OPR in Water in the Interstellar Medium

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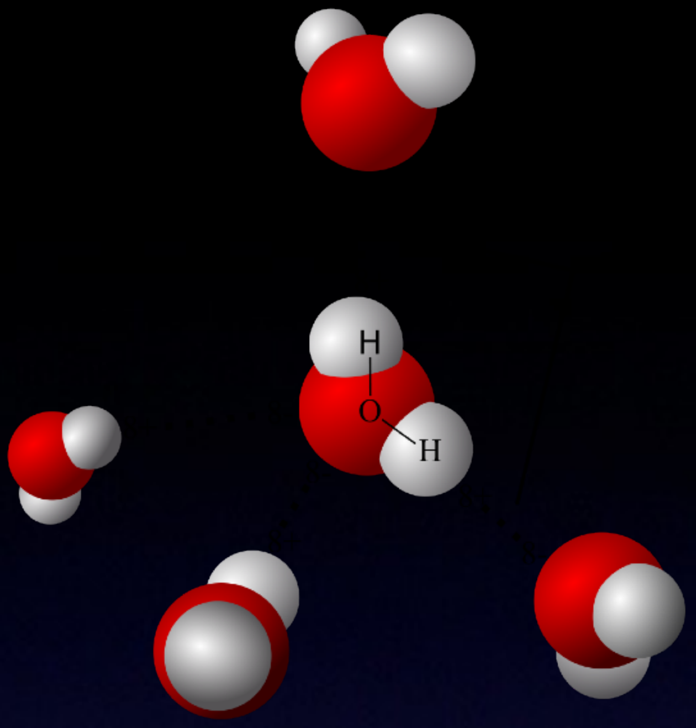
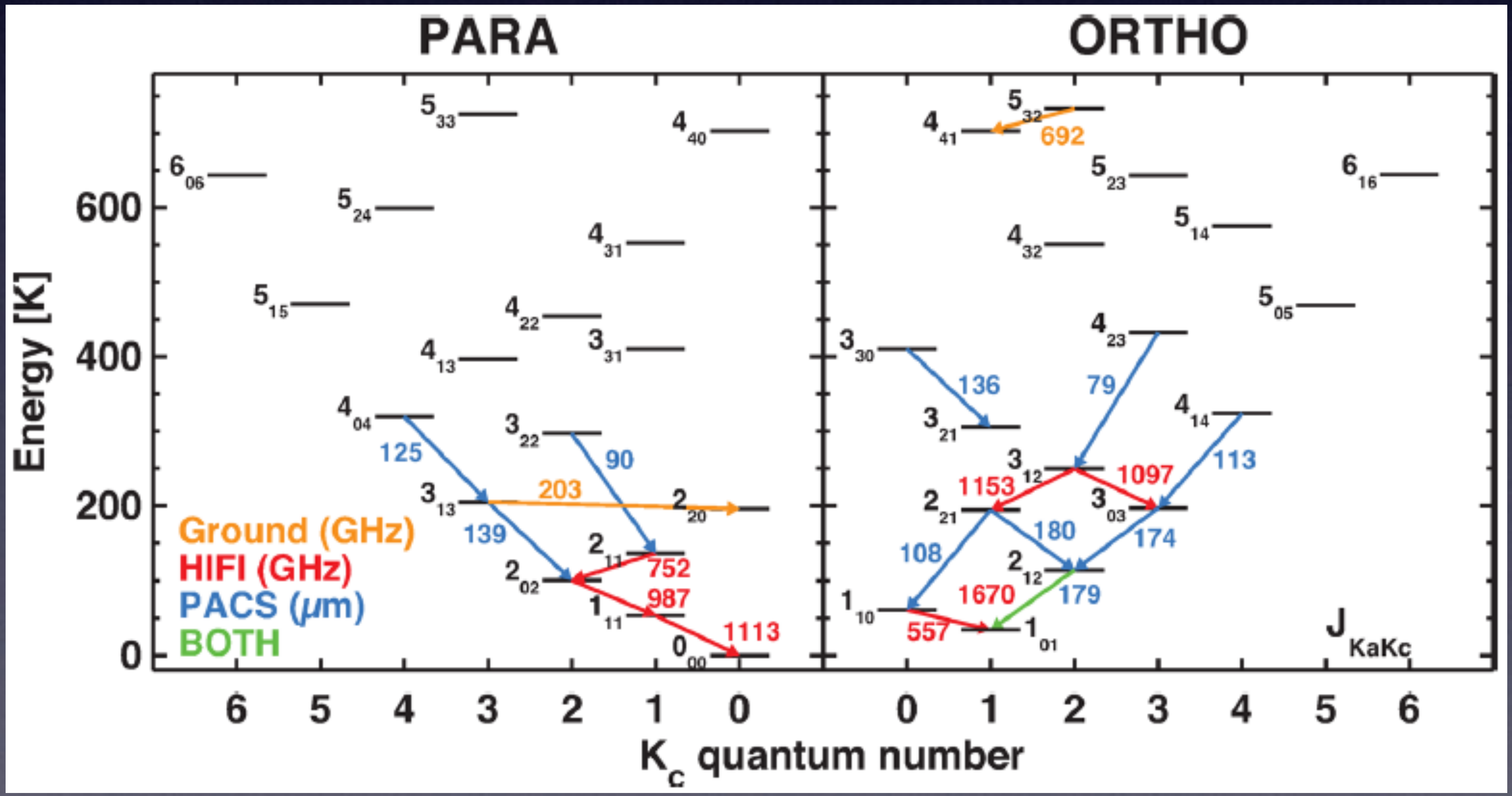
Grenoble, May 2, 2017



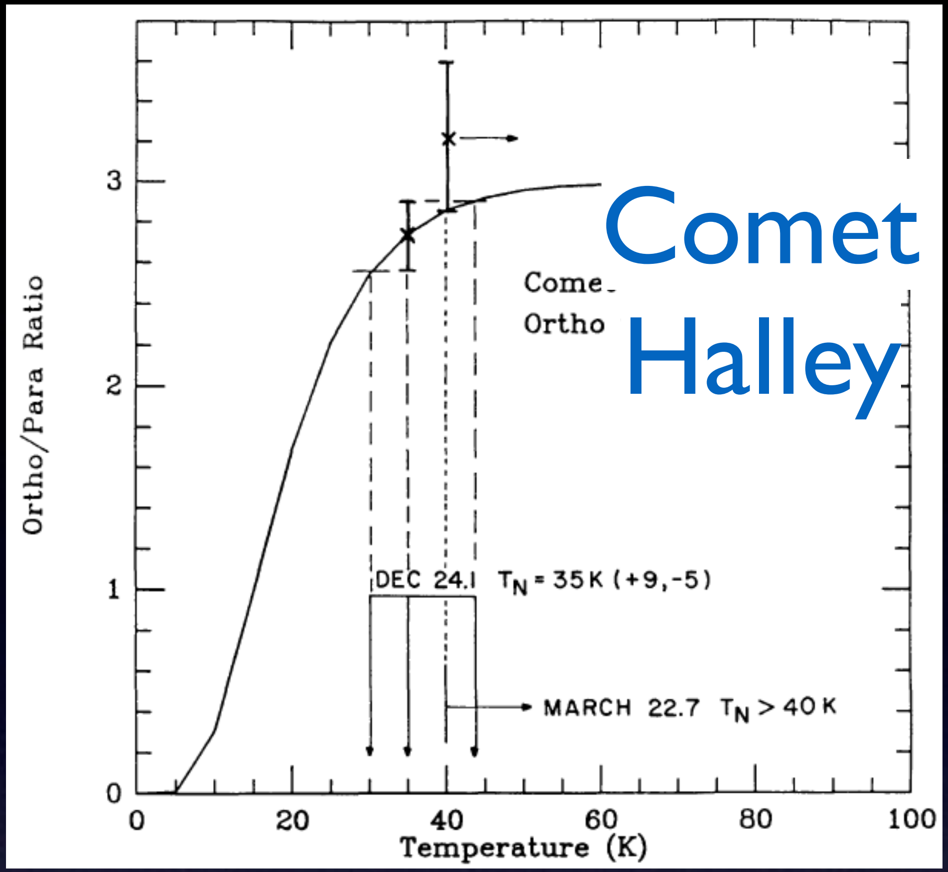
Water



van Dishoeck et al. 2013

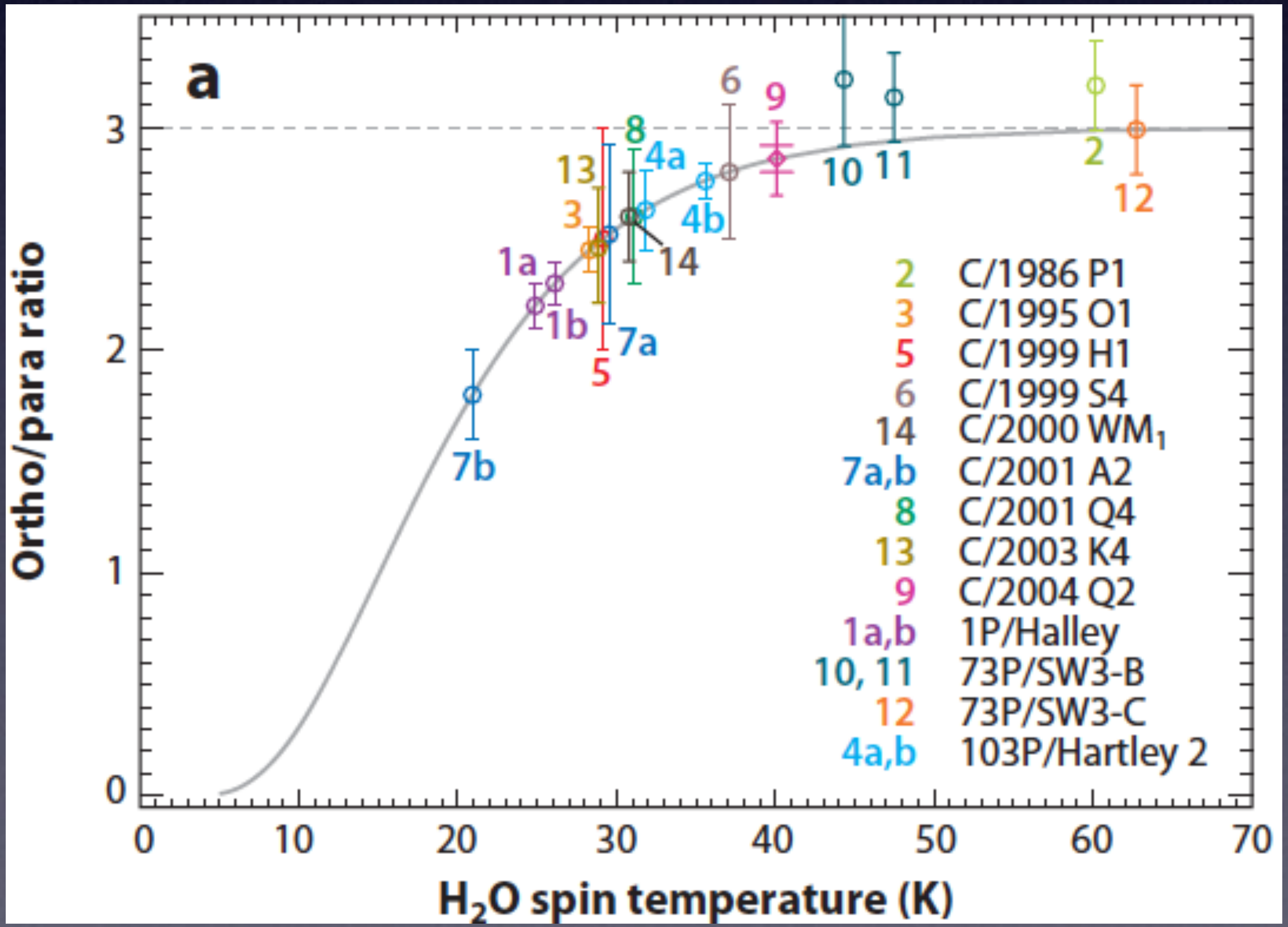
- Asymmetric top with two spin isomers: total hydrogen spin I=1 (ortho), I=0 (para)
- Energy difference 34.2 K
- High temperature limit OPR=3 (T>50 K)
- Spin temperature provides (maybe) some information about formation or condensation of water molecules on dust grains
- Herschel/HIFI has allowed for the first time high-resolution spectroscopy of the fundamental rotational transitions of both ortho- and para-water in the ISM

OPR in Cometary Water



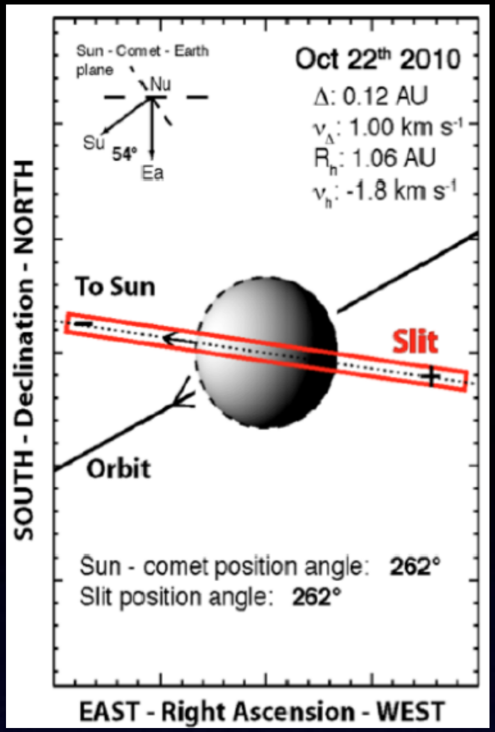
Mumma et al. 1987

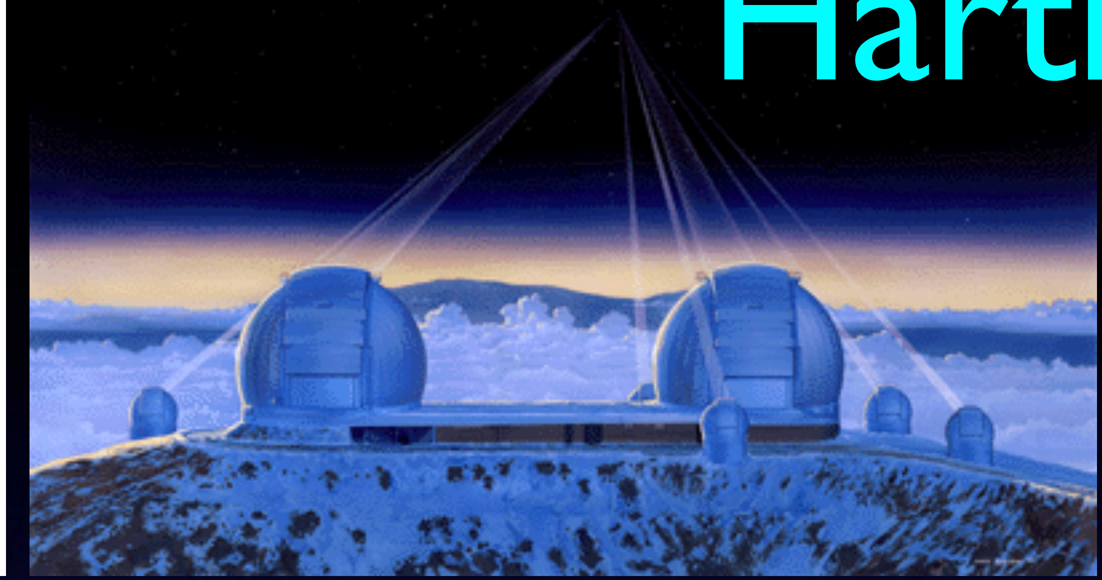
- OPR studied extensively in cometary atmospheres
- Optical or IR spectroscopy
- KAO, ISO, IRTF, Keck…
- Spin temperatures often ~30 K
- Some values consistent with LTE
- No values below ~20 K

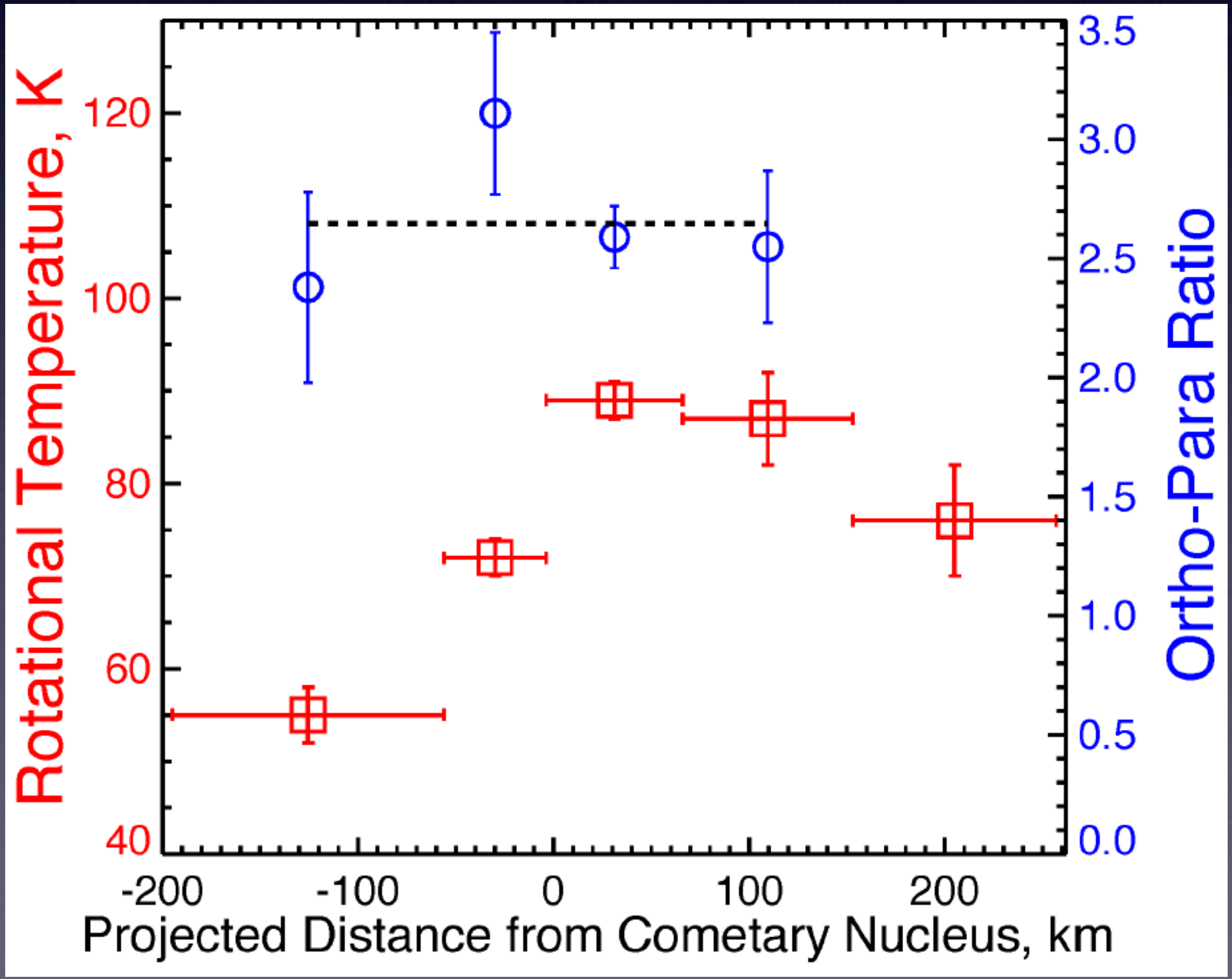


Mumma et al. 2011

Hartley 2 — Keck





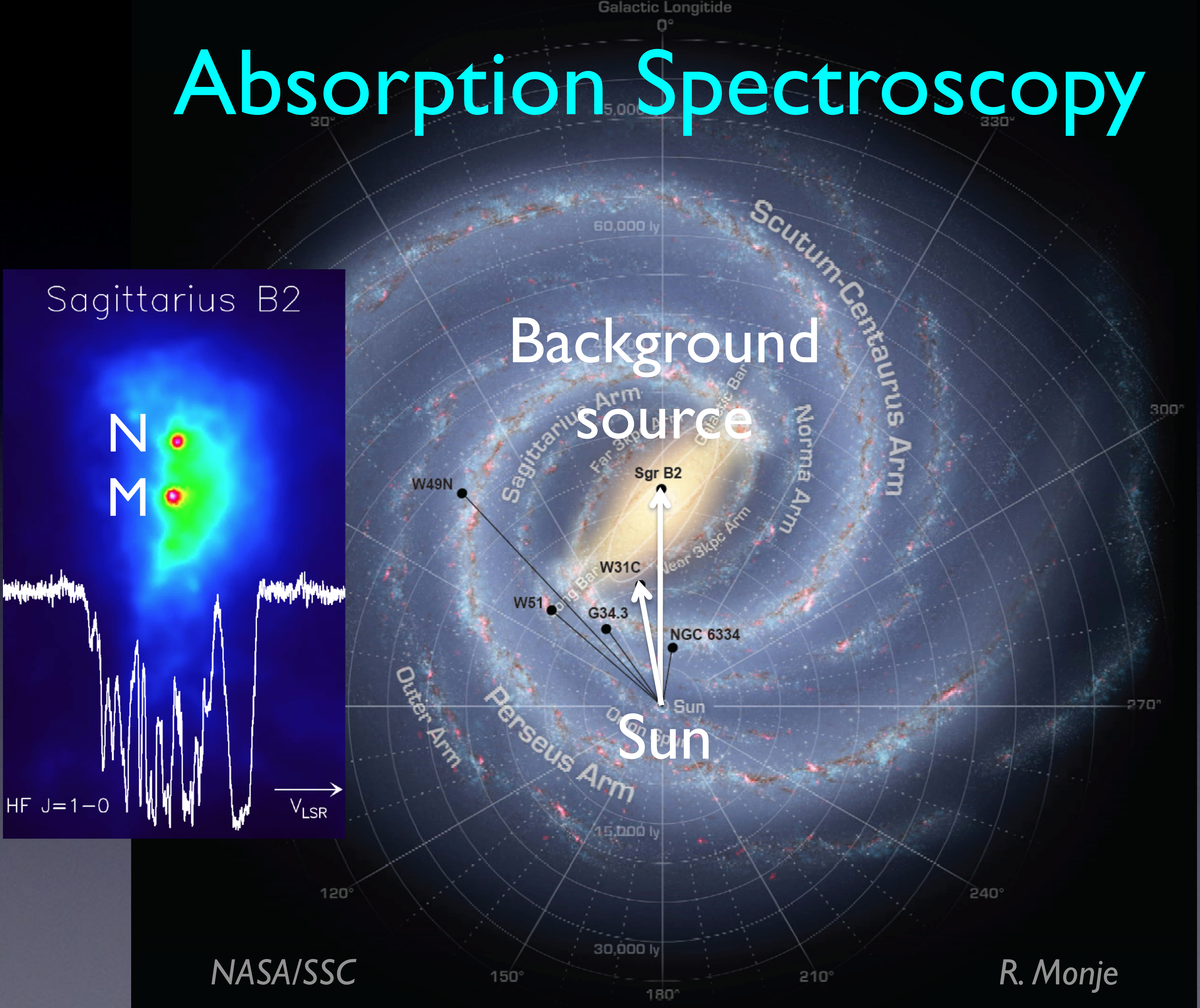


- Long-slit spectroscopy: measure OPR as a function of projected distance
- Most precise value 2.59±0.13, T_{spin} 31±3 K
- T_{rot} varies strongly with projected distance, but T_{spin} does not

- Solar nebula vs. ISM materials?
- Molecular abundances, isotopic ratios—OPR may provide additional useful information

Bonev et al. 2013, 2014

Absorption Spectroscopy

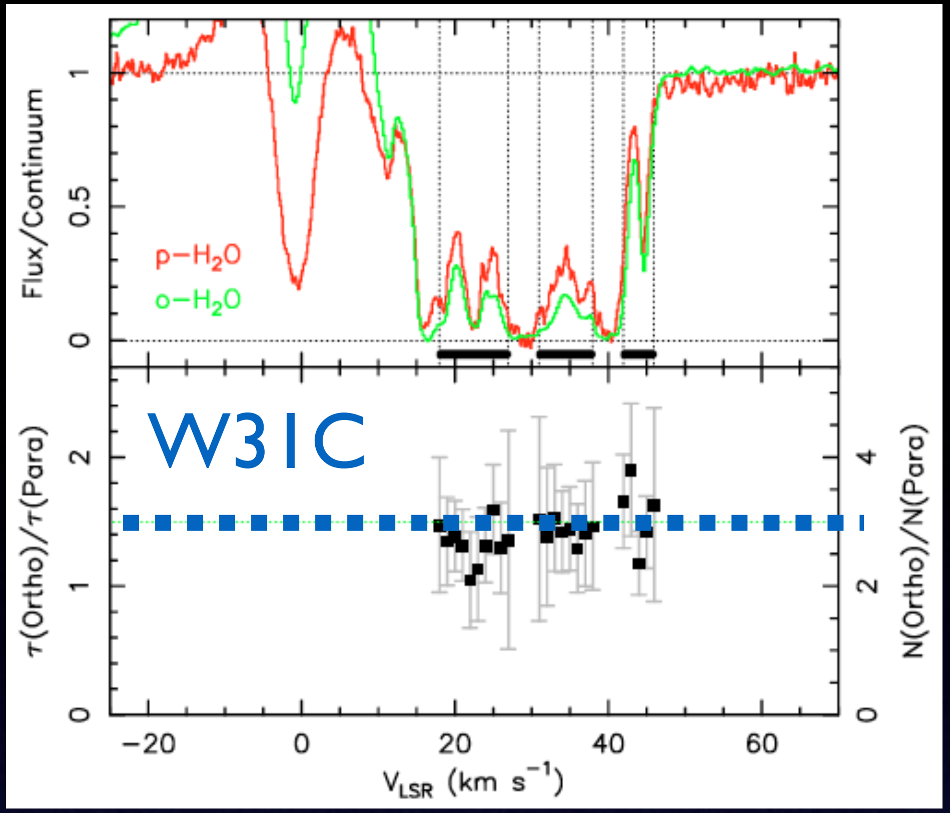


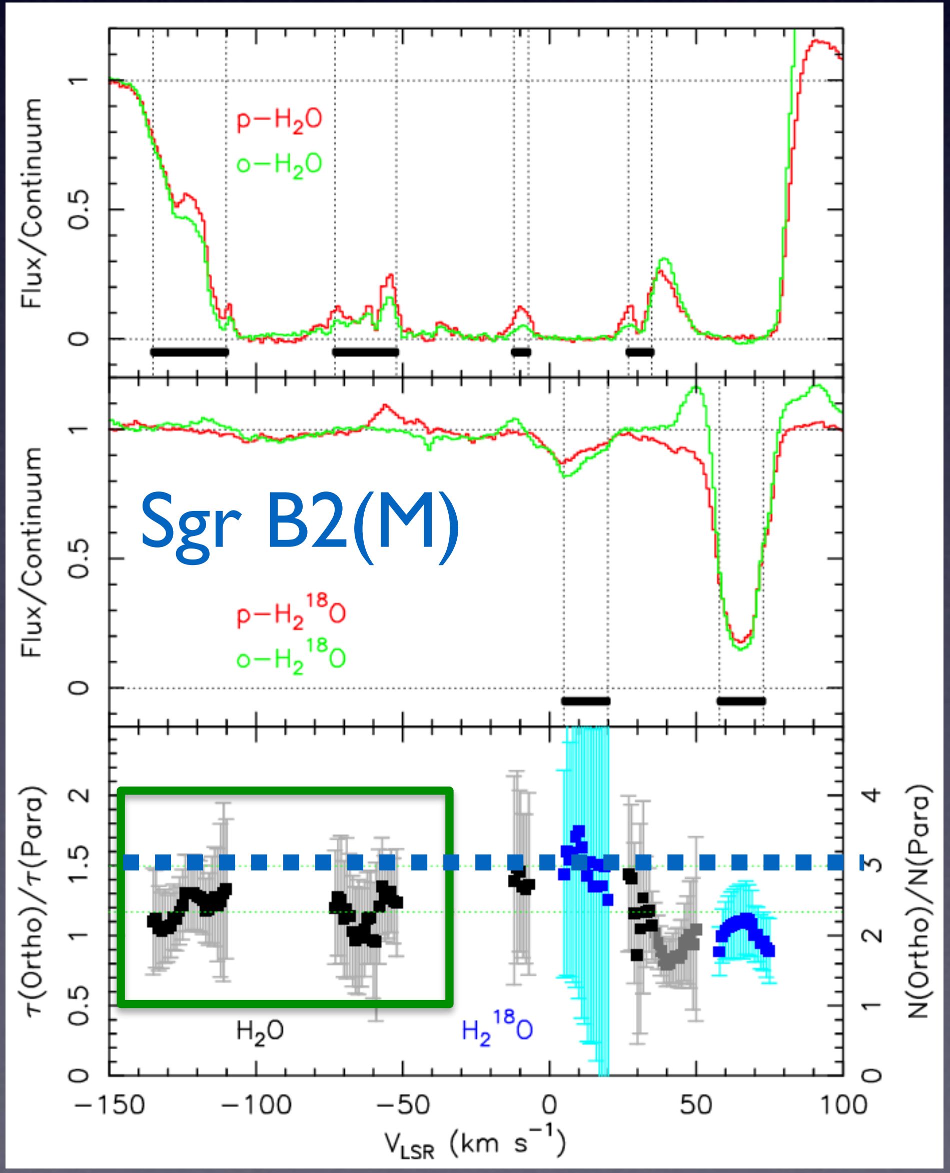
Background source

Sun

NASA/SSC

R. Monje





Early HIFI Results

- $H_2{}^{16}O$ spectra nearly completely saturated
- $H_2{}^{18}O$ absorption typically not detected

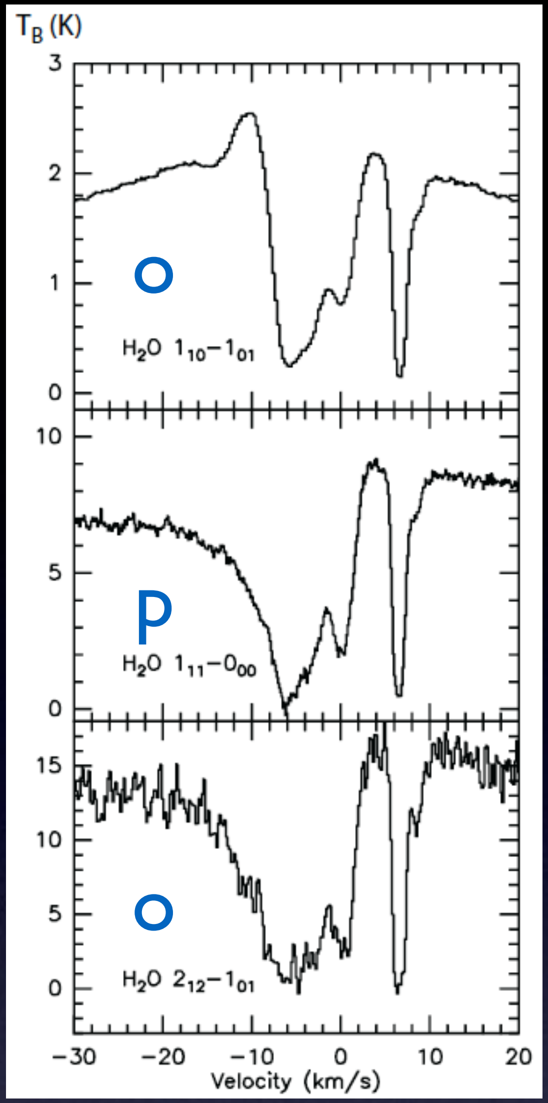
- Early results, based on the 557 and 1113 GHz data, showed that the OPR in most cases is consistent with the high-temperature limit (e.g., W31C)
- Possible exception: negative velocities in Sgr B2, corresponding to "expanding molecular ring"

- OPR 2.35±0.35, T_{spin}~27 K, similar to values measured in cometary atmospheres

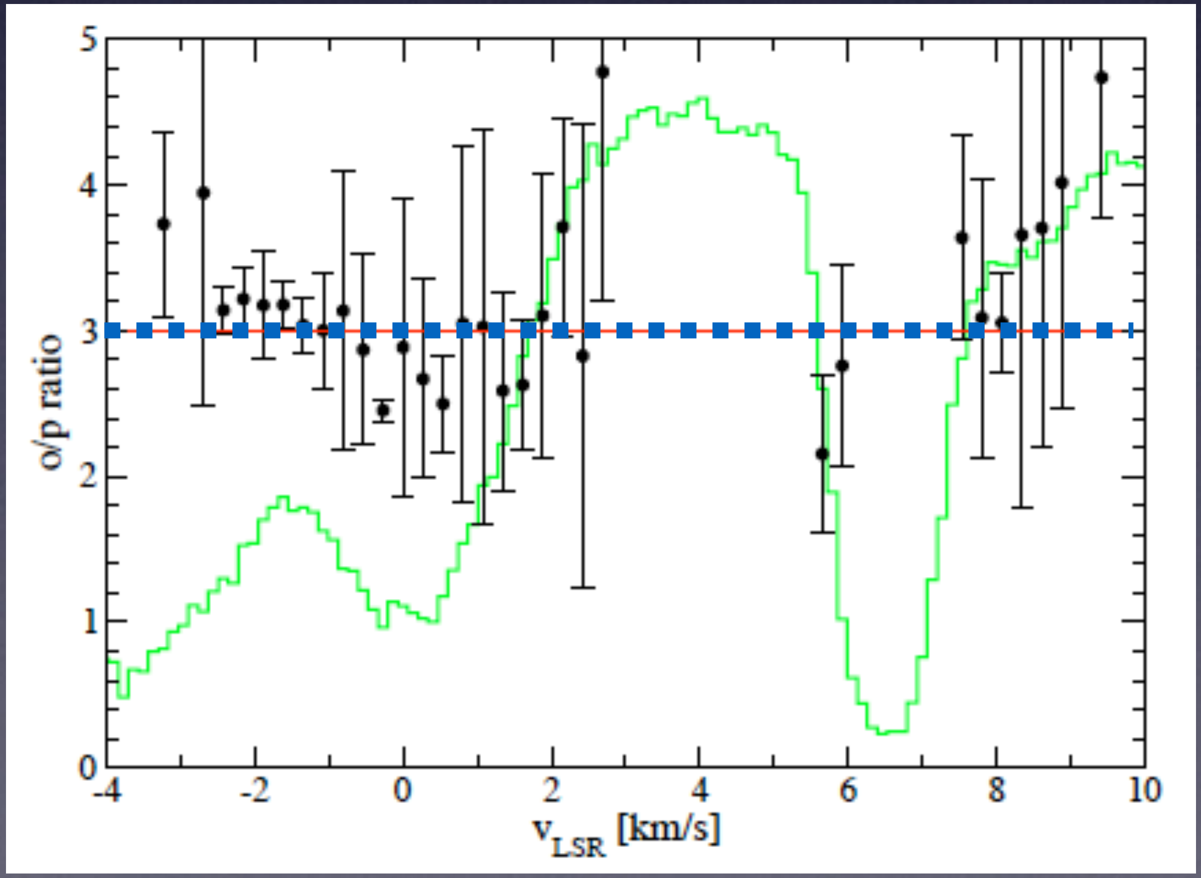
- *Difficult measurements*—have to get a good handle on *systematic effects* (e.g. baseline instabilities, sideband ratios), but also on *water excitation*

Lis et al. 2010

Molecular Excitation

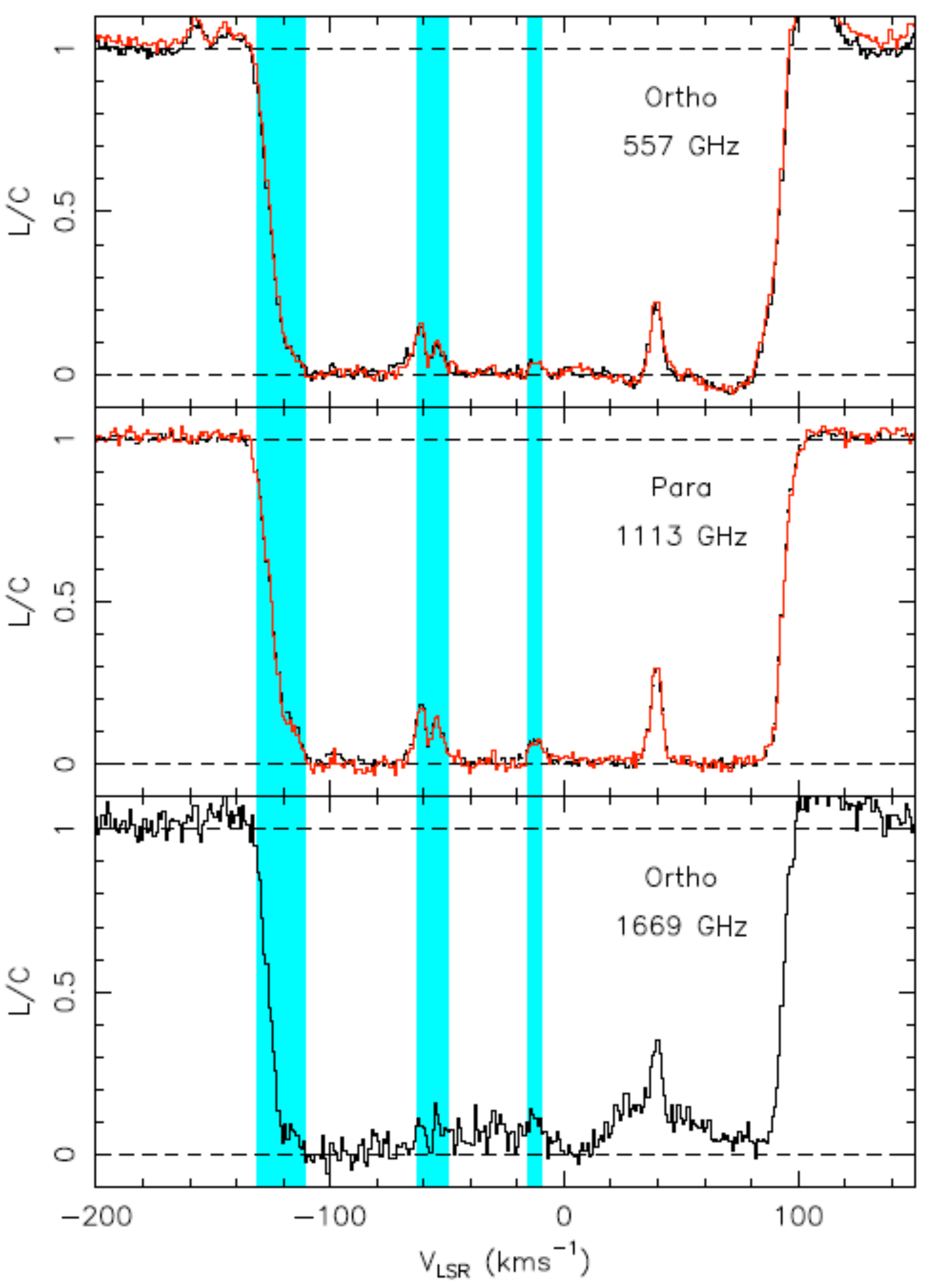


Emprechtinger et al. 2010, 2013



- Fundamental rotational transitions of light hydrides typically have very high critical densities
- Ortho-H_2O, 557 GHz, $n_{crit}=6x10^7$ cm^{-3}
- Assume all population in the ground rotational state in the diffuse ISM
- NGC6334I: OPR 1.6±1in the cold, quiescent gas, 2.5±0.8 in the outflow
- Addition of the 1669 GHz ortho-H_2O line allows *direct determination* of the excitation temperature
- NGC6334I: $T_{ex}=6.5$ K
- High for diffuse clouds, but absorption also seen in the ground state para-NH_3 line (tracer of dense gas)
- Revised OPR consistent with the high-temperature limit of 3

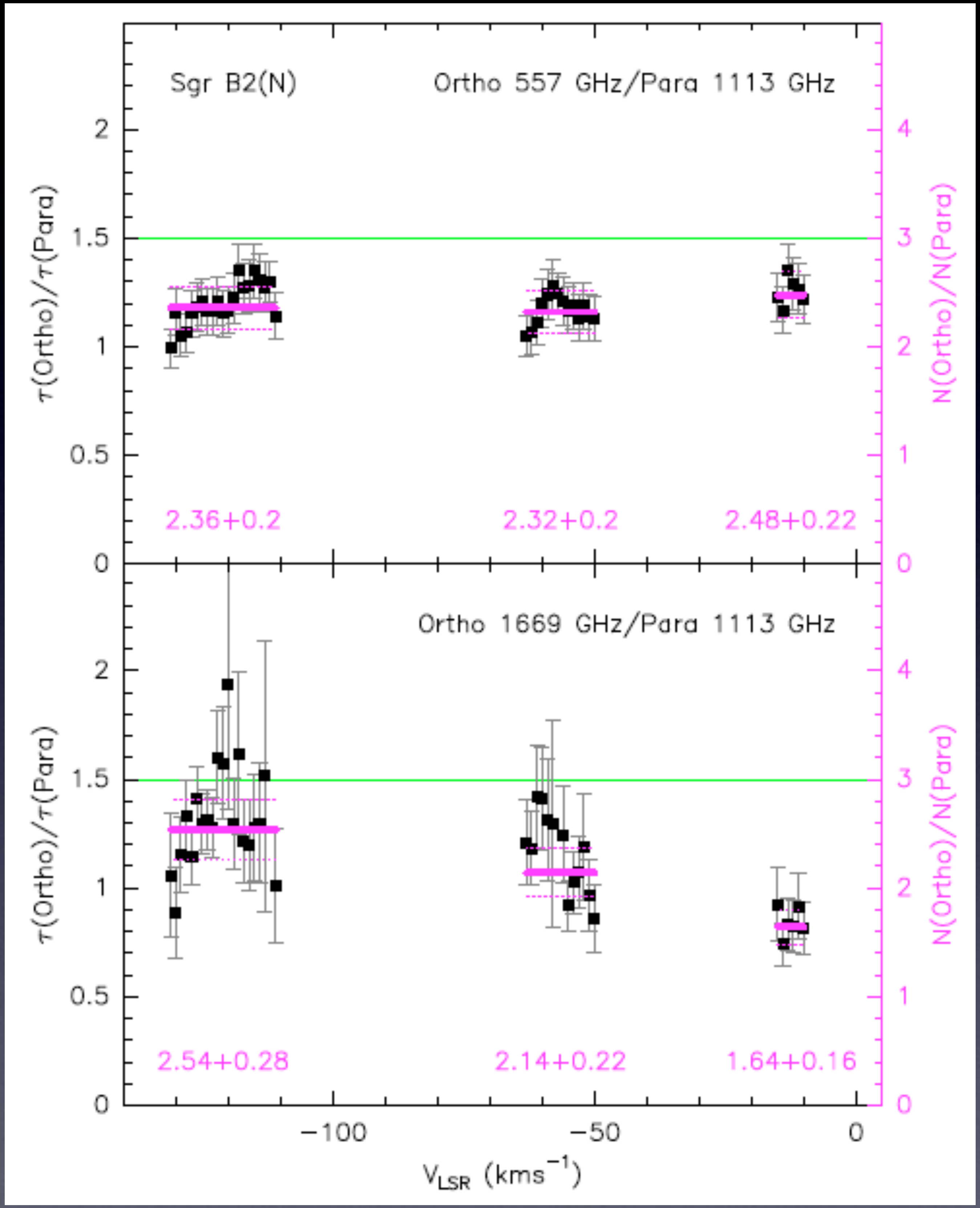
Sagittarius B2(N)



Lis et al. 2013

- Revisit Sagittarius B2
- Different line of sight, but nearby to Sgr B2(M) (tracing the same foreground gas)
- Independent measurement
- Better data reduction
- Redundant data set
- For the 557 and 1113 GHz lines: two independent measurements, using the HIFI mixer bands 1a/1b and 4b/5a
- Expect completely different systematics in terms of standing waves, sideband ratios etc.

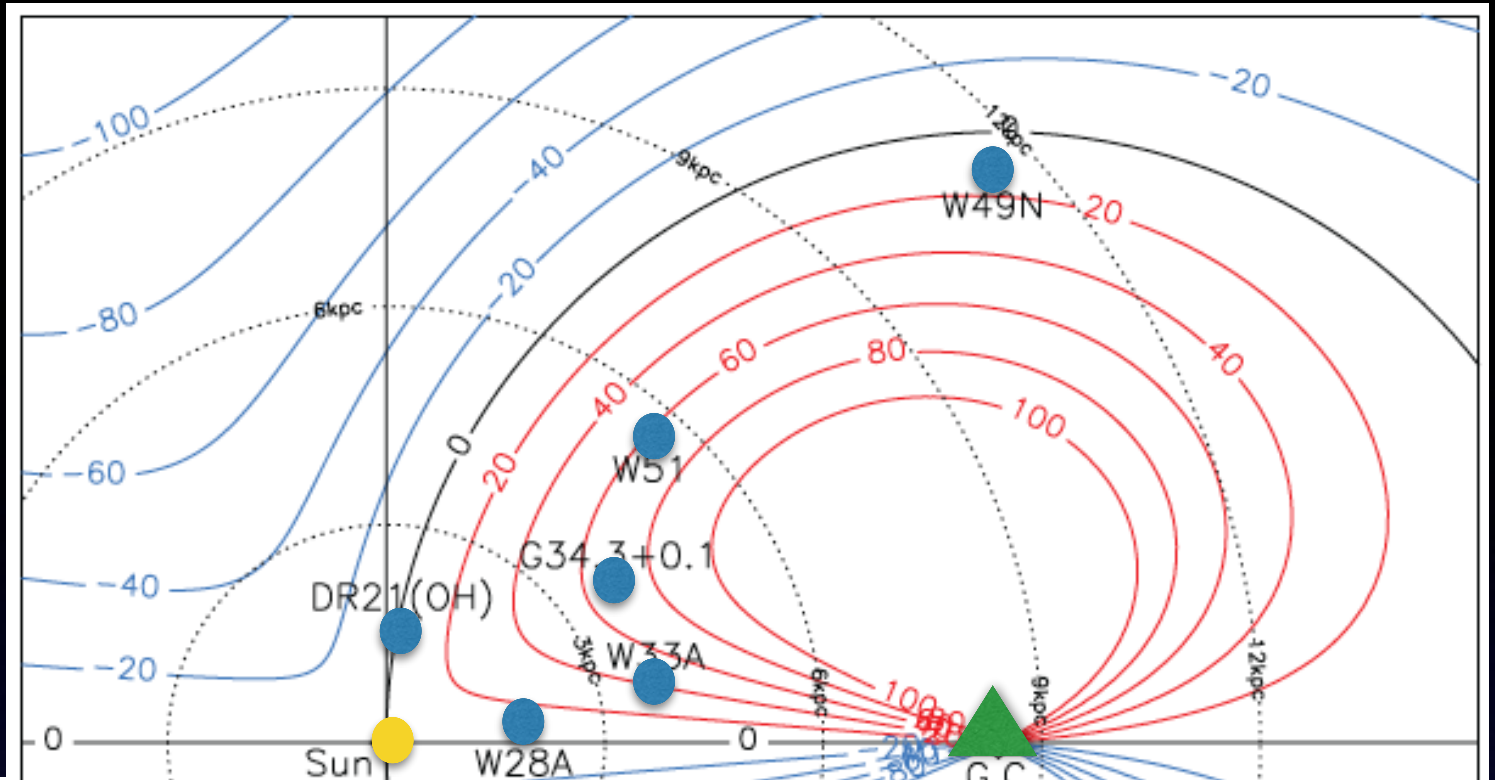
OPR in Sgr B2(N)

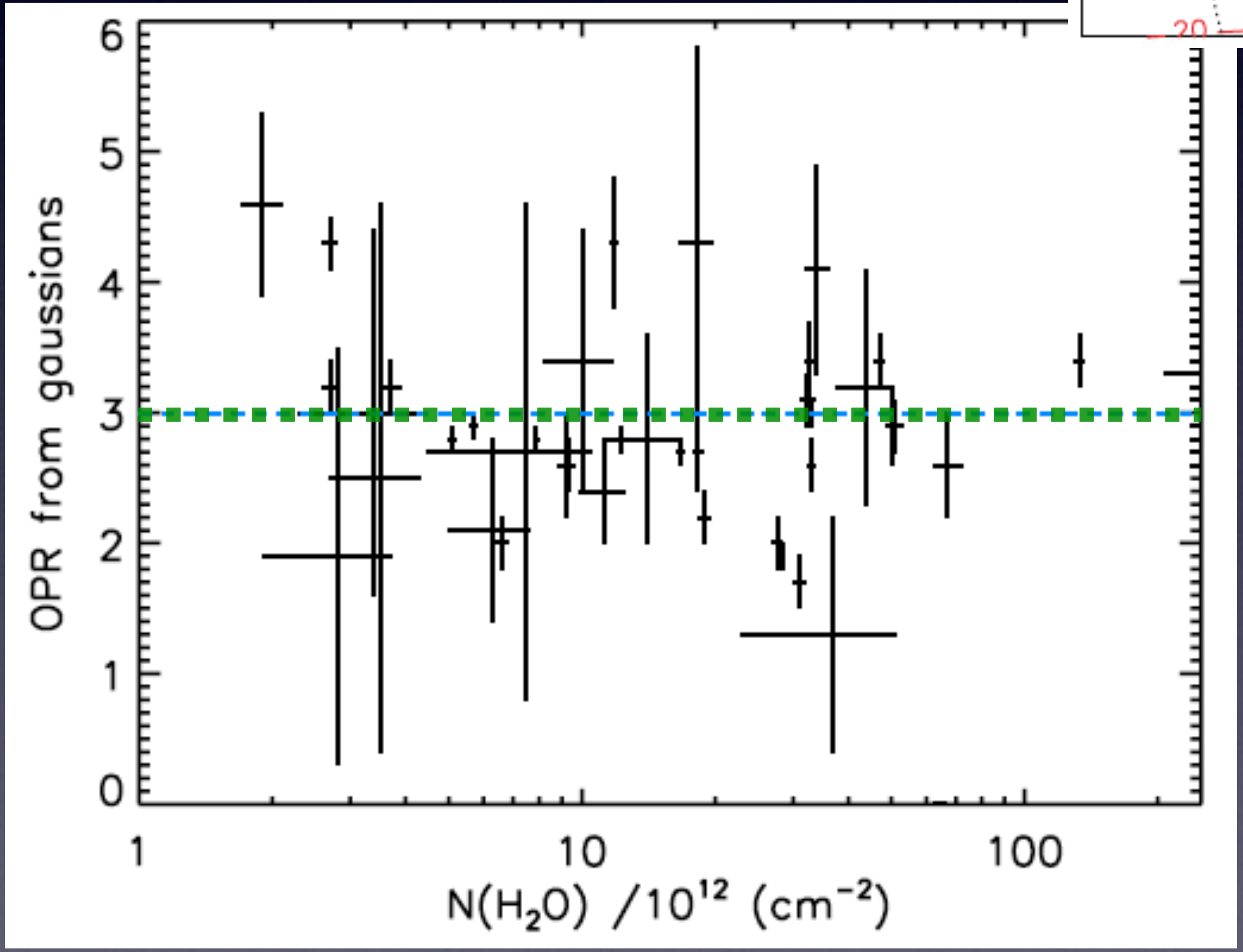


Lis et al. 2013

- With a good understanding of the correlated noise, we can derive accurate estimates of the uncertainties of the OPR in the three velocity intervals
- Confirms the earlier results that the OPR in water at negative velocities corresponding to the gas in the "x2" orbits is slightly lower than 3
- Same OPR based on observations of the 557 at 1669 GHz ortho-H_2O lines—assumption of low Tex justified for this line of sight
- Final value 2.34±0.35 (2σ)
- Spin temperature 24–32 K

Galactic Disk Sources

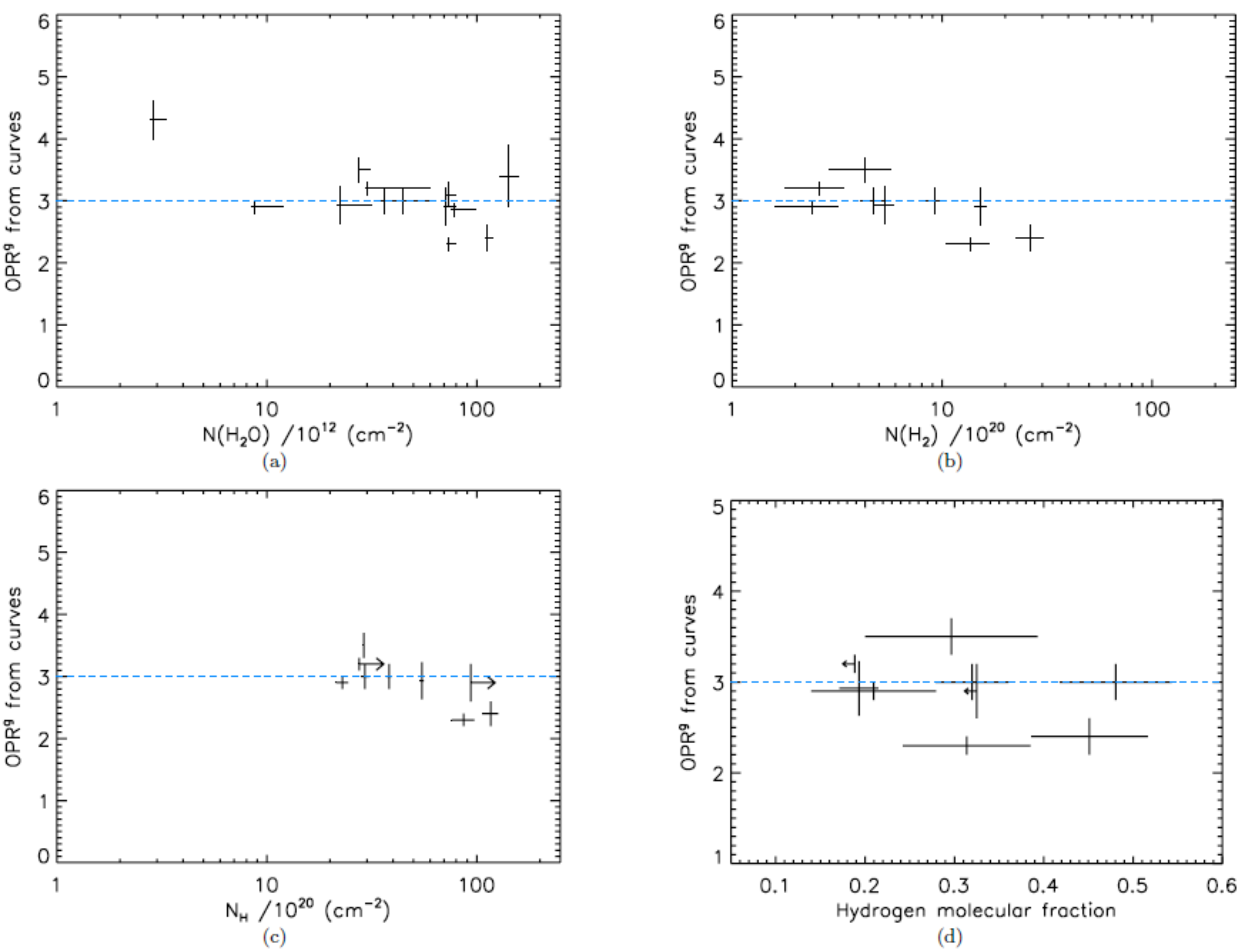




- Extensive compilations of PRISMAS observations of sources in the Galactic disk
- Different galactocentric distances, probe gas in different spiral arms
- H_2O/H_2 ~ 5 10^{-8} in diffuse clouds
- OPR generally consistent with 3, possibly with the exception of some components toward W49N

Flagey et al. 2013

No Apparent Trends

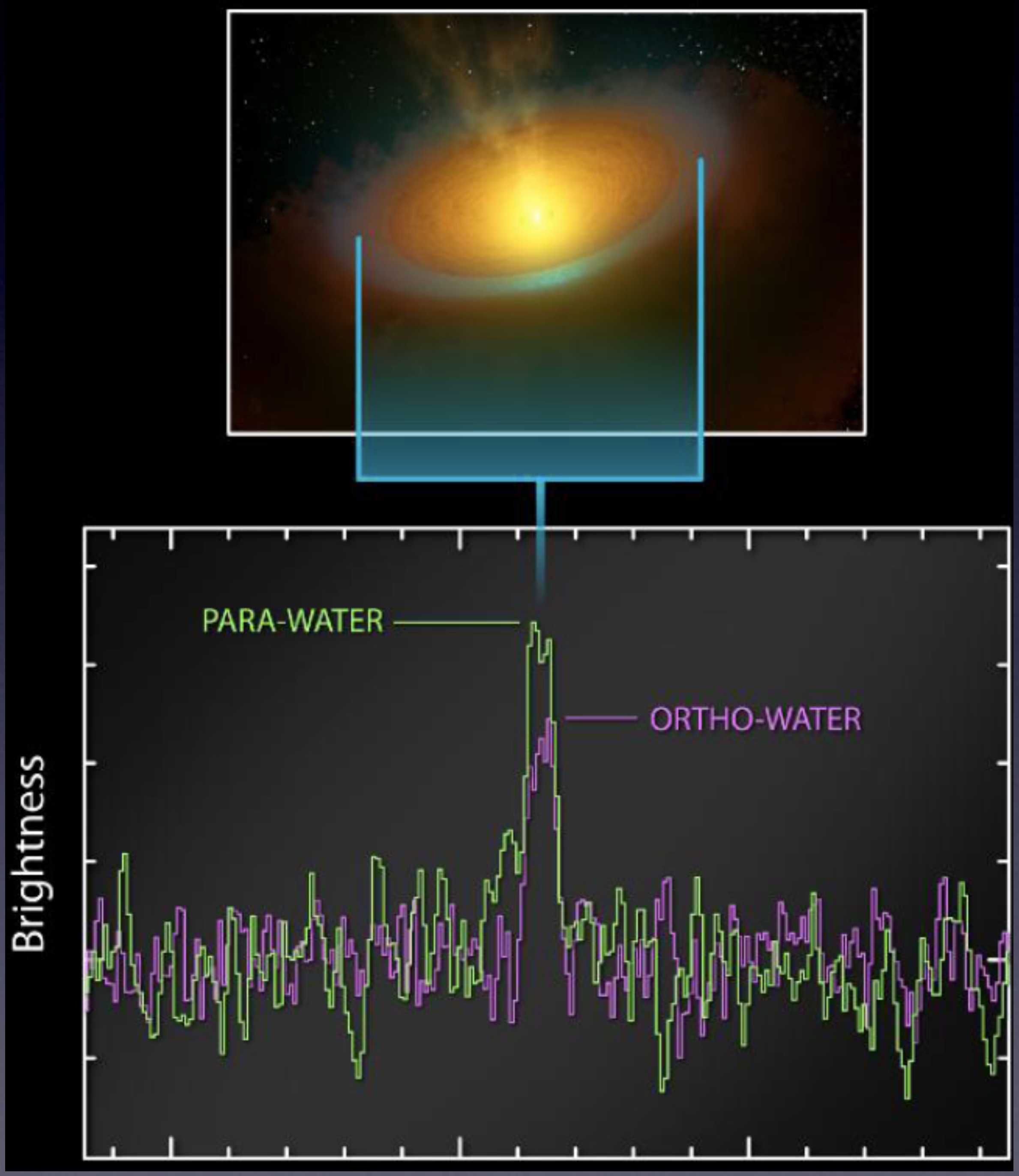


(a) (b) (c) (d)

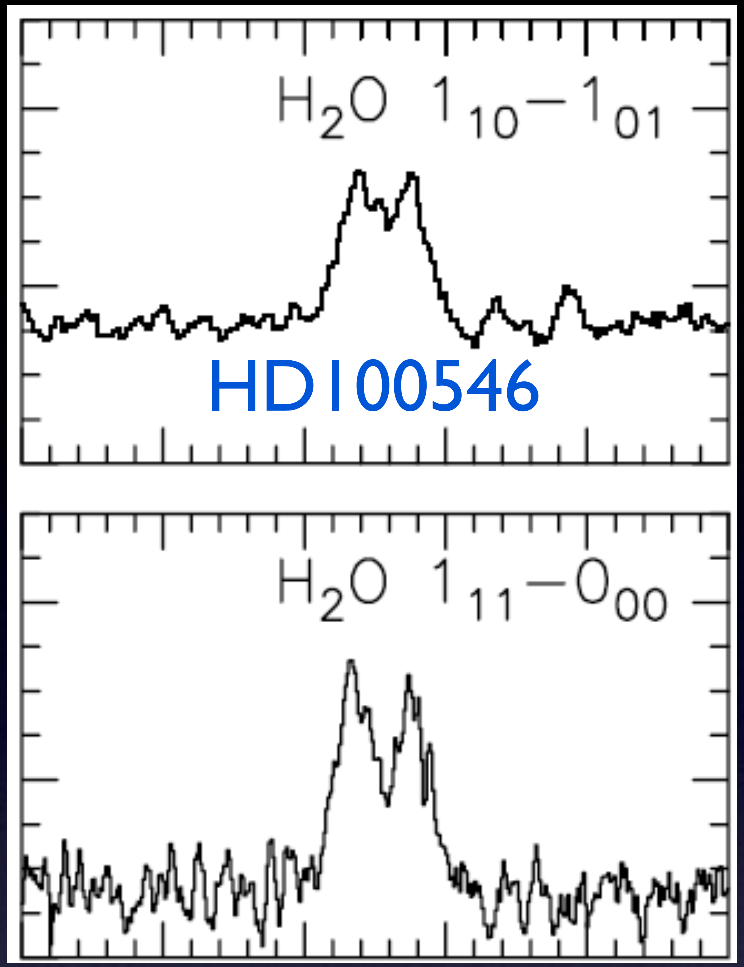
Flagey et al. 2013

Water in Disks

TW Hya

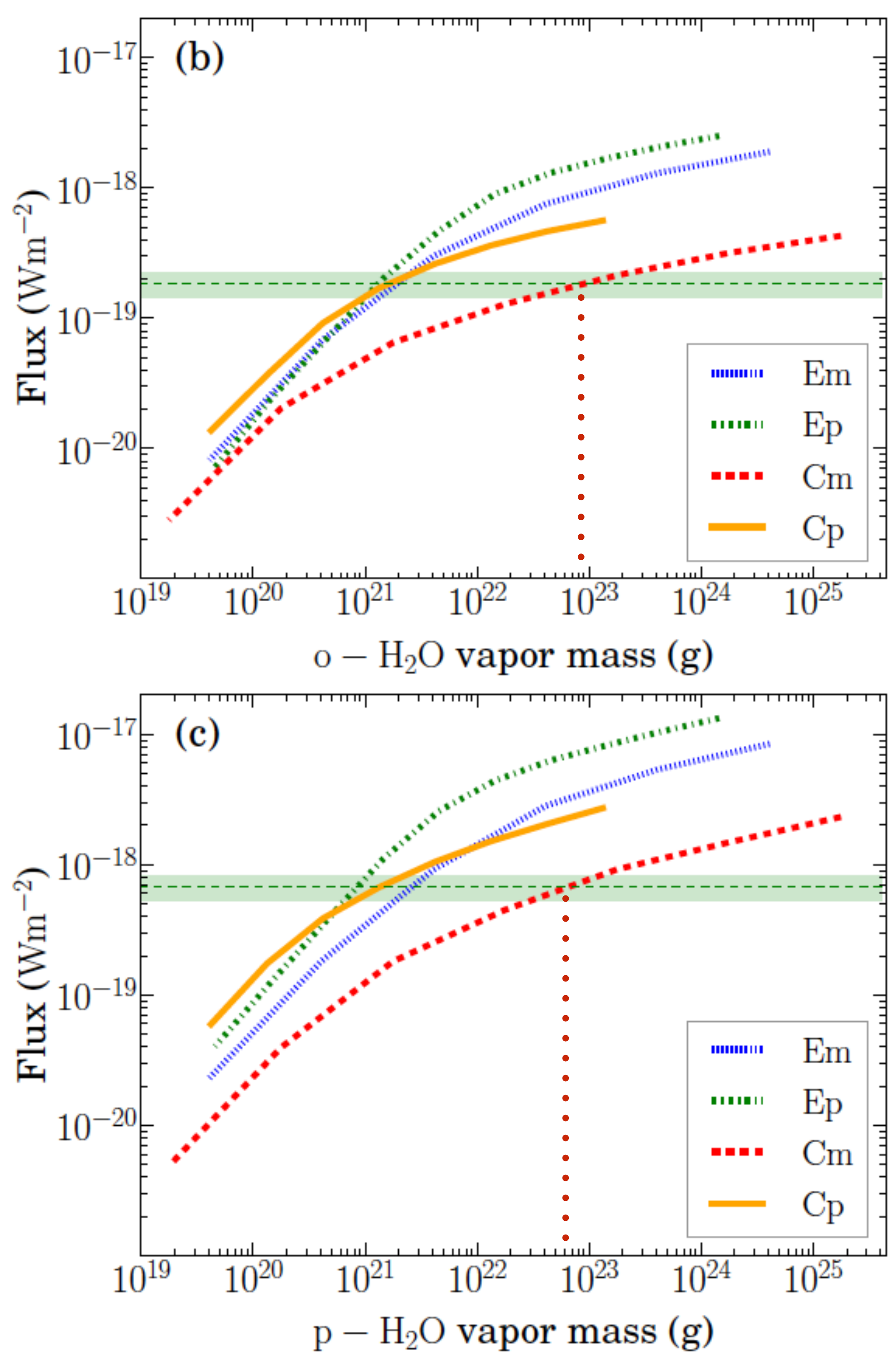


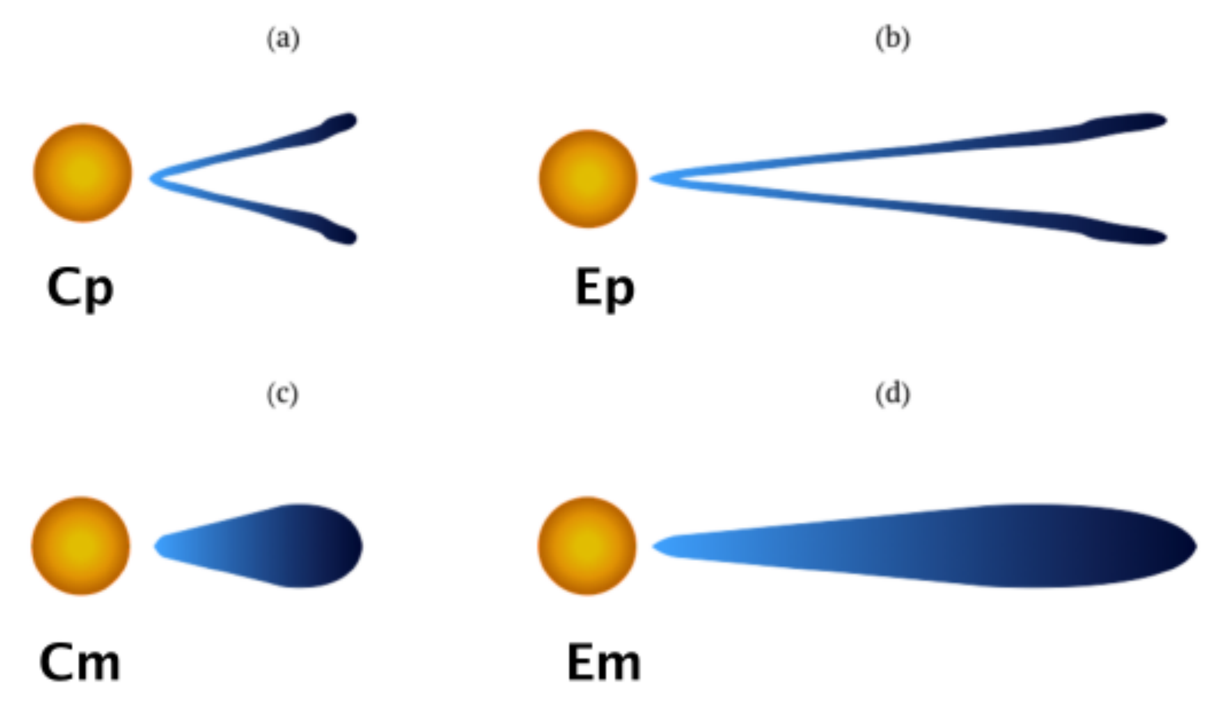
Hogerheijde et al. 2011



- Lines of ortho- and para-water detected for the first time with Herschel/HIFI in TW Hydrae
- 10 mln years old T Tauri star, 0.6 $M_\odot$ at 54 pc
- Lines seen in emission
- OPR 0.77+0.07 (1σ); T_{spin}=13.5 K
- Clearly lower than the cometary values!

TW Hya Revisited





- Simultaneous modeling of HIFI observations of water and ammonia
- Two classes of models
  - Desorption layer: compact and extended
  - Constant abundance: compact and extended
- Only model Cm gives an NH_3/H_2O ratio consistent with the low values observed in interstellar ices and solar system materials
- The same model is consistent within the errorbars with the H_2O OPR observed in the ISM and comets (OPR=1.4 +2.1/-1.15; mostly 20% calibration uncertainty)

Salinas et al. 2016

A&A 576, A85 (2015)
DOI: 10.1051/0004-6361/201322717
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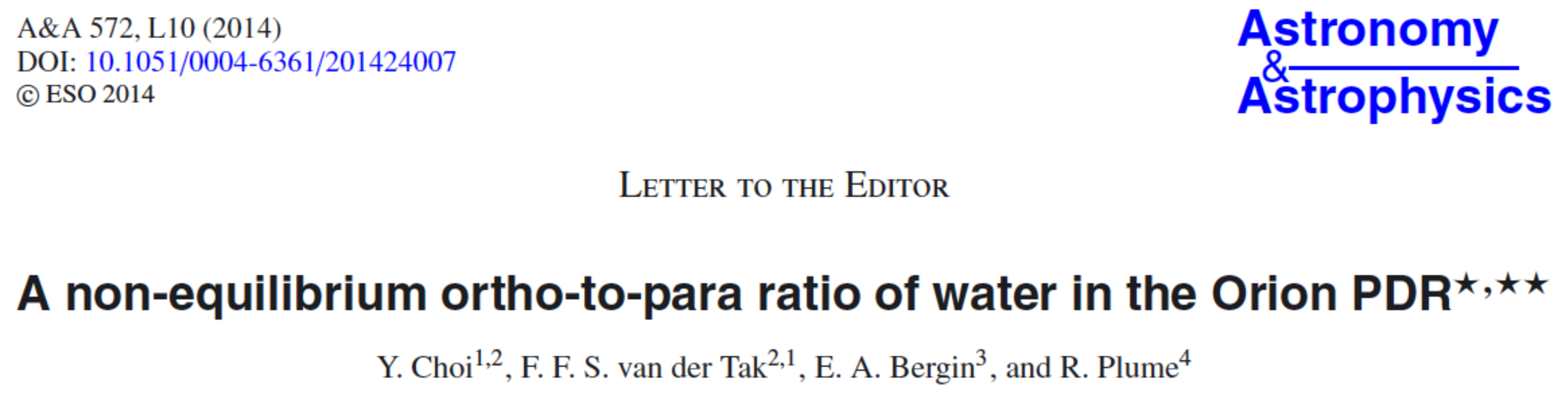
Astronomy & Astrophysics

Observations of water with *Herschel*/HIFI toward the high-mass protostar AFGL 2591★

Y. Choi[1,2], F. F. S. van der Tak[2,1], E. F. van Dishoeck[3,4], F. Herpin[5,6], and F. Wyrowski[7]

- Cold foreground absorption OPR=1.9±0.4, outflow 3.5±1



A&A 572, L10 (2014)
DOI: 10.1051/0004-6361/201424007
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Astronomy & Astrophysics

LETTER TO THE EDITOR

A non-equilibrium ortho-to-para ratio of water in the Orion PDR★,★★

Y. Choi[1,2], F. F. S. van der Tak[2,1], E. A. Bergin[3], and R. Plume[4]

- Orion S: OPR<2
- Orion Bar: OPR=0.1−0.5 — $H_2{}^{18}O$ lines seen in emission, single component LVG

Orion Bar

- Edge-on PDR illuminated by the Trapezium cluster
- Strong temperature and density gradients, clumping — single T, n model not applicable
- Use multi-line water observations (Choi, Bergin et al., in prep.) to constrain the physical conditions
- ISMDB — Online ISM Database, model grid calculated using the Meudon PDR code
- PhD thesis of Thomas Putaud at UPMC with Xavier Michaud

ISM DataBase - Inverse Search service Beta

https://ism.obspm.fr/

Grid of isobaric PDR 1.5.2 models *(2016-12-03)*

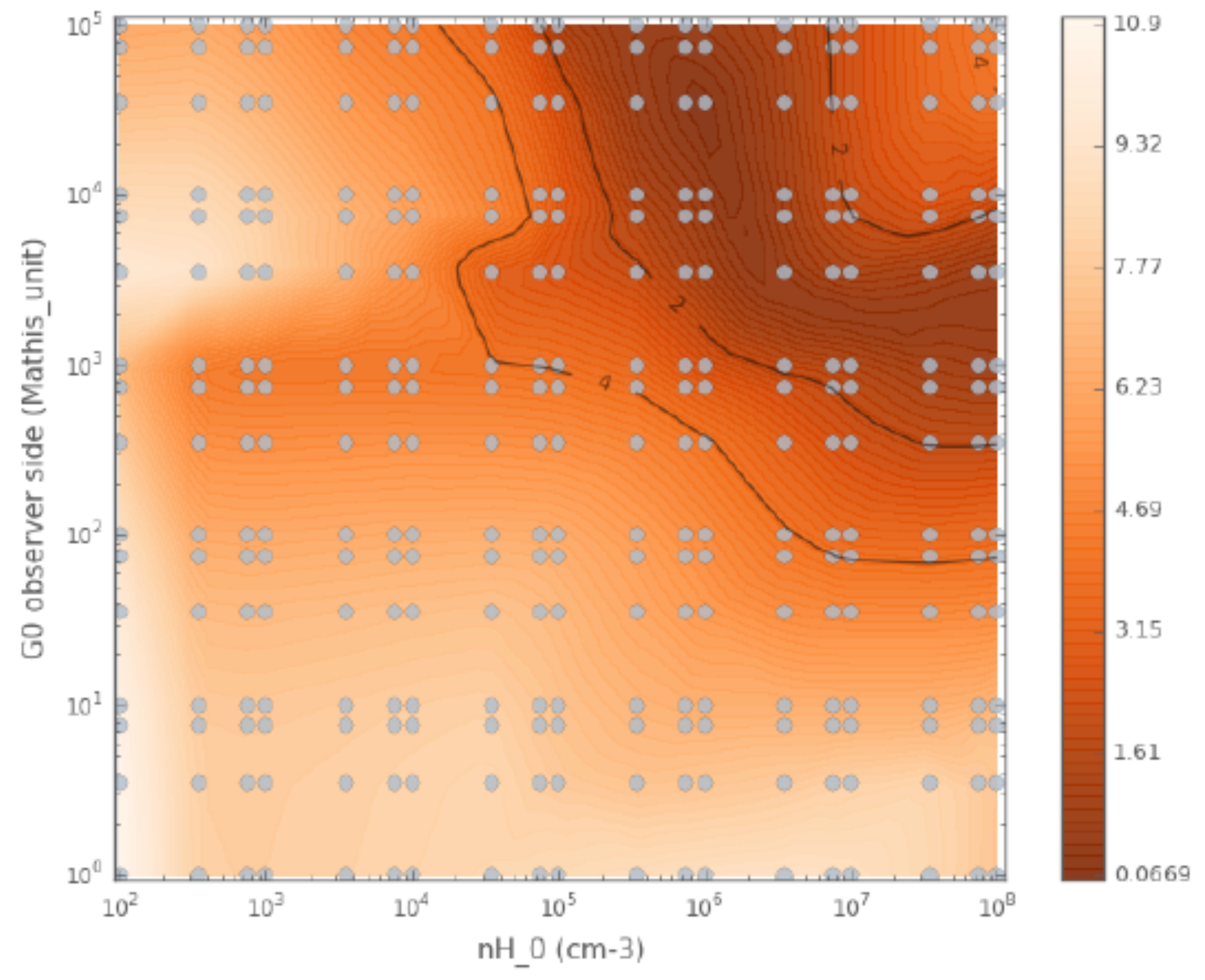
code: PDR 1.5.2 rev 1714

Parameters

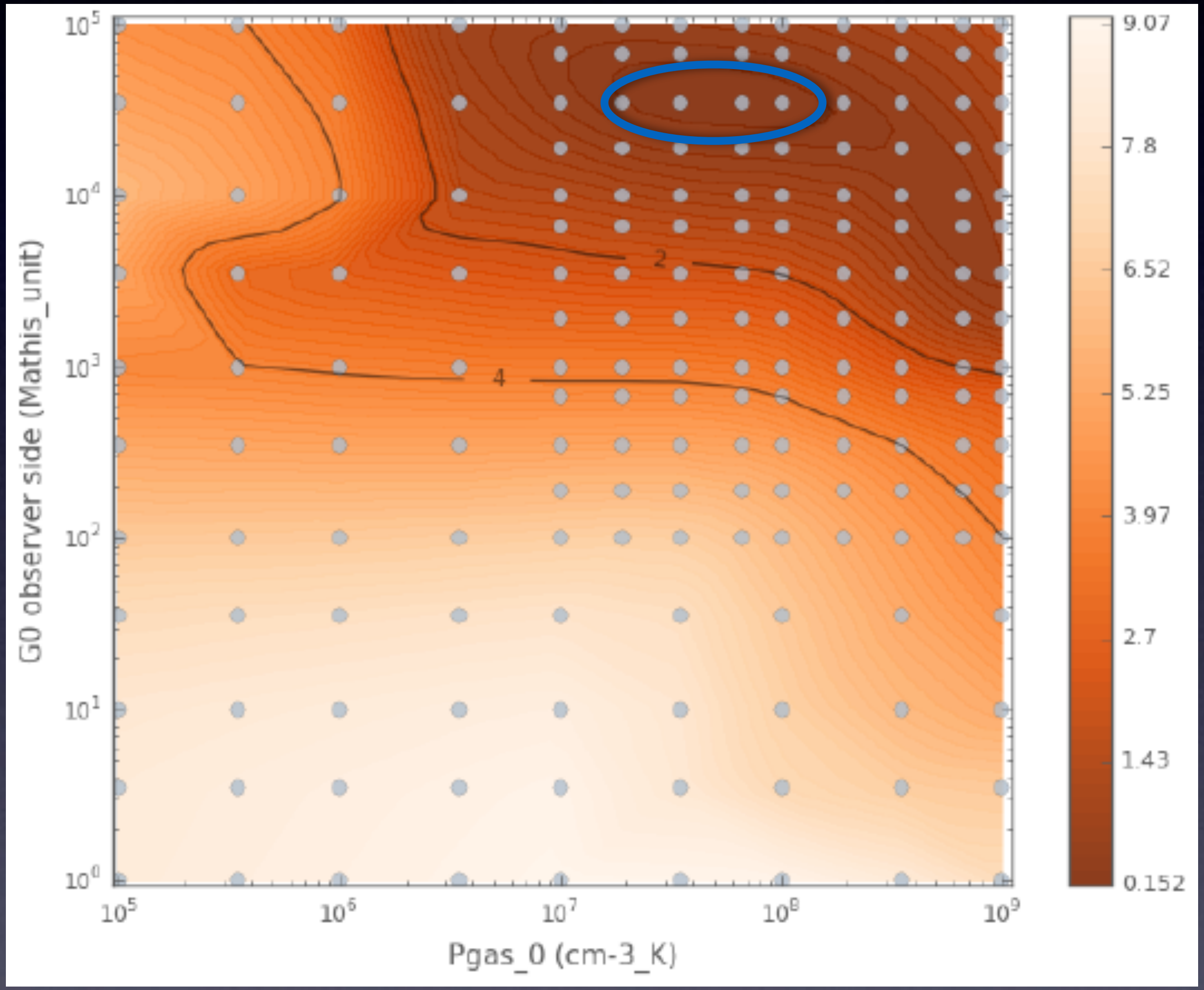
gas_pressure_input: from 1E5 to 1E9 (K cm-3)
radm_ini: from 1.0 to 1E5 (Mathis unit)
avmax: from 1.0 to 40.0 (mag)

Orion Bar — $H_2{}^{16}O$

Isochoric



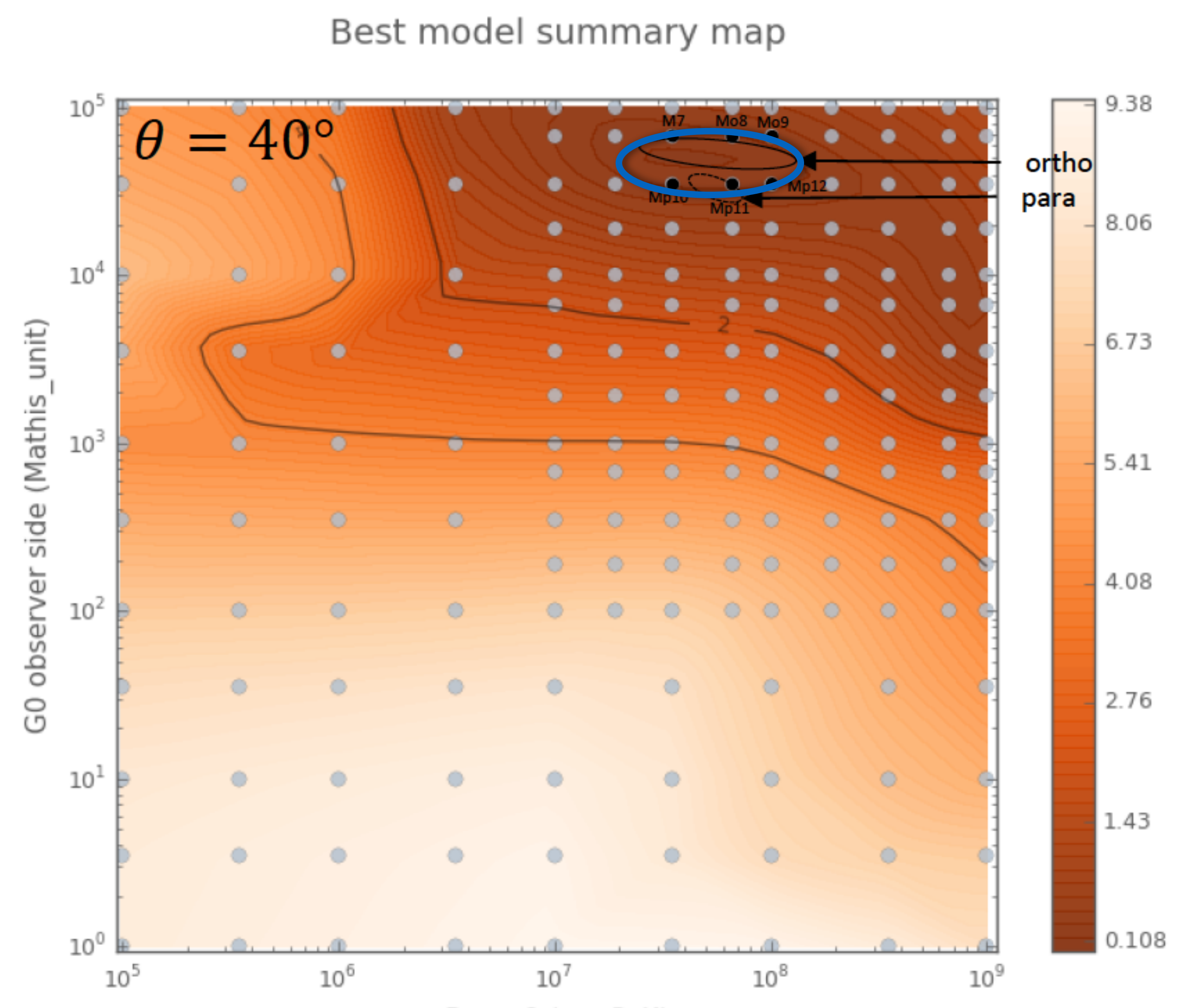
Isobaric

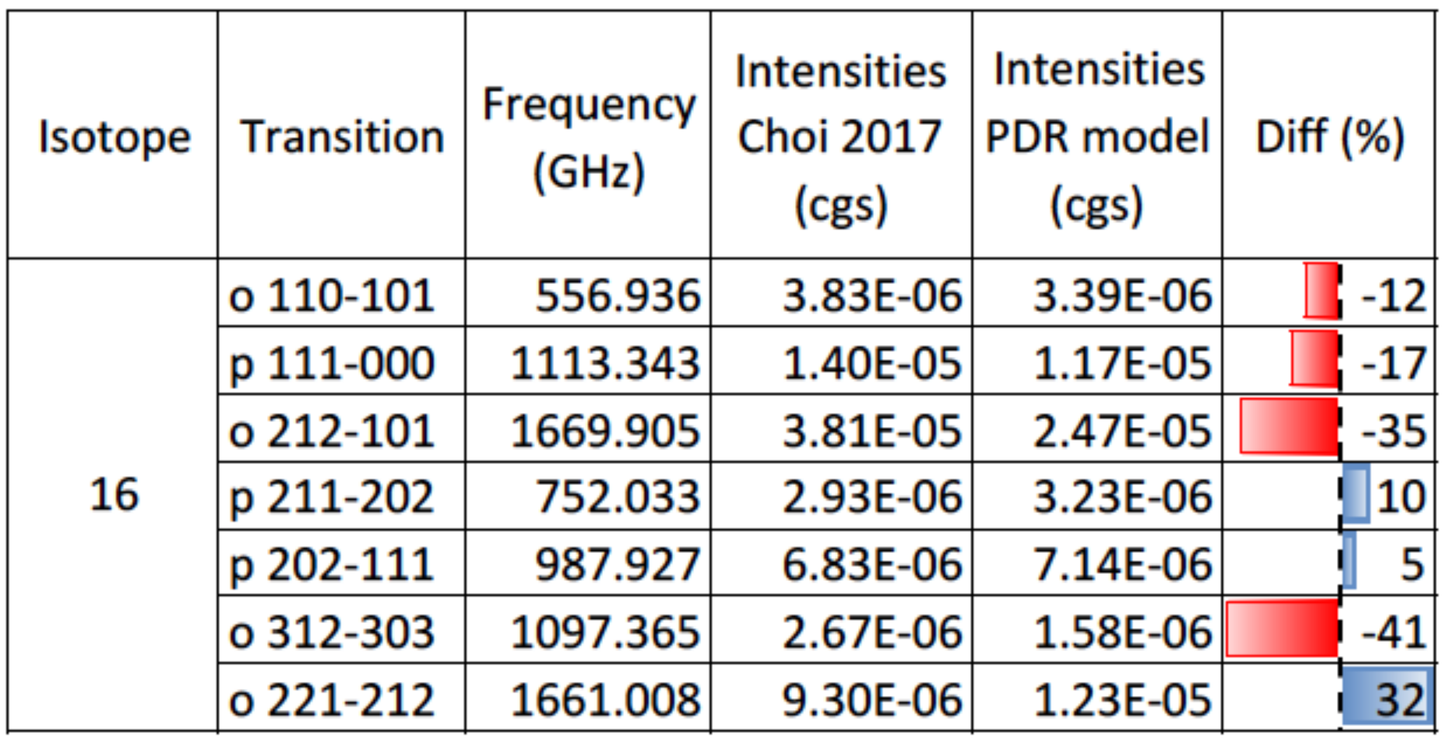


- No satisfactory solution
- Wide range of densities

- G_o and P relatively well constrained!
- See Marconi et al. (1998)

Best-Fit Isobaric Model $H_2^{16}O$

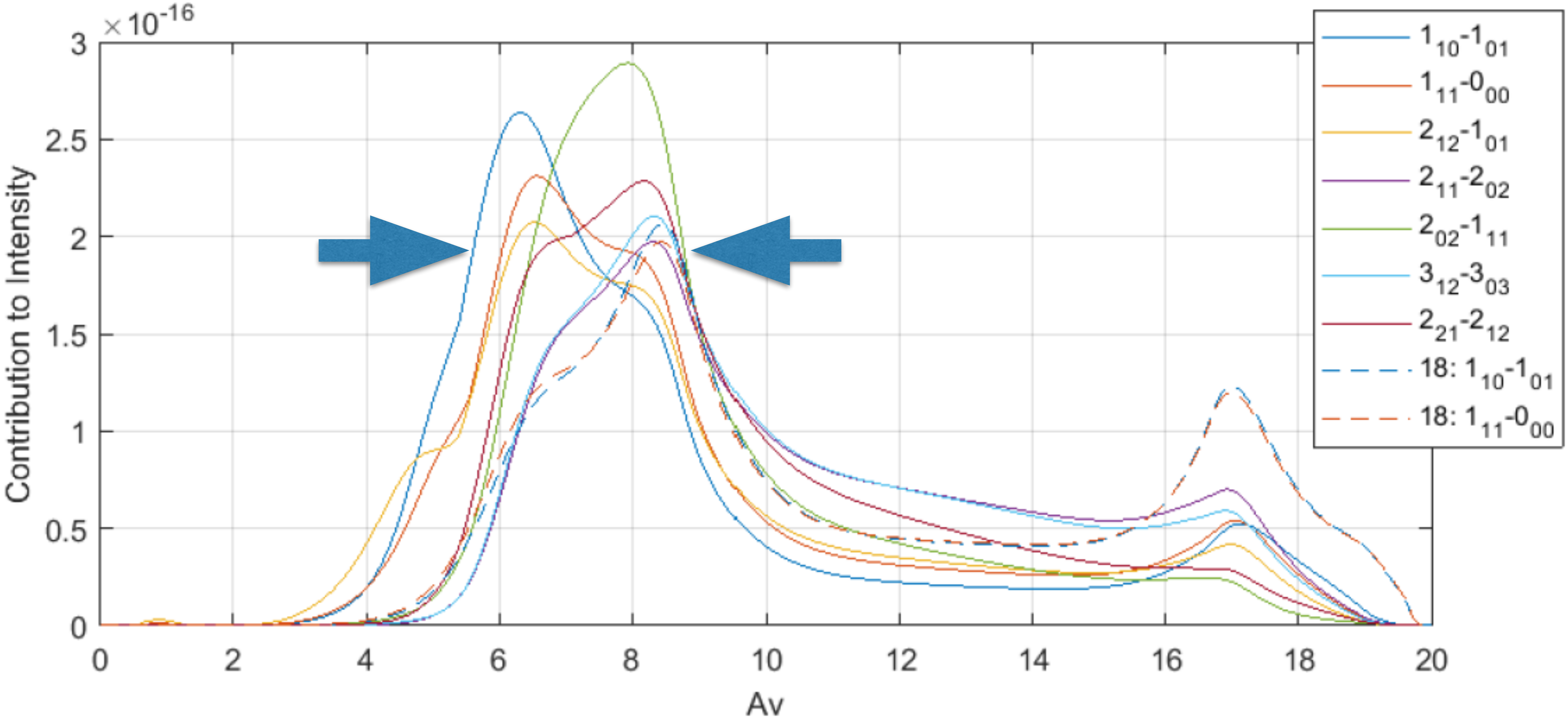




Isotope	Transition	Frequency (GHz)	Intensities Choi 2017 (cgs)	Intensities PDR model (cgs)	Diff (%)
16	o 110-101	556.936	3.83E-06	3.39E-06	-12
	p 111-000	1113.343	1.40E-05	1.17E-05	-17
	o 212-101	1669.905	3.81E-05	2.47E-05	-35
	p 211-202	752.033	2.93E-06	3.23E-06	10
	p 202-111	987.927	6.83E-06	7.14E-06	5
	o 312-303	1097.365	2.67E-06	1.58E-06	-41
	o 221-212	1661.008	9.30E-06	1.23E-05	32

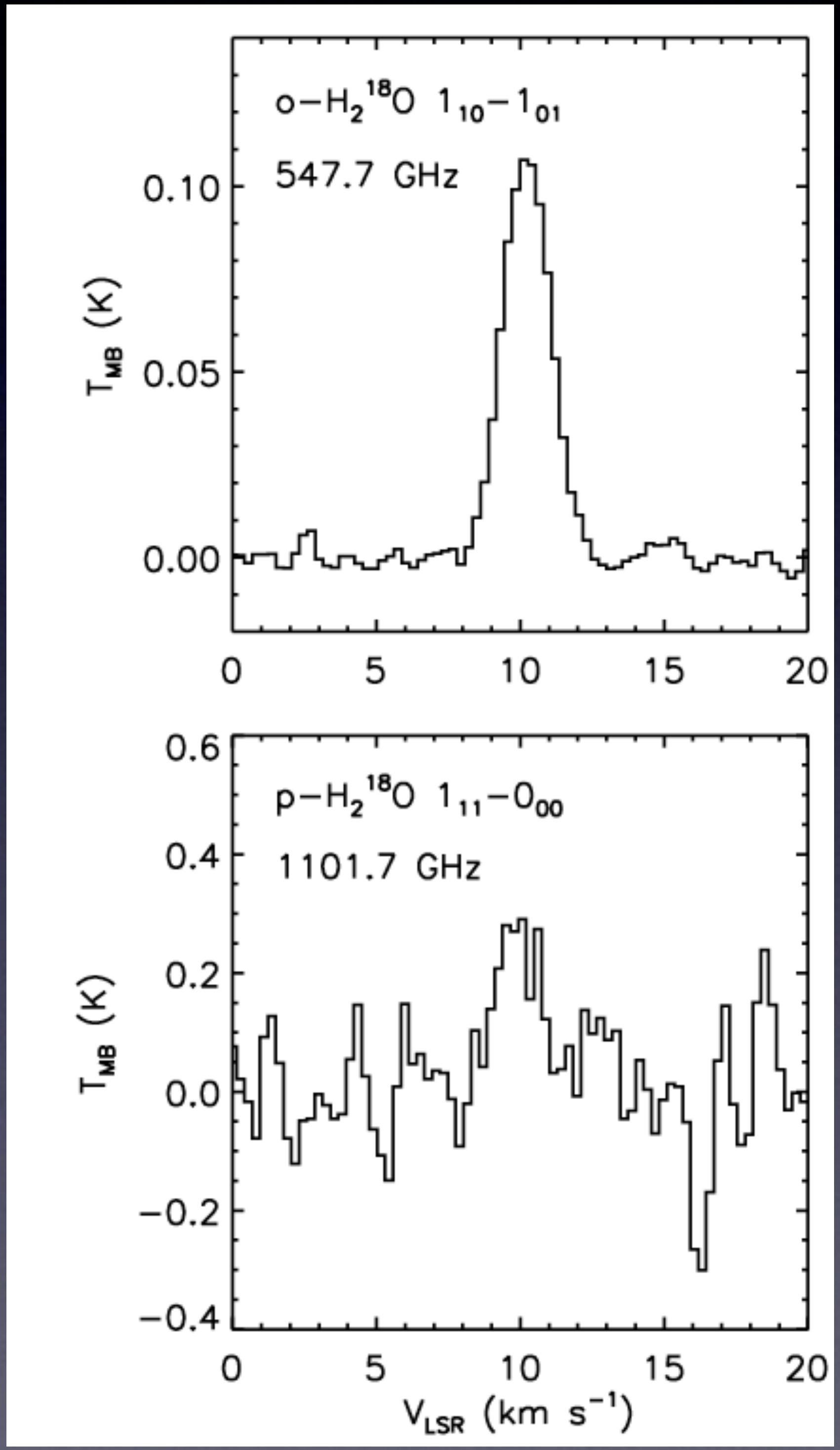
- Parameters: Go=4×10^4, P=4×10^7 cm^{-3}K, Av=20, inclination~40°
- Parameters largely consistent with what is know about the region (P ~ 1×10^8 cm^{-3}K in other studies)
- Reasonable fit — maximum discrepancies with $H_2^{16}O$ observations ~40%
- Fits both ortho and para lines

Where is Water Emission Coming From?

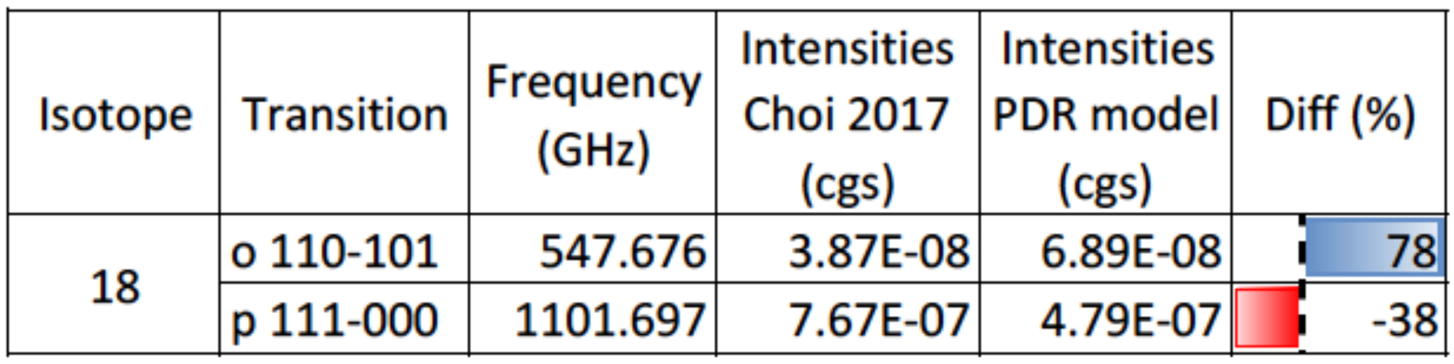


- Largest contribution ~5-9 A_V — T_{kin} ~30-35 K → OPR ~2.6

Model Predictions for $H_2{}^{18}O$



Choi et al. 2014



Isotope	Transition	Frequency (GHz)	Intensities Choi 2017 (cgs)	Intensities PDR model (cgs)	Diff (%)
18	o 110-101	547.676	3.87E-08	6.89E-08	78
	p 111-000	1101.697	7.67E-07	4.79E-07	-38

- $H_2{}^{18}O$ spectral and collisional data implemented into the Meudon PDR code
- Best fit $H_2{}^{16}O$ model (Go~4×10^4, P~4×10^7 $cm^{-3}K$):
  - $p-H_2{}^{18}O$ 1102 GHz under-predicted by 38% (but SNR only 4.7 in the data!)
  - $o-H_2{}^{18}O$ 547 GHz over-predicted by 78%
- Beam-dilution?
- Width of the Bar ~25”, beam size at 547 GHz 38” — beam dilution ~1.5 (linear correction)
- Affects optically thin $H_2{}^{18}O$ much more than optically thick $H_2{}^{16}O$

Summary

- There is a range of OPR values in water in the diffuse and dense ISM
- Most values are consistent with the high-temperature limit of 3, given the (relatively large) uncertainties
- There are some exceptions, e.g., gas on the "x2" orbits toward Sagittarius B2, where T_{spin}~24–32 K (2σ); also some velocity components toward W49N, Orion Bar
- There is no evidence for very low OPR values:
  - TW Hya—model dependent and consistent with OPR=3
  - Orion Bar—OPR may be lower than 3, but not likely as low as 0.1−0.5
- No trends seen in the OPR with the H_2O, H_2, or H column density, galactocentric distance, or molecular fraction
- Analysis of the existing Herschel data can still be improved
- All these conclusions are consistent with the latest cometary measurements