CO ON TITAN: MORE EVIDENCE FOR A WELL-MIXED VERTICAL PROFILE

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ABSTRACT

We report new interferometric observations of the CO (2 − 1) rotational transition on Titan. We find that the spectrum is best fit by a uniform profile of 52 ppm, with estimated errors of 6 ppm (40 to 200 km) and 12 ppm (200 to 300 km).

1. INTRODUCTION

The atmosphere of Titan exhibits a complex photochemistry, and many nitriles and hydrocarbons have been detected by Voyager spacecraft and from Earth. Until recently, however, only two oxygen-bearing species had been detected on Titan: CO$_2$ (observed by Voyager 1; Samuelson et al. 1983) and CO (observed from Earth; Lutz et al. 1983).

The presence of oxygenated molecules is interesting because the atmosphere of Titan is strongly reducing. The cold temperatures of the lower stratosphere and the troposphere imply that CO$_2$ condenses out of the lower atmosphere and is continuously deposited on the surface. To sustain the carbon dioxide abundance a source of oxygen is needed, and it is generally assumed to be supplied in water from bombardment of the upper atmosphere by icy grains. In this model vaporized water is quickly photolyzed to produce OH, and OH reacts with hydrocarbon radicals such as CH$_3$ to produce CO. CO in turn reacts with OH to produce CO$_2$ (Samuelson et al. 1983, Yung et al. 1984, Toublanc et al. 1993). While CO$_2$ has a short lifetime (order $10^3$–$10^4$ years), the photochemical lifetime of CO in the atmosphere of Titan is estimated to be very long ($\sim 10^9$ years; Yung et al. 1984, Chassefière and Cabane 1991).

Observationally the missing piece of the oxygen chemistry has been the source, water. Recently, water vapor was detected in the upper atmosphere of Titan by the Short Wavelength Spectrometer (SWS) aboard the Infrared Satellite Observatory (Coustenis et al. 1998). With observations of the three major components of oxygen chemistry, it is now possible to check the internal consistency of photochemical models, and to compare the oxygen chemistry and water infall rate of Titan with the other giant planets, particularly Saturn (Feuchtgruber et al. 1997, Coustenis et al. 1998).

Understanding the oxygen chemistry relies on accurate knowledge of the abundance and distribution of each species. A longstanding discussion regarding the CO distribution in Titan’s atmosphere, spanning more than a decade, has been primarily directed toward...
determining if CO is well-mixed (Marten et al. 1988; Gurwell and Muhleman 1993; Hidayat et al. 1998). Since the residence lifetime of CO is long compared to transport timescales, the molecular weight of CO is the same as for the dominant N\textsubscript{2} gas, and the atmosphere is never cold enough for CO to condense, carbon monoxide should be uniformly mixed in the Titan atmosphere to high altitudes.

Observational data, however, give conflicting results. Table 1 provides data on the CO abundance as measured by ground-based observers over the past 17 years. These observations have been sensitive to either the troposphere (near- and mid-IR) or the stratosphere (millimeter). The data in Table 1 show that no clear consensus has emerged regarding the CO abundance, either in the troposphere or the stratosphere.

In this Note, we present an analysis of new interferometric observations of the CO (2 − 1) line on Titan. The results of this study have important implications for our understanding of the oxygen budget and photochemistry of the stratosphere of Titan.

2. OBSERVATIONS AND DATA REDUCTION

Observations of the CO (2 − 1) rotational transition (rest frequency \( \nu_0 = 230.5380 \text{ GHz} \)) on Titan were made on November 11 and 12, 1999 with the Owens Valley Radio Observatory Millimeter Array, located near Big Pine, California. The Titan ephemeris data was generated using the Jet Propulsion Laboratory’s Horizons on-line system (Giorgini et al. 1996). Titan was approaching eastern elongation with respect to Saturn, with a separation increasing from \( \sim 145'' \) to more than \( 200'' \) over the two day period.

The interferometer was aligned in a fairly compact configuration, providing a synthesized beam of roughly \( 2'' \times 2.5'' \) at the observing frequency, while Titan’s apparent surface diameter was \( 0.86'' \) (at a distance of 8.2165 AU). Titan was observed on each night over a period of about 7 hours, when it was above 30° elevation. A single measurement on each baseline consisted of a three minute integration during which the complex visibility of the source was recorded. Amplitude and phase gain variations were monitored through observations of 0235+164 approximately every 20 minutes, and antenna pointing was checked about every two hours using 3C84. The total integration time spent on Titan equaled 238 minutes on each night.

The signal was detected for each antenna pair in two correlator systems: a wide-band analog cross correlator (\( \sim 1 \text{ GHz bandwidth} \)) and a digital spectrometer. The CO line is significantly wider than this system bandwidth, and we utilized two local oscillator tunings to provide better coverage of the line: on November 11 the digital spectrometer measured (in two secondary LO tunings) the line in the upper sideband from \( \Delta \nu = -656 \text{ MHz} \rightarrow +32 \text{ MHz} \), and on November 12 from \( \Delta \nu = -32 \text{ MHz} \rightarrow +656 \text{ MHz} \). Spectra in the image sideband, approximately 3 GHz lower in frequency, were also recorded. The sideband signals were isolated to better than 20 dB using a phase-switching cycle. The combination of two first and second LO tunings allowed us to ultimately measure \( \pm 650 \text{ MHz} \) of the center frequency of each sideband at 4 MHz resolution, and \( \pm 16 \text{ MHz} \) at 0.5 MHz resolution in the line core.

Calibration of the digital correlator passband was done through observations of 3C273 and an internal correlated noise source. The relative calibration of the sidebands was accurately measured from observations of Uranus, 3C273, 3C84, and 0235+164 (to \( \leq 1\% \)), since nearly all weather and instrumental effects impact each sideband in a similar manner. We note that the ability to isolate the astronomical signal sidebands and record independent spectra in each sideband represents a significant advantage for interferometric relative to single-dish observations of CO on Titan because the emission line is significantly broader than the spectrometer bandwidth. In this case the most precise measure of the line-to-continuum (LTC) ratio is provided by separating the sidebands. This relative sideband calibration then allows for the production of an accurate LTC spectrum, with one sideband sensing the continuum, and the other the line.

The Titan signal strength was sufficient for the application of phase self-calibration (see Thompson, Moran, and Swenson 1986) to remove atmospheric phase variations, which cause decorrelation of the signal, on timescales shorter than the standard calibration cycle.
unresolved (e.g. “zero-spacing”) spectrum for each ray was obtained by fitting the observed complex visibilities for each channel with a model of the Titan visibility function, correcting for the spatial sampling of the interferometer. The absolute flux scale was provided by scaling the continuum sideband intensity to equal the radiative transfer model flux of Titan at 227.5 GHz, corrected for the date and time of the observations (see below). The same scaling factor was applied to the emission line sideband, preserving the relative calibration.

The resulting combined spectrum of the CO (2 − 1) line on Titan is shown in Figure 1. The data clearly shows the CO (2 − 1) line is a strong emission feature in the spectrum of Titan. The image sideband spectrum is essentially flat except for a weak emission line due to the HC$_3$N (25 − 24) rotational transition at 227.419 GHz. This is particularly important because it shows that the sideband isolation procedure was effective to well below the noise level of the spectrum.

3. MODELING & ANALYSIS

The radiative transfer model used to analyze the new CO data is nearly identical to the one discussed in Gurwell and Muhleman (1995), and we only highlight important aspects.

The basic parameters of the Titan atmosphere were derived from revised Voyager 1 radio occultation results (Lindal et al. 1983, Lellouch 1990, Coustenis and Bézard 1995), including an atmospheric base at 2575 km from the center of Titan, with a surface pressure and temperature of 1460 millibar and 96.7 K. For the thermal profile of the atmosphere we used an equatorial profile determined by Coustenis and Bézard (1995, their profile A) based upon the occultation results and Voyager 1/IRIS spectra (Fig. 2) combined with model J of Yelle (1991) for the upper atmosphere; this same model was used by Hidayat et al. (1998) to analyze their results. This model is appropriate since the observations reported here are unresolved (whole-disk) spectra, which are heavily weighted by emission from equatorial and low latitudes.

The millimeter continuum opacity on Titan is due to collision induced dipole absorption by N$_2$ − N$_2$, N$_2$−Ar, and N$_2$−CH$_4$, and was modeled according to the results of Courtin (1988). The spectroscopic parameters for the CO (2 − 1) line were taken from the JPL catalog (Pickett et al. 1992; see also http://spec.jpl.nasa.gov). The full Voigt lineshape profile calculation using a fast computational method (Hu et al. 1978), integrated in pressure over atmospheric layers of constant temperature, was done using a collisional line-broadening coefficient for CO (2 − 1) in N$_2$ of γ = 2.21(T/300 K)$^{-0.74}$ MHz mbar$^{-1}$ (Semmoud-Monnanteuil and Colmont 1987). Radiative transfer calculations at appropriate frequencies were performed for a variety of radial steps, including limb-sounding geometries, and integrated over the apparent disk to provide the model whole-disk spectrum.

The contribution functions (W(ν) = e$^{-7dτ/dz}$) for several frequency offsets from the CO (2 − 1) line center are shown in Fig. 2, for a single raypath at the disk center. This function describes the relative contribution of different regions of the atmosphere to the emitted radiation at each frequency. The plotted functions assume a CO abundance of 50 ppm, constant with altitude. The ∆ν = −3000 MHz contribution function corresponds to the middle of the continuum (lower) sideband, and is dominated by the collision induced opacity of N$_2$. The other functions correspond to the emission (upper) sideband, and are dominated by CO (2 − 1) opacity. The full line senses the atmosphere from 40 km (the tropopause) to 400 km. However, the range from 200 to 400 km is sounded mostly in the inner 4 MHz of the line core. At 4 MHz spectral resolution we are limited to sensing the CO abundance from the tropopause to ∼200 km. The 0.5 MHz spectrum of the line core pushes this upper bound to near 350 km in the absence of noise. Thermal noise on the spectral measurements in practice limit our sensitivity to ∼ 300 km.

3.1. Best-fit Uniform CO Distribution

The radiative transfer model was run for a series of uniform CO distributions from $q$(CO)=10 to 90 ppm, in steps of 10 ppm. Resulting spectra are shown in Fig. 1 (in steps of 20 ppm for clarity). The model spectra have been convolved to the measurement spectral resolution of the data in each panel. The model calculations show that the continuum (lower) sideband emission is essentially unaffected by the CO distributions considered, and is an excellent continuum measurement. The model
gives a flux at 227.5 GHz of 1.565 Jy for the
gometry of the observations, equal to a
disk-average Rayleigh-Jeans brightness
temperature of 71.4 K.

Even by eye, the 50 ppm uniform model
provides an exceptionally good fit to the data at
both resolutions. The 50 ppm model gives an
RMS residual of 86.8 mJy for the 4 MHz data,
with models of 40 and 60 ppm giving RMS
residuals that are factors of 1.4 and 1.1 times
larger, respectively. Given that a large number
of channels are involved (324), even an 10%
crease in RMS residuals is quite significant.
The 0.5 MHz spectrum is also consistent with
this model. A rigorous least-squares analysis for
the best-fit uniform profile gives a formal
solution of 52±2 ppm from 40 to 300 km.

3.2. Best-fit Non-Uniform CO Distribution

An iterative least-squares inversion
algorithm (following Gurwell and Muhleman
[1995]) based on the radiative transfer model was
utilized to solve for a best-fit non-uniform CO
distribution. The logarithm of the CO
distribution was constrained to be a linear
function of altitude. This constrained solution
tests whether a gradient in the CO distribution
is consistent with the observed spectrum.

We find that the best-fit non-uniform profile,
with formal error, is 48±4 ppm at 40 km, rising
to 60±10 ppm at 300 km. The RMS residual is
86.1 mJy, representing less than 1%
 Improvement in the residual over the best-fit
uniform profile.

3.3. Error Estimates and the Best-fit CO
Distribution

The formal errors quoted in the above
sections are the direct results of the least-squares
analyses, and therefore do not take into account
errors in the radiative transfer modeling or the
 calibration of the spectrum.

To test whether the continuum emission
model is a serious source of error (since the
continuum is calibrated by referencing to the
continuum sideband data), we recomputed the
continuum emission at 227.5 GHz, scaling the
collision induced dipole absorption calculated
from the data of Courtin (1988) by factors of 0.5
and 2. The calculated emission results were
indistinguishable from the nominal model, which
can be explained as the result of two factors.

First, the collision induced continuum
absorption scales as the square of pressure, and
is therefore a very steep function of altitude.
Therefore, increasing (or decreasing) the
absorption coefficient even by factors of two will
only increase the peak of the contribution
function by a small fraction of a scale height.
Second, the peak of the contribution function is
right at the tropopause, where the temperature
gradient is near zero. The result is that the
emission change is very small, and we estimate
that this error is about 1%.

The spectrum sidebands were calibrated
assuming the QSO calibration sources had a
spectral index of -0.5 (e.g. flux ∝ ν^{-0.5}).
However, the spectral index of these types of
sources vary over the range of 0 to -1, and could
lead to a calibration error of approximately 1%
in the relative calibration over the 3 GHz
difference in the sidebands.

Adding the calibration errors in quadrature,
we find an error in the relatively calibrated
spectrum of about 1.4%. Using the uniform
distribution models discussed in section 3.1, we
find that a 3% error in the relative calibration
could lead to an error of roughly 10 ppm in a
worst-case situation (we note that this does not
include a refitting of the lineshape, which would
tend to reduce this error; hence this is a
worst-case estimate). The calibration error is
then about 6 ppm using this scaling. For the
uniform model solution, the formal error is
significantly smaller than this calibration error
 estimate, and we believe that the error of our
measurement is therefore about 6 ppm.

Noting that the non-uniform solution only
improves the RMS residuals by 1% at best, and
that the formal errors on the non-uniform
solution encompass our uniform solution, we
favor the uniform model for the CO distribution,
which is in agreement with the current
understanding of the chemistry of CO in the
atmosphere of Titan. The high resolution data
provides the information on altitudes above 200
km, and as can be seen in Fig. 1 this data has a
higher RMS noise (by a factor of ∼2); this
increases our error estimate by a factor of about
two over this altitude range. We therefore find
that the CO (2 – 1) spectrum is best fit by a
uniform profile of 52 ppm, with estimated errors
of 6 ppm (40 to 200 km) and 12 ppm (200 to 300
km).
4. DISCUSSION

The results presented here are nearly identical to our previous estimate of the CO distribution based on observations of the CO (1−0) transition [Gurwell and Muhleman 1993] and consistent with the original measurement of tropospheric CO [Lutz et al. 1983]. Taken together, these measurements suggest a vertical profile of CO that is constant with altitude, at about 52 ppm, from the surface to at least 300 km.

These results are at odds with the recent measurements of Noll (1996), who found a tropospheric abundance of 10 ppm, and Hidayat et al. (1998), who found a stratospheric CO abundance of around 27 ppm (Table 1). Noll (1996) explored the possibility that their simple reflecting layer was not the surface, but a higher altitude ‘haze’ layer. If the reflecting layer was at 0.9 bar (14 km) the spectrum was best fit with a CO abundance of 60 ppm. However, based on other evidence they found this model less satisfactory than a surface reflecting layer. The results of Hidayat et al. come from an analysis of several lines of CO, including the CO (1−0) and CO (2−1) lines; the discrepancy between their results and ours does not appear to be due to differences in modeling the atmosphere of Titan, but derives from differences in the measurement techniques and the resulting calibrated spectra (A. Marten, personal communication). However, we do point out that the interferometric method does offer advantages over single-dish observations for measuring the very broad lines of CO from the atmosphere of Titan.

We find the model of a uniform distribution of CO in the atmosphere of Titan provides a good fit to our data, but we cannot rule out a difference between the tropospheric and stratospheric CO abundance, since our data is insensitive to the lower atmosphere. A final confirmation of the abundance of CO and its vertical distribution requires further near- and mid-IR measurements of CO in the troposphere.

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TABLE 1. Observations of CO in Titan’s Atmosphere

| Altitude     | Mixing ratio (ppm)\(\text{a}\) | Wavelength | Reference                        |
|--------------|---------------------------------|------------|----------------------------------|
| Troposphere  | \(48^{+100}_{-32}\)            | 1.57 \(\mu\)m | Lutz et al. 1983                |
| Stratosphere | \(60^{\pm40}\)                 | 2.6 mm     | Muhleman et al. 1984            |
| Stratosphere | \(2^{+2}_{-1}\)                | 2.6 mm     | Marten et al. 1988              |
| Stratosphere | \(50^{\pm10}\)                 | 2.6 mm     | Gurwell and Muhleman 1998       |
| Troposphere  | \(10^{+10}_{-5}\)              | 4.8 \(\mu\)m | Noll et al. 1996                |
| Stratosphere | \(27^{\pm5}\)                 | 2.6, 1.3, 0.9 mm | Hidayat et al. 1998            |
| Stratosphere | \(52^{\pm6}\)                 | 1.3 mm     | this work                        |

\(\text{a}\) Mixing ratio defined as \(N(\text{CO})/N(\text{Total})\), i.e. \textit{not} referenced to \(N_2\).

\(\text{b}\) Reanalyzed by Paubert \textit{et al.} (1984): \(75^{\pm105}_{-105}\) ppm.

\(\text{c}\) Non-uniform model: \(29^{\pm5}\) ppm (60 km), \(24^{\pm5}\) ppm (175 km), \(4.8^{\pm2}\) ppm (350 km).

**Figure Captions**

**Fig. 1.**— Calibrated CO (2—1) spectrum obtained November 11–12, 1999 with the OVRO millimeter interferometer, and model spectra calculated assuming uniform profiles of \(q(\text{CO})=10, 30, 50, 70, \text{ and } 90\) ppm. The largest panel shows the full spectrum in both sidebands at 4 MHz resolution. The continuum sideband is flat except for a weak, narrow emission feature due to the \(\text{HC}_3\text{N}(25-24)\) rotational transition near \(\Delta \nu = -3119\) MHz. The larger inset concentrates on the upper sideband data, containing the CO emission feature (±650 MHz of the line center) at 4 MHz resolution. The small inset provides the inner ±16 MHz of the line core at 0.5 MHz resolution. For each panel, the model spectra are convolved to the spectral resolution of the data.

**Fig. 2.**— (left) Contribution functions for selected frequencies near the CO (2—1) line center for the Titan atmosphere, at normal incidence. These functions were calculated assuming a uniform profile \(q(\text{CO})=50\) ppm. (right) The model atmospheric temperature profile derived from Voyager 1 radio occultation measurements and IRIS spectra, and smoothly merged to fit a non-LTE model of the upper atmosphere (adopted from Coustenis and Bézard 1995).
Gurwell & Muhleman Fig. 2

Titan CO(2–1)

Altitude, km

Normalized Contribution Function, km⁻¹  Temperature, K