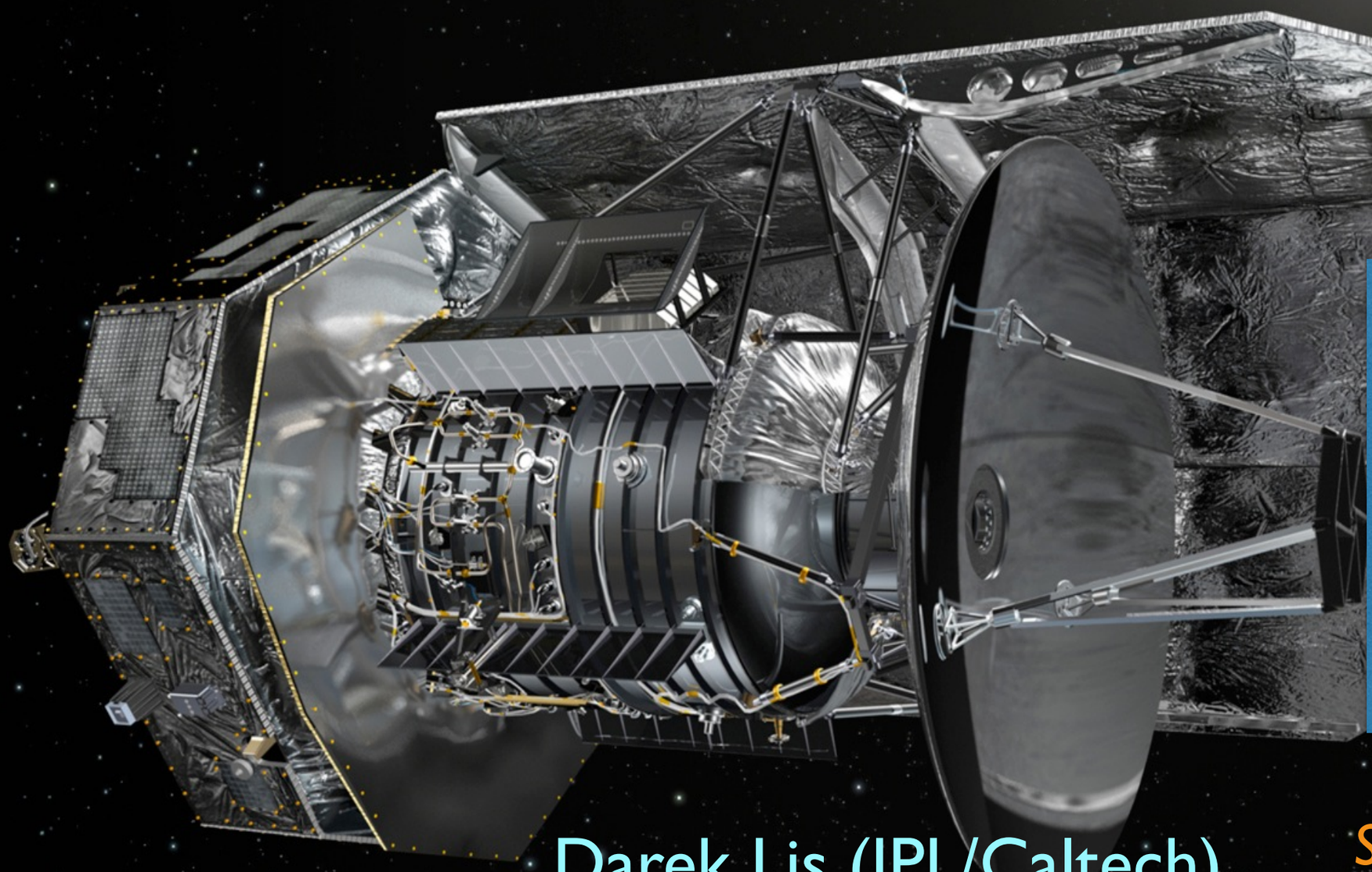
Ortho-Para Ratio in Water in the Interstellar Medium



Picture

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Jet Propulsion Laboratory
California Institute of Technology

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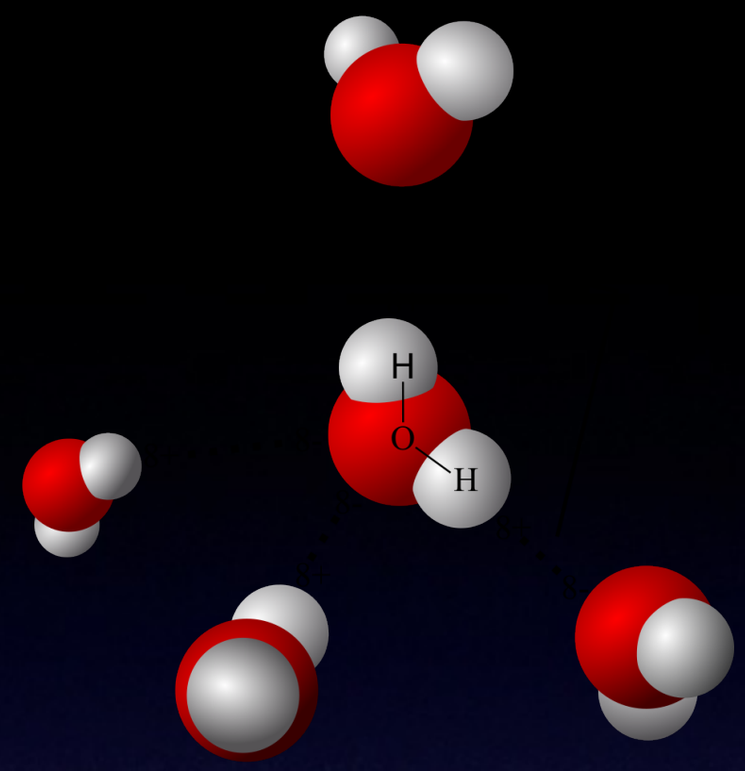
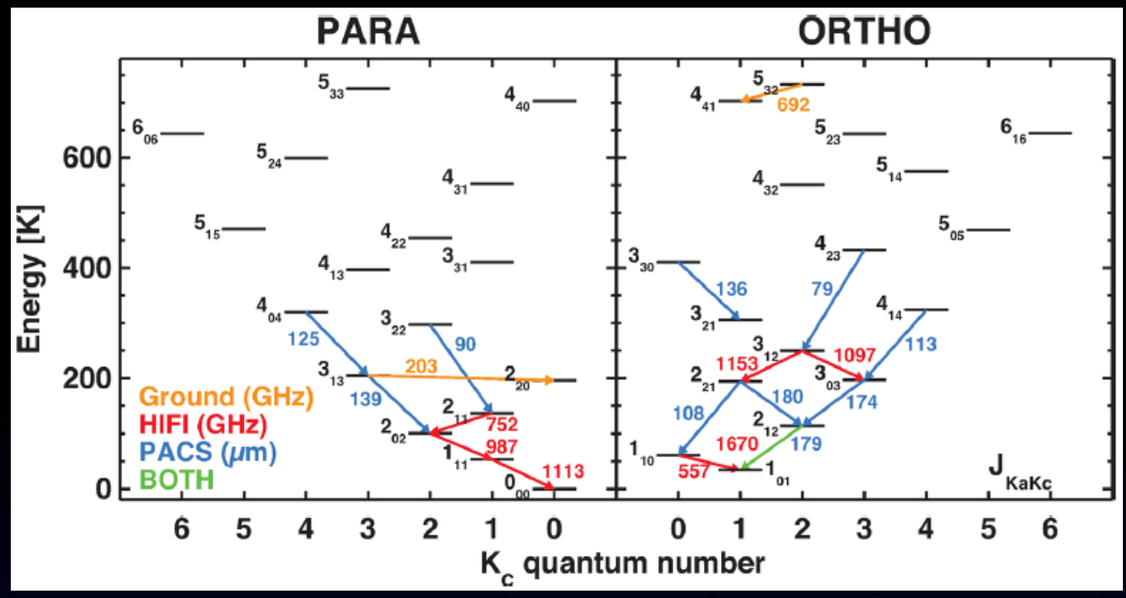
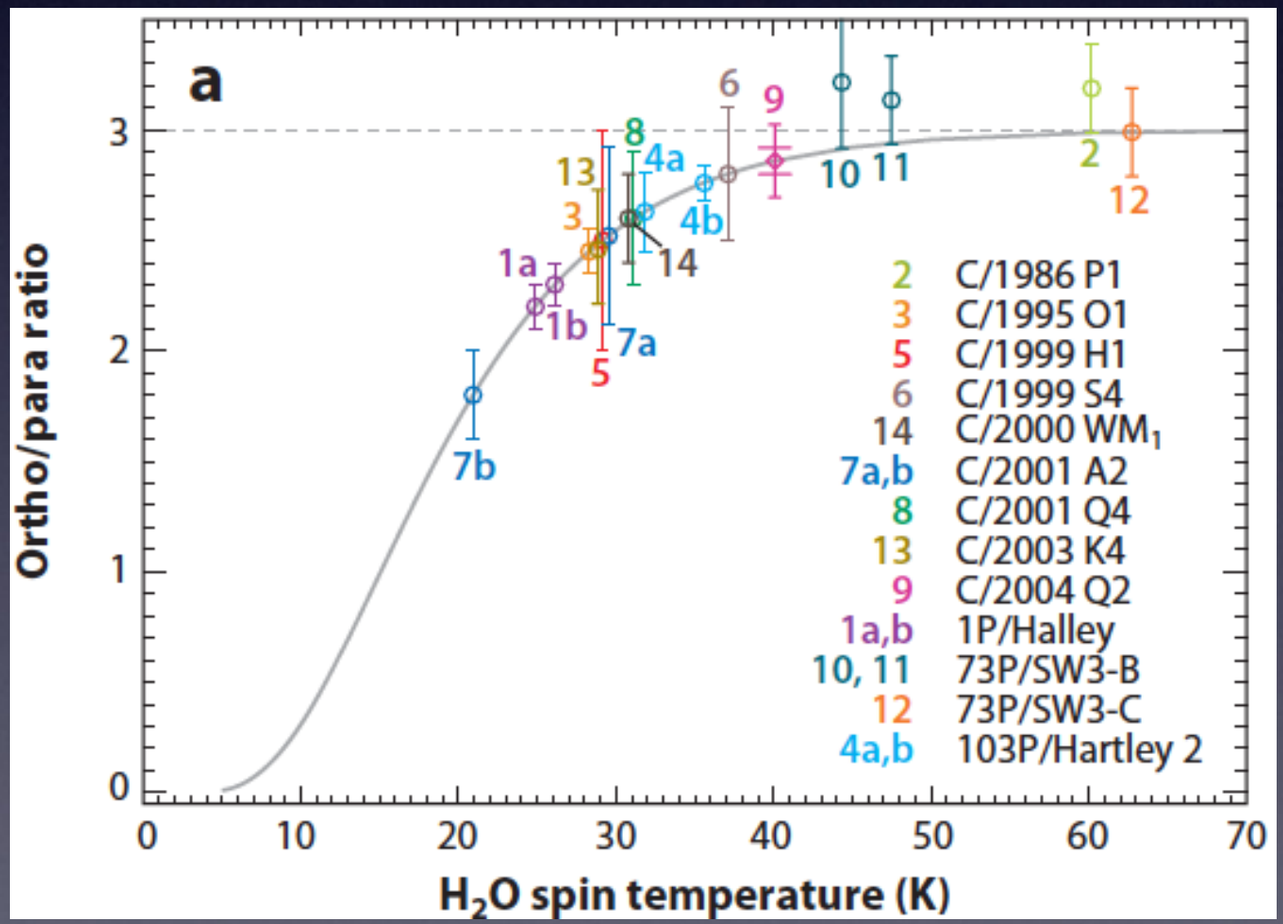
OPR in Water





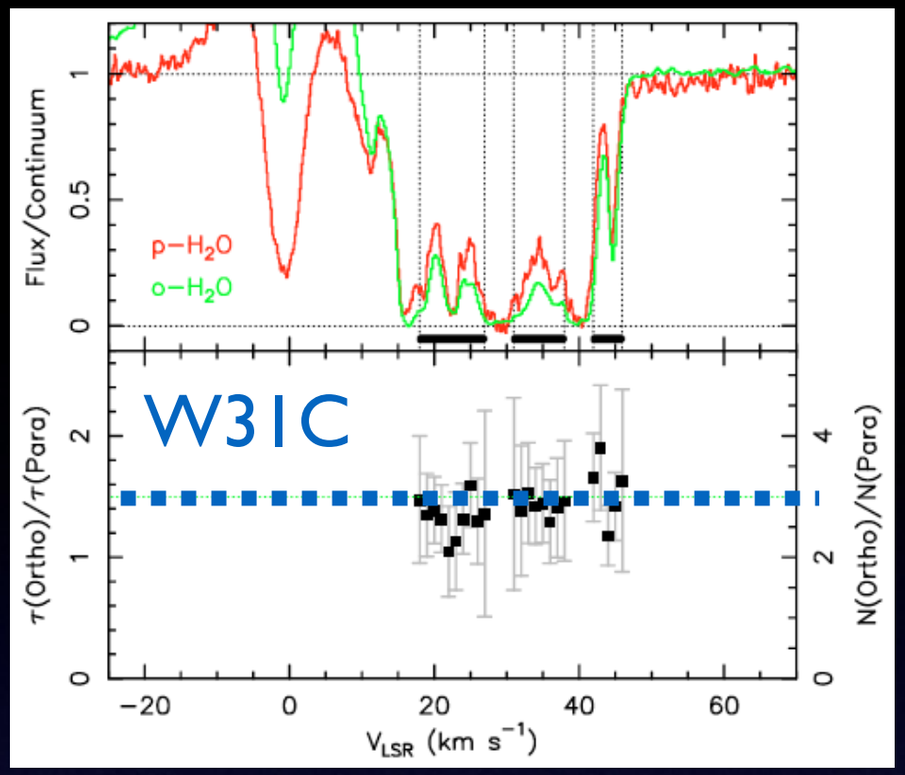
Van Dishoeck et al. 2013

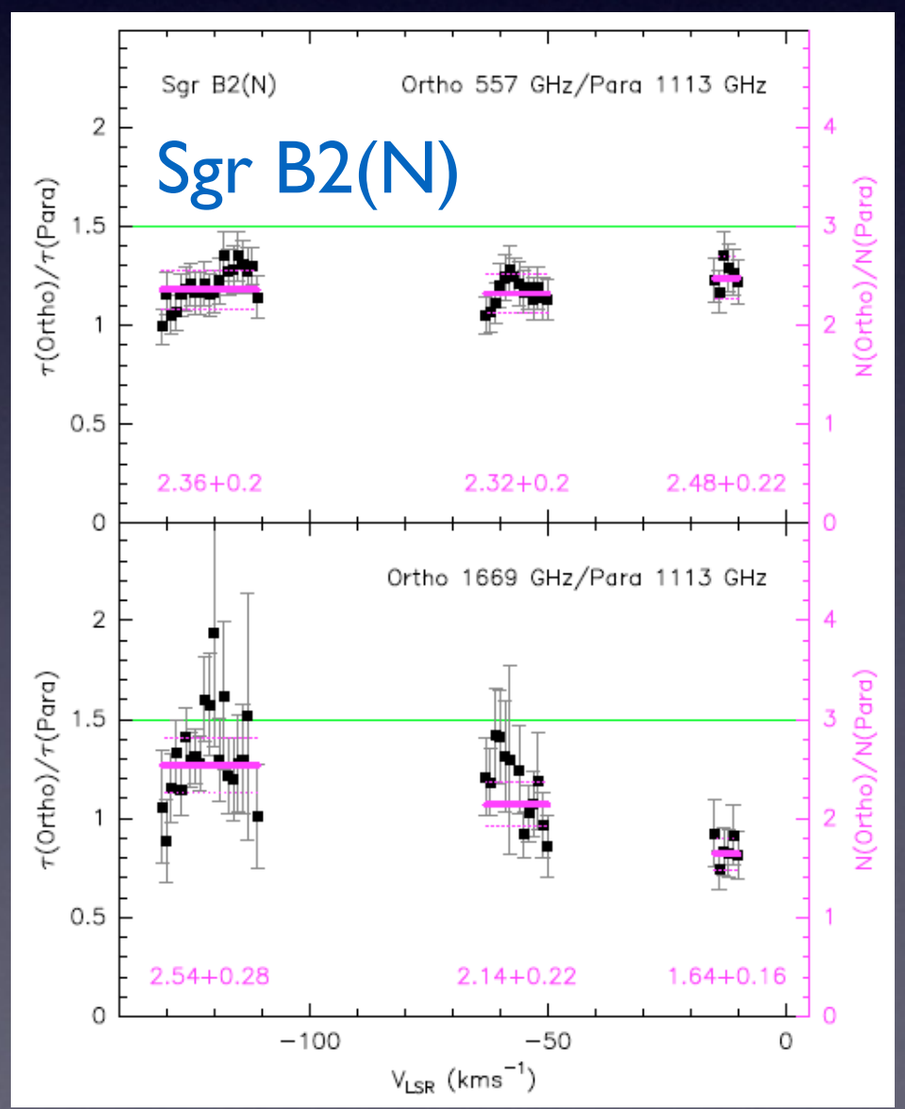
- Asymmetric top molecule with two spin isomers: total hydrogen spin I=1 (ortho), I=0 (para)
- Energy difference 34.2 K — high temperature limit (T>50 K) OPR=3
- Spin temperature provides (perhaps) some information about formation or condensation of water molecules on dust grains
- OPR studied extensively in cometary atmospheres using optical or IR spectroscopy — T_{spin}~30 K



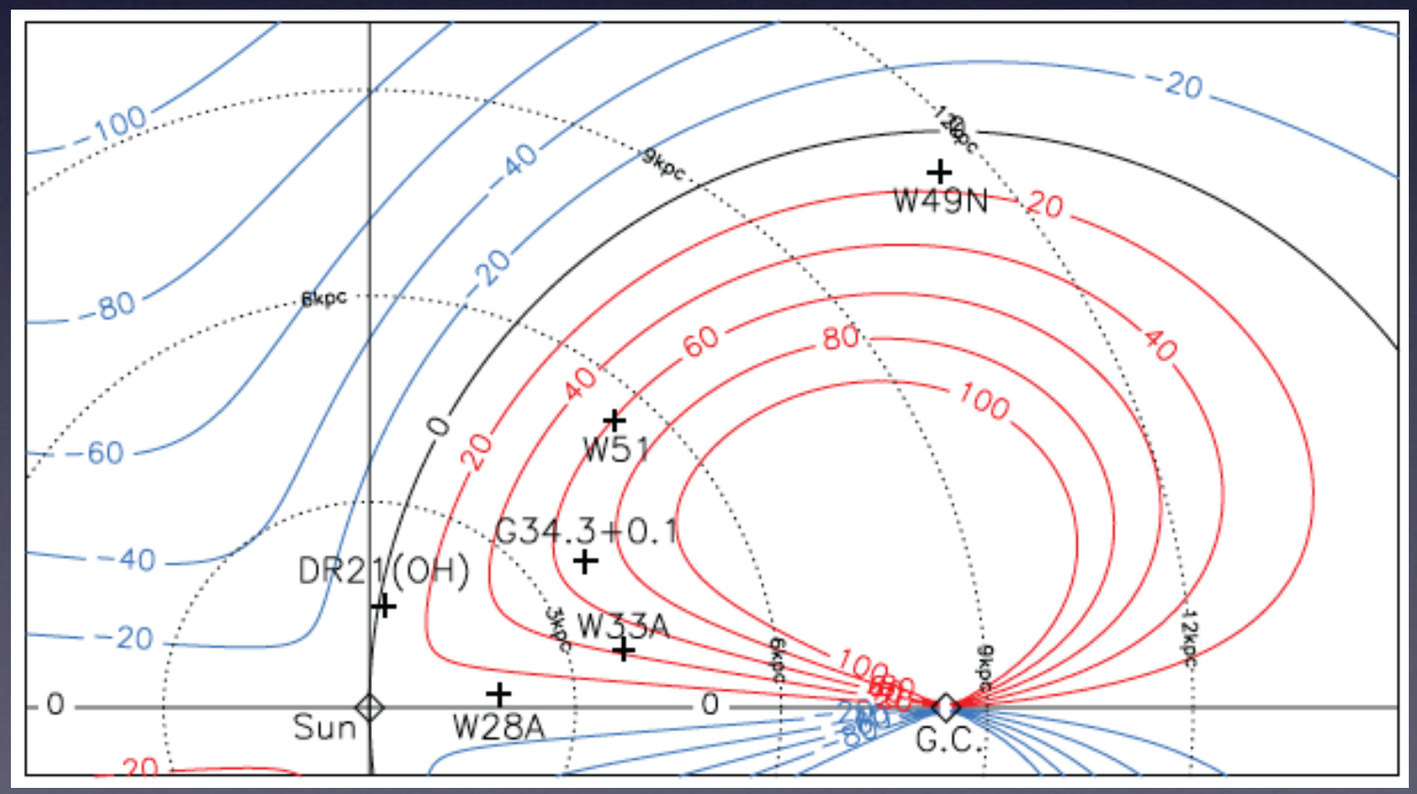
Mumma et al. 2011

Herschel Results





- Herschel/HIFI allowed studies of the OPR in the ISM, primarily using absorption spectroscopy
- $H_2O/H_2 \sim 5\ 10^{-8}$ in diffuse clouds
- OPR generally consistent with 3, with the exception of some velocity components toward Sgr B2 (OPR=2.35+0.35 2σ, T_{spin}~24-32 K) or W49N
- No apparent trends with column density, molecular fraction, galactocentric distance…

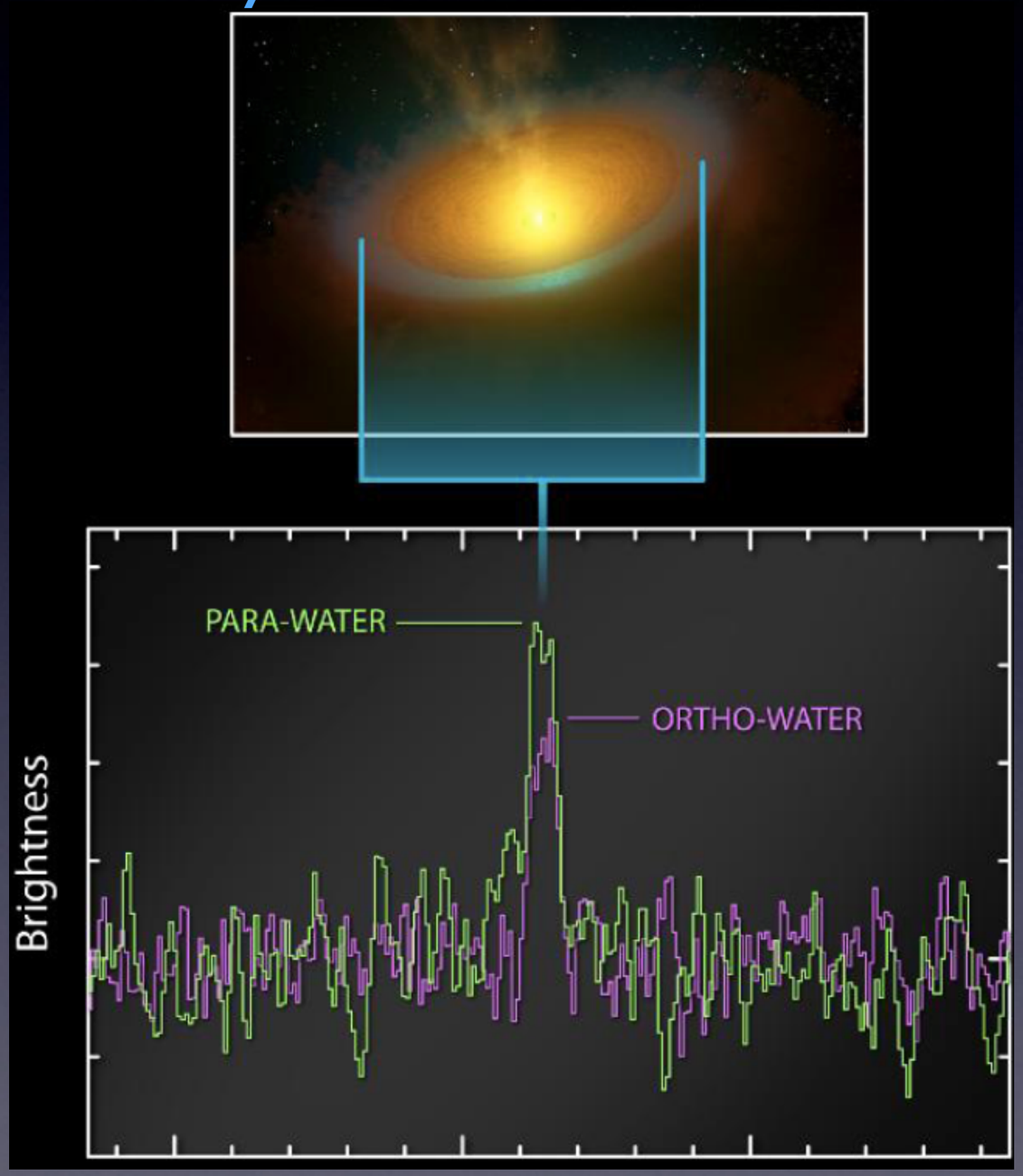


Lis et al. 2010, 2013; Emprechtinger et al. 2010, 2012; Flagey et al. 2013

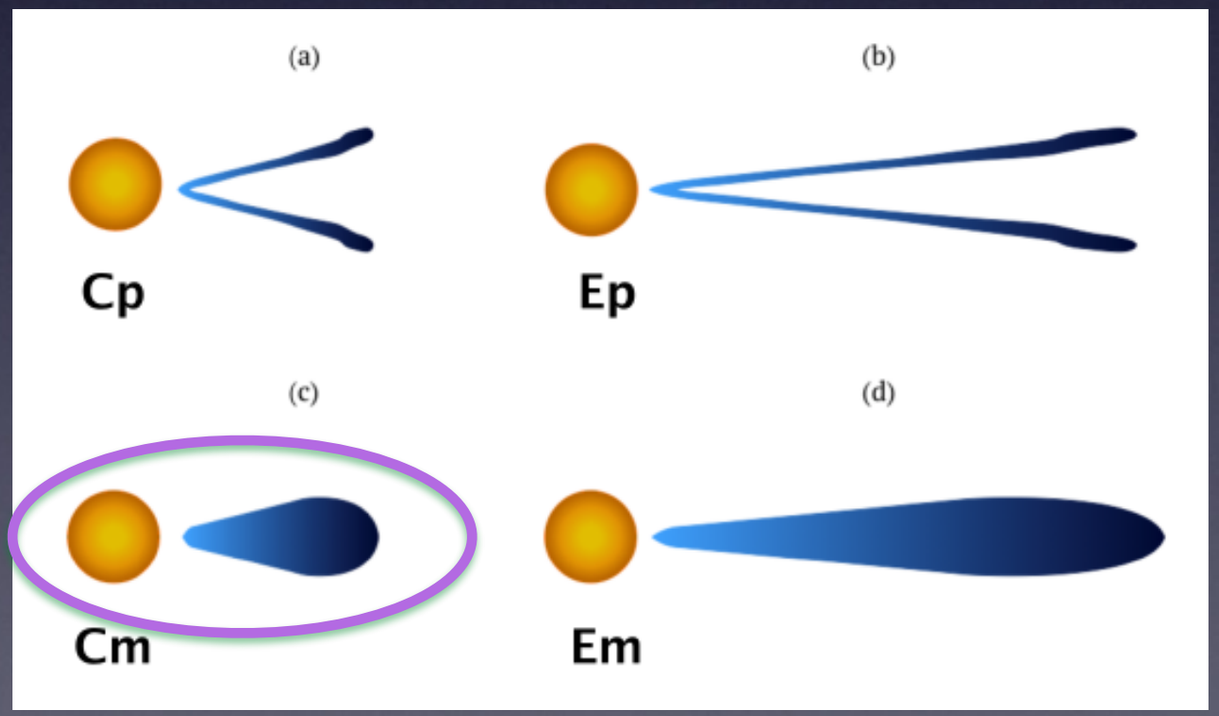
OPR in Disks

- A low OPR=0.77±0.07 (1σ) was initially reported in the TW Hydrae disk
- Lines seen in emission — results are strongly model dependent,
- Only one class of models gives an NH_3/H_2O abundance ratio consistent with the ISM and solar system values
- The same model is consistent within the errorbars with the high-temperature limit (OPR=1.4 +2.1/−1.15)

TW Hya



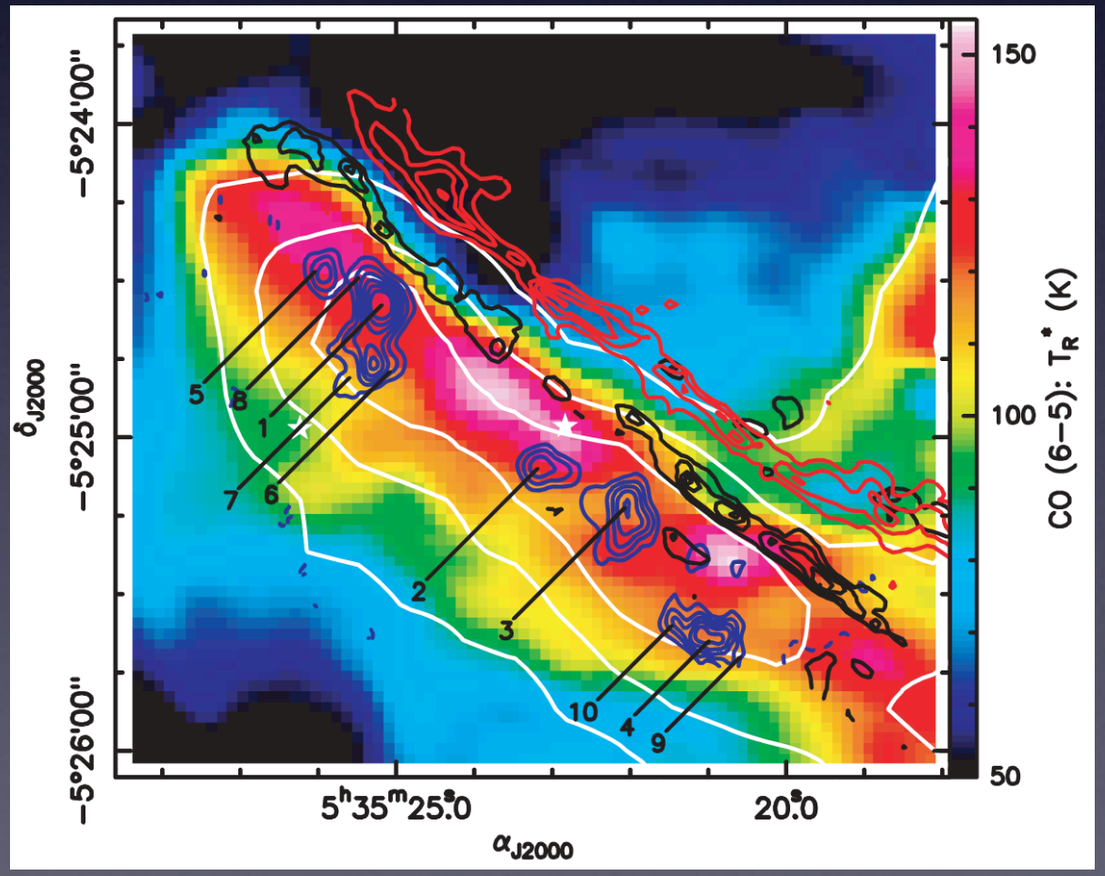
Hogerheijde et al. 2011



Salinas et al. 2013

Orion Bar

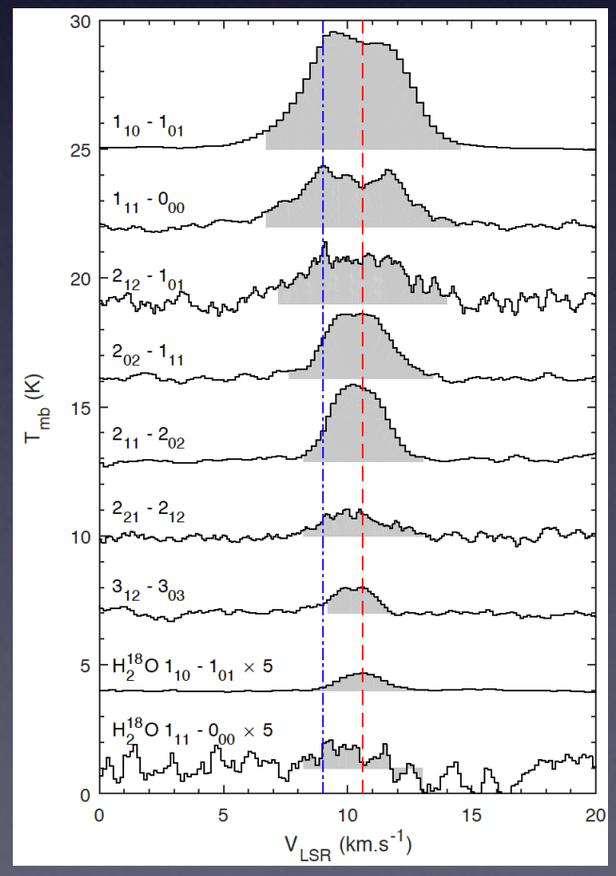
- A very low OPR=0.1−0.5 was derived in the Orion Bar (Choi et al. 2014) from observations two $H_2{}^{18}O$ *emission* lines, analyzed using a *single-slab* LVG model
- Edge-on PDR illuminated by the Trapezium cluster — strong temperature and density gradients, clumping — a uniform slab model not well adapted
- A more complete set of 8 lines was re-analyzed using the Meudon PDR code (Le Petit et al. 2006; ism.obspm.fr) as a part of the PhD thesis of Thomas Putaud



Lis & Schilke 2003

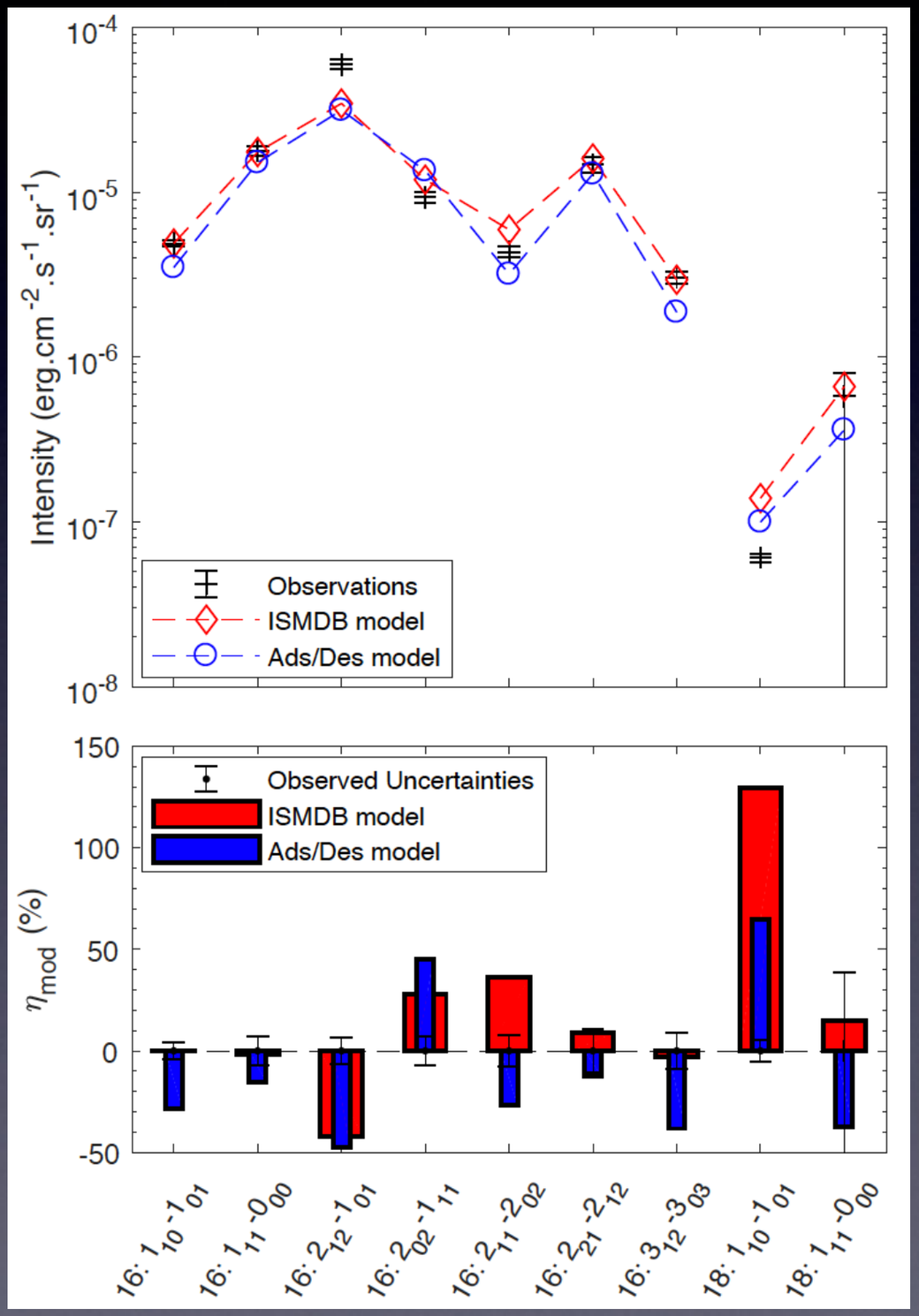
- Observations of a more complete set of 8 water lines were re-analyzed using the Meudon PDR code

Molecule	Transition	I_{Obs} [a] (K km s^{-1})
$H_2{}^{16}O$	$1_{10}-1_{01}$	21.13 ± 0.95
	$1_{11}-0_{00}$	10.28 ± 0.75
	$2_{12}-1_{01}$	8.91 ± 0.60
	$2_{02}-1_{11}$	8.06 ± 0.59
	$2_{11}-2_{02}$	7.82 ± 0.60
	$2_{21}-2_{12}$	2.62 ± 0.31
	$3_{12}-3_{03}$	1.85 ± 0.18
$H_2{}^{18}O$	$1_{10}-1_{01}$	0.29 ± 0.02
	$1_{11}-0_{00}$	<0.34 ± 0.15



Putaud et al. 2019

Results



- Model line intensities are in good agreement with observations, assuming that water molecules are formed with OPR corresponding to LTE at the local kinetic temperature of the gas
- Gas-phase water emission originates at Av~9
- Water abundance of ~2×10^{-7}
- Line-of-sight average OPR=2.8±0.2
- The resulting T_{spin}=36±2 is close to the kinetic temperature in the water-emitting gas
- More details:

The water line emission and ortho-to-para ratio in the Orion Bar photon-dominated region⋆

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Summary

- There is no compelling evidence for water OPR values significantly below the LTE value of 3 ($T_{spin} \lesssim 25$) to be present in the ISM:
  - TW Hya — OPR is model dependent and consistent with 3 within the uncertainties
  - Orion Bar — OPR=2.8±0.2, when taking into account the steep temperature and density gradients present in the region
- Herschel archives are a treasure trove of data that remain to be fully analyzed
- When launched, JWST will provide complementary information

Backup slides

Ortho-Para Conversion

- Gas phase: water forms with OPR=3
- Nuclear spin conversion (through proton exchange reactions with H^+, H_3^+) is slow, dependent on the local ionization rate and gas density (3×10^5 yr for 10^4 cm^{-3}, abundance of protonated ions 10^{-8})

- Water formation via grain-surface processes — need a mechanism to release water molecules back into the gas phase
- Molecular dynamics calculations of water photo-desorption (Andersson & van Dishoeck 2008) — only molecules "kicked-out" from the ice by energetic H atoms would preserve the OPR acquired in the ice — photodissociation followed by recombination resets the OPR
- Laboratory measurements of water desorbed from ice prepared as para-H_2O show the statistical OPR of 3 (Sliter et al. 2011; Hama et al. 2011, 2016, 2018…)