Meridional variations of C$_2$H$_2$ and C$_2$H$_6$ in Jupiter’s atmosphere from Cassini CIRS infrared spectra

C.A. Nixon$^a$, R.K. Achterberg$^b$, B.J. Conrath$^b$, P.G.J. Irwin$^c$, N.A. Teanby$^c$, T. Fouchet$^d$, P.D. Parrish$^e$, P.N. Romani$^f$, M. Abbas$^g$, A. LeClair$^b$, D. Strobel$^1$, A.A. Simon-Miller$^f$, D.J. Jennings$^f$, F.M. Flasar$^f$, V.G. Kunde$^a$

$^a$ University of Maryland, College Park, MD 20742, USA
$^b$ Department of Astronomy, Cornell University, Ithaca, NY 14853, USA
$^c$ Atmospheric, Oceanic and Planetary Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK
$^d$ LESIA, Observatoire de Paris, 5 Place Jules Janssen, 92195 Meudon Cedex, France
$^e$ Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109, USA
$^f$ NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA
$^g$ NASA Marshall Space Flight Center, SD50 NSSTC, Huntsville, AL 35812, USA
$^i$ University of Alabama, Huntsville, AL 35899, USA
$^h$ Departments of Earth and Planetary Sciences & Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

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Abstract

Hydrocarbons such as acetylene (C$_2$H$_2$) and ethane (C$_2$H$_6$) are important tracers in Jupiter’s atmosphere, constraining our models of the chemical and dynamical processes. However, our knowledge of the vertical and meridional variations of their abundances has remained sparse. During the flyby of the Cassini spacecraft in December 2000, the Composite Infrared Spectrometer (CIRS) instrument was used to map the spatial variation of emissions from 10 to 1400 cm$^{-1}$ (1000–7 µm). In this paper we analyze a zonally averaged set of CIRS spectra taken at the highest (0.48 cm$^{-1}$) resolution, firstly to infer atmospheric temperatures in the stratosphere at 0.5–20 mbar via the $\nu_4$ band of CH$_4$, and in the troposphere at 150–400 mbar, via the H$_2$ absorption at 600–800 cm$^{-1}$. Stratospheric temperatures at 5 mbar are generally warmer in the north than the south by 7–8 K, while tropospheric temperatures show no such asymmetry. Both latitudinal temperature profiles however do show a pattern of maxima and minima which are largely anti-correlated between the two levels. We then use the derived temperature profiles to infer the vertical abundances of C$_2$H$_2$ and C$_2$H$_6$ by modeling tropospheric absorption (∼200 mbar) and stratospheric emission (∼5 mbar) in the C$_2$H$_2$ $\nu_5$ and C$_2$H$_6$ $\nu_9$ bands, and also emission of the acetylene ($\nu_4 + \nu_5$) − $\nu_4$ hotband (∼0.1 mbar). Acetylene shows a distinct north–south asymmetry in the stratosphere, with 5 mbar abundances greatest close to 20° N and decreasing from there towards both poles by a factor of ∼4. At 200 mbar in contrast, acetylene is nearly flat at a level of ∼3 × 10$^{-9}$. Additionally, the abundance gradient of C$_2$H$_2$ between 10 and 0.1 mbar is derived, based on interpolated temperatures at 0.1 mbar, and is found to be positive and uniform with latitude to within errors. Ethane at both 5 and 200 mbar shows increasing VMR towards polar regions of ∼1.75 towards 70° N and ∼2.0 towards 70° S. An explanation for the meridional trends is proposed in terms of a combination of photochemistry and dynamics. Poleward, the decreasing UV flux is predicted to decrease the abundances of C$_2$H$_2$ and C$_2$H$_6$ by factors of 2.7 and 3.5, respectively, at latitude 70°. However, the lifetime of C$_2$H$_6$ in the stratosphere (3 × 10$^{10}$ s at 5 mbar) is much longer than the dynamical timescale for meridional mixing inferred from Comet SL-9 debris (5–50 × 10$^{8}$ s), and therefore the rising abundance towards high latitudes likely indicates that meridional mixing dominates over photochemical effects. For C$_2$H$_2$, the opposite occurs, with the relatively short photochemical lifetime (3 × 10$^7$ s), compared to meridional mixing times, ensuring that the expected photochemical trends are visible.

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* Corresponding author. Address for correspondence: Solar System Exploration Division, Planetary Systems Laboratory, Code 693, NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA. Fax: +1 (301) 286 0212.
E-mail address: conor.nixon@gsfc.nasa.gov (C.A. Nixon).

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1. Introduction

Methane (CH₄) is the primary carbon species found in Jupiter’s reducing atmosphere. In the stratosphere, production of acetylene (C₂H₂) and ethane (C₂H₆) is initiated by the photolysis of methane by light with wavelengths <160 nm. On Jupiter, methane photolysis is largely driven by solar Lyman-α at ~122 nm. The direct hydrocarbon products are methyl, CH₃, excited and ground state methylene, CH₂, and methylidyne CH. Excited methylene is rapidly converted to CH₃, and along with the primary CH₄, either recombines CH₄ via recombination with H, produces ethene via self recombination, or leads to higher order hydrocarbons by reacting with C₂ radical species. The ground state methylene and CH produce ethylene, C₂H₄, and acetylene.

Due to the high UV cross section of methane the photochemical reactions described above occur high in the atmosphere, just below the homopause. However, in the middle and lower stratosphere, the column density of C₂H₂ becomes large enough that unity optical depth is reached in the spectral region 170–200 nm. Acetylene photolysis produces either ethynyl, C₂H, or C₂. Ethynyl reacts predominately with H₂ and CH₄ producing H and CH₃ and reforming C₂H₂. C₂ does the same, except that instead of reforming C₂H₂, C₂H is produced. This secondary photosensitized methane destruction then leads to the production of C₂H₆ via CH₃ and is catalytic in the sense that C₂H₂ is reformed a majority of the time it undergoes photolysis. The H atoms produced in these reactions can lead to the conversion of unsaturated to saturated hydrocarbons.

Eventually the long-lived stable products of methane photolysis, ethane and other higher order hydrocarbons, are transported downward, out of the stratosphere, to balance the upward flux of CH₄ destroyed by the solar UV. Wildt (1937) first proposed that recycling of the photochemical products back to CH₄ in the deep hot interior of Jupiter enabled it to survive over the age of the solar system. Since then numerous authors have contributed to understanding the details of this process (e.g., Strobel, 1969, 1973, 1974; Gladstone et al., 1996; Moses et al., 2004).

Acetylene is a relatively short-lived species with a net lifetime (production-loss) of 3 × 10⁷ s at 5 mbar, and is therefore expected to show some meridional variations in abundance, if the horizontal mixing timescales are on the order of a jovian year (4 × 10⁸ s). Ethane on the other hand is a longer-lived species (3 × 10¹⁰ s at 5 mbar) and should therefore be more uniformly distributed in latitude as a result of planetary-scale transport processes. By examining the spatial trends in abundance of these molecules, in conjunction with theoretical models, we should be able to learn not only about the photochemistry, but also the dynamics of Jupiter’s upper atmosphere. A good set of hydrocarbon abundance measurements is thus the key to understanding multiple upper-atmospheric processes.

Since the first detection of C₂H₂ and C₂H₆ (Ridgway, 1974), many campaigns by ground-based (Sada et al., 1998, and references therein) and Earth-orbiting telescopes: International Ultraviolet Explorer (IUE) (Gladstone and Yung, 1983; Wagener et al., 1985), the Hopkins Ultraviolet Telescope (Morrissey et al., 1995), and the Infrared Space Observatory (ISO) (Encrenaz et al., 1996; Fouchet et al., 2000), have made great strides in elucidating disk-averaged vertical profiles of C₂H₂ and C₂H₆. Typically the stratospheric mixing ratios are in the ranges ~10⁻⁸–10⁻⁷ for C₂H₂ and ~10⁻⁶–10⁻⁵ for C₂H₆ (see also Table 7.1 of Moses et al. (2004) for a summary of recent measurements]. Recently, the stratosphere and upper troposphere at the equator were probed by the HST FOS (Bétrémieux et al., 2003), with a spatial resolution of ~3°. This study reached the contradictory conclusion that, while the UV spectra were best fitted with a minimum C₂H₂ abundance at the tropopause and a rising profile in the upper troposphere, that this type of profile was completely at odds with their high resolution IRTF spectra at 13.5 μm. This result will be discussed in more detail in Section 6.1.

The Voyager 1 and 2 spacecraft both made spatially resolved measurements of jovian hydrocarbons, during flybys on 5th March 1979 and 9th July 1979, respectively. The Voyager IRIS instrument observed the C₂H₂ 729 cm⁻¹ ν₉ band and the C₂H₆ ν₇ band at 821 cm⁻¹ at a resolution of 4.3 cm⁻¹ (Hanel et al., 1979a, 1979b). During the closer pass of Voyager 2, sufficient spectra were taken to enable a basic meridional trend in emission to be established from six latitudes. This indicated that the C₂H₂ and C₂H₆ mixing ratios appeared to decrease and increase respectively by a factor three from low northern latitudes to the north polar region, although a formal retrieval was not used (Maguire et al., 1984). Subsequent analysis of the IRIS Jupiter data has largely concentrated on the polar regions (Kim et al., 1985; Halthore et al., 1988; Drossart et al., 1993). The Voyager 2 UVS also made measurements of the equatorial hydrocarbon abundances at higher altitudes by stellar occultation, obtaining a value of 2.5 × 10⁻⁶ for C₂H₆ at 5 µbar, and an upper limit of 5 × 10⁻⁶ for C₂H₂ at 10 µbar (Festou et al., 1981).

Ground-based, spatially resolved measurements have been made by Kostiuk et al. (1987) using an ultra-high spectral resolution infrared heterodyne receiver at the McMath telescope at Kitt Peak. These permitted the retrieval of the abundance of ethane from the ν₁₀ band near 12 μm at a number of locations in the northern and southern hemisphere, if a temperature profile (from Voyager) was assumed. Livengood et al. (1993) followed up with a study of the same band in the region of polar auroral emission from ~50°–70° N using the NASA IRTF, constraining the temperature and C₂H₆ abundance around 1 mbar. More recently, the mass spectrometer on the Galileo probe has likely detected C₂H₂ and C₂H₆ peaks (Niemann et al., 1998; Hunten et al., 2000), but abundances have not yet been determined. The FOS instrument on the HST has also detected acetylene lines, but the error bars on this measurement were too large to determine a meridional trend (Edgington et al., 1998).

In summary, there has not, until now, been measured a large-scale, full-planet set of infrared spectra, from which both temperatures and hydrocarbon abundances can be found simultane-
ous. Unlike optical or UV data, this dual-information content is a particular advantage of the thermal IR regime.

The Cassini Millennium Flyby of Jupiter in December 2000 afforded an excellent opportunity to map the planet globally in the thermal infrared, using the Composite Infrared Spectrometer (CIRS) instrument, which covered the infrared range of IRIS, and beyond into the far-IR and sub-millimeter regime. Although the flyby was relatively distant, CIRS had sufficient spatial resolution to resolve the belts and zones, and also a longer period than the Voyagers in which to conduct mapping. The CIRS jovian dataset is therefore of great potential value in mapping the emissions and abundances of the more prevalent hydrocarbons.

In this paper we first describe the CIRS instrument and the Jupiter observations in detail. Next, we proceed to an explanation of the data modeling and analysis methods, leading to the results. The following section is a discussion of the implications of the current findings in the context of Jupiter science, and finally the conclusions of the article are summarized.

2. Observations

2.1. The CIRS instrument

The CIRS instrument onboard Cassini is a design evolved from the Voyager Infrared Interferometer Spectrometer (IRIS), but upgraded and improved in almost every respect. As the instrument has been described in detail in the literature (Kunde et al., 1996; Flasar et al., 2004a), only the most salient points are repeated here.

The instrument is actually two interferometers fed from a single telescope and foreoptics. The far-infrared (FIR) spectrometer is a Martin–Puplett type using wire-grid beam-splitters and thermopile detectors to collect radiation from 10–600 cm\(^{-1}\) (1000–17 µm) with a maximum resolution of 0.48 cm\(^{-1}\). The field of view (FOV) is circular, approximately a two-dimensional Gaussian response pattern with a FWHM of ~2.5 mrad.

The mid-infrared (MIR) spectrometer is a conventional Michelson type, with two parallel arrays of ten detectors each, each having approximately a square response 0.273 mrad across. One array (‘FP3’) is of photo-conductive detectors, sensitive to the 600–1100 cm\(^{-1}\) range, while the other (‘FP4’) is of the photo-voltaic type and sensitive from 1100–1500 cm\(^{-1}\). Both have a maximum apodized spectral resolution of 0.5 cm\(^{-1}\), however, FP4 is more sensitive (less noisy) than FP3 due to the nature of the detectors.

2.2. The Jupiter encounter

The Cassini Jupiter Millennium Flyby reached perijove around midday on 30th December 2000, at a distance of some 9.8 million km (137 \(R_J\)). This event occurred near the height of jovian northern summer, not long (1/5 of a jovian season) after the solstice on 2nd May 2000. The primary scientific part of the encounter ran from October 2000 to March 2001, during which time all four ‘optical’ remote sensing instruments, from the UV to the far-IR, were successfully operated. Results from the CIRS instrument have been reported by Abbas et al. (2004), Flasar et al. (2004b), Fouchet et al. (2004a, 2004b), Irwin et al. (2004), Kunde et al. (2004), Wong et al. (2004), achterberg et al. (2006), Simon-Miller et al. (2006), Lellouch et al. (2006).

2.2.1. Global emission maps

In early December 2000, during the approach phase of the flyby, CIRS obtained large numbers of high-resolution spectra. These were taken during ‘ride-along’ opportunities with the Cassini Imaging Science Subsystem (ISS), which was making high spatial resolution scans of the planet during November and early December for the purpose of making a movie.

The period from midnight on 1st December 2000 to midnight 15th December 2000 was selected as having sufficient spatial resolution, and also sufficient numbers of spectra at representative latitudes. This period encompassed approximately 13,000 spectra at the highest CIRS spectral resolution, equal to \(\Delta \nu = 0.48 \text{ cm}^{-1}\) apodized, while the spacecraft range from Jupiter was decreasing from 29.3–17.6 million km (410–246 \(R_J\)). The corresponding angular resolution on the disk of 0.27 mrad in the MIR equated to a spatial resolution of 6.0°–3.5° of great circle arc at the sub-spacecraft point, adequate for resolving jovian belts and zones.

Fig. 1 shows spatial maps of radiance at four individual wavelengths. The maps have good coverage between 60° S and 60° N latitude and at all longitudes. Note that while the MIR pixels have square projections at the sub-spacecraft point, the footprint becomes progressively more stretched in latitude towards the poles. Also, the airmass increases towards the poles.

The upper map, in the hydrogen collision-induced absorption spectral region, shows the temperature in the upper troposphere at 150–400 mbar. The equatorial and tropical zones and belts are seen clearly within ±30° latitude. The second map, in the methane \(v_3\) Q-branch, sounds the stratospheric temperature at 1–10 mbar, and clearly shows a different banding pattern from the troposphere. Also, a prominent north–south temperature asymmetry is seen, with the north appearing generally brighter than the south at this epoch. The retrieved temperatures reported by Flasar et al. (2004b) show the asymmetry to be largest near the 4-mbar level.

The third map shows the emission in the acetylene \(v_5\) Q-branch peak, with the nearby continuum subtracted. There appears to be a rise in emission from the equator to the northern mid-latitudes. It is not possible to tell merely from the emission whether the abundance is changing or not; temperature and geometric viewing effects first must be taken into account, which is the subject of this paper. Finally, the lower map shows the ethane \(v_6\) band emission. An overall rise in radiance is seen from equator to pole.

2.2.2. Equatorial spectrum

Fig. 2 shows an example averaged equatorial spectrum (15° S to 15° N) at 0.48 cm\(^{-1}\) resolution, with radiance converted to brightness temperature units, and demonstrates the main spectral features in the mid-infrared from 600 to 1400 cm\(^{-1}\).
Fig. 1. Global maps of Jupiter in the emissions of four different gas species. The upper two maps are plots of absolute radiance, whereas the lower two maps are the line emission with continuum emission subtracted using a nearby continuum-only wavelength for reference. All four maps were made by co-adding spectra from midnight 12/01/00 to midnight 12/15/00. Spectral resolution was 0.48 cm\(^{-1}\). Data has been spatially binned into 5° bins before mapping, with no additional smoothing applied. Each wavelength bin was a single apodized CIRS resolution element \(\Delta \nu = 0.5 \text{ cm}^{-1}\) in width.

The most prominent emission bands are acetylene \(\nu_5\) at 729 cm\(^{-1}\), ethane \(\nu_9\) at 822 cm\(^{-1}\), and methane \(\nu_4\) at 1304 cm\(^{-1}\). In addition, we note that ammonia absorption features, which are prominent beyond 850 cm\(^{-1}\), actually begin at lower wavenumbers and underlie the ethane spectrum. The isolated continuum below 670 cm\(^{-1}\) is due to the broad hydrogen S(1) line, and continues to dominate through to 800 cm\(^{-1}\).

However, this overall picture changes substantially with emission angle. At higher airmass (i.e., polewards for this dataset), the spectra sound higher in the atmosphere, thus reducing the contribution of condensible ammonia, found in the deeper levels, relative to hydrogen. This pushes the transition point from hydrogen-dominated continuum to ammonia-dominated to higher wavenumbers. The overall effect is that ammonia becomes less and less discernable in the 800–850 cm\(^{-1}\) spectrum away from the equator.

2.2.3. Zonally averaged spectra

The objective of this paper is to investigate the meridional variation of the abundances of \(\text{C}_2\text{H}_2\) and \(\text{C}_2\text{H}_6\), to which end a suitable set of zonally averaged mid-infrared spectra was first created from the data. The 0.48 cm\(^{-1}\) resolution spectra from December 1–14, 2000 were co-added in spatial bins of latitude 5° in width, from 70° S to 70° N. Beyond these latitudes, there
were insufficient high-resolution spectra to create useful averages. Also excluded were certain spatial regions containing enhanced emission due to the aurorae. These two areas were (60°–70° S, 330°–90° W) and (60°–70° N, 150°–210° W) (see Figs. 4 and 5 of Kunde et al., 2004).

All longitudes were represented evenly in the data (outside the deliberately excluded areas), but there were more spectra at lower latitudes than higher, due to the viewing angle effect coupled to steady scan rates. Table 1 gives a summary of the numbers and other details of FP3 and FP4 spectra which were averaged in each latitude bin. Also indicated is the mean emission angle in each bin, and the NESR in units of W cm⁻² sr⁻¹/cm⁻¹ at representative wavenumbers in each array. In calculating the mean emission angle, FP3 and FP4 were weighted by their respective numbers of spectra.

3. Forward model

This section describes the numerical ‘forward model’ used to calculate synthetic spectra that were used to model the jovian data. This comprises (i) a model atmosphere, based partly on previous experimental data and partly on (ii) a one-dimensional photochemical model used to produce initial hydrocarbon vertical abundance profiles, and (iii) a radiative transfer code used to calculate the spectra from the model atmosphere given the viewing geometry.

3.1. Model jovian atmosphere

The initial temperature profile used at all latitudes (Orton, private communication) was derived from the Galileo probe ASI results (Seiff et al., 1998) and extended from 4 bar to 0.4 µbar. Fig. 3 shows the initial temperature profile and also the initial abundance profiles of gaseous constituents.

![Graph showing meridional variations of C₂H₂ and C₂H₆ on Jupiter](image)
Hydrogen and helium were taken to be uniformly mixed at volume mixing ratios (VMRs) measured by the Galileo probe, 0.863 and 0.134, respectively (Niemann et al., 1998; von Zahn et al., 1998), and are not shown on the figure. The initial profiles of the three hydrocarbons: methane, acetylene and ethane, were calculated using a photochemical model, as described in the next section.

The ammonia profile was constructed from two variable parameters. The first parameter was the deep VMR value for NH₃, which was held constant from the profile base at 4 bar, through the troposphere to a ‘knee’ pressure of 0.7 bar. Above this level, the VMR decreased with a fractional scale height \( f \), according to
\[
q = q_0 \left( \frac{p}{p_0} \right)^{(1-f)/f},
\]
where \( q \) is VMR, and the subscript ‘0’ refers to values at the ‘knee’ pressure. Also, the VMR was constrained always to be less than the local saturation vapor pressure (SVP). The phosphine profile used the same scheme as NH₃, except that the change from constant to falling VMR occurred at 1.0 bar, and phosphine never reaches its SVP.

Table 2 summarizes the model parameters.

### 3.2. Photochemical model for hydrocarbon profiles

The initial hydrocarbon profiles were calculated using a one-dimensional photochemical model code based on Bishop et al. (1998), but with substantial modifications. Solar maximum Lyman-α flux was assumed, and the eddy diffusion parameter was as follows: (i) in the troposphere, \( K = 2.0 \times 10^2 \text{ cm}^2 \text{ s}^{-1} \); (ii) in the stratosphere, \( K \propto N^{-0.6} \) (\( N \) = number density of molecules); and (iii) \( K = 2.0 \times 10^6 \text{ cm}^2 \text{ s}^{-1} \) at the CH₄ homopause. Important updates to the chemistry schemes since the 1997 publication included the use of recent rate constant measurements for the CH₃–CH₃ reaction by Cody et al. (2003) and the CH₄ branching ratios measured by Heck et al. (1996). The model atmosphere was that of the Galileo probe (Seiff et al., 1998). Additionally, for the CH₄ profile, the deep abundance was shifted to match the results of the Galileo Probe Mass Spectrometer (GPMS) experiment (Niemann et al., 1996, 1998).

Fig. 3 shows the calculated vertical mixing profiles of CH₄, C₂H₂, and C₂H₆. Each of the three gases have substantially different vertical mixing gradients, which can be explained as follows. Methane is almost uniformly mixed up to 10 µbar, as the eddy mixing lifetime is much less than its photochemical lifetime. Within a scale height of the homopause the molecular diffusion lifetime of methane becomes similar to the eddy lifetime and the methane mixing ratio becomes controlled by diffusive equilibrium. Strict diffusive equilibrium does not occur as photolysis of methane reduces the mixing ratio profile below the diffusive equilibrium one. The majority (>80%) of the ethane production occurs for \( p < 0.5 \mu\text{bar} \). Once produced, ethane is photochemically stable. It can be destroyed by photons with

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**Table 2** Parameterization of physical quantities in the model atmosphere

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Parameters</th>
<th>A priori value</th>
<th>A priori error</th>
<th>Model variable</th>
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</thead>
<tbody>
<tr>
<td>NH₃</td>
<td>Deep abundance (2.19 \times 10^{-4})</td>
<td>1.00</td>
<td>±0.10</td>
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</tr>
<tr>
<td></td>
<td>Fractional scale height</td>
<td>0.15</td>
<td>±0.05</td>
<td>✓</td>
</tr>
<tr>
<td>PH₃</td>
<td>Deep abundance (6.00 \times 10^{-7})</td>
<td>1.00</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fractional scale height</td>
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<td>✓</td>
<td></td>
</tr>
<tr>
<td>C₂H₂</td>
<td>Profile</td>
<td>±50%</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>C₂H₆</td>
<td>Profile</td>
<td>±25%</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Temperature ( T_1 - T_7 )</td>
<td>±1 K at 0.4 bar to ±5 K at 0.4 µbar</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*a Supersaturation not allowed.
Meridional variations of \( \text{C}_2\text{H}_2 \) and \( \text{C}_2\text{H}_6 \) on Jupiter

\( \lambda < 169 \text{ nm} \), but methane absorbs out to \( \lambda = 160 \text{ nm} \), making for a small ethane absorption window in the atmosphere. Reactions between ethane and hydrocarbon free radicals often lead to products that can reform ethane. Ethane’s abundance in the lower stratosphere is then a balance between photochemical production aloft and the effective downward transport. Reducing the stratosphere–troposphere exchange rate then increases the ethane abundance in the stratosphere, while increasing the exchange rate decreases it. Acetylene is more reactive and can be photolyzed by photons out to 200 nm. Thus its profile is controlled by a combination of production (at low pressures), loss (at higher pressures) and transport connecting the two.

3.3. Calculation of synthetic spectra

The forward model uses the correlated-\( k \) method (e.g., Lacis and Oinas, 1991), and the \( k \)-tables were pretabulated in advance of the modeling runs. The computer code, developed at the University of Oxford, is derived from an earlier version used to model data from the Galileo NIMS instrument, and has been extensively tested against jovian spectra (Irwin et al., 1998, 2001; Nixon et al., 2001). The updated version for Cassini CIRS has now been successfully used to model Jupiter and Titan data. For more details see Irwin et al. (2004), Teanby et al. (2006).

The \( k \)-coefficients were computed on a grid of 15 temperature points from 70 to 300 K and 15 log pressure points from \(-8 \leq \log p \leq +5\) (\( p \) in mbar). The wavenumber grid was spaced at 0.125 cm\(^{-1}\) intervals with a Full Width to Half Maximum (FWHM) equal to 0.5 cm\(^{-1}\). \( k \)-Tables were produced for the band opacities of CH\(_4\) and its isotopes, \( \text{C}_2\text{H}_2 \), \( \text{C}_2\text{H}_6 \), PH\(_3\), and NH\(_3\). Gas line data for the \( k \)-table calculations were culled from a variety of sources. For \( \text{C}_2\text{H}_2 \) we used the HITRAN 2000 line atlas (Rothman et al., 2003), while for \( \text{C}_2\text{H}_6 \) we used the GEISA 2003 atlas (Jacquinet-Husson et al., 2005), both with \( \text{H}_2–\text{He} \) broadening. Lines for phosphine and ammonia in the mid-infrared were from Kleiner et al. (2003), and methane line data was taken from Brown et al. (2003). Also included was the collision-induced absorption of \( \text{H}_2–\text{H}_2 \) and \( \text{H}_2–\text{He} \) according to Borysow et al. (1985, 1988).

For each forward calculation, the model atmosphere was interpolated onto 71 layers equally spaced in log \( p \), for 4 bar \( \leq p \leq 0.4 \text{ mbar} \).

3.4. Information content of spectrum

The equatorial model atmosphere and radiative transfer forward code was now used to investigate the information content of the spectrum, as a preliminary step in order to inform the retrieval process. The emerging spectral radiance from the top of the atmosphere is given by

\[
I(\tilde{\nu}, x) = \int_0^{\zeta_0} \frac{d\tau(x, \zeta, \tilde{\nu})}{d\zeta} B(\tilde{\nu}, T(\zeta)) d\zeta,
\]

where \( \zeta = \ln p \) (log pressure), \( \tau \) is transmission, \( \tilde{\nu} \) is wavenumber, \( T \) is temperature, \( x \) is the set of model parameters. Local thermodynamic equilibrium (LTE) has been assumed at all levels.

We now define the functional derivative of the radiance with respect to some model parameter \( x_i \):

\[
\text{FD}(\tilde{\nu}, x_i) = -\frac{\partial I(\tilde{\nu}, x)}{\partial x_i}.
\]

Fig. 4 shows the functional derivative with respect to temperature in two representative spectral regions: the hydrogen S(1)

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Fig. 4. Functional derivatives for temperature, as a function of wavenumber. Lighter areas (solid contours) show a positive contribution, darker areas (dotted contours) show a negative contribution.
continuum and methane $\nu_4$ band. In these regions, the gas vertical abundance has been held constant to allow derivation of temperature information. The hydrogen continuum sounds only in the upper troposphere at 150–400 mbar. The methane $\nu_4$ band however is sensitive to two distinct stratospheric regions: strongly in the lower stratosphere (1–10 mbar) and weakly in the upper stratosphere (5 mbar), most notably in Q-branch lines.

Using H$_2$ and CH$_4$ spectral data we have the possibility of retrieving information in three distinct altitude regions of the atmosphere. However, the emission at 5 mbar is a small fraction of the overall emission (<10% at 1304 cm$^{-1}$ and less in the P- and R-branches) and hence will have a correspondingly large error associated with it.

Note that individual lines are still unresolved at the highest spectral resolution of CIRS, and appear as line manifolds. It should also be emphasized that these were calculated for a typical equatorial temperature profile (the nominal a priori profile used in later retrievals, see Section 3.1), and the relative strengths of the various contributions vary towards the poles, especially in the auroral regions where the upper atmosphere is heated by charged particle precipitation along magnetic field lines.

Fig. 5 shows the functional derivative of radiance with respect to acetylene vertical abundance. For the strongest emissions, which correspond to the P- and Q-branches of the $\nu_5$ band, the contribution peaks at around 5 mbar in the stratosphere, however there is also sensitivity at $\sim$0.1 mbar and 10 mbar. Note that the 0.1-mbar emissions are in many instances spectrally offset from the P- and Q-branch line manifolds, and are due to weaker ‘hotbands’ (non-ground-state transitions) rather than the $\nu_5$ band. For example, at $\sim$716.5 and $\sim$731.5 cm$^{-1}$, transitions of the $(\nu_4 + \nu_5) - \nu_4$ hotband (Jacquemart et al., 2001) are seen. These emissions are strongly dependent on temperature and therefore peak at a higher altitude level.

Finally, there is absorption at 100–400 mbar in the upper troposphere, discussed by Bétrémieux et al. (2003) in relation to their own analysis of the C$_2$H$_2$ $\nu_5$ band observations using the NASA Infrared Telescope Facility (IRTF), at $\sim$15× higher spectral resolution. We will return to this topic in Section 6.1. Fig. 6 is the result of a similar calculation for ethane, which shows a less complicated picture. The primary emission is again around 5 mbar, with absorption in the upper troposphere.

A key question for ethane and acetylene is whether the tropospheric absorption can be sufficiently distinguished from the stratospheric emission. A cross correlation of functional derivatives conducted by us indicates that the two levels are indeed spectrally correlated to a significant degree (>70%). However, substantial spectral differences remain, especially in the wings of the lines, and moreover the retrieval problem is non-linear, which led us to conduct several experiments with synthetic retrievals to assess the validity of separating these two levels, discussed in Section 4.3.

Additionally, the 0.1 mbar hot band emissions of C$_2$H$_2$ pose an interesting dilemma. While the spectral contribution at this level is undoubtedly different from the emissions in the lower stratosphere, the temperature is not constrained by the available information from the CH$_4$ $\nu_4$ spectrum. Fouchet et al. (2000) utilized the hot band information in their analysis of ISO
disk-average spectra, by assuming a temperature profile above 1 mbar, equal to a smoothed version of the Galileo Probe ASI instrument profile. From the hot bands and $\nu_5$ band, a vertical abundance gradient was thus derived.

In this analysis, we will allow a similar process to take place. In the 0.1 mbar region, the temperature profile is constrained mainly from information regions above (0.01 mbar) and below (1 mbar), and the a priori profile. The retrieved temperatures in this region therefore represent a smoothed ‘interpolation’ across the low-information region, and tied above and below to real information. Therefore, the retrieved acetylene abundances at 0.1 mbar will be subject to the caveat that there are based on ‘interpolated’ temperatures.

4. Data analysis

4.1. Method

A two-step method was followed. In the first step, selected spectral regions were analyzed to derive a temperature profile. As discussed previously, sections of spectral continuum due to the broad S(1) line of H$_2$ at 600–670 and 760–800 cm$^{-1}$ from FP3 were included to constrain upper tropospheric temperatures, whilst the P- and Q-branches of the methane $\nu_4$ band at 1225–1325 cm$^{-1}$ on FP4 were used to constrain temperatures in the stratosphere.

For each spectrum, corresponding to a single latitude bin, the forward model was calculated repeatedly, varying only the temperature profile to obtain a best fit according to a non-linear least-squares minimization technique (see Section 4.2). This process was repeated at 28 latitudes between 70° S and 70° N, using constant profiles for CH$_4$ and H$_2$. Since the methane mixing ratio profile is predominantly controlled by mixing and diffusive separation, this is equivalent to assuming a constant eddy mixing coefficient profile that is the same at all latitudes. This assumption was necessary to enable the stratospheric temperatures to be found.

When inverting the methane emission to find the temperature at 1–10 mbar, this assumption of $K$ uniform with latitude is not very restrictive. At this level, CH$_4$ is still close to its deep atmospheric value, unless $K$ was reduced by a factor of $\sim$100. However, the 5 µbar level is near, but below, the photolysis and the homopause region for CH$_4$ in our model and thus the mixing ratio of CH$_4$ at this level is sensitive to our choice of photochemical model parameters.

Once the temperature profiles were found, they were held fixed, and used to retrieve vertical abundance profiles for C$_2$H$_2$ and C$_2$H$_6$ in separate calculations. Spectral windows from 670–760 and 800–850 cm$^{-1}$ were modeled for this purpose. The gas profiles were initially set to calculated photochemical model profiles, and subsequently adjusted by the minimization technique to obtain a solution. Fig. 2 highlights the spectral regions used to derive information.

In this stage, the effect of varying ammonia, phosphine and haze profiles was also investigated. However, only variations in ammonia measurably improved the fit for ethane, hence phosphine and haze were fixed at a priori values. The scope of this paper does not extend to the retrieved profiles for NH$_3$. CIRS results for jovian NH$_3$, PH$_3$ and clouds/haze have been previously published in the literature (Irwin et al., 2004; Achterberg et al., 2006; Abbas et al., 2004; Fouchet et al., 2004a).
4.2. Retrieval/inversion scheme

The inversion scheme also derives its heritage from the Oxford NIMS retrieval code, again with some modifications for CIRS, and is based on the method of optimal estimation (Rodgers, 1976, 2000). The CIRS inversion scheme has been previously described in Irwin et al. (2004) and Teanby et al. (2006).

The measurement process may be written: \( y = F(x) + \epsilon \), where \( y \) is the measurement vector (spectrum), \( F \) is the forward model, \( x \) is the true atmospheric state, and \( \epsilon \) is the measurement error. The inverse problem therefore is to find a consistent atmospheric state \( \hat{x} \) such that \( F(\hat{x}) = y \pm \epsilon \).

We define a cost function, similar to a \( \chi^2 \) difference between model and data spectrum:

\[
\phi = (y - F(\hat{x}))^T S_\epsilon^{-1} (y - F(\hat{x})) + (\hat{x} - a)^T S_a^{-1} (\hat{x} - a),
\]

where \( S_\epsilon \) is the measurement error (matrix), \( S_a \) is the a priori error estimate (matrix), and \( a \) is the a priori state vector. Note the second term on the right, which adds a cost due to deviation from the a priori parameter set. The cost function therefore uses both data, and the a priori estimate of the state vector to constrain the inversion. If we set the a priori error to be large, then the model is largely constrained by the measured spectrum.

The matrix \( S_\epsilon \) is diagonal, having the square of the noise equivalent spectral radiance (NESR) of the average spectrum on the diagonal. This figure was initially calculated as a weighted average of the individual interferogram NESRs, accounting for the exact numbers of deep space and shutter reference spectra going into the calibration, as well as the number of on-target spectra (see Appendix A).

For the a priori error matrix \( S_a \), the diagonal elements were set to be the square of the estimated a priori errors (Table 2) for each of the continuous profiles to be retrieved: either temperature for the first retrieval, or acetylene or ethane for the second retrieval. Off diagonal elements were reduced from the diagonal values by a factor of \( \exp (-\zeta / CH) \), where \( \zeta = \log(p) \), \( H \) is the scale height in log-pressure units and \( C \) is the specified correlation length, set to 1.5. The effect is to decrease the off-diagonal error by a factor of \( 1/e \) for each increment of 1.5 scale heights, smoothing the retrieved profile.

For each iteration of the inversion, the forward model was computed, which allowed the calculation of the cost function for that set of parameter values. Then, the values were adjusted so as to attempt to reduce the cost function. Successive iteration minimized \( \phi \) using the Levenberg–Marquardt algorithm. When the cost function had converged to the required extent (changing by \(<0.2\%\)), we had a set of parameter values which gave the best estimate of atmospheric state consistent with data.

The retrieval error covariance is given by

\[
\hat{S} = (S_a^{-1} + K^T S_\epsilon^{-1} K)^{-1}
\]

and the RMS error by the square-root of the diagonal elements of \( \hat{S} \). \( K \) here is the matrix of functional derivatives associated with the forward model \( F(x) \).

4.3. Retrievals on synthetic and test spectral data

Before applying the inversion scheme to real data, it was first applied to synthetic data. The main objective here, beyond validating the basic functionality, was to examine experimentally whether the tropospheric absorption and stratospheric emission for both \( \text{C}_2\text{H}_2 \) and \( \text{C}_2\text{H}_6 \) could truly be separated.

The method was to begin with the a priori profile for temperature and gas VMR. Holding the temperature profile fixed, the gas VMRs were then perturbed, either in the troposphere, stratosphere or both. The new profile was used to calculate a spectrum using a single iteration of the forward model, and then random Gaussian noise was added equal to the actual NESR level at the equator. Finally, the synthetic spectrum was used as dummy ‘data’ for a retrieval calculation. The retrievals started with the gas profiles back at the a priori values and aimed to recover the new profiles.

Fig. 7 shows the results of a test perturbation in the troposphere, showing that the retrieved profile has indeed moved away from the a priori values in the troposphere and now approximates the artificial perturbation, although some ‘ringing’ is evident in the final deviation. As a further test, the retrieval was then performed on the same perturbation, but this time holding the tropospheric abundance fixed, in an attempt to force the retrieval into manipulating the stratospheric VMR. The result is shown in Fig. 8, in which the final profile is now wildly varying from the true profile. Fig. 9 shows the actual spectra and spectral residuals resulting from the previously described two types of retrievals based on the same tropospheric perturbation.

There remains however some concern as to whether or not these tests are truly representative of the retrieval process on real CIRS spectral data—that contains both random and systematic noises, and whose lines have not been artificially generated by the same code used to later model it. To this end, an equatorial average of CIRS spectra was created (as in Fig. 2) and trial retrievals were then run as before: firstly, allowing the entire VMR profiles to vary, and secondly, with no variation allowed in the troposphere.

Fig. 10 shows the outcome. For both acetylene and ethane, the spectral fits are substantially improved when the troposphere is allowed to vary—to a greater degree for ethane, but still significantly for acetylene as well. Hence, we conclude that our retrievals can indeed separate Jovian tropospheric from stratosphere variations and retrieve VMRs in both regions.

5. Results

5.1. Temperatures

Fig. 11 shows the calculated fit to the collision-induced S(1) line/continuum of \( \text{H}_2 \) at \( \sim 600–700 \text{ cm}^{-1} \) (left column), which sounds tropospheric temperatures between 150 and 400 mbar; and also fits to the \( \text{CH}_4 \nu_4 \) band at 1225–1325 cm\(^{-1}\) (right column) which sounds stratospheric temperatures in the 1–10 mbar region. The three spectra shown in each case are representative examples at mean planetographic latitudes 48° S, 3° S, and
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47° N. In all cases the retrieval has converged to a spectral mean
\[ \sum_{i=1}^{n} \chi_i^2 / n \leq 1, \]
where there are $n$ spectral points.

Fig. 12 displays temperatures retrieved from the 0.5 cm$^{-1}$
spectra described above. The temperatures are similar to those
reported by Flasar et al. (2004b) using $\Delta \tilde{\nu} = 3$ cm$^{-1}$ resolution
spectra obtained near Jupiter closest approach. The upper panel
shows the retrieved temperatures at 5 mbar in the stratosphere,
roughly in the center of sensitivity to $C_2H_2$ and $C_2H_6$. The over-

Fig. 7. Left column: a priori, perturbed and retrieved profiles for acetylene (top) and ethane (bottom). The equatorial NESR noise was added to the synthetic spectrum used as a retrieval target—see text for details. Right column: the percentage deviations of the perturbed and retrieved profiles from the a priori.

Fig. 8. Left column: a priori, perturbed and retrieved profiles for acetylene (top) and ethane (bottom) from synthetic spectra, as in previous figure but with no profile variation allowed in the troposphere. Right column: the percentage deviations of the perturbed and retrieved profiles from the a priori.
all temperature range between 70° S and 70° N is about 13 K, and the error on these measurements is about ±2.0 K. Firstly, we note that the north is warmer than the south, by 7–8 K at mid-latitudes. Also, the equator is warmer than the surrounding latitudes at ±15°, and the temperature rises again polewards in both directions. There is also some evidence of a second set of maxima and minima at ±30° and ±40° latitude, respectively.

Zonally averaged temperatures in the upper troposphere are shown in the lower panel of Fig. 12, at a level of 200 mbar. Again, this is median to the altitude range of sensitivity to C2H2 and C2H6. This time however, the overall temperature range on the plot is only ~5 K and the error bars are ~0.75 K. Also, the N–S temperature asymmetry of the stratosphere is not discernable.

The most dramatic difference is the apparent reversal, at many latitudes, of the local extrema in temperature from the stratosphere. This is true at 40° S, 30° S, 15° S, 0°, 15° N, but not at 30° N or 40° N. See Flasar et al. (2004b), Achterberg et al. (2006), Simon-Miller et al. (2006) for further discussion of jovian temperatures and dynamics from CIRS data.

5.2. Gas abundances

5.2.1. Acetylene

Fig. 13 shows the calculated fit to the C2H2 ν5 band at ~700–750 cm⁻¹ (left column) and corresponding residuals (data-model) in the right column. The residuals appear to be mostly random noise, showing that the model is fitting the spectral data extremely well. The notable exceptions to the fit are the large residual spikes at 717, 729, and 741 cm⁻¹. These are a well-known systematic noise in the instrument, occurring due to spacecraft data bus interrupts which cause a regular pattern of spikes in the interferograms at two second intervals. After the FFT transformation, the spacing becomes 12 cm⁻¹. Note the change from maximum to minimum, caused by the drifting phase of the spike pattern in the interferogram domain.

Fig. 14 shows retrieved vertical profiles of C2H2 at six representative latitudes, with retrieval error bars. The plot has been
cropped to the vertical range of 1 bar to 10 µbar, and the a priori profile is also depicted as a dashed line. The gray shaded region indicates the FWHM of the contribution function peaks: the upper tropospheric absorption, the lower stratospheric emission and the upper stratospheric hotband emission.

The upper panel of Fig. 15 shows the meridional variation of the acetylene VMR plotted at 5 mbar in the stratosphere. The trend is a decreasing abundance from 20° N to the poles in both directions, by a factor of ∼4. Overall, the abundances in the northern hemisphere low-to-mid latitudes are significantly higher than at corresponding southern latitudes. In the troposphere at 200 mbar (lower panel), the VMR is constant to within the error bars at ∼3 × 10^{-9}.

The hotband of acetylene at 716.5 cm$$^{-1}$$ yields VMRs near 100 µbar, assuming that the temperature at these altitudes is known. However, we have already noted that the sensitivity of the methane ν4 band to this region is small (Fig. 4), and so the temperatures at 100 µbar in our retrieved profiles are an ‘interpolation’ or smoothing (Section 3.4). We may use these temperatures as a ‘best guess,’ if we allow for appropriate errors.

The errors on the vertical temperature profiles, which were derived during the first retrieval stage, were propagated into the abundance retrieval by adding to the measurement covariance matrix as follows:

$$S'_x = S_x + K_n S_x K_n^T,$$

where $$S_x$$ is the previously retrieved temperature covariance matrix and $$K_n$$ is the temperature Jacobian calculated for the new wavelength range. Hence the final errors on the VMRs include the errors on the temperature profile.

The meridional variation of 100 µbar VMR is plotted in the upper panel of Fig. 16. The abundance is two orders of magnitude greater here than in the lower stratosphere, and the spatial variation is also different, having distinct peaks at northern and southern mid-latitudes. The lower panel of Fig. 16 shows the gradient $$-\frac{d \log q}{d \log p}$$ from 10 mbar to 100 µbar. The value is everywhere greater than unity, due to the rising abundance with altitude. A flat trend with latitude is consistent with the error bars, although there is some evidence for a peak towards southern mid-latitudes.
Fig. 11. Example spectral data and model fits for hydrogen S(1) and methane $\nu_4$ spectral regions.

Fig. 12. Retrieved zonally averaged stratospheric temperatures at 5 mbar (upper figure) and 200 mbar (lower figure).
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6.1. Comparison to other abundance determinations

6.1.1. Voyager IRIS

During the Voyager 2 flyby of 9th July 1979, the IRIS instrument, the conceptual predecessor of CIRS, made spatially resolved measurements of Jupiter at a spectral resolution of 4.3 cm$^{-1}$. The spectral range of IRIS, 200–1400 cm$^{-1}$ covers the same range as the CIRS FP3 and FP4 arrays, which have a higher spatial, as well as spectral, resolution. IRIS therefore was able to make spectrally unresolved measurements of the C$_2$H$_2$ $\nu_5$ band and C$_2$H$_6$ $\nu_9$ band.

By comparing the variation of the intensity ratios of the two band centers, Hanel et al. (1979a) showed that the 821 cm$^{-1}$/729 cm$^{-1}$ ratio was increasing away from the equator, in co-added spectra sets at comparable airmasses. A depletion of C$_2$H$_2$ towards the south pole was hypothesized. Both results are now confirmed by CIRS. Additionally, the IRIS team found a hemispheric asymmetry in the band ratio, which was higher in the north than the south. A similar ratio com-
computed for CIRS (Kunde et al., 2004) does not exhibit a strong north–south difference, but an equal rise towards both poles.

More recently, Maguire et al. (in preparation) have just finished revisiting the Voyager 1 IRIS data, and completed a study of the meridional variations of C$_2$H$_2$ and C$_2$H$_6$. These results...
Fig. 16. VMRs for C$_2$H$_2$ at 100 µbar in the stratosphere, and VMR gradients from 10 mbar to 100 µbar.

Fig. 17. Example spectral data and model fits for the C$_2$H$_6$ $\nu_9$ band (left) and residuals (right).
show that (i) ethane is constant, or increasing away from the equator, and (ii) acetylene is constant, or decreasing towards the poles. In short, their findings are in excellent qualitative agreement with our findings, although their results also hint that acetylene may not decrease in the north nearly so much as in the south (see Section 6.3).
6.1.2. Infrared Space Observatory (ISO)

Fouchet et al. (2000) inferred the abundances of C$_2$H$_2$ and C$_2$H$_6$ at two points in the stratosphere, using data from the ISO short wavelength spectrometer (SWS) taken in May 1997 close to solar minimum. The spectral resolution was similar to CIRS, and the data came from latitudes 30° S to 30° N. The spectral bands of methane and hydrogen used to retrieve temperatures, and the bands of acetylene and ethane used to determine abundances, were identical to the current paper.

For acetylene, their abundance of $q$(C$_2$H$_2$) = 1.1$^{+0.2}_{-0.1} \times 10^{-7}$ at 4 mbar is about three times our value at the same level: 3.8$ \pm 1.3 \times 10^{-8}$. Even though a disk-averaged figure for CIRS would be slightly higher, it would not exceed the peak value of (4.9$ \pm 1.6 \times 10^{-8}$) at 17° N, which still does not overlap with the ISO value. This seems to indicate that, for the lower stratosphere, either a real seasonal change in the mean acetylene abundance has occurred (see Section 6.2), or else the errors have been underestimated. It maybe relevant that the CIRS data was captured at a time of much higher solar activity: the solar (sunsot) cycle peaked in 2001.

Higher in the stratosphere sounded by the C$_2$H$_2$ hotbands, our estimated value of 1.7$ \pm 0.7 \times 10^{-6}$ at 0.3 mbar is around twice the ISO value of 8.9$^{+1.1}_{-0.6} \times 10^{-7}$, although the error bars are large enough for the numbers to marginally agree. For ethane the ISO vertical range of $q$(C$_2$H$_6$) = (10.0$ \pm $2.6) $\times 10^{-6}$ at 1–10 mbar is consistent with the CIRS abundance at low latitudes in the same pressure range (Fig. 18), in line with expectations that the longer-lived C$_2$H$_6$ might exhibit much less seasonal variation than C$_2$H$_2$.

6.1.3. Ground-based telescopes

Sada et al. (1998) observed Jupiter in the same four infrared spectral regions as in this paper, and the ISO group (Fouchet et al., 2000). They used a ground-based 1.5-m telescope and long-slit spectrograph in late 1994 and early 1995 to extract spectra spatially averaged from 58° S to 58° N. The results include a determination of $q$(C$_2$H$_2$) = (2.3$ \pm $0.5) $\times 10^{-8}$ at 8 mbar, in excellent agreement with our equatorial value, and $q$(C$_2$H$_6$) = 3.9$^{+1.9}_{-1.3} \times 10^{-6}$ at 5 mbar, which overlaps our value.

Kostiuk et al. (1987) made ultra-high spectral resolution measurements of the ethane ν$_3$ band at Kitt Peak with the McMath telescope, with a spatial resolution 1/20th of the apparent jovian disk. Using temperature profiles from the Voyager 2 IRIS data, they found an equatorial, mean stratospheric abundance to be 2.8$ \pm 0.6 \times 10^{-6}$, overlapping the CIRS range. They also detected an increasing abundance towards the south pole, in agreement with our findings.

Livengood et al. (1993) used the NASA IRTF in 1989 to determine an ethane abundance at 1 mbar of (3.8$ \pm $1.4) $\times 10^{-6}$ just outside the north polar aurora, at ~50° N, which is somewhat lower than our value of (11.6$ \pm $2.3) $\times 10^{-6}$, obtained 0.93 jovian years later. The retrieved temperature at this level (172 K) was identical to our result.

6.1.4. HST-FOS/IRTF

A recent study of the jovian UV spectrum has been published by Bétrémieux et al. (2003), investigating the complex interplay of NH$_3$, C$_2$H$_2$, H$_2$ and particulates in the spectral region near 200 nm. It was the conclusion of the authors that the spectrum both above and below 200 nm could not simultaneously be fitted by manipulating the stratospheric amounts of C$_2$H$_2$, rather, they found an improved fit when they introduced a profile which had increasing C$_2$H$_2$ below the tropopause, in contrast with photochemical expectations (see Section 3.2). As a caution however, they found that using such a profile would introduce deep absorption wings into the IR ν$_3$ band lines, e.g., at 743 cm$^{-1}$, which were not seen on IRTF equatorial spectra.

We concur that such a high tropospheric abundance (~1 $\times 10^{-7}$) of C$_2$H$_2$ would not be compatible either with CIRS spectra. Although we see a possibility of shallow absorption wings around the P- and R-branch lines, we do not see such deep wings as in their Fig. 10. We have also computed synthetic spectra with such absorber amounts at the lower spectral resolution of CIRS (0.48 cm$^{-1}$ versus 0.07 cm$^{-1}$), and in these we see small emission cores inside deep absorption features, at variance with our experimental data.

6.2. Seasons on Jupiter—insolation effects

Before considering the chemical causes of meridional abundance trends which may occur on Jupiter, it is important to have an appreciation of the seasonal cycles of insolation, which influence chemistry both directly, through photolysis, and indirectly, through ambient atmospheric temperature.

Although Jupiter has an obliquity of only ~3°, the northern summer solstice is nearly coincident with the perihelion of orbit (Beebe et al., 1986). This means that the 21% variation in insolation over the year due to heliocentric distance tends to reinforce the seasonal effect due to axial tilt in the north, but counteract it in the south. At 45° N the summer insolation exceeds the winter by 34%, but at 45° S the southern winter insolation is actually 9% higher than the ‘summer,’ defined by solar elevation.

Hanel et al. (1979b) found a substantial hemispheric temperature asymmetry in the stratosphere at the time of the Voyager encounters, when Jupiter was near northern fall equinox. At this time, the north was warmer than the south. The Cassini encounter was 1.75 jovian years later, just after northern summer solstice, and again the north was observed to be warmer than the south, by ~8 K. Furthermore, the time series data of Friedson (1999, Fig. 2) also appears to show a northern warming in 1988 of a similar magnitude, one jovian year before Cassini (ignoring the Quasi-Quadrennial Oscillation (QJO) area between ±20° latitude).

Hence, the temperature asymmetry appears to be nearly in phase or slightly lagging the insolation effect. This is somewhat perplexing, as the response time to radiative forcing of the atmosphere is expected to be close to a full season. We may define a thermal inertia parameter $\alpha_{\text{sea}x\text{rad}}$ (see Eq. (41) of Hunten et al., 1984), which is the ratio of the radiative time constant of the atmosphere at a given level to $T/2\pi$ ($T$ = 1 jovian orbital period). Conrath et al. (1990) calculated a value of ~5 for 5 mbar for this parameter, corresponding to a phase delay of ~80°.
6.3. Photochemistry and dynamics: interpretation

To understand the causes of the meridional hydrocarbon variations, we must consider the expected changes in chemistry with latitude, photochemical lifetimes, and meridional transport time. For equinoctial conditions, solar photodissociation rates are relatively flat for latitudes less than 45°. However at higher latitudes, the rates begin to drop substantially.

This reduction in photodissociation affects acetylene and ethane differently due to their different photochemistry. For both species the reduction in solar UV results in a lowered column chemical production from methane photolysis. Acetylene is also lost by photolysis so its loss rate also decreases towards the pole. However, for ethane, photolysis loss is less important (it can only be photolyzed in a narrow window). Thus the predicted C_2H_6 column drops off more than the predicted C_2H_2 one.

Note that for both acetylene and ethane their mixing ratios increase with height from the tropopause to ~10 µbar, the location of the CH_4 homopause. Thus these species have scale heights greater than the background atmospheric scale height. In the limit where the chemical time constant of a constituent equals or exceeds the dynamical time constant, the constituent becomes a tracer of atmospheric motion. Ethane certainly satisfies this requirement for large scale, meridional circulation, whereas acetylene probably fails to meet this criterion.

The photochemical production of acetylene and ethane coupled with globally averaged vertical mixing yields vertical mixing ratio profiles as shown in Fig. 3 from the one-dimensional photochemical model. Using this 1-D model, we can estimate the change in 5-mbar abundance expected with latitude. In the absence of meridional transport (or photochemical lifetime << meridional transport) the photochemical model (Section 3.2) predicts a 2.7-fold reduction in the C_2H_2 column from equator to 70° and a 3.5-fold reduction in the C_2H_6 column (both columns above 10 mbar). This predicted decrease is in reasonable agreement with our findings for C_2H_2 (Fig. 15), but not so for C_2H_6 where the abundance increases instead towards both poles (Fig. 19).

A plausible conclusion to draw from this is that the meridional transport time at 5 mbar must be faster than the ethane photochemical lifetime, 3 × 10^{10} s, so that transport processes eclipse the predicted latitude variation from photochemistry. But the meridional transport time must be slower than the acetylene photochemical lifetime, 5 × 10^7 s, or the observed acetylene variation with latitude would not be present.

The increase in ethane mixing ratio towards the poles indicates that the net downward transport of ethane is highest in the polar regions. This could be explained by a mean meridional circulation with subsidence in the polar regions, as has been used to explain the enhancement of trace gases in winter polar stratosphere on Earth (Bacmeister et al., 1995), and the enhancement of nitriles in the winter polar stratosphere of Titan (Lebonnois et al., 2001; Houdin et al., 2004).

The retrieved latitude variation of the C_2H_2 mixing ratios at 5 mbar and 100 µbar can be explained by simple photochemical modeling. For all latitudes the acetylene mixing ratio at 100 µbar is greater than that at 10 mbar (see Fig. 16), so we are retrieving the C_2H_2 mixing ratio below the location of its peak. Since the solar UV slant path increases towards the pole a 1-D photochemical model predicts that the location of the peak should shift to higher altitudes and the peak value will decrease. Both of these imply that the C_2H_2 mixing ratio at 100 µbar should drop from equator to pole, which is indeed seen for latitudes greater than 50° in Fig. 16. The data also suggest maxima at northern and southern mid-latitudes, however, it is difficult to say whether this is a true effect or not, in view of possible systematic temperature uncertainties in this region of the atmosphere.

6.4. Dynamics: existing observations and models

Current data relating to meridional transport are ambiguous. Sanchez-Lavega et al. (1998) found that debris (haze) from Comet SL-9 spread out both equatorward and poleward, from an initial post-impact range of 40°–60° S. The equatorward drift was faster, at 0.033° day^{-1}, than the poleward at 0.004° day^{-1}. Friedson et al. (1999) were able to model this flow using horizontal diffusive transport by large-scale eddies.

Lellouch et al. (2002) also considered the SL-9 event, looking at the distribution of tracers CO_2 and H_2O three years after impact with Jupiter. They computed an effective horizontal eddy diffusion co-efficient K_h = 2 × 10^{11} cm^2 s^{-1} at 0.5 mbar, which leads to a horizontal timescale τ_h = L^2/K_h (where L = 1.1 × 10^{10} cm, equator to pole distance) equal to 6.0 × 10^8 s, of similar order to the jovian orbital period (3.8 × 10^6 s). Moreno et al. (2003) derived a similar value for K_h from observations of CO, CS, and HCN from SL-9. We note that this would fall neatly between the expected acetylene and ethane photochemical timescales, and hence tend to support meridional motions combined with photochemistry as an explanation for the retrieved meridional trends in VMR.

Some earlier circulation models had found poleward drifting of air above 100 mbar similar to a Hadley circulation, with rising motions near the equator and subsidence at the poles, for example, Conrath et al. (1990) and the aerosol-free model of West et al. (1992). West et al. (1992) also calculated a global zonal mean meridional circulation in the presence of aerosols which was hemispherically asymmetric, and showed equatorward transport above 10 mbar and poleward below, with rising motion above 10 mbar at polar latitudes. However, this was based on Voyager and IUE data showing a hemispheric asymmetry in aerosols, so it is difficult to make pronouncements based on that work about the present epoch. Moreno and Sedano (1997) also calculated a zonal mean meridional circulation, using an aerosol distribution derived from near-UV HST imaging data. Their derived circulation differs considerably from that of West et al. (1992) in the stratosphere, with meridional transport generally from the equator to the poles, upwelling at low latitudes, and subsidence at high latitudes, except in the south where there is upwelling at high latitudes for pressures less than about 5 mbar.

Friedson (1999) modeled the ‘Quasi-Quadrennial Oscillation’ (QQO) in temperatures observed by Leovy et al. (1991)
and Orton et al. (1991). He concluded that mean meridional residual circulation existed between the equator and the mid-latitudes. Finally, Yelle et al. (2001) have emphasized the importance of photochemical species, especially C$_2$H$_6$, as stratospheric coolants between 0.2 and 20 mbar. The present work may hence be used in future global circulation calculations to provide additional constraints.

A more recent paper by Liang et al. (2005) has sought to model the published meridional line emission ratios (acetylene/ethane) of Kunde et al. (2004), from lower spectral resolution data (3 cm$^{-1}$) captured by Cassini/CIRS in early January 2001. Liang et al. (2005) used a pseudo 2-D coupled photochemical transport model that required that $K_h$ be constant in an attempt to match the observed latitudinal distribution of C$_2$H$_2$ and C$_2$H$_6$ intensities given in Kunde et al. (2004). They conclude that the meridional transport timescale must vary dramatically from ~10 years at or below 5–10 mbar, to as much as 1000 years above this level. We note here that their assumption that relative abundance variations with latitude will proportionally follow the relative variations of the line intensities is erroneous, due to saturation which can occur in the stronger emission lines. This means that the abundance variations are in fact somewhat greater than presumed in the paper.

Since the observations are latitudinal distributions, it would seem more plausible to explore latitudinal variations in $K_h$, rather than vertical variations. It should be noted that in the 5–10 mbar region their vertical transport and C$_2$H$_2$ loss time constants are ~10 years, precisely their derived timescale for horizontal transport. The loss time constant for C$_2$H$_6$ is ~2000 years in the vicinity of 5 mbar, so the ‘rapid’ horizontal mixing ensures negligible horizontal variation in the stratospheric C$_2$H$_6$ column density below 5 mbar. Above the 5-mbar level, their derived 1000-year horizontal transport timescale is much longer than the vertical transport timescale and the chemical loss time constants for C$_2$H$_2$ and C$_2$H$_6$. Thus, in this region, the slow horizontal mixing has a negligible effect on their latitudinal distributions which in their model are controlled by photochemistry (cf. their Fig. 3).

Lellouch et al. (2006) used a pseudo 2-D method to model the normalized latitudinal distribution of C$_2$H$_2$ and C$_2$H$_6$ at 5 mbar from Kunde et al. (2004). They found a satisfactory fit to the distribution with a uniform with latitude $K_h$ on the order of 10$^{10}$ cm$^2$ s$^{-1}$, i.e., a meridional mixing time on the order of 100 years (3 × 10$^9$ s). This agrees with Liang et al. (2005) who placed their transition from 10 to 1000 years at 5 mbar. More importantly, Lellouch et al. found that a latitudinally varying $K_h$ with rapid mixing at equatorial latitudes and severely inhibited mixing at polar latitudes coupled with equatorial advection could adequately describe the latitudinal redistribution of Comet SL-9 produced HCN and the latitudinal distributions which in their model are controlled by the slow horizontal mixing has a negligible effect on their latitudinal distributions which are not only sensitive to the stratospheric abundance at 0.5–20 mbar, but also to the abundance at 150–400 mbar in the upper troposphere. In the case of acetylene, there is additionally information via the hot bands peaking at 0.1 mbar, although modeling the data requires assumptions to be made regarding temperature in order to proceed.

Our main findings regarding the acetylene abundances from the retrievals are: (i) the stratospheric VMR at 5 mbar decreases sharply from a peak around 20$^\circ$ N towards both poles, by a factor ~4; (ii) the northern hemisphere stratosphere is apparently enriched compared to the southern hemisphere at the time of observation; (iii) in the upper troposphere at 200 mbar the abundance is near constant at ~3 × 10$^{-9}$. For ethane, the VMR in the equatorial stratosphere at 5 mbar is around 4 × 10$^{-9}$, in line with previous findings; and increases by factors of ~1.75 to 70$^\circ$ N and ~2.0 to 70$^\circ$ S. The tropospheric VMR at 200 mbar shows similar increases.

Photochemical considerations would lead us to a first-order expectation that C$_2$H$_4$ would decrease faster than C$_2$H$_2$ towards the poles, due to passage conditions. Why is this not observed? We seek to explain these meridional trends by noting that the typical lifetime of C$_2$H$_2$ is less than the expected horizontal mixing timescale, while the typical lifetime of C$_2$H$_6$ is greater. Hence, while C$_2$H$_2$ ‘reacts’ in a timely manner to insolation, the C$_2$H$_6$ response is delayed so much as to wash out any trends due to photochemistry. Indeed, ethane is observed rather to become more abundant towards the poles, which we hypothesize could be a redistribution of the species by a meridional circulation.

Furthermore, the fact that hemispheric differences are more pronounced in acetylene than in methane is probably due to a combination of the seasonal insolation effect, combined with the shorter photochemical lifetime, and therefore faster response time of the acetylene distribution to radiative forcing.

7. Conclusions and future work

7.1. Conclusions

In this paper we have analyzed infrared spectral data from the Cassini CIRS instrument taken during early December 2000, prior to the encounter with Jupiter. For the first time, the planet has been systematically mapped in the thermal infrared, with high spatial and moderate spectral resolution.

Our goal has been to derive the equator to pole abundance variations of C$_2$H$_2$ and C$_2$H$_6$, from zonally averaged spectral data. Close examination of the contribution functions of these gases has confirmed that, not only is there sensitivity to the stratospheric abundance at 0.5–20 mbar, but also to the abundance at 150–400 mbar in the upper troposphere. In the case of acetylene, there is additionally information via the hot bands peaking at 0.1 mbar, although modeling the data requires assumptions to be made regarding temperature in order to proceed.

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Photochemical considerations would lead us to a first-order expectation that C$_2$H$_4$ would decrease faster than C$_2$H$_2$ towards the poles, due to equinoxional conditions. Why is this not observed? We seek to explain these meridional trends by noting that the typical lifetime of C$_2$H$_2$ is less than the expected horizontal mixing timescale, while the typical lifetime of C$_2$H$_6$ is greater. Hence, while C$_2$H$_2$ ‘reacts’ in a timely manner to insolation, the C$_2$H$_6$ response is delayed so much as to wash out any trends due to photochemistry. Indeed, ethane is observed rather to become more abundant towards the poles, which we hypothesize could be a redistribution of the species by a meridional circulation.

7.2. Further work

The ethane line data in both HITRAN 2000 and GEISA 2003 are currently an impendence to the analysis of the v$_9$ emissions. Proposals to re-measure and improve the spectral line data in this region have been submitted and offer the possibility of greatly improved accuracy for spectral modeling in the next several years.

In the polar auroral regions (|l| > 70) the radiances of CH$_4$, C$_2$H$_2$, C$_4$H$_6$, C$_3$H$_2$, and other hydrocarbons are all dramatically enhanced, indicating a warming in the upper stratosphere. The ethane v$_9$ band emission is much less enhanced, seemingly because it lacks the sensitivity to the microbar region exhibited by the other molecules. Retrieval of gaseous abundances at
these latitudes and altitudes may be possible, but will require non-LTE considerations.

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Appendix A. NESR estimation

A.1. Noise in the mid-infrared calibration

CIRS is a two-temperature instrument, having an optics assembly at ~170 K and a passively cooled mid-infrared focal plane assembly (detectors) at ~75 K. In order to properly calibrate the interferogram (IFM) recorded when the instrument is pointing at a target object, two additional reference interferograms are needed, and must be recorded when pointing the instrument at known temperature targets. These are: space (2.73 K) and a shutter at the optics temperature (~170 K).

The basic calibration equation may be written as

$$S_{\nu} = \frac{\text{FFT}(I_{\text{TAR}} - I_{\text{SP}})_{\nu}}{R_{\nu}} = \frac{P_{(\text{TAR-SP})}}{R_{\nu}},$$

(A.1)

where $S_{\nu}$ is the spectrum, $I_{\text{TAR}}$ and $I_{\text{SP}}$ are the interferograms when looking at the target (planet) and cold space respectively, ‘FFT’ indicates the process of Fast Fourier Transform, the subscript $\nu$ indicates wavenumber dependence and $R_{\nu}$ is the responsivity defined as

$$R_{\nu} = \frac{\text{FFT}((I_{\text{SH}} - I_{\text{SP}})_{\nu})}{B_{\nu}(T_{\text{SH}}) - B_{\nu}(T_{\text{SP}})} = \frac{P_{(\text{SH-SP})}}{B_{\nu}(T_{\text{SH}}) - B_{\nu}(T_{\text{SP}})},$$

(A.2)

where $I_{\text{SH}}$ is the interferogram from pointing at the shutter target and $B_{\nu}$ is the Planck radiance function at the temperature of the shutter $T_{\text{SH}}$ or space $T_{\text{SP}}$. Henceforth, we will drop explicit reference to the wavenumber dependence of quantities $\nu$.

It is straightforward to show that the variance on the sum or difference of two uncorrelated quantities, e.g., the numerators of Eqs. (A.1) and (A.2), is the sum of the variances on the two measurements:

$$x = y + z \Rightarrow \sigma_x^2 = \sigma_y^2 + \sigma_z^2,$$

(A.3)

whereas for a quotient, allowing for cross terms, we have

$$x \equiv \frac{u}{v} \Rightarrow \sigma_x^2 = \sigma_u^2 + \sigma_v^2 - 2 \sigma_{uv}.$$  

(A.4)

If Eqs. (A.3) and (A.4) are now applied to the calibration of CIRS described above, we have

$$\sigma_n^2 = \sigma_{\text{TAR}}^2 + \sigma_{\text{SP}}^2,$$

(A.5)

$$\sigma_{uv}^2 = \sigma_{\text{TAR,SH}}^2 - \sigma_{\text{TAR,SP}}^2 - \sigma_{\text{SP,SH}}^2 + \sigma_{\text{SP,SP}}^2.$$  

(A.6)

In the last line above, all the cross terms on the RHS are uncorrelated and vanish except the last. Therefore, assuming that the temperatures $T_{\text{SH}}$ and $T_{\text{SP}}$ are well-known, then we can write

$$\left(\frac{\sigma_S^2}{S^2}\right) = \left(\frac{\sigma_{\text{TAR}}^2 + \sigma_{\text{SP}}^2}{P_{(\text{TAR-SP})}}\right) + \left(\frac{\sigma_{\text{SH}}^2 + \sigma_{\text{SP}}^2}{P_{(\text{SH-SP})}}\right) - 2\left(\frac{\sigma_{\text{SH}}^2}{P_{(\text{SH-SP})}}\right),$$

(A.7)

Multiplying through by $S^2$ and by substitution of

$$P_{(\text{TAR-SP})} = RS,$$

$$P_{(\text{SH-SP})} = R\left[B(T_{\text{SH}}) - B(T_{\text{SP}})\right] = R\Delta B,$$

we arrive at

$$\sigma_x^2 = \frac{1}{R^2} \left[\left(\sigma_{\text{TAR}}^2 + \sigma_{\text{SP}}^2\right) + \left(\frac{S}{\Delta B}\right)^2 (\sigma_{\text{SH}}^2 + \sigma_{\text{SP}}^2) - 2\left(\frac{S}{\Delta B}\right) (\sigma_{\text{SP}}^2)\right].$$

(A.8)

For convenience we define

$$\alpha \equiv \frac{S_{\nu}}{\Delta B_{\nu}},$$

(A.9)

and collecting similar terms we can write Eq. (A.11) in the form:

$$\sigma_x^2 = \frac{1}{R^2} \left[\sigma_{\text{TAR}}^2 + \alpha \sigma_{\text{SH}}^2 + (1 - \alpha \sigma_{\text{SP}}^2)\right].$$

(A.10)

We will now consider the meaning of the individual $\sigma_x^2$'s in more detail.

A.2. Calculation of NESRs on co-added interferograms

The random noise on a single interferogram may be assumed to be ‘white,’ i.e., it has the same variance at every point of the interferogram, and is also unaffected by the process of Fourier transform. Therefore we define the single-scan random noise variance in raw counts to be $\sigma_1^2$, and is identical regardless of target type. We will also ignore the dependence of this noise on detector temperature, while noting that in reality the amplitude will vary.

In the CIRS data processing pipeline target IFMs are calibrated into spectra individually, to allow for later combination/averaging in any possible combination desired. For these individual spectra, $\sigma_{\text{TAR}}^2 = \sigma_1^2$. However, it is not desirable to also use individual shutter and space interferograms where $\sigma_{\text{SH}}^2 = \sigma_{\text{SP}}^2 = \sigma_1^2$, because of the additional random noise thus added.

A much better approach is to use co-added, average IFMs for the shutter and space IFMs, which have lower random noise levels. When IFMs are co-added, the variance of the resulting mean IFM is reduced linearly by the number of IFMs $N$ in the
average:
\[ \sigma_{\mu}^2 = \frac{\sigma^2_I}{N}. \]  
\hspace{1cm} (A.14)

Therefore, by co-adding IFMs we aim to reduce \( \sigma_{\mu}^2 \) and \( \sigma_{\mu,SP}^2 \) to the lowest possible levels, and thereby ensure that the final noise on the single target calibrated spectrum is minimized (Eq. (A.13)), approaching the single-scan NESR limit \( \sigma_1 \) (square root of variance) due to \( \sigma_{\mu,SP}^2 \) alone.

The current algorithm allows for different space and shutter blocks to be used in the calibration over time, to allow for temporal effects (usually temperature) such as changing phase difference in the beamsplitter. The effect is that IFMs on a certain day may be calibrated with one space block, and those taken on another day with a different block.

However, we come to a point where we wish to co-add target spectra, over a period of days, months or even years, which have each been individually calibrated with different space and shutter blocks. The question then arises as to the final noise variance on the co-added spectrum. This is now derived from basic principles.

According to Bevington (1969) the most basic definition of the variance of a mean is
\[ \sigma_{\mu}^2 = \sum \left[ \sigma_I^2 \left( \frac{\partial \mu'}{\partial I_i} \right) \right]^2, \]  
\hspace{1cm} (A.15)

where \( \mu' \) is the sample mean:
\[ \mu' = \bar{I}(\bar{\nu}) \equiv \frac{1}{N} \sum_{i=1}^{N} I_i(\bar{\nu}). \]  
\hspace{1cm} (A.16)

In these equations, \( I_i \) is an interferogram and \( \bar{I} \) is the mean of a set of interferograms. Therefore
\[ \frac{\partial \mu'}{\partial I_i} = \frac{\partial}{\partial I_i} \left( \frac{1}{N} \sum_{i=1}^{N} I_i \right) = \frac{1}{N}. \]  
\hspace{1cm} (A.17)

Hence, Eq. (A.15) becomes
\[ \sigma_{\mu}^2 = \sum \left[ \sigma_I^2 \left( \frac{1}{N} \right) \right]^2 = \frac{\sigma^2_I}{N}, \]  
\hspace{1cm} (A.18)

which is the proof of Eq. (A.14). This formula holds for cases where all the IFMs co-added are unique.

Let us now consider a case where a sample of \( n_1 \) target IFMs have been individually calibrated using the same deep space block of \( m_1 \) IFMs co-added. A second sample of \( n_2 \) target IFMs have been calibrated against a co-added space IFM average of \( m_2 \) scans. For now, we will consider only noise due to target and space IFMs—the numerator of the calibration equation and therefore the first term in braces of Eq. (A.11)—but we will show in Appendix A.3 that the result is easily extended to include the other noise terms.

The noise on the first average due to the space alone is \( \sigma_1^2/m_1 \), the noise due to the target scans is \( \sigma^2_I/n_1 \), and the total noise is
\[ \sigma^2 = \sigma_1^2 \left( \frac{1}{n_1} + \frac{1}{m_1} \right). \]  
\hspace{1cm} (A.19)

and the second average is similar. But what happens when the two sets of target spectra are added together in a weighted average? The noise variance due to target scans is simply \( \sigma_I^2/(n_1 + n_2) \) because each interferogram is unique, but the noise component due to the space average is not so obvious, because of possible repetition. First we note that the weighted average of the two averages (working in IFM space) is
\[ \mu' = \bar{I} = \frac{1}{N} \sum_{j=1}^{K} I_j n_j, \]  
\hspace{1cm} (A.20)

where the \( j \)th deep space average is repeated \( n_j \) times and there are \( K \) distinct averages in all, for \( \sum n_j = N \). The derivative is
\[ \frac{\partial \mu'}{\partial I_j} = \frac{\partial}{\partial I_j} \left( \frac{1}{N} \sum_{j=1}^{K} I_j n_j \right) = \frac{n_j}{N}. \]  
\hspace{1cm} (A.21)

Now we can deduce the general form, by allowing for each of the individual \( I_j \) to be an average with variance \( \sigma_I^2/M_j \) (\( j = 1, \ldots, K \)), by substituting into Eq. (A.15):
\[ \sigma_{\mu}^2 = \sum \frac{\sigma^2_I}{M_j} \left[ \left( \frac{n_j}{N} \right)^2 \right] = \frac{\sigma^2_I}{N^2} \sum \frac{n_j^2}{M_j}. \]  
\hspace{1cm} (A.22)

This then replaces the simple form \( \sigma^2_I/m \) in Eq. (A.19) for cases where different deep space IFM averages have been used in a spectral average. The same formulation applies equally to shutter averages. We will now combine all the elements to give the total noise from target, space and shutter sources.

A.3. Effective total nesr on co-added spectral averages

Now we are in position to calculate the total variance on a calibrated spectrum in a quantitative way. Let us substitute:
\[ \sigma_{\mu,SP}^2 = \frac{\sigma_I^2}{N}, \sigma_{\mu,SH}^2 = \frac{\sigma_I^2}{M_{SH}}, \sigma_{\mu,SP}^2 = \frac{\sigma_I^2}{M_{SP}} \]  
into Eq. (A.13) yielding:
\[ \sigma_{\mu}^2 = \left( \sigma_{\mu,SP}^2 \frac{1}{R} \right)^2 \left[ \frac{1}{N} + \frac{\sigma_{\mu,SH}^2}{M_{SH}} + (1 - \alpha^2)^2 \right]. \]  
\hspace{1cm} (A.23)

Each of the individual \( M_j \)s represents an effective number of IFMs, defined as the dimensionless part of Eq. (A.22):
\[ \frac{M_{SH,SP}}{\sigma_{\mu,SP}^2} = \frac{\sigma_{\mu,SH,SP}^2}{\sigma_{\mu,SP}^2} = \frac{1}{N^2} \sum \frac{n_j^2}{M_j}. \]  
\hspace{1cm} (A.24)

This term is then easily computed during the process of spectral averaging, so long as knowledge of the calibration components has been carried forward in the pipeline processing.

References


