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# Laboratory procedure for simulating nadir measurements with the ACE-FTS

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**Abstract.** The Atmospheric Chemistry Experiment (ACE), or SCISAT mission, is a Canadian science satellite designed to investigate the chemical and dynamical processes that control the distribution of ozone in the stratosphere and upper troposphere. The ACE mission payload consists of two science instruments: a high-resolution infrared Fourier-Transform Spectrometer (FTS) and an ultraviolet/visible/near-infrared spectrometer. These instruments primarily function in occultation mode. However, during the dark portion of the orbit, the Earth passes between the Sun and the satellite. In this configuration, the ACE-FTS has the opportunity to acquire some nadir-view spectra of the Earth. Since the ACE-FTS was designed to view a hot source (i.e., the Sun) at high resolution using a single scan, it was necessary to determine if the ACE-FTS could also provide nadir spectra of the relatively cold atmosphere and surface with sufficient signal-to-noise ratio (SNR). As part of the pre-launch test program, laboratory measurements were performed to investigate this possibility. This paper reports the laboratory spectra of methane, ozone, and carbon monoxide gases measured with the ACE-FTS to determine the performance characteristics of the instrument when viewing a low-intensity blackbody source. From these results, it was shown that the ACE-FTS may be capable of measuring the column amounts of several abundant trace gases, such as methane, ozone, and nitrous oxide, in the atmosphere with sufficient SNR.

**Résumé.** L'Expérience sur la chimie atmosphérique (ACE), ou mission SCISAT, est un projet de satellite scientifique canadien conçu pour examiner les processus chimiques et dynamiques qui contrôlent la répartition de l'ozone dans la stratosphère et la troposphère supérieure. La charge utile de la mission ACE consiste en deux instruments scientifiques : un spectromètre infrarouge haute résolution à transformée de Fourier (FTS) et un spectromètre ultraviolet/visible/proche infrarouge. Ces instruments fonctionnent principalement en mode occultation; toutefois, au cours de la portion obscure de l'orbite, la Terre passe entre le Soleil et le satellite. Dans cette configuration, le capteur FTS de ACE a la capacité d'acquérir des spectres en visée nadir de la Terre. Étant donné que le FTS a été conçu-pour visionner une source chaude (c.-à-d. le Soleil) à une résolution élevée à l'aide d'un balayage unique, il a été nécessaire de déterminer si le FTS pouvait aussi acquérir des spectres en visée nadir de l'atmosphère et des surfaces relativement plus froides avec un rapport signal sur bruit (RSB) adéquat. Dans le cadre du programme de tests pré-lancement, des mesures en laboratoire ont été réalisées pour examiner cette possibilité. Dans cet article, on présente les résultats des spectres du méthane, de l'ozone et du dioxyde de carbone mesurés en laboratoire avec le FTS pour déterminer les caractéristiques de performance de l'instrument lorsque ce dernier est utilisé pour mesurer une source de corps noir de faible intensité. À partir de ces résultats, il a été démontré que l'instrument FTS peut mesurer des quantités intégrées sur la colonne de plusieurs gaz à l'état de trace abondants tels que le méthane, l'ozone et l'oxyde nitreux dans l'atmosphère avec un rapport signal sur bruit (RSB) adéquat.
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**Table 1.** ACE-FTS instrument settings for occultation and nadir measurements.

| Mode | Resolution ($cm^{-1}$) | Single scan duration (s) | Total measurement duration (s) | Spectral range ($cm^{-1}$) | Footprint (km) |
|---|---|---|---|---|---|
| ACE occultation measurement (high resolution) | 0.02 | 2 | 2 (1 scan) | 750–4400 | — |
| ACE nadir measurement (low resolution) | 0.4 | 0.1 | 16 (100 scans) | 750–4400 | 100 × 1 |
| IMG nadir measurement | 0.1 | 10 | 10 (1 scan) | 714–3030 | 8 × 8 |

# Introduction

The SCISAT satellite, carrying the Atmospheric Chemistry Experiment (ACE), was launched successfully on 12 August 2003. The satellite carries two science instruments: the ACE Fourier-Transform Spectrometer (ACE-FTS) (Bernath et al., 2005) and an optical spectrometer named the Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO) (McElroy et al., 2007). The SCISAT mission uses the occultation of the Sun by the Earth to make detailed determinations of the structure and chemistry of the atmosphere at heights ranging from cloud tops to 100 km above the Earth's surface (Bernath, 2006). The satellite orbits the Earth approximately 15 times each day providing an opportunity to observe sunlight that has passed through the Earth's atmosphere during the brief sunrises and sunsets, resulting in up to 30 sets of occultation observations each day.

However, in between the sunset and sunrise occultation, the ACE-FTS continuously points towards the dark side of the Earth and therefore has an opportunity to acquire nadir-view spectra of the Earth's atmosphere with a field of view of 1.25 mrad. This could provide additional atmospheric gas measurements (i.e., column gas amounts) for some satellite orbits (Clough et al., 1995). Column gas measurements provide similar information to those measured by the Interferometric Monitor for Greenhouse Gases (IMG) instrument, which operated for about 6 months in 1997 on board the Advanced Earth Observing Satellite (ADEOS) (Ogawa et al., 1994; Kobayashi et al., 1999). Thus, the nadir-view data could potentially contribute extra science to the ACE mission. For example, radiative trapping or the absorption of upwelling thermal radiation by the atmosphere can be observed for several greenhouse gases. This type of information is important to verify that climate models are correct in the forcing function aspect (Evans and Puckrin, 2001; IPCC, 2001; Harries et al., 2001). In addition, column amounts are useful for determining the presence of localized sources of pollution (Reichle et al., 1990). The potential science for future nadir missions could be evaluated as well. In the past, we have measured the radiative trapping from chlorofluorocarbon (CFC) 11 and CFC12 from IMG spectra. The radiative trapping from ozone, methane, nitrous oxide, and carbon dioxide also can be easily measured with good signal-to-noise ratio (SNR) from the IMG spectra, and column amounts of these gases can be measured from the same data.

Since the ACE-FTS was designed to view a hot source (i.e., the Sun) at high spectral resolution using a single scan, it was necessary to determine if the FTS could provide nadir spectra of the relatively cold atmosphere and surface (~300 K) with a sufficiently high SNR. Hence, preliminary tests were performed prior to launch using the ACE-FTS instrument and a background source that provided a radiative contrast of about 100 K to the gas in a laboratory cell, thereby approximately simulating the atmospheric temperature conditions of the Earth and its atmosphere. Methane, ozone, and carbon monoxide gases in a cell were used to determine the measurement characteristics of the ACE-FTS instrument for the Earth-viewing scenario. These measurements were compared with those from the IMG instrument, to evaluate whether the ACE instrument would have a sufficient SNR to measure the column amounts of trace gases in the atmosphere. These test measurements were carried out in the Space Instrument Calibration Facility at the University of Toronto on 12 March 2003. It should be emphasized that the ACE-FTS instrument conditions were not optimal for these measurements due to the contamination of the detectors with ice, which was discovered after the measurements were performed.

For the occultation measurements, the ACE-FTS operates at a resolution of 0.02 $cm^{-1}$ and records one interferogram every 2 s; however, to reduce the noise in the nadir observations of the Earth's atmosphere and surface, this resolution can be reduced to 0.4 $cm^{-1}$ with each interferogram taking 0.1 s to record, with the measurements co-added over 16 s, as summarized in **Table 1**. This configuration results in the acquisition of column gas amounts that represent an average measurement over a horizontal spatial scale of about 100 km at the Earth's surface.

# Experimental procedure

The ACE-FTS instrument is an adapted Michelson interferometer that uses an optimized optical layout (Soucy et al., 2002; Bernath et al., 2005). The high-resolution (0.02 $cm^{-1}$) FTS operates from 2 to 13 microns (750–4400 $cm^{-1}$) over two spectral bands. The first band covers a region ranging from 5.5 to 13 microns (750–1800 $cm^{-1}$) with a mercury-cadmium-telluride (MCT) detector, whereas the second band is from 2 to 5.5 microns (1800–4400 $cm^{-1}$) with an indium antimonide (InSb) detector. The interferometer uses two corner cubes rotating on a center flex pivot to produce the optical path difference (OPD). A folding mirror placed inside the interferometer is used to increase the OPD.

Normally, a high-temperature 3000 K blackbody is used during the ACE test measurements for the purpose of simulating the occultation scenario (Dufour et al., 2005). However, to reduce the amount of thermal radiation entering the ACE-FTS and thus simulate more realistically the nadir scenario, the blackbody temperature was reduced to 1273 K and two attenuators with a transmission of 30% each were added in the optical path, as shown in **Figure 1**. This configuration had the effect of decreasing the total radiance to the level corresponding to a blackbody at 400 K at 1000 cm$^{-1}$; however, the intensity of the Planck function at 2000 cm$^{-1}$ departed significantly from that corresponding to a 400 K source, as illustrated in **Figure 2**. Here, the radiance for the attenuated blackbody was about 10 times greater than for a 400 K blackbody.

The gas cell used for the test measurements had a path length of 20 cm and was fitted with zinc selenide (ZnSe) windows (Dufour et al., 2006). The gases used for the measurements included methane, ozone, and carbon monoxide. The ACE-FTS was installed in a vacuum chamber and configured to measure the transmission of the cells using 100 co-additions (50 in the forward scan direction and 50 in the reverse direction) over a time of 16 s at a resolution of 0.4 cm$^{-1}$ for each gas in the cell. In addition, the spectrum of an empty cell was acquired, as well as a spectrum of a liquid nitrogen cooled blackbody target. The latter was used to characterize the thermal self-emission of the instrument. The raw interferograms from ACE-FTS were transformed into corrected spectra (level 1b) by software supplied by the instrument contractor, ABB-Bomem. The spectra were corrected for instrument self-emission, and then transmission spectra were computed by dividing each gas cell spectrum by the empty cell spectrum.

For comparison purposes, FTS measurements of the cell transmission were also made with a bench model spectrometer (Magna 550, Nicolet Instruments) to determine the quantity of gas in the cell. The spectrometer was operated at a resolution of 0.5 cm$^{-1}$ with an MCT detector and a globar source at a temperature of 1500 K. The transmission measurements were first made with the Magna instrument, then by the ACE-FTS, and then repeated in the Magna FTS to ensure stability of the gas amount in the cell and the reproducibility of the measurement. The high-purity methane and carbon monoxide gases were purchased from Matheson Gases.

The ozone gas was generated in the cell by a simple and inexpensive approach (Puckrin and Evans, 2003). The apparatus essentially consisted of the gas cell with a metal electrode inserted through a stopper, which plugged one of the apertures to the cell, as shown in the schematic diagram in Figure 2 of Puckrin and Evans (2003). The cell was first filled with pure oxygen gas and then a Tesla coil with a typical electrode voltage of about 40 000 V was placed next to the glass wall of the cell near the internal electrode. Atomic oxygen was produced subsequently in the path of the arc inside the cell, which reacted with molecular oxygen in the presence of a third body to form ozone. The process required about 15 min of arcing to produce about 150 Dobson units (1 DU = 2.73 × $10^{16}$ molecules/cm$^2$) of ozone in the cell, which is about half the amount found in the atmospheric column. The ozone generated in the cell had a half-life of several hours. The background transmission spectrum of the cell was obtained by purging completely with oxygen gas.

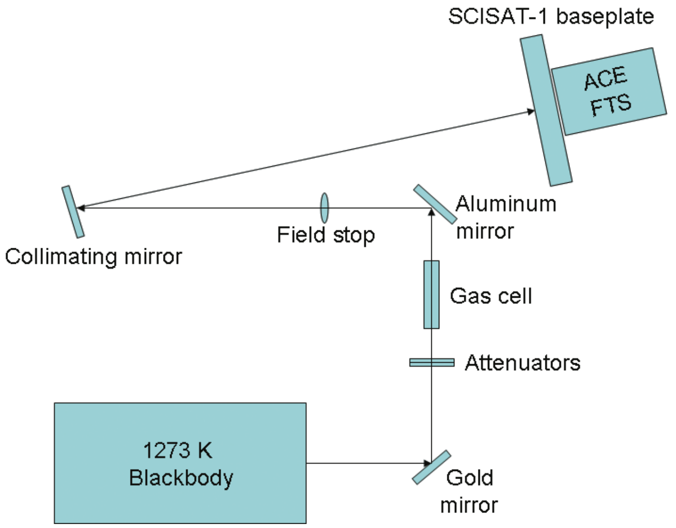

**Figure 1.** Schematic diagram of the testing configuration used for the nadir measurements with the ACE-FTS. The attenuator consisted of two individual meshes each with a transmission of 30%. The blackbody was operated at a temperature of 1273 K.

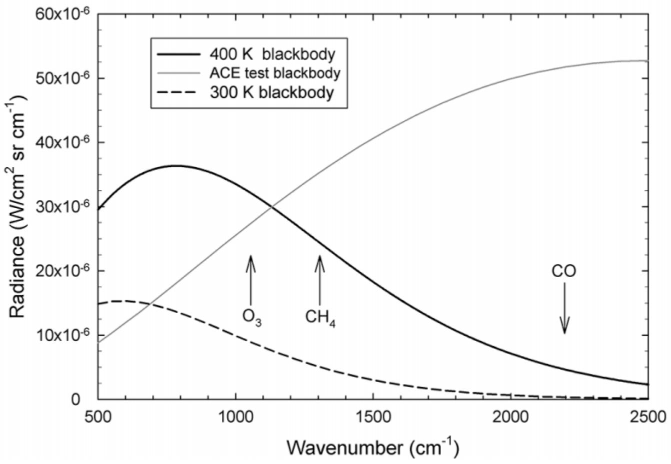

**Figure 2.** Source intensity for the nadir-testing configuration. A 1273 K blackbody with two attenuators with a transmission of 30% each and a beamsplitter were used to simulate a blackbody at a temperature of 400 K. The Planck function for a temperature of 300 K is also shown, which is typical of the Earth's surface temperature.

An example of an ozone transmission spectrum obtained from the gas cell containing about 6.5 × $10^{18}$ molecules/cm$^2$ (or ~240 DU) of ozone is shown in **Figure 3**. The spectrum was measured at a temperature of 26 °C and at a resolution of 0.5 cm$^{-1}$ using the Magna 550 FTIR spectrometer. A simulation of the ozone transmission spectrum using the line-by-line radiative transfer model (LBLRTM) (Clough et al., 2005) is also shown for comparison to help identify the ozone absorption bands. The primary absorption by ozone occurs in the 9.6 μm band, and other bands are present at 700, 1700,

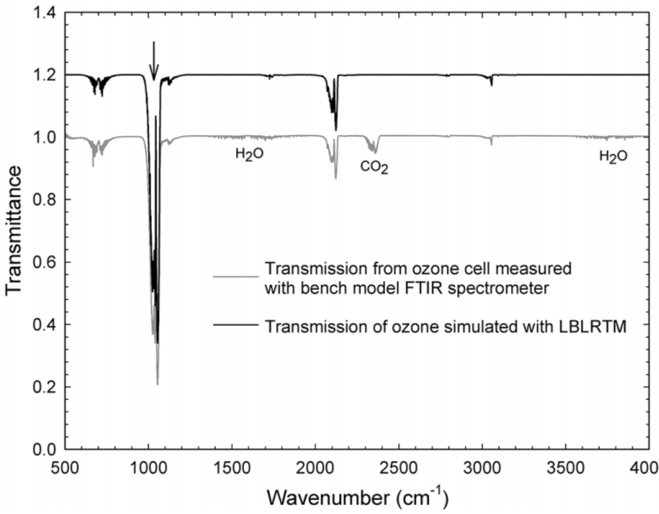

**Figure 3.** A survey spectrum of the gas cell containing ozone, as measured at a resolution of 0.5 cm$^{-1}$ using the Magna FTIR spectrometer. The LBLRTM simulation, which has been shifted upwards for clarity, shows the major ozone absorption bands in the thermal infrared region. The arrow indicates the primary ozone absorption at 9.6 µm. The water and carbon dioxide bands in the measured spectrum are due to residual gases in the sample compartment of the spectrometer. The cell contains about 6.5 × 10$^{18}$ cm$^{-2}$ (~240 DU) of ozone.

2100, 2800, and 3050 cm$^{-1}$. The absorption features by water vapour and carbon dioxide that are present in the spectrum are due to residual gases, which remained in the desiccated sample compartment of the FTS.

## Results and discussion

The quantity of methane, ozone, and carbon monoxide gases used in the gas cell were roughly equivalent to the column amounts found in the 1976 US standard atmosphere (Anderson et al., 1986). The simulated transmission spectra for these gases are represented in **Figure 4**. The LBLRTM was used to simulate these nadir transmission spectra at a resolution of 0.4 cm$^{-1}$ for an altitude regime from 40 km to the surface. The line transition parameters incorporated in the LBLRTM were taken from the High-Resolution Transmission (HITRAN) 2000 molecular database (Rothman et al., 2003). In addition to the spectra for methane, ozone, and carbon monoxide, simulations of the nadir transmission were performed for carbon dioxide and nitrous oxide to show the possibility for the measurement of these important greenhouse gases. All of the gases in **Figure 4** have transmission spectra of the order 50% and therefore have the potential of being detected in the nadir measurements. An example of the raw test spectrum measured with the ACE-FTS is shown in **Figure 5**. This corresponds to the transmission through a cell of methane using the 1273 K blackbody source attenuated to the approximate level of a 400 K source. The result of the measurement of the empty cell is also shown, as well as the instrument self-emission obtained from a cold target source. The spectra from the cell containing methane and from the empty cell are directly superimposed on each other, except in the region between 1200 and 1400 cm$^{-1}$ where methane absorbs energy. Removing the instrument self-emission contribution and dividing the spectrum of the filled cell by that of the empty cell results in the transmission measurement shown in **Figure 6A**. The transmittance of about 10% is approximately the level that one would find for the US standard atmosphere shown in **Figure 4**. Also shown in **Figure 6A** is the transmission result measured with the Magna FTS. The maximum absorption near 1300 cm$^{-1}$ from the two measurements agrees within about 5%. **Figure 6B** shows the corresponding absorbance spectrum calculated for the ACE

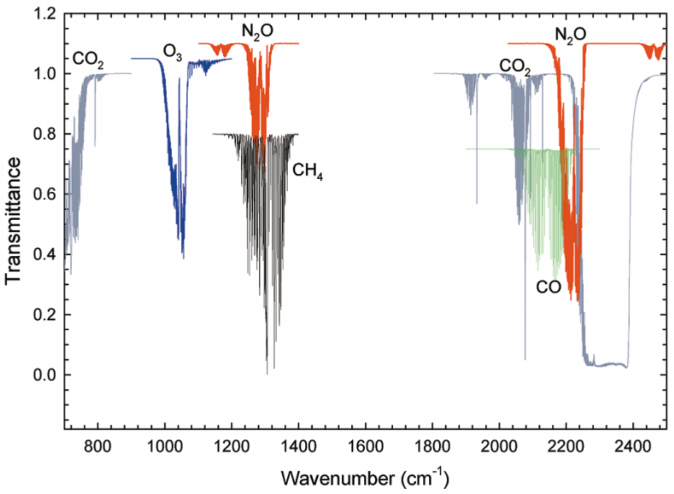

**Figure 4.** Nadir transmission of several gases simulated with the LBLRTM at a resolution of 0.4 cm$^{-1}$ for the 1976 US standard atmosphere. The spectra have been offset in transmittance to improve the clarity.

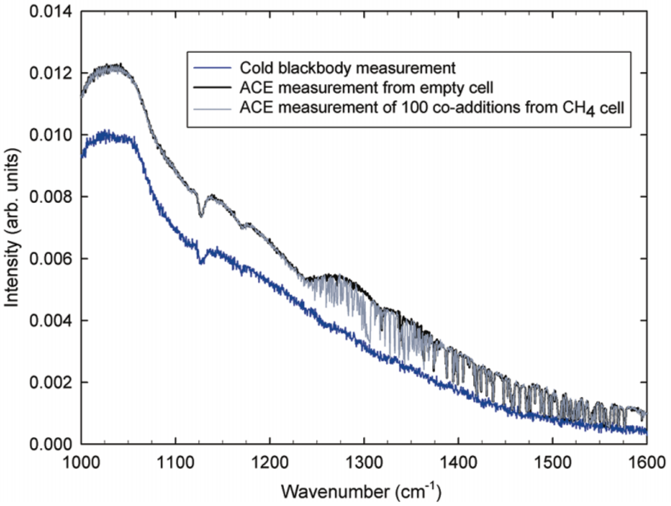

**Figure 5.** The raw spectra measured with the ACE-FTS for the nadir-view configuration. The infrared source consisted of a 1273 K blackbody attenuated by a beamsplitter and two mesh filters with an overall transmission of 9%.

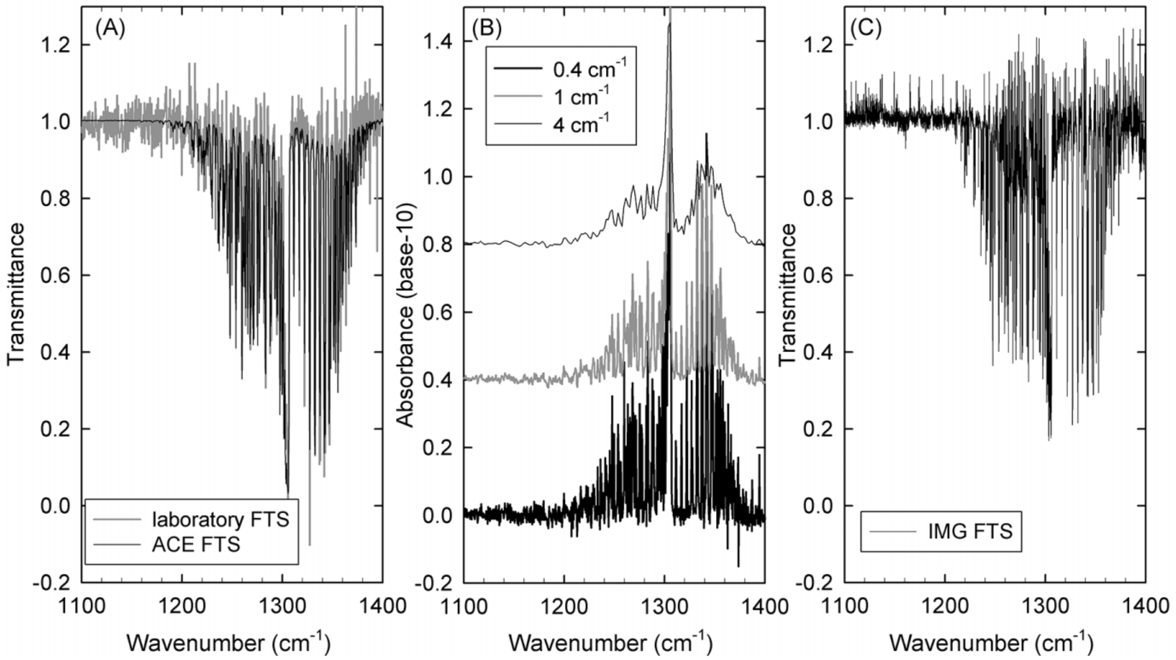

**Figure 6.** (A) The transmission spectra of methane measured with the ACE and Magna FTS. (B) ACE absorbance spectra calculated at three different spectral resolutions. The spectra have been shifted upwards for clarity. (C) The transmission spectrum of methane measured with the IMG instrument at a resolution of 0.1 cm$^{-1}$.

methane measurement at three resolutions: 0.4, 1, and 4 cm$^{-1}$. The degraded results at 1 and 4 cm$^{-1}$ were obtained by truncating the ACE-FTS interferogram recorded at 0.4 cm$^{-1}$ and then recomputing the spectra. The respective peak SNR values at the three resolutions are 52:1, 99:1, and 192:1. It should be noted that the blackbody intensity for these measurements was about 1.5 times greater than would be expected for a 400 K source (**Figure 2**, blue curve versus black curve at 1300 cm$^{-1}$); hence, the resulting SNR values should be approximately decreased by a corresponding amount. **Figure 6C** shows the nadir transmission measured by the IMG spectrometer on the ADEOS satellite. It was measured at a spectral resolution of 0.1 cm$^{-1}$ and has a SNR of about 50:1 in the 1150 cm$^{-1}$ region, which is also comparable to the ACE measurement at 0.4 cm$^{-1}$. This result demonstrates that nadir spectra measured with the ACE-FTS should produce methane total column amounts of the Earth's atmosphere with an adequate precision.

A similar analysis has been performed for ozone, as shown in **Figure 7A**, where a comparison is made between the transmittance of the ozone absorption band at 9.6 microns. The maximum absorption measured near 1050 cm$^{-1}$ with the two instruments agrees within about 5%. **Figure 7B** shows the corresponding absorbance spectrum calculated for the ACE ozone measurement at three resolutions: 0.4, 1, and 4 cm$^{-1}$. The respective peak SNR values at the three resolutions are 61:1, 102:1, and 194:1. It should be noted that the blackbody intensity for these measurements was about 1.2 times less than would be expected for a 400 K source (**Figure 2**, blue curve versus black curve at 1050 cm$^{-1}$); hence, the resulting SNR values should be approximately increased by a corresponding amount. **Figure 7C** represents the nadir transmission measured by the IMG spectrometer. It was measured at a spectral resolution of 0.1 cm$^{-1}$ and has a SNR of about 50:1 in the 1100 cm$^{-1}$ region, which is also comparable to the ACE measurement at 0.4 cm$^{-1}$. This demonstrates that nadir spectra measured with the ACE-FTS should produce ozone total column amounts of the Earth's atmosphere with an adequate precision.

Finally, the analysis performed for carbon monoxide is shown in **Figure 8A**, where a comparison is made between the transmittance of the absorption bands at 2200 cm$^{-1}$. The maximum absorption features at 2100 and 2180 cm$^{-1}$ in the measurements obtained with the two instruments agree again within about 5%. **Figure 8B** shows the corresponding absorbance spectrum calculated from the ACE-FTS carbon monoxide measurement at three resolutions: 0.4, 1, and 4 cm$^{-1}$. The respective peak SNR values at the three resolutions are 34:1, 29:1, and 28:1. In this case, there is little advantage to be gained in the SNR by manually degrading the resolution of the spectrum, since the intensity of the carbon monoxide signal decreases at approximately the same rate as the noise level of the measurement. It should also be noted that the blackbody intensity for these measurements was about 10 times greater than would be expected for a 400 K source (**Figure 2**, blue curve versus black curve at 2200 cm$^{-1}$); hence, the resulting SNR values should be decreased to a value of about 3:1. It is therefore doubtful that the ACE-FTS operating in a nadir configuration would be able to measure accurately the total column amount of carbon monoxide in the atmosphere. For

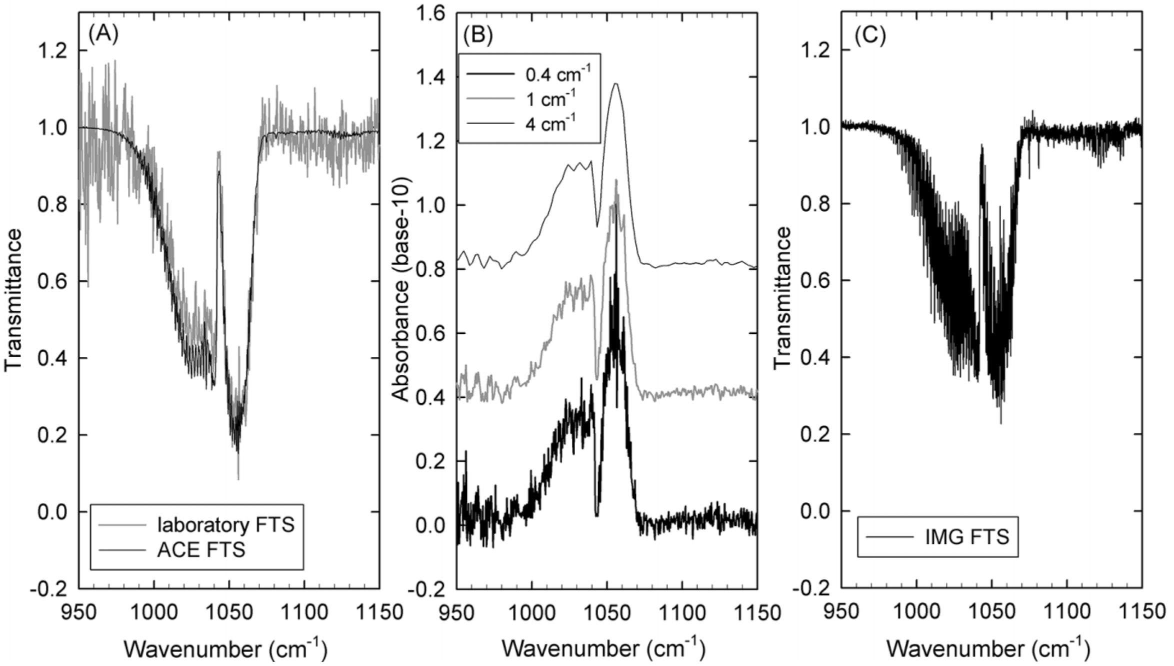

**Figure 7.** (A) The transmission spectra of ozone measured with the ACE and Magna FTS. (B) ACE absorbance spectra calculated at three different spectral resolutions. The spectra have been shifted upwards for clarity. (C) The transmission spectrum of ozone measured with the IMG instrument at a resolution of 0.1 cm$^{-1}$.

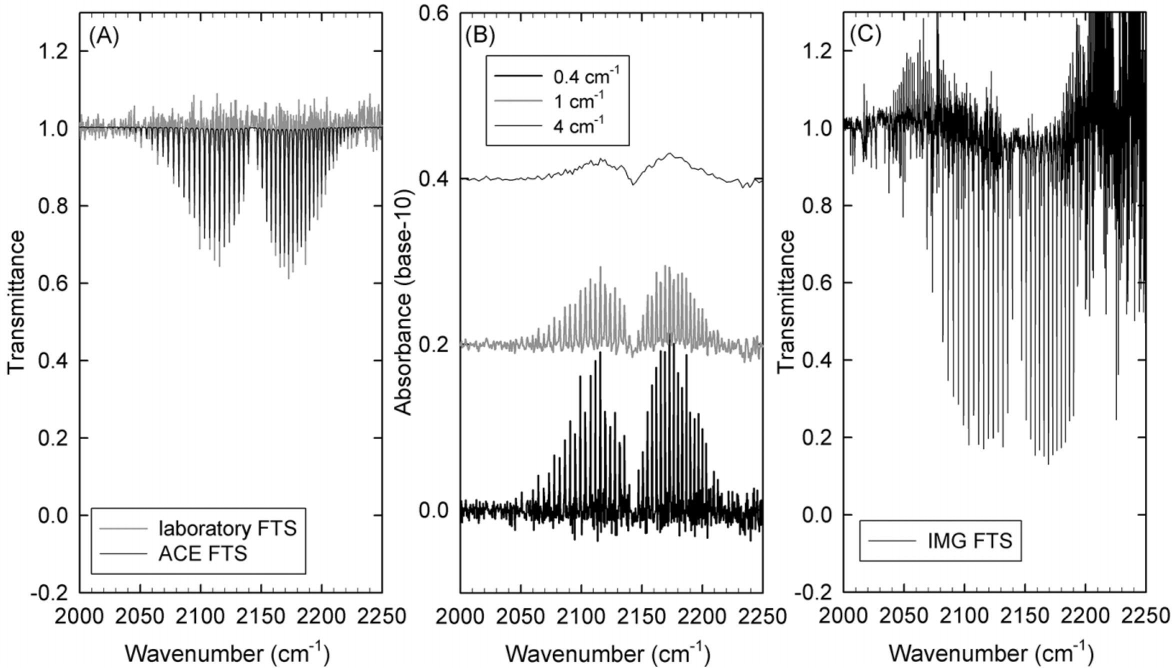

**Figure 8.** (A) The transmission spectra of carbon monoxide measured with the ACE and Magna FTS. (B) ACE absorbance spectra calculated at three different spectral resolutions. The spectra have been shifted upwards for clarity. (C) The transmission spectrum of carbon monoxide measured with the IMG instrument at a resolution of 0.1 cm$^{-1}$.

comparison, **Figure 8C** represents the nadir transmission of carbon monoxide measured by the IMG spectrometer with SNR of about 90:1. The carbon monoxide transmittance is lower in the case of the IMG spectrum due to the higher resolution at which the measurement was made.

## Conclusions

Laboratory transmission measurements of several gases have been measured successfully with the ACE-FTS instrument. From a comparison with a standard bench model FTS instrument, and using the LBLRTM, it is apparent that these measurements show that the retrieval of nadir column amounts should be possible for methane and ozone, and possibly nitrous oxide. Gases such as carbon monoxide may prove to be too difficult to measure due to insufficient SNR. The SNR of the ACE-FTS measurements for methane and ozone were comparable to those measured at a higher spectral resolution of 0.1 $cm^{-1}$ with the IMG instrument onboard the ADEOS satellite. These results are important since they demonstrate that extra science can be acquired potentially from this occultation-viewing instrument, including information on the phenomena of global warming and air pollution, through the measurement of gas column amounts.

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