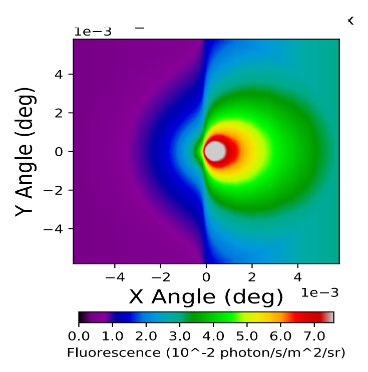
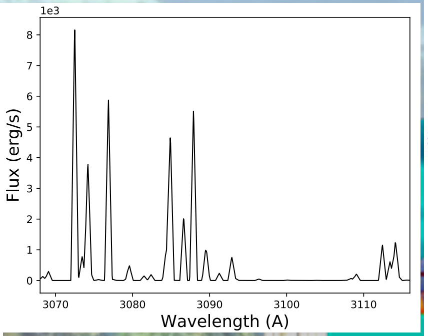
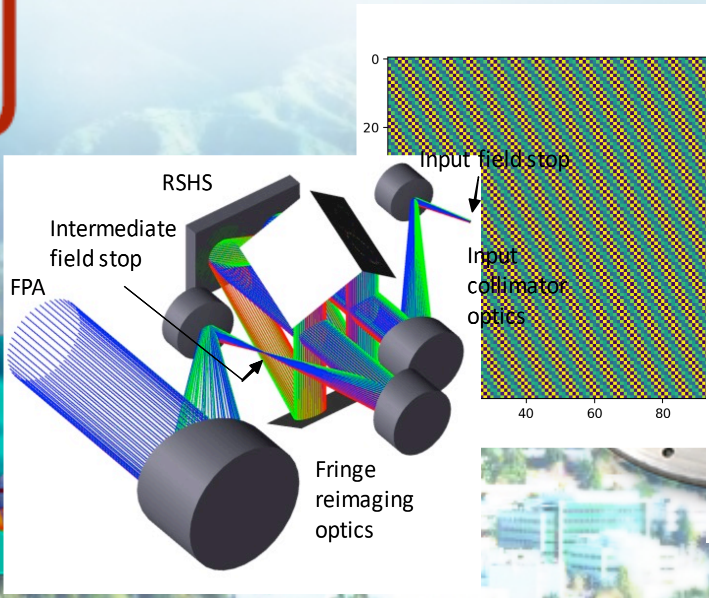
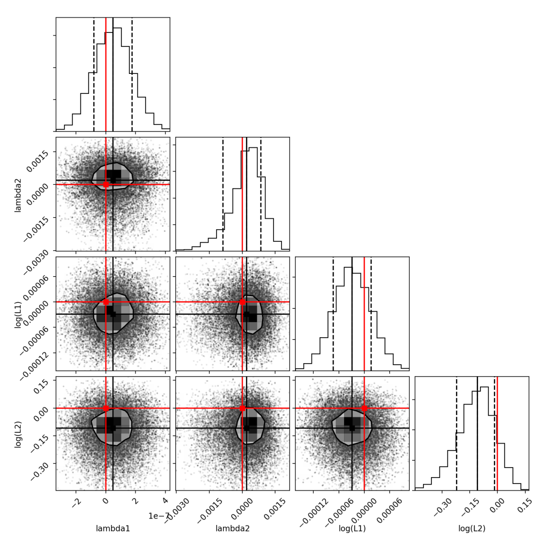
# RPC 2020









# Virtual Research Presentation Conference

## D/H in Comets: A VVUQ Approach for JPL Mission Concepts

**Principal Investigator: Robert West (3222)**
**Co-Is: Paul von Allmen (3980) Sona Hosseini (3224) Gaël Roudier (3262)**
**Program: (Topic)**

Assigned Presentation # RPC-071

**Jet Propulsion Laboratory**
California Institute of Technology

# Tutorial Introduction

## Abstract

In this work we address two issues of importance to JPL. As the title indicates, we (1) develop a VVUQ (Verification Validation Uncertainty Quantification) methodology for a Science Traceability Matrix for (2) mission concepts to measure the deuterium to hydrogen ratio in comets. This is the second year of a two-year study. In the first year we looked at a sub-mm Discovery-class concept with instrument PI Imran Mehdi. In FY 20 we studied a near-UV Discovery-class heterodyne spectrometer concept with instrument PI Sona Hosseini. The measure of D/H continues to be a high-science-value topic, as evidenced by publications in Science and Nature, as recently as the 28 August 2020 issue of Science. Because of its large fractionation effect D/H is potentially a valuable indicator of cosmochemistry in the early solar system and much work has focused on the origin of the earth's oceans. But cometary measurements are few and the statistics are poor. **Our concept missions could triple or quadruple the number of comets with measured D/H by remote measurements of cometary spectra over a 3-year period. By contrast, to achieve the same number of samples via comet flyby would require 20 or more missions.**

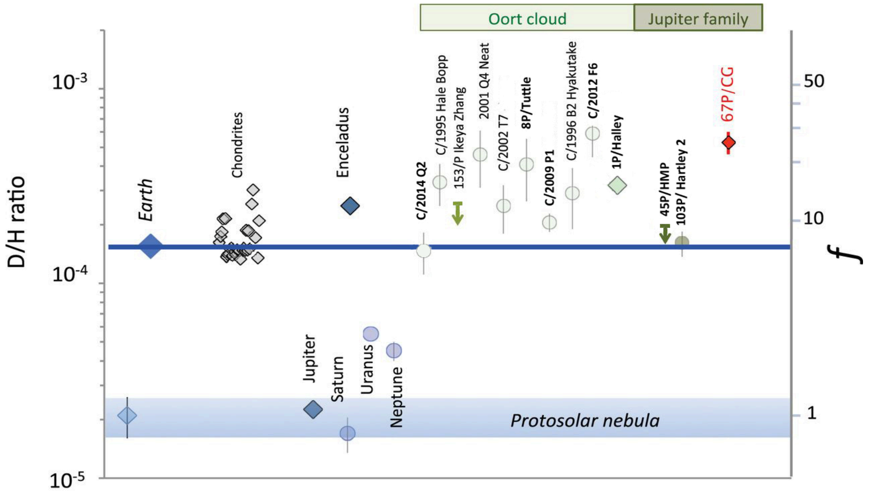


Fig. 1. Inventory of D/H for the solar system from Altwegg et al. (2015),but modified to add two results from Biver et al. (2016). The parameter f is the ratio relative to the protosolar nebula.

# Problem Description (no audio – relevant audio in previous time step)

a) Context: Because the D/H isotopic mass ratio is very much larger than other observable isotopic ratios, chemical fractionation is also very much larger than for other observable ratios. We can therefore expect to glean important insights into the processes that took place during the formation of the solar system because the D/H ratio is relatively sensitive to formation conditions, especially temperature, during the formation of the planets, meteorites, asteroids, and comets. Since the earth formed inside the snow line it is not clear how it acquired its oceans, and for a long time the leading proposal was late-formation delivery by comets. But now that we have some samples of D/H in comets (mostly higher than for the earth) we must seriously consider that the origin of earth’s water is from meteorites or the rocky material that formed the bulk earth. Unfortunately the sample size is still small (see Fig. 1) and the a cometary origin is still in play. In order to make a significant advance we seek to measure D/H in many more comets.

b) SOA: There have been a few ground-based spectroscopic measurements and a few in situ measurements of D/H in comets. The mission concepts we worked on would increase the sample size by a factor of three or four over a three-year mission duration, by remote space-based telescopic observations in the sub-mm (H2O and HDO, studied in FY 2019) or near-UV (OH and OD). OH emissions (studied in FY 2020) are among the brightest cometary emissions

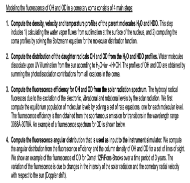
c) Relevance to NASA and JPL: The work we performed put JPL on a path for the advancement of two possible Discovery (or smaller) missions. We examined instrument capabilities and uncertainties in detail, and we applied UQ methodology to the construction of elements of potential Science Traceability Matrices for these missions. We have also identified areas that could most benefit from technology development for both sub-mm and near-UV.

# Methodology

a) Formulation, theory: Our FY 2020 study comprised the following three major areas: (1) calculation of the comet emissions and uncertainties – Paul von Allmen, (2) Instrument configuration and uncertainties, and an instrument simulator in software – Sona Hosseini and Robert West, and (3) combining these into a Bayesian formulation showing uncertainties and correlations using Monte Carlo Markov Chain (MCMC) methods – Gaël Roudier. These are detailed in subsequent slides (with audio from the lead co-investigators von Allmen, Hosseini, and Roudier) for each major task, respectively.

b) Innovation, advancement: The major advancements in the corresponding areas from above are (1) calculation of fluorescence of OH and OD lines and their dependencies on solar heliocentric velocity and distance from the sun, (2) selection of instrument/telescope parameters to calculate components of the observational signal/noise, the creation of an instrument simulator in software to accurately address the mapping of input photons to output detector, accounting for all uncertainties, and (3) the combination of uncertainties from both areas, and the simulation of the signal as input to Bayesian inference and MCMC. These will be apparent in the following slides.

# Results: Coma and Fluorescence Models



Modeling the fluorescence of OH and OD in a cometary coma consists of 4 main steps:

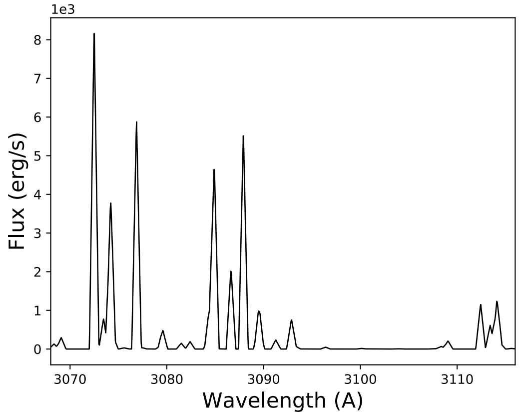
1. **Compute the density, velocity and temperature profiles of the parent molecules $H_2O$ and HDO.** This step includes 1) calculating the water vapor fluxes from sublimation at the surface of the nucleus, and 2) computing the coma profiles by solving the Boltzmann equation for the molecular distribution function.
2. **Compute the distribution of the daughter radicals OH and OD from the $H_2O$ and HDO profiles.** Water molecules dissociate upon UV illumination from the sun according to $H_2O+h\nu \rightarrow H+OH$. The profiles of OH and OD are obtained by summing the photodissociation contributions from all locations in the coma.
3. **Compute the fluorescence efficiency for OH and OD from the solar radiation spectrum.** The hydroxyl radical fluoresces due to the excitation of the electronic, vibrational and rotational levels by the solar radiation. We first compute the equilibrium population of molecular levels by solving a set of rate equations, one for each molecular level. The fluorescence efficiency is then obtained from the spontaneous emission for transitions in the wavelength range 3068Å-3078Å. An example of a fluorescence spectrum for OD is shown below.
4. **Compute the fluorescence angular distribution that is used as input to the instrument simulator.** We compute the angular distribution from the fluorescence efficiency and the column density of OH and OD for a set of lines of sight. We show an example of the fluorescence of OD for Comet 12P/Pons-Brooks over a time period of 3 years. The variation of the fluorescence is due to changes in the intensity of the solar radiation and the cometary radial velocity with respect to the sun (Doppler shift).

# Results: Coma and Fluorescence Models

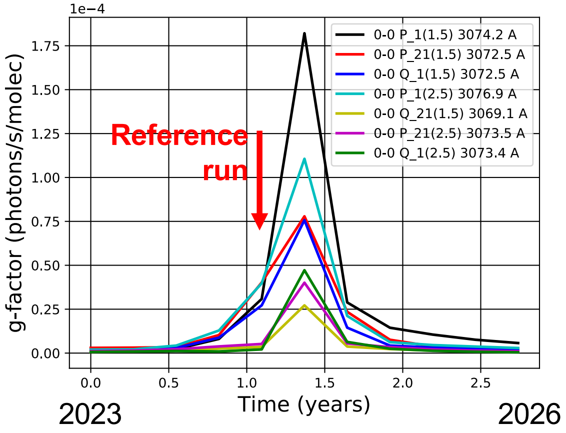
Significance and next steps

We developed a model for the fluorescence of OH and OD and studied a few of the sources of uncertainty (branching ratio for OD formation and uncertainty on the molecular transition probabilities) as a proof of concept (a first estimate of the model error is 7%). This model is ready to be used for more detailed analysis in support of a future Discovery (or smaller) missions. Next steps include a more detailed study of the model error sources that can be used for the MCMC retrievals.

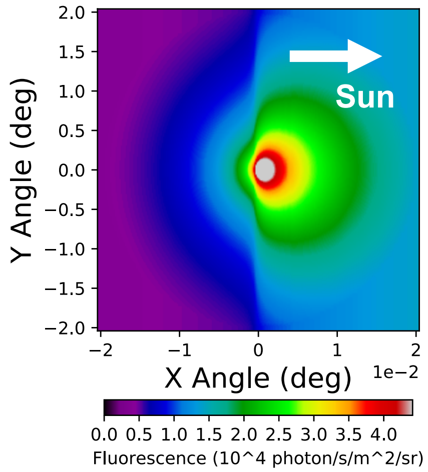
Typical OD fluorescence spectrum



Fluorescence efficiency for OD in comet 12P



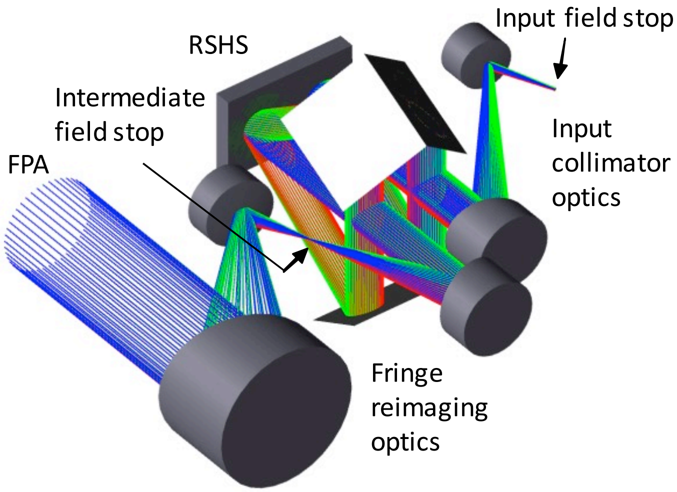
Angular distribution of OH fluorescence



# Results: Spatial Heterodyne Spectrometry (SHS) technique

We developed an instrument concept model for the telescope and the spectrometer (with the all-reflective SHS design) with a set of parameters for spectral bandwidth, spectral resolution, field of view, étendue, detector array size and instrument efficiency.

Next steps include designing the SHS instrument with optical raytracing programs to simulate the instrument parameters, the stray light and instrumental error sources to verify the instrument parameters and the system efficiency and for the MCMC retrievals.



*Assumptions:*

Telescope: 2 reflections
SHS: 6 reflections and two diffractions

Mirror reflectivity: ~%98
Grating first diffraction: ~%35
Grating second diffraction: ~%20
Sensor QE > %80

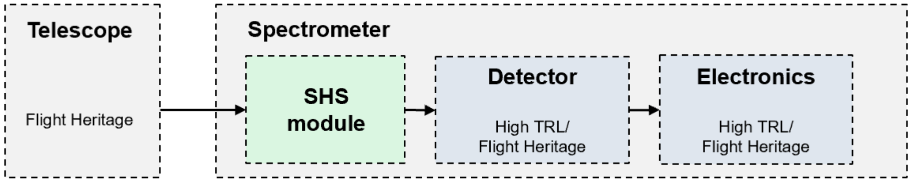
# Results: Instrument Parameters and technique

**No audio**

In choosing the instrument technique and parameters for measuring the OD/OH in a cometary coma we considered the below assumptions:

1. **Technique:** The instrument used here is based on Spatial Heterodyne Spectrometer (SHS) technique. SHS obtains high spectral resolution measurements over a narrow targeted spectra with no moving parts.

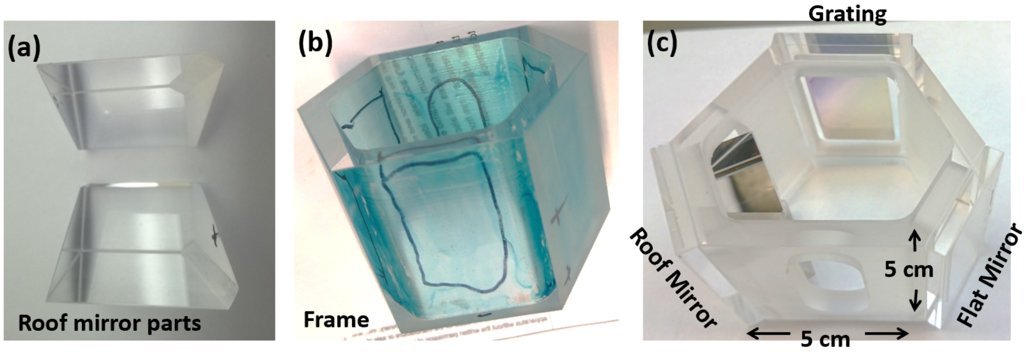
2. **System block diagram:** The spectrometer consists of three modules. Light collected by the telescope enters the SHS module. The array detector records the interference fringe.



3. **Reference mission, Discovery:** We chose to adopt a Discovery mission class concept for the comparison with sub-mm technology study that was done in the first year of this study in FY19. Our reference payload includes an SHS instrument observing the targeted 308 nm bandpass for OH and OD spectral lines. SHS instruments can be build ultra-compact but for the purpose of this study, in a Discovery mission concept, we did not look into optimizing SHS for smaller telescopes or compact formats.

4. **Telescope aperture size:** According to the JPL internal costing report (2011), the largest telescope size that would fit in a discovery cost cap is about 1.5 m. Our design uses telescope diameter 1 m, providing margin. The large telescope enables us to focus on the maximum signal shown in slide #6 which is near the comet nucleus.

# Extra material (no audio)



Here we show the picture of the breadboard hardware in our lab. The SHS module in here is ~155 grams. **(a)** The flat mirror, roof mirror and the grating are separately fabricated and coated. **(b)** The datum block's outer hexagon is machined from a solid block of Fused Silica. The inner hollow area is removed, then the port holes are removed using Ultra-Sonic CNC machining. A small chamfer is added to some of the edges to prevent chipping. **(c)** The optical elements are contact-bonded to the datum block, effectively creating one solid block of glass as shown here for our TRL 3 OH-SHS in 3073 Å.

# Uncertainty Quantification Approach

The objective of our approach is to connect instrument specifics with our science parameter, D to H ratio, through Monte Carlo simulations. Each simulation includes a recovery from simulated data which is in essence a two step process:

1. Given an instrument configuration (7 parameters see below) and an error budget → dataset
2. What is the accuracy of a D/H recovery (Markov Chains) based on previously simulated data → D/H recovery relative accuracy

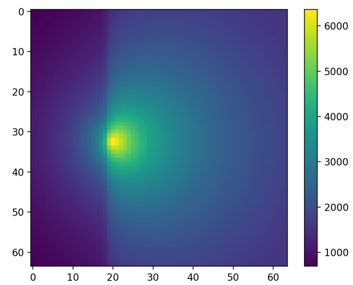
Varying one or multiple elements in (1) throughout Monte Carlo simulations informs on the propagation of design choices and associated uncertainties on our science parameter (D/H).

Such a tool would naturally supports a STM. For this example we take the case of comet 12P/Pons-Brooks

| Parameter | Value |
|---|---|
| Detector format | 256 x 256 pixels |
| Grating efficiency | 0.2 |
| Central Wavelength | 307.3195 nm |
| Tilt angle | 4.8e-4 rad |
| Size of the grating | 200 mm |
| # lines/mm | 1700 |
| Telescope diameter | 1 m |

# Simulated Data/Retrieval

Fluorescence Model
(OH emission 3072.95 A)



~ 68 arcsec

Map to focal plane

Zoom on (detector is 256*256 pixels) OD + OH fringe pattern, dominated by OH

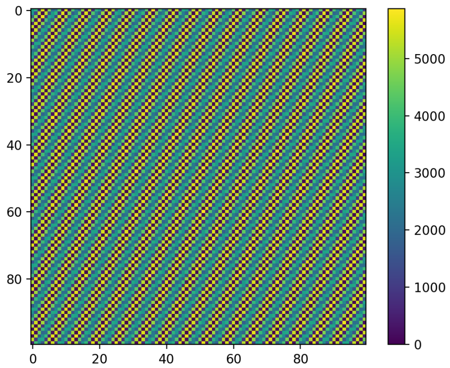
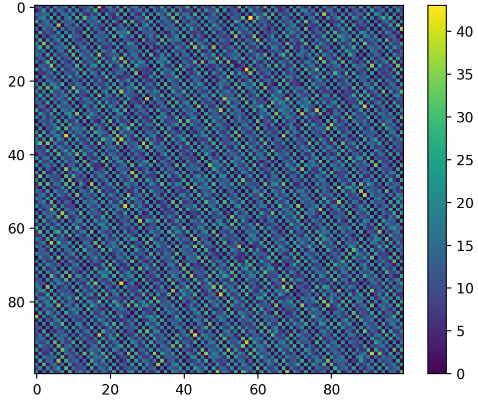


Photo e- quantization

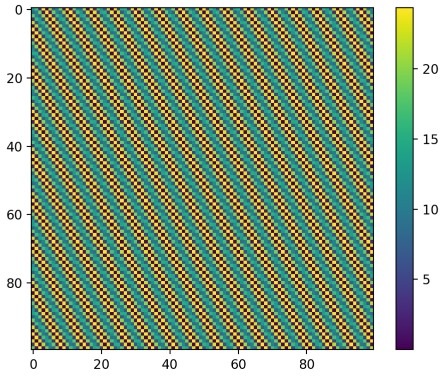
Zoom on simulated OD fringe pattern contribution, with noise



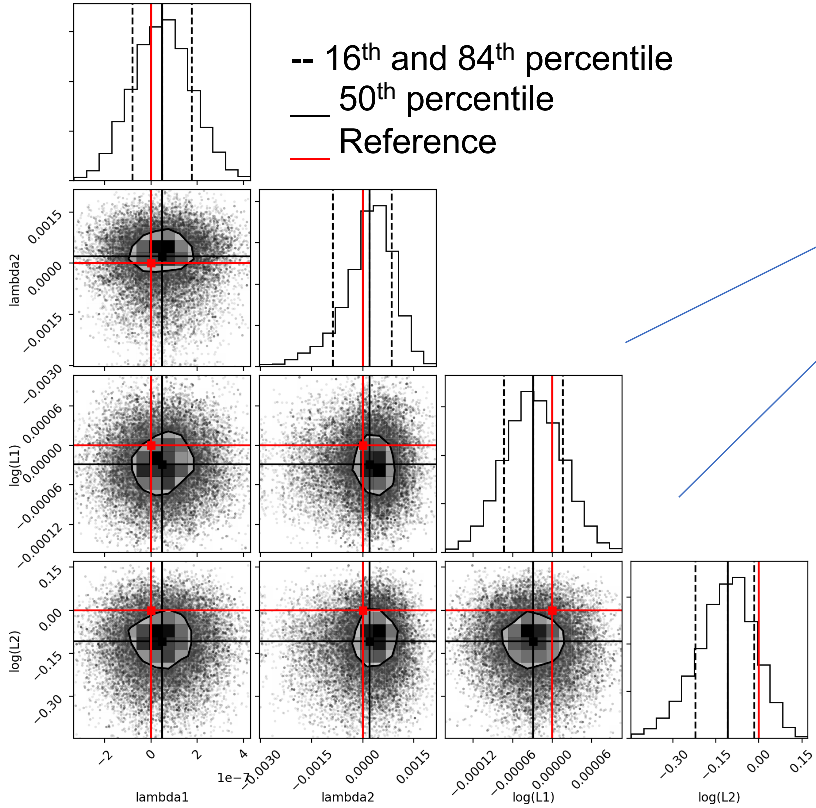
MCMC parameter recovery is done on the total (all pixels combined) fringe pattern, including quantization effects.

Pattern Matching

Zoom on OD noiseless forward model pattern used in the retrieval

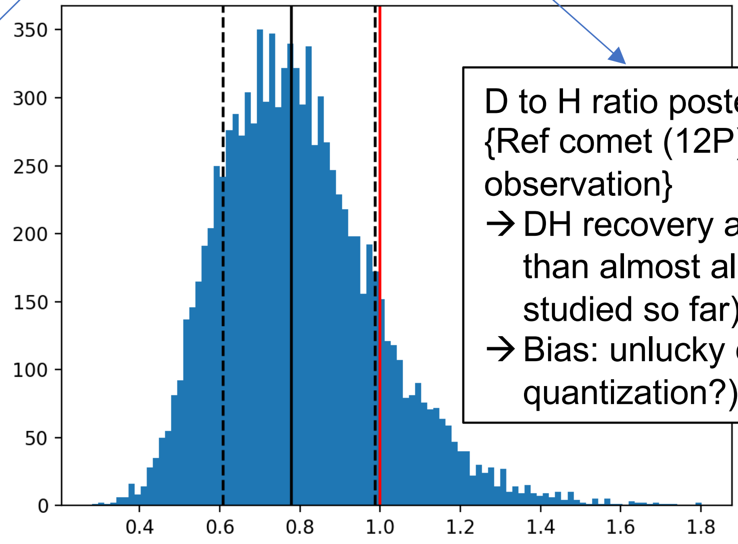


# MCMC Recovery



-- 16th and 84th percentile
__ 50th percentile
__ Reference

Sampling from posterior on the recovered line intensities and adding fluorescence model errors in quadrature (7%)



D to H ratio posterior distribution {Ref comet (12P), Ref design, 10 days observation}

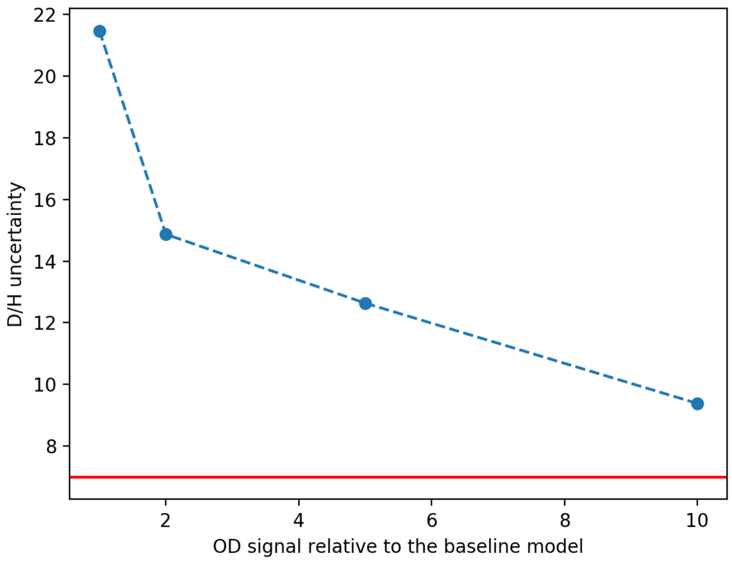
→ DH recovery accuracy ~20% (better than almost all comet samples studied so far)

→ Bias: unlucky case (photon quantization?)

# Perspectives (no audio)

D/H recovery performances in [%] as a function of OD signal. The plot shows how uncertainty drops for higher D fluorescence, either because D/H is higher, or if a comet is closer to the sun or more active than our example 12P/Pons-Brooks. Alternatively, if integrations times longer than 10 days are feasible we can reduce uncertainty that way.

- Target (ref.: 12P/Pons-Brooks)
- Design (see table slide 10)
- Observation period (ref 10 days)



Potential future application:
Isolate the effect of grating photon efficiency (0.2) and mirror size (1m) and report similarly the D/H uncertainty changes.

Fluorescence model lower limit (7%)

# References

K. Altwegg, et al., 67P/Churyumov-Gerasimenko, a Jupiter family comet with a high D/H ratio. Science (2015). doi:10.1126/science.1261952

N. Biver, et al., Isotopic ratios of H, C, N, O, and S in comets C/2012 F6 (Lemmon) and C/2014 Q2 (Lovejoy). Astronomy & Astrophysics 589, article A78 (2016).

S. Hosseini, Characterization of cyclical spatial heterodyne spectrometers for astrophysical and planetary studies. Appl. Opt. 58, https://doi.org/10.1364/AO.58.002311 (2019).