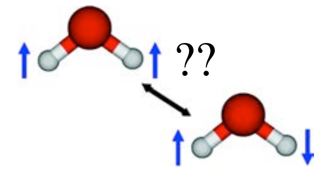
Spin Ratios in Comets: Complexity of Measurements, Post-2014 Updates, and Prospects

Boncho P. Bonev

Nuclear Spin Effects in Astrochemistry 2017
Université Grenoble Alpes

Comet Hale-Bopp Image Credit: Terry Acomb

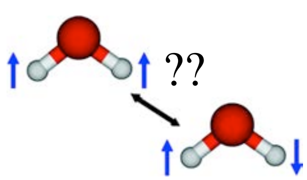
Outline



- An often underappreciated point:
  Complexity of measurements and **uncertainties** beyond stochastic noise.

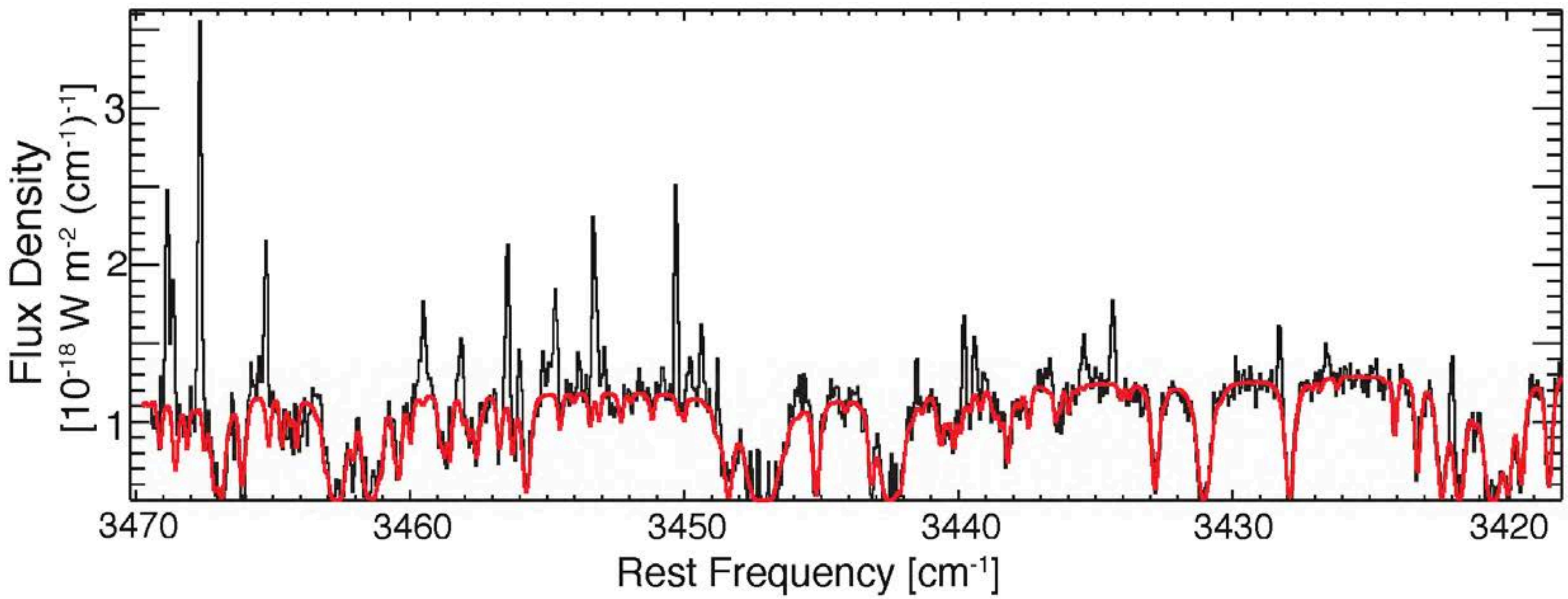
IMAGE CREDIT: Sliter et al. 2011

- **Improved methodology** for ground-based retrievals.
- The database of **H_2O OPRs**.
- Recent measurements of **H_2CO OPRs** (in progress)
- Prospects: new spectrographs to measure spin ratios.
- **Open questions and the need for continuing synergy with laboratory and theoretical work** …

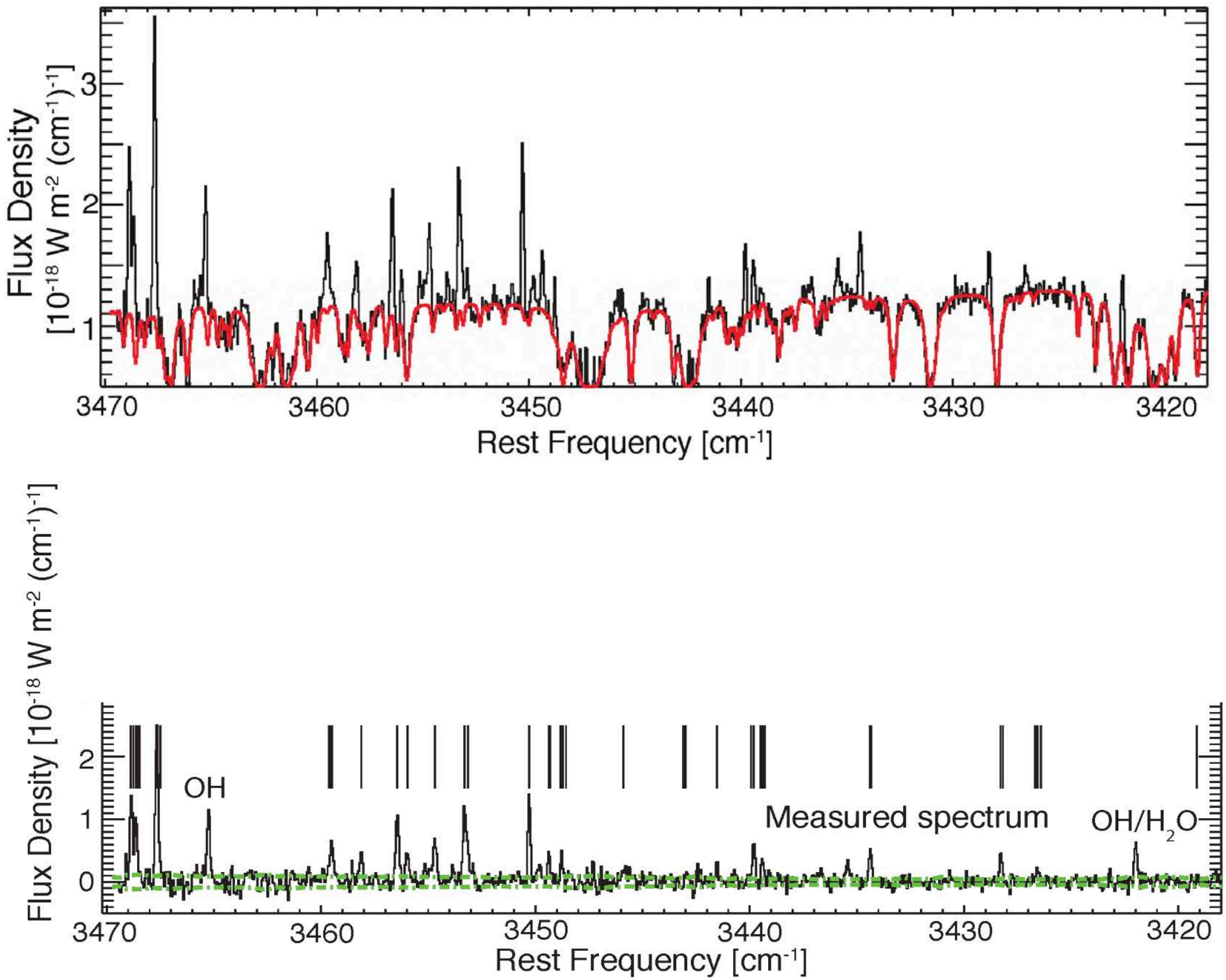


Related TALK: G. Villanueva – comparing spin temperatures of H_2O and H_2CO with those of other molecules.

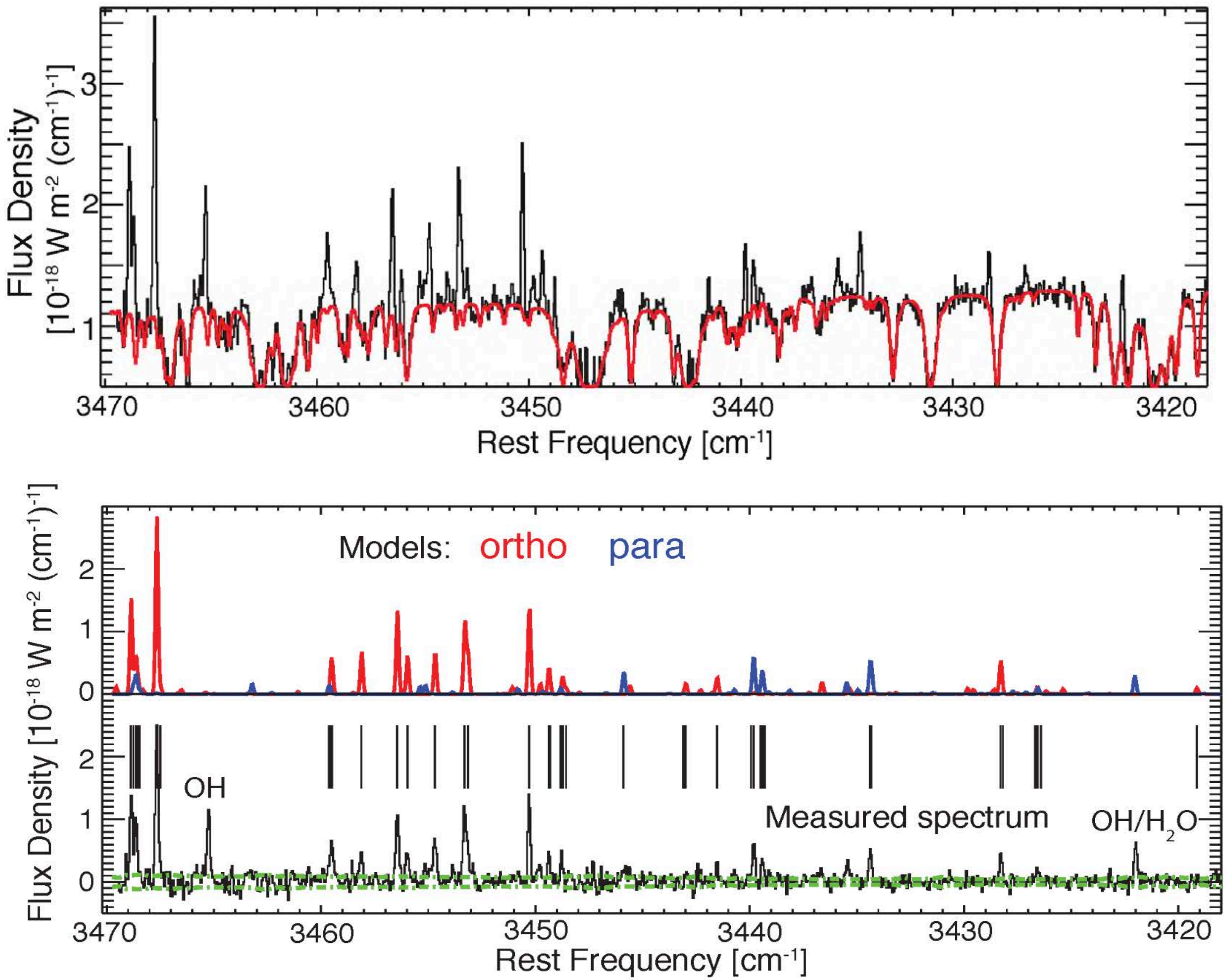
Example of OPR Retrieval (Near-IR, ground-based)



Example of OPR Retrieval (Near-IR, ground-based)



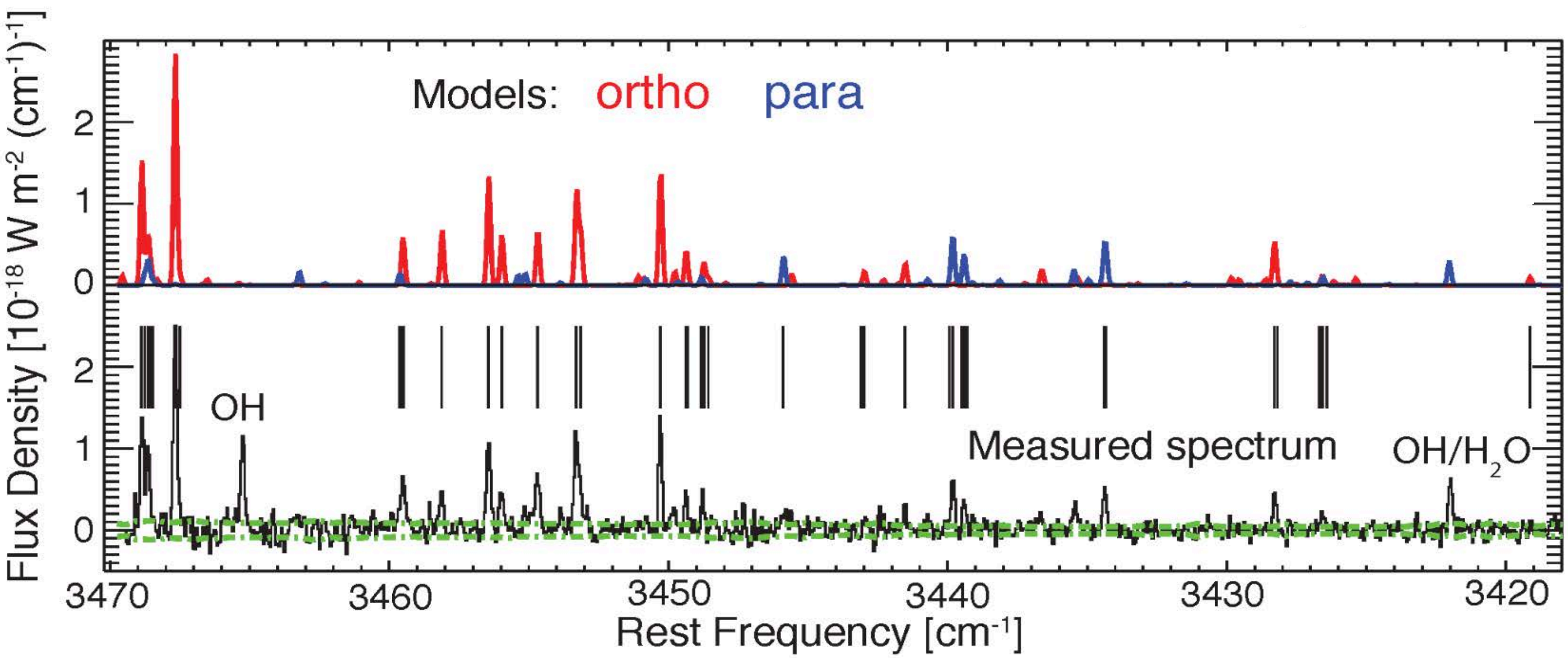
Example of OPR Retrieval (Near-IR, ground-based)



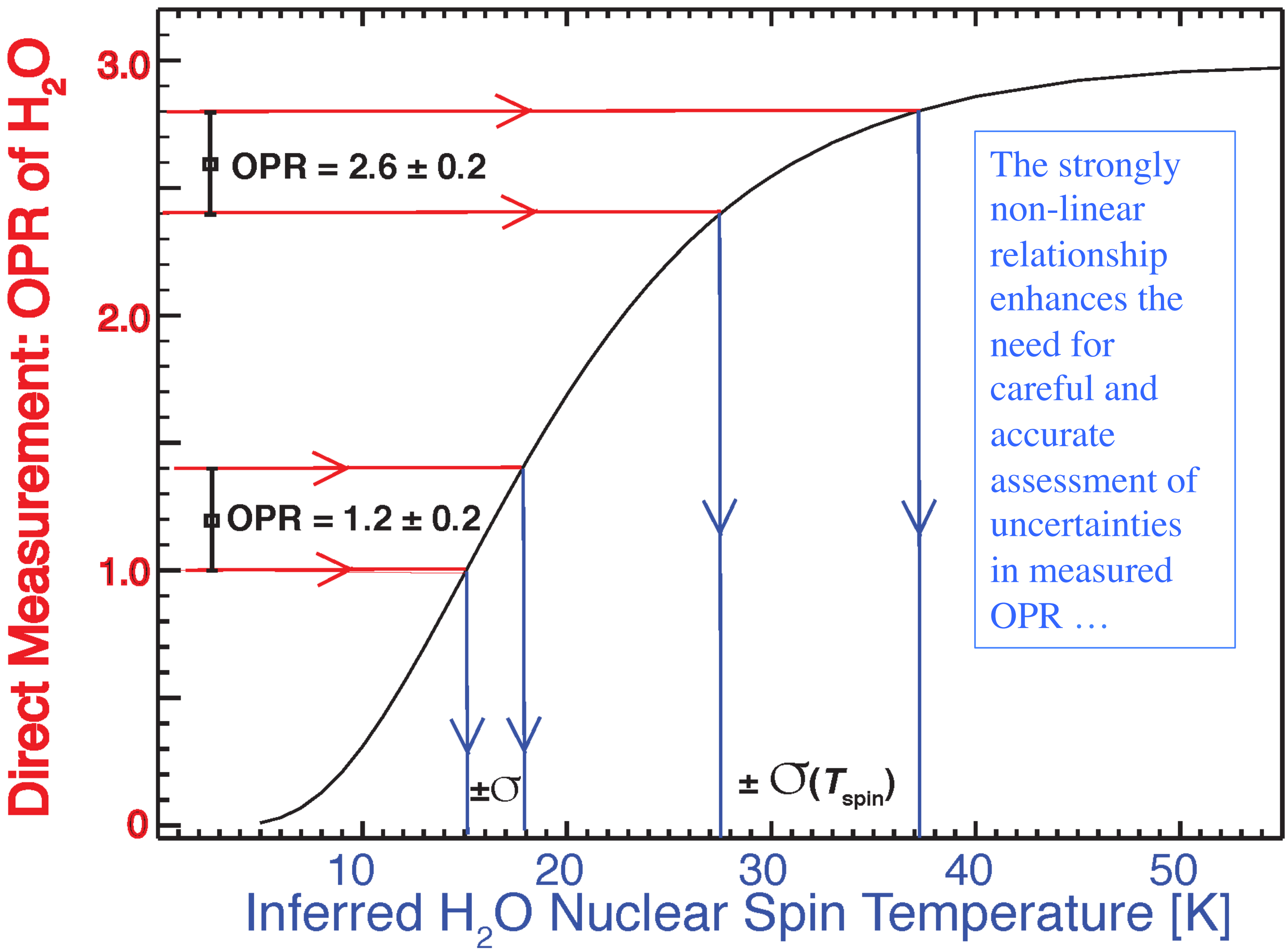
Bonev et al. 2013, Icarus

Fluorescence Models Include Separately the Effects of Gas Rotational Temperature (T_{rot}) and Spin Ratio

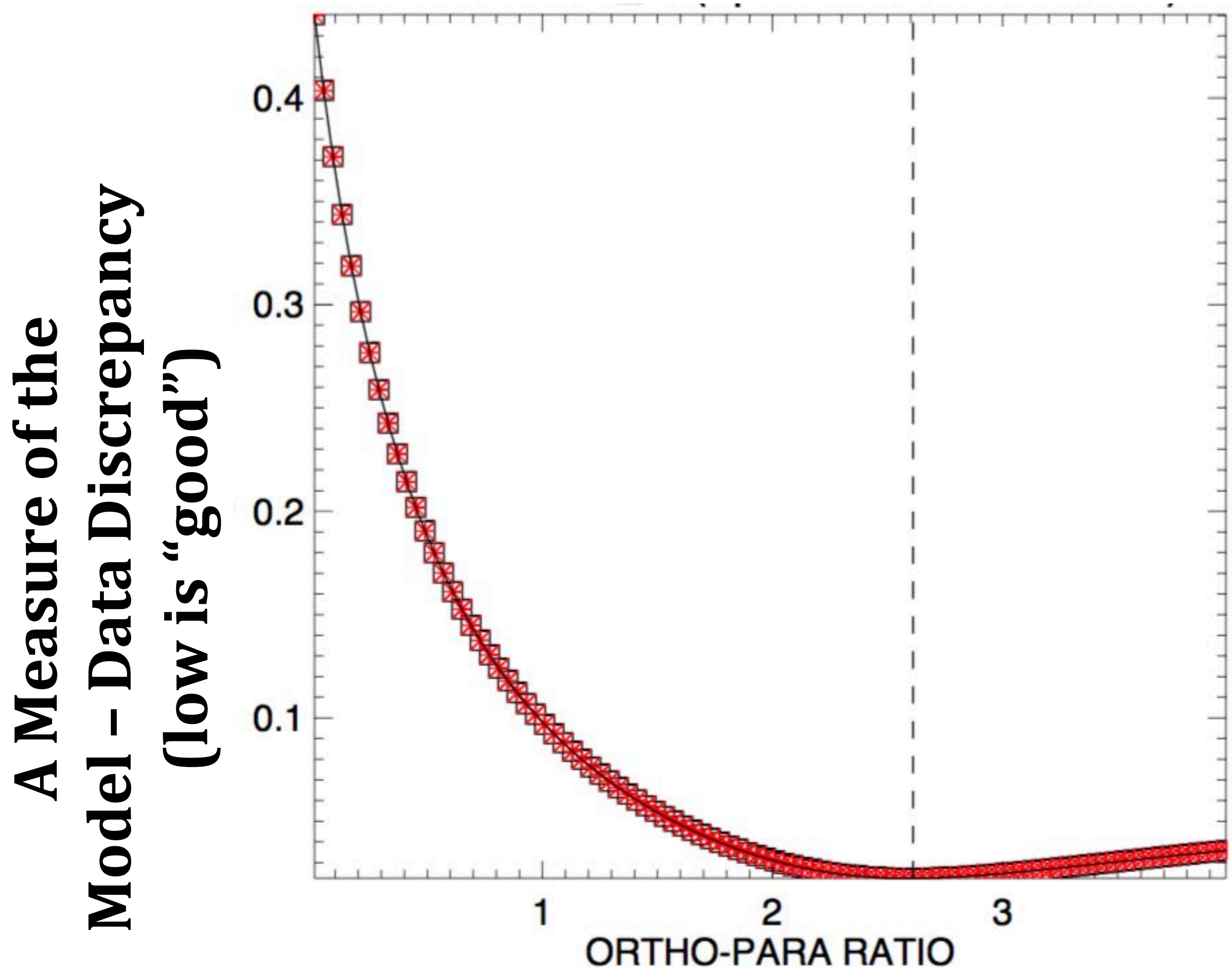
- T_{rot} – easier to retrieve
- Spin ratio – more challenging measurement

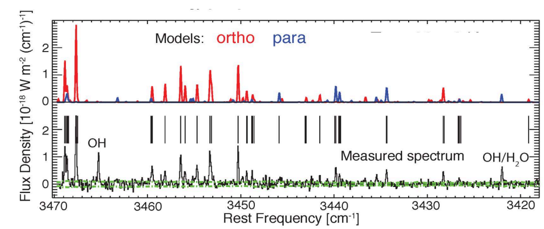


The Importance of Accurate OPR Uncertainties Near the High-T_{spin} Limit



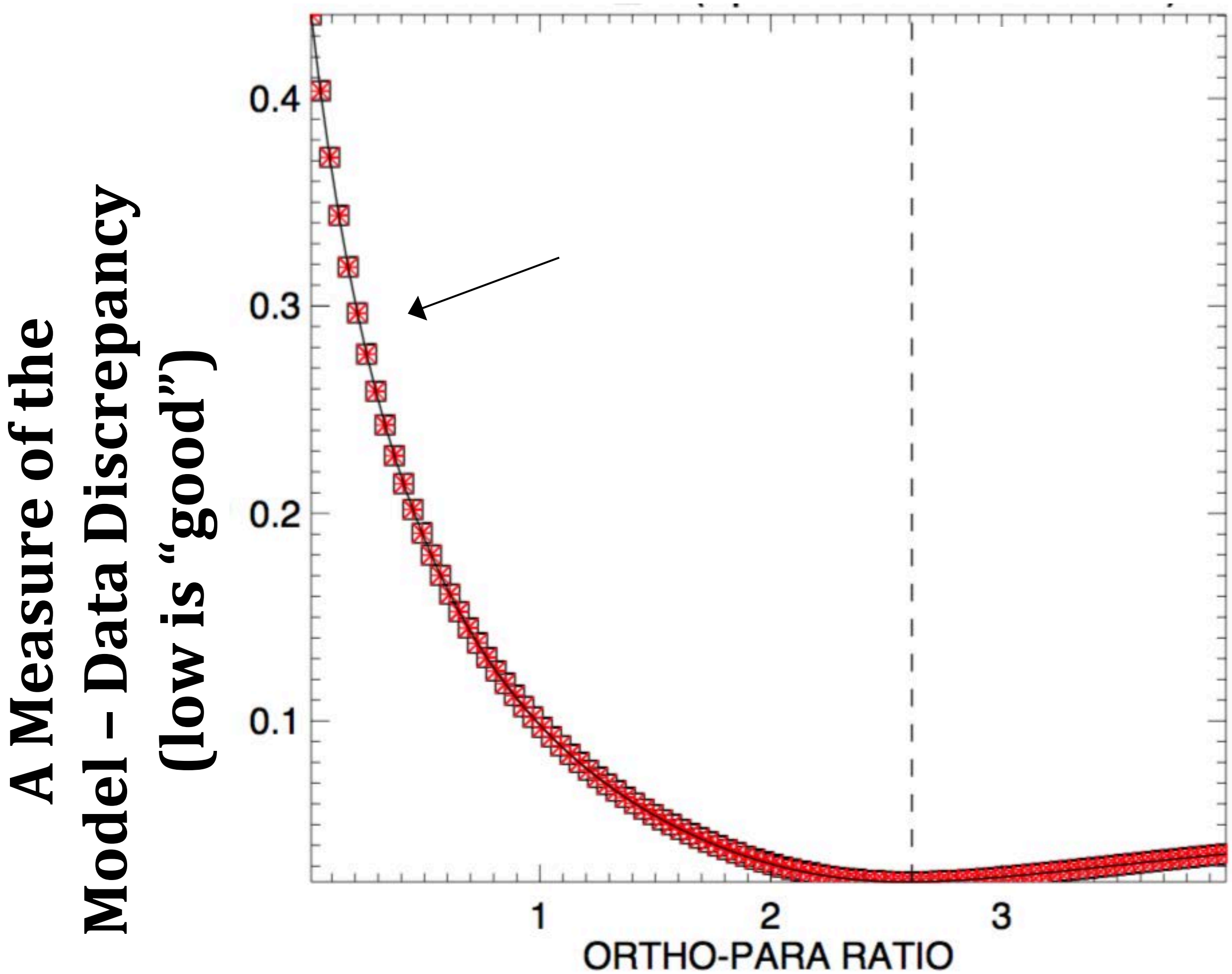
The Importance of Accurate OPR Uncertainties Near the High-T_{spin} Limit (2)

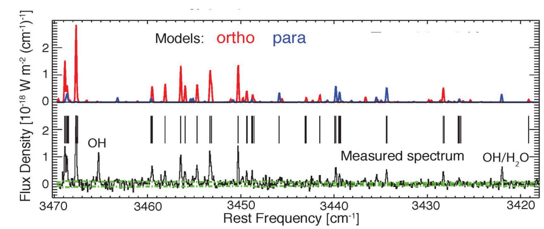




- OPR as a free parameter is not restricted to ≤ 3.0 [the statistical equilibrium value] to avoid a measurement bias - see also **G. Villanueva's talk tomorrow**.

The Importance of Accurate OPR Uncertainties Near the High-T_{spin} Limit (2)

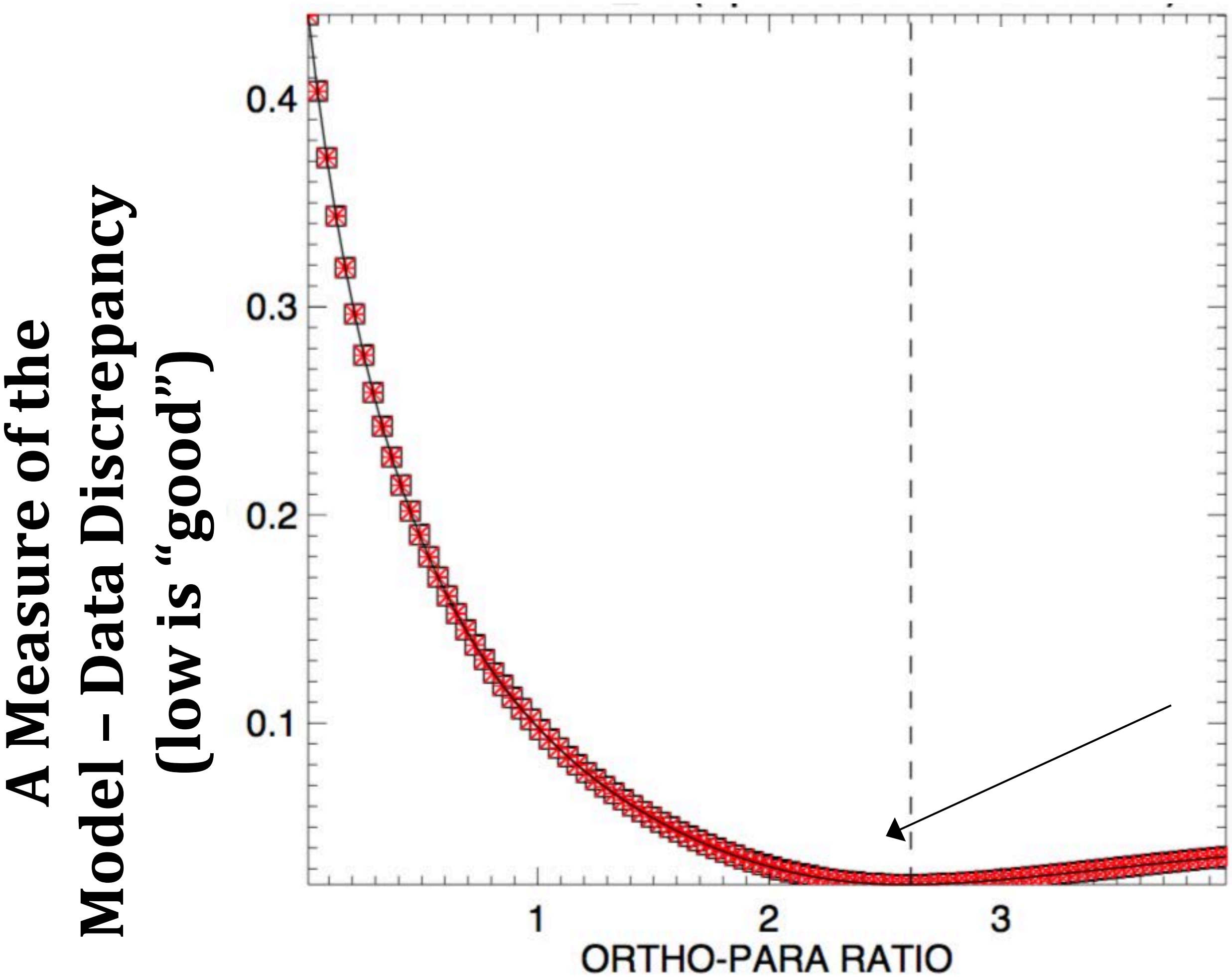


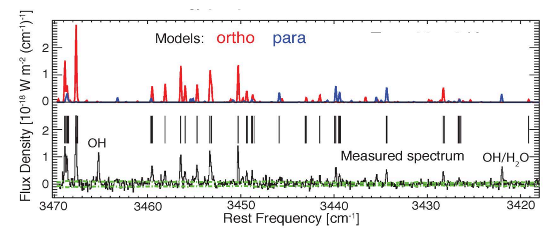


- **Modeled line intensities are very sensitive to OPR in the low T_{spin} limit …**

- OPR as a free parameter is not restricted to ≤ 3.0 [the statistical equilibrium value] to avoid a measurement bias - see also **G. Villanueva's talk tomorrow**.

The Importance of Accurate OPR Uncertainties Near the High-T_{spin} Limit (2)

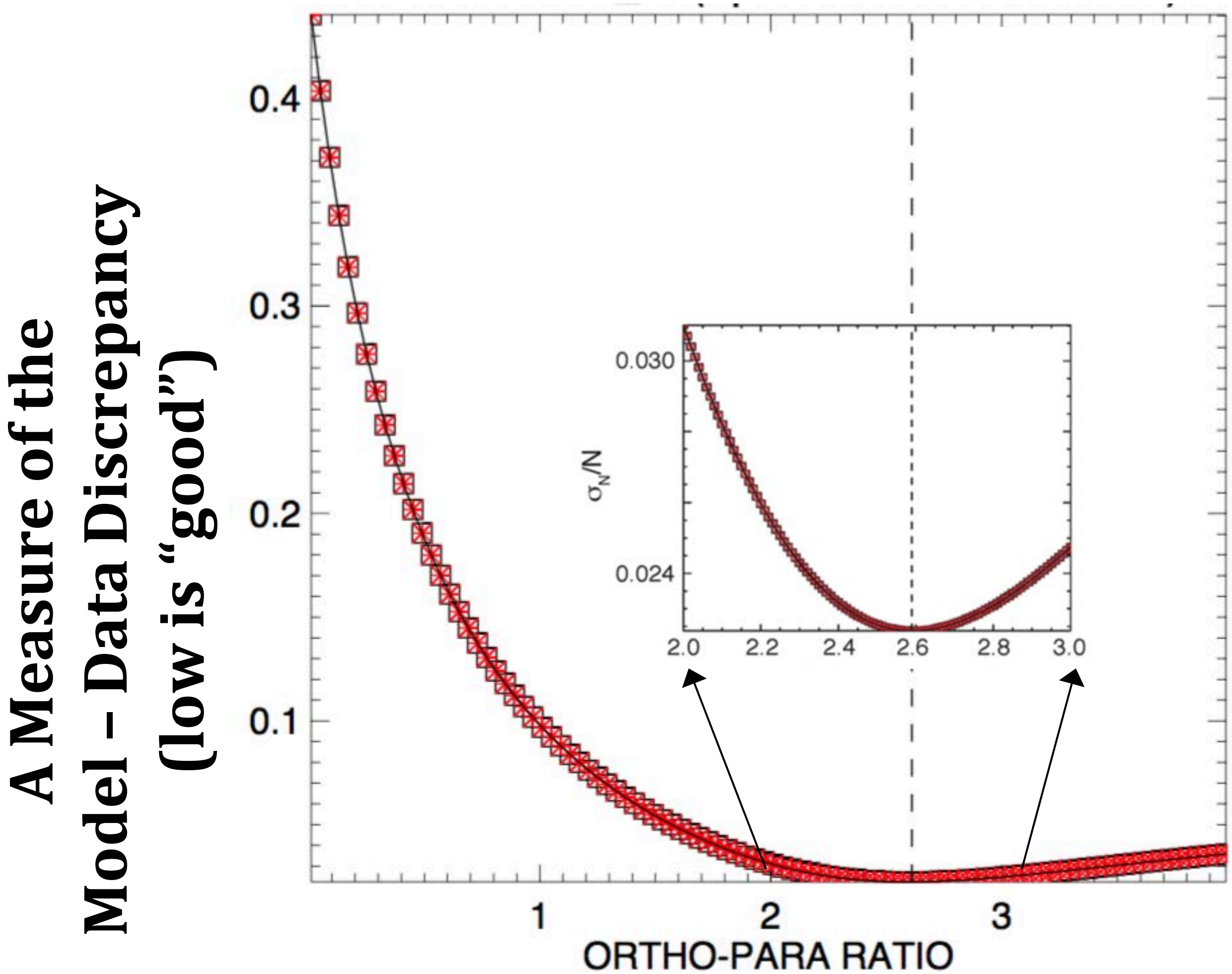


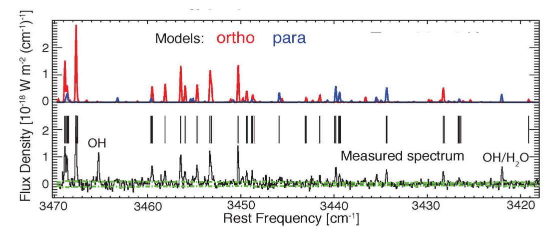


- **Modeled line intensities are very sensitive to OPR in the low T_{spin} limit …**
- **Varying the OPR parameter produces smaller changes in the quality of the model-data fit at the high T_{spin} limit.**

- OPR as a free parameter is not restricted to ≤ 3.0 [the statistical equilibrium value] to avoid a measurement bias - see also **G. Villanueva's talk tomorrow**.

The Importance of Accurate OPR Uncertainties Near the High-T_{spin} Limit (2)

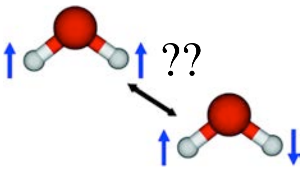




- **Modeled line intensities are very sensitive to OPR in the low T_{spin} limit …**
- **Varying the OPR parameter produces smaller changes in the quality of the model-data fit at the high T_{spin} limit.**

- OPR as a free parameter is not restricted to ≤ 3.0 [the statistical equilibrium value] to avoid a measurement bias - see also **G. Villanueva's talk tomorrow**.

Spin Ratios from Ground-Based Observations



2004 - basic methodology for H_2O completed and applied to several comets (Dello Russo et al. 2004, 2005; Bonev 2005)

GOALS:

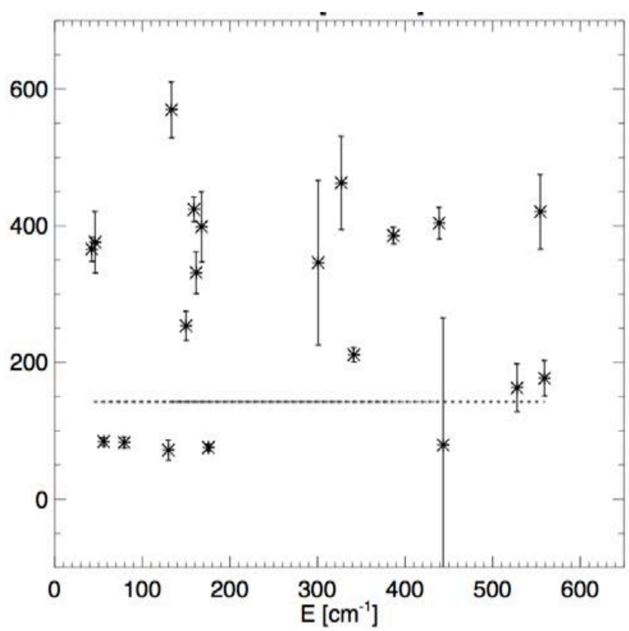
- improve not only precision, but also the accuracy of measurements;
- understand and evaluate multiple sources of uncertainty;
- build a coherent database of spin ratios

Gradual implementation of improved methodology:

(1) Emphasis of **uncertainties beyond stochastic noise** (Dello Russo et al. 2005, Bonev 2005, Bonev et al. 2007, 2008) ...

Each plot will show H_2O abundance measured independently from each individual spectral line:

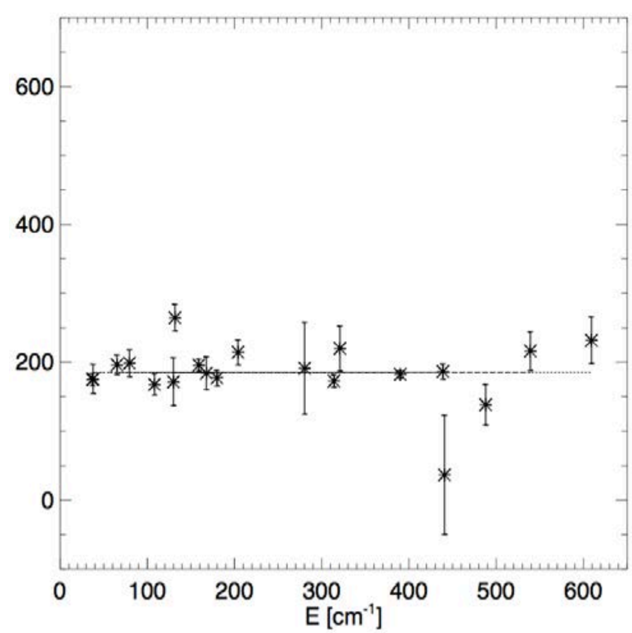
- OPR is varied as a **free parameter**, not restricted to ≤ 3.0



OPR = 0.5

σ (stoch) = 2 %

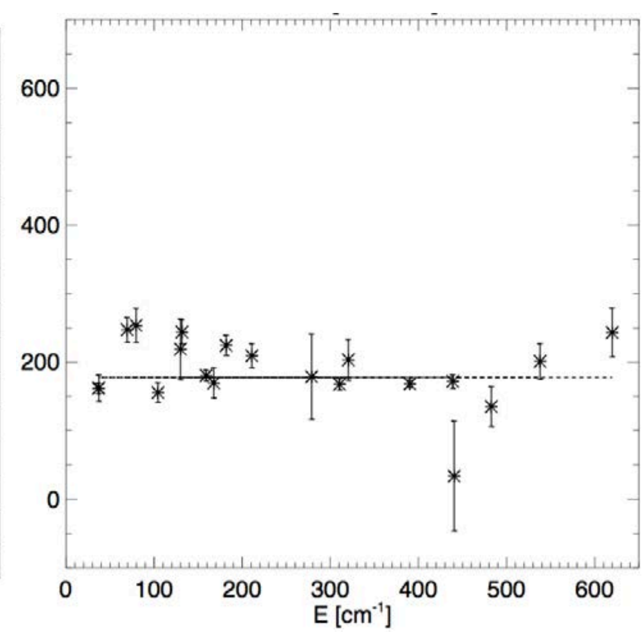
σ (line-by-line variance) =19 %



OPR = 2.6

σ (stoch) = 2 %

σ (line-by-line variance) = 2 %



OPR = 3.4

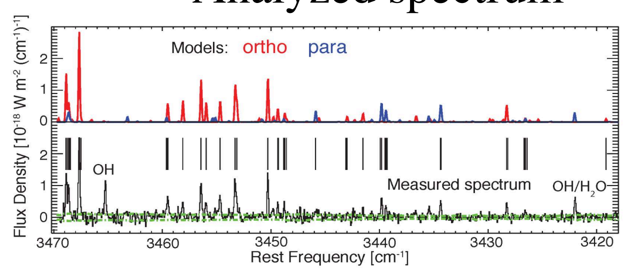
σ (stoch) = 2 %

σ (line-by-line variance) = 3 %

→ Uncertainties are in % of the mean …

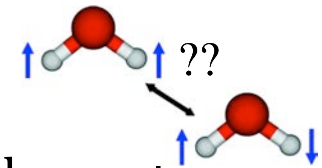
- Stochastic errors depend on SNR (which is important!) and do not change, regardless quality of the modeling.
- Line-by-line spread is important for evaluating accurate OPRs.

Analyzed spectrum



How to reduce the scatter in line-by-line measurements?

Spin Ratios from Ground-Based Observations



2004 - basic methodology for H_2O completed and applied to several comets (Mumma et al. 2003; Dello Russo et al. 2005; Bonev 2005)

GOALS:

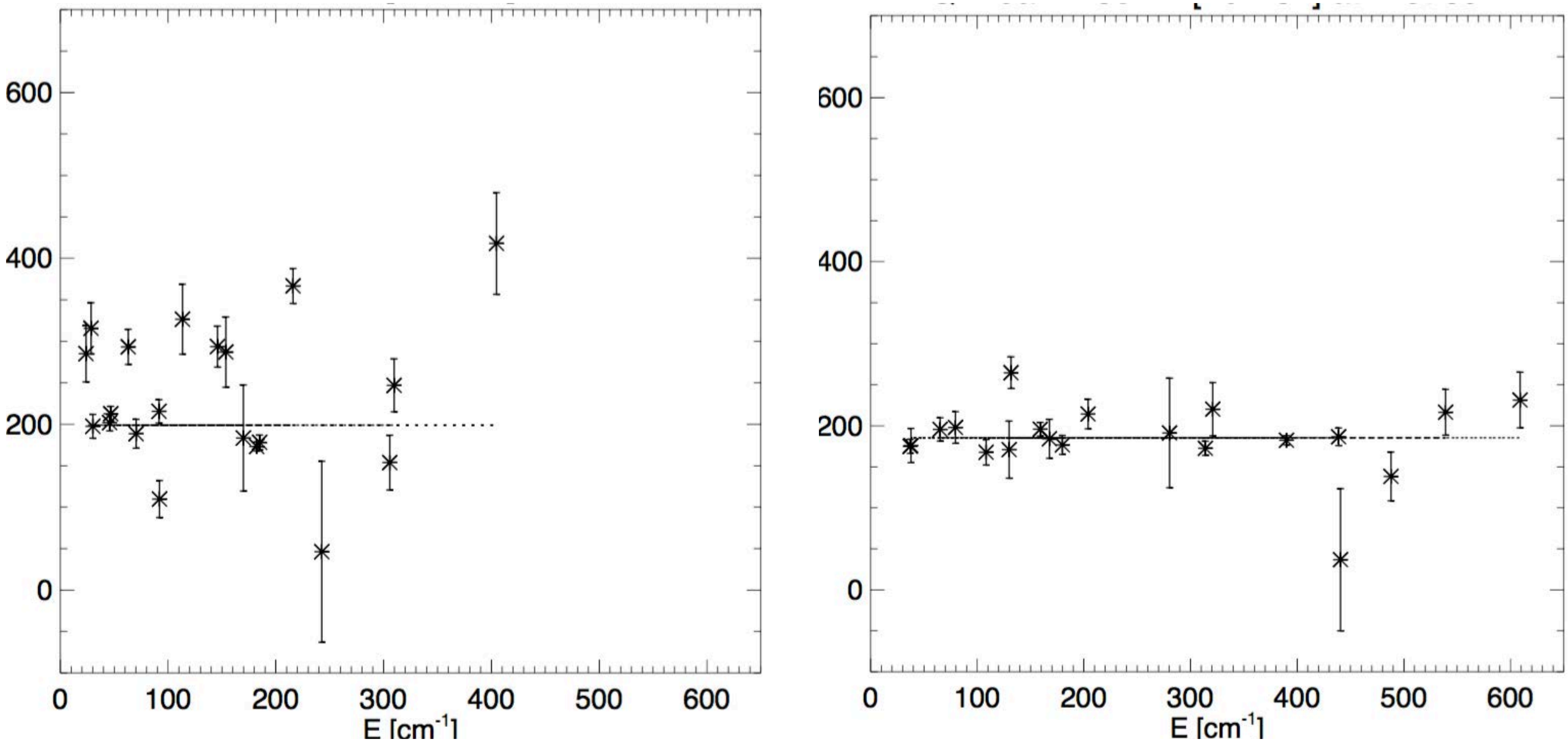
- improve not only precision, but also the accuracy of measurements;
- understand and evaluate multiple sources of uncertainty;
- build a coherent database of spin ratios

Gradual implementation of improved methodology:

(1) Emphasis of **uncertainties beyond stochastic noise** (Dello Russo et al. 2005, Bonev 2005, Bonev et al. 2007, 2008) …

(2) Advanced telluric transmittance models (Villanueva et al. 2008, 2012) and advanced **cometary fluorescence models** (Villanueva's talk) → **greatly reduced uncertainties**.

H_2O model pre-2012 ... post-2012

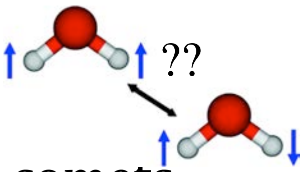


Water in planetary and cometary atmospheres: H_2O/HDO transmittance and fluorescence models

G.L. Villanueva [a,b,*], M.J. Mumma [a], B.P. Bonev [a,b], R.E. Novak [c], R.J. Barber [d], M.A. DiSanti [a]

[a] *Solar System Exploration Division, Mailstop 690.3, NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA*
[b] *Department of Physics, Catholic University of America, 20064 Washington, DC, USA*
[c] *Department of Physics, Iona College, New Rochelle, 10801 NY, USA*
[d] *Department of Physics and Astronomy, University College London, UK*

Spin Ratios from Ground-Based Observations



2004 - basic methodology for H_2O completed and applied to several comets (Mumma et al. 2003; Dello Russo et al. 2005; Bonev 2005)

GOALS:

- improve not only precision, but also the accuracy of measurements;
- understand and evaluate multiple sources of uncertainty;
- build a coherent database of spin ratios

Gradual implementation of improved methodology:

(1) Emphasis of **uncertainties beyond stochastic noise** (Dello Russo et al. 2005, Bonev 2005, Bonev et al. 2007, 2008) ...

(2) Advanced telluric transmittance models (Villanueva et al. 2008, 2012) and advanced **cometary fluorescence models** (Villanueva's talk) → **greatly reduced uncertainties**.

(3) Complimentary methods to retrieve T_{rot} and OPR using **global fits** to spectra and **line-by-line analysis** (reviewed in Bonev et al. 2014).

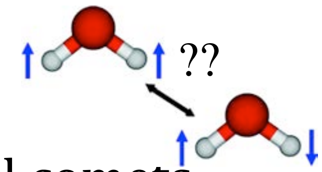
- Employing several methods to retrieve T_{rot} and OPR is not redundant:

1. Levenberg–Marquardt χ^2 minimization (Villanueva et al. 2008).
2. Spectral correlation analysis (Bonev 2005; DiSanti et al. 2006).
3. Zero slope excitation analysis (Dello Russo et al. 2004, 2005; Bonev 2005).
4. $F/g\,(T_{rot})$ variance minimization (Bonev et al. 2008, 2013); →→→ F is the flux of an individual line and $g(T_{rot})$ is its fluorescence g-factor.

- The sources of uncertainty (beyond photon noise) often propagate differently for each method.

- Thus divergent results among methods reveal that one or more systematic errors are skewing the measurement.

Spin Ratios from Ground-Based Observations



2004 - basic methodology for H_2O completed and applied to several comets (Mumma et al. 2003; Dello Russo et al. 2005; Bonev 2005)

GOALS:

- improve not only precision, but also the accuracy of measurements;
- understand and evaluate multiple sources of uncertainty;
- build a coherent database of spin ratios

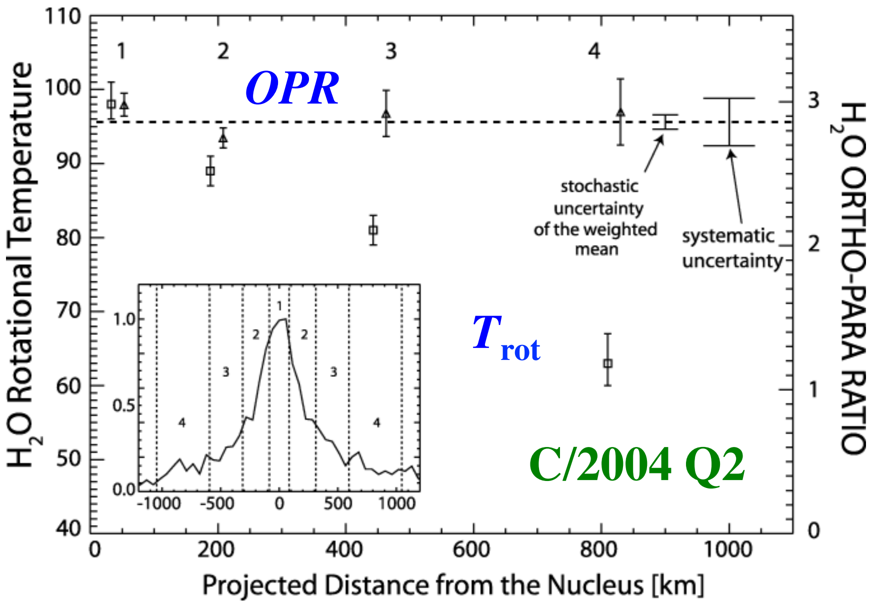
Gradual implementation of improved methodology:

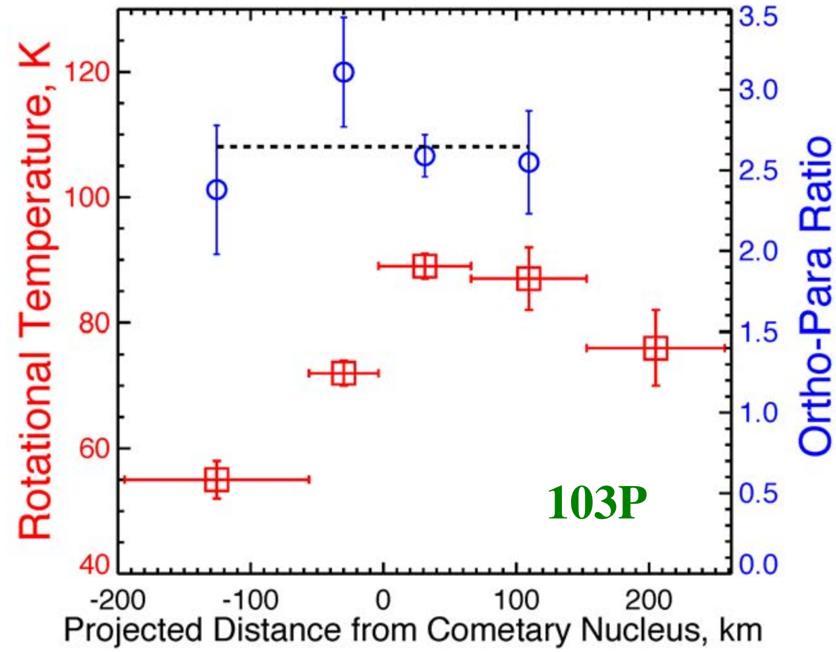
(1) Emphasis of **uncertainties beyond stochastic noise** (Dello Russo et al. 2005, Bonev 2005, Bonev et al. 2007, 2008) …

(2) Advanced telluric transmittance models (Villanueva et al. 2008, 2012) and advanced **cometary fluorescence models** (Villanueva's talk) → **greatly reduced uncertainties**.

(3) Complimentary methods to retrieve T_{rot} and OPR using **global fits** to spectra and **line-by-line analysis** (reviewed in Bonev et al. 2014).

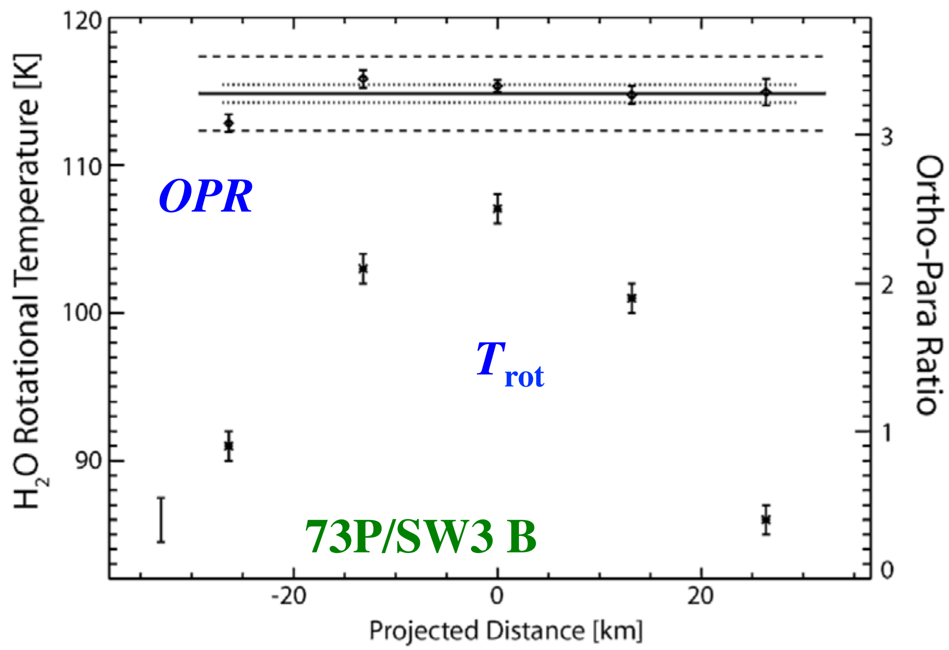
(4) **Spatially-resolved** spin ratios …





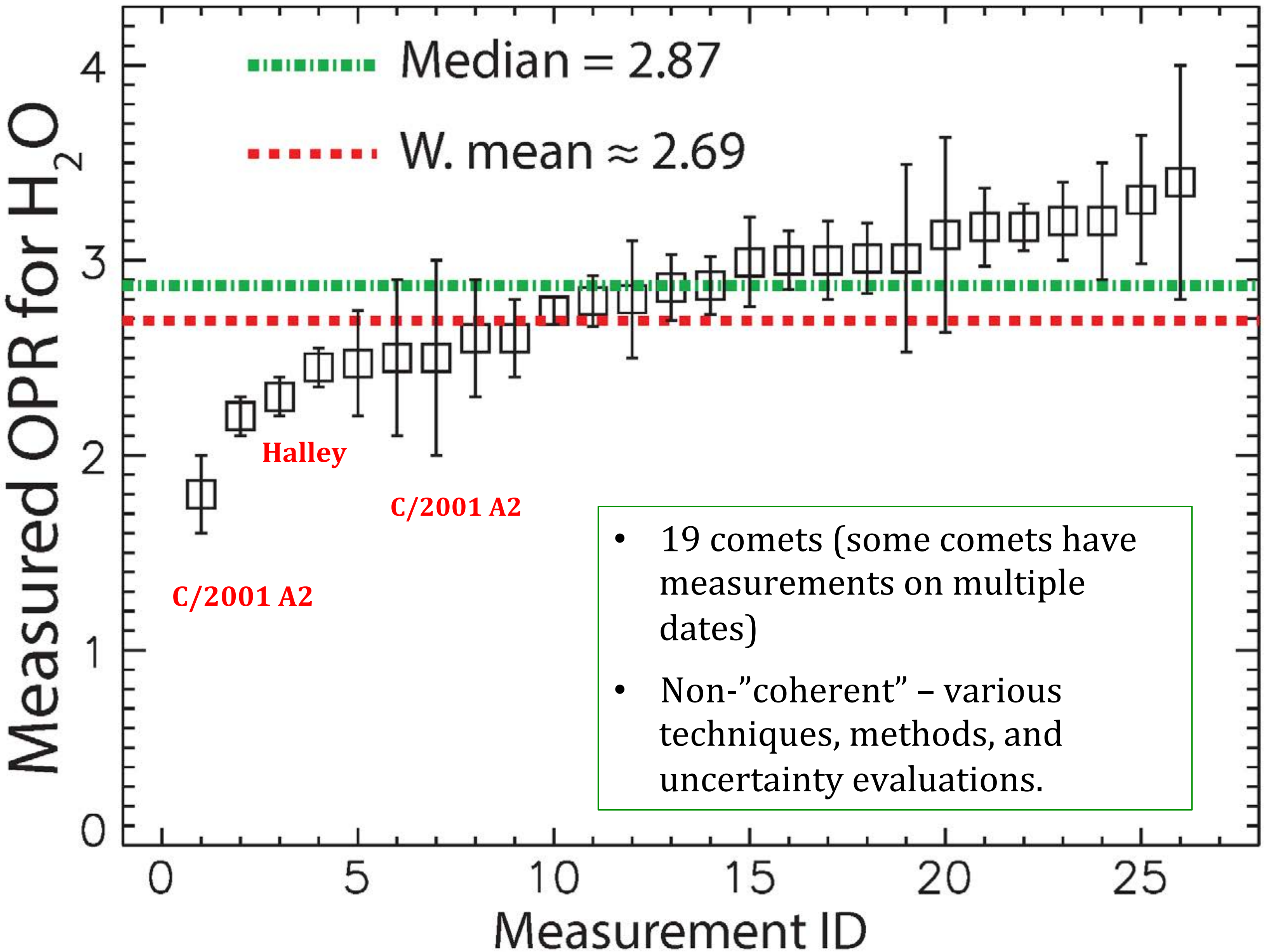
(1) Improved accuracy of retrieval – correlated line-by-line diagrams reveal systematic uncertainties …

(2) No evidence for nuclear spin conversion in the coma on the spatial scales of ~1000 km (C/2004 Q2), ~100 km (103P), and ~30 km (73P/SW3 B).



Bonev et al. 2007, 2008, 2013; see also Woodward et al. 2007

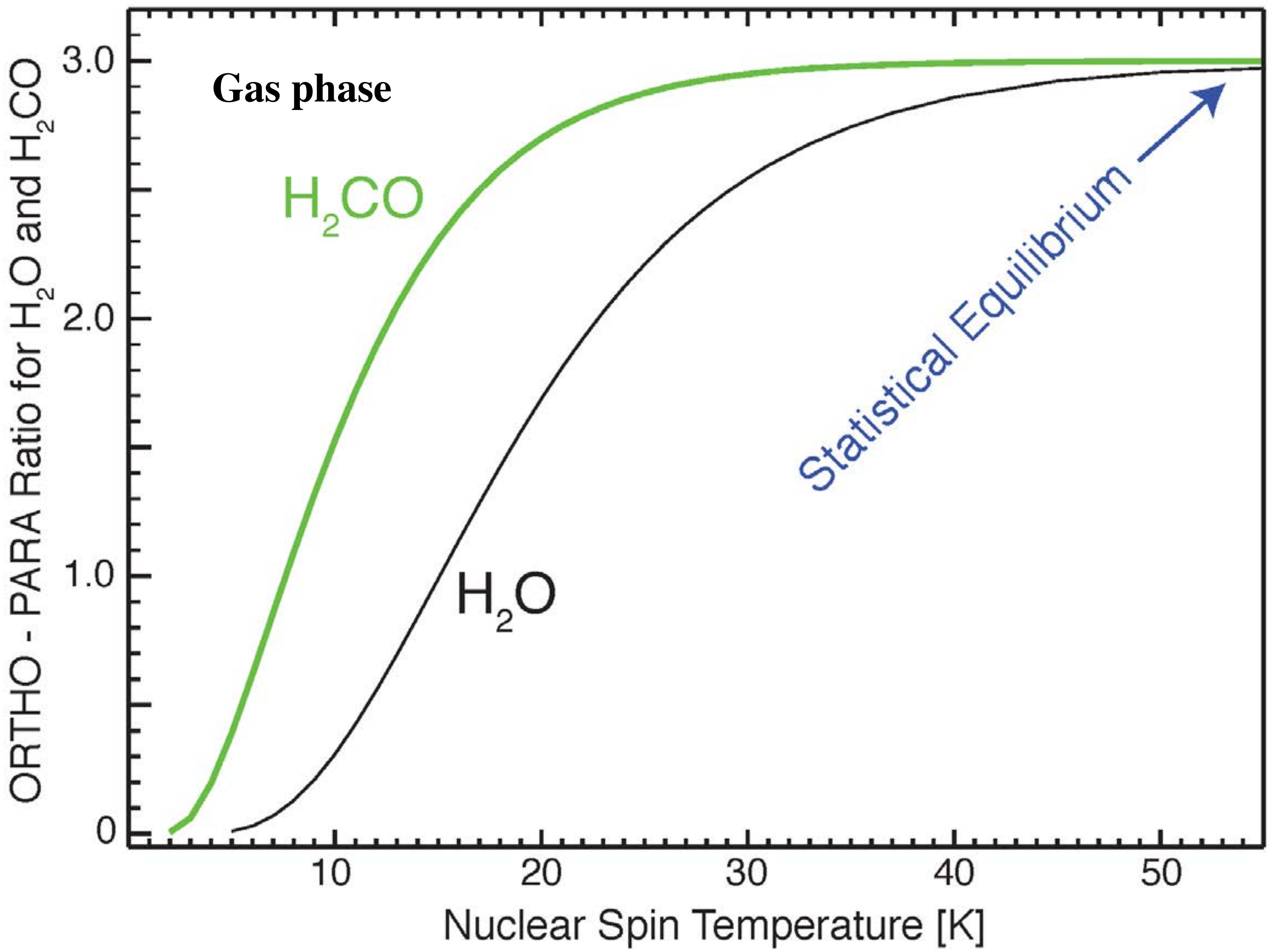
The database of H_2O Spin Ratios in Comets



- 19 comets (some comets have measurements on multiple dates)
- Non-”coherent” – various techniques, methods, and uncertainty evaluations.

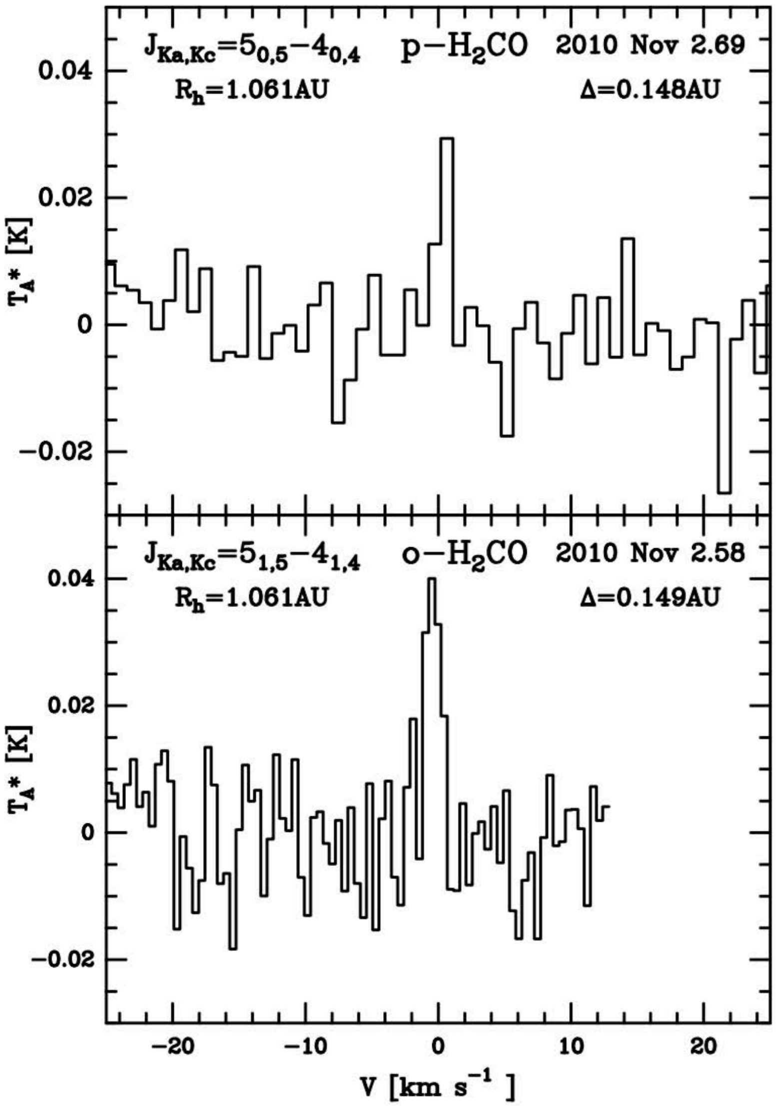
Preliminary analysis of the database

OPR of Formaldehyde



GROUND-BASED MULTIWAVELENGTH OBSERVATIONS OF COMET 103P/HARTLEY 2

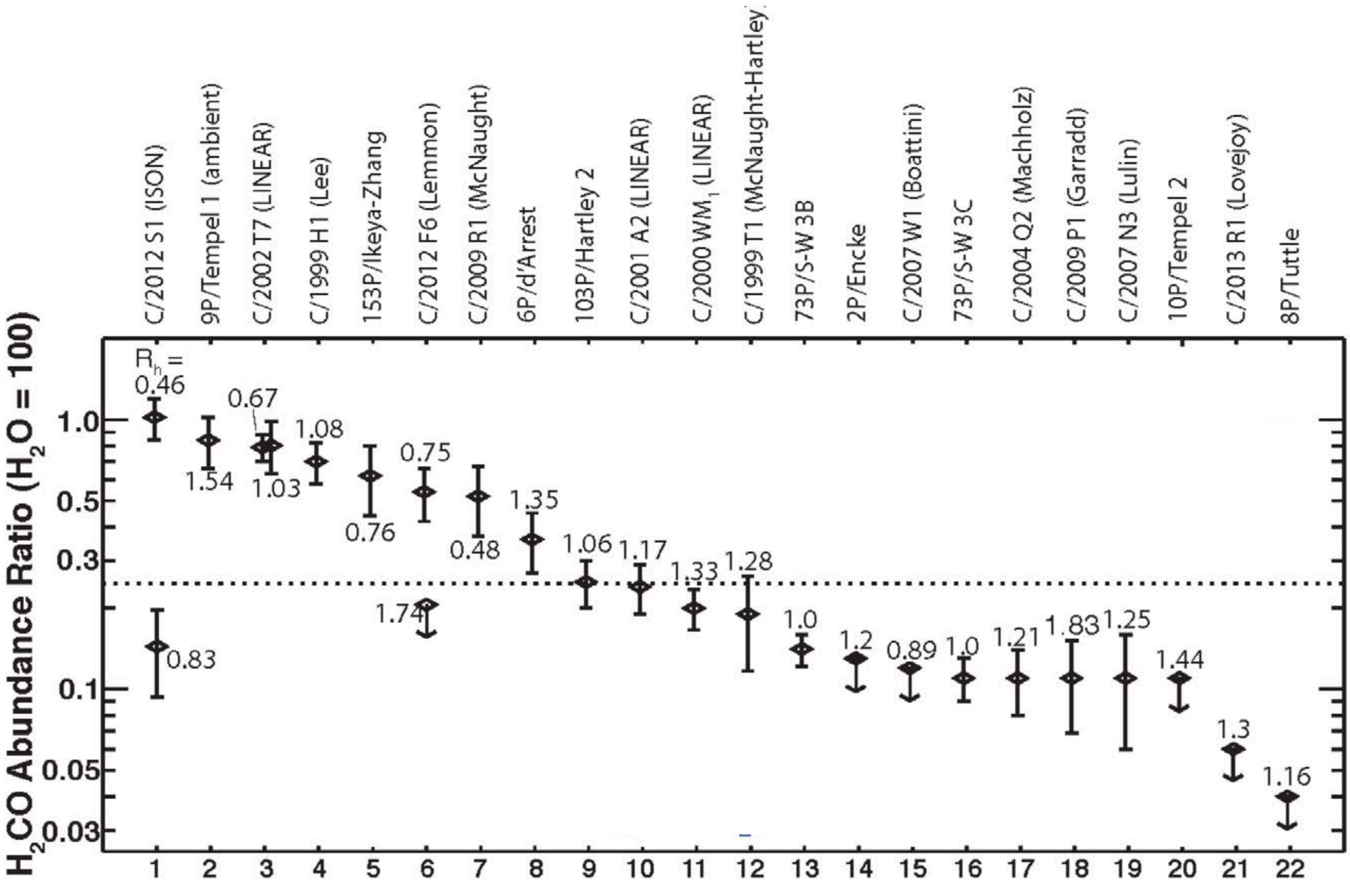
A. Gicquel[1,2], S. N. Milam[2], G. L. Villanueva[1,2], A. J. Remijan[3], I. M. Coulson[4], Y.-L. Chuang[5], S. B. Charnley[2], M. A. Cordiner[1,2], and Y.-J. Kuan[5,6]



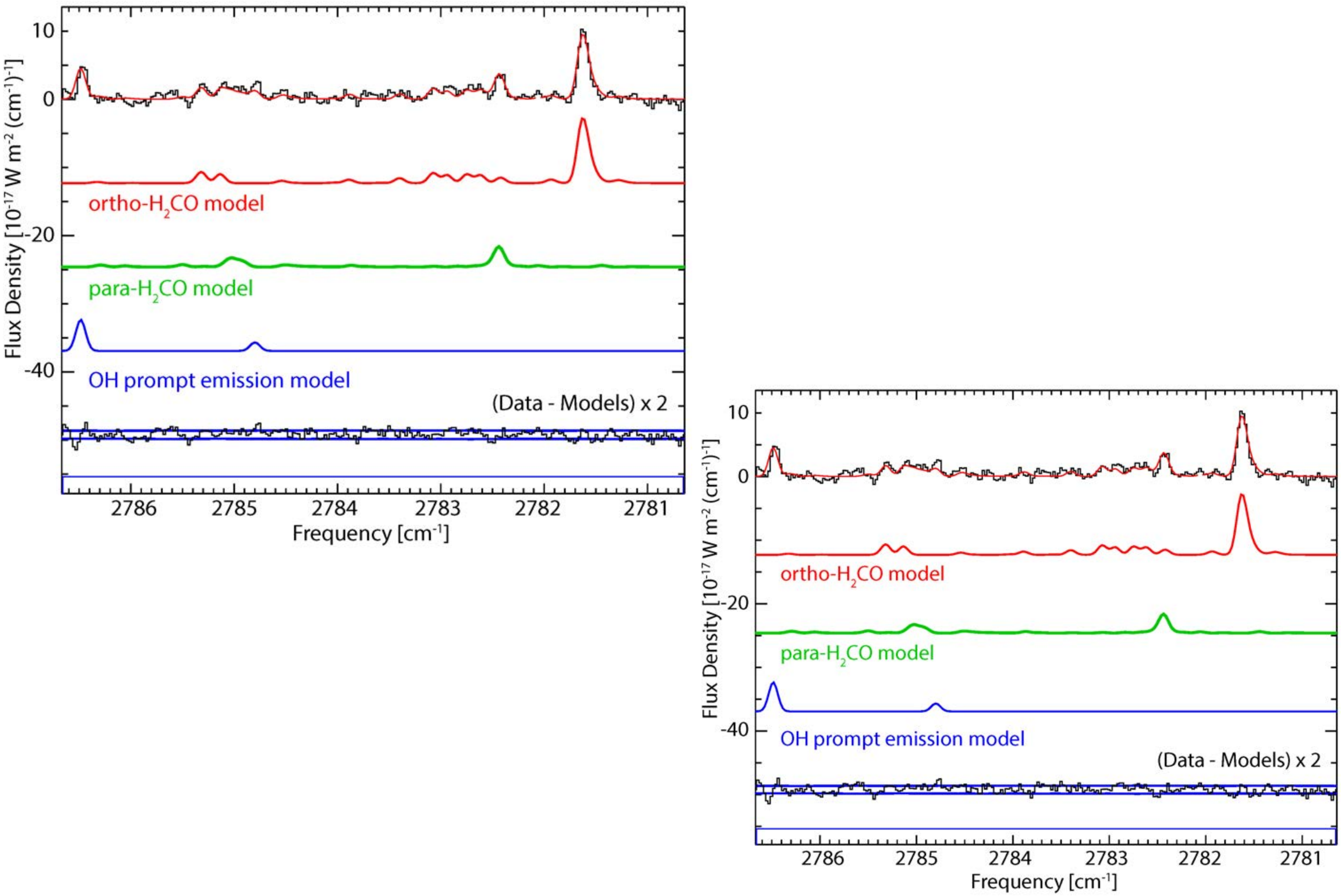
Radio Techniques (JCMT)

OPR ≈ 2.12 ± 0.59 (1σ), corresponding to T_{spin} > 8 K (2σ)

Spin Ratio of H_2CO through IR observations requires moderately bright comet AND high H_2CO / H_2O relative abundance:



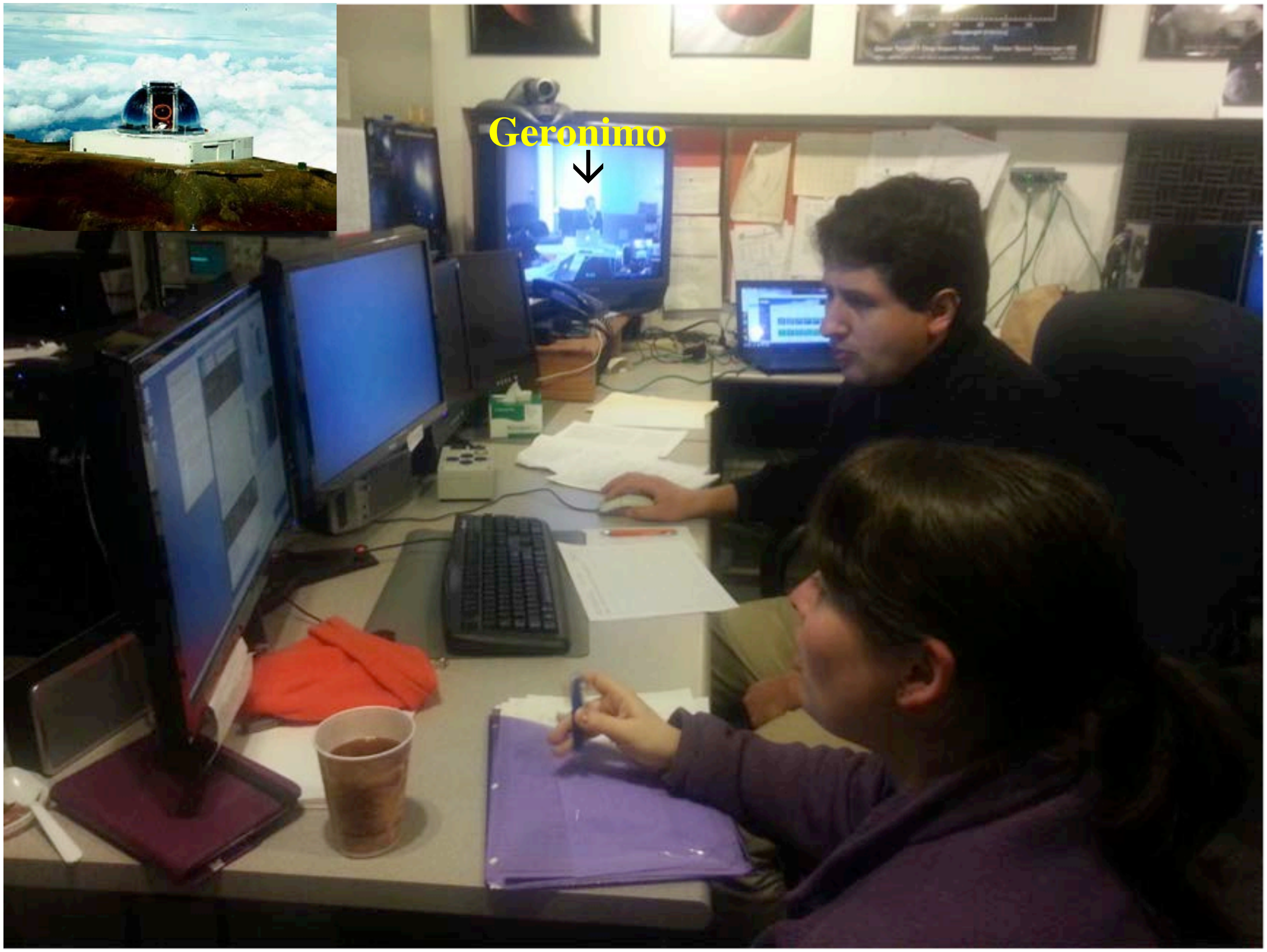
Compilation by Mike DiSanti (see also DiSanti et al. 2016, 2005).



Bonev, DiSanti, Villanueva – preliminary results

Prospects …

NASA Infrared Telescope Facility (NASA IRTF) and beyond …



The Need for Continued Theoretical and Laboratory Work in Synergy with Cometary Observations

- Can spin ratios measured in comets test predictions for nuclear spin conversion (or lack thereof) ?

J.-H. Fillion *et al.*: Experimental Study of Ortho-Para Ratios

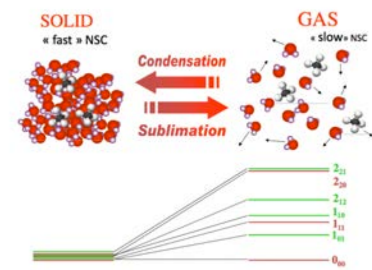


Fig. 4. Picture of gas-solid interplay and NSC dynamics.

✓ upon phase transition ?

- direct sublimation from the cometary nucleus
- **sublimation of icy-mantled grains in the cometary atmosphere (N. Fougere, PhD thesis, U. Mich)**

- **in the gas phase in cometary environments**?
  - **Gas + dust …**
  - **Implication for species (e.g. H_2CO) that might be products of more complex precurosors in the inner-most atmosphere of the comet?**

Discussion after the talk (incomplete)

We have invested a significant effort to improve the accuracy of the measurements, as detailed in this talk. With improved measurements, we can then use the comet as **a natural laboratory** to help better understand nuclear spin conversion. Experimental work presented in this workshop suggests that stat. equilibrium spin ratios (OPR $\sim$ 3.0, etc.) should be measured for molecules after sublimation from the cometary nucleus. Our goal is to test this through measuring spin ratios of multiple species (see also G. Villanueva and H. Kawakita's talks) and on as many comets as we can.

Acknowledgements

Geronimo Villanueva
Mike DiSanti
Neil Dello Russo
Erika Gibb
Mike Mumma
Hideyo Kawakita
Hermann Boehnhardt
Gerd Buntkowsky
Martin Cordiner
Hans-Heinrich Limbach
Karen Magee-Sauer
Lucas Paganini
Nathan Roth
Ron Vervack
Keara Wright

Support

AST-1616306

NNX17AC86G


SPECIAL THANKS TO THE ORGANIZING COMMITTEES FOR A VERY PRODUCTIVE WORKSHOP!
This was a very well organized meeting in a beautiful town.