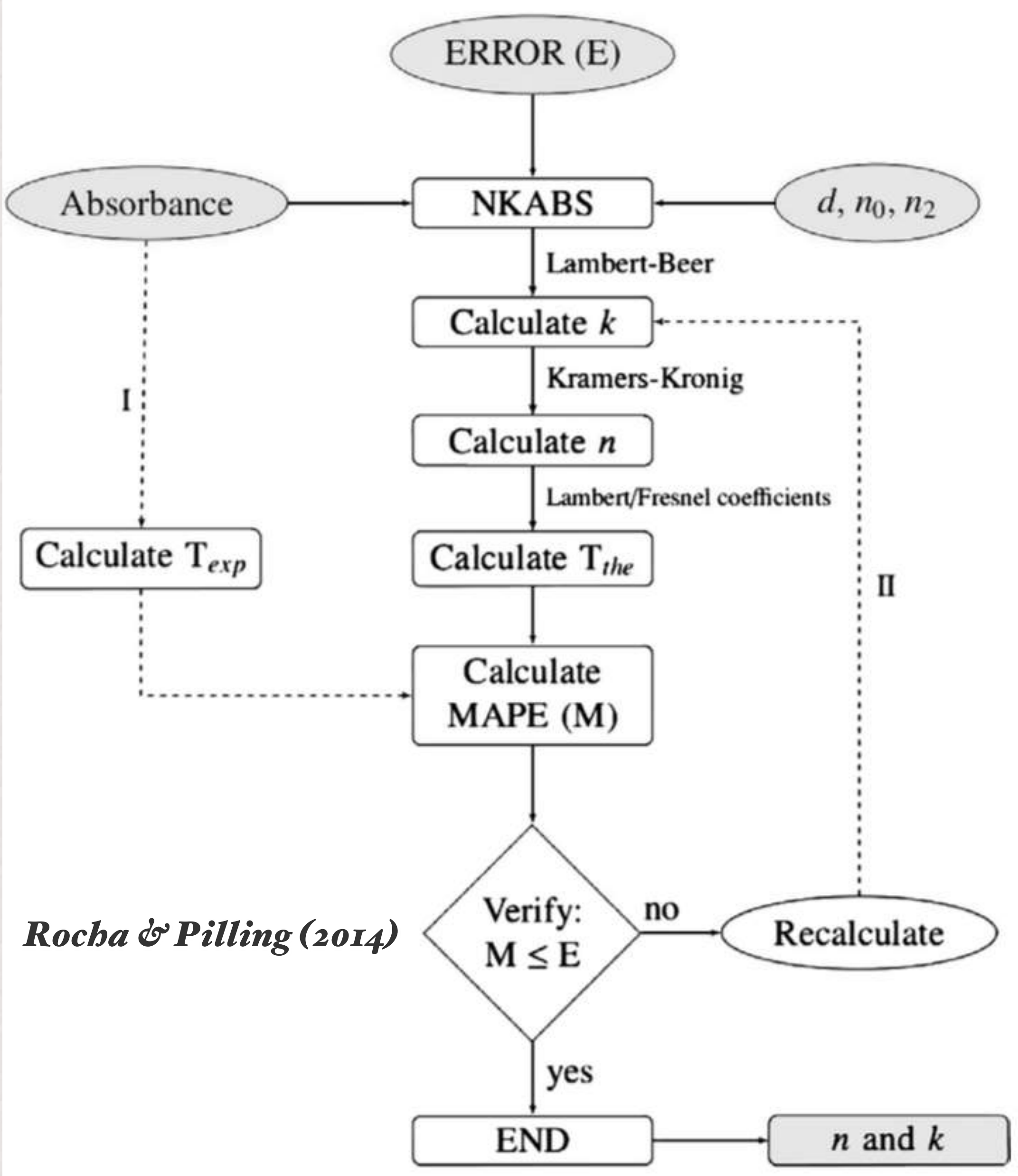


1 - Bruker Vertex 70v FTIR spectrometer
2 - External IR transfer optics chamber
3 - External MCT detector chamber
4 - Main chamber
5 - Pfeiffer QMS
5a - QMS probe
6 - Gas dosing mechanism
6a - Doser tube
7 - CsI Sample substrate
8 - Cryostat cold head
9 - Gas mixing line

How the CRI are calculated?
Part II



Vasconcelos, Pilling, Rocha+ (2017)

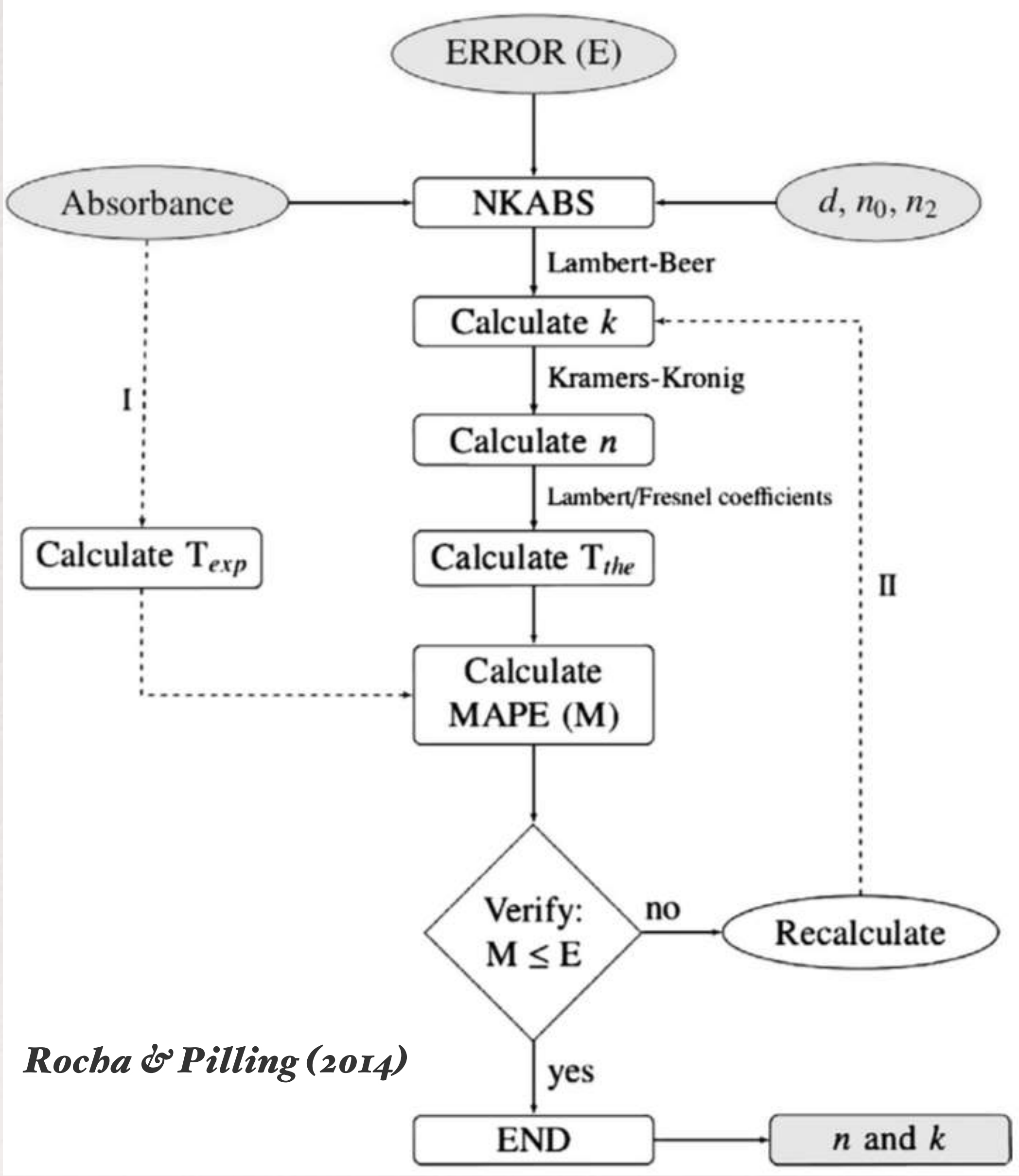


Rocha & Pilling (2014)

Available to download at:

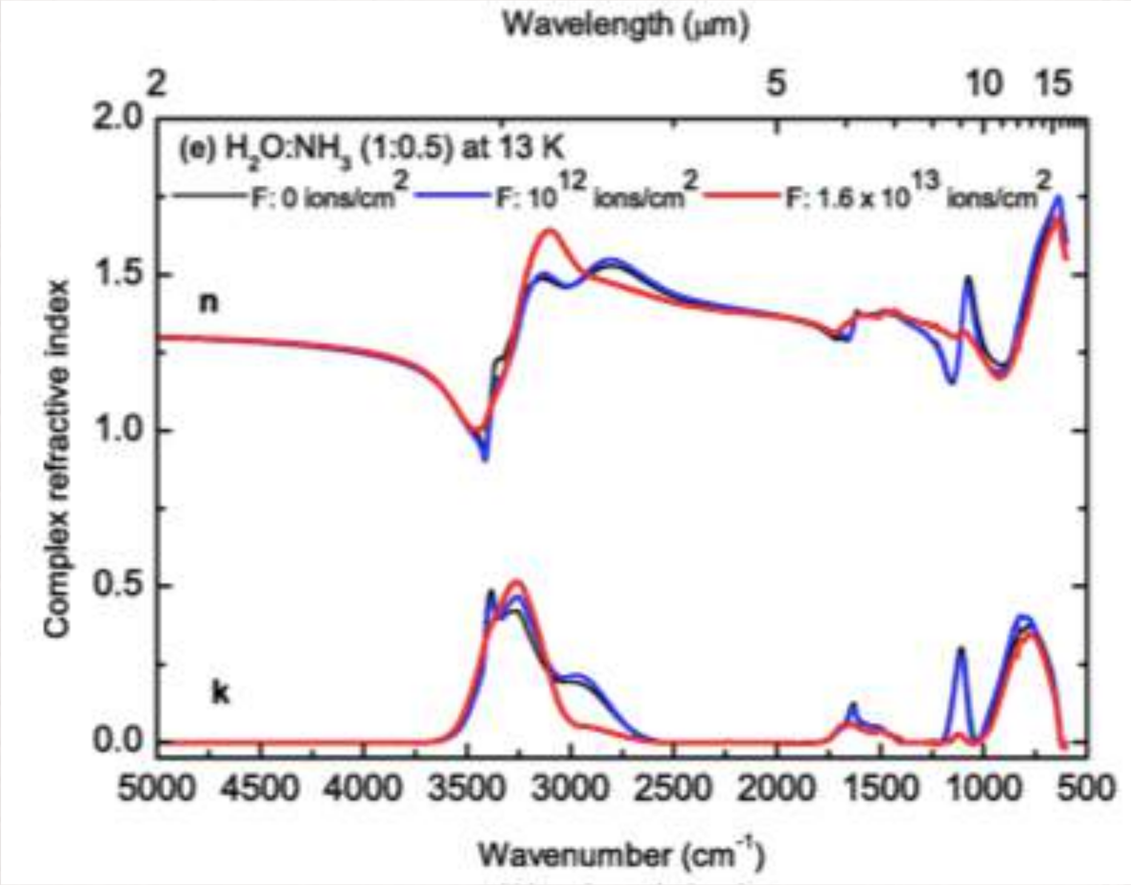
https://sites.google.com/view/astrowill/codigos-computacionais/nkabs

How the CRI are calculated?
Part II



Rocha & Pilling (2014)

Available to download at:
https://sites.google.com/view/astrowill/codigos-computacionais/nkabs

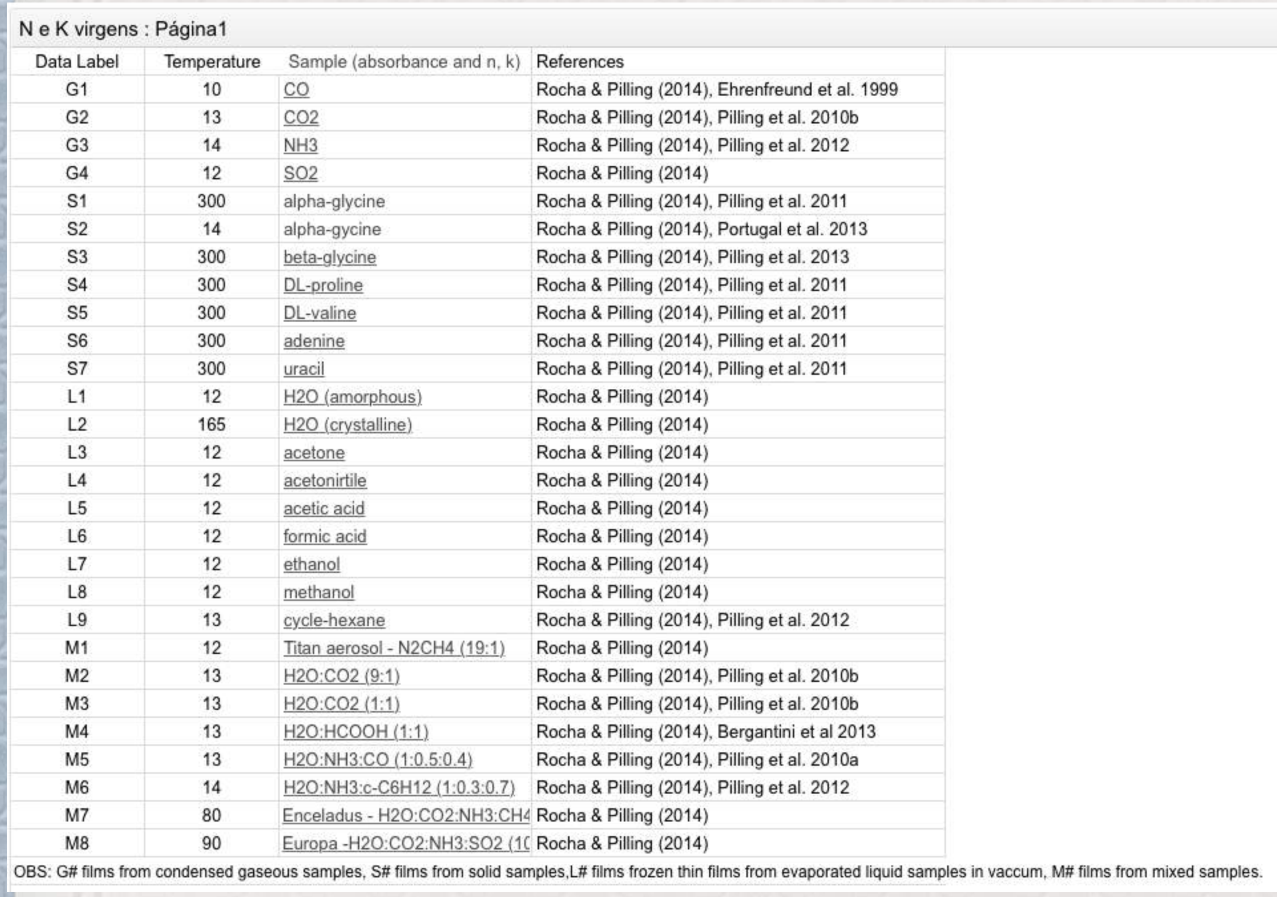


Rocha+(2017)

Public database of Complex Refractive Index of astrophysical ices

- *Leiden: https://www.strw.leidenuniv.nl/lab/databases/isodb/isodb.html*
- *NASA: https://science.gsfc.nasa.gov/691/cosmicice/constants.html*
- ***Me (special ☺): https://sites.google.com/view/astrow-en/research/databases (Rocha & Pilling 2014, Rocha et al. 2017). ICES PROCESSED BY CRs!!!***
- *Other (not ascii format): http://www.astro.spbu.ru/JPDOC/1-dbase.html*

Public database of Complex Refractive Index of astrophysical ices

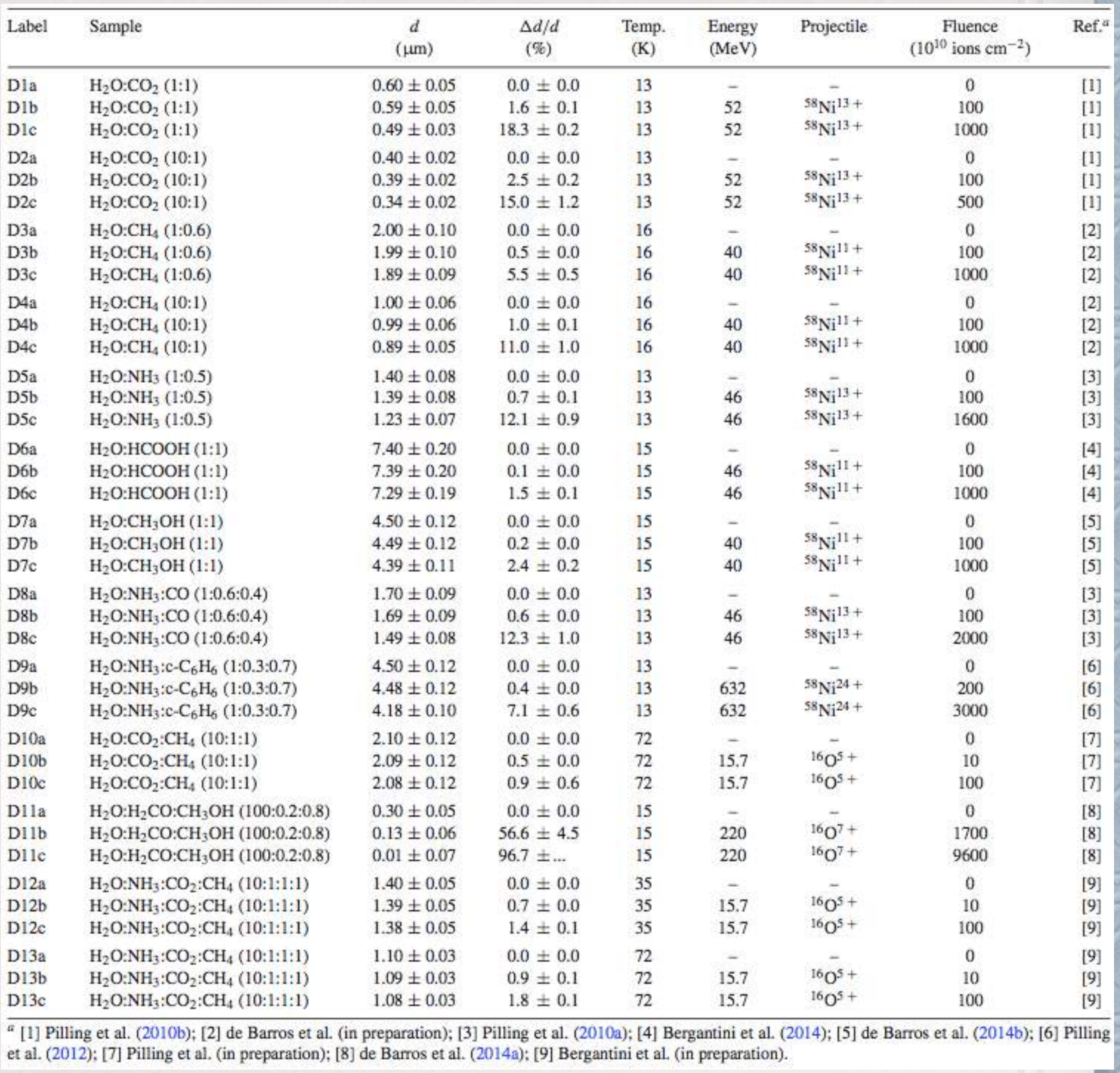


N e K virgens : Página1

Data Label	Temperature	Sample (absorbance and n, k)	References
G1	10	CO	Rocha & Pilling (2014), Ehrenfreund et al. 1999
G2	13	CO2	Rocha & Pilling (2014), Pilling et al. 2010b
G3	14	NH3	Rocha & Pilling (2014), Pilling et al. 2012
G4	12	SO2	Rocha & Pilling (2014)
S1	300	alpha-glycine	Rocha & Pilling (2014), Pilling et al. 2011
S2	14	alpha-gycine	Rocha & Pilling (2014), Portugal et al. 2013
S3	300	beta-glycine	Rocha & Pilling (2014), Pilling et al. 2013
S4	300	DL-proline	Rocha & Pilling (2014), Pilling et al. 2011
S5	300	DL-valine	Rocha & Pilling (2014), Pilling et al. 2011
S6	300	adenine	Rocha & Pilling (2014), Pilling et al. 2011
S7	300	uracil	Rocha & Pilling (2014), Pilling et al. 2011
L1	12	H2O (amorphous)	Rocha & Pilling (2014)
L2	165	H2O (crystalline)	Rocha & Pilling (2014)
L3	12	acetone	Rocha & Pilling (2014)
L4	12	acetonirtile	Rocha & Pilling (2014)
L5	12	acetic acid	Rocha & Pilling (2014)
L6	12	formic acid	Rocha & Pilling (2014)
L7	12	ethanol	Rocha & Pilling (2014)
L8	12	methanol	Rocha & Pilling (2014)
L9	13	cycle-hexane	Rocha & Pilling (2014), Pilling et al. 2012
M1	12	Titan aerosol - N2CH4 (19:1)	Rocha & Pilling (2014)
M2	13	H2O:CO2 (9:1)	Rocha & Pilling (2014), Pilling et al. 2010b
M3	13	H2O:CO2 (1:1)	Rocha & Pilling (2014), Pilling et al. 2010b
M4	13	H2O:HCOOH (1:1)	Rocha & Pilling (2014), Bergantini et al 2013
M5	13	H2O:NH3:CO (1:0.5:0.4)	Rocha & Pilling (2014), Pilling et al. 2010a
M6	14	H2O:NH3:c-C6H12 (1:0.3:0.7)	Rocha & Pilling (2014), Pilling et al. 2012
M7	80	Enceladus - H2O:CO2:NH3:CH4	Rocha & Pilling (2014)
M8	90	Europa -H2O:CO2:NH3:SO2 (1(	Rocha & Pilling (2014)

OBS: G# films from condensed gaseous samples, S# films from solid samples,L# films frozen thin films from evaporated liquid samples in vaccum, M# films from mixed samples.

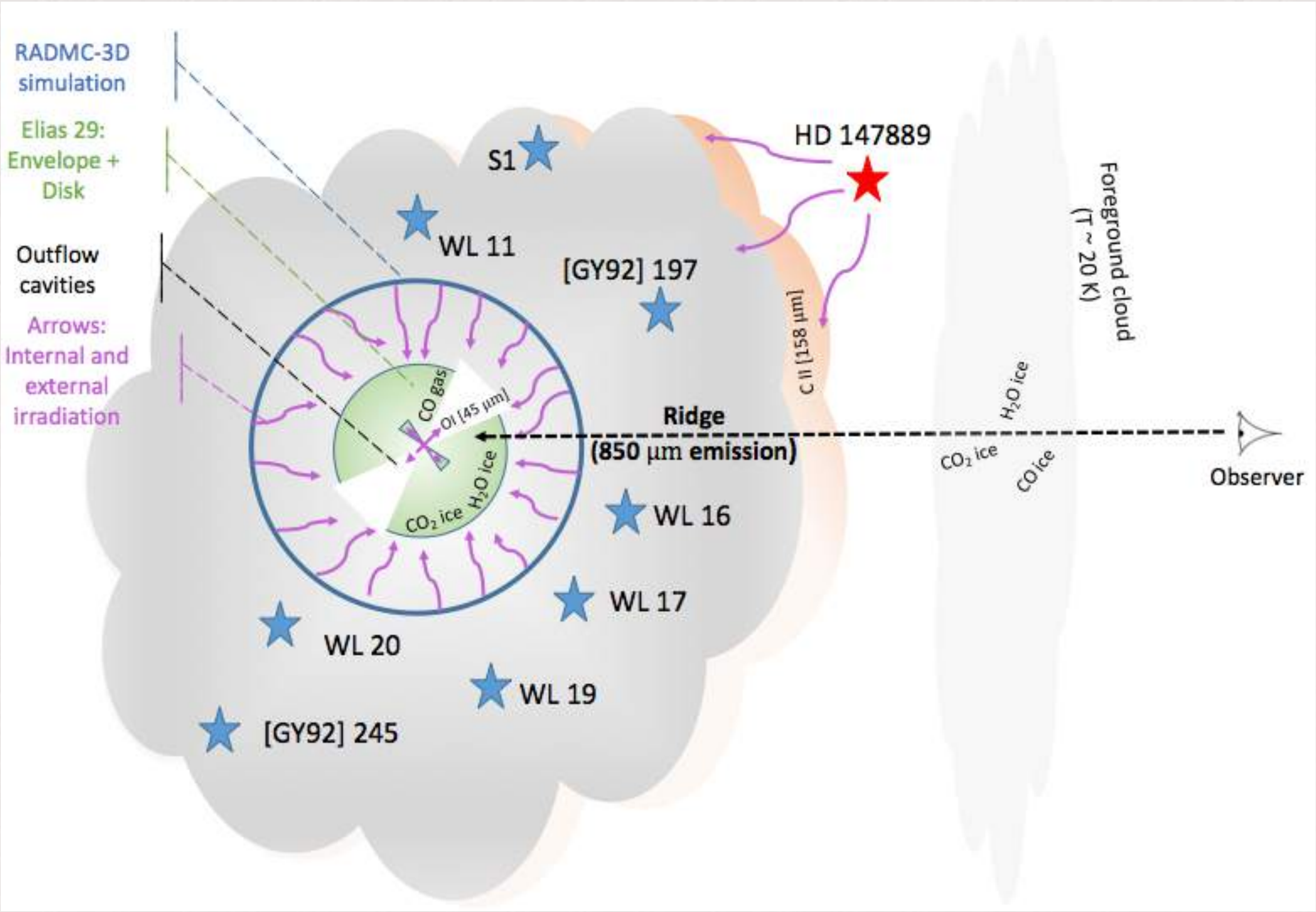
Rocha+ (2014, 2017)



Label	Sample	d (μm)	$\Delta d/d$ (%)	Temp. (K)	Energy (MeV)	Projectile	Fluence (10^{10} ions cm^{-2})	Ref.[a]
D1a	$H_2O:CO_2$ (1:1)	0.60 ± 0.05	0.0 ± 0.0	13	–	–	0	[1]
D1b	$H_2O:CO_2$ (1:1)	0.59 ± 0.05	1.6 ± 0.1	13	52	$^{58}Ni^{13+}$	100	[1]
D1c	$H_2O:CO_2$ (1:1)	0.49 ± 0.03	18.3 ± 0.2	13	52	$^{58}Ni^{13+}$	1000	[1]
D2a	$H_2O:CO_2$ (10:1)	0.40 ± 0.02	0.0 ± 0.0	13	–	–	0	[1]
D2b	$H_2O:CO_2$ (10:1)	0.39 ± 0.02	2.5 ± 0.2	13	52	$^{58}Ni^{13+}$	100	[1]
D2c	$H_2O:CO_2$ (10:1)	0.34 ± 0.02	15.0 ± 1.2	13	52	$^{58}Ni^{13+}$	500	[1]
D3a	$H_2O:CH_4$ (1:0.6)	2.00 ± 0.10	0.0 ± 0.0	16	–	–	0	[2]
D3b	$H_2O:CH_4$ (1:0.6)	1.99 ± 0.10	0.5 ± 0.0	16	40	$^{58}Ni^{11+}$	100	[2]
D3c	$H_2O:CH_4$ (1:0.6)	1.89 ± 0.09	5.5 ± 0.5	16	40	$^{58}Ni^{11+}$	1000	[2]
D4a	$H_2O:CH_4$ (10:1)	1.00 ± 0.06	0.0 ± 0.0	16	–	–	0	[2]
D4b	$H_2O:CH_4$ (10:1)	0.99 ± 0.06	1.0 ± 0.1	16	40	$^{58}Ni^{11+}$	100	[2]
D4c	$H_2O:CH_4$ (10:1)	0.89 ± 0.05	11.0 ± 1.0	16	40	$^{58}Ni^{11+}$	1000	[2]
D5a	$H_2O:NH_3$ (1:0.5)	1.40 ± 0.08	0.0 ± 0.0	13	–	–	0	[3]
D5b	$H_2O:NH_3$ (1:0.5)	1.39 ± 0.08	0.7 ± 0.1	13	46	$^{58}Ni^{13+}$	100	[3]
D5c	$H_2O:NH_3$ (1:0.5)	1.23 ± 0.07	12.1 ± 0.9	13	46	$^{58}Ni^{13+}$	1600	[3]
D6a	$H_2O:HCOOH$ (1:1)	7.40 ± 0.20	0.0 ± 0.0	15	–	–	0	[4]
D6b	$H_2O:HCOOH$ (1:1)	7.39 ± 0.20	0.1 ± 0.0	15	46	$^{58}Ni^{11+}$	100	[4]
D6c	$H_2O:HCOOH$ (1:1)	7.29 ± 0.19	1.5 ± 0.1	15	46	$^{58}Ni^{11+}$	1000	[4]
D7a	$H_2O:CH_3OH$ (1:1)	4.50 ± 0.12	0.0 ± 0.0	15	–	–	0	[5]
D7b	$H_2O:CH_3OH$ (1:1)	4.49 ± 0.12	0.2 ± 0.0	15	40	$^{58}Ni^{11+}$	100	[5]
D7c	$H_2O:CH_3OH$ (1:1)	4.39 ± 0.11	2.4 ± 0.2	15	40	$^{58}Ni^{11+}$	1000	[5]
D8a	$H_2O:NH_3:CO$ (1:0.6:0.4)	1.70 ± 0.09	0.0 ± 0.0	13	–	–	0	[3]
D8b	$H_2O:NH_3:CO$ (1:0.6:0.4)	1.69 ± 0.09	0.6 ± 0.0	13	46	$^{58}Ni^{13+}$	100	[3]
D8c	$H_2O:NH_3:CO$ (1:0.6:0.4)	1.49 ± 0.08	12.3 ± 1.0	13	46	$^{58}Ni^{13+}$	2000	[3]
D9a	$H_2O:NH_3:c\text{-}C_6H_6$ (1:0.3:0.7)	4.50 ± 0.12	0.0 ± 0.0	13	–	–	0	[6]
D9b	$H_2O:NH_3:c\text{-}C_6H_6$ (1:0.3:0.7)	4.48 ± 0.12	0.4 ± 0.0	13	632	$^{58}Ni^{24+}$	200	[6]
D9c	$H_2O:NH_3:c\text{-}C_6H_6$ (1:0.3:0.7)	4.18 ± 0.10	7.1 ± 0.6	13	632	$^{58}Ni^{24+}$	3000	[6]
D10a	$H_2O:CO_2:CH_4$ (10:1:1)	2.10 ± 0.12	0.0 ± 0.0	72	–	–	0	[7]
D10b	$H_2O:CO_2:CH_4$ (10:1:1)	2.09 ± 0.12	0.5 ± 0.0	72	15.7	$^{16}O^{5+}$	10	[7]
D10c	$H_2O:CO_2:CH_4$ (10:1:1)	2.08 ± 0.12	0.9 ± 0.6	72	15.7	$^{16}O^{5+}$	100	[7]
D11a	$H_2O:H_2CO:CH_3OH$ (100:0.2:0.8)	0.30 ± 0.05	0.0 ± 0.0	15	–	–	0	[8]
D11b	$H_2O:H_2CO:CH_3OH$ (100:0.2:0.8)	0.13 ± 0.06	56.6 ± 4.5	15	220	$^{16}O^{7+}$	1700	[8]
D11c	$H_2O:H_2CO:CH_3OH$ (100:0.2:0.8)	0.01 ± 0.07	96.7 ±...	15	220	$^{16}O^{7+}$	9600	[8]
D12a	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.40 ± 0.05	0.0 ± 0.0	35	–	–	0	[9]
D12b	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.39 ± 0.05	0.7 ± 0.0	35	15.7	$^{16}O^{5+}$	10	[9]
D12c	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.38 ± 0.05	1.4 ± 0.1	35	15.7	$^{16}O^{5+}$	100	[9]
D13a	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.10 ± 0.03	0.0 ± 0.0	72	–	–	0	[9]
D13b	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.09 ± 0.03	0.9 ± 0.1	72	15.7	$^{16}O^{5+}$	10	[9]
D13c	$H_2O:NH_3:CO_2:CH_4$ (10:1:1:1)	1.08 ± 0.03	1.8 ± 0.1	72	15.7	$^{16}O^{5+}$	100	[9]

[a] [1] Pilling et al. (2010b); [2] de Barros et al. (in preparation); [3] Pilling et al. (2010a); [4] Bergantini et al. (2014); [5] de Barros et al. (2014b); [6] Pilling et al. (2012); [7] Pilling et al. (in preparation); [8] de Barros et al. (2014a); [9] Bergantini et al. (in preparation).

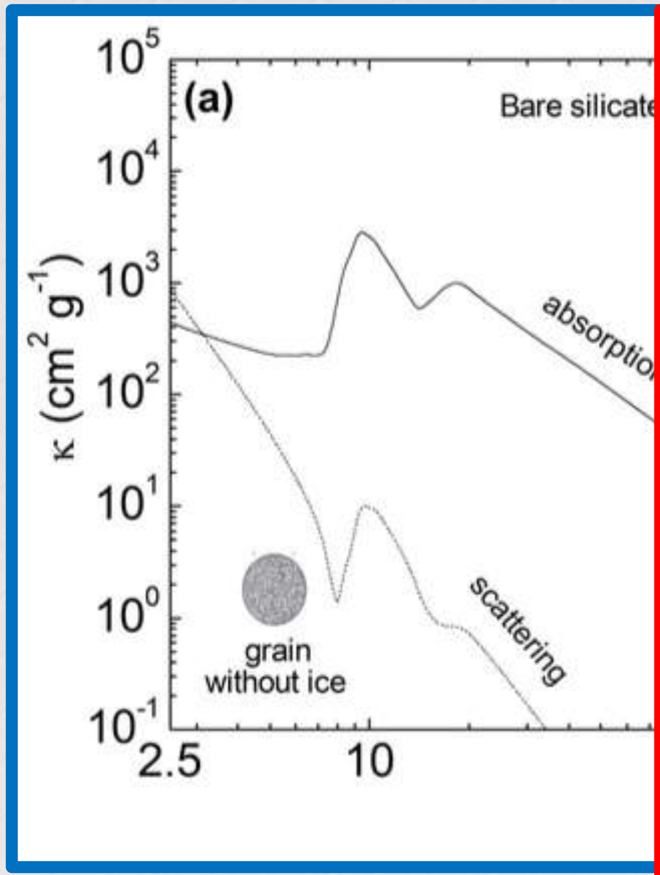
Ices in Class I object

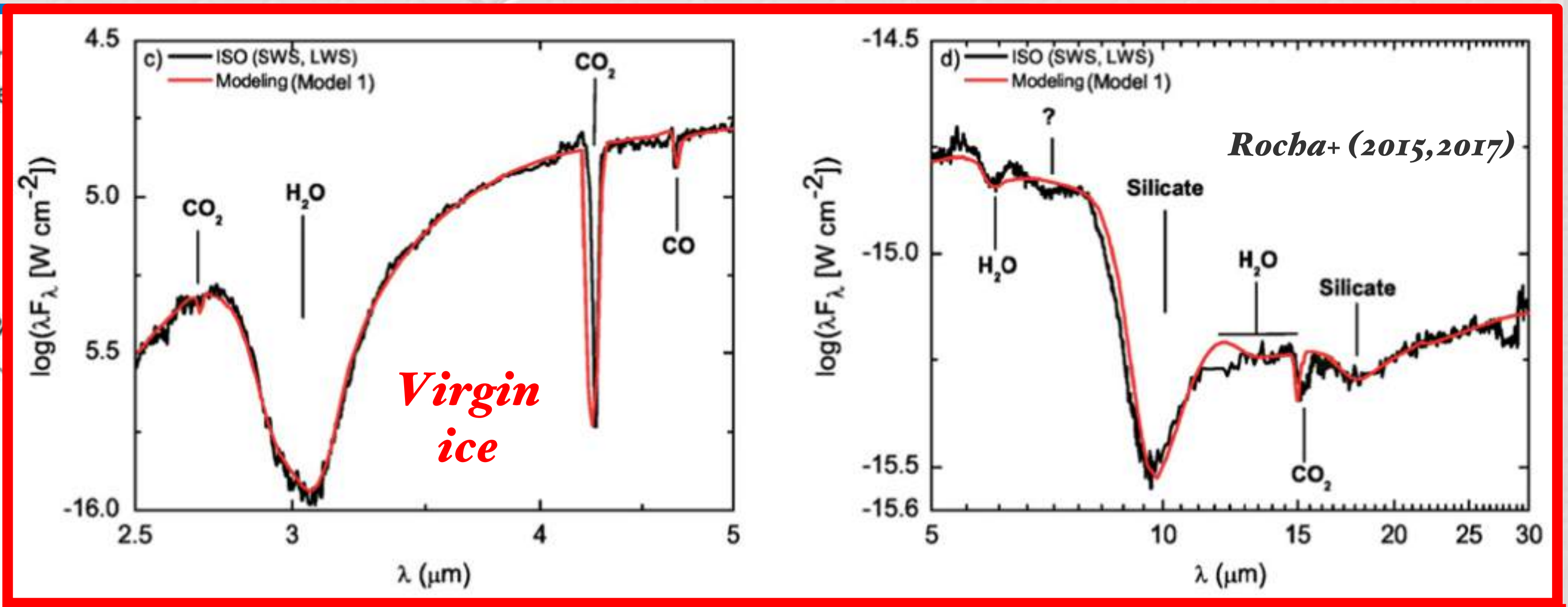


Rocha,Pilling (submitted)

~70% of ices in the foreground clouds (Boogert+2002, Rocha,Pilling 2015)

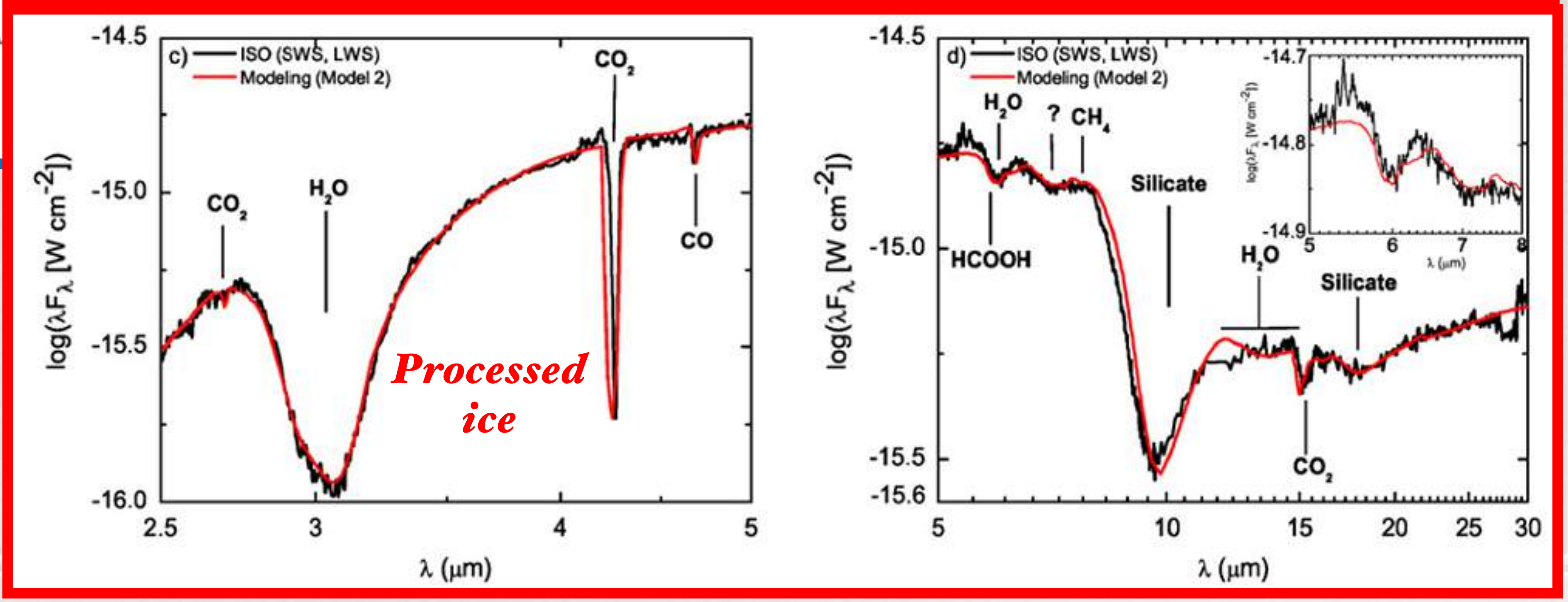
Ices in Class I object





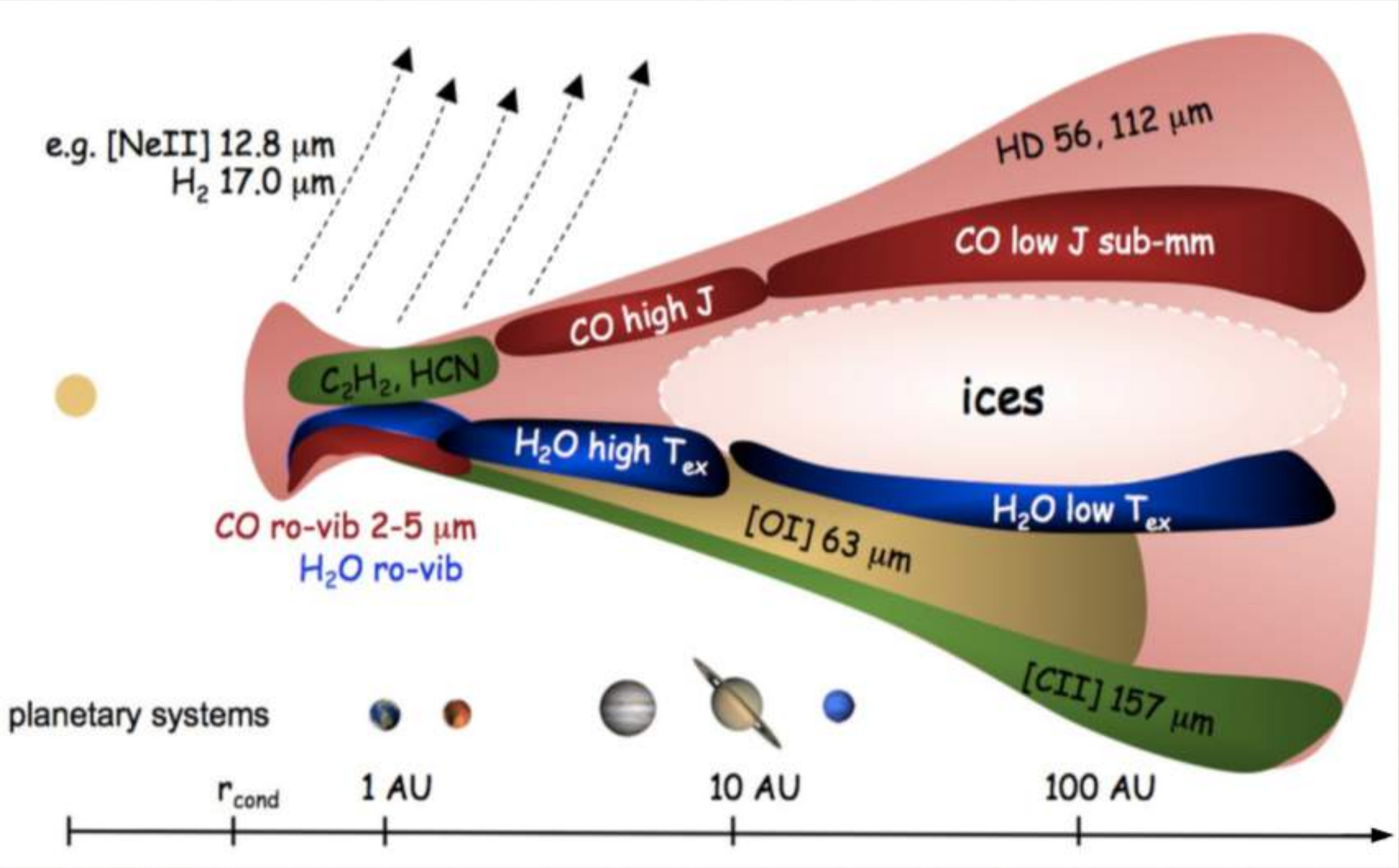
Virgin ice

Rocha+ (2015,2017)



Processed ice

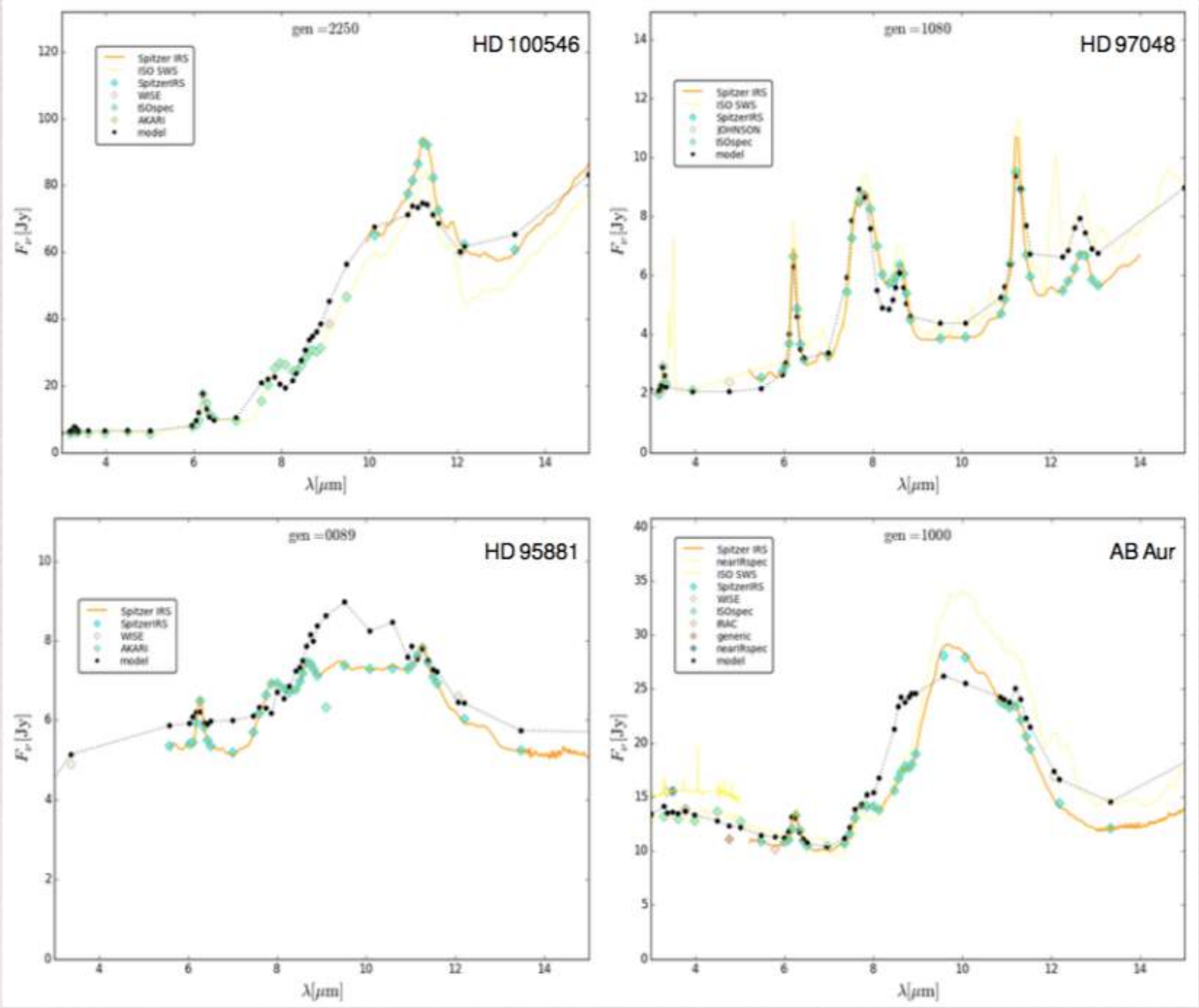
Ices in PPDs



Kamp+ (2015)

- Ice reservoir in very embedded regions;
- Models have shown very large visual extinctions (Aikawa et al., Bergin et al., Willacy et al., Woitke et al., Kamp et al., Thi et al., Glassgold et al., Meijerink et al., Najita et al., Semenov et al., Walsh et al., ...)

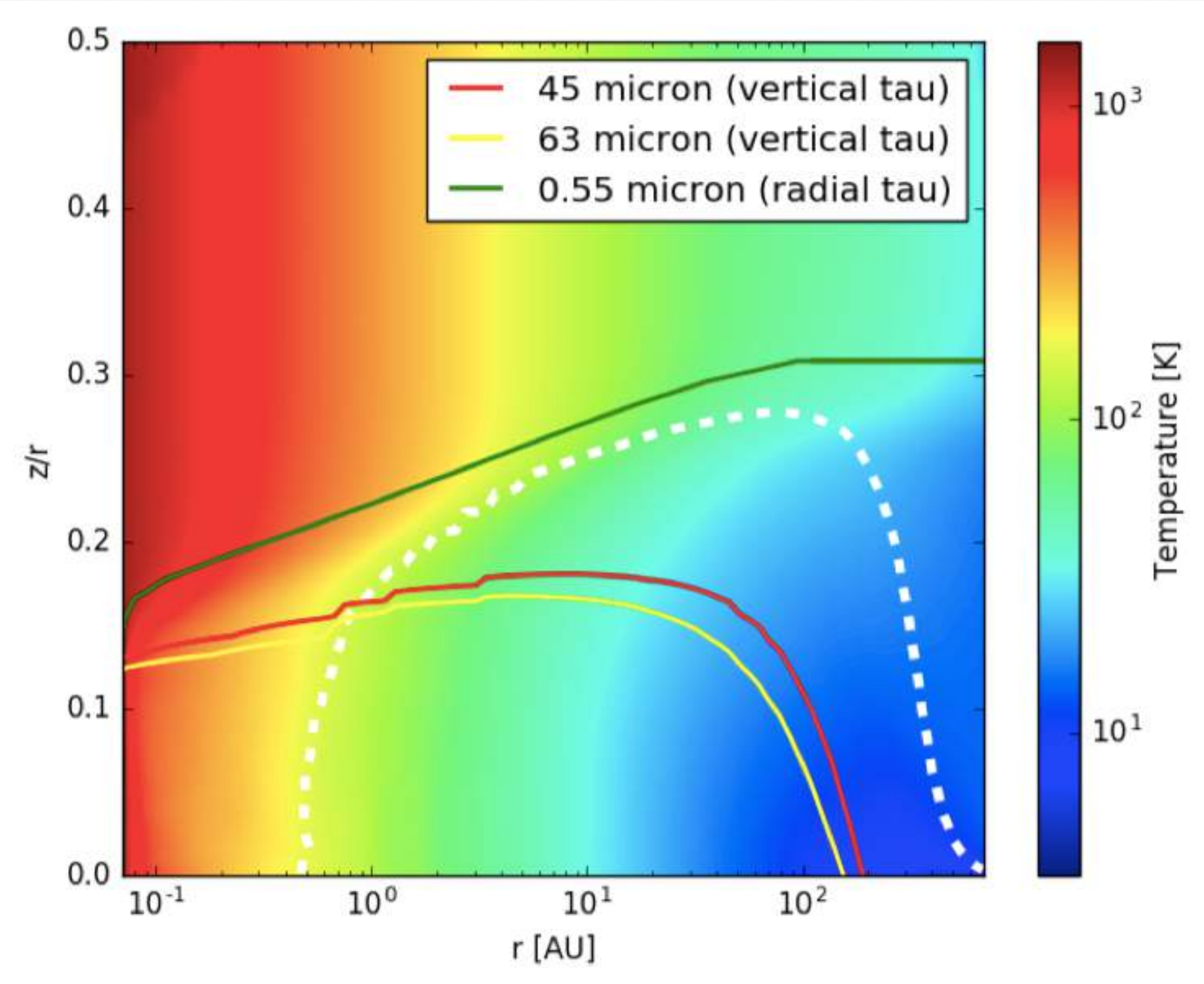
Ices in PPDs



- Results from DIANA project (Woitke+2016, Kamp+2017, Woitke+ subm).
- No ices in mid-IR observed in PPDs!!!
- Silicate and PAHs emission.

Ices in PPDs

Kamp+ (2018)



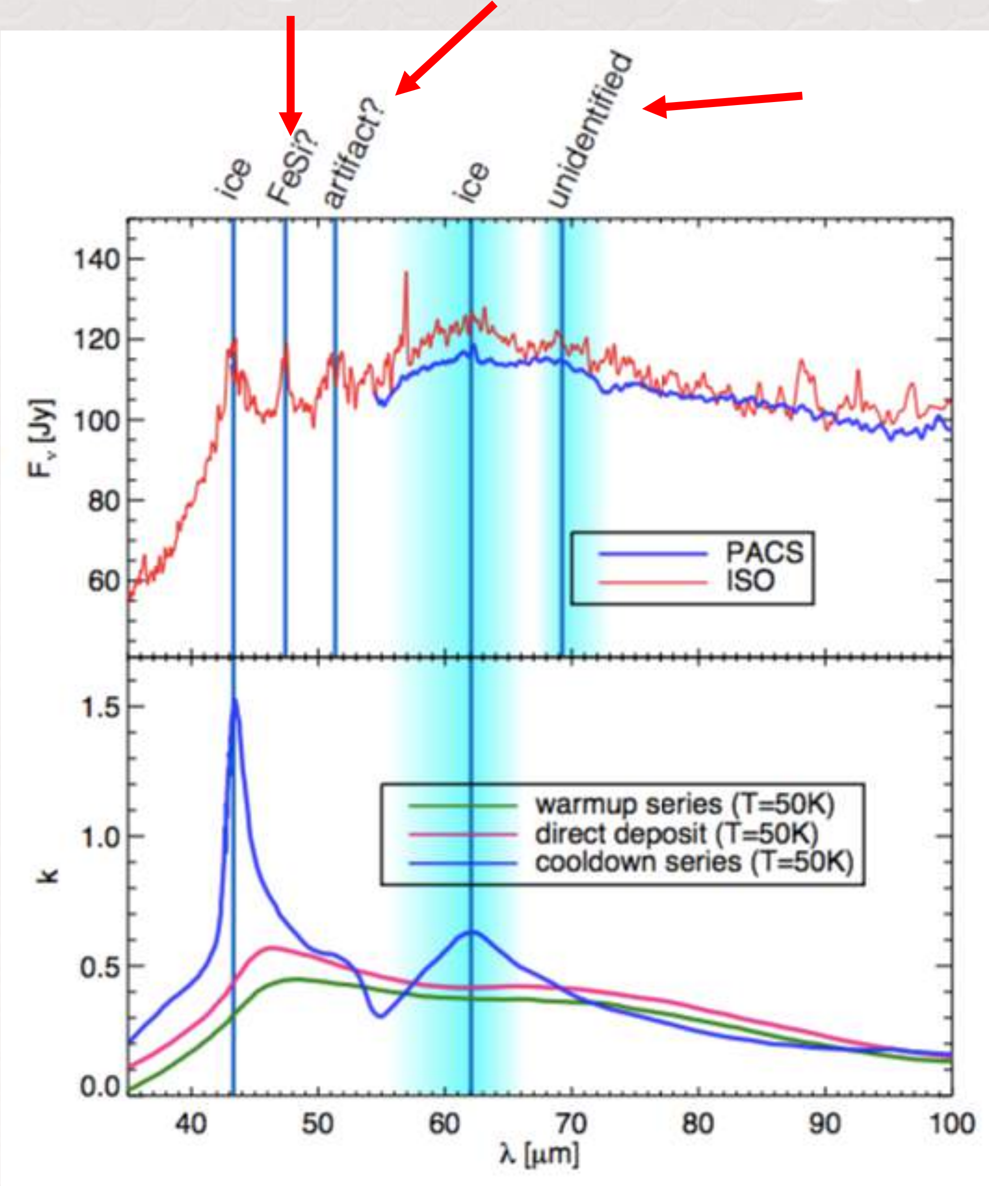
- Ices very embedded in the midplace;
- Not observable in optical;
- We must move to far-IR. Problem: lack of quality spectrum, although Herschel helps a lot.

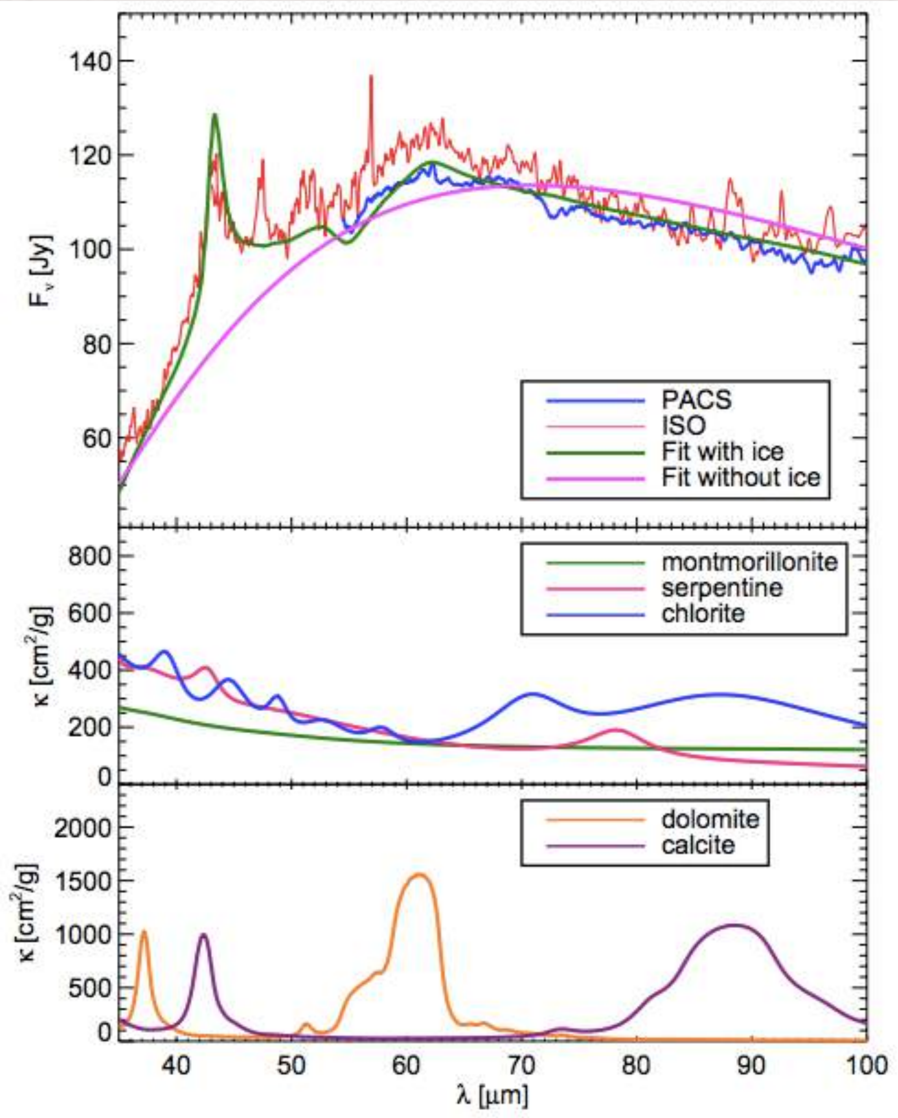
Computational modelling of ices in PPDs

Recent (unique?) modeling of ices in mid-IR (HD 142527)

Min+2016

MCMax
+
ProDiMo



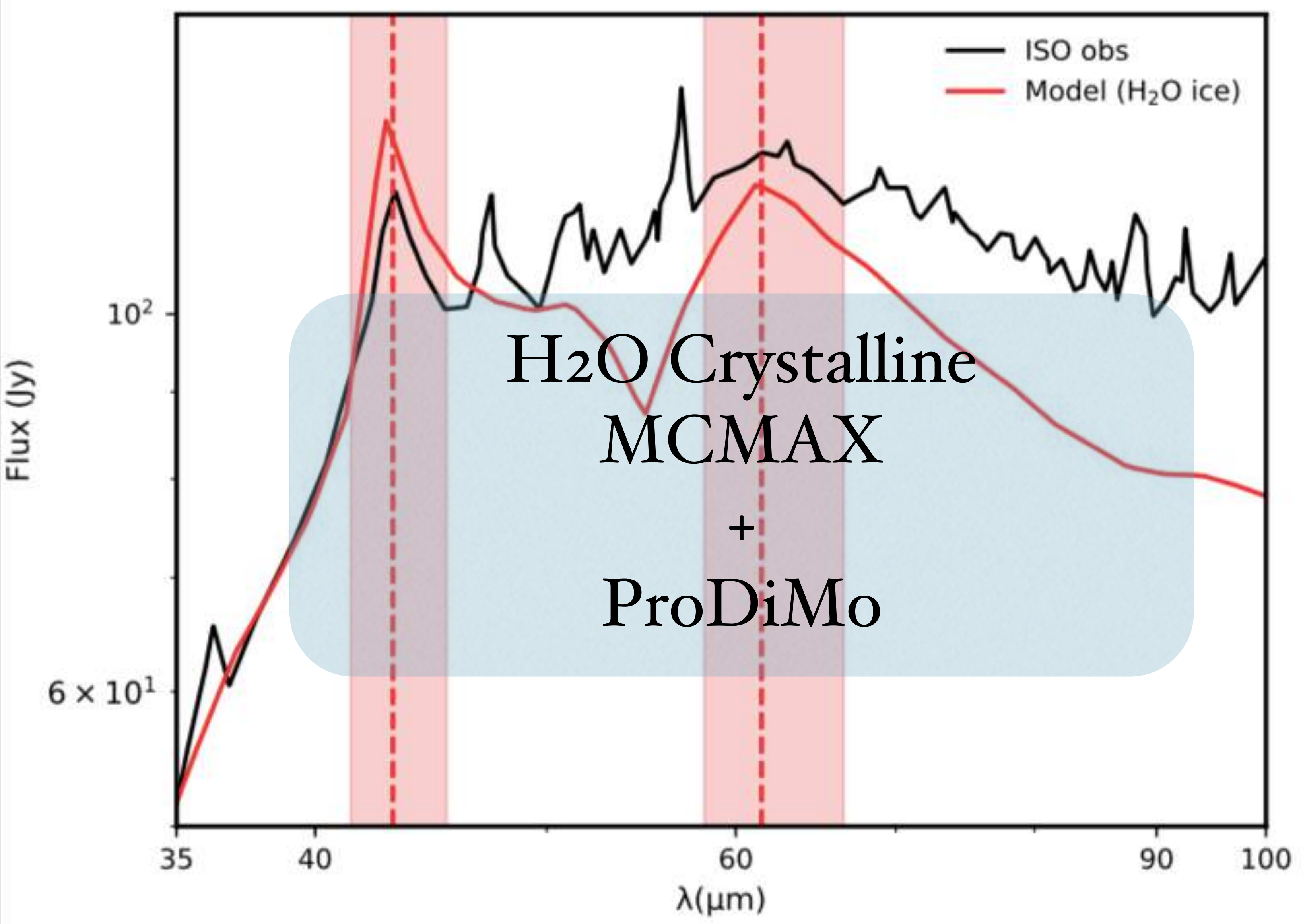


Computational modelling of ices in PPDs

- Collected laboratory data in FIR from:
  - McGuirre et al. (2016)
  - Moore & Hudson (1994, 1995)

Seeing ices in PPDs

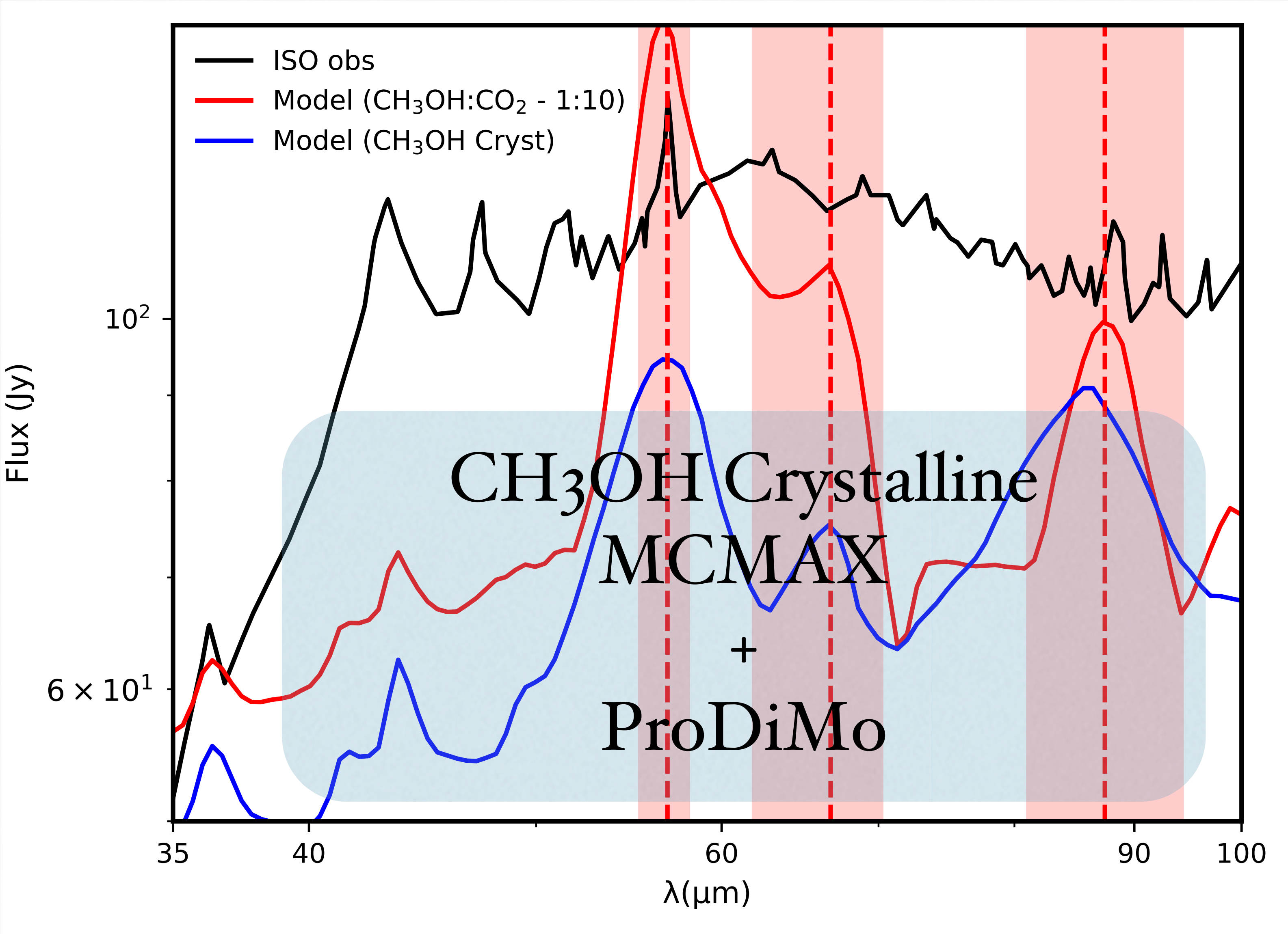
H_2O Crystalline



H_2O Crystalline
MCMAX
+
ProDiMo

Seeing ices in PPDs

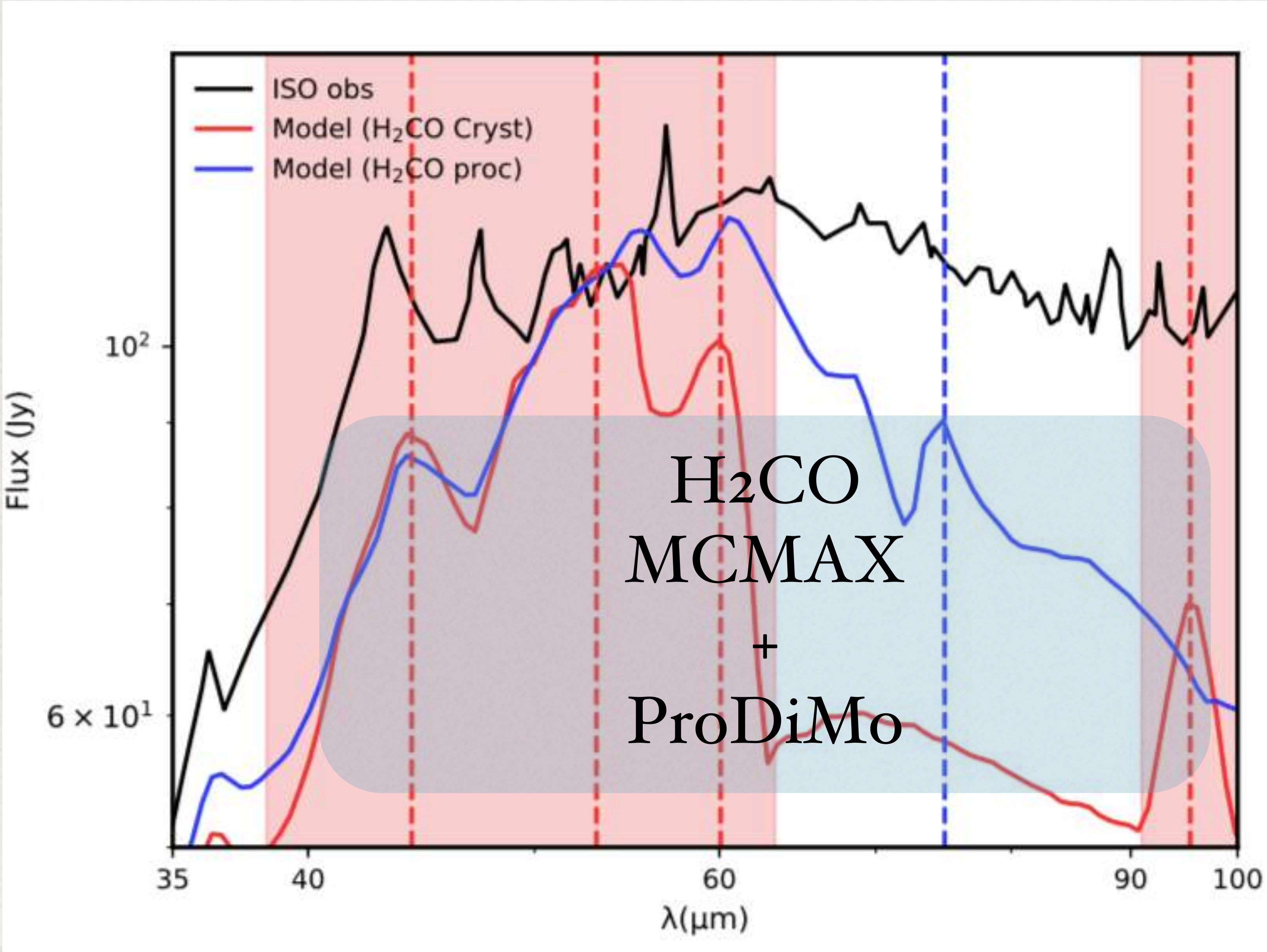
CH_3OH



CH3OH Crystalline
MCMAX
+
ProDiMo

Seeing ices in PPDs

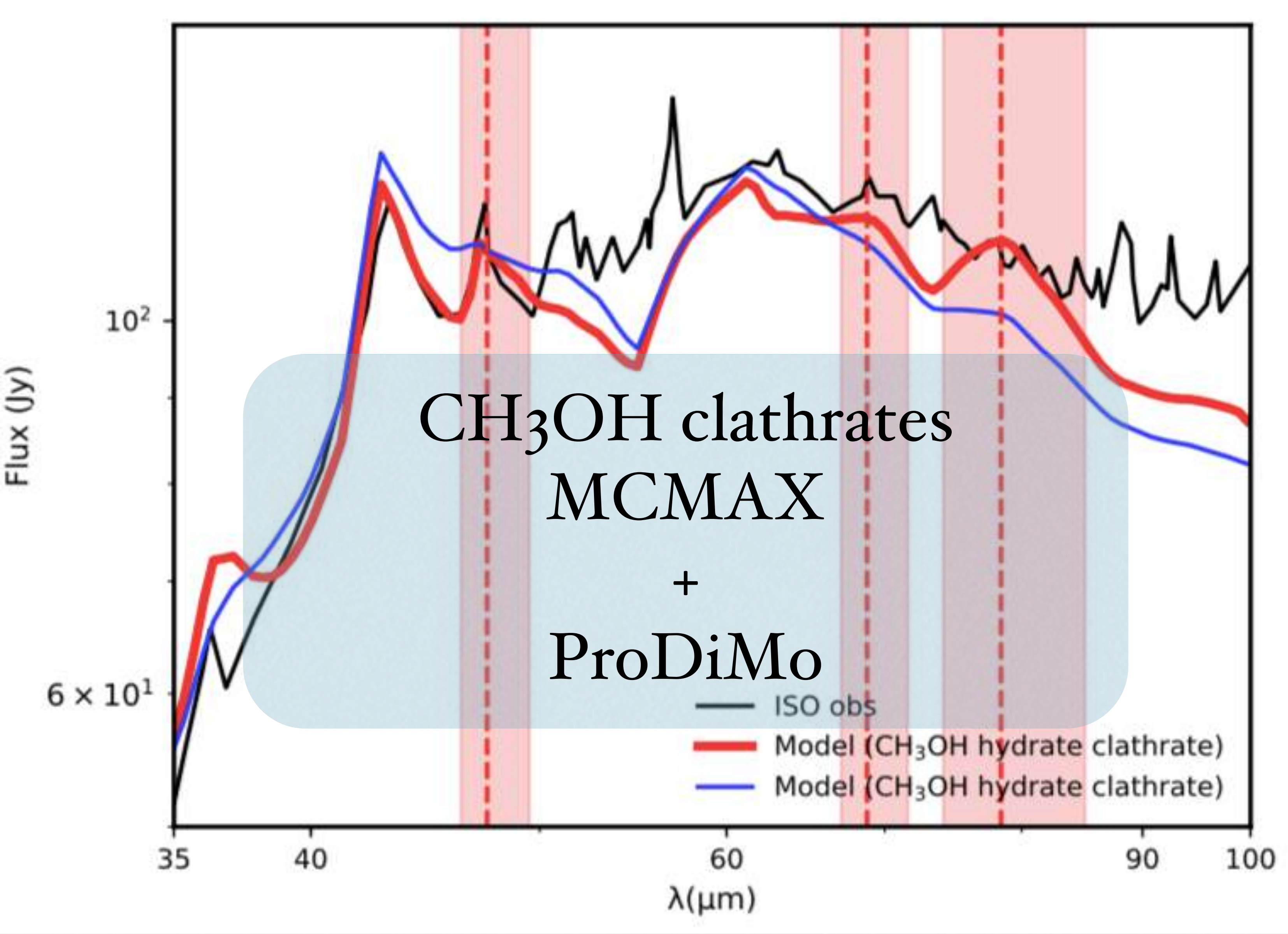
H_2CO



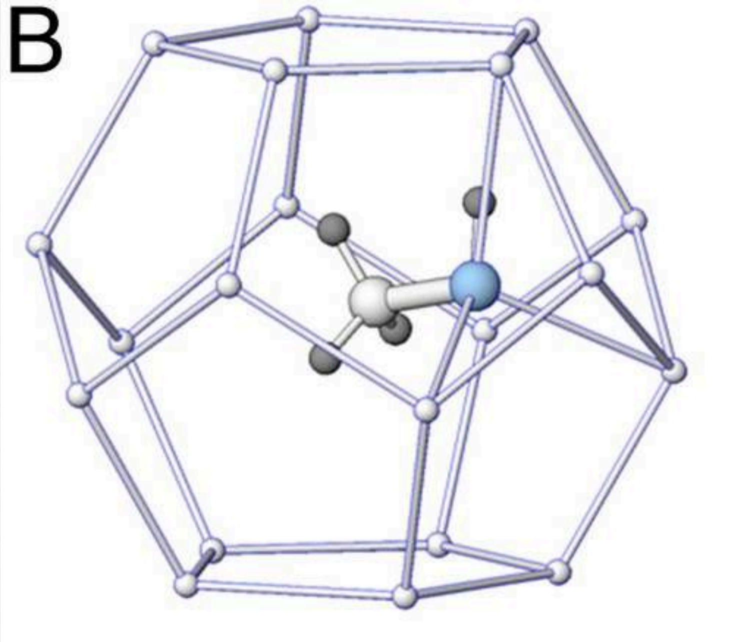
H_2CO
MCMAX
+
ProDiMo

Seeing ices in PPDs

CH_3OH Clathrates (This is gonna be the first evidence of ice processing



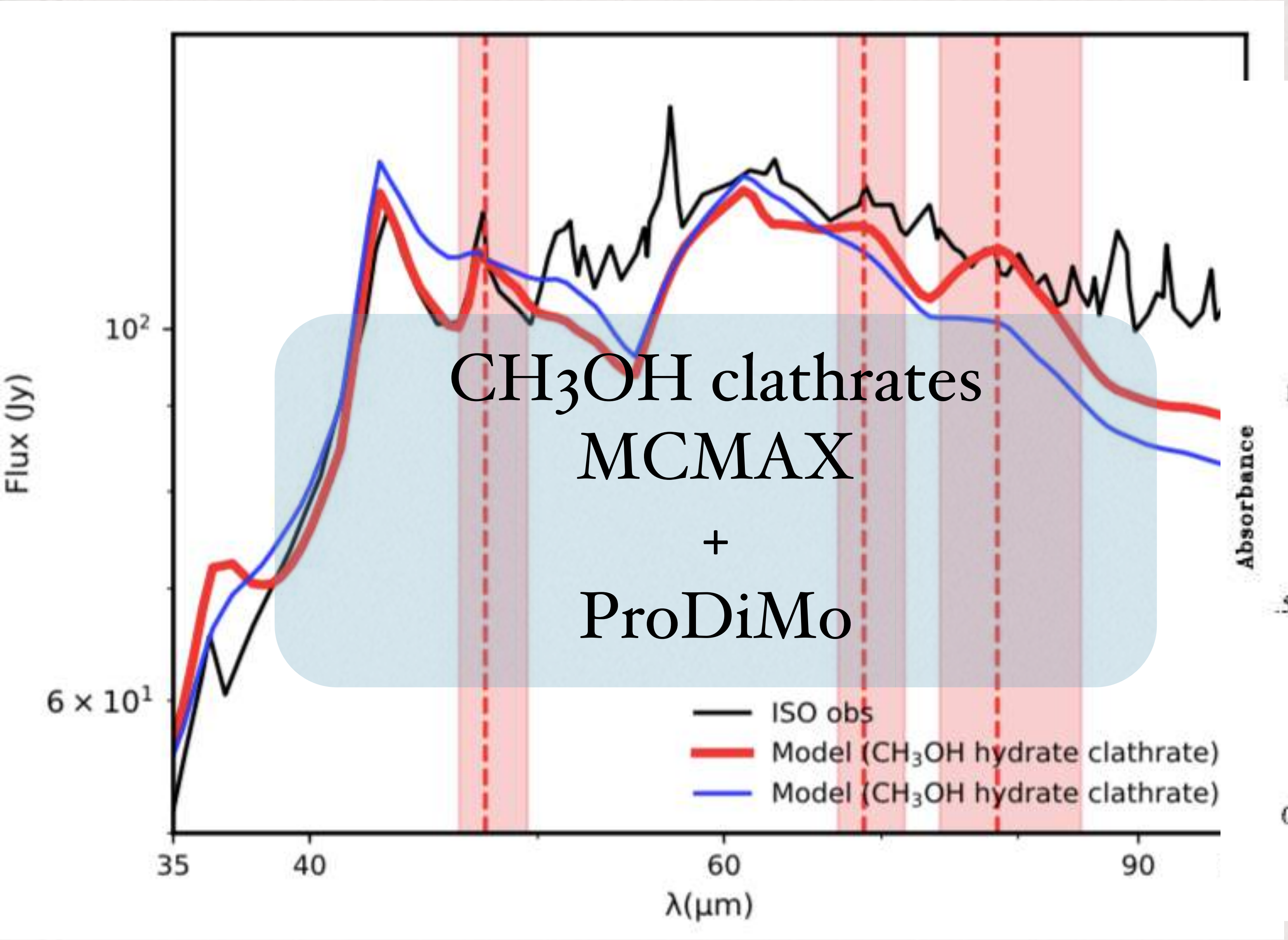
CH_3OH clathrates
MCMAX
+
ProDiMo



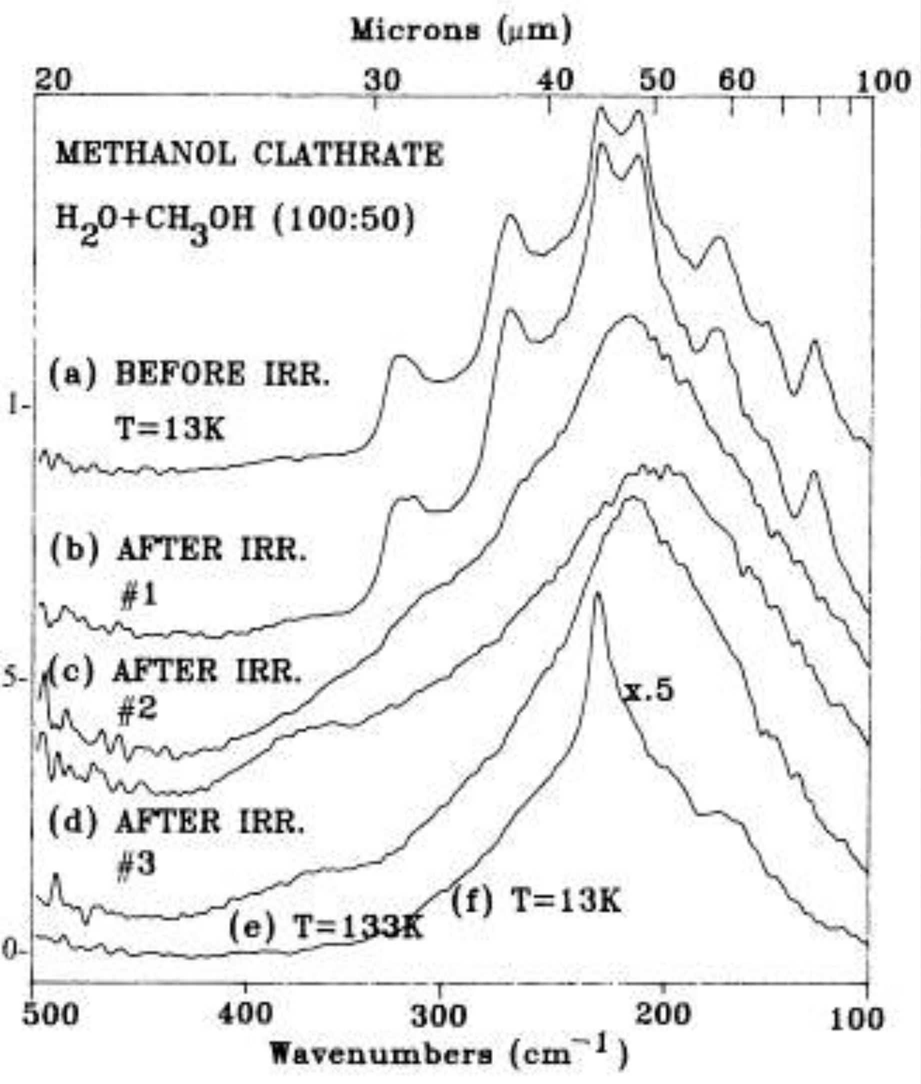
Shin+ (2013)

Seeing ices in PPDs

CH_3OH Clathrates (This is gonna be the first evidence of ice processing



CH_3OH clathrates
MCMAX
+
ProDiMo



Final remarks

- CRI are powerful tools to reproduce the chemical evolution of ices in YSOs;
- Realistic models are required to simulate PPDs properly;
- It seems that CH_3OH clathrates is going to be the first evidence of ice processing inside PPDs (*wow!!!*)
- Opacity models containing ice processing is going to be essential to match future observations with JWST (Bible citation: *...And men do not put new wine into old wine-skins*).