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LETTER

Letter to the Editor

Evidence for water vapor in Titan's atmosphere from ISO/SWS data*

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Abstract. The infrared spectrum of Titan around 40 μm was recorded in the grating mode of the Short Wavelength Spectrometer (SWS) of ISO, with a resolving power of about 1900. Two emission features appear at 43.9 and 39.4 μm, where pure rotational water lines are expected. Line strengths are about 8 times the 1σ statistical noise level. The H_2O vertical profile for water suggested by the photochemical model of Lara et al. (1996), rescaled by a factor of about $0.4^{+0.3}_{-0.2}$, is compatible with the data. The associated water mole fraction is about $8^{+6}_{-4} \times 10^{-9}$ at an altitude of 400 km (column density of $2.6^{+1.9}_{-1.6} \times 10^{14}$ mol cm^{-2} above the surface). The inferred water influx at 700 km in Titan's atmosphere is in the range (0.8–2.8) $\times 10^6$ mol cm^{-2}s^{-1}.

Key words: planets and satellites: Titan – infrared: solar system

1. Introduction

Two oxygen compounds were identified in Titan's atmosphere over 15 years ago: CO_2 (observed by Voyager 1/IRIS; Samuelson et al., 1983) and CO (observed from the Earth; Lutz et al., 1983). The derived abundance of CO_2 strongly suggests the presence of stratospheric water vapor as the required source of oxygen, though its detection has proven difficult.

Since the recent discoveries of CO_2 and H_2O in the stratospheres of the giant planets (Feuchtgruber et al., 1997; Lellouch et al., 1997), there has been a renewed interest in oxygen chemistry in reducing atmospheres. The essentials of the process were first outlined in Samuelson et al. (1983; see also Yung et al., 1984). Water ice enters the atmosphere in the form of icy particles. Vaporization and subsequent photolysis produce OH, which reacts with various hydrocarbon radicals (principally CH_3) to produce CO. The CO in turn reacts with OH, producing CO_2. Another possibility is that CO_2 is directly injected into the atmosphere (Feuchtgruber et al., 1997). Losses of CO_2 by photolysis and reaction with the methylene radical occur, but at rates insufficient to overcome CO_2 production. A steady state for CO_2 is reached when condensation and attendant precipitation of CO_2 ice halts a further buildup. The response time for the system on Titan is $\sim 4 \times 10^3$ years. In contrast, CO has a much longer equilibrium time constant (doubling time $\sim 10^9$ years), and its steady-state abundance is roughly proportional to the abundance of CH_3 and almost independent of the H_2O influx. Intercomparisons of observed abundances of the various oxygen and hydrocarbon species provide crucial tests for these ideas.

To date water vapor has been found in the stratospheres of all four giant planets. Two major sources of meteoritic H_2O are likely. One is the interplanetary component (IC) pervading the outer solar system and the other is a local component (LC) arising from sputtering and collisions associated with local icy satellites and rings. One of the goals for the search for water vapor on Titan is to determine the relative H_2O influxes at Saturn and Titan. The hope is to separate the relative contributions of the IC and LC in the Saturn system, which in turn will lead to a better understanding of the role these sources play in injecting water into the atmospheres of the other major planets. Another goal is to better understand the oxygen chemistry occurring in Titan's atmosphere and to set some constraints on the H_2O and CO_2 profiles.

Synthetic high resolution spectra of Titan demonstrated the potential value of the ISO spectrometers to study the satellite's atmosphere (Coustenis et al. 1993). Titan was observed with ISO in January and December 1997. The 7–45 μm spectrum recorded in January 1997 was used to infer the disk-average temperature and composition of Titan (Coustenis et al. 1998).

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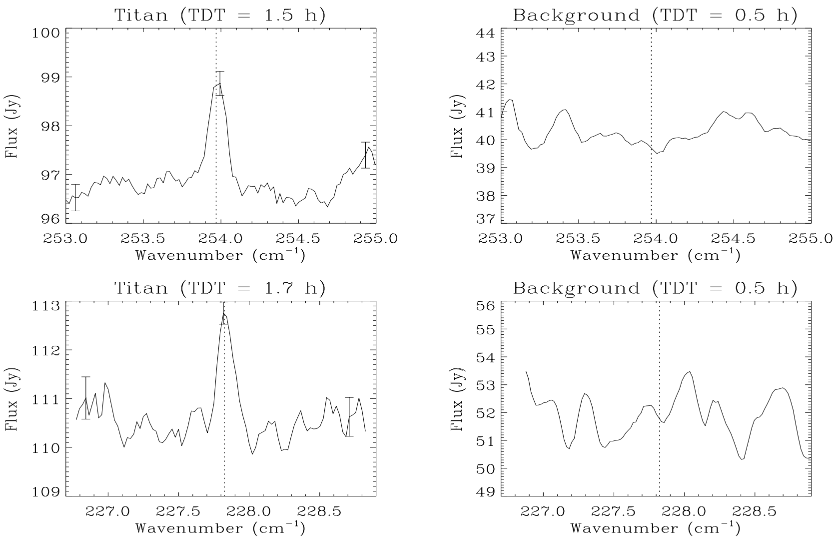

Fig. 1. Titan observations with SWS/Grating of two water lines at 227.8 and 254 cm^{-1} (43.9 and 39.4 μm respectively), along with the off-source spectra. The background plots correspond to 3 times less total integration time than the on-Titan (1 hr instead of 3.2 hrs). The 1σ error bars are of the order of 0.2 Jy and 0.25 Jy for the 254 and 227.8 cm^{-1} lines respectively.

2. Observations

Titan observations in the spectral region around 40 μm, which contains water vapor lines, were performed using the Short Wavelength Spectrometer (SWS) of ISO in the grating mode on December 27, 1997, when Titan was at its Greatest Eastern Elongation with respect to Saturn.

2.1. Strategy for data acquisition

For the detection of the weak water lines near 40 μm, we have used an ISO observational mode that corresponds to grating line profile scans optimized for sensitive observations of one or more single lines (de Graauw et al., 1996). Thus, on December 27, 1997, a total of 4.2 hours were allocated for the detailed search of water on Titan. Integration times of 3.2 hr and 1.0 hr were devoted to on-source and off-source observations, respectively (Fig. 1). The 3.2 hr spectrum on Titan is composed of 23 up-down scans on the 39.37 μm line and 26 up-down scans on the 43.89 μm line. The scans are overlapping, covering about 24 resolution elements and consist of pairs of scans in opposite directions in order to overcome detector transient effects.

Maximum sampling is reached by moving the scanners one step at a time. For each position, 8 resolution elements are imaged onto the 12 element detector array, which is aligned along the dispersion direction. This results in a staggered coverage of the wavelength range; the line and nearby continuum are recorded by all 12 detector elements, whereas the outer parts of the continuum are recorded by a gradually decreasing number of detector pixels. Thus, the statistical errors grow near the scanned borders with respect to the center. Any residual unidentified features appearing in the spectra at the 1% level (Fig. 1) might be attributed to the residuals of the instrumental artifacts such as: (a) glitches and spikes caused by the high energy radiation, (b) transient response of the detector in the presence of moderately high flux sources, and (c) tracking and pointing jitter on the tail of the beam profile associated with the stray light from Saturn. Additional uncertainty may result from residuals present in the SWS Relative Spectral Response file (for a general discussion of the SWS calibration and description of the main residual instrumental artifacts, see Salama et al., 1997, and references therein). In the case of the 3.2 hr observation of Titan, this results in around 1500 independent data points for the 39.37 μm line in a single resolution element at the line center.

SWS does not use spatial chopping; hence all spectra will contain some contributions from zodiacal light and galactic background as well as diffuse light from Saturn. In order to take these unwanted contributions into account we have acquired independent background spectra close to the source. These off-source observations are performed at a position on the sky chosen in such a way that (*i*) Titan is far away from the SWS slit, (*ii*) Saturn is at the same relative position with respect to the slit center as for the on-Titan observation, (*iii*) no other target is present in and around the SWS slit.

2.2. Reduction of the data

The reduction of the Titan observations was performed within the SWS Interactive Analysis environment. The main processing pipeline modules were run from the raw data telemetry (ERD) on each individual grating scan, with particular attention given to the detector dark current subtraction steps and to the removal of the spikes by use of the interactive tool. The effects of the ISO Solar System tracking and of the detector transients during each scan were treated by flatfielding (with a second order polynomial) each detector scan to the same continuum shape. This shape was determined from previous observations obtained in January 1997 over a larger wavelength range (29.5 to 45 μm) and well approximated by flat lines in the small wavelength ranges scanned here. Each scan was regridded to the instrumental resolution (0.14 cm^{-1} at 254 cm^{-1} and 0.11 cm^{-1} at 227.8 cm^{-1} respectively). Residual spikes in the data were removed by computing the median of each bin in the grid and clipping away data that exceeded the median by more than 3σ. These last two operations were iterated twice.

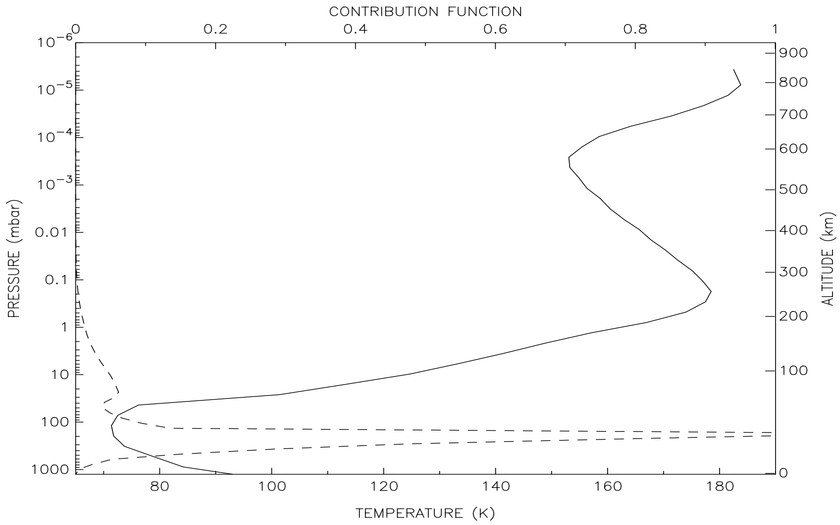

Fig. 2. Contribution functions of continuum (dashed line) and nominal thermal profile for Titan from ISO (full line).

The final spectrum was regridded to a resolution equal to five times the instrumental resolution. For each point in the grid, the median of the fluxes and their statistical standard deviation (=$\sigma/\sqrt{n}$) were computed. The data containing the two water lines at 227.8 and 254 cm^{-1} (43.9 and 39.4 μm respectively) are shown in Fig. 1. We subtracted the means of the background spectrum provided by the off-source measurements (also shown in Fig. 1) from the corresponding on-source Titan data. These means are on the order of 40 Jy for the 39.37 μm line and 52 Jy for the 43.89 μm line. This yields continuum fluxes at Titan of $\sim$ 56.5 Jy at 39.4 μm and $\sim$ 59.5 Jy at 43.9 μm, with corresponding peak fluxes of 2.2 and 2.5 Jy.

From the stray light contributions from Saturn (via the off-source measurements) and the strengths of the water lines at Saturn obtained by Feuchtgruber et al. (1997), we can estimate the contributions due to Saturn water, even though we do not observe them directly in the off-source spectra. We find these contributions to be on the order of 0.6 Jy for the 39.37 μm line and 0.5 Jy for the 43.89 μm line. The remaining peak fluxes associated with the Titan water lines are then about 1.6 and 2.0 Jy for each line, respectively.

A statistical analysis suggests peak intensities above the continuum of $\sim 8\sigma$ for the two water lines. Other features also appear above the formal 3σ level. These features lie near the ends of each spectral range and are probably due to increased noise, a result of the reduced number of detector pixels contributing to the signal there.

3. Modelling and results

The infrared continuum around 40 μm on Titan is determined mainly by collision-induced N_2-N_2, N_2-CH_4, and CH_4-CH_4 emissions in the upper troposphere, and aerosol emission in the lower stratosphere. Superimposed on this continuum are pure rotational lines of H_2O, as well as spectral signatures of emission bands of C_4H_2 and C_2N_2 at 220 cm^{-1} and 233 cm^{-1}. Calculations show that only the C_4H_2 contribution affects the inferred strength of the 227.8 cm^{-1} (43.89 μm) water line.

The spectrum of this region is sensitive to atmospheric temperature, collision-induced absorption between 15 and 40 km, and aerosol opacity between 40 and 200 km (Fig. 2). The emission observed in the C_4H_2 lines originates mainly from the 70–150 km range. The rotational water lines, however, are indicative of the upper stratosphere of Titan at altitudes of several hundred kilometers. These weak, optically thin lines ($\tau \sim$ 0.53 at 43.9 μm and $\sim$ 0.29 at 39.4 μm) do not provide constraints on the vertical profile of H_2O, but allow us to test pre-existing photochemical models. Their broad contribution functions peak near the 0.01 mbar level on Titan (around an altitude of $\sim$ 400 km), extending between 1 and 10^{-5} mbar (between 200 and 700 km; see Fig. 3).

Accordingly, a theoretical water vapor spectrum was computed for Titan, with spectroscopic parameters from the GEISA'97 data bank (Husson et al. 1997). The nominal and extreme temperature profiles used in the calculations are derived for the stratosphere (up to about 400 km) from analyses of the ν_4 methane band at 7.7 μm (1304 cm^{-1}), also observed by ISO/SWS (Coustenis et al., 1998). These profiles are calculated for methane abundances of 1.9% in the stratosphere (nominal) and between 0.5 and 3.4% for the extreme values (Lellouch et al., 1989). They are then extrapolated in the upper atmosphere so that they join the recommended model of Yelle et al. (1997) and references therein (the nominal profile is plotted in Fig. 2).

In our modelling, contributions from C_4H_2 (with a mixing ratio of 1.5 $\times 10^{-9}$, derived from its other band at 628 cm^{-1}), and from estimated water lines from Saturn (simulated with a Gaussian profile and based on values by Feuchtgruber et al., 1997) were included.

We find that a synthetic spectrum using a constant H_2O mole fraction of 4 $\times 10^{-10}$ above the saturation level is compatible with the observed SWS/ISO data.

We have also calculated theoretical profiles of the two lines based on the vertical distribution of H_2O predicted by the photochemical model of Lara et al. (1996, their Fig. 12). We find that the H_2O profile of Lara et al. (1996), multiplied by factors of 0.35 and 0.45 gives a satisfactory fit to the observations in the

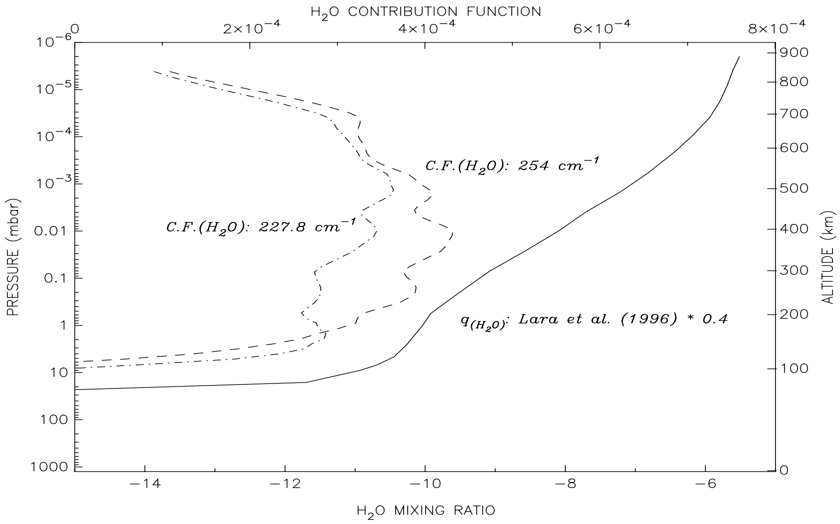

Fig. 3. Water vapor contribution functions and vertical profile used in the calculations for the best fit, equal to 0.4× that of Lara et al. (1996).

227.8 and 254 cm^{-1} lines respectively (Fig. 4). On this value, uncertainties due to instrumental noise, position of the continuum level in the data, and atmospheric modelling (notably the uncertainty on the thermal profile as mentioned earlier) need to be included. Our final water vapor profile is a mean value of $0.4^{+0.3}_{-0.2}\times$ the Lara et al. profile (Fig. 3). The associated water vapor mole fraction at 400 km (where the contribution functions peak) is then $8^{+6}_{-4} \times 10^{-9}$. The corresponding H_2O column density is $2.6\ ^{+1.9}_{-1.6} \times 10^{14}$ mol cm^{-2}.

4. Discussion

With our evidence for water vapor in Titan and the detection of CO_2 and H_2O in Saturn (de Graauw et al., Feuchtgruber et al. 1997), all three major oxygen compounds (CO, CO_2, H_2O) appear to be present in both the atmospheres of Titan and Saturn, and intercomparisons of the associated oxygen chemistry become possible. In particular, estimates of the relative rates of H_2O injection into the two atmospheres follow from abundance determinations and photochemical modelling.

The Lara et al. H_2O profile was calculated by using a water external flux of 6.2×10^6 mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$ referred to the tropopause for an eddy diffusion coefficient at the homopause $k_{hom} \sim 10^7$ $\mathrm{cm}^{-2}\mathrm{s}^{-1}$. A linear scaling of this model suggests that the water vapor flux that best fits our data is $2.5^{+1.8}_{-1.3}\times 10^6$ mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$. The meteoroid ablation model of English et al. (1996) suggests that meteoritic water should be deposited in Titan's atmosphere over a broad range of altitudes centered around 700 km. Referring the water flux to 700 km then yields an H_2O influx at Titan $\sim 1.6 \times 10^6$ mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$. Due to a large intrinsic uncertainty, the actual value lies somewhere in the range $8 \times 10^5 - 2.8 \times 10^6$ mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$, not including any uncertainties associated with the eddy diffusion coefficient.

No significant spatial variations in the H_2O distribution are expected, inspite the fact that the incoming micrometeorite flux is expected to be much larger on the leading than on the trailing side of Titan. The reason is that the lifetime of H_2O in the atmosphere is considerably long (on the order of 5 years), compared to the horizontal mixing duration: for a zonal wind of 100 m/s, material can be transported around Titan in very short periods of time (about 2×10^5 sec, that is a thousand times faster). This remains true even if the zonal wind decreases with altitude.

For Saturn, Feuchtgruber et al. (1997) find H_2O fluxes of $3 \times 10^5 - 5 \times 10^6$ mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$, depending primarily on the eddy diffusion profile. Using the most recent estimate of Saturn's eddy diffusion coefficient by Parkinson et al. (1997) ($K_{hom} = 10^8$ $\mathrm{cm}^2\mathrm{s}^{-1}$), the H_2O flux into Saturn is then (1.5–5) $\times 10^6$ mol $\mathrm{cm}^{-2}\mathrm{s}^{-1}$. Consequently, the Saturn/Titan flux ratio is then in the range 0.5 to 6.2.

It is not possible at this time to assert with certainty the relative importance of the local (LC) and interplanetary (IC) components in supplying water to the atmospheres of Saturn and Titan. The H_2O influx we derive from the data appears to be in basic agreement with that inferred from the ablation model of English et al. (1996) for the leading side of Titan (integrated value of $\sim 2 \times 10^6$ mol cm^{-2} s^{-1}), and is therefore in reasonable accord with what is expected for the IC. Also, the fact that the flux into Saturn is not much larger than that into Titan suggests that the LC is not overly dominant. Indeed, gravitational energetics greatly favors Saturn as the recipient of water originating from the inner icy satellites and rings (see e.g. Connerney and Waite, 1984; Connerney, 1986; Northrop and Connerney, 1987 for discussions of the influx into Saturn of water eroded from Saturn's rings). Note however that sputtering of H_2O ice from Phoebe, Iapetus, and Hyperion might provide preferential sources for Titan.

On the other hand, even the IC is expected to be enhanced at Saturn as the result of gravitational focussing. Specifically, the flux into a planet is enhanced, with respect to its value away from the gravitational pull of the planet, by a factor $f = 1 + (v_{esc}/u)^2$, where v_{esc} is the escape velocity from the planet and u is the relative particle-planet velocity. Following Moses (1992), we adopt for u the heliocentric escape velocity at Saturn's orbit (13.7 km/s). This leads to f = 7.8 for Saturn and f = 1.02 for Titan, i.e. a ratio equal to 7.5. This value is slightly outside the error bars on the Saturn/Titan influx ratio given before, but

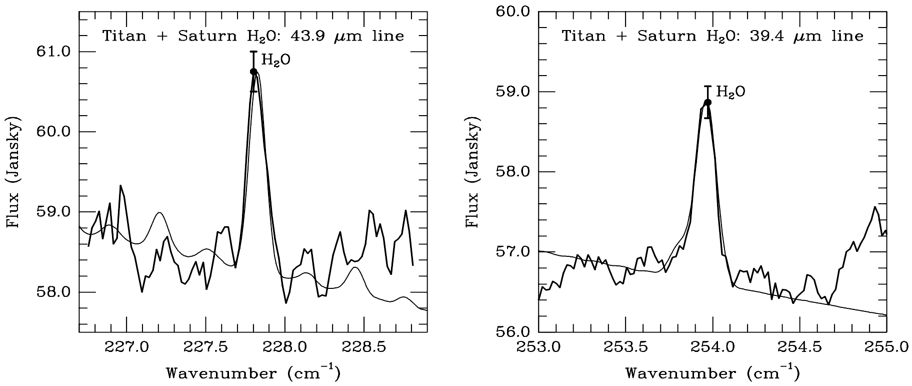

Fig. 4. Synthetic spectra calculated with 0.35 and 0.45 times the water vertical profile predicted by the photochemical model of Lara et al. (1996), to fit the 227.8 and 254 cm^{-1} lines respectively.

could be reconciled by a moderate change in the velocity of the icy particles. However, the above reasoning ignores possible electrical charging of the dust from ion collisions in Saturn's magnetosphere. The resulting precipitation of highly charged ice particles into Saturn's atmosphere along magnetic lines of force will enhance the H_2O influx at Saturn relative to that at Titan.

A partial test of the Lara et al. (1996) photochemical model entails comparing the calculated abundances of H_2O and CO_2 with those suggested by the observations. The H_2O flux in the Lara et al. model was adjusted in order to fit the CO_2 emission observed by Voyager 1/IRIS, for an assumed CO mole fraction of 5×10^{-5}. As mentioned previously, the H_2O profile they propose (their Fig. 12) corresponds to an external flux of water of 6.2×10^6 $cm^{-2}s^{-1}$, referred to the tropopause. However, the CO_2 profile calculated simultaneously (and shown also in their Fig. 12) is a factor of two too high when compared with observations. In fact, there appears to be an inconsistency between Figs. 11 and 12 of this article. Re-examination of the calculations by L. M. Lara (priv. comm.) reveals that Fig. 11 has a wrong caption and that the CO_2 Voyager observations are indeed matched with an H_2O flux of 3.1×10^6 mol $cm^{-2}s^{-1}$. The H_2O flux that we find hereabove to give the best match of our observations (2.5×10^6 mol $cm^{-2}s^{-1}$) is then in good agreement with the value required for CO_2. Although there remains considerable uncertainty on the stratospheric abundance of CO (Noll et al., 1996, and references therein), we note that this agreement holds regardless of the adopted value for CO, since, to first order, the CO_2 abundance is independent of the abundance of CO as long as the latter is near equilibrium.

In conclusion, the observations of two independent water lines gives evidence for H_2O vapor in the atmosphere of Titan. We have inferred the total H_2O column density, the associated value for its abundance around the 10 μbar level, and the H_2O flux. Although further work will be needed to reconcile all observables and to disentangle local and interplanetary sources of water, our observations imply progress is being made toward understanding Titan's oxygen chemistry, and that the complicated issues involved with dust transport in the Saturn system can now be addressed with growing confidence.

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