National Aeronautics and Space Administration

Cosmic Origins of Earth's Oceans

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Program: FY21 R&TD **Strategic Focus Area: The Science of Water in the Universe**

Objectives

Water is a central theme of NASA's vision. The Decadal Survey *Vision and Voyages* explicitly identified "determining the deuterium/hydrogen and other crucial isotopic ratios in multiple comets" as key measurements for understanding Solar System beginnings. We will identify and quantify the confounding factors that affect the accuracy of such measurements through (1) Development and implementation of improved coma excitation models; (2) Calculation and experimental verification of water-water and water-heavy water collision rates; and (3) Detailed parameterization of water vaporization processes at low temperatures, which may affect isotopic ratios in the gas phase.

Background

Measurements of the D/H ratio (Fig. 1), and oxygen isotopic ratios, in comets provide key constraints on the origin and history of water molecules, and the contribution of comet-like bodies to Earth's oceans. The precision of the existing isotopic ratio measurements is currently limited by statistical and calibration uncertainties and is of order 5-10% (1σ) for most accurate space measurements. Future space missions will provide much higher accuracy, but modeling uncertainties will become a limiting factor. In addition, good understanding of fractionation processes during water sublimation from ices is required to ensure that the isotopic composition of the coma accurately represents the bulk composition of the nucleus.

Approach and Results

1. We assembled a comet modeling package that computes line profiles in a non-spherical coma, including collisions and non-gravitational forces, using the physical properties of the nucleus sub-surface (ice content, dust layer thickness, mass density, grain size) as input parameters to the model (Figure 2). We incorporated a non-linear optimization algorithm to enable the retrieval of model parameters within the optimal estimation approach, including uncertainty quantification.
2. We assembled a molecular collision modeling package capable of extending computations of collisional cross sections to rare isotope molecular systems such as HDO-H_2O. For laboratory validation we refurbished a cryocooled collisional apparatus and confirmed the capability for the system to measure the Lamb (or saturation) dip phenomenon.
3. We assembled a modular mm-wave cavity spectrometer capable of low-pressure H_2O and HDO measurements in JPL's ice lab sublimation chamber (Figure 3). The system is capable of measuring saturation vapor density at temperatures 50K lower than existing measurements of H_2O saturation. These measurements will allow careful tracking of deuterium gradients and system residence time periods as functions of temperature, extent of sublimation, and surface area (solid vs. granular ice of controlled particle size).

Significance/Benefits to JPL and NASA

This effort will enable observing programs for existing (SOFIA) and future (JWST, SPHEREx) NASA facilities and improve JPL's technical capabilities for executing planetary or astrophysics spectroscopic missions, ranging from SIMPLEx concepts, to larger Discovery, Explorer, or Probe class missions, by providing firm scientific predictions and hypotheses that can be tested by future observations.

Publications

N. Biver, et al., "Molecular composition of short-period comets from millimetre-wave spectroscopy", A&A, **651**, A25 (2021); N. Roth, et al., "Leveraging the ALMA Atacama Compact Array for Cometary Science", Ap. J., in press (2021; arXiv:2104.03210).

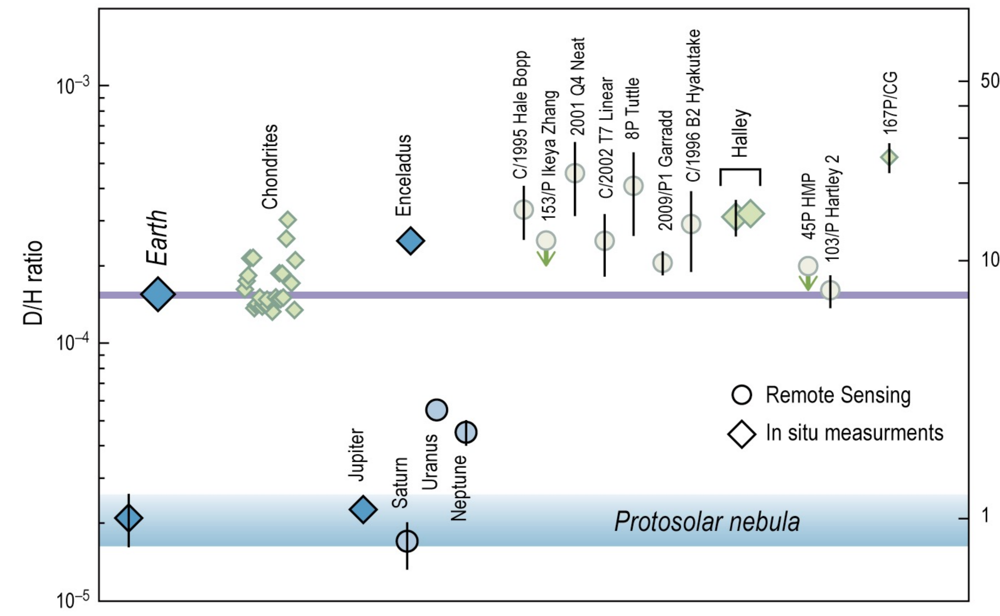

Figure 1. D/H ratios in the Solar System.

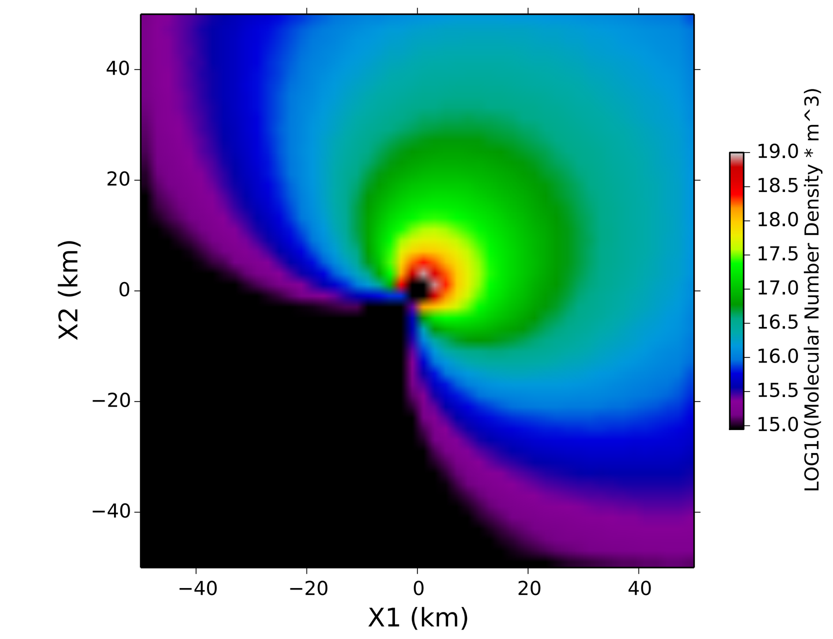

Figure 2. Computed profile of the $H_2{}^{16}O$ vapor density in the coma of a comet.

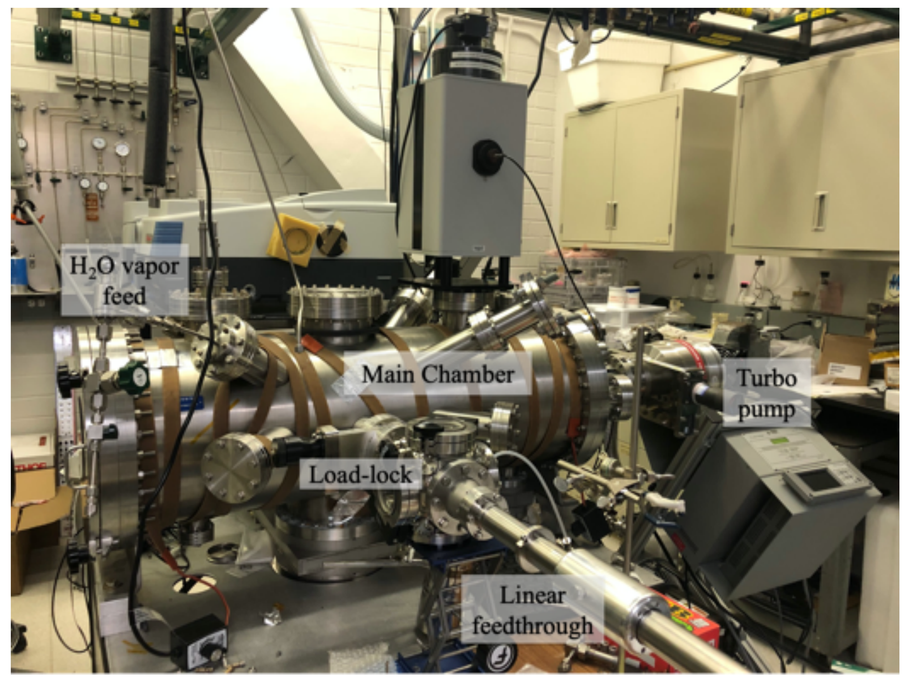

Figure 3. JPL large-volume, high-vacuum cryogenic chamber.

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