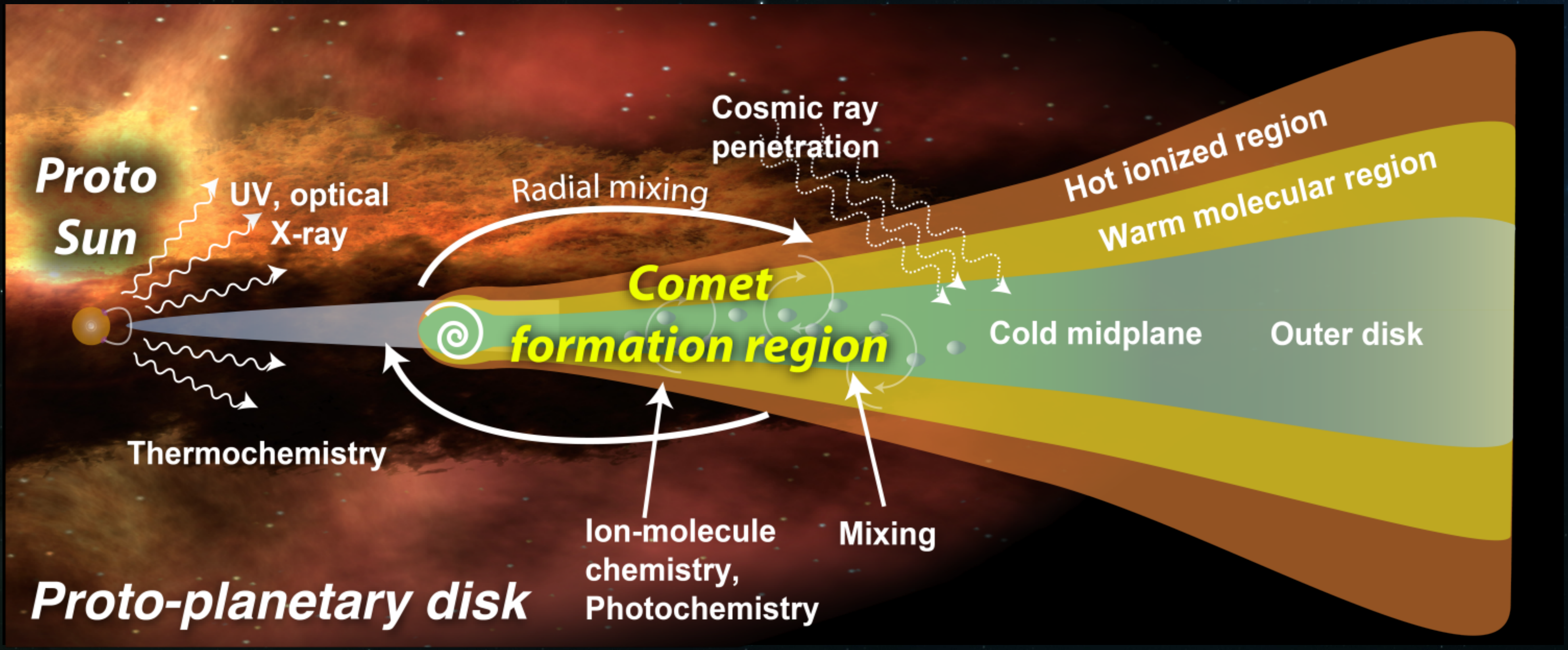
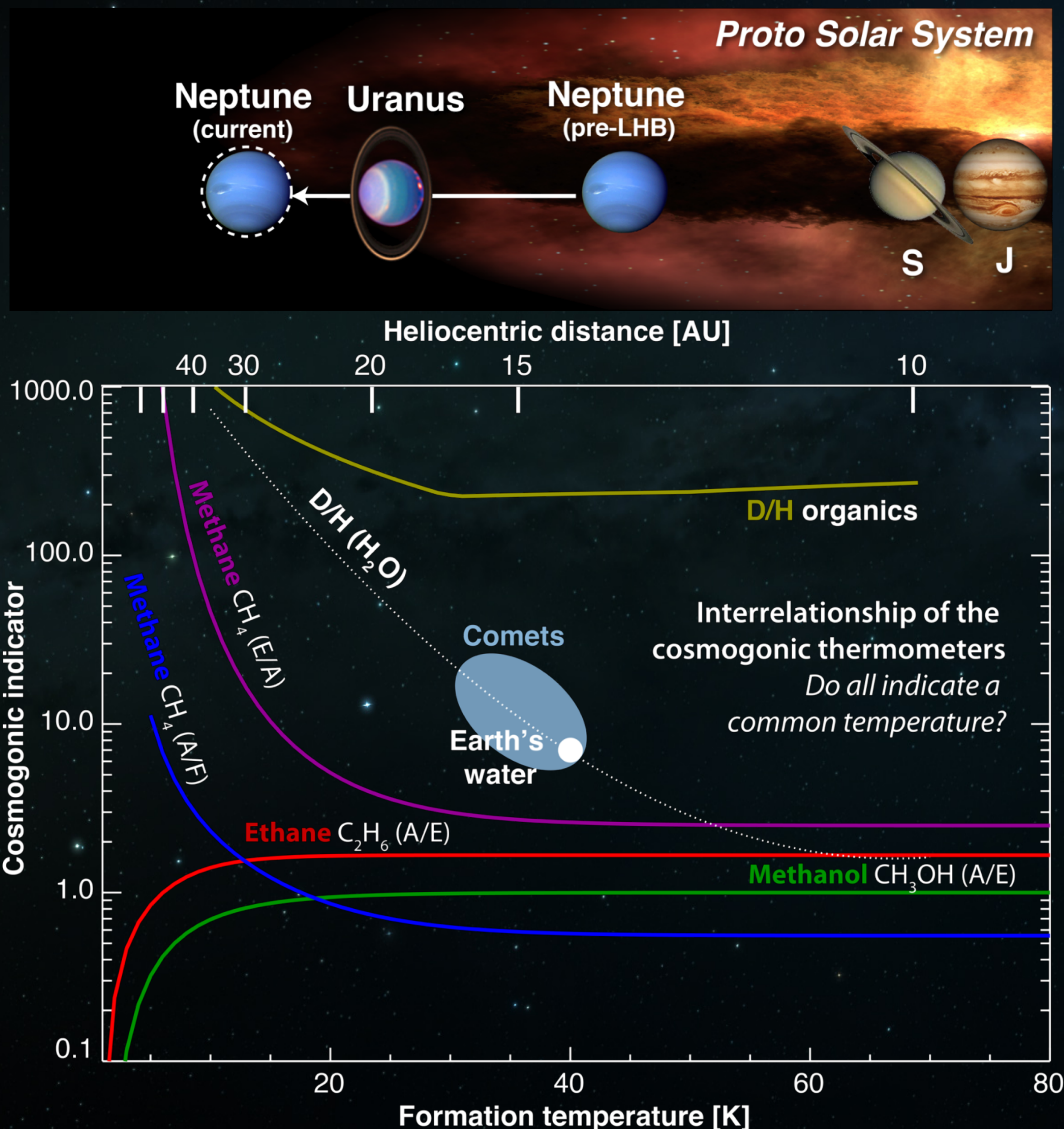
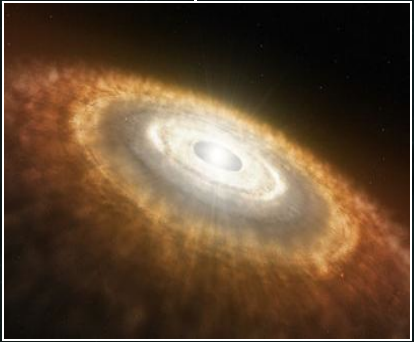
Spin Temperatures in comets
Cosmogonic indicator?

Geronimo Villanueva
NASA Goddard Space Flight Center


Proto Sun
UV, optical
X-ray
Thermochemistry
Radial mixing
Cosmic ray penetration
Hot ionized region
Warm molecular region
Comet formation region
Cold midplane
Outer disk
Ion-molecule chemistry, Photochemistry
Mixing
Proto-planetary disk

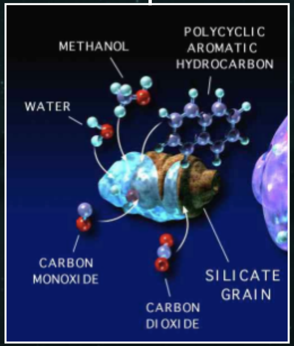

Proto Solar System
Neptune (current)
Uranus
Neptune (pre-LHB)
S
J
Heliocentric distance [AU]
40 30 20 15 10
1000.0
100.0
10.0
1.0
0.1
Cosmogonic indicator
D/H organics
D/H (H_2O)
Methane CH_4 (E/A)
Methane CH_4 (A/F)
Comets
Earth's water
Ethane C_2H_6 (A/E)
Methanol CH_3OH (A/E)
Interrelationship of the cosmogonic thermometers
Do all indicate a common temperature?
20 40 60 80
Formation temperature [K]

4.6 Ga 3.7 Ga Present



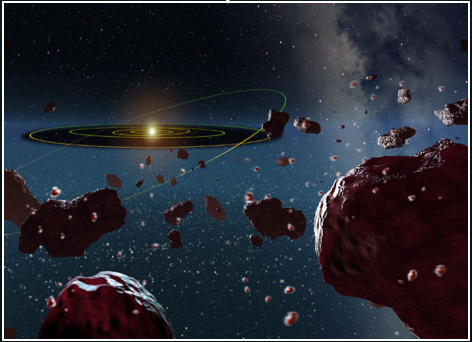
Gas-phase chemistry

$T_{gas} \sim 10\text{-}30K$



Icy grain formation

$T_{ice} \sim 10K$



Storage in Oort Cloud / Kuiper belt

$T_{reservoir} \sim 3K$

Sublimation

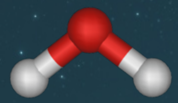
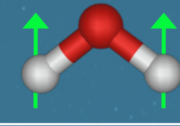
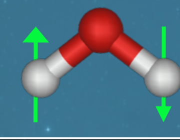
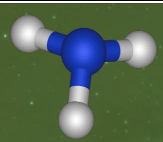
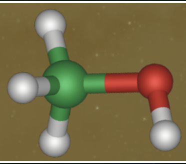
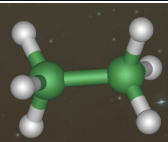
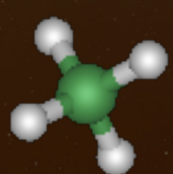
$T_{coma} \sim 50\text{-}150K$

$T_{surface} \sim 100\text{-}200K$

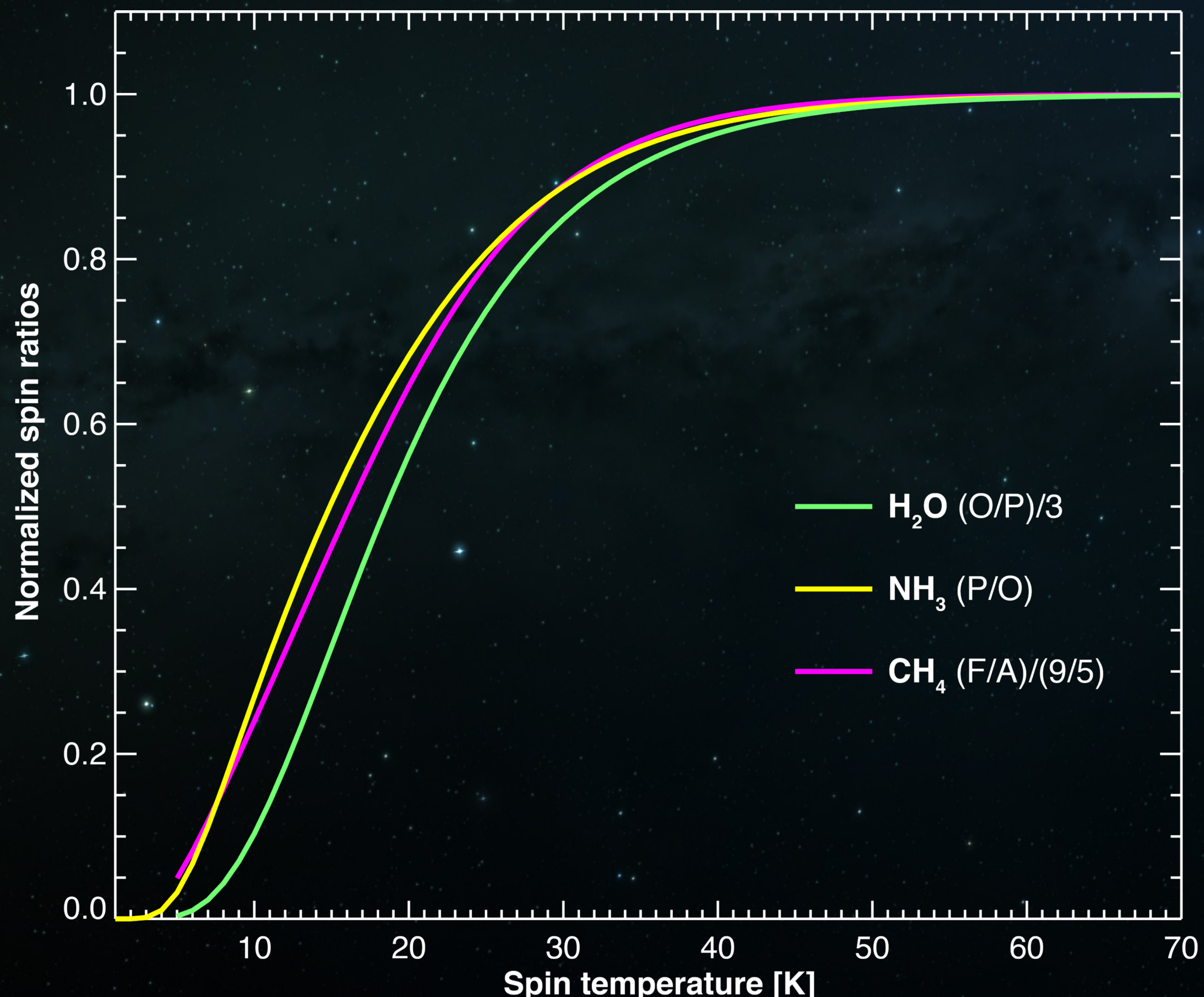
$\mathbf{T_{spin}} = ???$

The **complexities** of deriving **Tspin** from **OPR** measurements

List of spin species

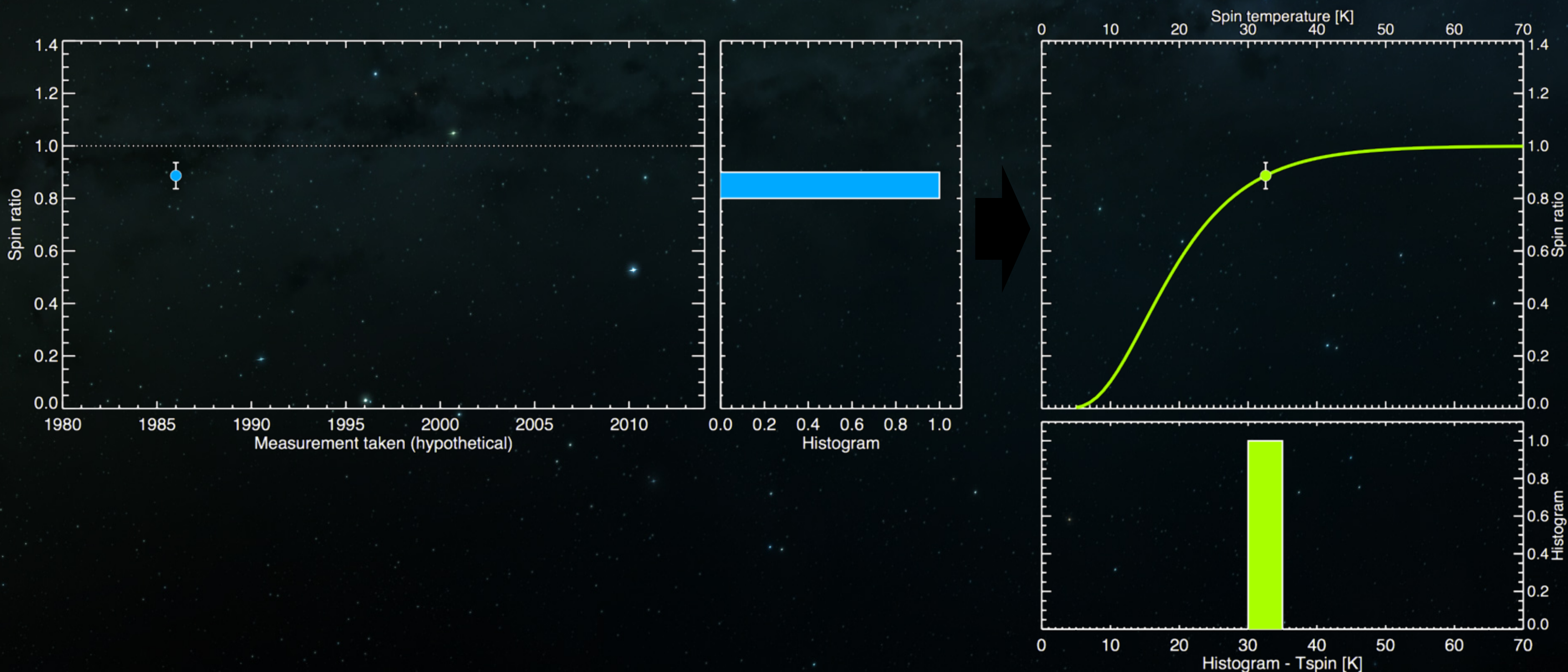
	Species	Nuclear Spin Isomers	Point Group
	Water (H_2O)	 Ortho (A)	C_{2v}
		 Para (B)	
	Ammonia (NH_3)	Ortho (A_2)	C_{3v}
		Para (E)	
	Methanol (CH_3OH)	A symmetries	C_{3v}
		E symmetries	
	Ethane (C_2H_6)	E_g symmetry	D_{3d}
		A_g symmetry	
	Methane (CH_4)	A symmetries	T_d
		F symmetries	
		E symmetries	

H_2O, **NH_3** and **CH_4** T_{spin} curves become asymptotic at "**30K**"



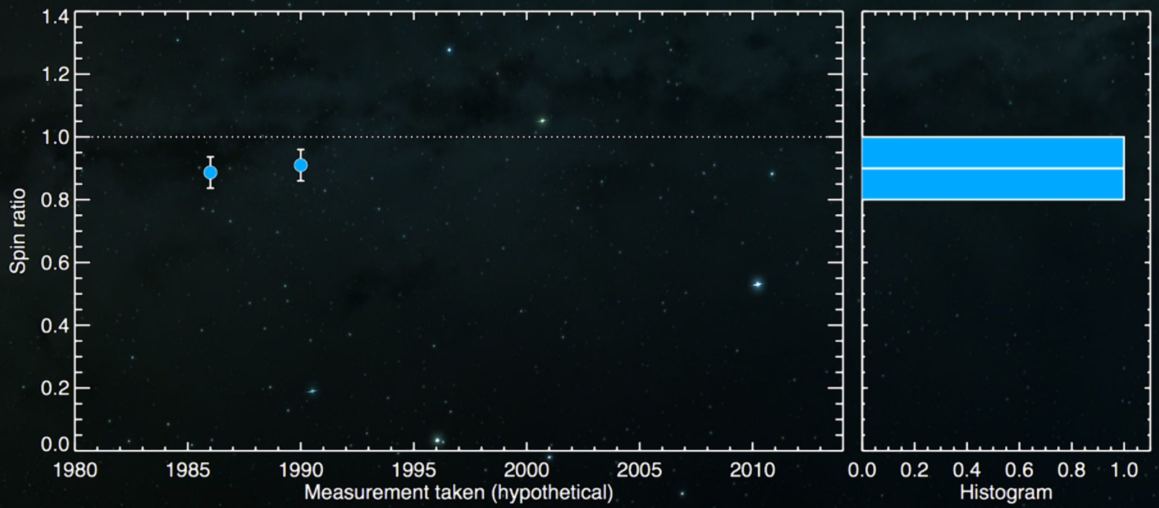
Let's imagine spin populations are in **equilibrium** (normalized spin ratio = 1) and we attempt to measure this "equilibrium"

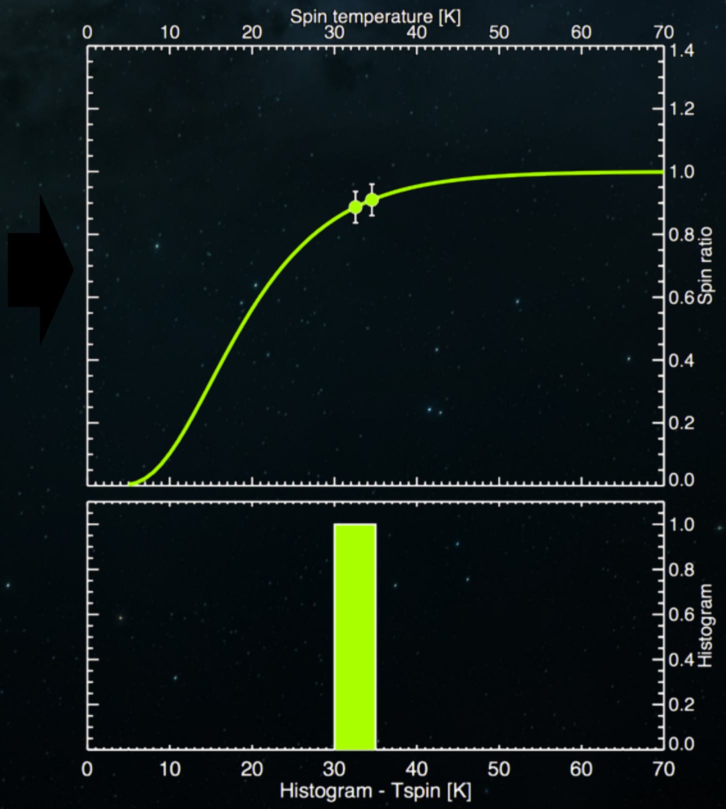
1 hypothetical measurement



Let's imagine spin populations are in **equilibrium** (normalized spin ratio = 1) and we attempt to measure this "equilibrium"

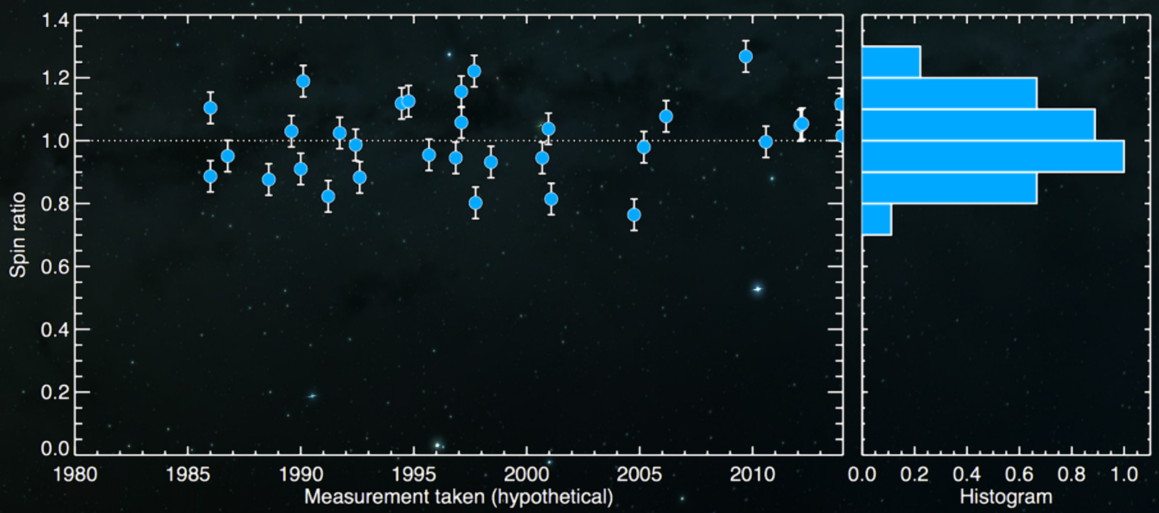
2 hypothetical measurements

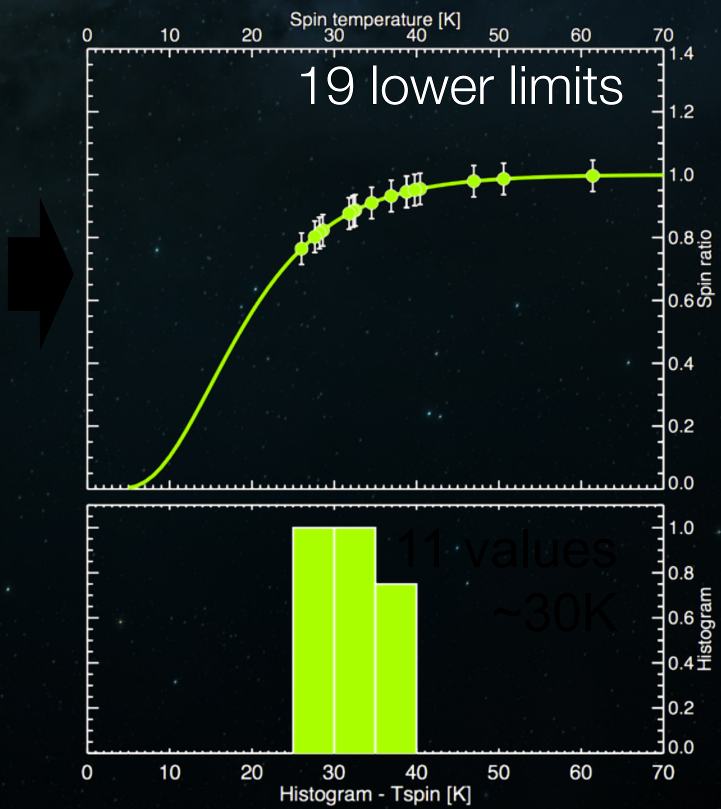




Let's imagine spin populations are in **equilibrium** (normalized spin ratio = 1) and we attempt to measure this "equilibrium"

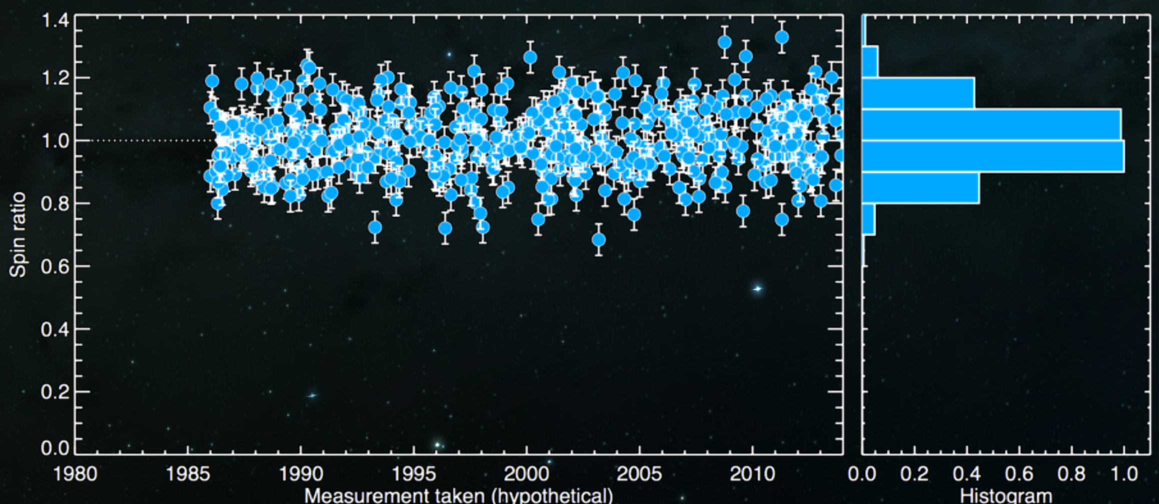
30 hypothetical measurements of **equilibrium**

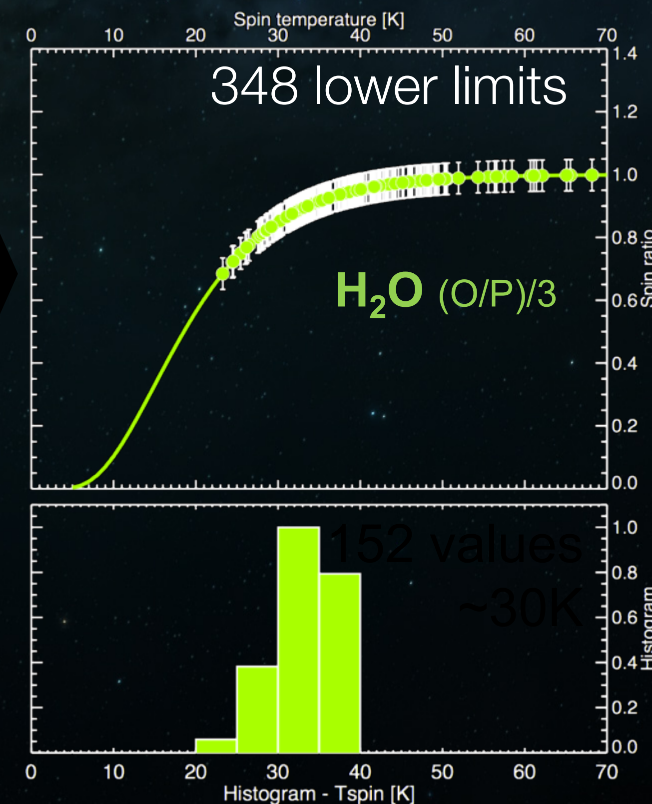




Let's imagine spin populations are in **equilibrium** (normalized spin ratio = 1) and we attempt to measure this "equilibrium"

500 hypothetical measurements of **equilibrium**





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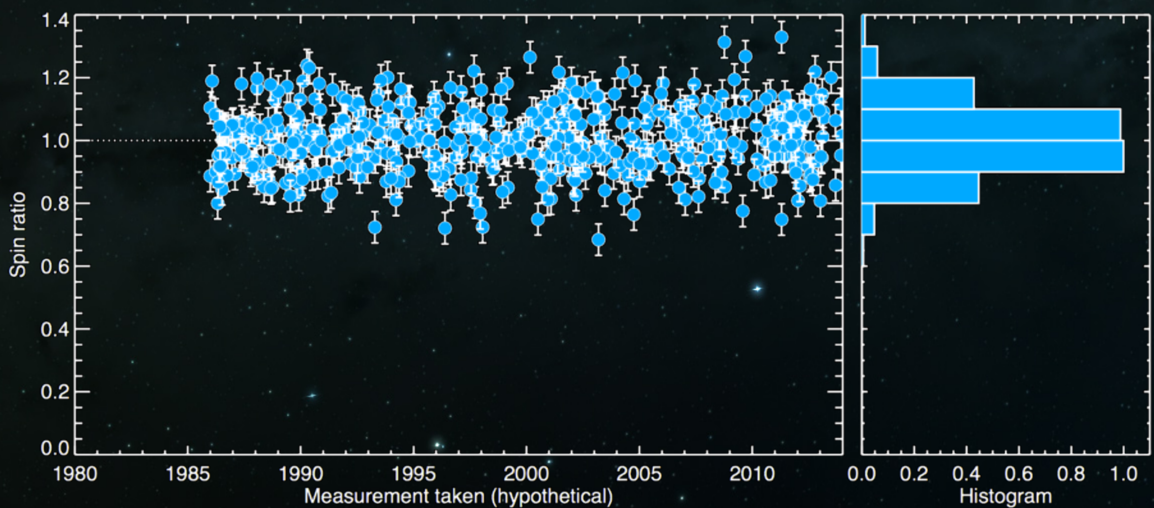
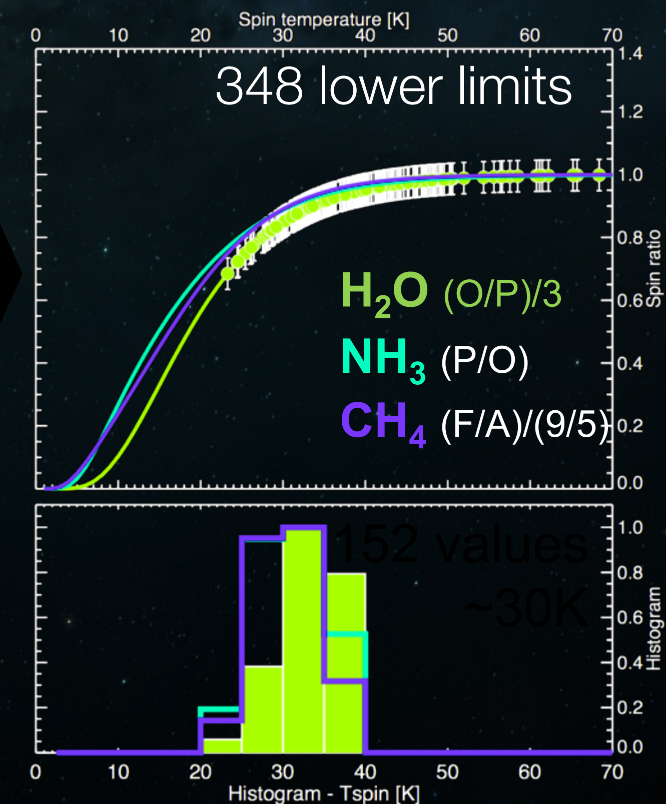
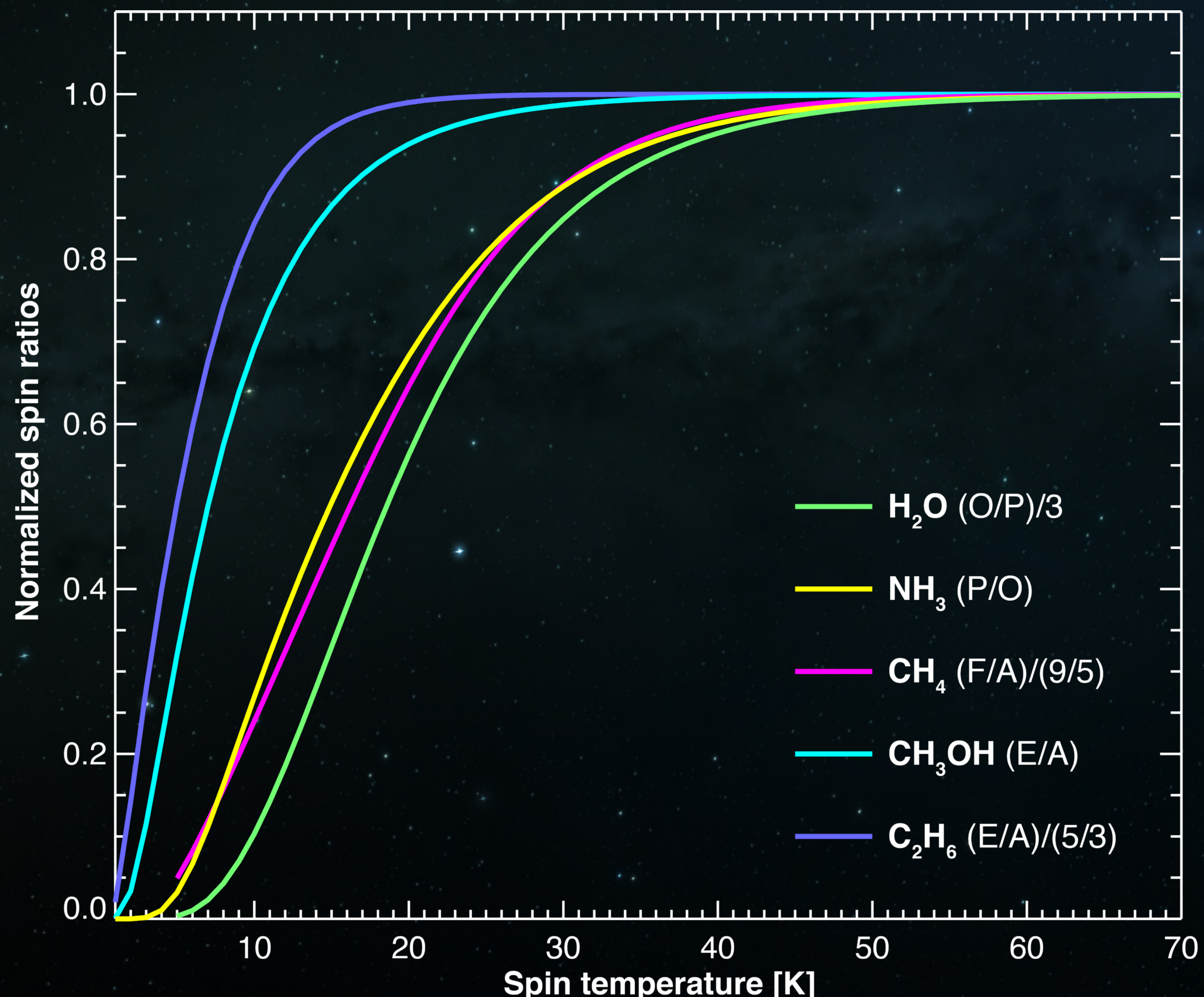
500 hypothetical measurements of **equilibrium**





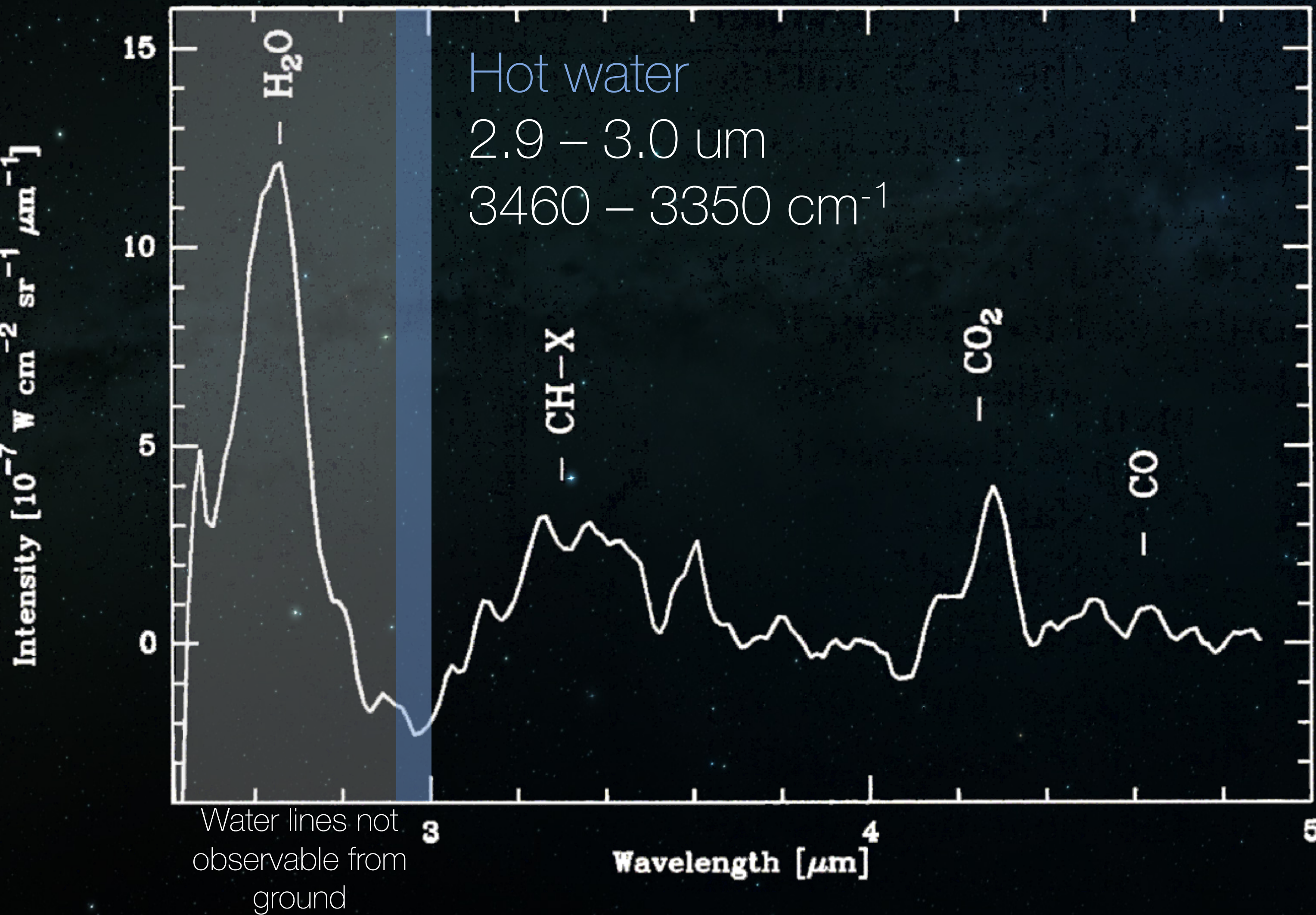
New measurements for CH_3OH and C_2H_6 will "reveal" ~10K ?

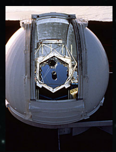


New models and retrievals
Does the "**30K**" paradigm hold?

Infrared spectrum of comet 1P/Halley

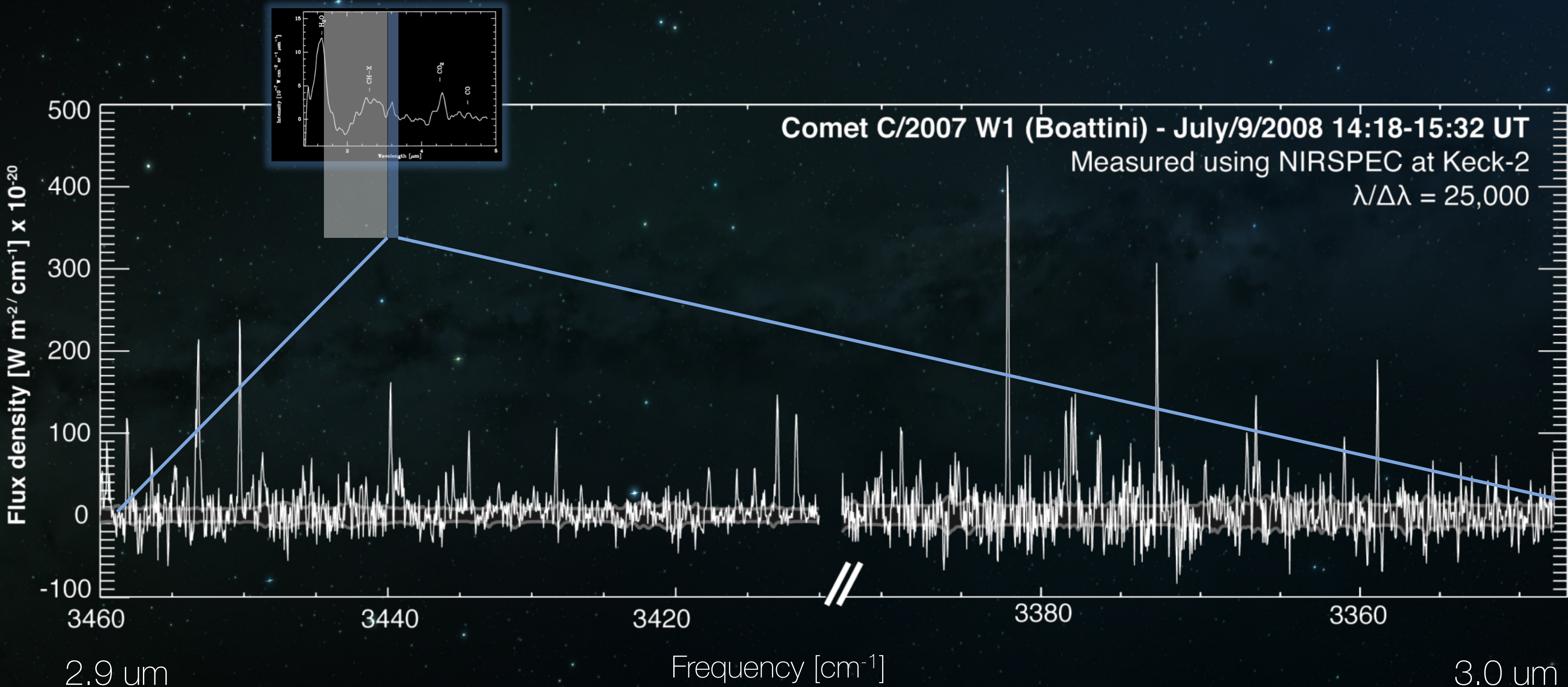
Combes+1988, VEGA/IKS space probe

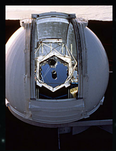




Modern high-resolution ground-based astronomy

Keck/NIRSPEC – Villanueva+2011





Modern high-resolution ground-based astronomy

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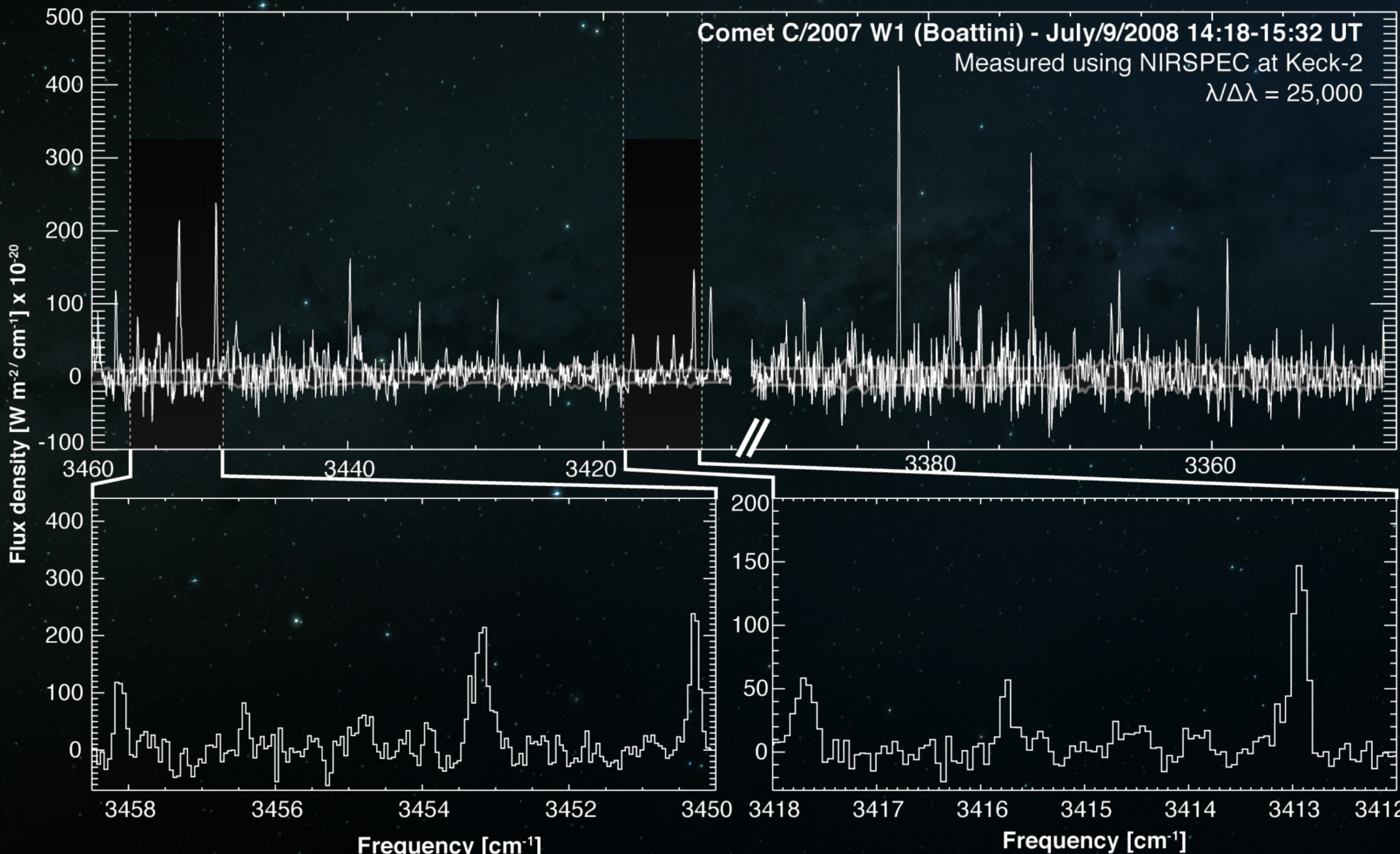
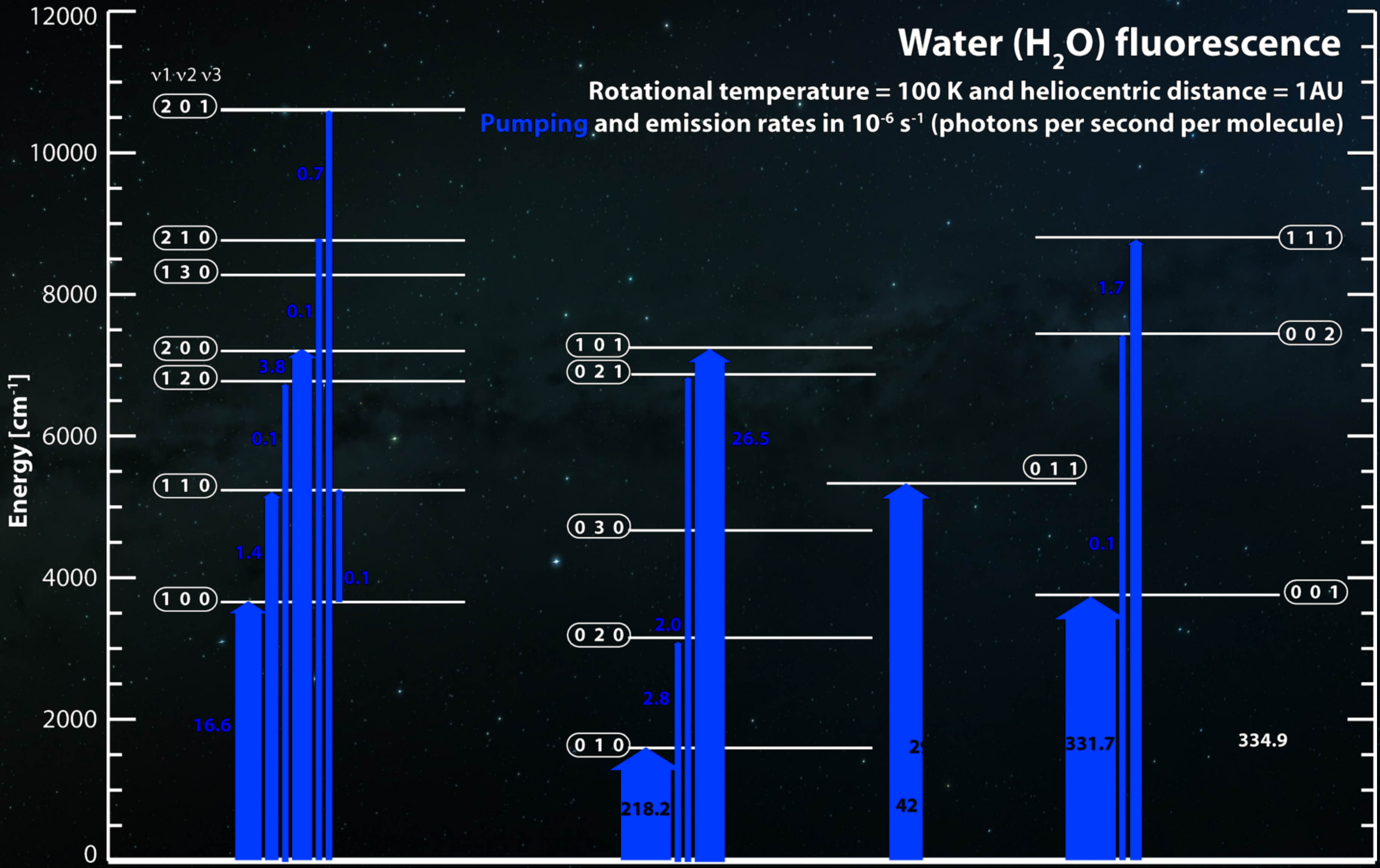


Water (H_2O) fluorescence

Rotational temperature = 100 K and heliocentric distance = 1AU
Pumping and emission rates in 10^{-6} s^{-1} (photons per second per molecule)



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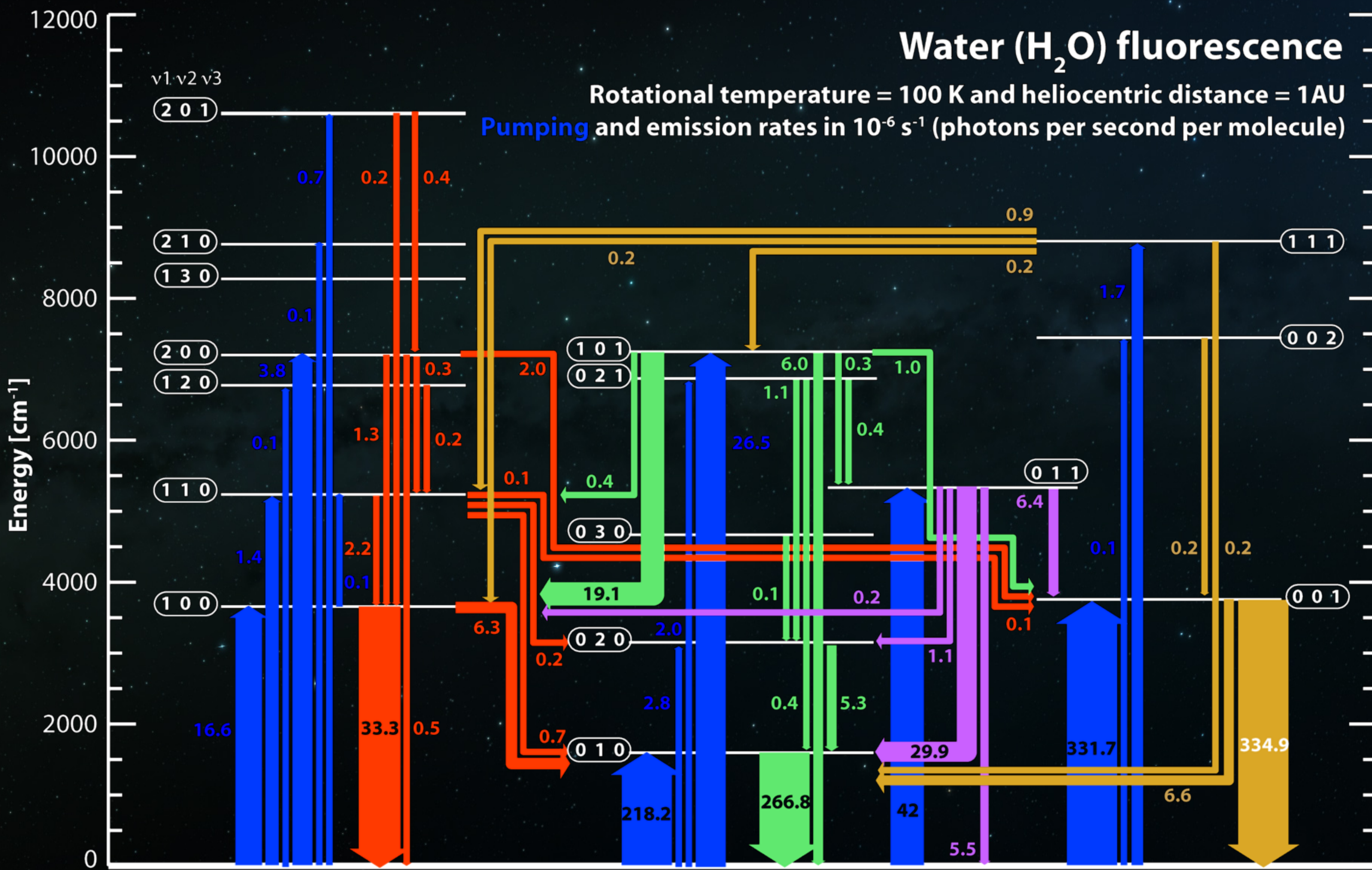
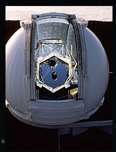


700 million ro-vibrational lines - Villanueva et al. JQSRT 2012



Modern high-resolution ground-based astronomy

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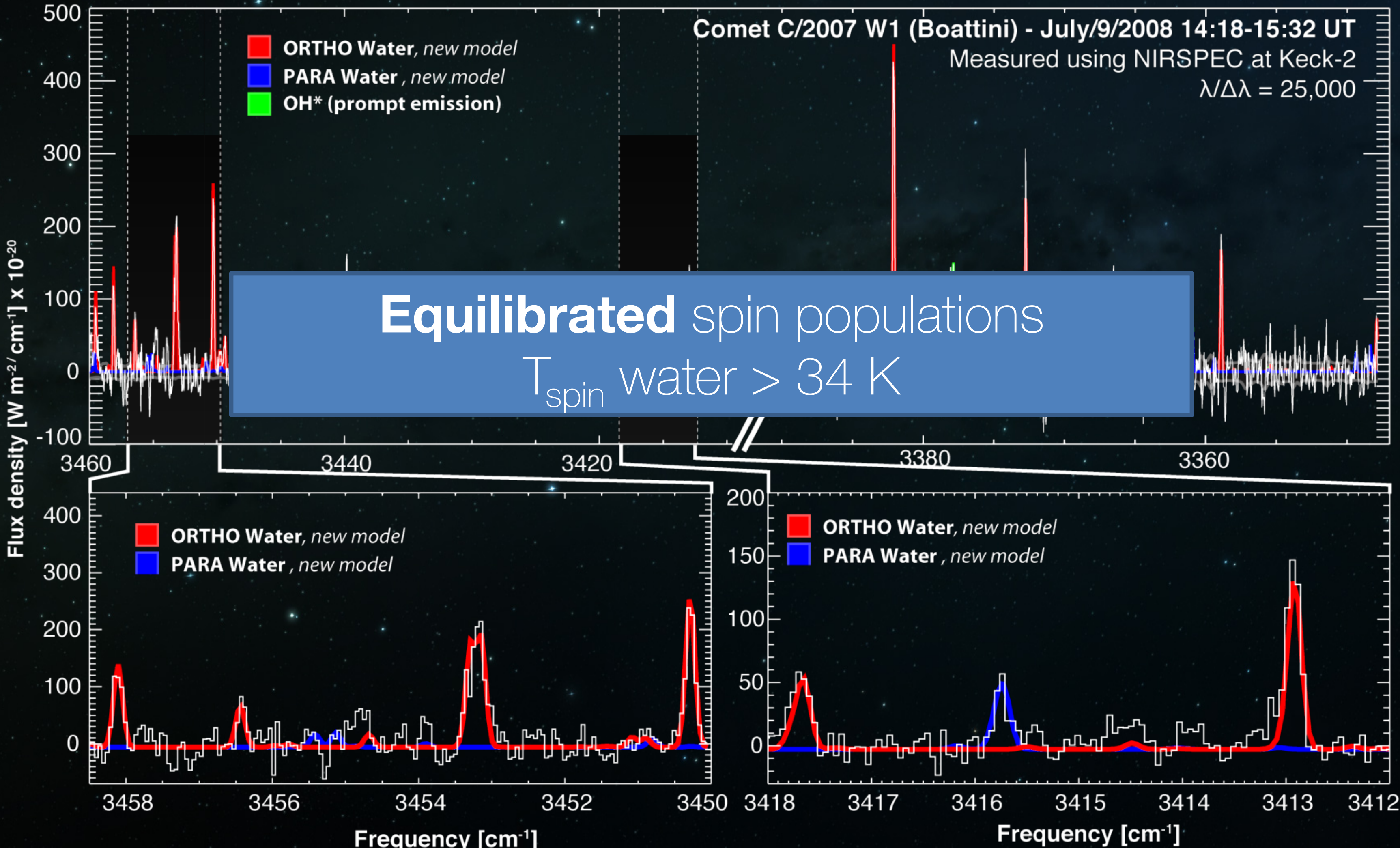
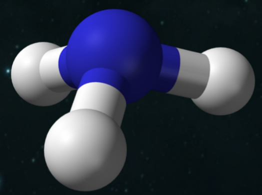


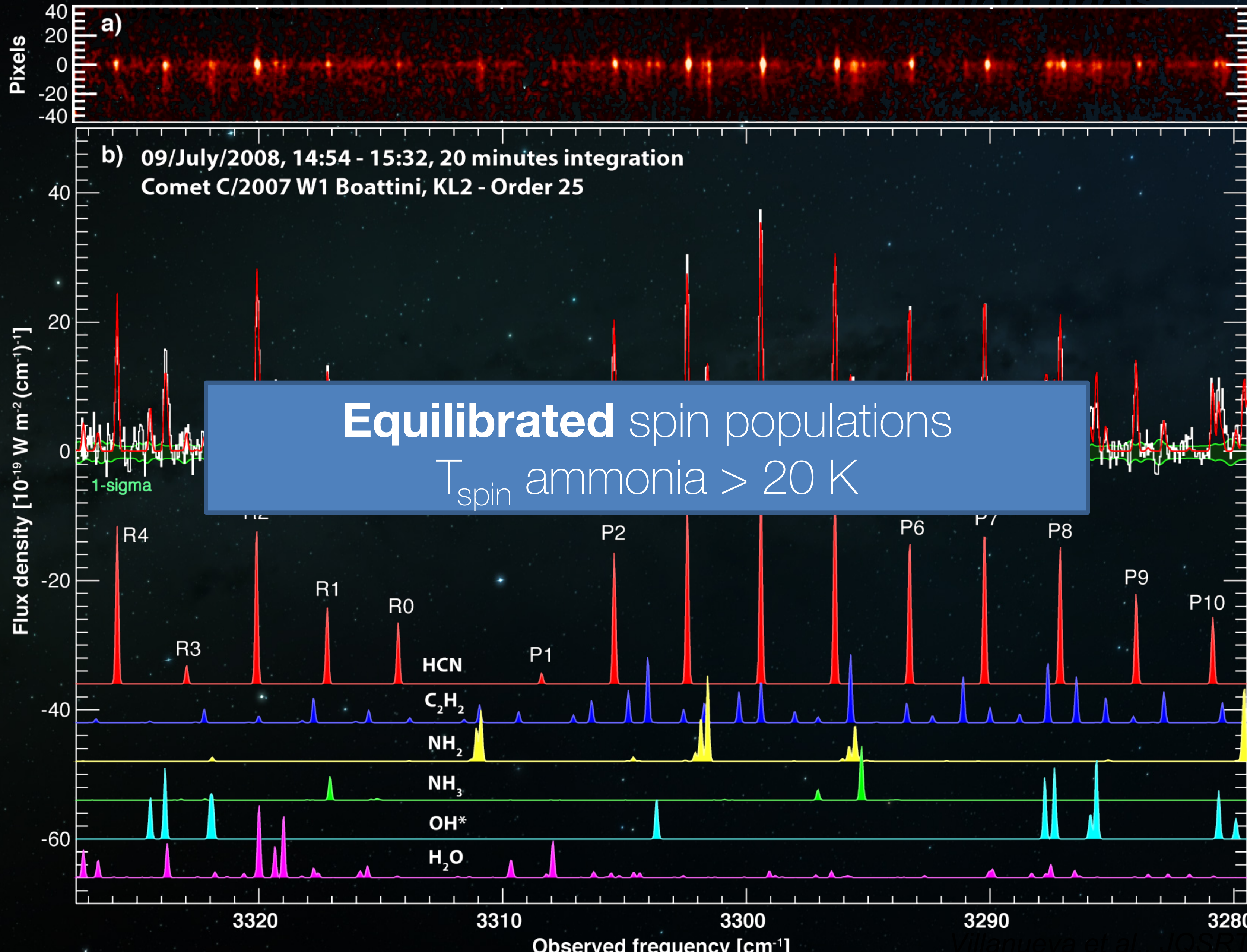
Equilibrated spin populations

T_{spin} water > 34 K

A new model for ortho and para ammonia (NH_3)

With 1,100 million spectral lines





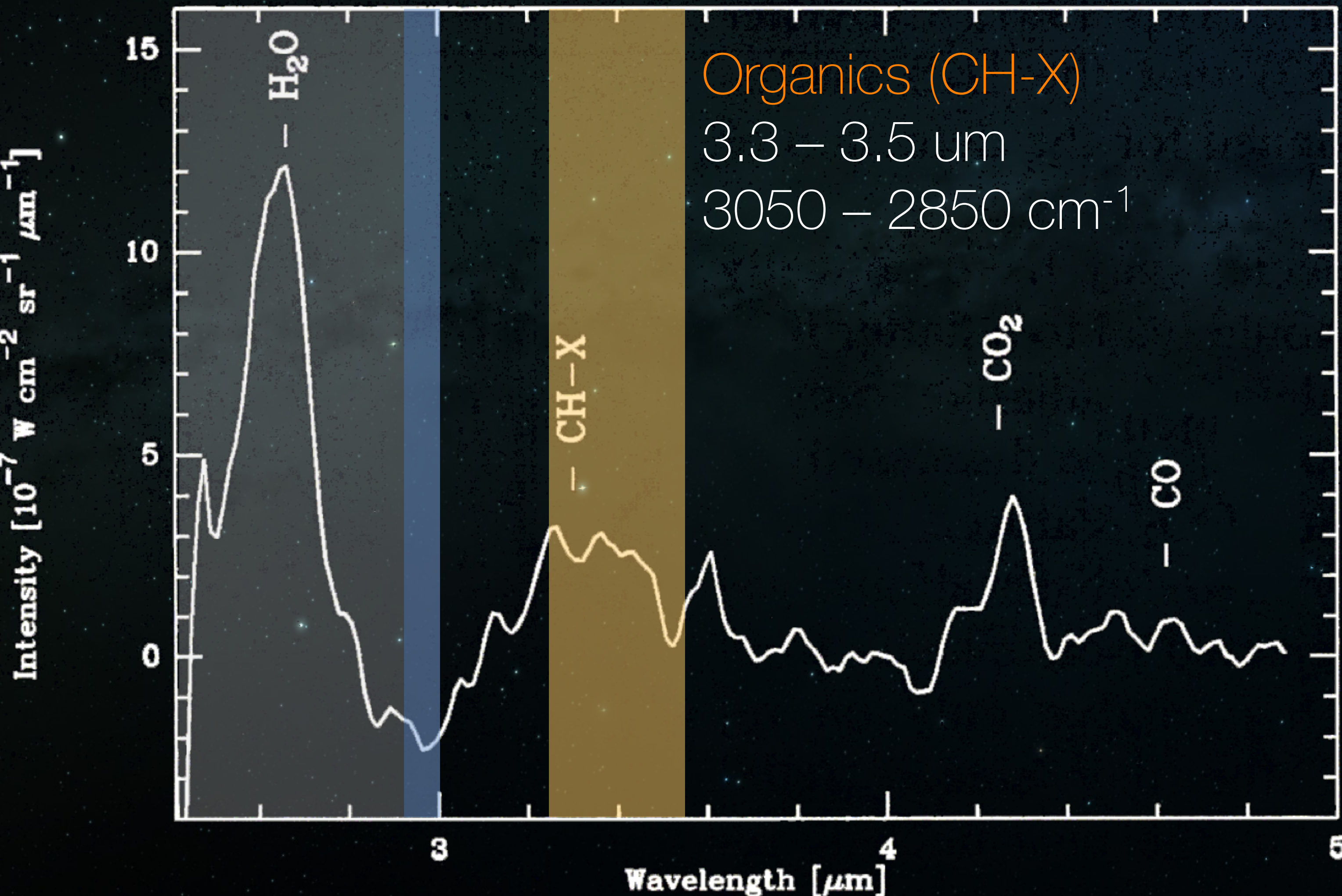
Equilibrated spin populations

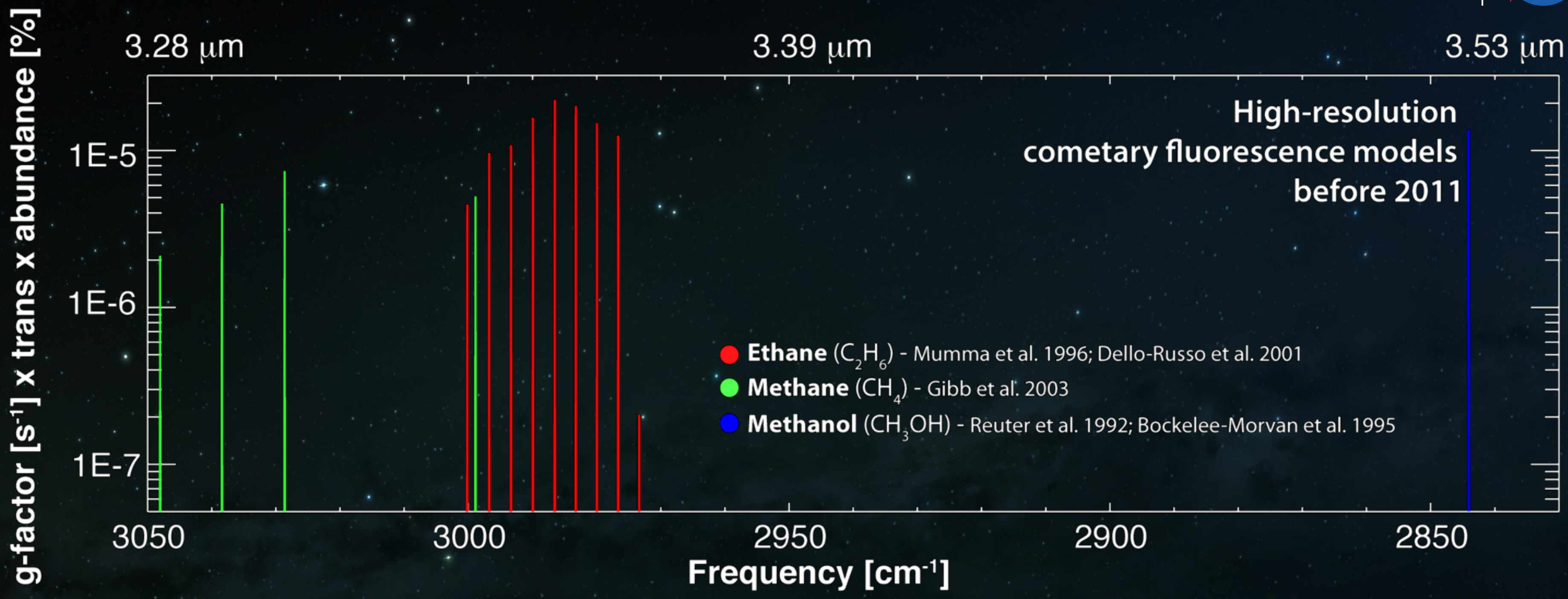
T_{spin} ammonia > 20 K

Testing Tspin in **organics**

Infrared spectrum of comet 1P/Halley

Combes+1988, VEGA/IKS space probe




3.28 µm
3.39 µm
3.53 µm
High-resolution cometary fluorescence models before 2011
1E-5
1E-6
1E-7
g-factor [s-1] x trans x abundance [%]
Ethane (C2H6) - Mumma et al. 1996; Dello-Russo et al. 2001
Methane (CH4) - Gibb et al. 2003
Methanol (CH3OH) - Reuter et al. 1992; Bockelee-Morvan et al. 1995
3050
3000
2950
2900
2850
Frequency [cm-1]

Spin Temperatures in comets: Cosmogonic?

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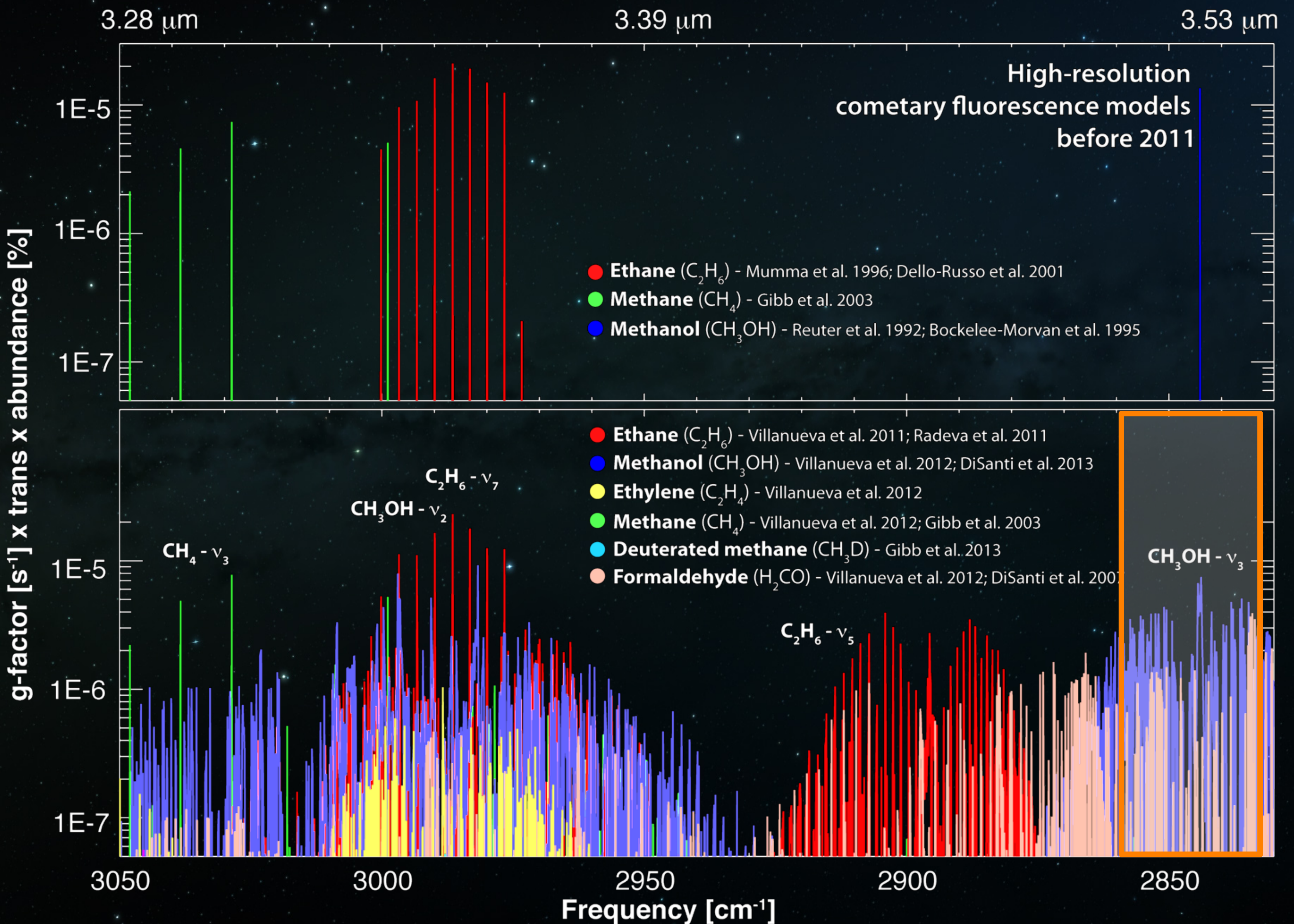
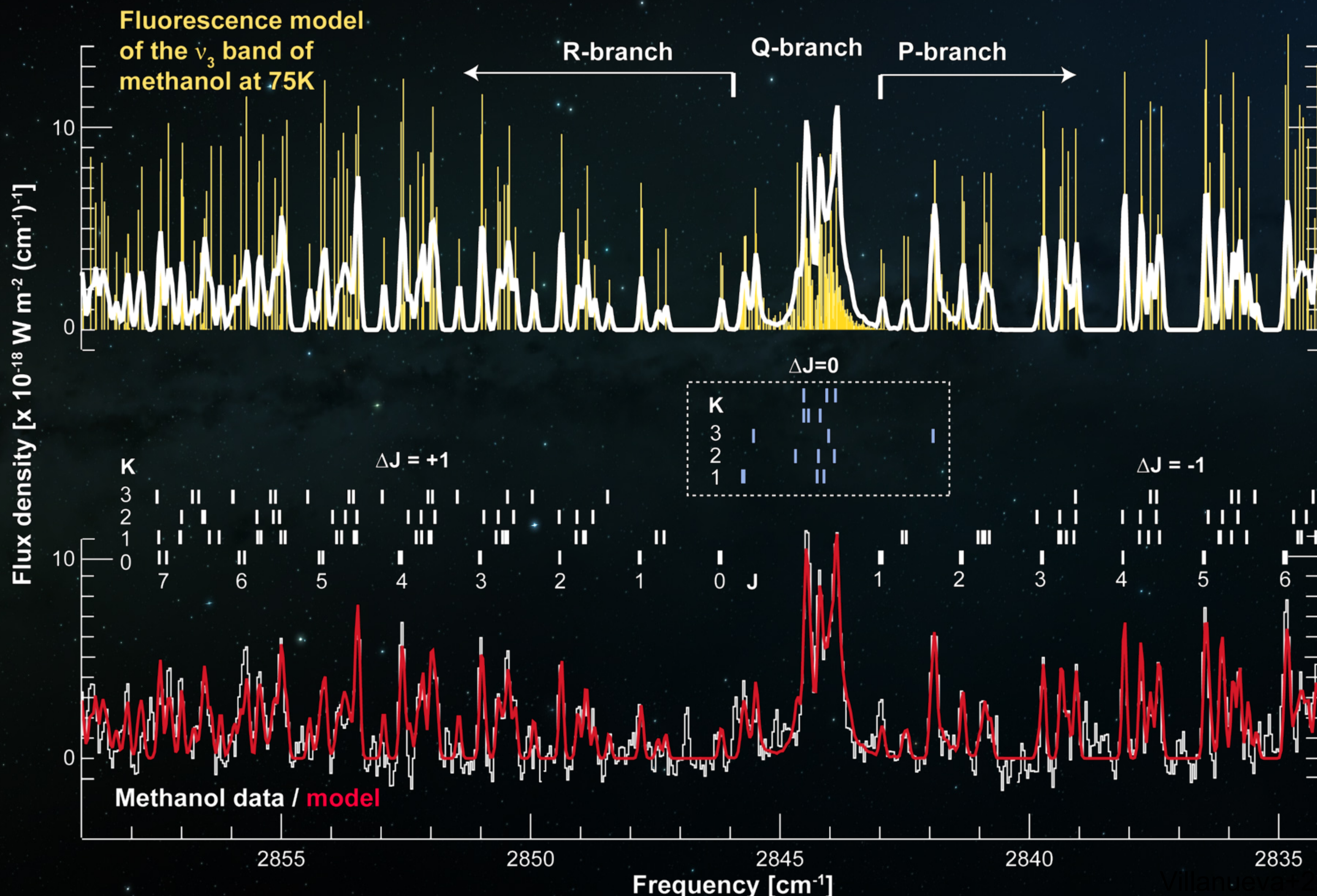
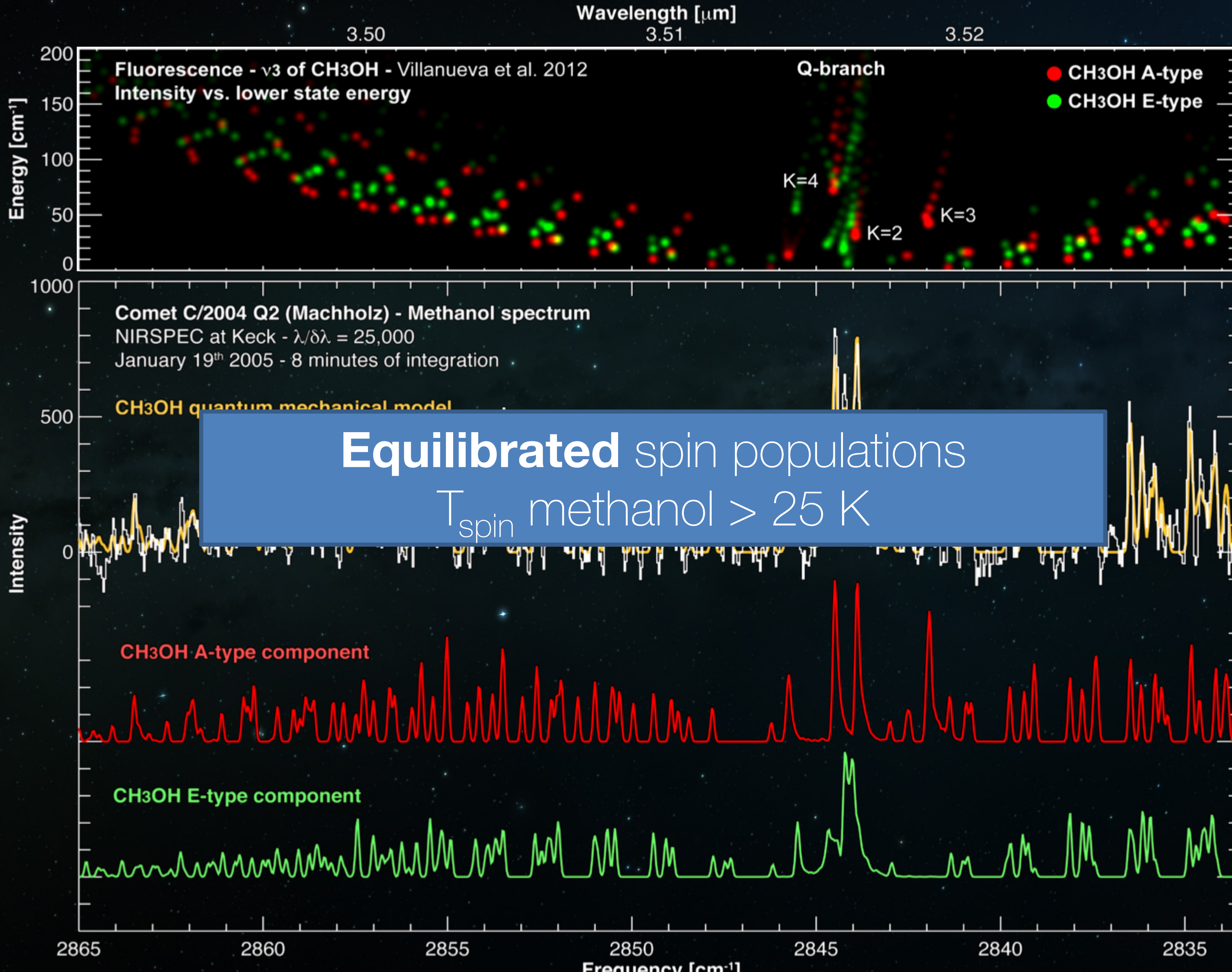


C/2004 Q2 (Machholz), January/19/2005, NIRSPEC at Keck II



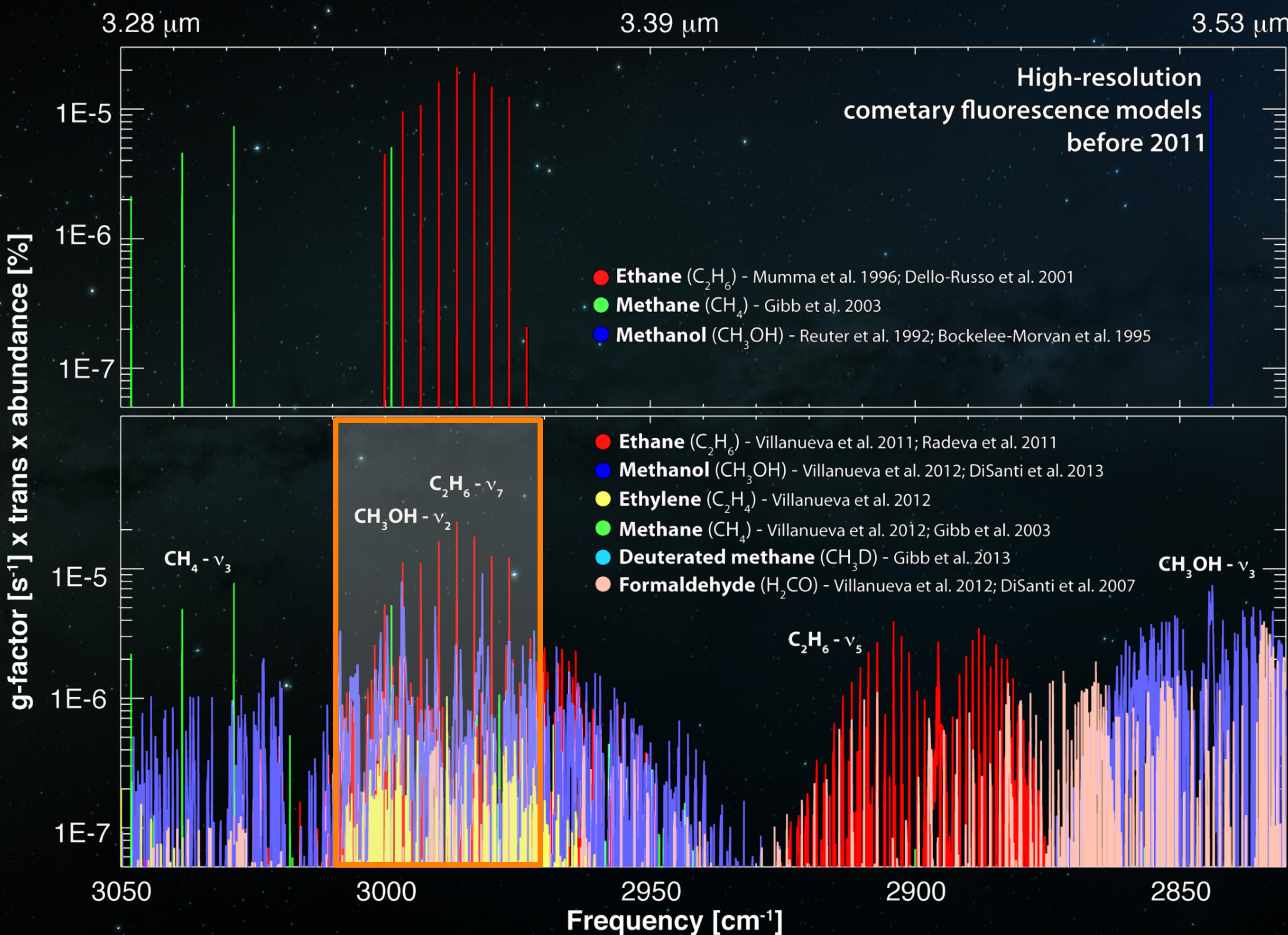


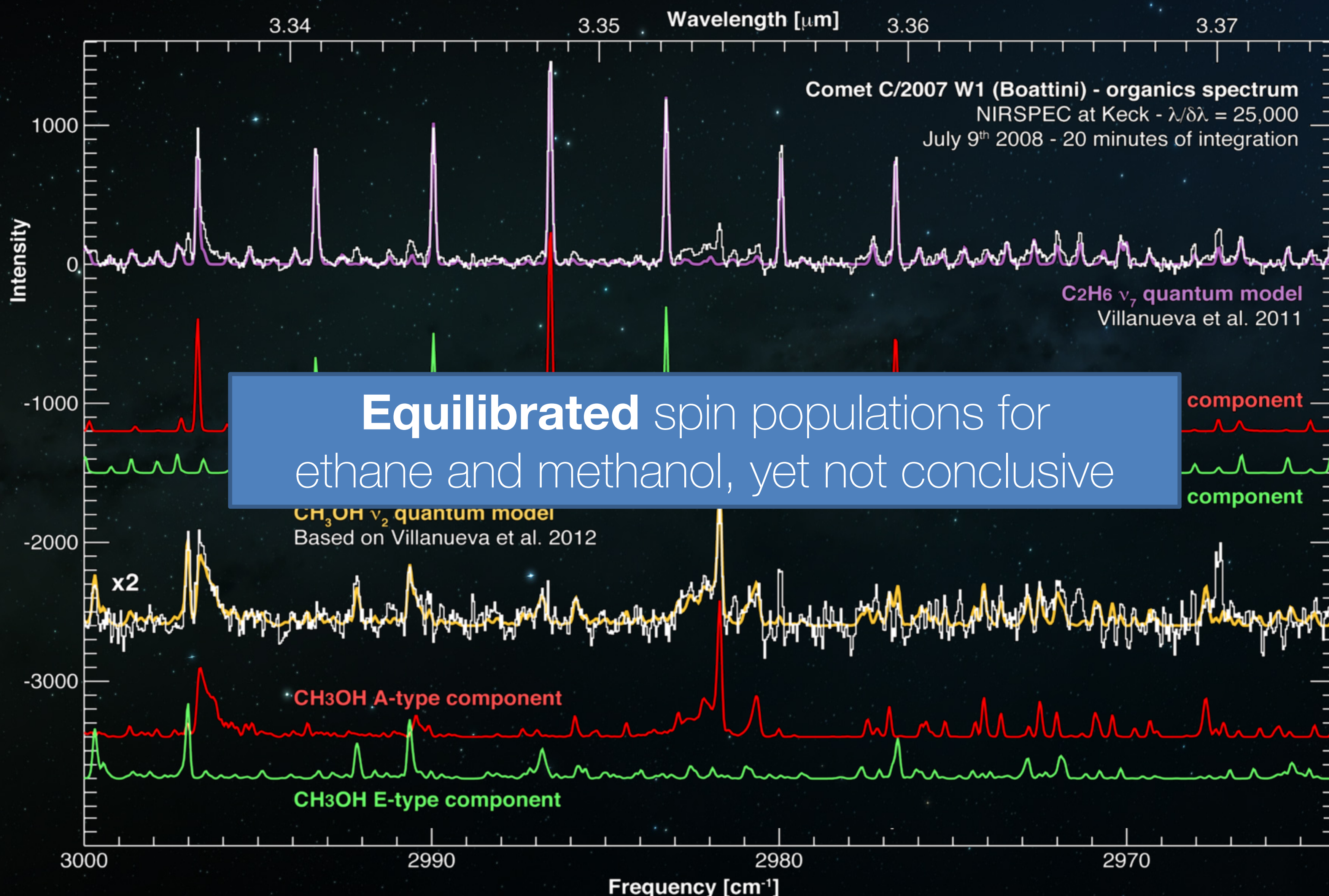
Equilibrated spin populations

T_{spin} methanol > 25 K

Spin Temperatures in comets: Cosmogonic?

Villanueva – Goddard Space Flight Center





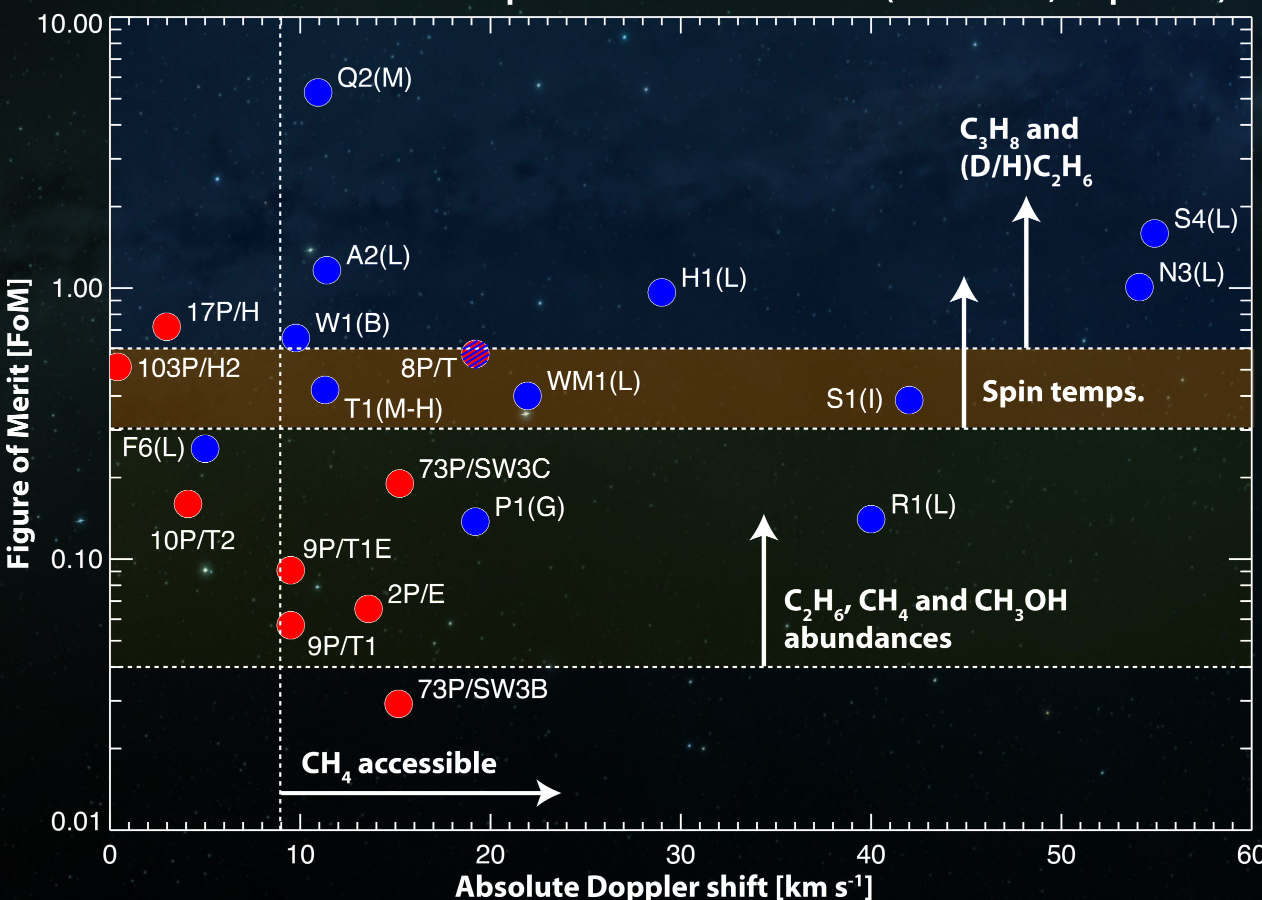
Equilibrated spin populations for ethane and methanol, yet not conclusive

Future steps:

Systematic probe of Tspins in many **comets** / **molecules**

- Awarded ~$400K (2016-2019) from NASA to probe Tspin and D/H of CH_4, C_2H_6, CH_3OH, C_3H_8 and H_2O in our survey of 20 comets.
- Hired a new post-doc (**Manuela Lippi**)

Our NIRSPEC/Keck II spectral database of comets (Oort-Cloud, Kuiper Belt)



Keck / VLT
Diameter: 10m
Optical to 5um
High-resolution
Adaptive optics

ALMA
66 antennas of 12m
Radio / THz
High-resolution
Interferometer

GMT
Diameter: 25 m
Optical to 2.5 μm
Four first light inst.
Adaptive optics

E-ELT
Diameter: 39 m
Optical to 14 μm
Six phase-A inst.
AO, WF, spec, MOS

TMT
Diameter: 30 m
Optical to 2.5 μm
Three phase-A inst.
AO, WF, spec, MOS

Hubble (HST)
Diameter: 2.4m
0.1 to 1.7 μm
Moderate resolution
Diverse inst. suite

TESS
Diameter: 0.1m
FOV 24 x 24 degree^2
Imaging / photometry
No spectroscopy

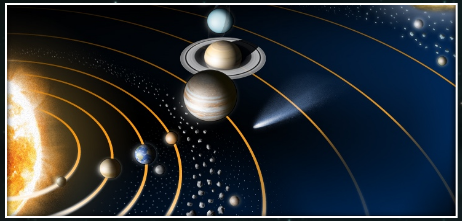
JWST
Diameter: 6.5m
0.6 to 28.5 μm
Moderate resolution
Diverse inst. suite
Ultra-cold (50K)

WFIRST
Diameter: 2.4m
0.4-1 μm
Wide-field camera
Coronagraph
Contrast 10^{-9}

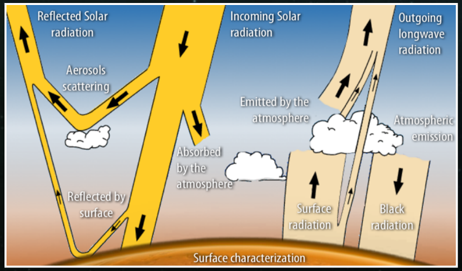
LUVOIR
Diameter: >9m
UV, Optical, IR
Coronagraph
Wide-field camera
UV and O/IR insts.

To **synthesize** planetary spectra with **any** of these facilities, a new tool is now **online** (Planetary Spectrum Generator, **PSG**):

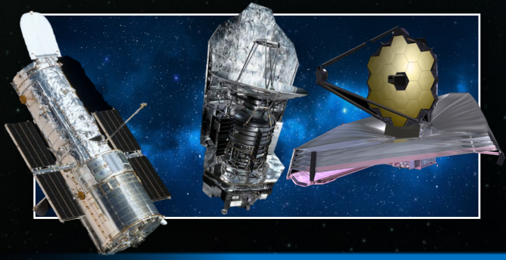
Spectra of **comets**, **planets**, **exoplanets** and **small-bodies** from 0.1 µm to 100 mm (UV/Vis/near-IR/IR/far-IR/THz/sub-mm/Radio) from any observatory (e.g., JWST, ALMA, Keck, SOFIA), any orbiter (e.g., ExoMars, Cassini, New Horizons).



The tool has a **3D orbital calculator** for **all bodies** in the Solar system, and **all confirmed exoplanets**. Observing geometries are: observatory, from surface, nadir, limb, occultation.

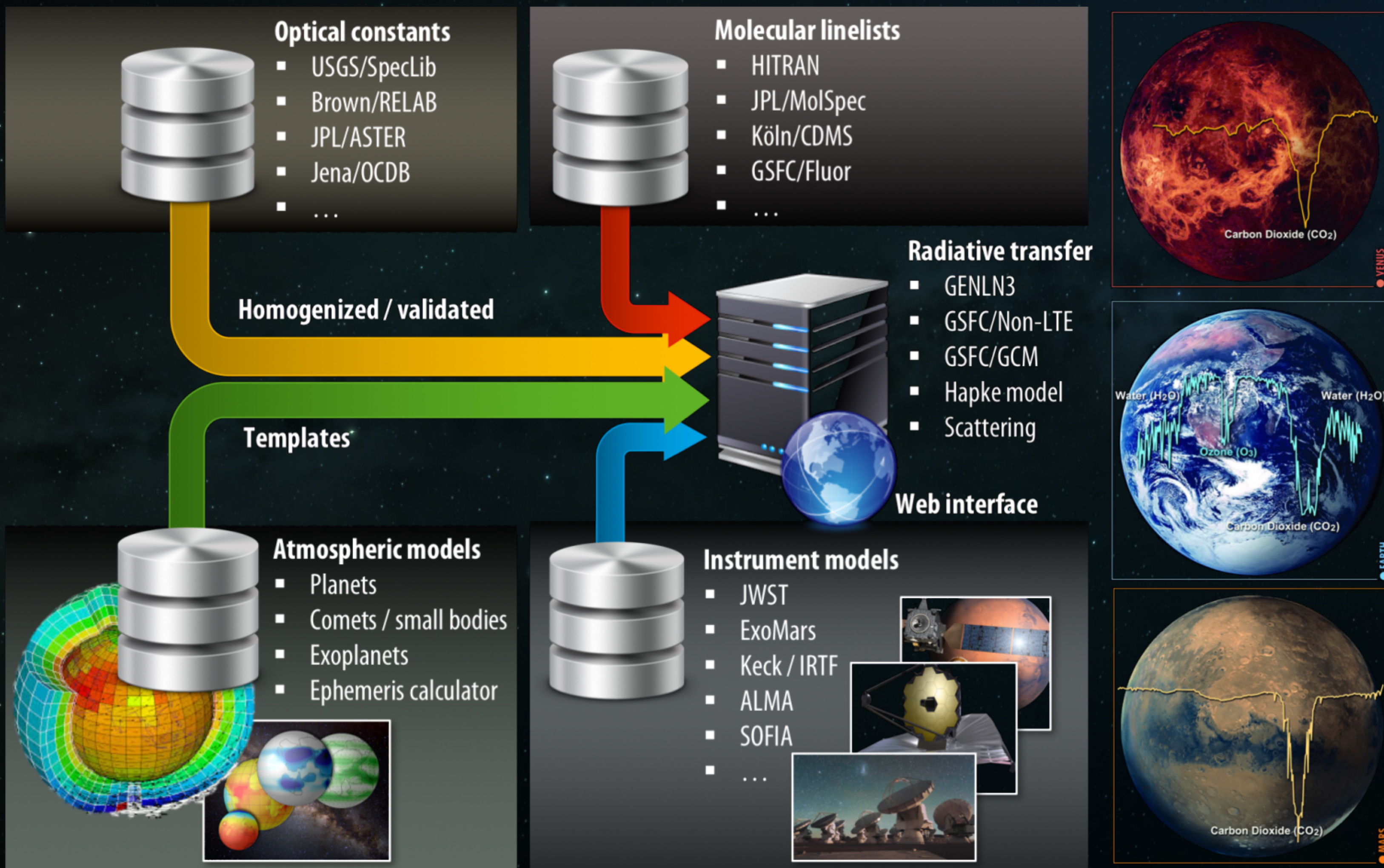


Radiative transfer performed with several models: line-by-line, correlated-K, non-LTE fluorescence, and surface models



It includes a noise and signal-to-noise calculator for quantum and thermal detectors, at any observatory.

http://ssed.gsfc.nasa.gov/psg


Optical constants
USGS/SpecLib
Brown/RELAB
JPL/ASTER
Jena/OCDB
...
Molecular linelists
HITRAN
JPL/MolSpec
Köln/CDMS
GSFC/Fluor
...
Homogenized / validated
Templates
Radiative transfer
GENLN3
GSFC/Non-LTE
GSFC/GCM
Hapke model
Scattering
Web interface
Atmospheric models
Planets
Comets / small bodies
Exoplanets
Ephemeris calculator
Instrument models
JWST
ExoMars
Keck / IRTF
ALMA
SOFIA
...
Carbon Dioxide (CO_2)
VENUS
Water (H_2O)
Water (H_2O)
Ozone (O_3)
Carbon Dioxide (CO_2)
EARTH
Carbon Dioxide (CO_2)
MARS

Conclusions

- Current measurements of **spin temperature** in comets may be **biased** towards **30K**.
- **Under-reporting of high OPRs**, may bias our impression of a 30K domain in Tspin for H_2O, NH_3 and CH_4.
- **Under-estimating of error-bars** may lead to strong Tspin constraints, but modeling errors, extended excitation field-of-views, etc. should be also taken into consideration.
- A **systematic** (many comets, many molecules, same instrument / FOV / time) is **necessary** to shed light on the **significance** of Tspin in comets.

Collaborators

Boncho Bonev
Michael Mumma
Michael DiSanti
Lucas Paganini
Karen Magee-Sauer
Erika Gibb

Thank you