SUB MILLIMETER OBSERVATIONS OF TITAN: GLOBAL MEASURES OF STRATOSPHERIC TEMPERATURE, CO, HCN, HC₃N, AND THE ISOTOPIC RATIOS ¹²C/¹³C AND ¹⁴N/¹⁵N

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ABSTRACT

Interferometric observations of the atmosphere of Titan were performed with the Submillimeter Array on two nights in 2004 February to investigate the global average vertical distributions of several molecular species above the tropopause. Rotational transitions of CO, isomers of HCN, and HC₃N were simultaneously recorded. The abundance of CO is determined to be 51 ± 4 parts per million (ppm), constant with altitude. The vertical profile of HCN is dependent on the assumed temperature but generally increases from 30 parts per billion at the condensation altitude (~83 km) to 5 ppm at ~300 km. Furthermore, the central core of the HCN emission is strong and can be reproduced only if the upper stratospheric temperature increases with altitude. The isotopic ratios are determined to be ¹²C/¹³C = 132 ± 25 and ¹⁴N/¹⁵N = 94 ± 13 assuming the Coustenis & Bézard temperature profile. If the Lellouch temperature profile is assumed, the ratios decrease to ¹²C/¹³C = 108 ± 20 and ¹⁴N/¹⁵N = 72 ± 9. The vertical profile of HC₃N is consistent with that derived by Marten et al.

Subject headings: planets and satellites: individual (Titan) — radio lines: solar system — submillimeter — techniques: interferometric

1. INTRODUCTION

The atmosphere of Titan is cold, dense, and nitrogen-dominated. Water, CO, nitriles, and hydrocarbons have been detected by the Voyager spacecraft and from Earth. Understanding this unique atmosphere is a major focus in planetology, particularly with the imminent arrival of the Cassini spacecraft with the Huygens probe destined for Titan. Studies of the photochemistry of Titan’s atmosphere have been ongoing since the Voyager era and have become increasingly sophisticated (e.g., Yung et al. 1984; Toublan et al. 1995; Lara et al. 1996; Lébonnois et al. 2001, 2003). These models rely on accurate observational data as primary constraints.

Trace molecules such as CO and nitriles contribute many emission features that can be used to probe the vertical structure of its atmosphere. As access to the millimeter and submillimeter wavelength bands has improved, there has been a series of ground-based observational studies of Titan’s atmosphere (e.g., Muhleman et al. 1984; Tanguy et al. 1990; Gurwell & Muhleman 1995, 2000; Hidayat et al. 1997, 1998; Marten et al. 2002). The Submillimeter Array (SMA) is well suited for observing Titan.

2. OBSERVATIONS AND DATA REDUCTION

We utilized the SMA to obtain high-precision spectroscopy of the atmosphere of Titan on 2004 February 1 and 2004 February 21. Parameters for these observations are in Table 1; we briefly discuss here a few important points.

The nearly 2 GHz total bandwidth/sideband allowed for several molecular transitions to be observed. The lower sideband (LSB) includes the CO (3–2), H¹³CN (4–3), HC¹³N (4–3), and HC₃N (38–37) rotational transitions. The upper sideband (USB) covered both the ground and vibrationally excited HCN (4–3) ν₂ = 0, 1 transitions and the HC₃N (39–38) transition.

The large separation between Saturn and Titan relative to the primary beam size severely downweighted the integrated flux of Saturn. In addition, Saturn is highly resolved on the baselines used, further reducing any contribution from Saturn. We consider any contamination from Saturn negligible.

Data from each night were independently calibrated to remove instrumental gain drifts over time and to correct the complex bandpass response. Titan’s signal strength was sufficient for application of phase self-calibration. The flux scale was initially determined using relatively line-free regions of the Titan spectrum. In the absence of molecular lines, the emission from Titan in the submillimeter band comes from the region near the tropopause (~40 km, 71 K), and this “continuum” emission provided the primary flux calibration reference. Further adjustments to the flux scale were performed during analysis.

Spatially unresolved (e.g., “zero-spacing”) spectra for each night were obtained by fitting the visibility data for each channel with a model, correcting for the spatial sampling of the interferometer. To minimize errors associated with this model fitting, only baselines less than 125 m (corresponding to angular scales greater than 1′.4) were used. The relative sideband scale in the average spectra is better than 0.5%. The spectra from the 2 days were scaled to reflect a common apparent size of 0′.866 then added to increase the signal-to-noise ratio. Figure 1 presents the final calibrated spectra.

3. ANALYSIS, RESULTS, AND DISCUSSION

The measured line shape from a planetary atmosphere is a complex function of the vertical profiles of temperature and absorber abundances. This information is “encoded” in the line shape through pressure broadening and can be retrieved within certain bounds through suitable numerical inversion or radiative transfer modeling. We updated and expanded our iterative least-squares inversion algorithm, previously used to measure the atmospheric abundance of CO on Titan (Gurwell & Muhleman 1995, 2000), to allow analysis of the rotational lines observed for this work.

The base thermal profile model was the equatorial profile A determined by Coustenis & Bézard (1995) based on Voyager II/
TABLE 1

| **Titan Observational Parameters** | 2004 Feb 01 | 2004 Feb 21 |
|-----------------------------------|-------------|-------------|
| LO frequency (GHz)                | 349.95      | 349.95      |
| Total bandwidth/sideband (MHz)    | 1968        | 1968        |
| Channel spacing (MHz)             | 0.8125      | 0.8125      |
| Primary beam half-power beamwidth (arcsec) | 33          | 33          |
| Synthesized resolution (arcsec)   | ~0.5        | ~0.5        |
| Calibration sources               | Ceres, Callisto | Ceres, Callisto |
| Number of antennas                | 5           | 6           |
| Integration time (minutes)        | 257         | 232         |
| Zenith atmospheric opacitya       | 0.18–0.28   | 0.15–0.20   |
| Titan diameterb                    | 0.866       | 0.841       |
| Separation from Saturn (arcsec)   | 171–182     | 113–126     |
| Sub-Earth longitude               | 233.4–240.5 | 324.4–331.1 |
| Sub-Earth latitude                | ~25.66      | ~25.82      |

a At LO frequency.

b For surface; assumes radius of 2575 km.

IRIS spectra of methane and the Voyager radio occultation results; we refer to this as profile A as well.3 We investigated two ad hoc temperature profiles related to profile A. Profile B is isothermal at 180 K above 230 km, and profile C is isothermal at 180 K from 230 to 350 km, with a positive temperature gradient above 350 km. Profile D is an older profile from a reanalysis of the Voyager radio occultation data (Lellouch 1990; see Fig. 2a). The base molecular abundance model has CO uniformly mixed at 52 parts per million (ppm; Gurwell & Muhleman 2000), the HCN and HC₃N profiles following the results of Marten et al. (2002), and isotopic ratios of ¹²C/¹³C = 89 (Hidayat et al. 1997) and ¹⁴N/¹⁵N = 65 (Marten et al. 2002).

3 Also used in Hidayat et al. (1997, 1998), Gurwell & Muhleman (2000), and Marten et al. (2002). This model is appropriate since the observations are of unresolved (whole-disk) spectra, which are heavily weighted by emission from equatorial and low southern latitudes.

3.1. CO

CO has a long chemical lifetime in the atmosphere of Titan (∼10⁹ yr; Yung et al. 1984) and is expected to be uniformly mixed from the surface to high altitude. Observational evidence has shown this to be the case, although there is disagreement regarding the value (Gurwell & Muhleman 1995, 2000; Hidayat et al. 1998). Here we assumed that the CO profile is constant with altitude and iteratively fitted the LSB spectrum for the stratospheric CO abundance.

There is a modest error associated with the overall flux scale of the spectrum, which was set using a basic model of the Titan spectrum in a relatively line-free region near 344.0 GHz. This error was calibrated by scaling the current model spectrum to best fit the observed spectrum at each iterative step. This essentially eliminates the effect of an overall error in the flux density scale by forcing a best fit to the normalized line shape.
Fig. 2.—(a) Model temperature profiles used in inversion analysis. (b) HCN best-fit profile solutions assuming temperature models A, B, C, and D, and the HCN profile (M) determined by Marten et al. (2002). The gray scale represents the error envelope for solutions A, B, and C. (c) Observed and best-fit HCN line center spectra for HCN profiles A, D, and M. (d) Observed and best-fit HCN line core spectra for HCN profiles A, B, and C.

rather than to a fixed flux scale spectrum. This calibration is robust for interferometric observations, which preserve the relative line to continuum of the source emission. The output of the iterative inversion is the best-fit CO abundance and a best-fit correction to the overall flux scale. This scale factor is applicable to both sidebands.

The best-fit CO abundance is insensitive to the different temperature models, with solutions of 50.6, 51.5, 51.8, and 52.0 ppm (all \(10^3\) ppm) obtained with temperature models A, B, C, and D, respectively. Taking the uncertainty of the upper atmospheric temperature, we consider all of these solutions as equally valid and adopt a mean stratospheric CO abundance of 51 ppm. This agrees well with the previous stratospheric CO4 measurements of Gurwell & Muhleman (2000; ppm),52 ppm Gurwell & Muhleman (1995; ppm), and Muhleman et al. (1984; ppm), as well as the initial measurement of ppm on Titan from near-IR observations (Lutz et al. 1983; in the troposphere). However, these values are at odds with other recent measurements, such as those of Hidayat et al. (1997; Marten et al. 2002). Radiative transfer modeling using the HCN profile of Marten et al. (2002) results in a poor fit to the HCN line wings, indicating that the profile is overabundant in HCN below \(180\) km. The nearly constant HCN profile above \(180\) km does not provide enough contribution to the central \(50\) MHz of the HCN line shape, resulting in a poor fit to the line center (see Fig. 2c). Our results strongly favor a steadily increasing HCN mixing ratio from the condensation altitude to at least \(300\) km.

3.3. HCN: Upper Atmospheric Temperature

None of the calculations using temperature models A or D provide a good fit to the HCN (4–3) line core, which exhibits strong emission in the central \(5\) MHz. We find no manipulation of the HCN mixing ratio profile that can reproduce this line core assuming these standard temperature profiles. Yelle & Griffith (2003) present a reanalysis of 3 \(\mu\)m HCN fluorescence observations obtained by Geballe et al. (2003). They find the observations can be fitted assuming the HCN profile determined by Marten et al. (2002) up to \(450\) km and a temperature profile similar to model A. Their temperature model (from Yelle et al. 1997) was constructed to satisfy a variety of observational and theoretical constraints. In relation to this work, a key component of this temperature profile is a smooth decrease from about \(180\) K near \(250\) km (250 \(\mu\)bar) to a mesopause temperature of \(135\) K near \(600\) km (0.2 \(\mu\)bar), a trait shared with model A below \(450\) km.

The HCN spectrum presented here is clearly incompatible with the Yelle et al. (1997) and model A temperature profiles. A negative temperature gradient above \(250\) km results in a line core in absorption (see Fig. 2d). An isothermal upper atmosphere (model B) can account for some of the strong core emission, but not all. The progression of model fits shown in...
Figure 2d suggests that the only way to fit the intense line core is to have an upper stratosphere that is warmer than the stratosphere near 250 km. Model C has such a profile and provides the closest fit to the data.

There is little observational evidence for a temperature maximum occurring only near 250 km (250 μbar). The thermal profile below 180 km (1 mbar) is measured from IR and radio observations (e.g., Coustenis et al. 2003), and the thermospheric temperatures are constrained by UV occultation measurements (Smith et al. 1982). Several lines of evidence point to a mesopause around 600 km, above 1 μbar. Thermal profiles determined from occultations of star 28 Sgr by Titan do sense the 300–500 km altitude range (Hubbard et al. 1993) and especially for the southern hemisphere are relatively consistent with an isothermal atmosphere below ~350 km, although the large scatter in the inversion results for different data sets makes a definitive statement difficult, and a positive temperature gradient from 300 to 350 km is possible.

We propose here that the strong HCN emission core is solid evidence for a significantly warmer atmosphere above 250 km compared to the profiles from Yelle et al. (1997) and Coustenis et al. (2003). The possibility of a mesopause above 1 μbar is not precluded, but we find that the profile likely cannot have a negative temperature gradient below roughly 450 km.

### 3.4. Isotopic Ratios

Iterative solutions for the ratios of HCN/H13CN and HCN/H15N were obtained assuming that the less abundant isomers had the same vertical profile shape as HCN and that the isomer ratios reflect the overall ratios of 12C/13C and 14N/15N in the atmosphere. The solutions we obtain show that retrievals of H13CN and HC15N are less sensitive than that of HCN to the assumed temperature profile below 300 km. Therefore, there is a dependence of the isotopic ratios on the assumed temperature profile. For models A, B, and C (which are identical below 230 km), we find 12C/13C = 132 ± 25 and 14N/15N = 94 ± 13. Both ratios decrease assuming model D to 12C/13C = 108 ± 20 and 14N/15N = 72 ± 9.

Terrestrial values for the carbon and nitrogen isotopic ratios are 89 and 272, respectively (Fegley 1995). Our observations are consistent with nitrogen being enriched in the heavier isotope by a factor of 2.9 and carbon being depleted in the heavier isotope by a factor of 0.5, relative to terrestrial values. In contrast, using model A, Hidayat et al. (1997) derived 12C/13C = 95 ± 25 and Marten et al. (2002) derived 14N/15N = 65 ± 5. These previously measured isotopic ratios are consistent with results we obtain assuming temperature profile D but are not consistent with results for profiles A, B, and C.

### 3.5. HCN

Previous observations of HCN have shown it is most abundant above 300 km (Marten et al. 2002). The observations presented here are unresolved at a resolution of 0.8125 MHz, which is consistent with an abundance limited to altitudes above 300 km. Since we did not resolve the line shapes, retrieval of a profile was not practical. We instead modeled the overall column abundance assuming that the shape of the profile determined by Marten et al. (2002) was correct. We find that the HCN transitions we observed are consistent with the Marten et al. (2002) profile for all the model temperature profiles.

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