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AN EXTERNAL ORIGIN FOR CARBON MONOXIDE ON URANUS FROM *HERSCHEL*/SPIRE?*

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ABSTRACT

Previous studies have demonstrated an external source of CO on Jupiter, Saturn, and Neptune. However, it has not been possible to demonstrate this on Uranus because of its low CO abundance, low upper-tropospheric temperatures, and low stratospheric thermal gradient, which make detection very challenging. Here we use 17 *Herschel*/SPIRE observation sequences spanning 3 yr (2009–2012), which cover 14.6–51.8 cm^{−1} with a combined integration time of 5 hr. These spectra were originally taken for routine calibration purposes, so were corrected for continuum offsets prior to analysis. The final stacked spectra had an extremely low noise level of 10–50 pW cm^{−2} sr^{−1}/cm^{−1}. Despite this, CO was not observed, but we were able to obtain stringent 3 σ upper limits at the 0.1–0.2 bar level of 2.1 ppb for a uniform profile, and 9.4 ppb for a stratosphere-only profile—an order of magnitude improvement over previous studies. Comparison with observed CO fluorescence by Encrenaz et al. suggests the majority of Uranus' stratospheric CO has an external origin. It thus appears that external supply of oxygen species—via comets, micrometeorites, or dust—is an important process on all giant planets in our solar system.

Key word: planets and satellites: atmospheres

1. INTRODUCTION

Over the past few decades there has been much debate about the source of carbon monoxide (CO) on the outer planets. Carbon monoxide has been observed on Jupiter (Beer 1975; Bézard et al. 2002), Saturn (Noll et al. 1986; Cavalié et al. 2009, 2010), Uranus (Encrenaz et al. 2004), Neptune (Rosenqvist et al. 1992; Marten et al. 1993; Lellouch et al. 2005; Hesman et al. 2007; Fletcher et al. 2010; Luszczyk-Cook & de Pater 2013; Irwin et al. 2013), and Titan (Lutz et al. 1983; Gurwell 2004; Teanby et al. 2010). CO on Uranus is the least well characterized of all the outer planets, with only a single confirmed observation (Encrenaz et al. 2004). CO could be sourced from the deep interior via vertical mixing processes, externally sourced via impacts of comets, micrometeorites, ring material and dust, or a combination of all these processes.

Internal and external sources can be distinguished by measuring the abundance at different atmospheric levels. An external source would result in a higher abundance in the upper atmosphere than in the lower atmosphere due to dilution and mixing processes, whereas an internal source would result in a more uniform vertical profile. Note that unlike many trace species, CO does not condense until extremely low temperatures: 50 K at 0.1 bar partial pressure (Haynes 2011), which is colder than the minimum temperature measured on Uranus of 53 K (Lindal et al. 1987). Therefore, condensation at the tropopause cold trap is not expected to affect the profile.

Measured tropospheric abundances in Jupiter and Saturn of around 1 parts per billion (ppb) are consistent with an internal source (Fegley & Lodders 1994). However, greater abundances observed in their stratospheres suggest an external contribution is also required (Bézard et al. 2002; Cavalié et al. 2010). Neptune has the largest observed CO abundance of any giant planet at around 0.1 parts per million (ppm) in the troposphere and 1 ppm in the stratosphere; subsequently it has the most well-

defined vertical profile (see Luszczyk-Cook & de Pater 2013, for a summary). Therefore, both internal and external components are required to explain existing outer planet observations. This idea is also consistent with measurements of other oxygen species (CO₂ and H₂O) by Feuchtgruber et al. (1997) and Burgdorf et al. (2006), which also require an external origin.

A consistent picture requiring combined internal and external CO sources is now emerging—at least for Jupiter, Saturn, and Neptune. Uranus' CO inventory provides an important and currently missing piece to this picture. However, it has so far not been possible to constrain the vertical profile of CO on Uranus. There is only one positive identification of CO, from stratospheric CO fluorescence observed by Encrenaz et al. (2004), which implied a volume mixing ratio of 30⁺³⁰_{−15} ppb at pressures below 0.1 bar. However, a uniform profile with a volume mixing ratio of 20⁺²⁰_{−10} ppb fitted the data equally well. It is not possible to distinguish internal versus external source based on this single observation. Submillimeter studies have attempted to identify CO spectroscopically, but have so far been unsuccessful (Rosenqvist et al. 1992; Marten et al. 1993; Cavalié et al. 2008). However, these studies were able to constrain the maximum CO abundance: the most stringent of which being Cavalié et al. (2008) who obtained upper limits of <18 ppb for a uniform profile and <27 ppb for a profile restricted to the stratosphere (pressures less than 0.1 bar). Unfortunately, given the large uncertainties on the Encrenaz et al. (2004) detection, these upper limits are not sufficient to constrain the vertical profile and CO source.

In this Letter, we use new measurements from the SPIRE instrument (Griffin et al. 2010) on board the *Herschel Space Observatory* (Pilbratt et al. 2010) to gain extremely precise measurements of Uranus' submillimeter spectrum. These observations allow us to improve over previous CO abundance determinations to better constrain the vertical profile and origin.

2. OBSERVATIONS

Observations were taken with *Herschel*'s SPIRE Fourier Transform Spectrometer (FTS) instrument (Griffin et al. 2010;

* *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

Table 1
Summary of *Herschel*/SPIRE Observations

Obs.ID	Start Time (UT)	Integration Time (s)	Dist. (AU)	Disc (")
1342187880	2009 Dec 8 23:46:24.0	876.0	19.97	3.53
1342197472	2010 Jun 1 12:45:24.0	3597.0	20.41	3.45
1342197485	2010 Jun 1 16:38:09.0	559.0	20.41	3.45
1342198273	2010 Jun 13 12:04:43.0	839.0	20.21	3.49
1342198274	2010 Jun 13 12:18:53.0	865.0	20.21	3.49
1342199261	2010 Jun 28 14:13:46.0	865.0	19.96	3.53
1342200174	2010 Jul 10 19:36:53.0	865.0	19.76	3.57
1342210844	2010 Dec 5 17:23:26.0	839.0	19.84	3.55
1342212338	2011 Jan 5 11:38:52.0	839.0	20.37	3.46
1342222864	2011 Jun 19 22:41:56.0	839.0	20.17	3.49
1342237013	2012 Jan 10 13:25:43.0	839.0	20.37	3.46
1342237014	2012 Jan 10 13:39:52.0	1052.0	20.37	3.46
1342237018	2012 Jan 10 14:47:12.0	1171.0	20.37	3.46
1342246974	2012 Jun 11 21:05:22.0	1052.0	20.35	3.46
1342247100	2012 Jun 17 05:31:39.0	1052.0	20.26	3.48
1342247618	2012 Jul 2 11:59:43.0	1052.0	20.00	3.52
1342247767	2012 Jul 8 11:20:22.0	1052.0	19.90	3.54

Notes. All observations were taken with the SPIRE FTS at 0.01 cm^{-1} sample spacing. Total integration time is 5.07 hr. “Dist.” is the *Herschel*–Uranus distance and “Disc” is Uranus’ apparent equatorial diameter.

Swinyard et al. 2010). The SPIRE FTS covers the spectral range $14.6\text{--}51.8 \text{ cm}^{-1}$ ($685\text{--}193 \mu\text{m}$) using two separate detector arrays: the short-wave spectrometer array (SSW) $31.2\text{--}51.8 \text{ cm}^{-1}$ and the long-wave spectrometer array (SLW) $14.6\text{--}33.3 \text{ cm}^{-1}$. At these wavelengths, *Herschel*’s 3.5 m diameter mirror had field-of-view diameters of $11''\text{--}19''$ for the SSW and $18''\text{--}40''$ for the SLW. Uranus’ disc typically had a diameter of $3''.5$ during 2009–2012, resulting in disc-averaged spectra.

SPIRE periodically observes Uranus for calibration, resulting in a large number of repeat observations over *Herschel*’s 3 yr mission—it is this large calibration data set that we use here. We selected all Level 2 calibration data that had a sample spacing of 0.01 cm^{-1} from the *Herschel* Science Archive, which resulted in a data set of 17 observation sequences. Observations had a native resolution comprising a sinc instrument function with an FWHM of 0.048 cm^{-1} . These Level 2 data were apodized prior to analysis using a Hamming instrument function with a FWHM of 0.074 cm^{-1} to remove any spectral ringing. Each of the 17 observations was comprised of the sum of many individual spectra, which were combined to give a mean radiance and variance at each wavenumber (Swinyard et al. 2010). Observations are summarized in Table 1 and represent a total of 5.07 hr on-source integration time. The primary purpose of these calibration observations is to set the SPIRE baseline, so there is inevitably some variation in the level of the spectra and also some continuum rippling that needs to be addressed before the data can be used. This is evident in Figures 1(a)–(d). Fortunately for our analysis, narrow spectral features, such as the CO absorption lines are unaffected by broad spectral variations such as these and can still be robustly studied in the calibration spectra.

3. METHODS

To determine CO abundance, our analysis comprises four main steps: (1) create a synthetic reference spectrum based on existing knowledge of Uranus’ atmosphere; (2) use the reference spectrum to correct continuum offsets and broad ripples on

the individual observations; (3) form a stacked overall high signal-to-noise spectrum; and (4) perform a χ^2 -analysis to determine limits on CO abundance from the stacked spectrum.

3.1. Reference Spectrum

First we defined a reference atmosphere, based on the pressure–temperature profile in Lindal et al. (1987), which covers 0.25 mbar to 2.3 bar. This profile was extended to higher pressures (2.3–20 bar) by assuming a lapse rate of 0.85 K km^{-1} based on the moist adiabat, and lower pressures ($1\text{--}30 \mu\text{bar}$) by using stellar occultation measurements from Sicardy et al. (1985). Composition profiles were identical to those used by Irwin et al. (2012a) and had 0.1 bar volume mixing ratios of major atmospheric species of 0.85 for H_2 and 0.15 for He (Conrath et al. 1987). Note that methane is condensed at the tropopause, but was assumed to have a deep abundance of 0.016 (Sromovsky & Fry 2008). We tested the effect of this assumption on the reference spectrum by comparison with a trial synthetic with a deep methane abundance of 0.032 from Karkoschka & Tomasko (2009). Increasing deep methane reduced the continuum level by up to $0.1 \text{ nW cm}^{-2} \text{ sr}^{-1}/\text{cm}^{-1}$ for the smallest wavenumber considered (15 cm^{-1}), but the change in CO absorption feature depth was $<2 \text{ pW cm}^{-2} \text{ sr}^{-1}/\text{cm}^{-1}$ for a representative 10 ppb uniform CO profile, i.e., about 10 times less than the noise level. Therefore, for the observations in this Letter, assumed deep methane abundance has negligible effect on CO abundance determinations. We did not include clouds or aerosols as these also have negligible effect in the submillimeter.

Spectroscopic parameters for atmospheric gases were from the HITRAN2012 database (Rothman et al. 2013). However, we replaced the HITRAN2012 air-broadened Lorentz line widths and temperature exponents with hydrogen/helium broadened values derived from an abundance-weighted mean of measured line parameters in Sung & Varanasi (2004) and Mantz et al. (2005). In the submillimeter spectral region, atmospheric opacity is dominated by collision-induced absorption of pair-wise combinations of H_2 , He, and to a lesser extent CH_4 , for which we used the formulations of Borysow et al. (1985, 1988), Borysow & Frommhold (1986, 1987), and Borysow (1991).

A synthetic reference spectrum was then created using the Nemesis retrieval tool (Irwin et al. 2008), which employs the correlated- k approximation (Lacis & Oinas 1991). Previously, we have used this code extensively to model Uranus’ spectrum in the near-IR (e.g., Irwin et al. 2007, 2012b, 2012a) and Titan’s submillimeter spectra (e.g., Teanby et al. 2010, 2013). A Hamming instrument function with a FWHM of 0.074 cm^{-1} was incorporated directly into the k -tables, so that the synthetic spectrum had the same spectral resolution as the apodized observations. We generated a disc-averaged reference spectrum using 21 field-of-view points spread across Uranus’ disc from zero emission angle at the sub-*Herschel* point (SHP) to an offset of 26,000 km (441 km above the 1 bar pressure surface) following the method outlined in Teanby et al. (2013) and Teanby & Irwin (2007). Most points were clustered around offsets of 24,000–26,000 km from the SHP, where the spectrum changes most rapidly due to limb darkening.

3.2. Continuum Correction

Individual Uranus spectra were first re-scaled from janskys to spectral radiance units ($\text{W cm}^{-2} \text{ sr}^{-1}/\text{cm}^{-1}$) following Teanby et al. (2013) (Figures 1(c) and (d)). This conversion accounted for orbital variations in the *Herschel*–Uranus distance.

Figure 1. SPIRE FTS data from the long-wave spectrometer (SLW) and short-wave spectrometer (SSW). Panels (a) and (b) show the Level 2 data extracted from the Herschel Science Archive in raw radiance units (janskys). Panels (c) and (d) have been converted into spectral radiance units following Teanby et al. (2013) in order to account for variations in distance. Panels (e) and (f) show the spectra corrected for baseline shifts and long-wavelength continuum ripples using a reference synthetic. The large-scale offsets between observations have been removed, but the small-scale noise, which determines the sensitivity to sharp CO emission/absorption features, has been retained. Panels (g) and (h) show the final averaged spectrum (black line, left axis) and uncertainty (gray line, right axis). The SLW has about half the noise level of the SSW and overlaps with stronger CO lines so provides greatest sensitivity.

However, discrepancies still existed between the continuum levels of each spectra with magnitudes of $<5\%$ for the SLW and $<15\%$ for the SSW. These are consistent with the absolute calibration uncertainties discussed by Fletcher et al. (2012). Therefore, we performed an absolute calibration by rescaling the averaged radiance in the central 10 cm^{-1} of each spectrometer range to match that of the reference spectrum. Consequently, scaling factors of 0.95–1.04 were applied to the SLW observations and scaling factors of 0.97–1.17 were applied to the SSW observations. This corrected for gross continuum offsets, but continuum rippling was still present.

Remaining broad-scale continuum ripples were corrected as follows. First, the residual between the reference spectrum and each measured spectrum was calculated. Second, the predicted positions of CO absorption features were masked out and a smooth cubic b -spline curve (Teanby 2007; Teanby et al. 2013) was fitted to the residuals using a knot spacing of 0.5 cm^{-1} (equivalent to an overall basis function width of 2 cm^{-1}). Finally, this smooth fit to the residual, including the interpolation

across the CO features, was removed from the measured spectra (Figures 1(e) and (f)).

3.3. Stacked Spectrum

Once corrected, individual spectra were stacked using an error-weighted mean to account for the different noise levels (due to different observation durations); resulting in an overall high signal-to-noise composite spectrum (Figures 1(g) and (h)). Error bars on the composite spectrum were calculated using the weighted standard error (Bevington & Robinson 1992) of the 17 individual spectra and were of order $10\text{--}30\text{ pW cm}^{-2}\text{ sr}^{-1}/\text{cm}^{-1}$ for the SLW and $30\text{--}50\text{ pW cm}^{-2}\text{ sr}^{-1}/\text{cm}^{-1}$ for the SSW.

3.4. Misfit (χ^2) Calculation

CO abundance was determined using a χ^2 minimization analysis. Following Cavalié et al. (2008), two CO volume mixing ratio profiles were investigated: one with uniform

Figure 2. (a) Temperature profile assumed throughout the analysis. (b) Relative contributions functions at CO line centers. Solid curves show SLW CO lines and dashed curves show the weaker SSW CO lines. Peak sensitivity of the SPIRE observations is at 0.2 bar, with an FWHM spanning 0.6–0.06 bar (indicated by horizontal dashed lines). (c) Predicted radiance difference (ΔR) between synthetic spectra with 0 and 10 ppb CO (uniform profile assumed). CO lines are in absorption and the strongest lines occur in the SLW range.

Figure 3. Change in χ^2 as a function of CO volume mixing ratio (VMR). Panels (a) and (b) are for a uniform CO profile representing an internal source, whereas (c) and (d) are for a profile containing CO only for pressures less than 0.1 bar representing an external source. Dashed horizontal lines represent changes required for a 3σ CO detection ($\Delta\chi^2 = -9$) and a 3σ upper limit ($\Delta\chi^2 = +9$). CO is not detected in these spectra and the most stringent upper limits are from the SLW: 2.1 ppb (uniform) and 9.4 ppb (external source). All CO lines within the SLW and SSW ranges were used to derive the upper limits: 19.22, 23.07, 26.91, and 30.75 cm^{-1} for the SLW; and 34.59, 38.43, 42.26, 46.10, and 49.93 cm^{-1} for the SSW.

abundance at all pressure levels representing a well-mixed profile with an internal source; and a second with uniform abundance for pressures less than 0.1 bar (stratosphere) and zero abundance for higher pressures (troposphere) representing an external source. Contribution functions over the range of abundances investigated peaked at 0.2 bar for the uniform profile and were truncated at 0.1 bar for the stratosphere-only profile, indicating that our observations are sensitive to CO abundance in the upper troposphere and lower stratosphere (Figure 2). The CO abundance α in each profile was incrementally varied from 0 to 100 ppb, a synthetic spectrum $f(v, \alpha)$ was created, and the

misfit $\chi^2(\alpha)$ calculated according to

$$\chi^2(\alpha) = \frac{\sum_{i=1}^N (\bar{s}(v_i) - f(v_i, \alpha))^2}{4\bar{\sigma}^2(v_i)}, \quad (1)$$

where v_i are the N measured wavenumbers, $\bar{s}(v_i)$ is the stacked measured spectrum, and $\bar{\sigma}$ is the error on the stacked spectrum. The factor of four in the denominator is to account for the four times oversampling of the raw spectra. This process was repeated for both SSW and SLW spectra.

Figure 4. Comparison of measured stacked spectra with synthetic spectra including CO abundances of: 0 ppb; 3σ CO upper limit; and five times the CO upper limit to emphasize the features. The regions around the three strongest CO lines are plotted for each spectrometer. No consistent CO absorption features are seen for either spectrometer, which agrees with the lack of detection from the formal χ^2 analysis. Curves for external profiles are offset by $+0.5 \text{ W cm}^{-2} \text{ sr}^{-1} \text{ cm}^{-1}$ for clarity. Note that the external profile results in narrower features due to reduced pressure broadening effects. At the resolution of SPIRE, CO stratospheric emission cores—which typically have FWHMs less than 0.0001 cm^{-1} (3 MHz)—are not resolved. Errors on the measured spectra are represented by the width of the gray line.

4. RESULTS

The variation of χ^2 as a function of CO volume mixing ratio α for both the SLW and SSW is shown in Figure 3 for uniform and stratosphere-only vertical profiles. For a detection of CO with 3σ significance, the minimum misfit $\chi^2_{\min}$ must satisfy $\chi^2_{\min} < \chi^2(0) - 9$ (Press et al. 1992). It can be seen from the figure that there are no significant minima in χ^2 for either the SSW or SLW observations; including CO in the synthetic spectrum worsens the fit. In this case formal 3σ upper limits are defined by the abundance $\alpha_{3\sigma}$ which satisfies $\chi^2(\alpha_{3\sigma}) = \chi^2(0) + 9$. The SLW provides the best constraint and gives a 3σ upper limit of <2.1 ppb for the uniform mixing ratio profile and <9.4 ppb if CO is only present above the tropopause. The SSW had greater noise and weaker CO lines so is less constraining at <7.6 ppb (uniform profile) and <43.6 ppb (stratosphere-only profile). Figure 4 compares the SLW and SSW measurements with synthetics including CO profiles with these abundances. No CO absorption features are apparent in the data.

5. DISCUSSION AND CONCLUSIONS

The *Herschel*/SPIRE observations used here provide 3σ upper limits on Uranus' CO abundance of 2.1 ppb (uniform profile) and 9.4 ppb (stratosphere-only profile). This is an order of magnitude improvement over previous determinations (Cavalié et al. 2008; Marten et al. 1993) and allows a direct comparison with Encrenaz et al. (2004) to give insight into the vertical profile. Encrenaz et al. (2004) found 30^{+30}_{-15} ppb CO, which they report is applicable to pressures below 0.1 bar, but they could also model their data with a uniform CO profile with 20^{+20}_{-10} ppb CO. The large error bars were due to uncertainties in fluorescence modeling. This is much larger than our tropospheric upper limit of 2.1 ppb, and our stratosphere-only upper limit of 9.4 ppb—even when the large error bars on the Encrenaz et al. (2004) result are taken into account.

In order to explain this apparent discrepancy, we must consider the very different contribution functions of the two data sets. Our measured *Herschel*/SPIRE spectra were sensitive to CO abundance around the tropopause, with a peak sensitivity at

0.2 bar and an FWHM spanning 0.6–0.06 bar. If Encrenaz et al. (2004)’s abundances are confirmed, we suggest that CO fluorescence may in fact originate at lower pressures than their quoted maximum pressure of 0.1 bar. This would be consistent with a CO profile that increases with altitude, which would provide the low abundances necessary at 0.6–0.06 bar to be consistent with our observations, while skewing the fluorescence emission to lower pressures (higher altitudes) where CO is more abundant.

Another possibility is that Encrenaz et al. (2004) observed Uranus immediately after a large comet impact and the CO produced has since dissipated. However, given the photochemical stability of stratospheric CO, such a dissipation is unlikely between the time of the Encrenaz et al. (2004) observations (late 2002) and our *Herschel* observations (2009–2012). For example, Moreno et al. (2003) monitored the distribution of CO on Jupiter after the SL-9 impact and found no detectable change in the total mass of stratospheric CO during the four years following impact.

We thus infer that CO abundance increases with decreasing pressure on Uranus, which implies an external origin is required. This suggests CO is sourced from comets and/or micrometeorites and is consistent with derived CO sources on Jupiter, Saturn, and Neptune. Therefore, it seems that significant external CO sources exist for all outer planets.

Finally, it is interesting to compare CO on Uranus to that on Neptune, which has a similar bulk composition (Irwin 2009). Neptune is inferred to have an internal source resulting in around 0.1 ppm CO in the upper troposphere and an external cometary source resulting in around 1 ppm in the upper stratosphere (Luszcz-Cook & de Pater 2013). An abundance of 0.1 ppm CO would be easily detected on Uranus. The observed low tropospheric abundance is consistent with Uranus’ sluggish atmospheric overturning and lack of significant internal heat source. Therefore, our data suggest that vertical mixing processes caused by convection in the troposphere are at least 50 times less effective on Uranus than on Neptune, which severely limits the amount of CO dredged up from the interior. Further progress requires more sensitive observations combined with higher spectral resolution to obtain more detailed information on the vertical profile.

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Facility: Herschel

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