



Titania's Deuterium Abundance and the Origin of Its Water

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Abstract

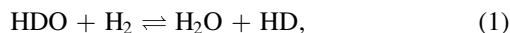
Models of our solar system's protoplanetary disk account for processes such as the infall of water-ice-rich grains from the surrounding molecular cloud, the reprocessing of some infalling water-ice in the hot inner disk, and water's outward migration in the disk. These models predict deuterium abundance in water as a function of heliocentric distance. The James Webb Space Telescope (JWST) enables us to test these models by measuring the abundance of deuterium on icy outer solar system bodies through spectroscopic observations of the semiheavy water (HDO) band near 4.1 μm . However, a hurdle to measuring deuterium abundances from JWST spectra is the lack of optical constants for HDO. We present the separated contributions of HDO and H₂O to the optical constants of crystalline water-ice that contains both isotopologues. In addition, we combine these effective optical constants, a radiative transfer model, and a JWST spectrum of the Uranian satellite Titania to measure its deuterium abundance in water, finding $\text{D}/(\text{H}+\text{D}) = (2.8 \pm 0.5) \times 10^{-4}$ in agreement with the model by L. Yang et al. Using a simple model, we estimate that most of Titania's water originated from thermally processed inner-disk water, and only a minor portion came from inherited molecular-cloud water. By combining our Titania measurement with Saturnian satellite and comet measurements in the literature, we suggest that outer-satellite water came from a more homogeneous reservoir than comets, and perhaps accreted over a shorter time interval than comets. Furthermore, Titania's deuterium abundance suggests that it formed in a lower-temperature, hydrogen-poor circumplanetary disk rather than a higher-temperature, hydrogen-rich disk.

Unified Astronomy Thesaurus concepts: [Uranian satellites \(1750\)](#); [James Webb Space Telescope \(2291\)](#); [Surface ices \(2117\)](#); [Infrared spectroscopy \(2285\)](#); [Radiative transfer \(1335\)](#); [Isotopic abundances \(867\)](#); [Astrochemistry \(75\)](#)

1. Introduction

Studies of interstellar chemistry in cold molecular clouds have shown that water becomes enriched in deuterium relative to molecular hydrogen through ion-molecule and grain-surface reactions at temperatures $T < 50$ K. These models suggest $0.001 < \text{D}/(\text{H}+\text{D}) < 0.01$ for water in cold molecular clouds (P. D. Brown & T. J. Millar 1989; T. J. Millar et al. 1989; H. Roberts & T. J. Millar 2000; H. Roberts et al. 2004; C. Ceccarelli et al. 2014).

During the formation of the solar system, not all water remained enriched in deuterium because some of it was delivered into the hot, inner regions of the protoplanetary disk. At high temperatures in the inner disk, the rapid isotopic exchange reaction,



erased much of the deuterium enrichment. Water equilibrated with hydrogen, resulting in $\text{D}/(\text{H}+\text{D}) = 2.0 \times 10^{-5}$ in the inner disk. In the cold outer disk, water retained its deuterium enrichment from the cold molecular cloud (J. Geiss & H. Reeves 1981; C. Lécluse & F. Robert 1994; A. Drouart

et al. 1999; O. Mousis et al. 2000; F. Hersant et al. 2001; J. Horner et al. 2007; J. J. Kavelaars et al. 2011).

L. Yang et al. (2013) studied an earlier phase of the disk's evolution than the models discussed above. Specifically, they combined isotopic exchange and material transport, as in earlier models, but also included the ongoing infall of deuterium-enriched molecular cloud water into the evolving protoplanetary disk.

In this paper, we describe our measurement of $\text{D}/(\text{H}+\text{D})$ in water on Titania's icy surface, compare it to the model of L. Yang et al. (2013) and deuterium abundances of other outer solar system bodies, and describe the implications of the comparison for the origin of Titania's water.

This paper is organized as follows. In Section 2, we briefly describe our observations of Titania with the James Webb Space Telescope (JWST). In Section 3, we describe our experimental configuration and procedures for measuring the separate contributions of HDO and H₂O to the optical constants of crystalline water-ice, which are necessary for analyzing the Titania spectrum. We refer to these separate contributions as effective optical constants rather than optical constants. It is important to note that our effective optical constants for HDO differ from optical constants for pure HDO. For pure HDO, each HDO molecule is surrounded by HDO molecules. For the effective optical constants we present here, each HDO molecule is overwhelmingly surrounded by H₂O molecules. In Section 4, we describe our analysis of the Titania



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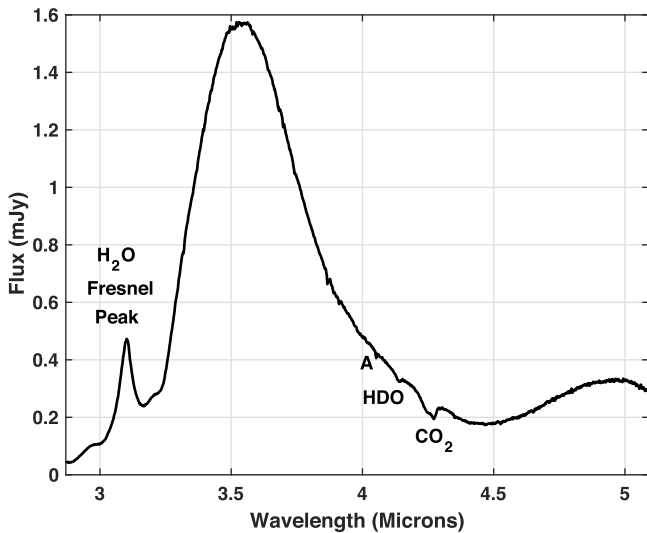


Figure 1. Spectrum of Titania’s leading hemisphere taken with JWST and NIRSpec (R. J. Cartwright 2026). Peak absorptions of the weak HDO and CO₂ bands are observed at 4.14 and 4.27 μm , respectively. An artifact (A) of the data reduction process appears at 4.05 μm . The HDO band is distinct from the artifact and CO₂ band. The feature at 3.1 μm is the H₂O Fresnel peak.

spectrum with the Hapke model and the resulting deuterium abundance. In Section 5, we discuss the implications of our deuterium measurement for the origin of Titania’s water. In Section 6, we give our conclusions.

2. Observations

We obtained observations of Titania’s leading hemisphere with JWST and the Near Infrared Spectrograph, i.e., NIRSpec (P. Jakobsen et al. 2022; T. Böker et al. 2023), as part of General Observer Program 1786. We made observations on 2023 September 10, starting at 01:03:46 UT. We used a total integration time of 2567.6 s. The mid-observation subobserver longitude was 103°. The spectrum covered the 2.87–5.25 μm wavelength range using the G395M grating with a resolving power $R \sim 1000$. Details of the data reduction procedures are given in R. J. Cartwright (2026).

In Figure 1, we plot the spectrum of Titania’s leading hemisphere. We observe peak absorptions from the semiheavy water (HDO) and CO₂ bands at 4.14 and 4.27 μm , respectively. An artifact of the data reduction process appears at 4.05 μm and is marked with an “A.” We note that the weak HDO band is isolated from the artifact and the CO₂ band, providing a well-defined baseline. The feature at 3.1 μm is the H₂O Fresnel peak.

3. Effective Optical Constants

Measuring the deuterium abundance on Titania using the spectrum in Figure 1 requires optical constants, where n_λ is the real part and k_λ is the imaginary part, along with a radiative transfer model. Unfortunately, there are no published effective optical constants for HDO, and effective optical constants for the weak H₂O band coincident with the HDO band may be subject to large uncertainties (R. M. Mastrapa et al. 2009).

Therefore, we obtained effective optical constants for HDO and H₂O in the Astrophysical Materials Laboratory (AML) and the Process, Environments, and Astrochemistry on Extraterrestrial Surfaces (PEAXS) Laboratory, respectively,

both in the Department of Astronomy and Planetary Science at Northern Arizona University.

3.1. HDO Experiments

To measure the effective optical constants for HDO, we used the vacuum system previously described by S. C. Tegler et al. (2024). To prepare samples, we used separate reservoirs and leak valves (Pfeiffer model number EVN 116) for heavy water (D₂O) and H₂O. We pumped on each reservoir to remove any air above the liquids. Proton–deuteron exchange between H₂O and D₂O was dominant, favoring HDO over D₂O in the manifold between the leak valves and the chamber. We chose a D₂O concentration of 1% to obtain a HDO concentration of 2% because we observed that D₂O was not fully converted to HDO at higher concentrations. This low concentration is consistent with the highly diluted environment expected in astrophysical ices, where each HDO molecule’s nearest neighbors are overwhelmingly H₂O molecules, and provides sufficient absorption for confident analysis of our data. The effective optical constants presented below are valid only for low HDO abundances in an H₂O ice. We background-deposited the vapor onto the cold substrate at 150 K, while monitoring the pressure with an INFICON Bayard-Alpert Pirani combination gauge sensor (model number BPG-400), and the areal mass with an INFICON IC 6 optically flat, gold-plated quartz crystal microbalance (QCM). During deposition, we first opened the D₂O reservoir to a chamber pressure of 6.0×10^{-8} torr. We then quickly opened the H₂O reservoir to a pressure of 6.0×10^{-6} torr. We simultaneously deposited both gases for about 20 minutes, with the partial pressures yielding an HDO abundance of 2%. As our base pressure prior to deposition was $\sim 3.0 \times 10^{-9}$ torr, we estimate our HDO composition is accurate to $\sim 5\%$.

During deposition, we measured the sample thickness using an AvaSpec Avantes Fiber-Optic Spectrometer. A fiber emitted an ultraviolet–visible beam 45° to the surface normal. A second fiber received the reflected beam and sent it to the spectrometer (Figure 2). Interference between light reflected from the substrate–ice and ice–vacuum interfaces produced a wavelength-dependent variation in the intensity of the reflected light that depended on the sample thickness. We compared our laboratory ultraviolet–visible spectrum to a Markov Chain Monte Carlo (MCMC) model-generated reflectance spectrum to obtain thickness (P. R. Behr et al. 2020; R. A. Carmack et al. 2023). The reflectance model used the same mathematical formalism as described in detail in S. C. Tegler et al. (2024), but it assumed transparent ice and an index of refraction for the ice approximated by the Sellmeier equation. In Figure 3, we plot our laboratory spectrum (blue line) of $2.0\% \pm 0.1\%$ HDO in crystalline H₂O ice at $T = 80$ K and the most likely MCMC model spectrum (red line), yielding a sample thickness of 1.02 ± 0.01 μm , where the uncertainty comes from the 1σ spread of the MCMC-derived distribution of thicknesses. We note that the thickness measurement is particularly sensitive to fringe spacing with wavelength, rather than to amplitude. We suspect that a small amount of scattering in our sample, not accounted for in our model, is responsible for the lower amplitude of the measurements relative to the model in Figure 3.

We obtained infrared spectra of samples using a Thermo-Nicolet iS50 Fourier transform infrared (FTIR) spectrometer. The FTIR was configured to emit an external beam, which was

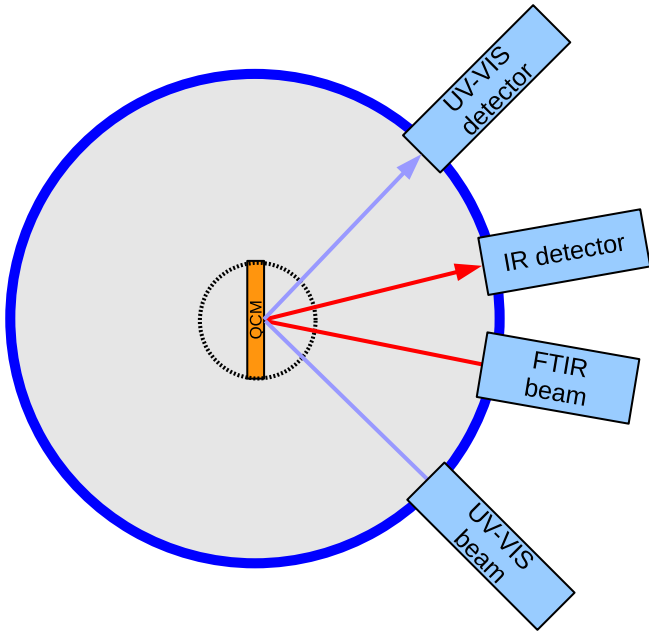


Figure 2. A schematic cross section of our vacuum chamber, as seen from above, that illustrates the light paths of our ultraviolet-visible fiber-optic spectrometer and our FTIR spectrometer. Samples reside on the side of the QCM facing the spectrometers.

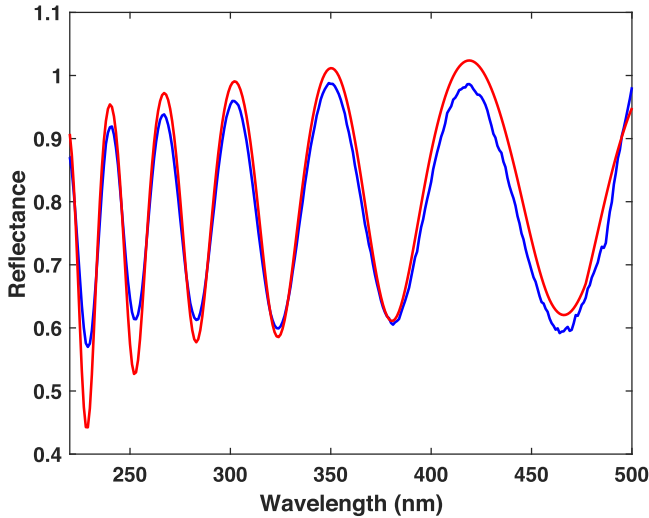


Figure 3. An ultraviolet-visible spectrum of 2.0% $\pm$ 0.1% HDO embedded in crystalline H₂O-ice at 80 K (blue line) and the model of the spectrum, which gives a most likely thickness of 1.02 $\pm$ 0.01 μ m for the sample (red line).

focused by a gold-coated parabolic mirror onto the sample at an angle of incidence of 8.5° relative to the surface normal. Upon reflection, the beam was refocused by an additional mirror onto a mercury cadmium telluride type A (MCT-A) detector (Figure 2). All experiments covered a wavenumber, $\tilde{\nu}$, range from 6000 cm^{-1} (1.7 μ m) to 650 cm^{-1} (15 μ m) at a resolution of 0.5 cm^{-1} . We averaged 125 scans per sample and per reference (bare substrate) spectrum.

The experimental procedure was as follows. The substrate was cooled to 150 K. Reference spectra of the bare substrate were recorded with both the FTIR and the ultraviolet-visible spectrometer. The sample was then background-deposited at 150 K, briefly heated to 165 K to ensure uniform mixing of HDO, and cooled back to 150 K. FTIR and ultraviolet-visible

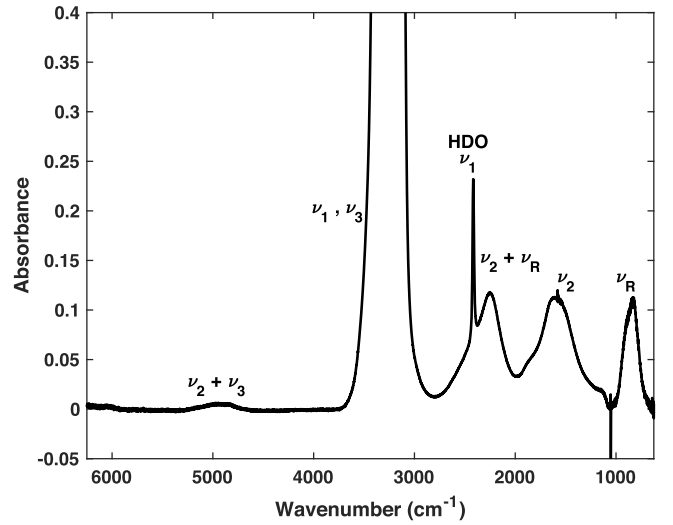


Figure 4. The absorbance spectrum of a 2% HDO and 98% H₂O sample at 80 K. The HDO ν_1 (O–D stretch) band is clearly visible at 2416 cm^{-1} (4.14 μ m). The remaining features are H₂O bands labeled with their vibrational modes, except for the feature at 1052 cm^{-1} , which is an artifact in the data. The H₂O feature near 3333 cm^{-1} (3 μ m) is saturated, so we cannot compute optical constants for this band.

spectra of the sample were recorded from 150 to 10 K at 10 K intervals. Three experiments were performed over the 150 to 10 K interval to assess reproducibility.

We removed instrumental effects from each raw sample spectrum, R_{sam} , by dividing it by the raw reference (bare substrate) spectrum, R_{ref} , and then we calculated absorbance using

$$\text{Absorbance} = -\log_{10}(R_{\text{sam}}/R_{\text{ref}}). \quad (2)$$

In Figure 4, we plot the absorbance spectrum of a sample composed of 2% HDO and 98% H₂O by mole at 80 K with a thickness of 1.02 μ m. The HDO ν_1 (O–D stretch) band is clearly visible at 2416 cm^{-1} (4.14 μ m). The remaining features are H₂O bands labeled with their vibrational modes.

3.2. Effective Optical Constants for HDO

As optical constants from a laboratory absorbance spectrum cannot be computed analytically, we use the usual iterative approach, varying the optical constants n_λ and k_λ in a model until we achieve excellent agreement between the model and the laboratory spectra (S. C. Tegler et al. 2024). In Figures 5(a) and (b), we plot n and k as a function of wavenumber from the best-fit model for the HDO band and the underlying H₂O band. In Figure 5(b), we also show the linear interpolation used to isolate the HDO k -values. To allow comparison to and quantification of remote sensing observations (see below), we multiplied the isolated HDO k -values in Figure 5(b) by 50 to represent 100% HDO k -values (see Figure 5(c)). We note that these effective optical constants are not specific to our 2% HDO experimental concentration. For example, if our experimental concentration was 1%, we would have multiplied by 100, yielding the same effective optical constants in Figure 5(c). The multiplicative factor corrects for concentration and preserves the HDO band shape for highly dilute mixtures. Ó. Gálvez et al. (2011) show different HDO band shapes for 0.8%, 4%, and 20% HDO in H₂O. Our effective optical constants apply to modeling any icy astrophysical body composed of crystalline water-ice, where molecules

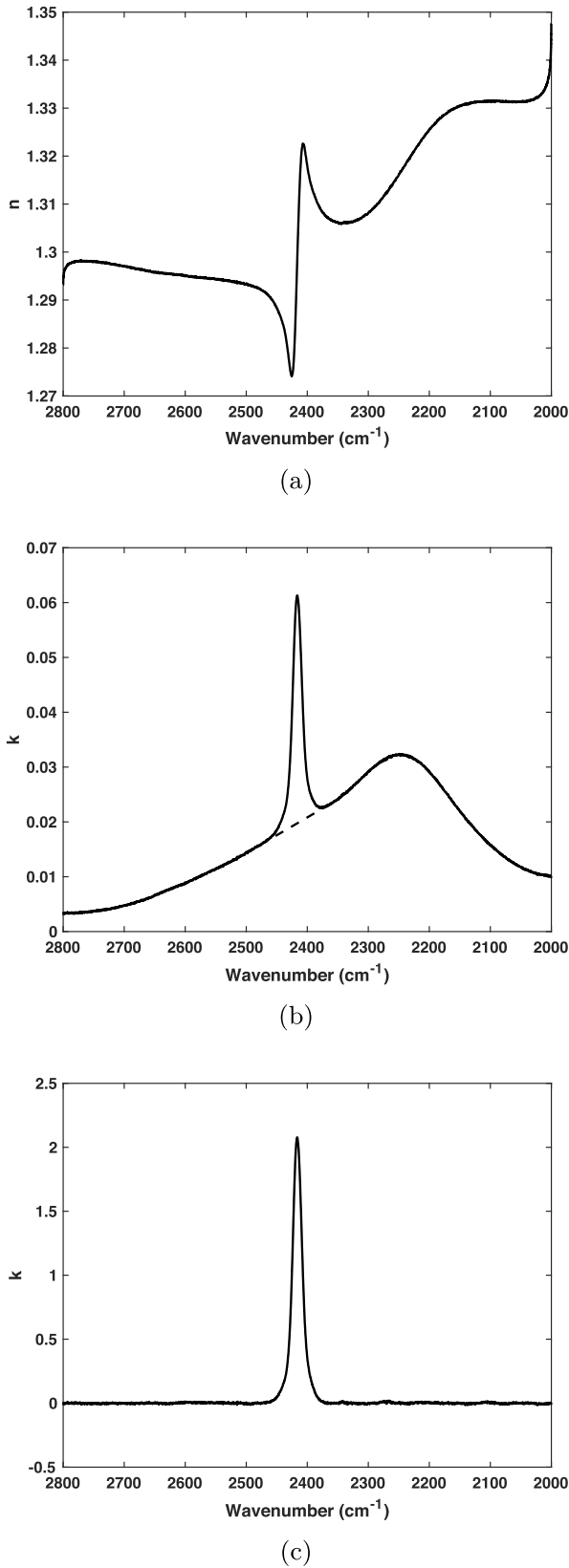


Figure 5. (a) The real component of the effective optical constants, n , as a function of wavenumber from a 2% HDO and 98% H₂O sample at 80 K. (b) The imaginary component of the effective optical constants, k , for the same sample, and the interpolation to separate the HDO band from the H₂O band. (c) Theoretical 100% HDO k -values derived by multiplying the baseline-subtracted k -values in Figure 5(b) by 50. We used these values as an endmember for our Hapke modeling, keeping in mind that it will only be valid for samples with low HDO concentrations (see the main text).

neighboring each HDO molecule are overwhelmingly H₂O, say, <2% HDO. W. M. Grundy et al. (2011) obtained the effective optical constants for CH₃D in CH₄ as if it were pure CH₃D, in the same way we do here for HDO in H₂O.

In Figure 6, we plot k as a function of T for HDO in crystalline water-ice at temperatures from 150 to 10 K. From the plot, we observe no evidence of D₂O absorption at 2447 cm⁻¹ and 2367 cm⁻¹ (G. Ritzhaupt et al. 1978; R. L. Hudson et al. 2025). In addition, the HDO bands become stronger and shift to lower wavenumbers as the temperature decreases.

Because the HDO band is symmetrical, it is possible to derive analytical expressions that represent the band as a function of temperature. Such expressions will aid JWST spectrum modelers by treating T as a continuous variable rather than relying on our discrete band profiles, which are separated by 10 K steps. In Figure 7, we compare the best-fitting Gaussian (dashed-dotted line), Lorentzian (dotted line), and Voigt (dashed line) band profiles to the HDO band (red line) from a sample at 80 K. The Voigt profile provides a much closer fit than the Gaussian and Lorentzian profiles. The percent differences in area between the fitted profiles and the HDO band profile were 7%, 8%, and 1% for the Gaussian, Lorentzian, and Voigt profiles, respectively.

We describe the Voigt fitting algorithm here. The input spectrum consisted of the measured wavenumber, ν_i , and corresponding optical constant values, k_i . The fit was performed using a nonlinear least-squares minimization routine with four free parameters: the band center ν_0 , the Lorentzian half-width at half-maximum γ , the Gaussian standard deviation σ , and the band amplitude A .

The Voigt profile was evaluated using the real part of the Faddeeva function, $\Re[w(z)]$,

$$V(\nu) = \frac{1}{\sigma\sqrt{2\pi}} \Re[w(z)], \quad (3)$$

where

$$z = \frac{(\nu - \nu_0) + i\gamma}{\sqrt{2} \sigma}. \quad (4)$$

In the implementation used here, the Faddeeva function was evaluated numerically through the MATLAB function (`fadef`).⁶

The profile was normalized to unit peak and then multiplied by a scale factor A , such that

$$V_{\text{fit}}(\nu) = A \frac{V(\nu)}{\max[V(\nu)]}. \quad (5)$$

The best-fit parameters were obtained by minimizing the residuals between the measured spectrum and the model profile,

$$\chi^2 = \sum_i [k_i - V_{\text{fit}}(\nu_i)]^2, \quad (6)$$

as implemented by the least-squares fitting routine (`lsqcurvefit`) in MATLAB.

We fit Voigt profiles to the HDO band at 15 temperatures between 150 and 10 K. In Figure 8, we plot the best-fit parameters as a function of temperature (solid circles). Next, we fit polynomials to each Voigt parameter as a function of temperature (solid black lines). The polynomials for the Voigt

⁶ <https://www.mathworks.com/matlabcentral/fileexchange/47801-the-voigt-complex-error-function-second-version/files/fadef.m>

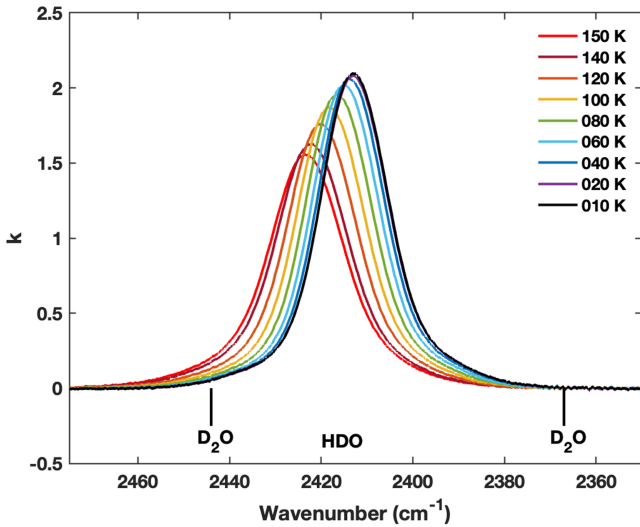


Figure 6. The imaginary component of the effective optical constants, k , for HDO in a crystalline H_2O ice centered on the HDO ν_1 (O–D stretch) band. The band peak shifts to lower wavenumbers and becomes stronger as the temperature decreases. There is no trace of D_2O absorption at 2447 cm^{-1} and 2367 cm^{-1} .

parameters are given by Equation (7) and the coefficients in Table 1. Combined with the Voigt profile in Equations (3)–(6), the polynomials provide the k -values required to model the HDO band over the temperature range from 150 to 10 K.

$$\begin{aligned} \nu_0 &= a_3 T^3 + a_2 T^2 + a_1 T + a_0 \\ A &= b_3 T^3 + b_2 T^2 + b_1 T + b_0 \\ \sigma &= c_3 T^3 + c_2 T^2 + c_1 T + c_0 \\ \gamma &= d_3 T^3 + d_2 T^2 + d_1 T + d_0. \end{aligned} \quad (7)$$

3.3. H_2O Experiments

Initially, we used H_2O optical constants from R. M. Mastrapa et al. (2009) in our Hapke model fit to the H_2O $\nu_2 + \nu_R$ band near 2250 cm^{-1} ($4.44\text{ }\mu\text{m}$), which overlaps the HDO band in the Titania spectrum. The model band shape did not match the band in the Titania spectrum, so we remeasured these optical constants.

We obtained reflectance spectra of H_2O in the AML. However, we observed a small perturbation to the weak H_2O $\nu_2 + \nu_R$ band at 2250 cm^{-1} . We suspect this perturbation arose from the reflectance geometry—specifically, the oblique angle of incidence on a metallic substrate—which enhances the surface-normal electric field component and distorts the band shape of the strong $3\text{ }\mu\text{m}$ H_2O complex, possibly producing a weak shoulder feature. Such a shoulder is not expected in a normal-incidence transmission experiment. We therefore measured the optical constants of H_2O using the PEAXS Laboratory (P. D. Tribbett et al. 2021; P. D. Tribbett & M. J. Loeffler 2022), which was recently modified to enable transmission measurements.

We used the same general procedure as with HDO, except that we deposited $2.38\text{ }\mu\text{m}$ of H_2O onto our KBr substrate and we did not anneal to 165 K.

3.4. Effective Optical Constants for H_2O

We calculated the H_2O optical constants in a manner similar to that used for HDO. However, because we conducted a transmission experiment, we compared the absorbance spectra

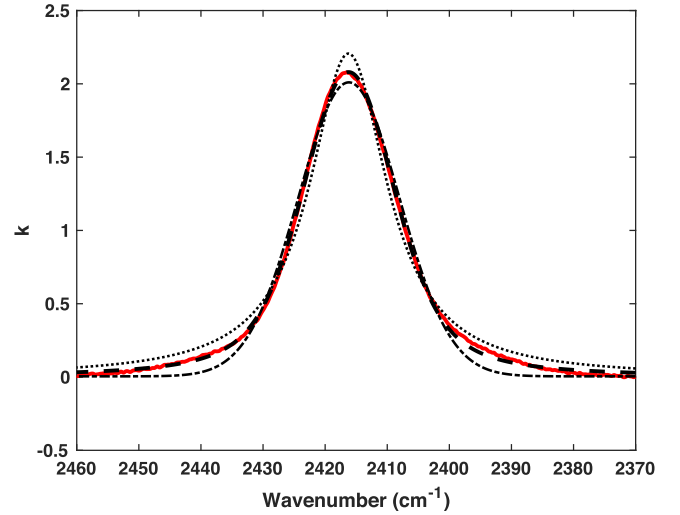


Figure 7. Comparison of the best-fitting Gaussian (dashed–dotted line), Lorentzian (dotted line), and Voigt (dashed line) band profiles to the HDO band measured at 80 K (red line). The Voigt profile provides a closer match to the HDO band than the Gaussian or Lorentzian profile, thereby enabling us to provide analytical expressions for HDO effective optical constants using Equations (3)–(7) and Table 1.

to the transmission model of P. A. Gerakines & R. L. Hudson (2020) rather than to the reflectance model of S. C. Tegler et al. (2024).

In Figure 9, we plot the resulting k -values as a function of wavenumber for $40\text{ K} < T < 150\text{ K}$. The H_2O bands become slightly stronger and shift to slightly higher wavenumbers as the temperature decreases. Naturally occurring HDO appears as a weak band near 2420 cm^{-1} ($4.13\text{ }\mu\text{m}$). The HDO band becomes stronger and shifts to lower wavenumbers as temperature decreases, consistent with the behavior observed for HDO in Figure 6.

Next, we derived k -values for deuterium-free H_2O between 150 and 20 K, i.e., effective optical constants for H_2O . For each band at a given temperature, we subtracted the HDO band at the corresponding temperature until no residual HDO band remained in the resulting spectrum. Figure 10 shows an example of the deuterium-depleted H_2O band at 80 K (solid black line). The tiny wiggles at wavenumbers smaller than 2400 cm^{-1} are due to incomplete cancellation of CO_2 vapor in the path of the FTIR beam. We note that these wiggles are well separated from the HDO band.

In Figure 10, we plot our k -values (solid black line) alongside those of R. M. Mastrapa et al. (2009) (dashed black line) at 80 K. The Mastrapa transmission spectra exhibit strong scattering effects that require adjustments to the continuum level and slope. Mastrapa notes that the largest uncertainties in their k -values occur in transparent regions, i.e., regions with low k -values, such as the H_2O $\nu_2 + \nu_R$ band. Thus, in the analysis that follows, we adopt our effective optical constants for this H_2O band.

3.5. Ground Truth Test of the Effective Optical Constants

As a ground truth test, we used our HDO effective optical constants to measure the deuterium abundance in a water sample. Accurate HDO effective optical constants should produce a deuterium abundance consistent with the terrestrial value.

We deposited a water sample on a KBr crystal and measured the sample's thickness and optical constants as described

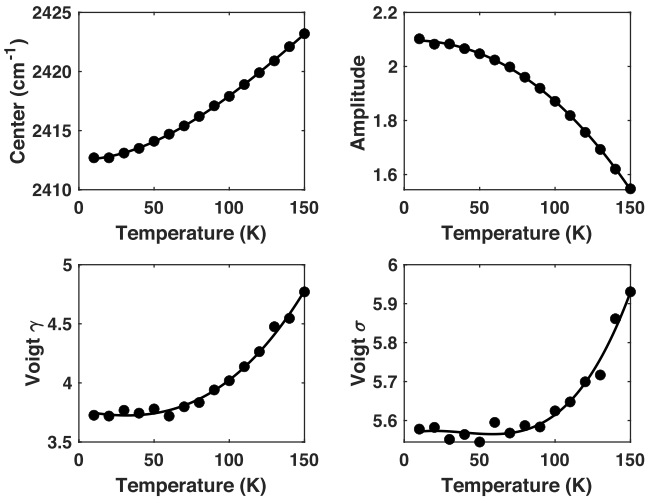


Figure 8. Best-fitting Voigt parameters as a function of temperature (solid black circles). Polynomial fits to the parameters using Equation (7) and the values in Table 1 (black line). A Voigt function and these polynomials reproduce the HDO band at any temperature between 150 and 10 K.

Table 1
Coefficients for Voigt Parameters

Coeff.	Value	Coeff.	Value
a_3	$-1.2988(-6)$	b_3	$-2.8146(-8)$
a_2	$6.6255(-4)$	b_2	$-2.1567(-5)$
a_1	$7.6642(-4)$	b_1	$1.8459(-4)$
a_0	$2.4125(3)$	b_0	$2.0965(-0)$
c_3	$2.9152(-7)$	d_3	$2.1993(-7)$
c_2	$-3.4283(-5)$	d_2	$2.8585(-5)$
c_1	$1.0179(-3)$	d_1	$-2.4966(-3)$
c_0	$5.5645(-0)$	d_0	$3.7683(-0)$

Note. Coefficients for Equation (7). Values in parentheses are the powers of 10, e.g., $(-6) = \times 10^{-6}$.

above. Assuming the HDO and H₂O molecules are intimately mixed, we obtained the deuterium abundance in the sample using

$$k_{\text{H}_2\text{O},\text{eff}} = k_{\text{meas}} - 2f_{\text{D}}(1 - f_{\text{D}})k_{\text{HDO},\text{eff}}, \quad (8)$$

where

$$f_{\text{D}} = \frac{\text{D}}{(\text{H} + \text{D})} \quad (9)$$

is the deuterium abundance, k_{meas} comes from the water sample measurements, $k_{\text{HDO},\text{eff}}$ comes from our measured HDO effective optical constants, $2f_{\text{D}}(1 - f_{\text{D}})$ gives the probability of a HDO molecule in the sample, and $k_{\text{H}_2\text{O},\text{eff}}$ are the deuterium-free water effective optical constants.

In Figure 11, we plot k_{meas} (black line), the interpolated baseline across the HDO band (dashed red line), and the best HDO subtraction and resulting deuterium-free effective optical constants for water, $k_{\text{H}_2\text{O}}$ (blue line), corresponding to $\text{D}/(\text{H} + \text{D}) = (1.58 \pm 0.05) \times 10^{-4}$. Both the sample and HDO effective optical constants were at 120 K. The deuterium abundance in the water sample aligns well with the terrestrial value of about 1.56×10^{-4} (R. Hagemann et al. 1970), thereby increasing our confidence in our procedures and in the resulting HDO effective optical constants.

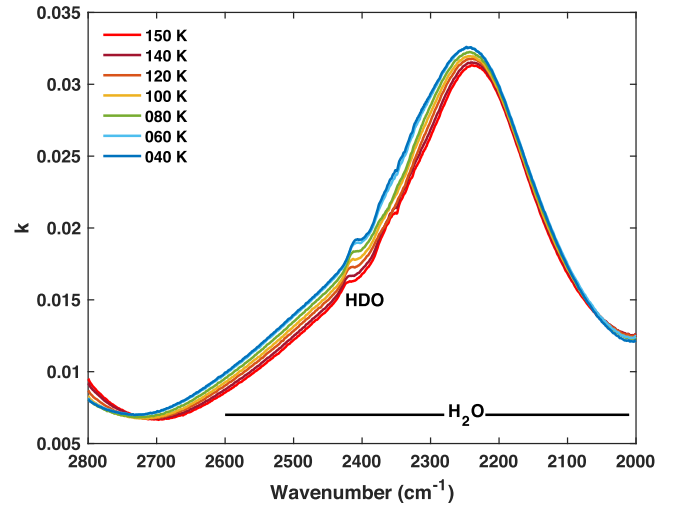


Figure 9. The imaginary part of the optical constants for the H₂O $\nu_2 + \nu_R$ band as a function of wavenumber. The band shows a slight increase in strength and a shift to higher wavenumbers as the temperature decreases. Naturally occurring HDO is visible near 2420 cm^{-1} . It shows the same increase in strength and shift to lower wavenumbers with decreasing temperature as seen in the HDO sample in Figure 6.

4. Hapke Modeling of Titania

The leading hemisphere of Titania showed the highest signal-to-noise detection of solid HDO in our JWST spectroscopic survey of the Uranian satellites (R. J. Cartwright 2026). We quantified Titania's HDO abundance by first converting the spectrum in Figure 1 from flux to geometric albedo, and then modeling the resulting spectrum with the Hapke radiative transfer model (B. Hapke 2012).

We used the Hapke model to account for light scattering by small surface particles on Titania. The most fundamental parameters in our Hapke model were the single-scattering albedo, ω_λ , which describes the fraction of light not absorbed by a single particle, and the single-scattering phase function, $P(g)$, which describes the angular distribution of light scattered by a particle at phase angle g . To obtain ω_λ , we used Hapke's equivalent slab model, the new k -values for crystalline H₂O and HDO embedded in crystalline H₂O ice described above, $n = 1.30$ at 4 μm for H₂O, and two particle sizes weighted by their fractional contribution to the surface area. For the single-scattering phase function, $P(g)$, we used a double Henyey-Greenstein function evaluated at the phase angle seen by JWST, $g = 2.69$, and clear, nearly spherical particles (i.e., Hapke parameters, $b = 0.63$ and $c = -0.60$).

We computed the optical constants for our Hapke model, k_{mod} , by assuming that HDO molecules were intimately mixed with H₂O molecules and weighting each effective optical constant by the probability of an H₂O, HDO, or D₂O molecule. Specifically,

$$k_{\text{mod}} = (1 - f_{\text{D}})^2 k_{\text{H}_2\text{O},\text{eff}} + 2f_{\text{D}}(1 - f_{\text{D}})k_{\text{HDO},\text{eff}} + f_{\text{D}}^2 k_{\text{D}_2\text{O},\text{eff}}. \quad (10)$$

The probability factors in front of the k -values in Equation (10) sum to one, as they should. For the expected small value of f_{D} , we ignored the presence of D₂O molecules.

For the remaining Hapke parameters, we used values typical of other investigations of icy outer solar system objects, see, e.g., A. J. Verbiscer et al. (2022) and W. M. Grundy et al. (2024). We set the macroscopic roughness, opposition width,

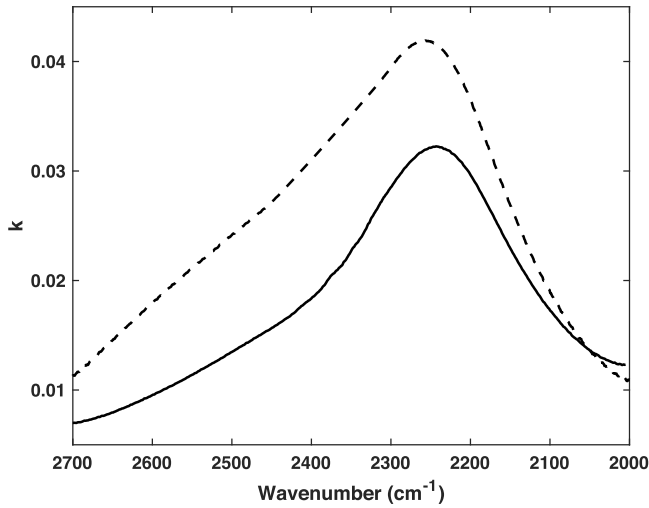


Figure 10. Deuterium-free k -values for the $\text{H}_2\text{O } \nu_2 + \nu_R$ band as a function of wavenumber. A significant difference exists between our values (solid black line) and those of R. M. Mastrapa et al. (2009) (dashed black line). The Mastrapa values have the largest uncertainties for weak bands such as this one due to scattering effects.

and opposition amplitude to $\bar{\theta} = 20^\circ$, $h = 0.057$, and $B_o = 0.36$, respectively.

We explored the parameter space of the key Hapke parameters using a Markov Chain Monte Carlo technique. The analysis employed 256 independent samplers (“walkers”) that traversed the parameter space, with each walker taking 512 sequential trial steps (“jumps”) to sample the posterior probability distribution. Particle diameters of 162 and 28 μm , a volumetric fraction of about 0.50 for each particle, effective optical constants at $T = 80$ K, and $\text{D}/(\text{H} + \text{D}) = (2.8 \pm 0.5) \times 10^{-4}$, all integrated over Titania’s hemisphere facing JWST, produced the best-matching geometric albedo spectrum (black line) to Titania’s spectrum (red line) in Figure 12.

For comparison, we plot the same model with $\text{D}/(\text{H} + \text{D}) = 1.56 \times 10^{-4}$ (dashed black line), i.e., the deuterium abundance of Vienna Standard Mean Ocean Water (VSMOW; R. Hagemann et al. 1970), and $\text{D}/(\text{H} + \text{D}) = 5.3 \times 10^{-4}$ (dotted-dashed black line), i.e., the deuterium abundance of comet 67P/C-G (D. R. Müller et al. 2022). The comparison indicates that Titania is enriched in deuterated water relative to Earth’s ocean water, but not as much as water in the coma of comet 67P/C-G.

Before discussing the implications of our deuterium measurement for the origin of Titania’s water, we take a step back and consider whether another compound could contribute to the absorption seen at 4.14 μm . The Near Infrared Mapping Spectrometer (NIMS) on the Galileo spacecraft found an absorption feature near 4 μm in Callisto spectra, which was attributed to sulfur dioxide, SO_2 (T. B. McCord et al. 1997). In Figure 13, we plot the laboratory absorbance spectrum of H_2O and HDO from Figure 4, along with laboratory absorbance spectra of $\text{H}_2\text{O} + \text{SO}_2$ at 100 and 50 K (M. J. Loeffler & R. L. Hudson 2010). Comparing the spectra in Figure 13, it is clear that SO_2 absorption occurs at shorter wavelengths than HDO absorption and therefore cannot contribute to the 4.14 μm band in our Titania spectrum. More recent NASA Infrared Telescope Facility (IRTF) and SpeX spectra of Callisto were compared to laboratory spectra of calcium carbonate (CaCO_3) and

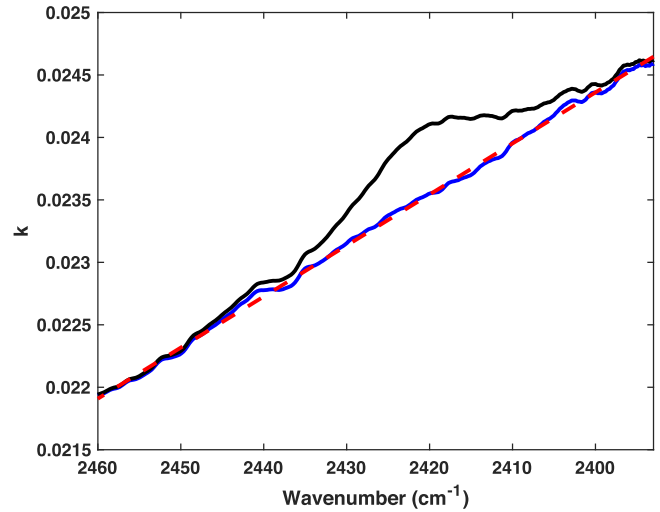


Figure 11. The imaginary component of the optical constants, k , for a water sample at 120 K (black line). Naturally occurring HDO appears as the broad band near 2420 cm^{-1} (4.13 μm). The interpolated baseline across the HDO band (dashed red line). The best HDO band subtraction and resulting deuterium-free effective optical constants for water (blue line) using Equations (8) and (9), corresponding to $\text{D}/(\text{H} + \text{D}) = (1.58 \pm 0.05) \times 10^{-4}$. Our deuterium abundance is in good agreement with the terrestrial value, which increases our confidence in our procedures and in the resulting HDO effective optical constants.

sodium carbonate (Na_2CO_3) (R. J. Cartwright et al. 2020). By inspecting their Figure 3, we found that these carbonates absorb at about 4.02 μm , wavelengths shorter than those of SO_2 , so they also do not contribute to the absorption observed in our Titania spectrum. Given the abundance of water on Titania (R. J. Cartwright 2026), HDO is likely exclusively responsible for the 4.14 μm absorption we see in our Titania spectrum.

5. Discussion

5.1. Origin from Protoplanetary Disk Water

Measuring the deuterium abundance in water on the icy surfaces of outer solar system bodies provides a powerful means of constraining their origin. In a model that combined isotopic exchange, outward migration of material in the protoplanetary disk, and infall of molecular cloud water, L. Yang et al. (2013) predicted $\text{D}/(\text{H} + \text{D}) \sim (3\text{--}4) \times 10^{-4}$ for water in the outer solar system, after 1 Myr of protoplanetary disk evolution (see their Figure 4). The close agreement with our measured value of $\text{D}/(\text{H} + \text{D}) = (2.8 \pm 0.5) \times 10^{-4}$ suggests that Titania’s water came from a combination of water inherited from the cold molecular cloud and water processed in the hot inner regions of the protoplanetary nebula. Titania’s deuterium abundance is in stark contrast to $\text{D}/(\text{H} + \text{D}) = (98 \pm 6) \times 10^{-4}$ in water for interstellar object 31/Atlas, a visitor from an ancient planetary system (M. Cordiner et al. 2026).

Additional evidence in the literature supports the idea that water in the outer solar system originated from a combination of processed inner-disk water and pristine molecular-cloud water. Using an HDO and H_2O band ratio technique pioneered by R. N. Clark et al. (2019) because HDO effective optical constants were not available, M. E. Brown et al. (2025) measured the deuterium abundance for the Saturnian satellites Mimas,

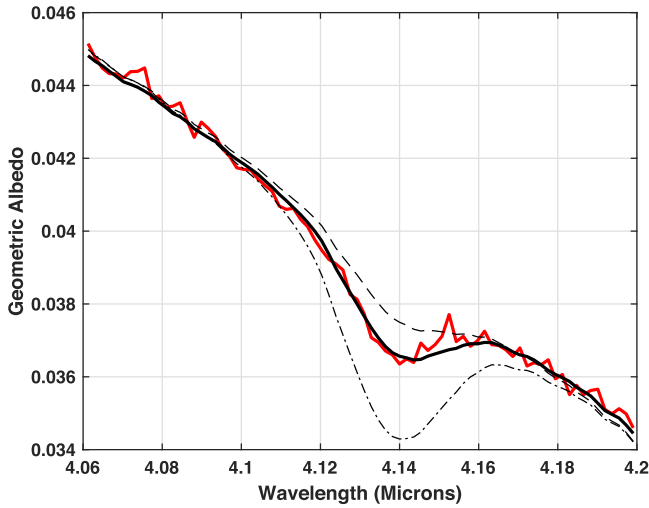


Figure 12. The geometric albedo spectrum of Titania from JWST and NIRSpec (red line). The best-fit model with $D/(H+D) = (2.8 \pm 0.5) \times 10^{-4}$ (solid black line). A model with $D/(H+D) = 1.56 \times 10^{-4}$ (dashed black line), i.e., the deuterium abundance of Vienna Standard Mean Ocean Water (R. Hagemann et al. 1970). A model with $D/(H+D) = 5.3 \times 10^{-4}$ (dotted-dashed black line), i.e., the deuterium abundance in water for comet 67P/C-G (D. R. Müller et al. 2022).

Tethys, Dione, Rhea, Hyperion, and Iapetus. They found $D/(H+D) = (2.3 \pm 0.5) \times 10^{-4}$. While it is possible that the Uranian satellites are slightly enriched in deuterium relative to Saturn’s moons, the existing measurements of $D/(H+D)$ overlap, supporting a broad degree of homogeneity over large distances in the outer solar system. These results support the L. Yang et al. (2013) protoplanetary disk model, which predicts consistent deuterium abundances at the heliocentric distances of Saturn and Uranus; however, it is important to reevaluate the deuterium abundances for Saturn’s satellites now that HDO effective optical constants are available.

Assuming water in the outer solar system formed as described by L. Yang et al. (2013), we used a simple model to estimate the fraction of Titania’s water from the molecular cloud, f_{cloud} , and the fraction from the inner protoplanetary disk ($1 - f_{\text{cloud}}$). Specifically,

$$(D/H)_{\text{measured}} = f_{\text{cloud}}(D/H)_{\text{cloud}} + (1 - f_{\text{cloud}})(D/H)_{\text{processed}}. \quad (11)$$

In Equation (11), we used $0.001 < (D/H)_{\text{cloud}} < 0.01$ and $(D/H)_{\text{processed}} = 2 \times 10^{-5}$, as described in L. Yang et al. (2013). The range in $(D/H)_{\text{cloud}}$ reflects observations of different clouds. In Figure 14, we plot the fraction of water-ice inherited by Titania from the molecular cloud as a function of the deuterium abundance of water in the molecular cloud. For all $(D/H)_{\text{cloud}}$ values, the fraction of Titania’s water inherited from the molecular cloud is a minority component, ranging from about 25% down to only a few percent. This simple model suggests that most of Titania’s water is reprocessed material from the warm inner disk that was transported outward.

Comparing the deuterium abundance of Titania to other solar system objects provides some further constraints on the origin of its water. In Figure 15, we plot $D/(H+D)$ for bodies across the solar system. Well-known patterns are recognizable. The low deuterium abundance of the Sun,

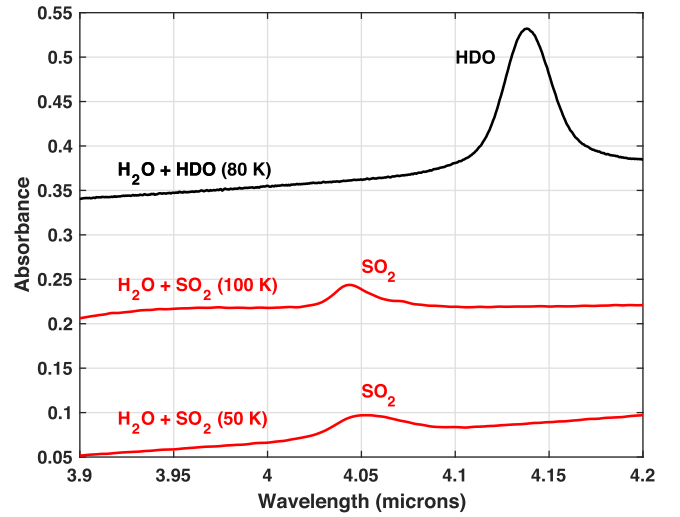


Figure 13. A comparison of laboratory absorbance by $H_2O + HDO$ from Figure 4 and $H_2O + SO_2$ at 100 and 50 K from M. J. Loeffler & R. L. Hudson (2010). SO_2 absorption does not overlap the HDO absorption. Carbonates absorb at shorter wavelengths than SO_2 , see, e.g., Figure 3 in R. J. Cartwright et al. (2020), so they too do not contribute to the 4.14 μm absorption in our Titania spectrum. Because of the abundance of water on the surface of Titania, it is likely that the absorption in our spectrum of Titania is exclusively due to HDO. The spectra are vertically offset for clarity.

Jupiter, and Saturn is the result of their originating from bulk nebular material rich in hydrogen gas and poor in water (J. Geiss & G. Gloeckler 1998). Uranus and Neptune are slightly enriched in deuterium due to their inheritance of some deuterium-rich water from cold molecular cloud material; see, e.g., H. Feuchtgruber et al. (2013). Earth’s water is enriched in deuterium relative to the protosolar value, likely reflecting the accretion of a combination of nebular material and hydrated, carbonaceous chondrite-like material during planet formation, and subsequent isotopic fractionation driven by preferential loss of hydrogen through atmospheric escape processes (H. Genda & M. Ikoma 2008; C. M. O. Alexander et al. 2012; B. Marty 2012). We note that the goal of Figure 15 is to present key contextual markers for the Titania deuterium measurement and not to provide a comprehensive summary of deuterium abundances in the solar system.

As seen in Figure 15, Saturnian satellites and Titania show less scatter in their deuterium abundances than comets; see the review of comet deuterium abundances by K. Altwegg et al. (2019). A possible reason for the relative uniformity of the satellite deuterium measurements is that homogeneous material, perhaps from a limited heliocentric zone and over a relatively limited time window, fed the circumplanetary disks. On the other hand, the scatter of deuterium abundances of comets suggests they accreted across a range of places and times in the protoplanetary disk.

It is also possible that, because most comet measurements come from the coma rather than the nucleus, some of the scatter could be due to fractionation occurring during sublimation (D. C. Lis et al. 2019). Recently, K. E. Mandt et al. (2024) observed ice-covered dust grains in the coma of 67/P that markedly enriched the coma deuterium abundance over the nucleus value. They reported $D/(H+D) = (2.59 \pm 0.36) \times 10^{-4}$ for the nucleus of 67/P.

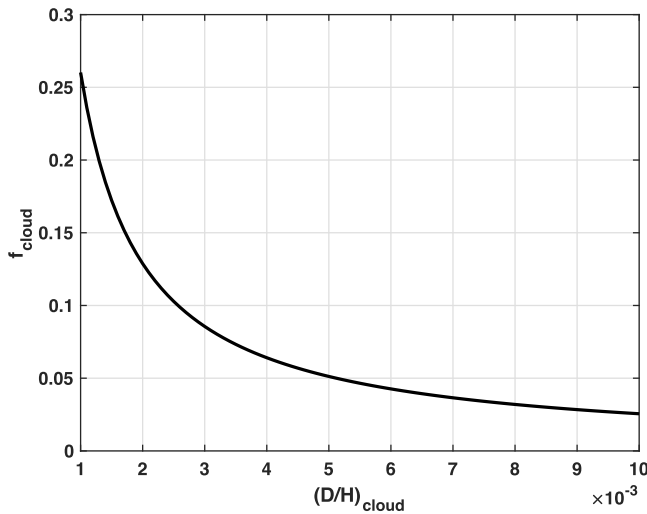


Figure 14. The fraction of Titania’s water-ice inherited from the molecular cloud, f_{cloud} , as a function of the deuterium abundance of water in the cloud, $(D/H)_{\text{cloud}}$. The range of deuterium abundances reflects the range of values in models and observations, as described in L. Yang et al. (2013). Most of Titania’s ice comes from reprocessed ice in the inner protoplanetary disk that was radially transported into the outer parts of the disk.

5.2. Formation in a Lower Temperature, Hydrogen-poor Circumplanetary Disk

The deuterium abundance of Titania also helps us discriminate between two scenarios for the formation of Uranus’ regular satellites. In the framework of O. Mousis (2004), the formation of the Uranian satellites is linked to a circumplanetary disk produced following a giant impact, often invoked to explain Uranus’s extreme obliquity. In their lower-temperature scenario, a solid-dominated disk is envisioned, fed by icy impactor debris and possibly by infalling solid solar-nebula material, in which isotopic exchange with hydrogen is inefficient because water is frozen and the disk contains little hydrogen, and water retains its elevated outer-solar-nebula $D/(H+D)$ value. In their higher-temperature scenario, satellites form within a hydrogen-rich disk in which water is initially present as vapor and undergoes efficient isotopic exchange with hydrogen, driving the $D/(H+D)$ ratio of water toward near-protosolar values. As the disk cools, water condenses into ice that has been isotopically reset, limiting the deuterium enrichment to $D/(H+D) < 1 \times 10^{-4}$. Our measured value for Titania, $D/(H+D) = 2.6 \times 10^{-4}$, exceeds the upper limit predicted for the higher-temperature scenario, and therefore disfavors a strong isotopic reset within a hydrogen-rich disk. Our result is more consistent with the incorporation of deuterium-enriched material from the outer solar nebula, broadly in line with the evolution models of L. Yang et al. (2013).

6. Conclusions

We measured the first effective optical constants for HDO and combined them with new effective optical constants for H_2O , a Hapke model, and a JWST spectrum of Titania to compute the deuterium abundance in the ice on the surface of Titania. We found that our deuterium abundance $D/(H+D) = (2.8 \pm 0.5) \times 10^{-4}$ is consistent with the model of L. Yang et al. (2013), suggesting that Titania’s water originated

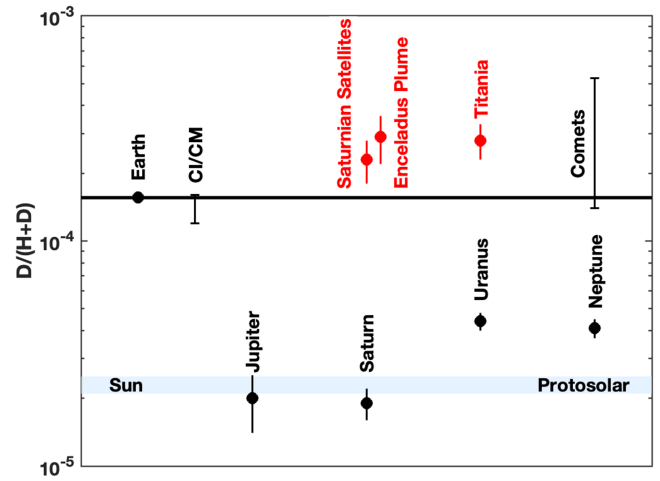


Figure 15. Deuterium abundances across objects in the solar system. Our measurement of $D/(H+D)$ for Titania, the average and standard deviation of twelve different $D/(H+D)$ measurements for seven different Saturnian satellites by M. E. Brown et al. (2025), and Enceladus plume measurements by J. H. Waite et al. (2009) are plotted in red and show less scatter than that of comets, suggesting a more homogeneous reservoir for water in forming outer-planet satellites than in forming comets. Values for the Sun/protosolar nebula are from J. Geiss & G. Gloeckler (1998); values for the Earth are from H. Craig (1961); values for carbonaceous chondrites (CI/CM) are from C. M. O. Alexander et al. (2012); values for Jupiter are an average from P. R. Mahaffy et al. (1998), C. Gapp et al. (2024), and H. Wiesemeyer et al. (2024); values for Saturn are an average from L. N. Fletcher et al. (2009) and J. D. R. Pierel et al. (2017); values for Uranus and Neptune are from H. Feuchtgruber et al. (2013); the range of values for comets are from K. Altwegg et al. (2019), and references therein.

from inherited molecular-cloud water and thermally processed inner-disk water that migrated outward. A simple end-member model suggests that most of Titania’s water came from processed inner-disk water. By comparing Titania’s deuterium abundance with those of Saturnian satellites and comets in the literature, we suggest that outer-satellite water came from a more homogeneous reservoir, and perhaps accreted over a shorter time interval, than comets. Lastly, Titania’s deuterium abundance suggests that it formed in a lower-temperature, hydrogen-poor circumplanetary disk rather than in a higher-temperature, hydrogen-rich disk.

The HDO and H_2O effective optical constants described in this paper are available at the OpenKnowledge@NAU archive.⁷

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⁷ <https://openknowledge.nau.edu/id/eprint/6359>

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