A submm-wave comet explorer for water isotopic composition measurements

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ABSTRACT

Remote submm-wave spectrometers have the capability of providing statistically significant numbers of isotopic composition measurements within the budget constraints of available planetary missions. This talk will present a mission and instrument concept that would enable an accurate measurement of the D/H ratio on not one but several dozens of comets in a four-year mission lifetime. The instrument would utilize advanced cryogenic detectors that would allow us to measure the abundance of the para and ortho spin states of water and its isotopologues. State of the art superconducting heterodyne receivers have been developed that provide detection sensitivities approaching the quantum limit in the 500 GHz frequency range enabling the measurement of D/H ratio on around 50 comets from an observatory stationed for example at the thermally benign Lagrange point L2.

Keywords: water isotopic ratio, D/H ratio, comet water isotopic ratio, SIS technology, heterodyne receivers, superconductive detectors

1. INTRODUCTION

It is widely accepted that fossil record of our initial solar nebula is captured in small bodies, with the isotopic composition of water being the most sensitive to 1) the thermal history of the forming solar system (through D/H ratio) and 2) the origin and composition of volatile reservoirs (through O isotopes). NASA's Planetary Decadal Survey concluded that isotopic composition measurements of comets are an important means to unravel the mysteries involving the origin of Earth's water and the evolution of our solar system [1]. Figure 1 shows the D/H ratio of various planetary bodies, including recent results for Comet 67P [2,3]. A factor of 3 variation exists in the very limited data set available to date for comets. Figure 2 shows the oxygen three-isotope plot, including the measurement for Comet 67P obtained with the ROSINA instrument on Rosetta [4], and how it relates to the fractionation lines for other solar system bodies. While measurements of D/H ratios in comets have provided some clues to the potential origins of Earth's water, due to limited samples and unknown redistribution of small bodies during solar system formation, it is currently impossible to draw definitive conclusions from the limited set of data.

The potential of submm-wave heterodyne remote sensing instruments has recently been highlighted by significant science data return from Astrophysics-centric instruments such as *Herschel's* Heterodyne Instrument for the Far-Infrared (HIFI) & the German Receiver for Astronomy at Terahertz Frequencies (GREAT) on the Stratospheric Observatory for Far-Infrared Astronomy (SOFIA), as well as planetary instruments such as the Microwave Instrument for the Rosetta Orbiter (MIRO). One of the common themes of these instruments is their ability to measure molecular abundances and production rates of a large body of different molecules (e.g. carbon monoxide, ammonia, water). A MIRO-like instrument, with room temperature detectors, lacks the sensitivity for making isotopologue ratio measurements for distant comets, while SOFIA-GREAT will not have sufficient observation time to make the long integrations necessary to detect faint lines from a varied sample of comets of different types.

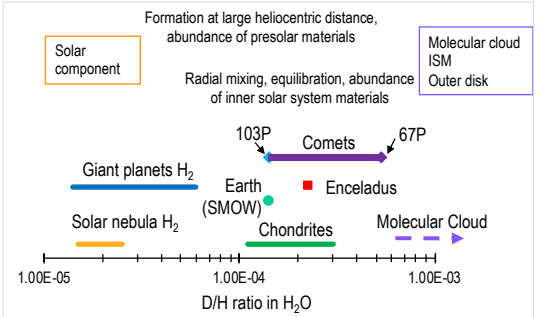

Figure 1: Measured D:H ratios indicate a large range for comets with only a handful of data points.

With this in mind, a possible mission, ORigins And Composition of comets Lagrange Explorer (ORACLE) is being investigated that would for the first time measure the isotopic composition of water and additional major comet volatiles on a statistically significant number of comets. Remote submm-wave spectrometers have the capability of providing statistically significant numbers of isotopic measurements within the budget constraints of available

planetary missions. This talk will present a mission and instrument concept that would enable a more accurate measurement of the D/H ratio on not one but several dozens of comets in a four-year mission lifetime. The instrument would utilize advanced cryogenic detectors that would allow us to measure the abundance of the para and ortho spin states of water and its isotopologues.

ORACLE would consist of three bands covering, 500-560, 890-990, and 1100-1280 GHz respectively. These bands would enable measurement of both ortho as well as para $H_2{}^{16}O$ lines along with isotopologues $H_2{}^{17}O$ and $H_2{}^{18}O$, and the singly deuterated species. The cryogenic receiver system would utilize advanced SIS devices for all three bands providing close to quantum-limit detection capability. The sensitivity would be enhanced by simultaneous observations of line combinations and dual polarization operation. The mission concept would also be effective in addressing important astrophysical questions such as the enhancement of water in shocks produced by young stars, the collapse of dense cores to form a protostar & protoplanetary disk (through measurements of the H_2O line profile), thus linking this program to the important and timely topics of star formation and exoplanets.

2. DETERMINATION OF NUMBER OF TARGET COMETS

Our goal is to determine how many target comets could be measured given realistic trade space of a submillimeter-wave observatory for the optimal detection of H_2O and HDO in comets. The observation period was fixed to 4 years for this study based on nominal cryogen usage of a comet observing mission. We made progress toward that goal by computing the variation with telescope diameter of the signal to noise ratio (SNR) for the measurement of the 110-101 water emission line for a fixed noise temperature, bandwidth, and integration time. The general approach is to use scaling laws for the water production rate together with reference measurements of the molecular line strengths to compute the maximum signal for all known comets over the duration of the four-year observation campaign.

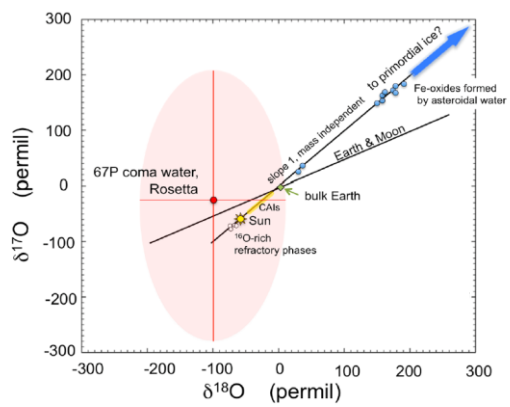

Figure 2: Oxygen three-isotope plot with Rosetta measurement for comet 67P.

We first retrieved the physical parameters needed for this study, such as the orbital parameters and visual magnitude coefficients, for the 3,366 comets in the JPL Horizons database (ssd.jpl.nasa.gov). We then excluded from this set all the comets with a heliocentric distance at periapsis larger than 3 AU or an orbital period larger than 200 years because we don't expect these comets to be detectable in the timeframe of our prospective mission concept. Figure 3 shows a histogram of the perihelion heliocentric distance for the remaining 558 comets. The large peak at around 0.9 AU corresponds to the fragments of 73P/Schwassmann-Wachmann.

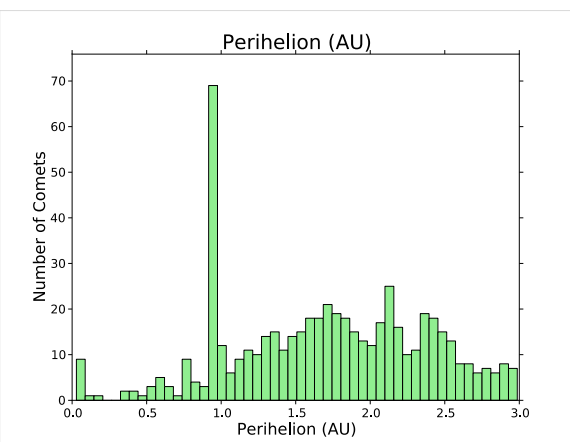

Figure 3: Heliocentric distance at perihelion for 558 comets retrieved from the JPL Horizons database.

The next step is to compute the water production rate for the 558 comets over the duration of the mission. The Horizons database provides for each comet the parameters M_1 and K_1 that can be used in the following expression to compute the apparent magnitude when the heliocentric distance is r_h and the range to the observer δ:

$$M = M_1 + 5\log_{10}(\delta) + K_1 \log_{10}(r_h)$$

The units of r_h and δ are AU. We then assume that the logarithm of the water production rate varies linearly with the apparent magnitude, following the work of Jorda 2008 [5]:

$$\log_{10}(Q_{H_2O}) = a + bM(\delta = 1)$$

The two linear coefficients are given by a=30.675±0.007 and b=-0.2453±0.0013 [5]. These coefficients were obtained from ground based observations of the OH production rates for a set of 37

comets. It is interesting to compare the production rates obtained from this expression with recent direct observations of the water production rate with space telescopes for comets 45P/Honda-Mrkos-Pajdušáková with HIFI on Herschel [6] and 67P/Churyumov-Gerasimenko with MIRO on Rosetta [7]. The result of this comparison is shown in Table 1.

Table 1. Measured water production rates on two comets are used for calibration.

Comet	r_h (AU)	δ_{obs} (AU)	M@$\delta = 1AU$	Q_{obs} (s^{-1})	Q_{Jorda} (s^{-1})
67P	2.99	0.025	16.81	7 10^{25}	3.6 10^{26}
45P	1.03	0.06	14.33	9.1 10^{26}	1.4 10^{27}

The HIFI observation of 45P is within the 1-σ error bar on the Jorda 2008 expression while the MIRO observation of 67P is outside of the 3- σ error bar. It should be noted that the MIRO observation is in good agreement with the results obtained with the other instruments on Rosetta, ROSINA and VIRTIS.

Since it is scattering of sun light on the dust that makes the comets visible at short wavelengths, the apparent magnitude is ultimately proportional to the dust density around the comet. Measurements with GIADA on Rosetta indicate that the dust-to-gas ratio for 67P is markedly larger than for other comets (4 versus a 0.1-1 range). This is consistent with the larger value of the water production rate obtained with the coefficients from Jorda 2008 compared with the value measured by the Rosetta instruments. This topic deserves more detailed investigation that we plan to undertake in the next phase of this study. In the meantime, we will use the coefficients presented in [5].

The second step in computing the SNR for the water emission line is to determine the amplitude of the signal corresponding to a given outgassing rate. For the MIRO observations, we will use the first measurement of the $H_2{}^{16}O$ line on June 6-7, 2014 when the heliocentric distance was r_h=3.93 AU (Fig. 4).

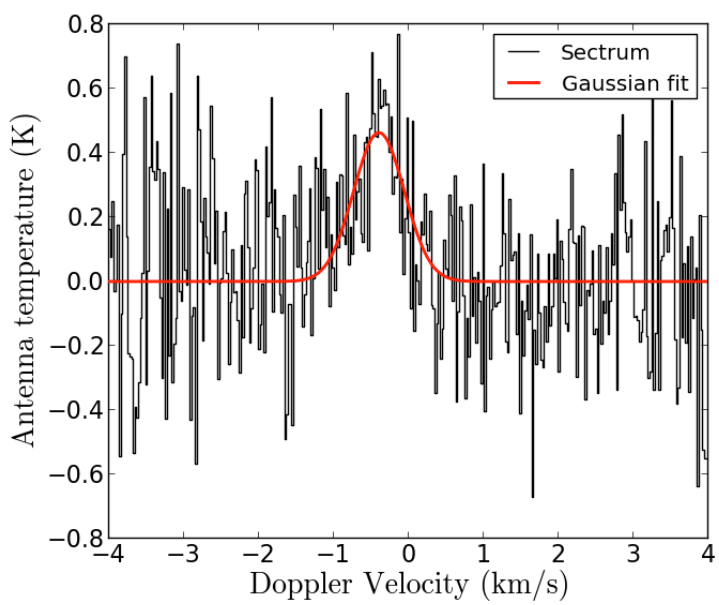

Figure 4: First MIRO observation of the $H_2{}^{16}O$ line on June 6-7, 2014.

The maximum peak amplitude is approximately S_{ref} = 0.42 K. We use this early measurement to ensure as much as possible that the line is optically thin, meaning that the peak amplitude is proportional to the gas column density and hence the global production rate. The outgassing rate for this observation is computed following the procedure described above,

using the expression of Jorda 2008, and is Q_{ref} = 3.1 10^{25} s^{-1}. The signal (maximum peak amplitude) is then computed using the following expression:

$$S = S_{ref} \frac{Q}{Q_{ref}} \frac{D^2}{D_{ref}^2} \frac{\delta_{ref}^n}{\delta^n} \qquad (3)$$

The reference telescope diameter for MIRO is D_{ref} = 0.3 m and the reference distance to the comet is δ_{ref} = 0.0025 AU. The power of the variation with the range depends on the extent the comet fills the antenna beam. If the comet is a point source $n = 2$ and if it fills the beam $n < 2$ (extended source). Explicit radiative transfer calculations for a model comet show that n can become as small as 0.5 for small ranges. We will use $n = 1$, which we expect to be appropriate for most ranges under consideration.

The signal amplitude measured with a telescope of diameter D, at a distance δ of a given comet and a heliocentric distance for the comet of r_h is now given by expression (3) with the production rate Q given by (2) and the magnitude M by (1). The heliocentric distances and ranges to Earth (assuming that the telescope is near the Earth) for the 558 comets selected from the Horizons data base are computed using the SPICE kernels (JPL SPICE kernels are composed of navigation and other ancillary information that has been structured and formatted for easy access, https://naif.jpl.nasa.gov/naif/data.html), which are also retrieved from the Horizons database. The noise on the measurement is computed assuming a DSB heterodyne detection process similar to the one on MIRO and HIFI and is given by the following expression:

$$N = \frac{2T_{noise}}{\sqrt{2Bt_{int}}}$$

The receiver noise temperature is taken as T_{noise} = 50 K, the bandwidth B = 300 kHz (sufficient to detect water emission peak) and the integration time t_{int} = 10 days. This sensitivity is now realized, as will be shown later, the bandwidth is assumed to be sufficiently narrow for the detection of the water emission peak, and the integration time attainable with a mission that would be dedicated to a detailed exploration of outgassing from comets. In the next step of the analysis, the SNR is calculated for the 558 comets at an interval of one day between 2023-Jan-01 and 2027-Jan-01. The time with the largest SNR is recorded for each comet and the corresponding heliocentric distance, range to Earth and SNR are plotted in Fig. 5.

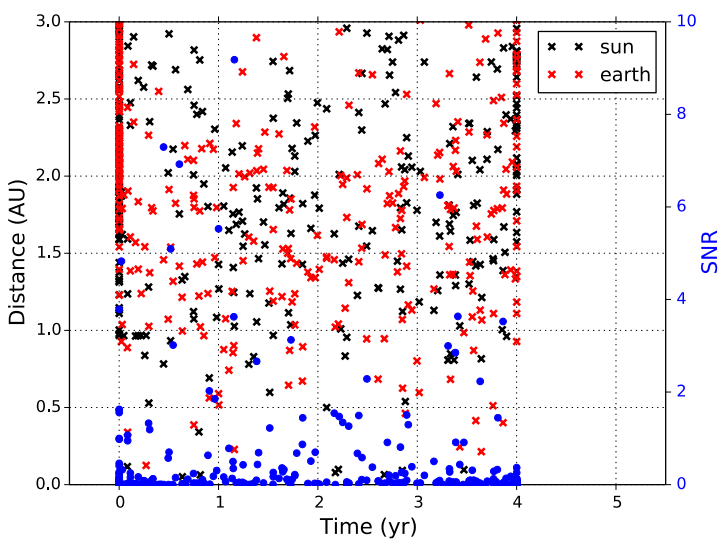

Figure 5: Distance to sun and Earth, and SNR (see text) for the 558 comets selected from the Horizons database, at the times where the SNR is largest between 2023-Jan-01 and 2027-Jan-01.

If it is assumed that a SNR of 1 is needed to measure the $H_2{}^{16}O$ production rate, we can compute the number of comets that satisfy this condition when the diameter of the telescope (or any other parameter of the observing instrument) is varied.

If the production rate of HDO is also to be measured, the SNR needs to be larger than about 2,000 for a D/H of 5 10-4 (Rosetta data for 67P) or 6,700 for a D/H ratio of 1.5 10-4 (SMOW). The corresponding number of detectable comets is shown in Figures 6. We note that D/H can be measured for over 70 comets over a period of 4 years with a telescope diameter of 3 m, assuming a D/H ratio close to that observed at 67P.

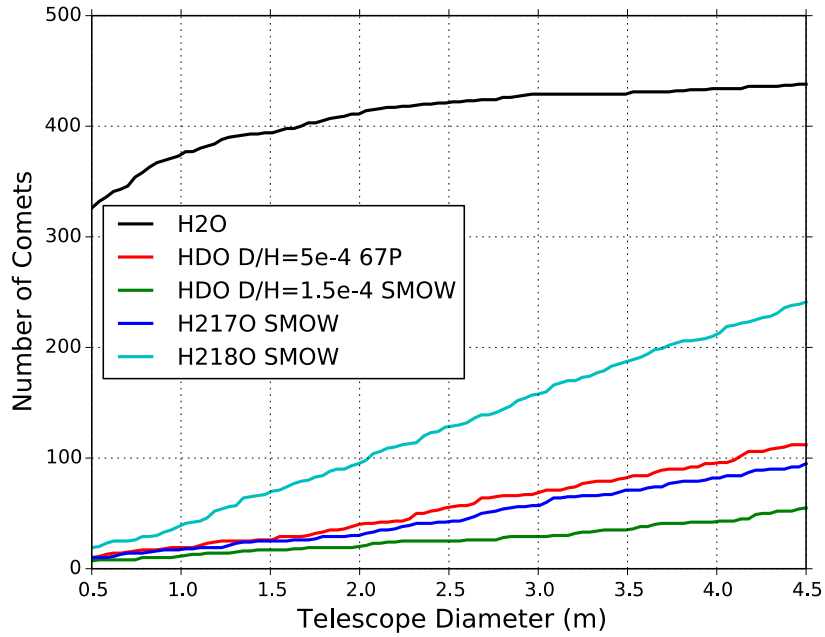

Figure 6: Number of detectable comets as a function of the telescope diameter for various water isotopologues.

3. HETERODYNE DETECTOR CAPABILITY

Heterodyne detectors provide a true and tested way of measuring water in all its form. For ORACLE, a three-channel heterodyne instrument is envisioned which would provide the required sensitivity to quantitatively measure water and its isotopologues. A number of different technologies could be utilized to make the detectors. For example, Schottky diode mixers, such as that used on MIRO, provide room temperature operation but cannot provide the required sensitivity. Superconducting-insulator-superconducting (SIS) tunnel junction mixers provide the highest sensitivity up to around 1.4 THz [8]. Our recent focus has been to develop the receiver for Band 1 which covers the 500 – 600 GHz frequency range, which is just below the 690 GHz superconducting energy gap of niobium.

The SIS devices are fabricated on 4- and 6 μm Silicon-on-Insulator (SOI) substrate. This allows for arbitrary shaped 'wet-etched' geometric features that facilitate alignment in the mixer block. Design of the devices is based on critical modeling of the superconducting junction along with careful microwave circuit design to provide optimum impedance matching. The block diagram of the Band 1 receiver is shown in Fig. 7. The Band 1 SIS mixer utilized an Nb/Al-O_x/Nb high-current density (Jc ~ 25 kA/cm^2) tunnel junction. The ground and wire layers are Nb. Au beam leads are employed to provide the ground and IF contacts. The RF choke provides approximately 40 dB of RF isolation, and thus exactly where the ground beam leads are tagged down is not critical. A fabricated chip, mounted inside the waveguide block is shown in Fig. 8.

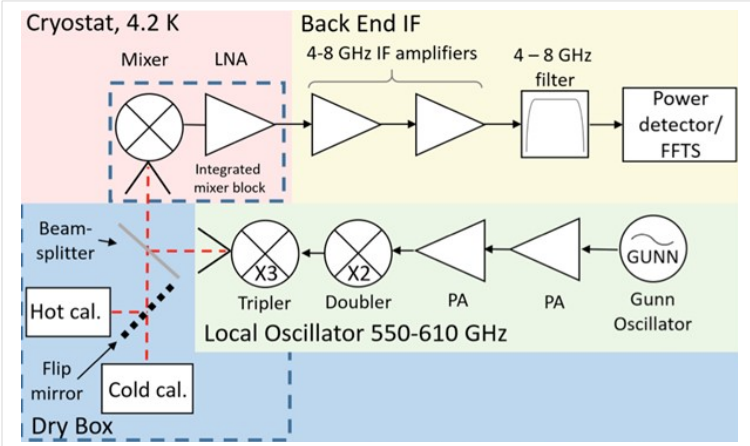

Figure 7:Band 1 receiver is built using freqeuncy multipliers and SIS based mixer. A commercial cryogenic LNA is used for the IF.

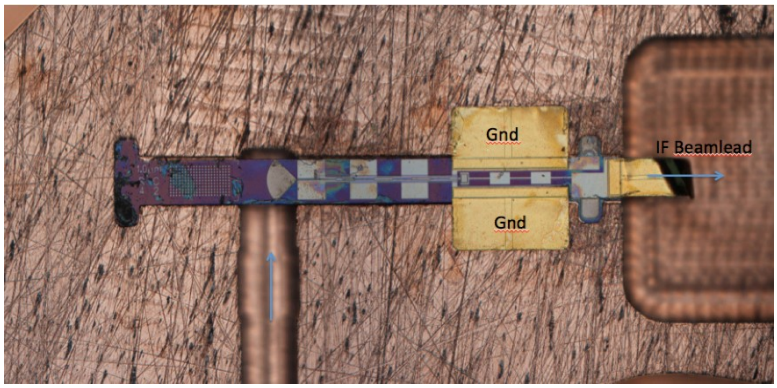

Figure 8: A completed mixer chip is mounted in a waveguide block for measurment.

Measured results of the Band 1 double sideband (DSB) receiver are shown in Fig. 9. These data were taken in an open lab enviornment with no consideration for correcting for the loss due to water vapor. In future, we will contruct a Nitrogen 'dry-box' around the receiver test-setup to reduce the effect of water vapor on the measurements. Once corrected for the front-end optics loss and measured IF noise temperature and derived mixer conversion loss (not shown) we obtain the mixer noise temperature as shown in right panel of Fig. 9. Within the error-bars the mixer noise hugs the theorectical quantum noise limit (hf/e), which at this frequency is ~ 28K. This demonstrates that we can achieve the required sensitivity as described in the previous section.

Mixer band 2 (890-1000 GHz) and Mixer band 3 (1100-1280 GHz) are well above the energy gap of Niobium. For this reason we are working on develooping the NbTiN-Nb/Al-AlN/NbTiN-Al material system to achieve high current density devices for the higher bands. The Nb/Al-AlN/NbTiN junctions have an expected energy gap around 3.5 meV which allows biasing the mixers around 3 mV, thereby avoiding the overlapping photon step from the negative side of the I/V curve.

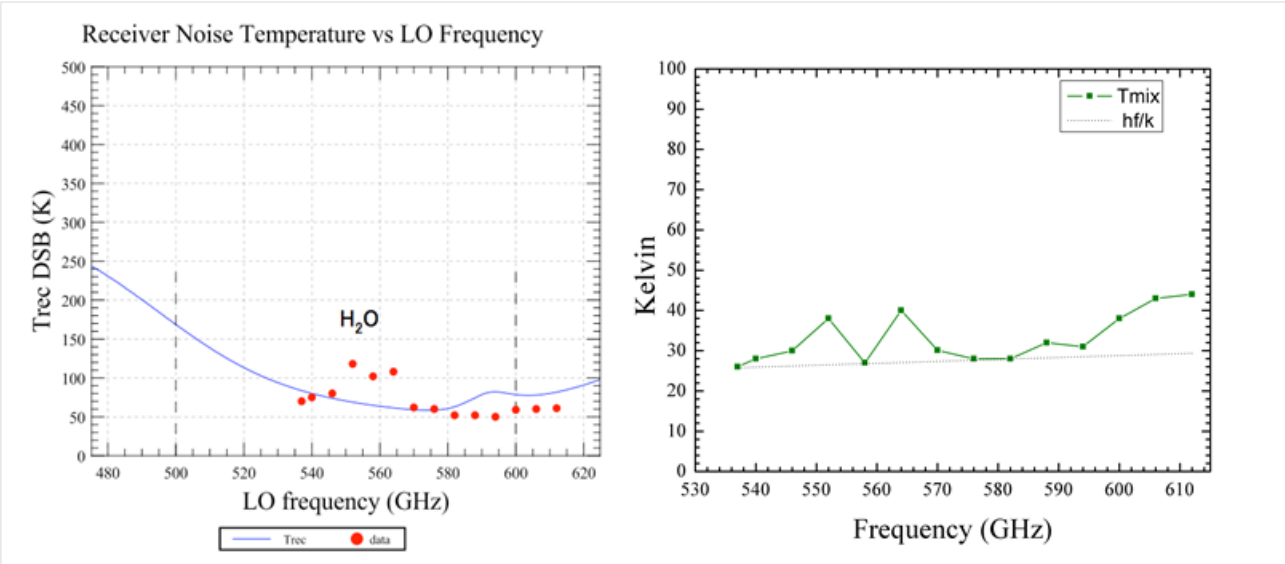

Figure 9: Measured and predicted band 1 double sideband (DSB) receiver (right panel) and mixer (left panel) noise temperature. The simulation was done at a fixed mixer bias (2.2 mV), whereas to achieve optimal noise the mixer bias is in fact varied at each frequency, thus explaining the discrepancy between the theory and measurement. The ground state 557 GHz H_2O absorbtion line is clearly visible in the mesurement. To remove the H_2O line a Nitrogen 'dry-box' will be utilized in future measurements.

4. SUMMARY

A rigorous comet model was developed that can determine the number of possible target comets given the distance to the telescope, detector sensitivity and telescope diameter. This model predicts that over a 4-yr time period it would be possible to measure water isotopologue ratios on >50 comets with a 3-meter telescope. This provides the basis for envisioning a Discovery class mission for measuring the water isotopologues in comets. Superconducting junction detectors have been demonstrated for Band 1 with sensitivities approaching the quantum limit. This technology development would allow us to measure dozens of comets with a dedicated mission.

5. ACKNOWLEDGEMENTS

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