The Solar Spectrum: an Atmospheric Remote Sensing Perspective

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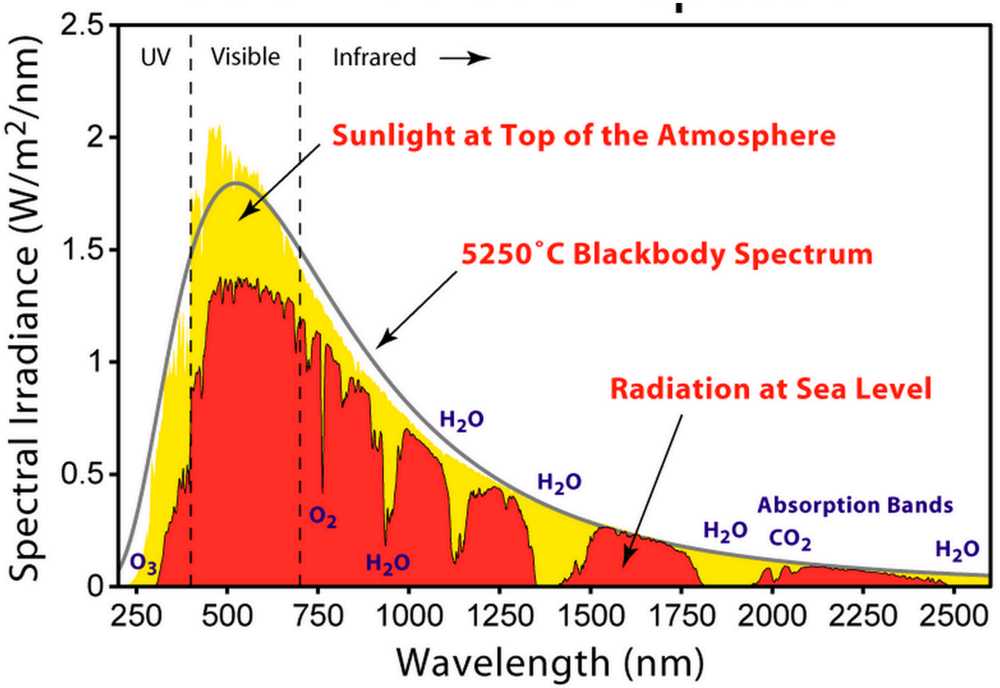
Background

Astronomers hate the Earth's atmosphere – it impedes their view of the stars and planets. Forces them to make corrections for its opacity.

Atmospheric scientists hate the sun – the complexity of its spectrum:

- Fraunhofer absorption lines
- Doppler shifts
- Spatial Non-uniformities (sunspots, limb darkening)
- Temporal variations (transits, solar cycle, rotation, 5-minute oscillation)



all of which complicate remote sensing of the Earth using sunlight.

In order to more accurately quantify the composition of the Earth's atmosphere, it is necessary to better understand the solar spectrum.

Motivation

Solar radiation is commonly used for remote sensing of the Earth:

- the atmosphere
- the surface

Both direct and reflected sunlight are used:

- Direct: MkIV, ATMOS, ACE, SAGE, POAM, NDACC, TCCON, etc.
- Reflected: OCO, GOSAT, SCIAMACHY, TOMS, etc.

Sunlight provides a bright, stable, and spectrally continuous source.

As accuracy requirements on atmospheric composition measurements grows more stringent (e.g. TCCON), better representations of the solar spectrum are needed.

Historical Context

Until 1500 (Copernicus), it was assumed that the Sun orbited the Earth.

Until 1850 sun was assumed 6000 years old, based on the Old Testament.

Sunspots were considered openings in the luminous exterior of the sun, through which the sun's solid interior could be seen.

1814: Fraunhofer discovers absorption lines in visible solar spectrum

1854: von Helmholtz calculated sun must be ~20MY old based on heating by gravitational contraction.

1868: Helium emission seen in solar spectrum (not seen on Earth until 1895).

Late 1800's: Geologists realized that Earth was far older then 20MY.

Early 1900's: Sir Authur Eddington calculated central temperature of 10MK.

1930's: realization that solar energy source must be nuclear. Hans Bethe et al. proposed that solar energy was from fusion: $4\ {}^{1}H \rightarrow {}^{4}He + 2e^{+} + 2\gamma + 2\nu$

1939: Wildt proposes that H^{-} ions are the main source of photospheric opacity

1968-1998: Solar neutrino deficiency mystery.

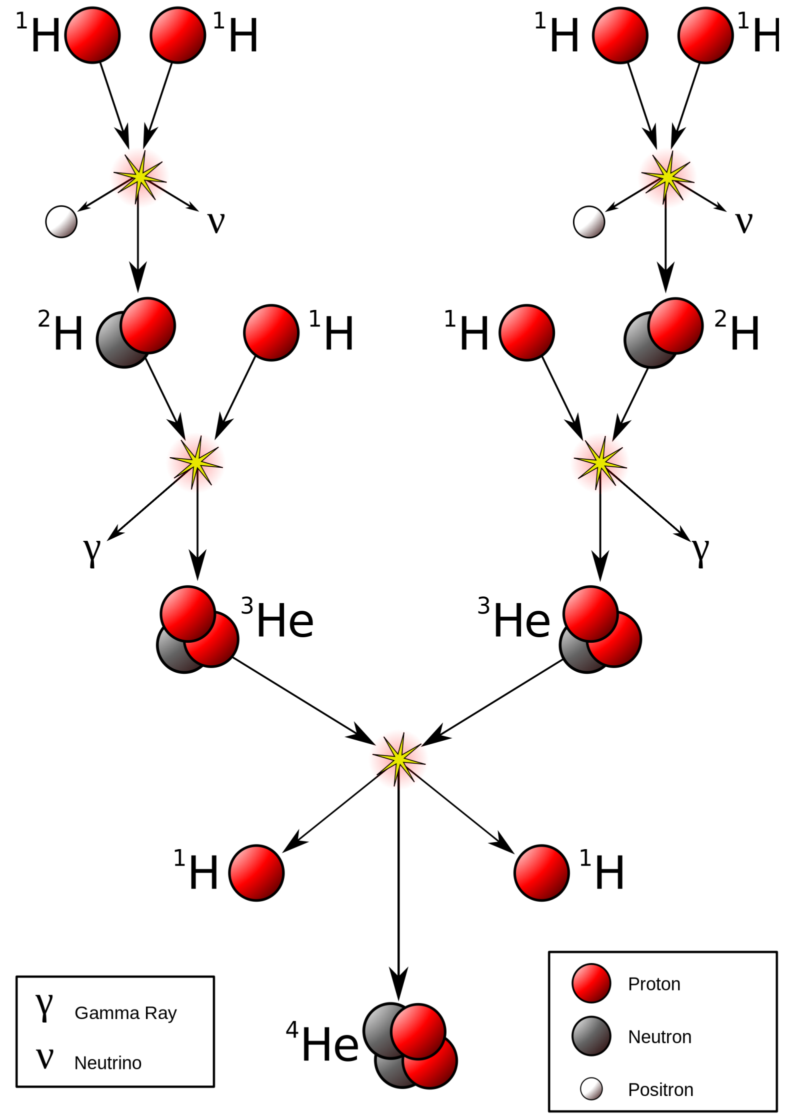
Nuclear fusion in the sun

Energy production at the sun's core is 275 W/m^3, about the same as a typical compost heap.

So why is the sun so hot? Because it is huge: energy production varies as r^3, but the energy can escape only through the surface, whose area varies as r^2. So the energy escaping per unit area (and hence T) increases with r.

At temperatures of ~15 MK (with help from quantum tunneling) two protons can occasionally overcome their electrostatic repulsion and fuse together under the strong nuclear force, emitting a positron and a neutrino. This is the rate-limiting step to the proton-proton reaction chain (right), from which our sun generates most of its power.

The net result is to convert 4 protons into a ^4He nucleus, two positrons, two neutrinos, and γ-rays, with a loss of 0.7% of the initial mass.

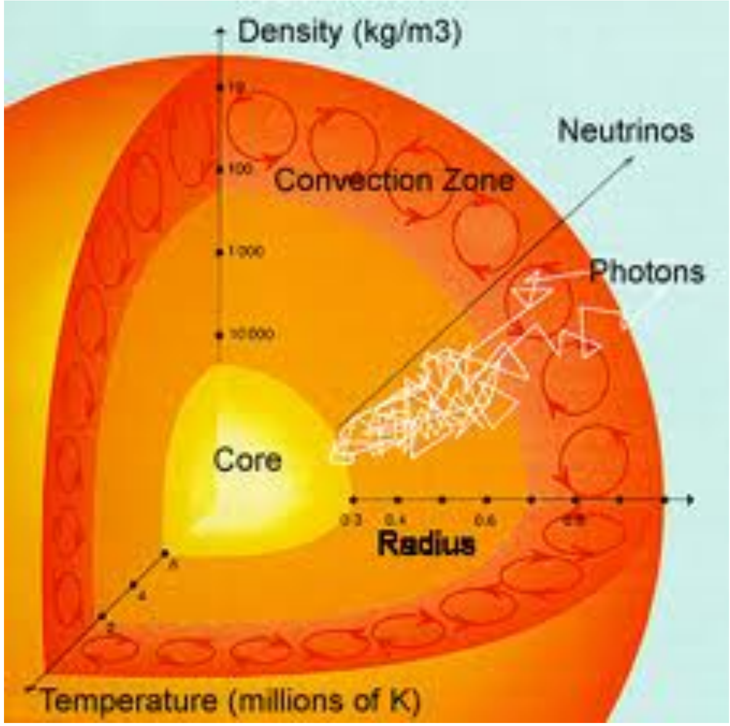


Nuclear fusion in the sun

Only the innermost 25% of the sun (1.5% by volume) actually generates energy.

Most of the energy produced in the sun's core is gamma rays. This has a MFP of only a couple of mm, and are absorbed and re-emitted (at slightly lower energies) gazillions of times in a random walk before the radiation reaches the surface.

No gamma rays are emitted by the sun. They are all absorbed and re-emitted as lower energy radiation (e.g., X-ray, UV, Vis, IR).



Radiation starting at the core (as gamma rays) takes ~10M years to reach the surface (as visible radiation), despite travelling at the speed of light the whole time. So the sun's core is extremely well insulated. In fact, diffusion of radiation is so slow that convection is faster.

Neutrinos, on the other hand, take just 2s to escape the sun, + 8 min to reach Earth. If sun goes out, we'll find out first from the neutrinos.

Issues Addressed in this Presentation

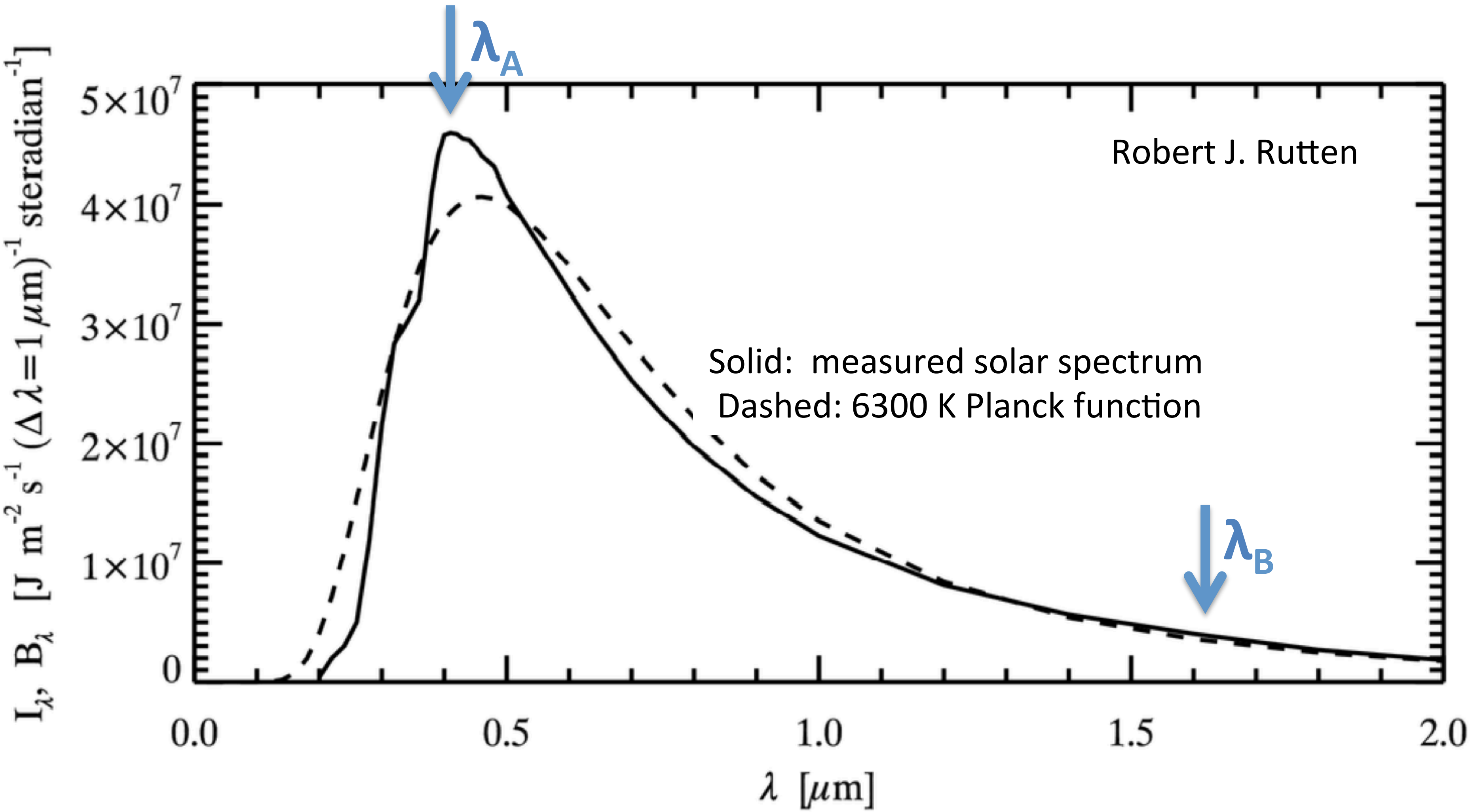
1. Low-resolution solar spectrum
    - Resemblance to a 6000K black body
    - Limb darkening

2. High Resolution solar spectrum
    - Fraunhofer absorption lines
    - Doppler shifts
    - Disk-Center vs Disk-Integrated

3. Efforts to parameterize the solar spectrum
    - Distinguishing solar from telluric lines
    - Solar linelist and model

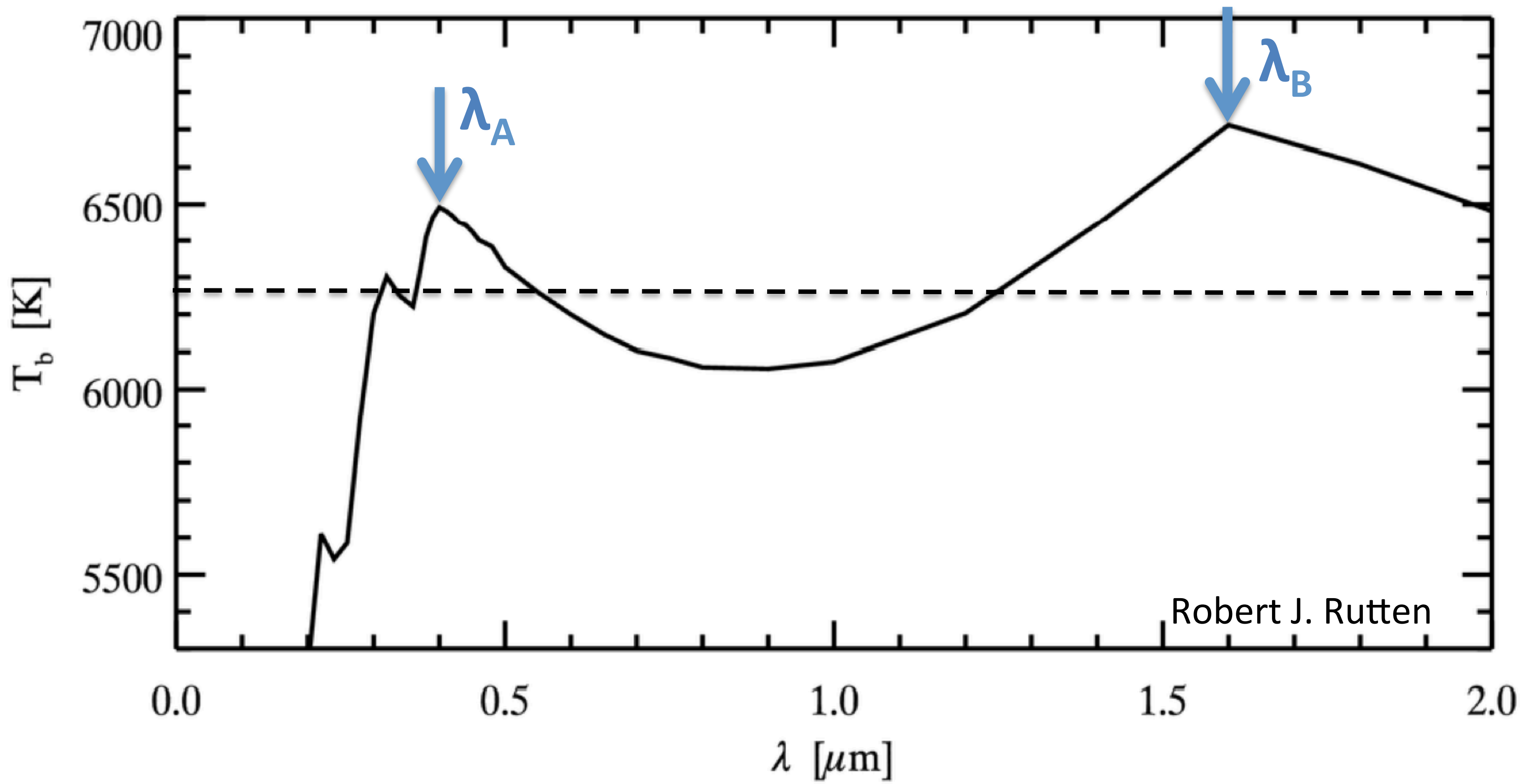
4. Implications for Earth remote sensing

The Solar Spectrum – Low Resolution



Can be approximated well by a Planck Function
At which wavelength is solar radiation hottest?

Effective Solar Brightness Temperature

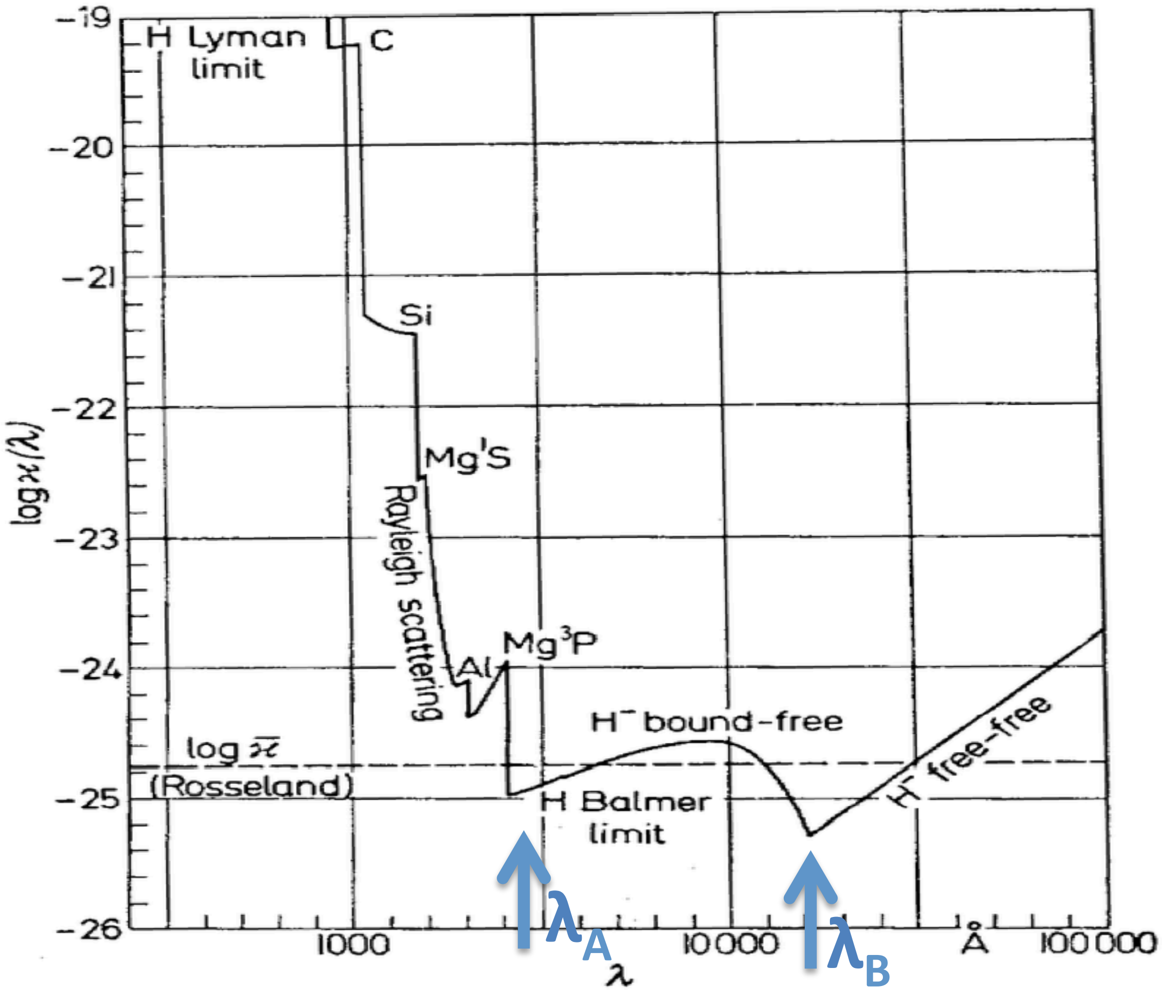


Why is sun hottest (i.e. most transparent) at 1.6 um ?

Why is the solar spectrum so close to a black body curve anyway?

The sun is just a bunch of H & He atoms, transparent in the IR and Vis at 6000K

Solar Photospheric Opacity

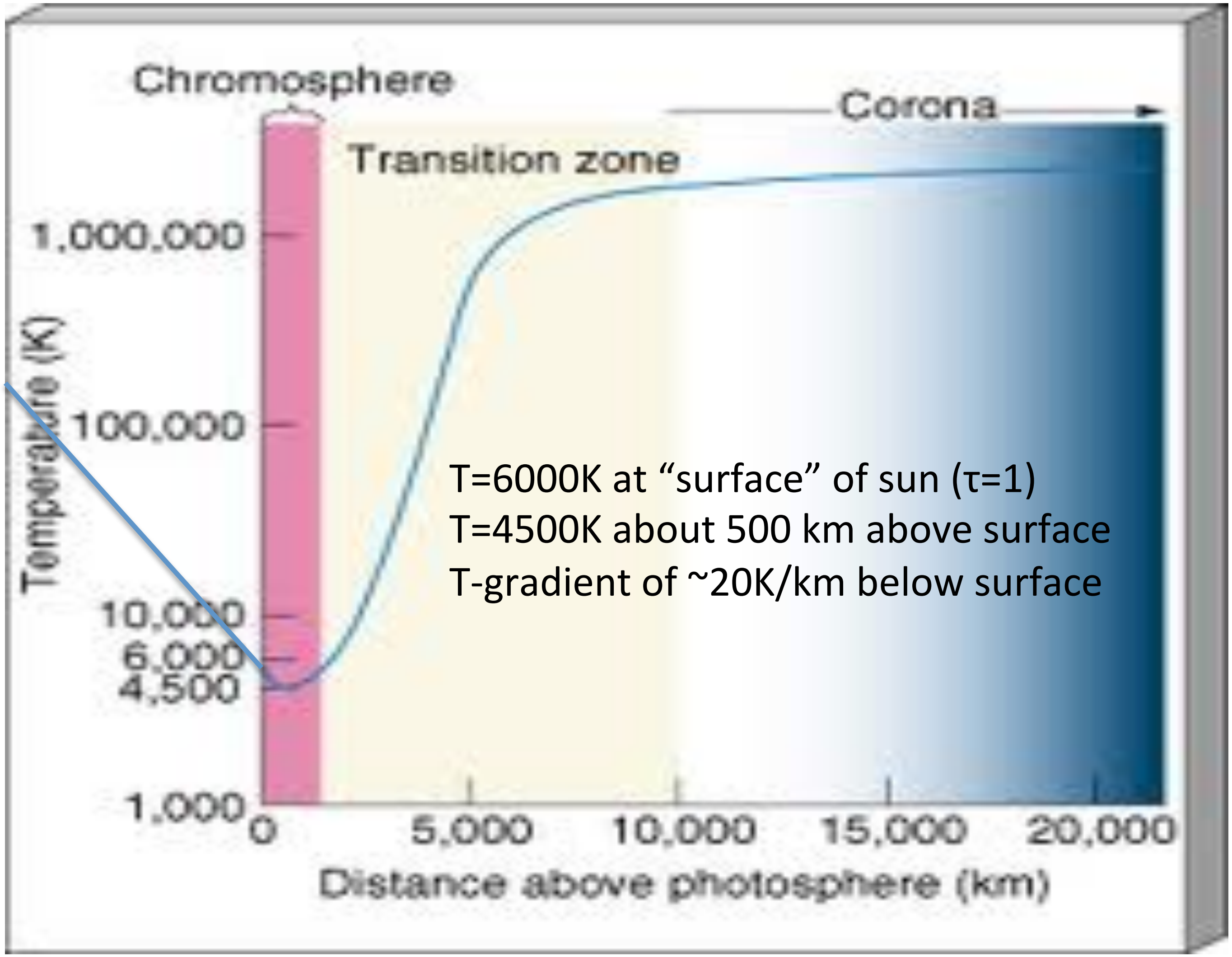


H Lyman limit:
1→ ∞ 91 nm

H Balmer limit:
2→ ∞ 365 nm

In the visible and IR, H^- ions are the dominant source of solar opacity.
Without H^- ions, we would see much deeper into the sun (hotter, brighter)

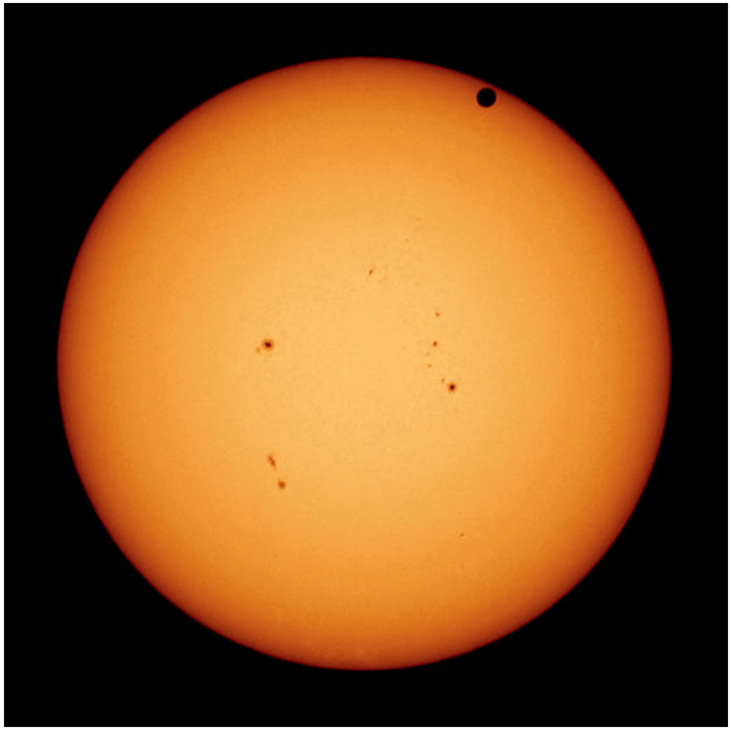
The Solar Temperature Profile

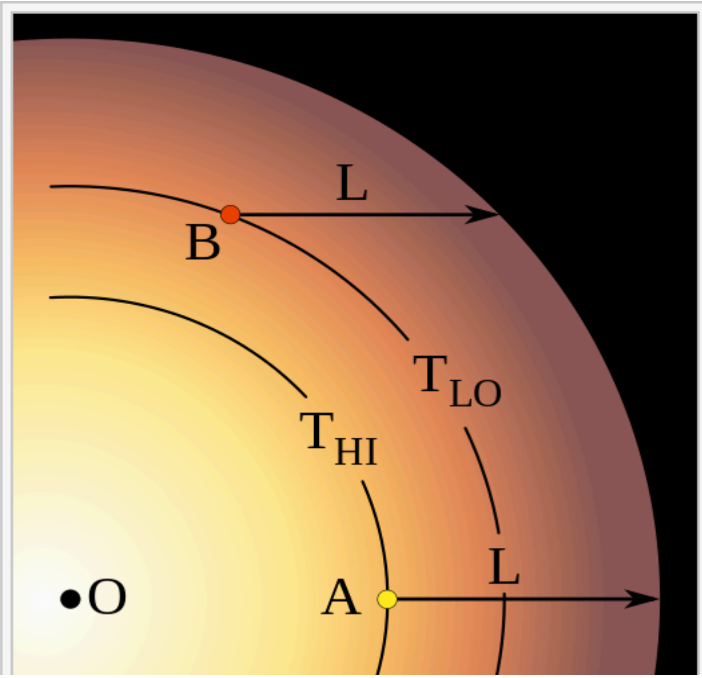


The T decrease from 0 to 500km above the "surface" has important implications

Solar Limb Darkening

Confirms the decrease of temperature with altitude in photosphere. At normal incidence, we see deeper into the sun (hotter & brighter). Viewing the limb, unit opacity occurs at a higher altitude, where it's cooler. Limb/Center intensity Ratio ≅ Planck(4500,v)/Planck(6000,v)





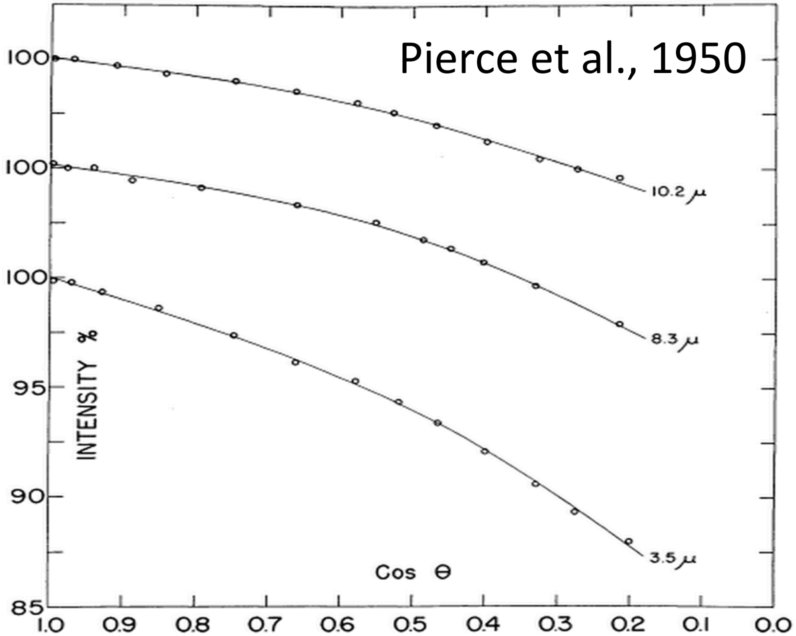
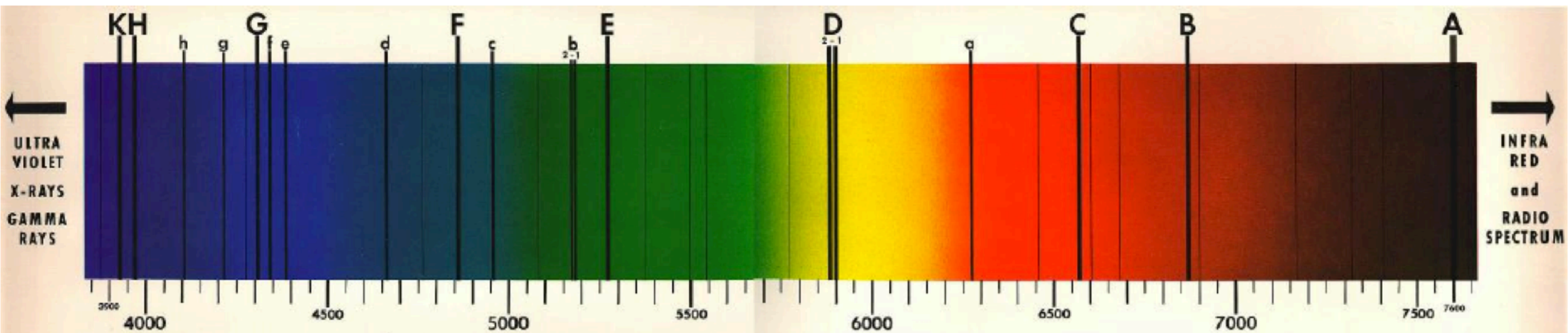


Fig. 4.—Solar limb-darkening-curves for the region 3.5–10.2 μ

The Solar Spectrum – High Resolution

In 1814, Fraunhofer invented the spectroscope, and discovered 574 dark lines appearing in the solar spectrum. They are still called Fraunhofer lines. Kirchhoff and Bunsen showed in 1859 that they are atomic absorption features providing diagnostics-at-a-distance of the local conditions in the atmospheres of the Sun and other stars.



scale in Ångstrom; 1 Å = 0.1 nm

K & H: resonance lines of calcium ions

G: rotation-vibration band of CH molecules

F: Balmer-β line of hydrogen atoms

b: three lines of magnesium atoms

E: a group of lines of iron atoms

D: two resonance lines of sodium atoms (the same as in street lights)

C: Balmer-α line of hydrogen atoms

B & A: rotation-vibration band of oxygen molecules in the Earth atmosphere

Solar Absorption lines at high resolution

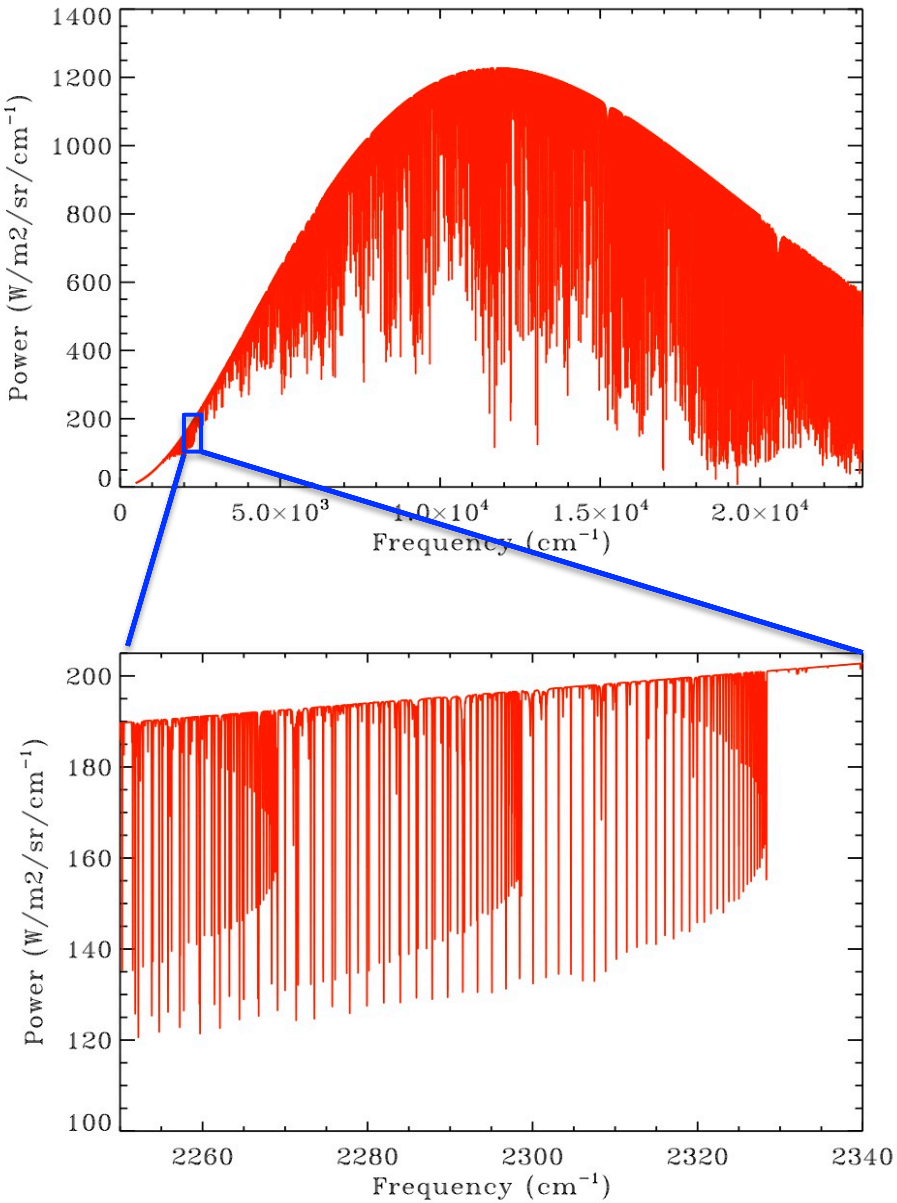
At high spectral resolution, the solar spectrum has over 40,000 documented discrete absorptions.

These represent photons emitted from the sun's surface and then absorbed during their passage through the 4500K temperature minimum above the photosphere.

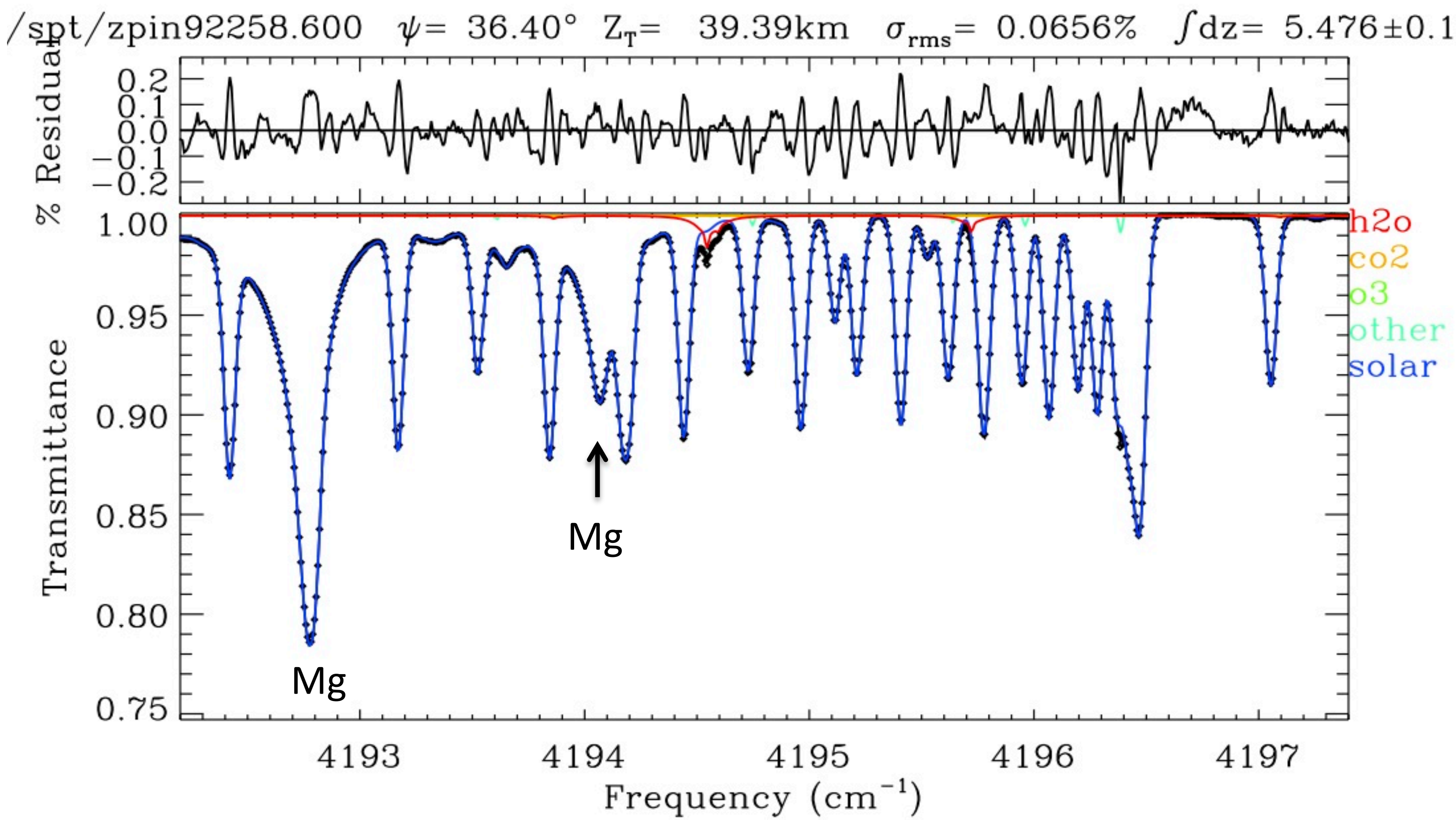
In the IR they are mostly due to molecules (CO, CH, OH).

In the NIR and Vis they are mostly due to atomic and ionic transitions (Fe, Ni, Si, Mg, Na, K, C, H, He). These are what Fraunhofer saw.

[For high-res discussion, use ν not λ]

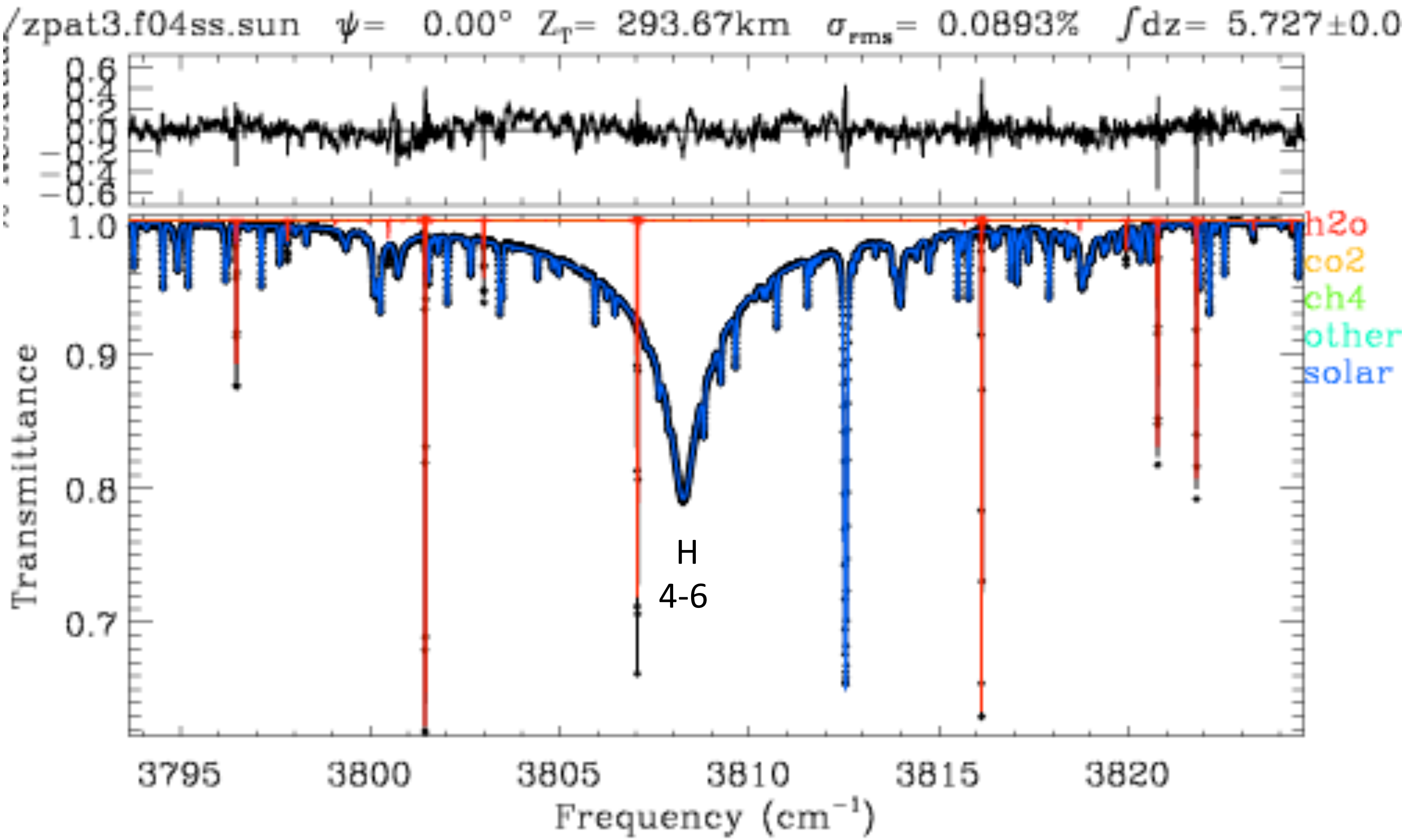


Atomic versus Molecular Absorption

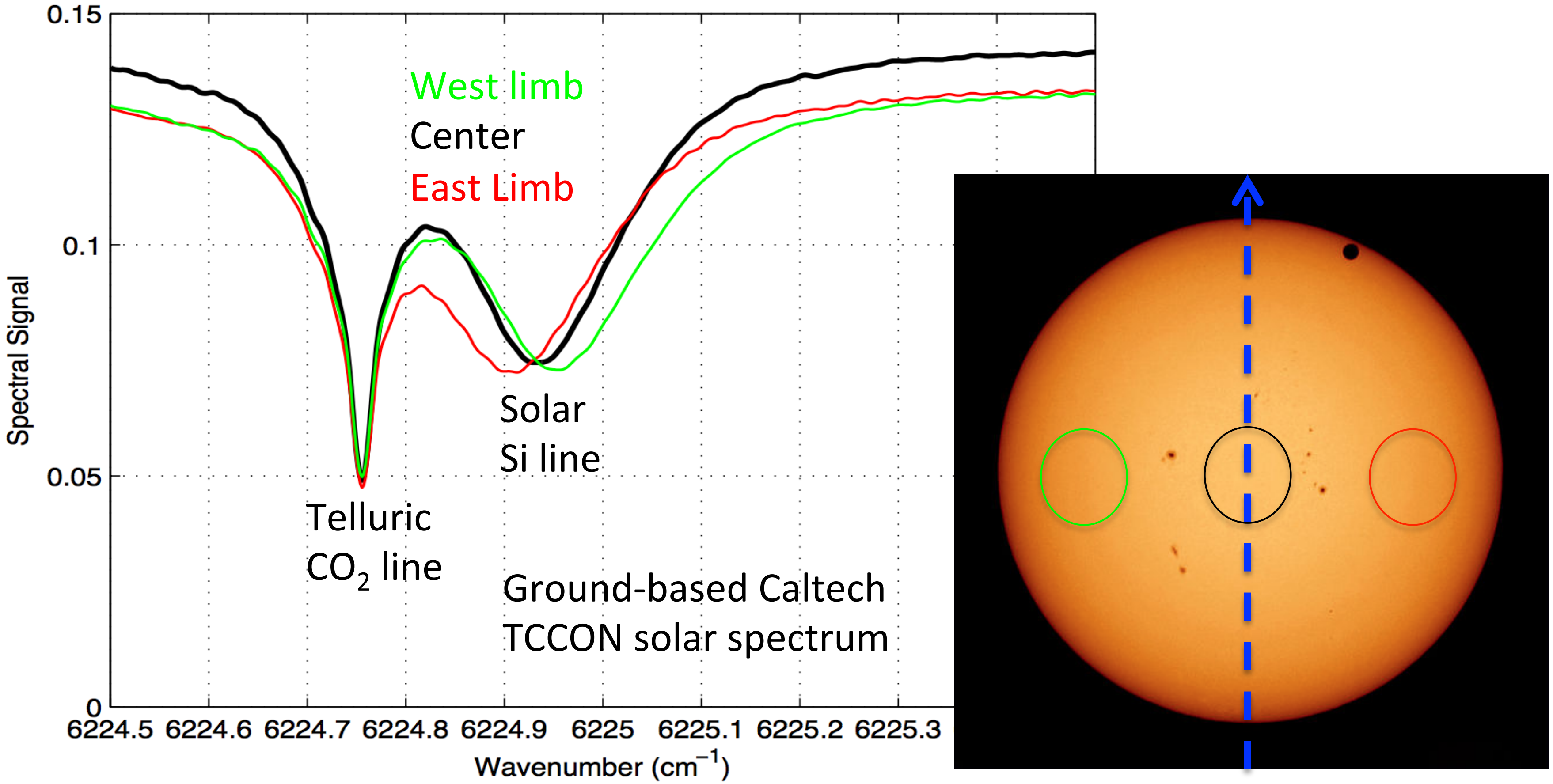


Molecules (e.g. CO, OH, NH, HF) only exist at the coolest temperatures (~4500K) and therefore have narrow lines. Atoms (H, Ca, Mg, Si, Fe, Ni) can exist at cool and hot temperatures and therefore have cusp-shaped absorption lines, reflecting larger P/T deeper inside the sun.

Example: H-atom absorption lines

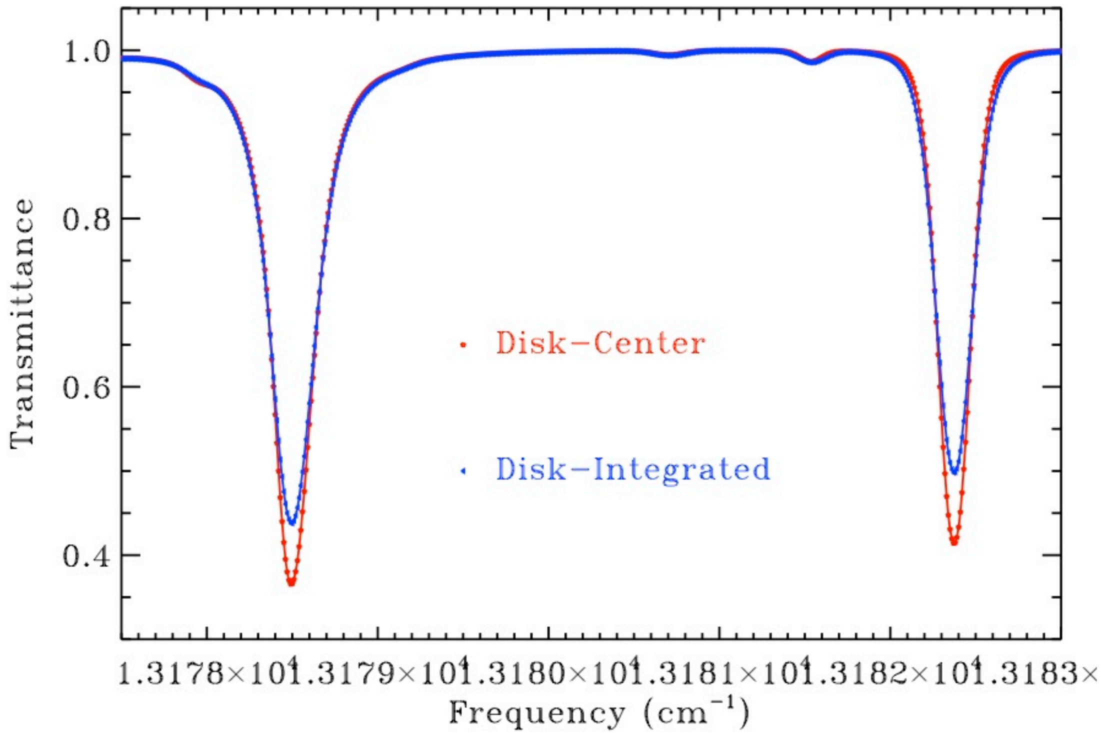


Solar-spin–induced doppler shifts



East & West limbs of sun doppler shifted relative to disk center.
Continuum level reduced (limb darkening).
Disk-integrated spectrum (average of red/black/green) would therefore have broader, shallower solar lines than disk-center spectra. [0.06/6000 cm^{-1} = 10^{-5} = 3000 m/s]

Disk-Center versus Disk-Integrated



Sensors using direct sunlight (MkIV, ACE) generally use only a small portion of the solar disk near the center, to prevent degradation of spectral/vertical resolution.

Sensors that use reflected sunlight receive photons from the entire solar disk.

We already know that the center of the solar disk is brighter than the limb because unit optical depth occurs deeper and hence at a higher temperature.

The absorption lines are shallower and broader in the disk-integrated spectrum

Modeled Center-to-limb behavior of Fraunhofer lines

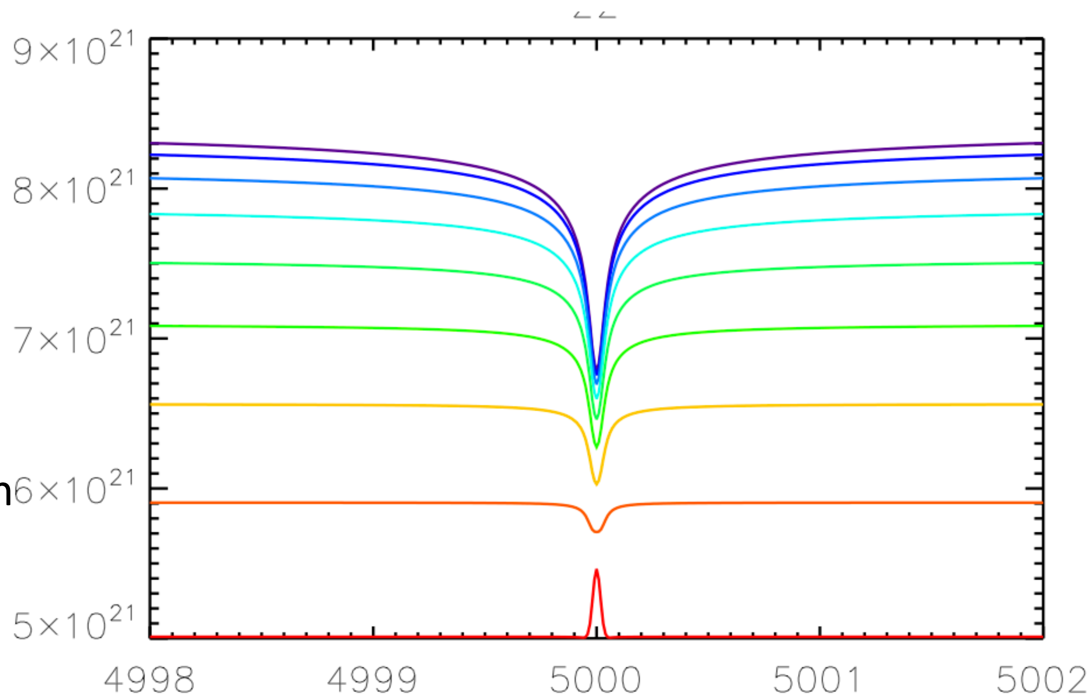
Nearly all solar lines are shallower, as a fraction of the continuum level, in limb spectra than disk center spectra.

This may seem paradoxical to scientists familiar with remote sensing of the Earth's atmosphere, where absorption lines get stronger/deeper towards the limb.

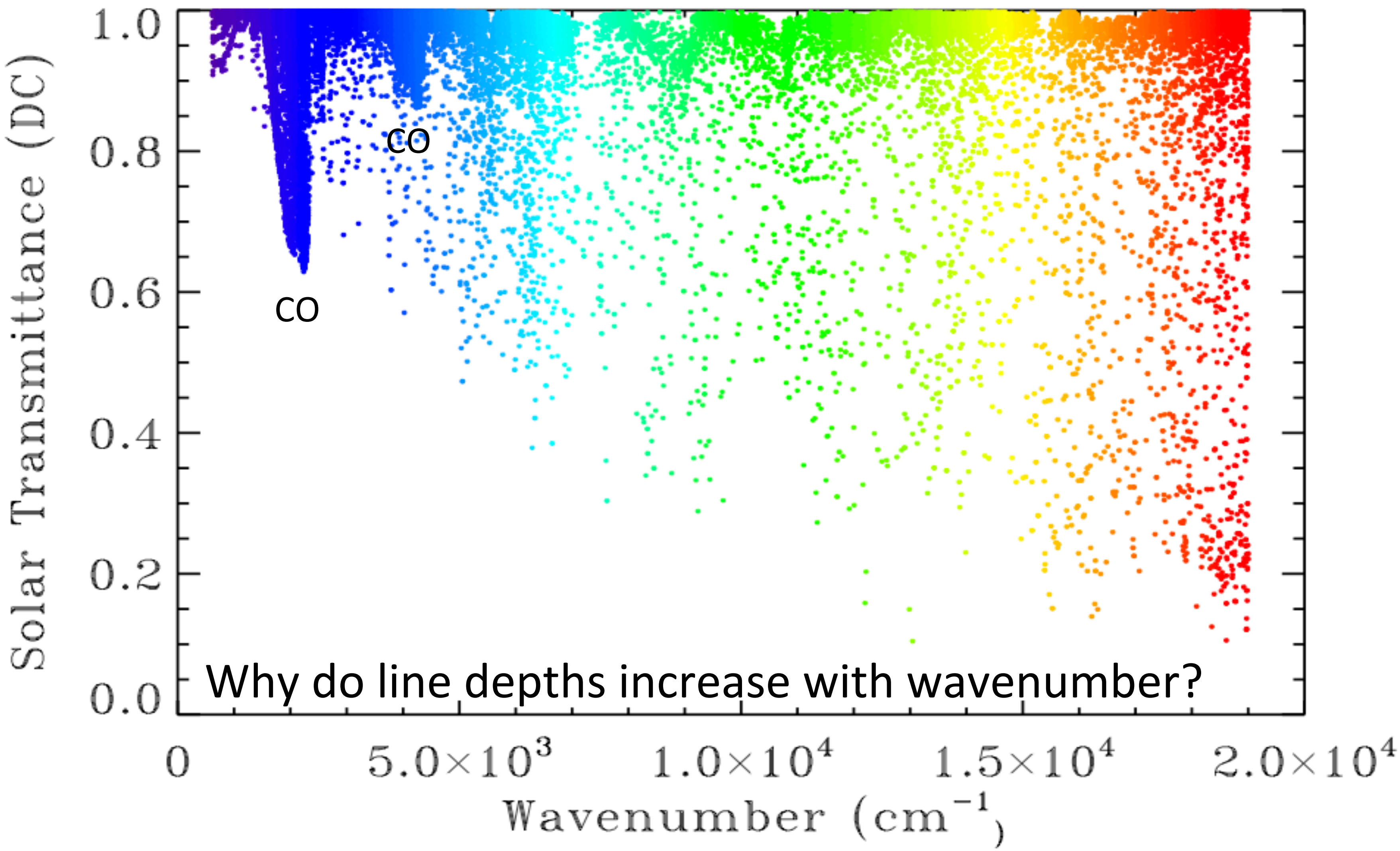
In the continuum, unit optical depth occurs at T=6000K for the disk center spectrum and T=4500K for the limb.

For the strong line absorption itself, unit optical depth happens at higher altitude near the temperature minimum, perhaps 5000K for disk center and 4800K for limb.

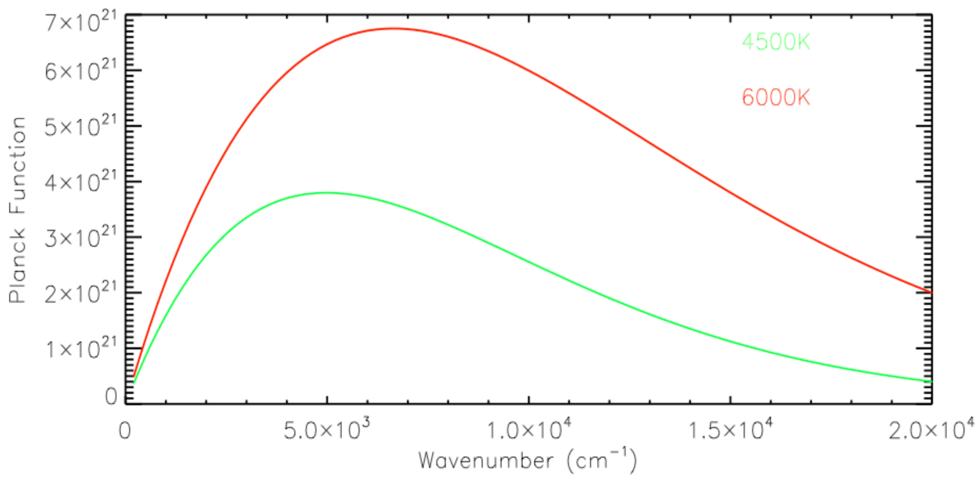
So the temperature contrast between the disk-center and limb is greater in the continuum regions than in the absorption lines.

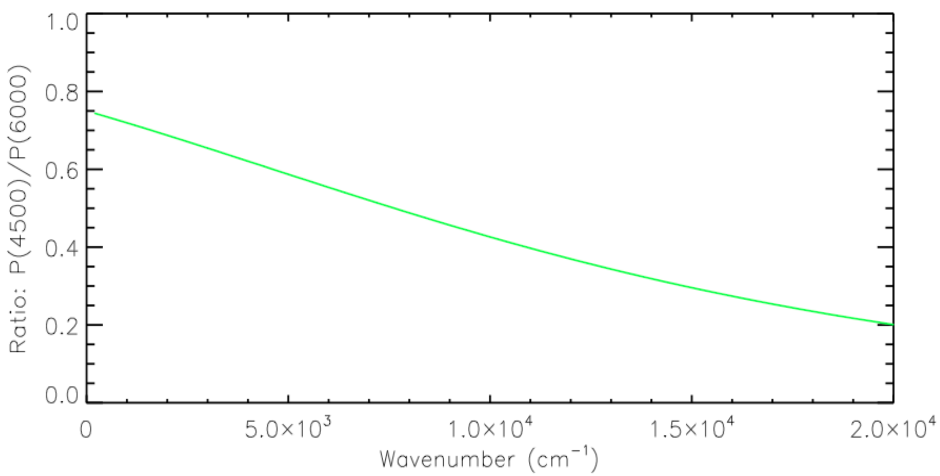


Measured Solar Line Depths



Solar Planck Functions





The 6000K Planck function (red) represents the solar continuum.

The 4500K Planck function (green) represents the emission from the centers of strong absorption lines.

Solar emission spectrum must lie between these two curves.

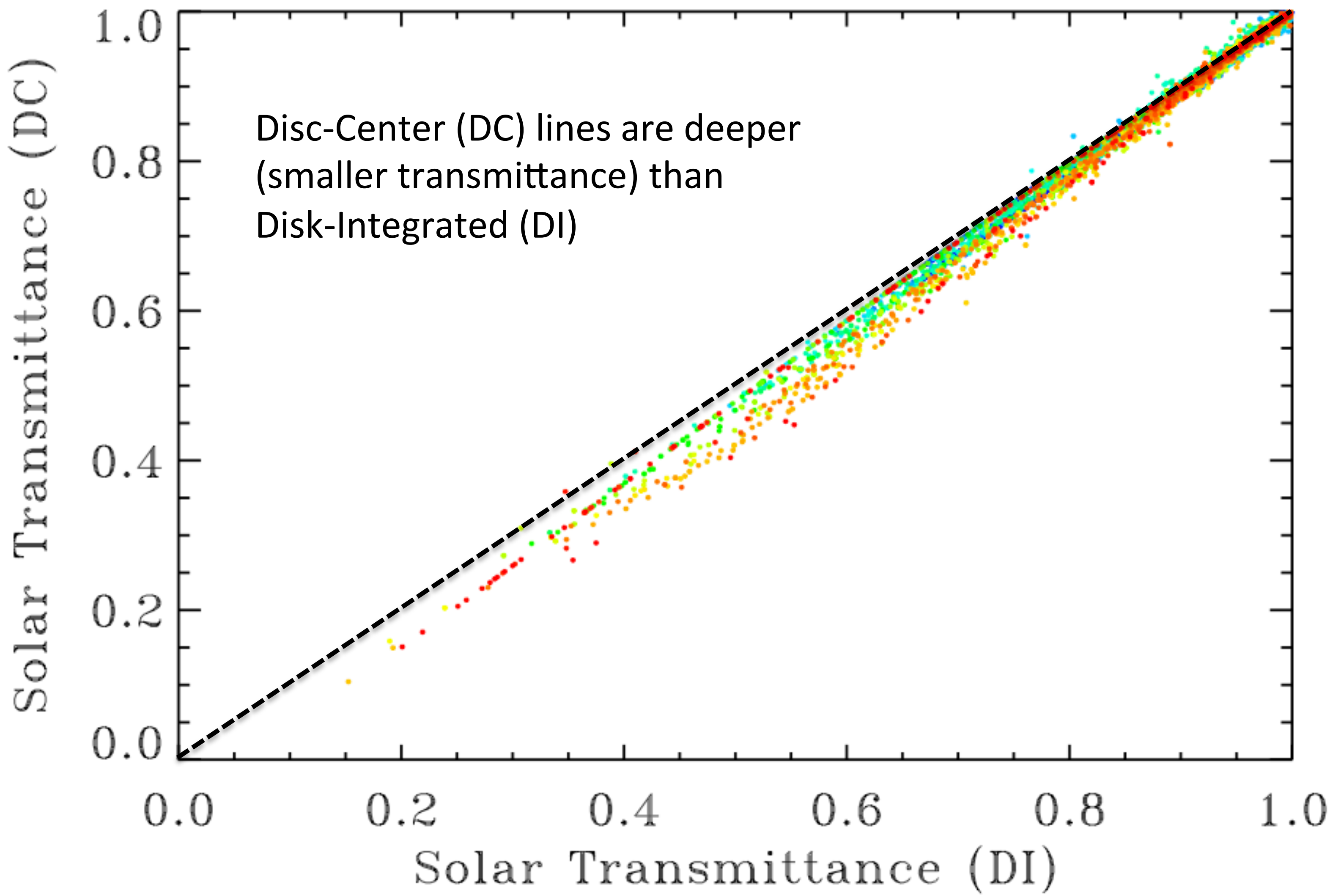
No matter how strong an absorption line, its emission can never fall below the 4500K Planck function, that of the temperature minimum.

The ratio of the 4500K and 6000K Planck functions decreases with ν.

This is main reason for the increasing solar absorption line depths with wavenumber.

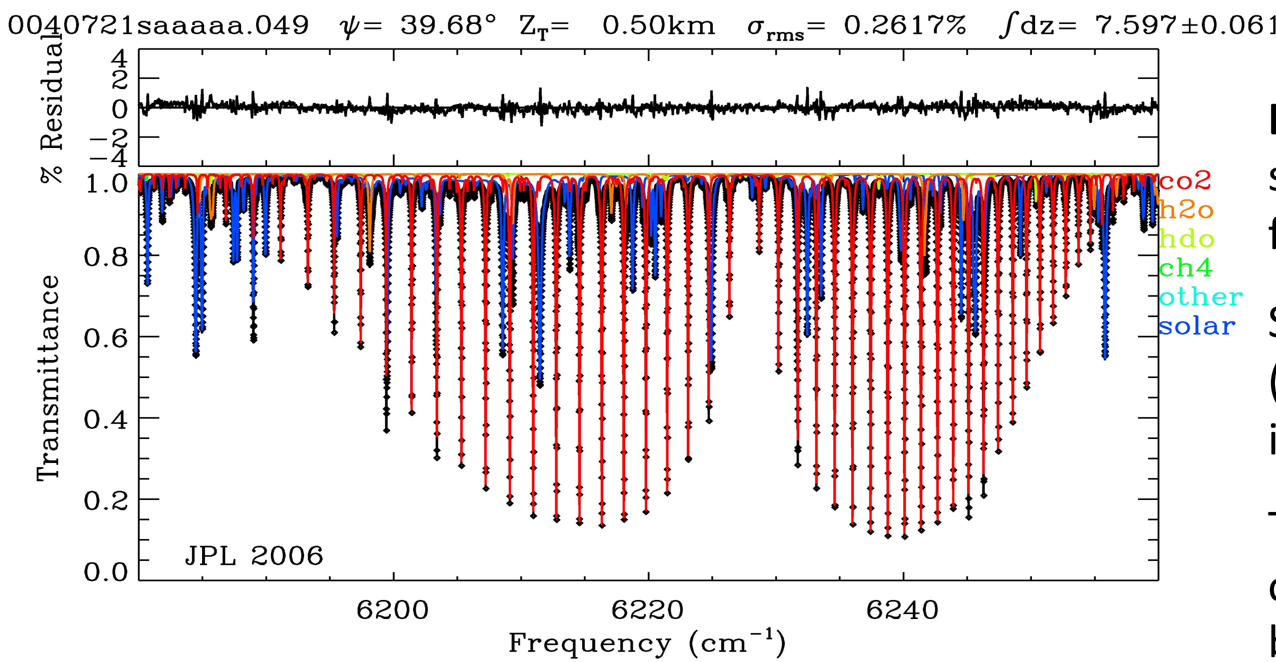
And limb darkening.

Measured Solar Line Depths



Efforts to Parameterize the Solar Spectrum

The majority instruments don't have exo-atmospheric spectra to calibrate their atmospheric spectra. The high resolution solar structure must therefore somehow be accounted for in the forward model used to fit the atmospheric spectra.



Left: Fit to ground-based solar spectrum measured from Park Falls, Wisconsin.

Solar Fraunhofer lines (blue) are up to 50% deep in the NIR.

To achieve fitting residuals of 0.25%, solar lines must be accurately represented.

If science goal is to measure atmospheric CO_2 to 0.1% precision (Carbon Cycle modeling) then solar lines must be accurately represented in terms of their position, depth & shape.

How do we know which absorptions are solar versus telluric?

Four Methods to determine Solar Spectrum

1. Theoretical. Spectroscopic calculation of solar spectrum based on knowledge of atomic/molecular energy levels and solar P/T & composition (Kurucz, 2005)

- Difficult, but can be applied to any star

2. Exo-Atmospheric. Measure a solar spectrum from high above the atmosphere (e.g. ATMOS: Farmer & Norton, 1989; ACE: Hase et al. 2005, 2010),

- By far best approach (telluric absorptions are negligible).
- ATMOS/ACE/GOSAT spectra have limited spectral coverage and/or resolution

Will not discuss these two further. Neither ATMOS or ACE cover NIR or Vis. And instruments that do are at poor spectral resolution

Four Methods to determine Solar Spectrum

3. Zero Airmass Extrapolation. Measure a series of solar spectra over a range of airmasses and then use the Bouger (-Langley) method to extrapolate to zero airmass (e.g., Langley, 1881; Arvesen at al., 1969; Kurucz, 2008, Livingston and Wallace, 1991)

- Requires unchanging atmospheric conditions (P/T, gas & aerosol)
- Under-resolved atmospheric absorptions not fully removed if non-linear
- independent of telluric spectroscopy

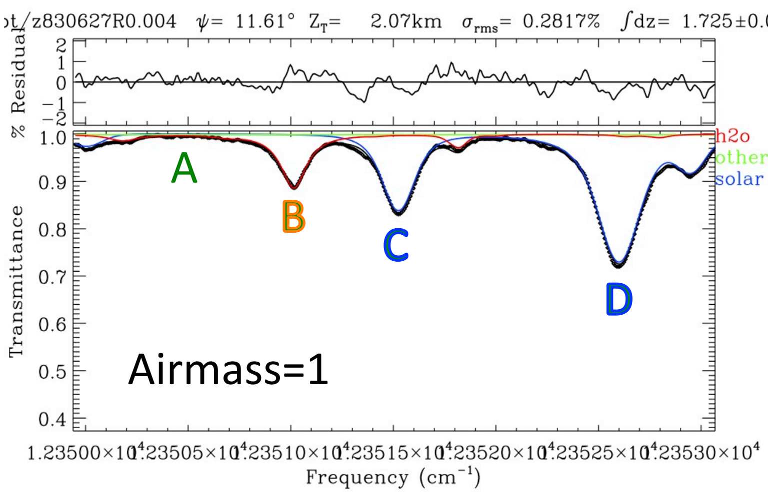
4. Telluric Subtraction. Measure low-airmass solar spectra. Fit calculated atmospheric transmittance spectrum. Dividing the measured spectrum by the calculated atmospheric transmittance, yielding solar/instrumental component (Hase et al., 1996; Chance and Kurucz, 2010)

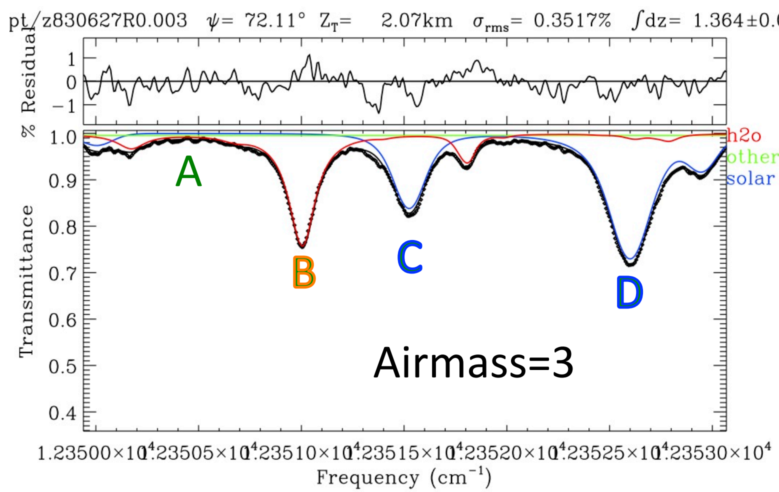
- Requires good spectroscopic linelist and atmospheric model & fitting software
- More flexiblity handling different observations and varying atmosphere

Will now discuss these two.

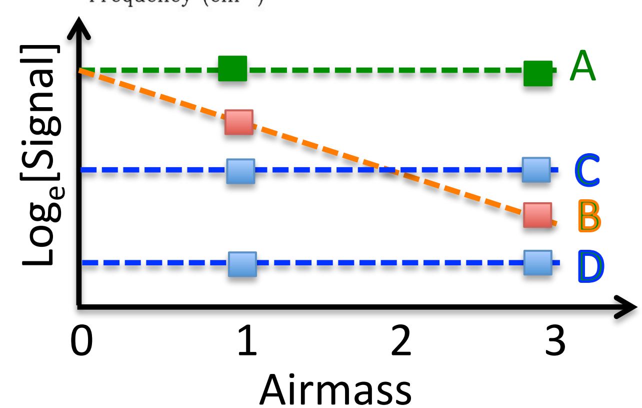
Zero Airmass Extrapolation - Theory

Before the satellite era, people derived solar spectra from ground-based and aircraft measurements, by exploiting the fact that telluric absorption line depths increase with airmass as Exp[-k_v.a], whereas solar absorptions remain constant. So plotting $\log_e$(Signal) versus airmass (Langley plot) distinguishes solar/telluric.

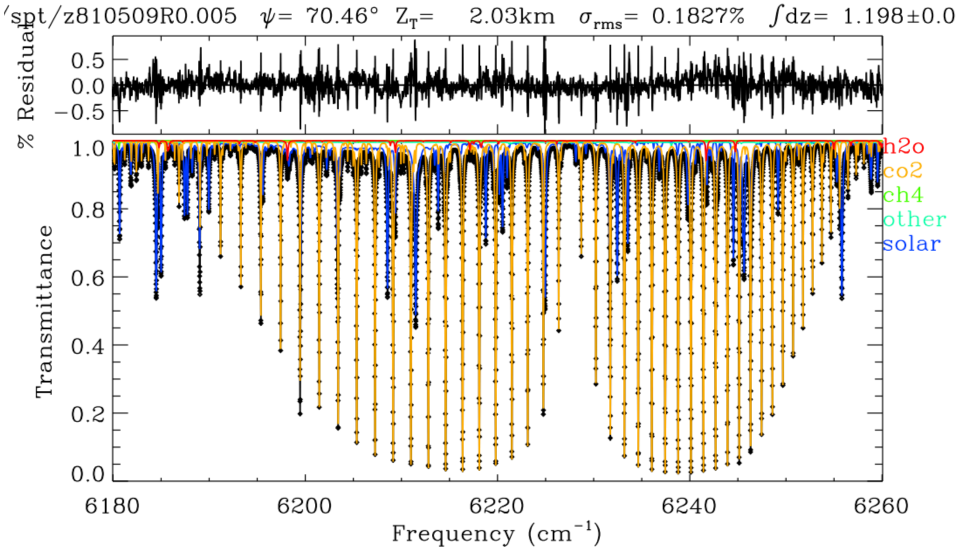




- Atmospheric absorption must remain unchanged between low & high airmass (T/P, gas & aerosol)
- Absorption features must be weak or fully resolved
- Useless in blacked out spectral regions
- *Didn't need any spectroscopy knowledge*

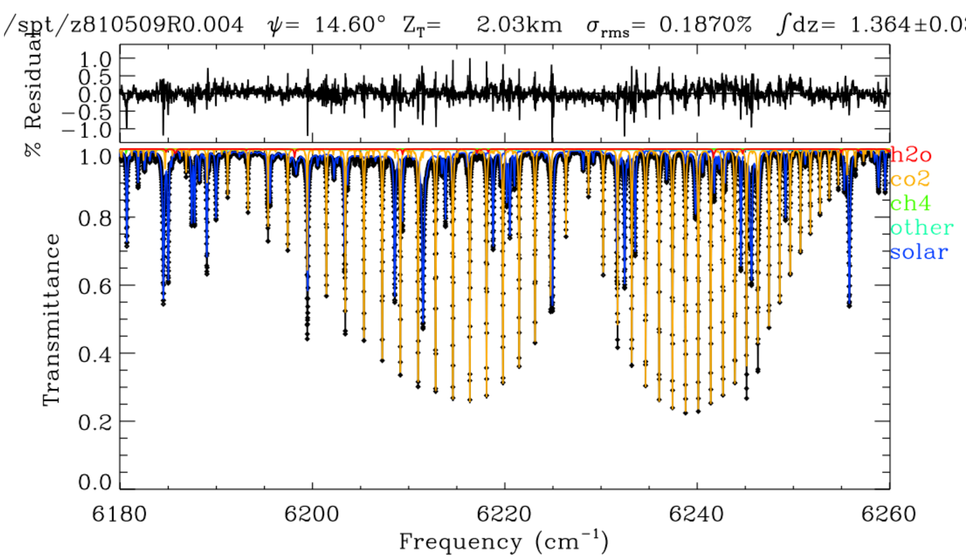


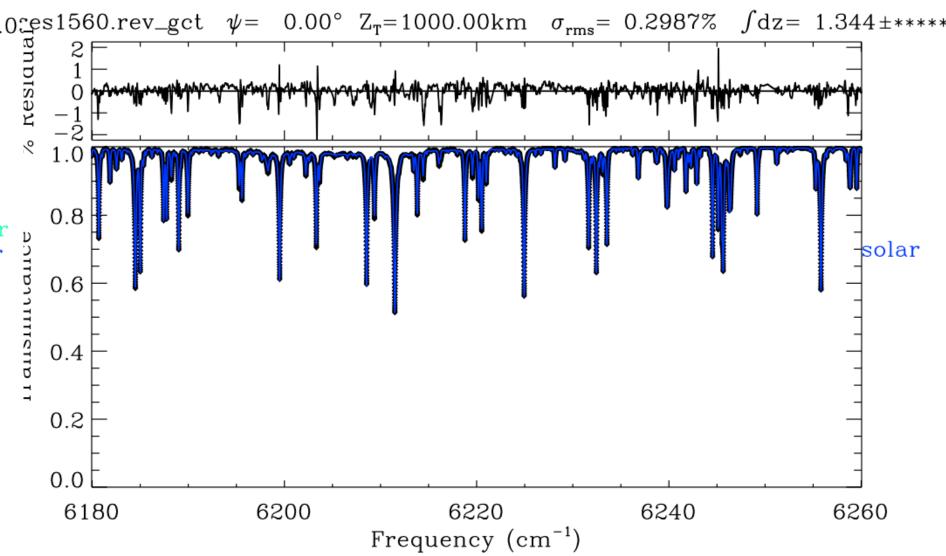
Zero Airmass Extrapolation - Example



Left: Low and high-airmass ground-based Kitt Peak spectra in the 6220 cm^{-1} region used for TCCON CO_2 retrievals.

Below: The zero-airmass-extrapolated solar spectrum calculated from these by Kurucz [2005], fitted using a solar model spectrum.





Telluric Subtraction Method

Utilize a variety of low-airmass solar spectra measured under different conditions (disk center, disk integrated,).

Fit calculated telluric transmittance spectrum.

Divide each measured spectrum by the fitted atmospheric transmittance

What is left is the solar (and instrumental) component.

Improved spectroscopy and telluric modeling/retrieval capabilities in recent years make this possible.

Promises greater flexibility (earth atmosphere not assumed constant)

Solar Spectrum versus Solar Model

Previously-discussed methods will give you a solar spectrum, but it may not be applicable to your needs in terms of:

- Fraction of the disk observed & pointing location on sun
- Spectral coverage
- Earth-Sun doppler shift
- Spectral resolution of the observing instrument
- Phase of the solar cycle (Vis/UV)

So in the absence of a large library of solar spectra representing different measurement conditions (wavenumber ranges, spectral resolutions, fraction of solar disk), a single high-quality solar spectrum isn't always going to be useful.

For example, the ATMOS and ACE solar spectra represent a great achievement. But they cannot easily be extrapolated to other conditions (e.g. disk-integrated) outside those of the original measurement.

To be able to generate a more generally applicable solar spectrum, you need a solar model based on a wide variety of measured solar spectra.

New Solar Model

Based on the Telluric Subtraction approach, an empirical solar linelist has been developed containing 40,000 lines covering the 600-20000 cm^{-1} region.

Together with a model that encodes a simple solar lineshape function, the linelist can be used to generate a solar pseudo-transmittance spectrum on any spectral grid for any fraction of the solar disk observed.

Kitt Peak spectra form the backbone of the new solar spectrum/linelist:

- Available at all frequencies of interest (MIR, NIR, & visible)
- Disk-center and disk-integrated
- Solar lines are fully resolved

In the mid-IR, the linelist is based on MkIV balloon and ATMOS shuttle spectra.

In the O_2 A-band region it is based primarily on Denver University balloon spectra.

This solar linelist & model are currently used for consistent analysis of ground-based TCCON spectra (disk-center) and of GOSAT spectra (disk-integrated).

Available FTS Measurements

Instrument	Advantages	Disadvantages
#GOSAT (650 km) (2009-present)	Disk-integrated (3 bands)	0.2-0.5 cm^{-1} resolution Disk-integrated only
ATMOS (350 km) 1985-1994	600-4800 cm-1 (3 filters) 0.015 cm-1 resolution	Slight H2O contamination Disk-center only
#ACE (650 km) (2003-present)	700-4400 cm-1 simultaneously High SNR. Contamination-free	0.04 cm-1 resolution (apodized) Disk-Center only
MkIV balloon 1989-	650-5650 cm^{-1} simultaneously 0.01 cm-1 resolution	39 km altitude, residual gas absorption. Disk-center only
Denver University 2000 32 km	12930-13250 cm-1 (O2 A-band) 0.02 cm-1 resolution	Telluric O2 absorption
Kitt Peak 1978-2006)	Disk-Center & Disk-Integrated 600-35000 cm-1 @ 0.01 cm-1	2 km altitude Telluric interference.
TCCON	3900-15500 cm-1 Center-to-limb observations	0-2 km altitude H2O contamination

Used for validation purposes only

These solar spectra have different attributes. Combine them in such a way that their strengths are emphasized and weaknesses hidden.

Empirical Solar Lineshape Model

By making some assumptions about the shape of the solar Fraunhofer lines, and their variation from center to limb, develop an empirical solar model.

$$f(\nu - \nu_0) = e^{-\frac{(\nu-\nu_0)^2}{\sqrt{d^4+(\nu-\nu_0)^2 w^2}}}$$

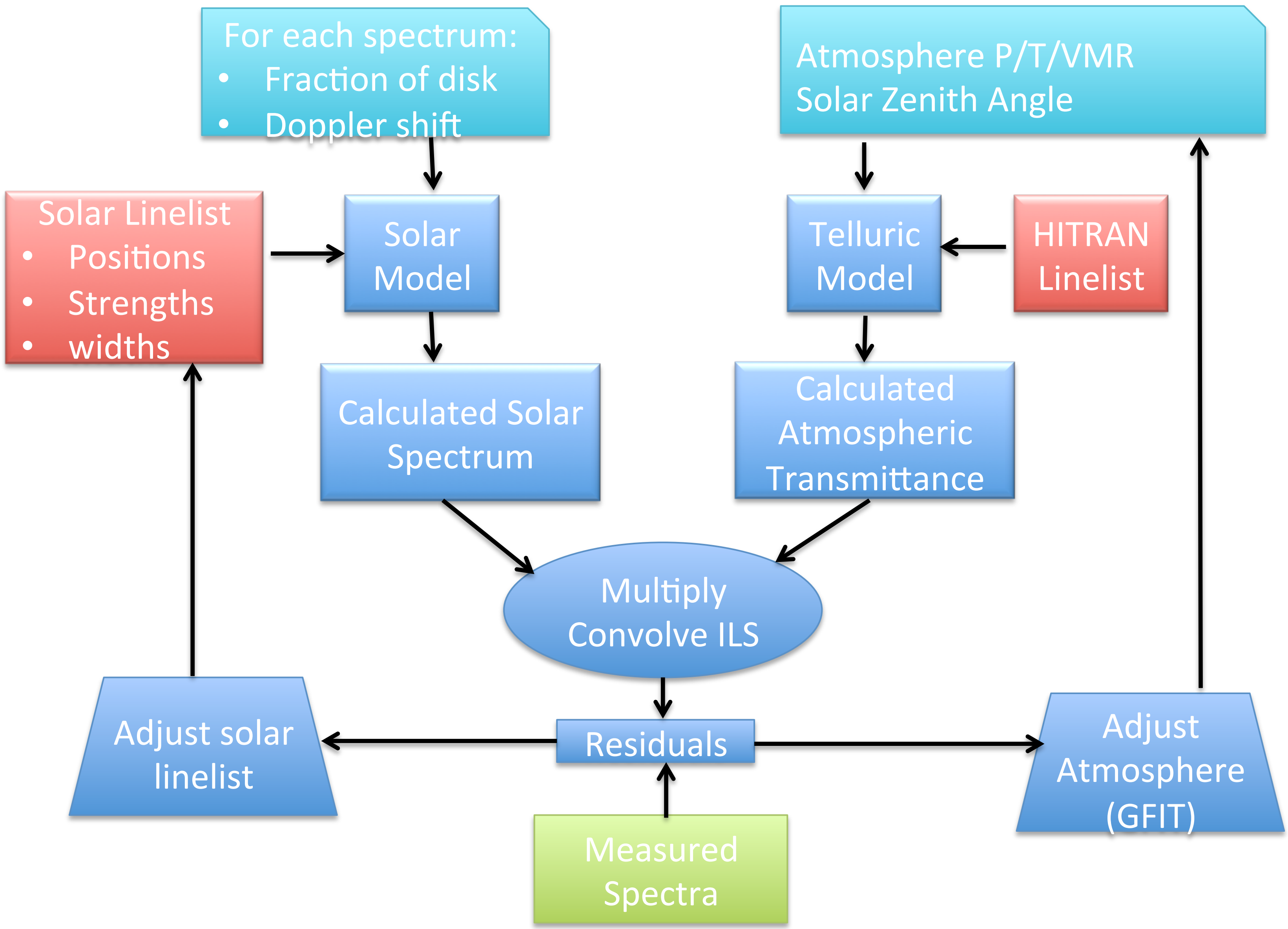
This choice of lineshape has no physical basis, but seems to provide a reasonable representation is nearly all cases.

The various measured solar spectra can then be fitted using the solar model, after accounting for the:

1. Earth atmosphere (observation altitude, zenith angle, gas vmr profiles)
2. Fraction of solar disk observed (broadening)
3. Time of observation (doppler shift)
4. ILS of the measuring FTS spectrometer

Solar line positions, intensities, widths (DC & DI) are determined using ALL spectra. Using diverse set of measured input spectra helps expose inconsistencies.

Solar Linelist Generation Flowchart



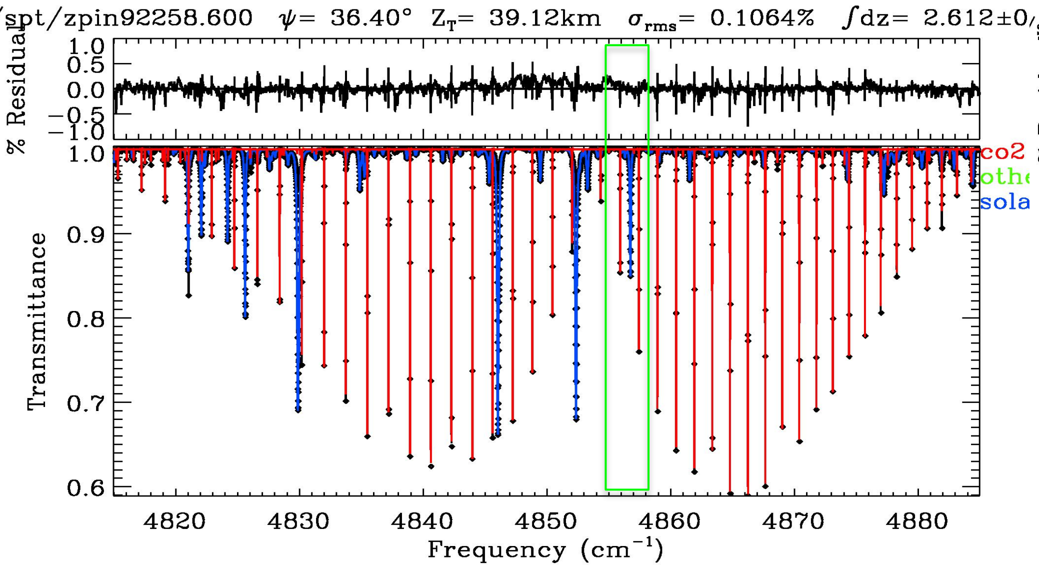
Advantages over previous Empirical Solar Reference Spectra/Linelists

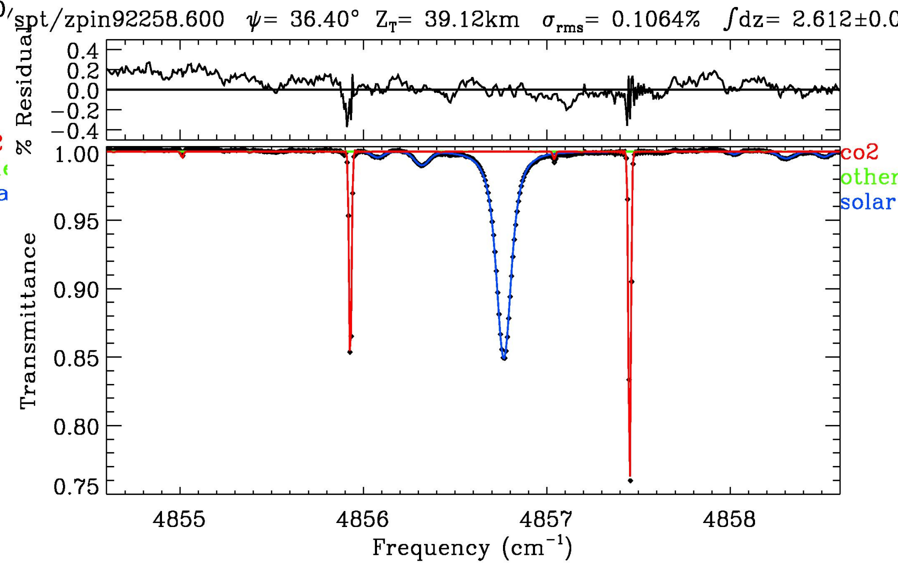
- Covers a much broader spectra region (600-15500 cm^{-1}) then previously
- Also uses high-resolution, high-altitude balloon spectra
- Can be calculated on arbitrary spectral grids
- Calculates disk-center, the integrated solar disk, and intermediate cases

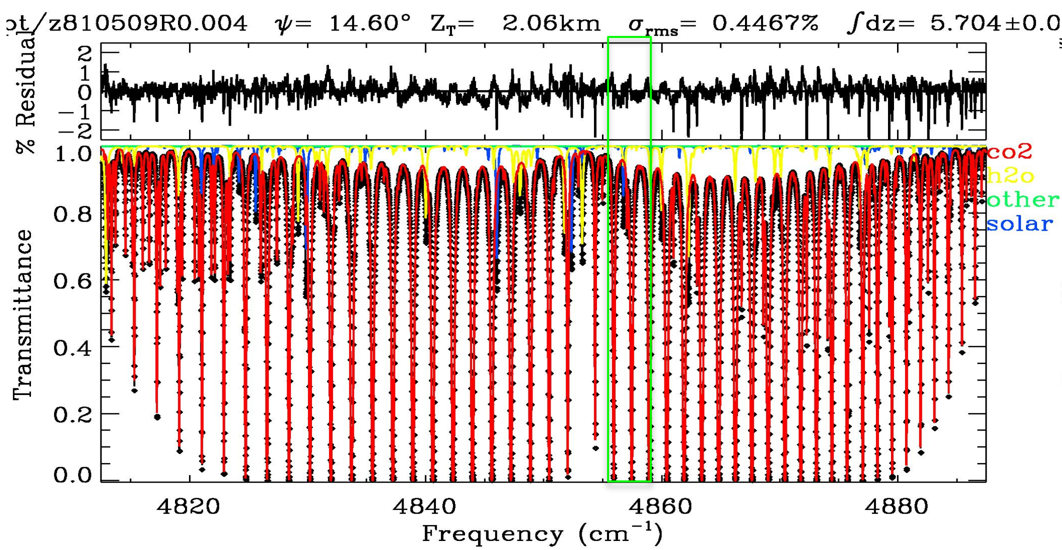
Currently being used for analysis of MkIV, TCCON, GOSAT (and OCO-2) spectra.

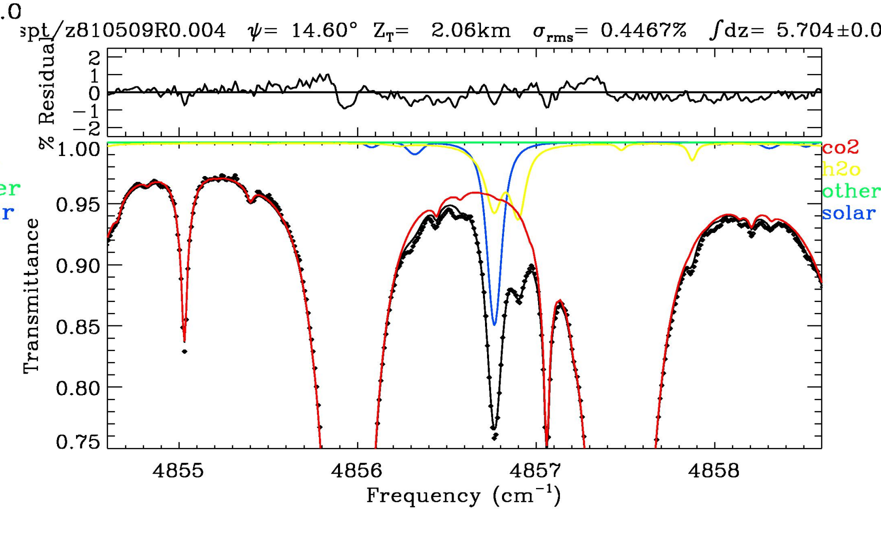
Model-generated disk-center and disk-integrated solar transmittance spectra vailable from: http://mark4sun.jpl.nasa.gov/toon/solar/solar_spectrum.html

Example – Comparing Kitt Peak & Balloon









Conclusions

Over the past 20 years there have been substantial improvements in our ability to predict the high-resolution structure of the solar spectrum. This is due to:

- Spectroscopic improvements (telluric lines)
- Improved atmospheric and solar models
- New high-altitude observations (ATMOS, Balloon, ACE)

An empirical solar linelist, together with a solar lineshape model, has been derived by the telluric absorption method.

Based on a variety of measured spectra as input with different:

- Observation geometries and telluric contamination amounts
- Spectral resolutions and coverages
- Solar doppler shifts and fractions of solar disk observed

Fitting to model exposes inconsistencies between measured input spectra.

Artifacts (e.g. ILS, ZLO, CF, gas absorptions) can removed in the fitting process.

This has improved our ability to represent solar absorption features, especially in the NIR from 4800 – 15500 cm-1, essential for Earth remote sensing by sunlight.

Acknowledgements

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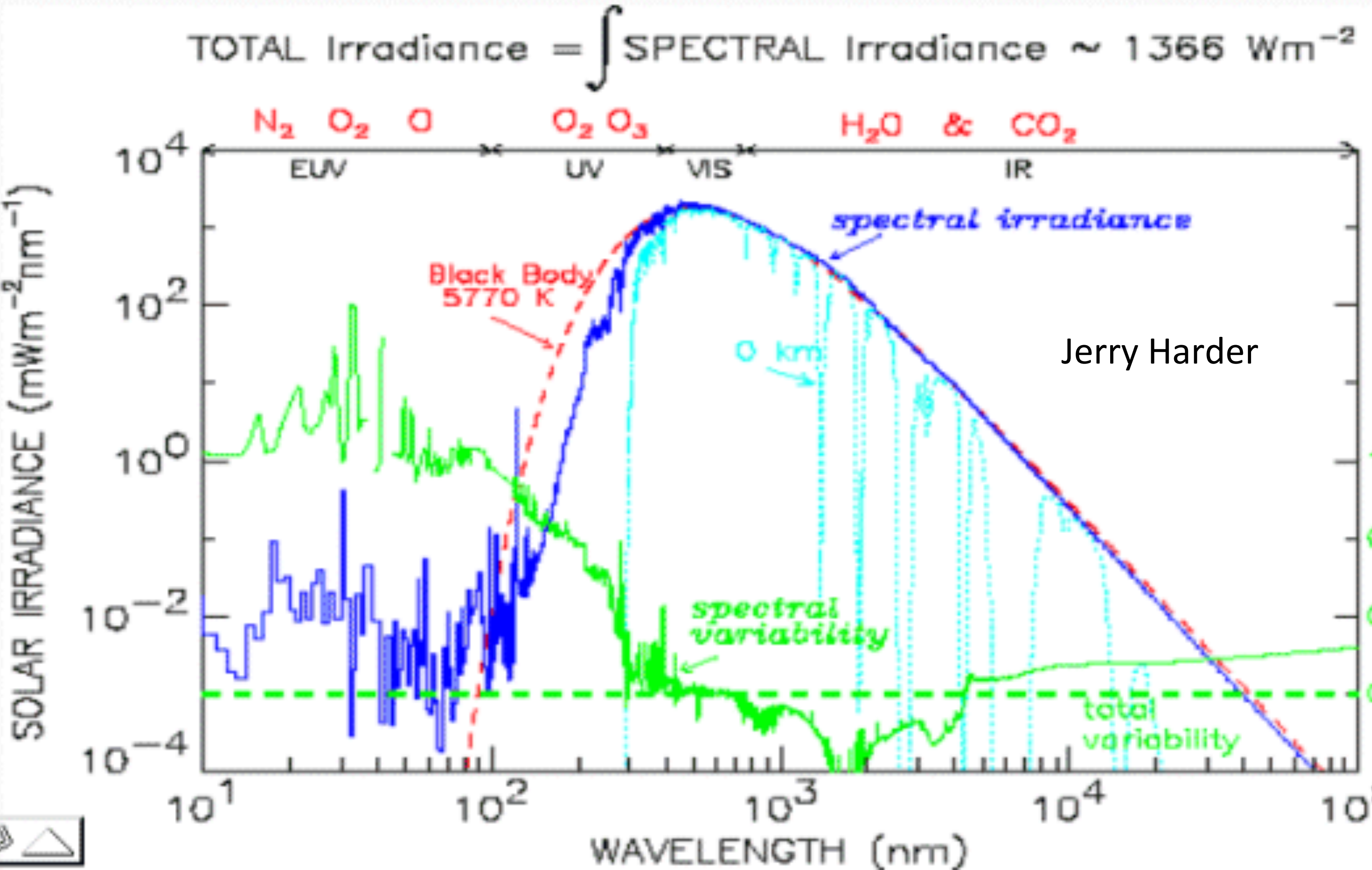
The many people involved in building FTS and acquiring solar spectra

- ATMOS
- ACE
- Kitt Peak
- MkIV
- TCCON
- GOSAT

Supplemental Material

SOLAR SPECTRUM, VARIABILITY and ATMOSPHERIC ABSORPTION



Implications for remote sensing

Sun is a bright and stable source, especially in the IR.

This assumes that you are looking at the same part of the sun all the time.

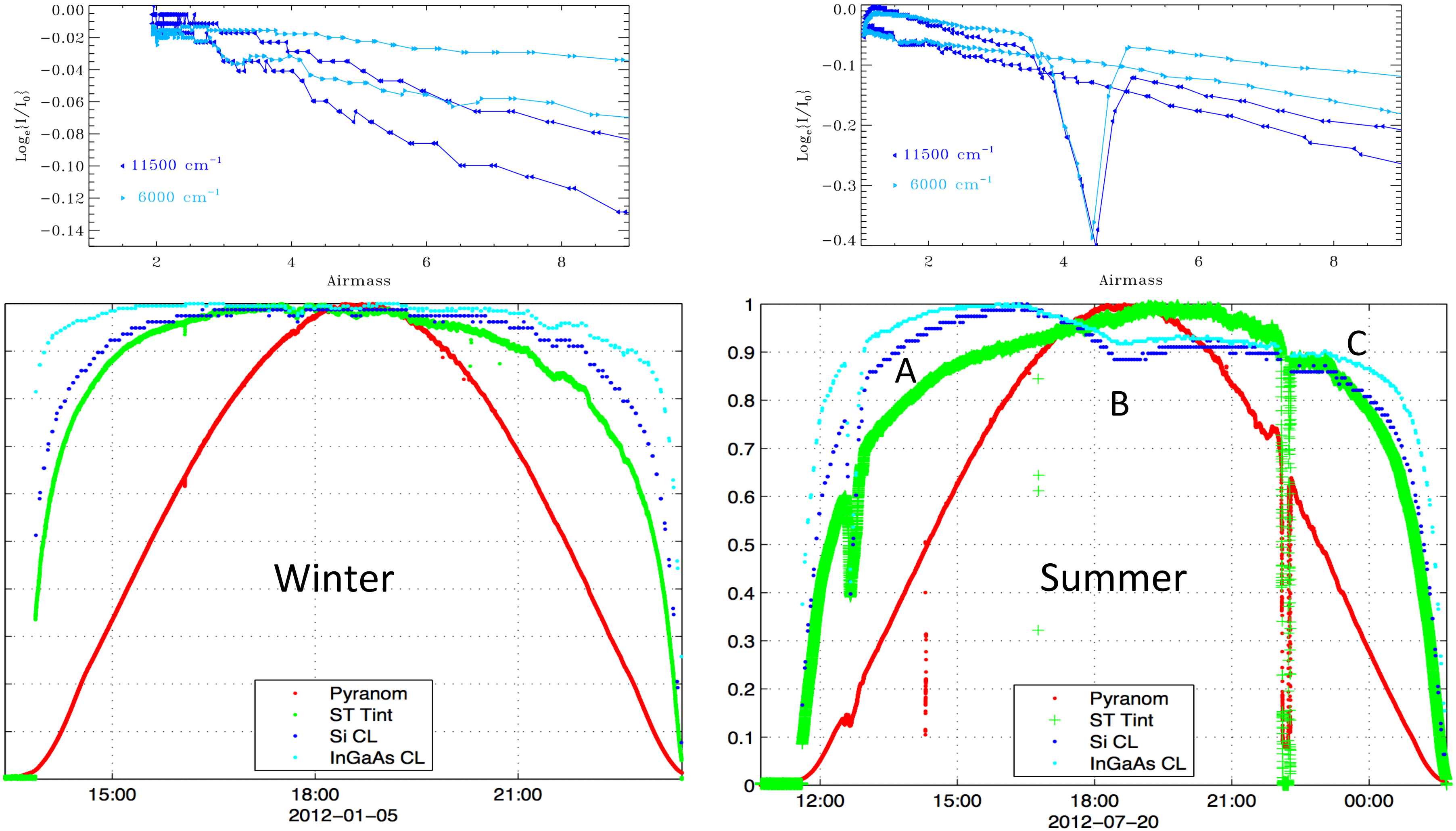
If only using a fraction of the full solar disk, spatial inhomogeneities (sunspots, limb darkening, doppler shifts) make accurate pointing important.

Mis-pointing will cause:

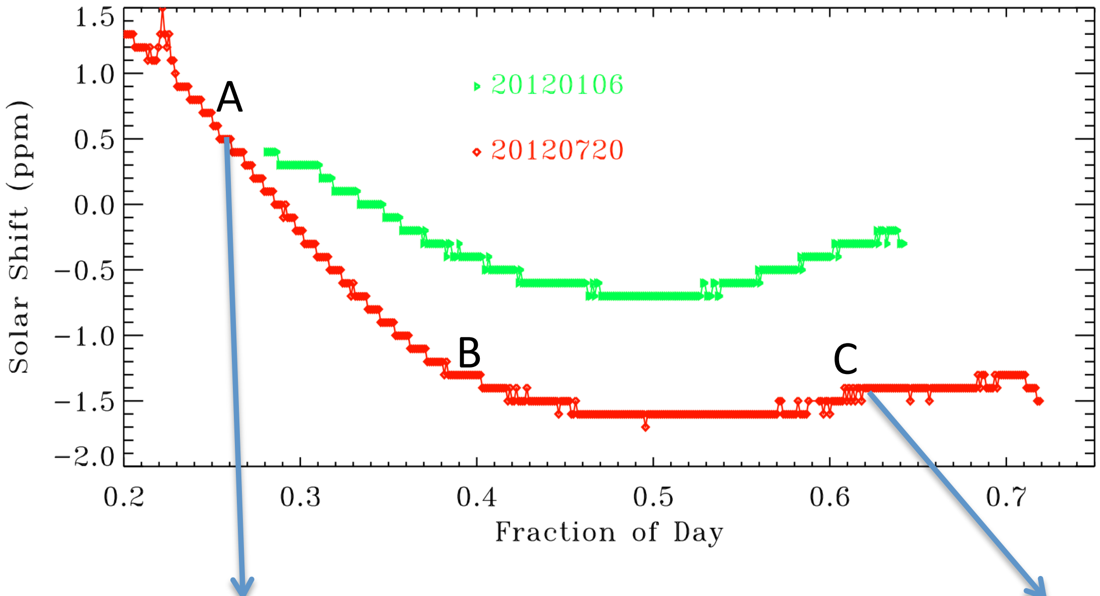
- Spurious variations in the solar intensity (limb darkening) and solar line depths
- Doppler shifts of the solar lines
- Spurious detections of gases on the sun (e.g. H_2O, HF, CO)

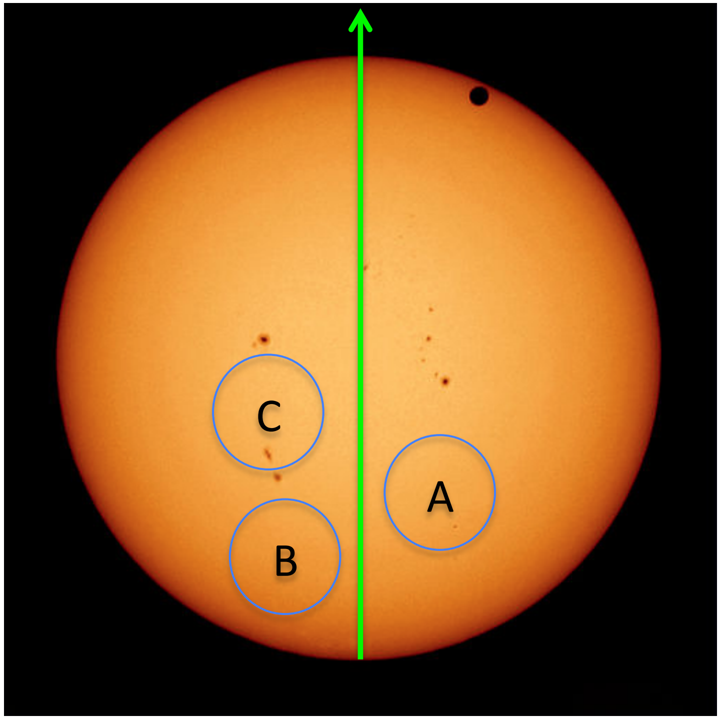
Effects of Limb Darkening

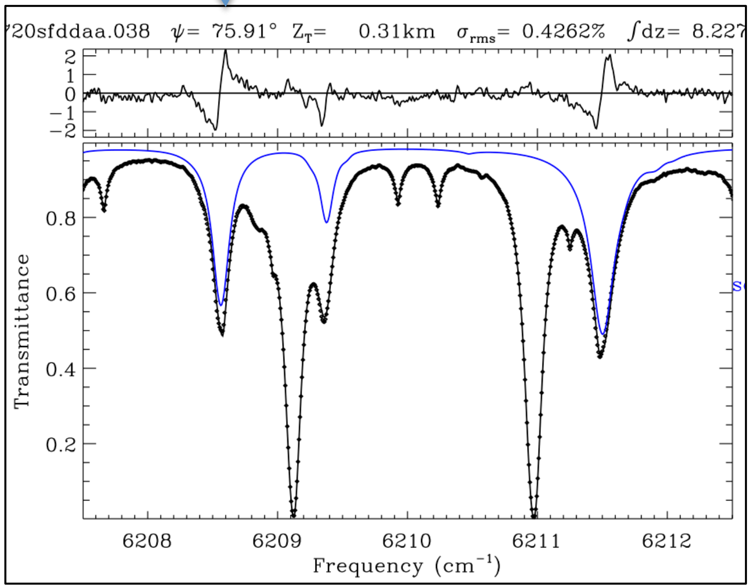
Mis-tracking of the high sun causes noon-time summer dip in solar signal, complicating efforts to derive aerosol extinction from $Log_e(I/I_0)$ vs airmass

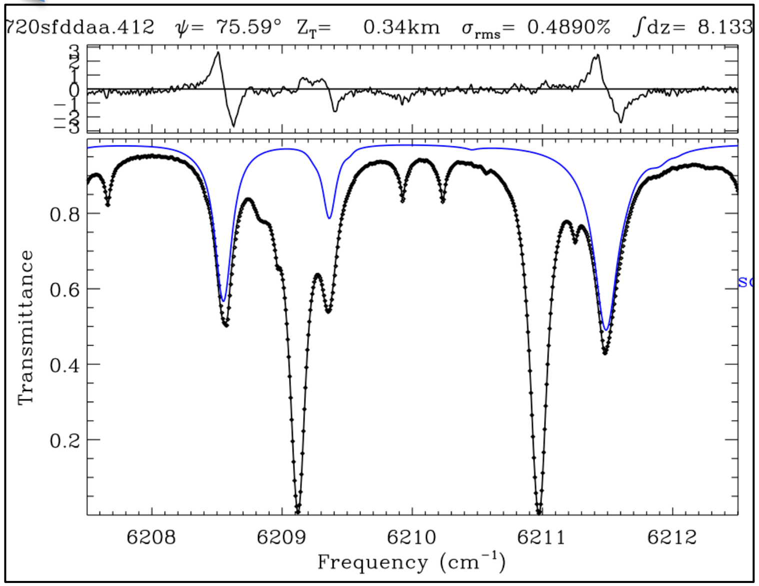


Doppler Shifts









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Disentangling chlorophyll fluorescence from atmospheric scattering effects in O_2 A-band spectra of reflected sun-light

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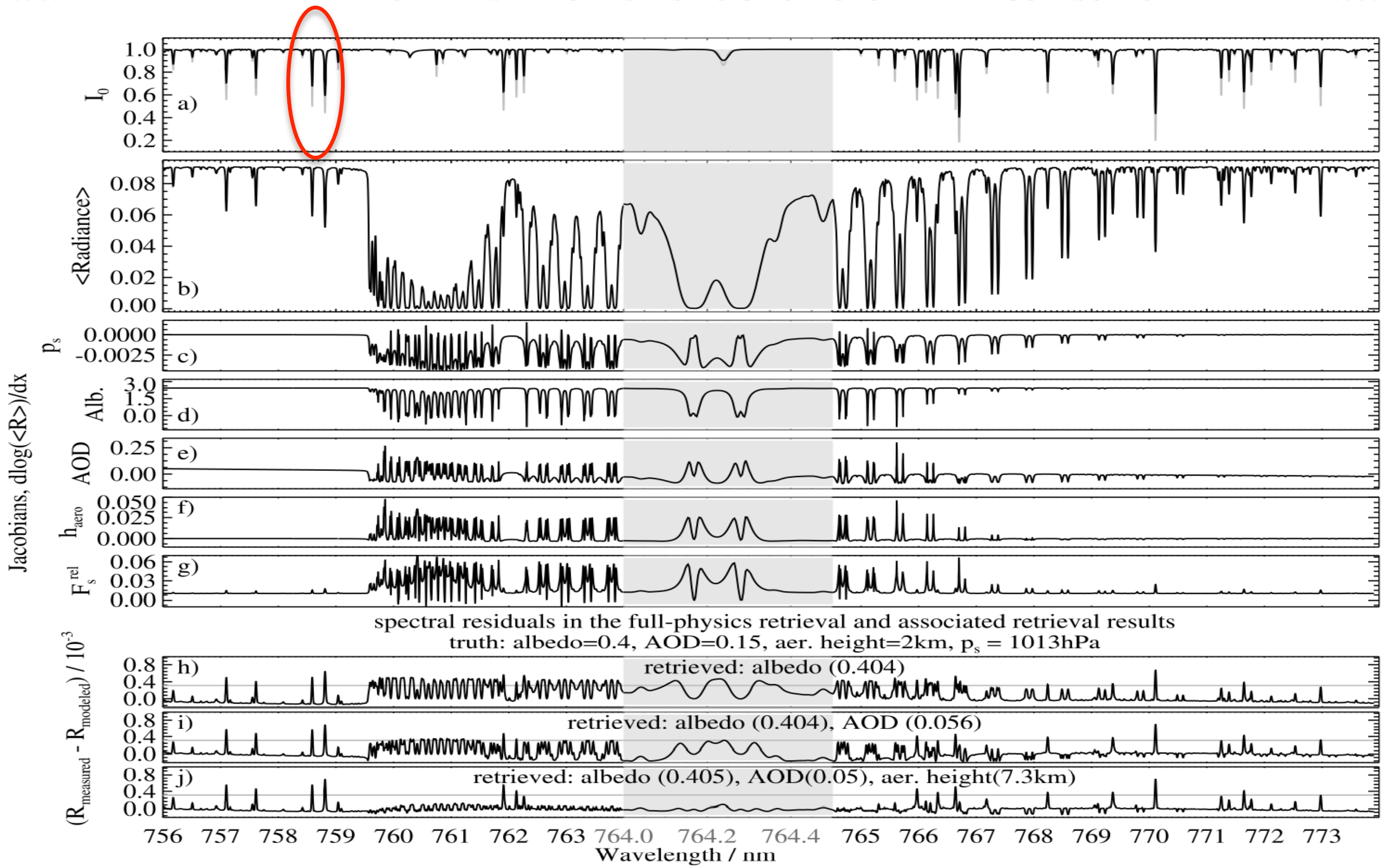
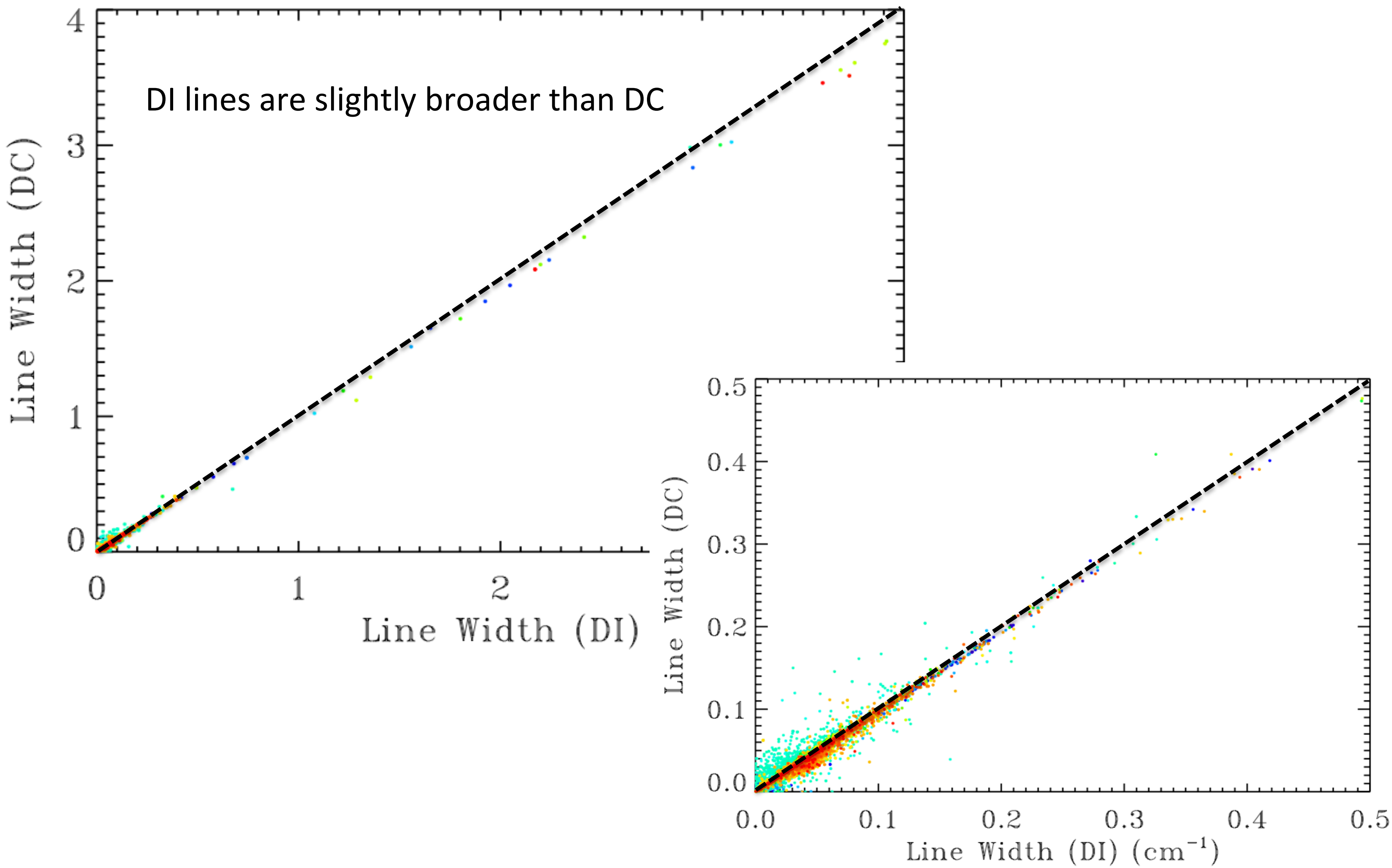
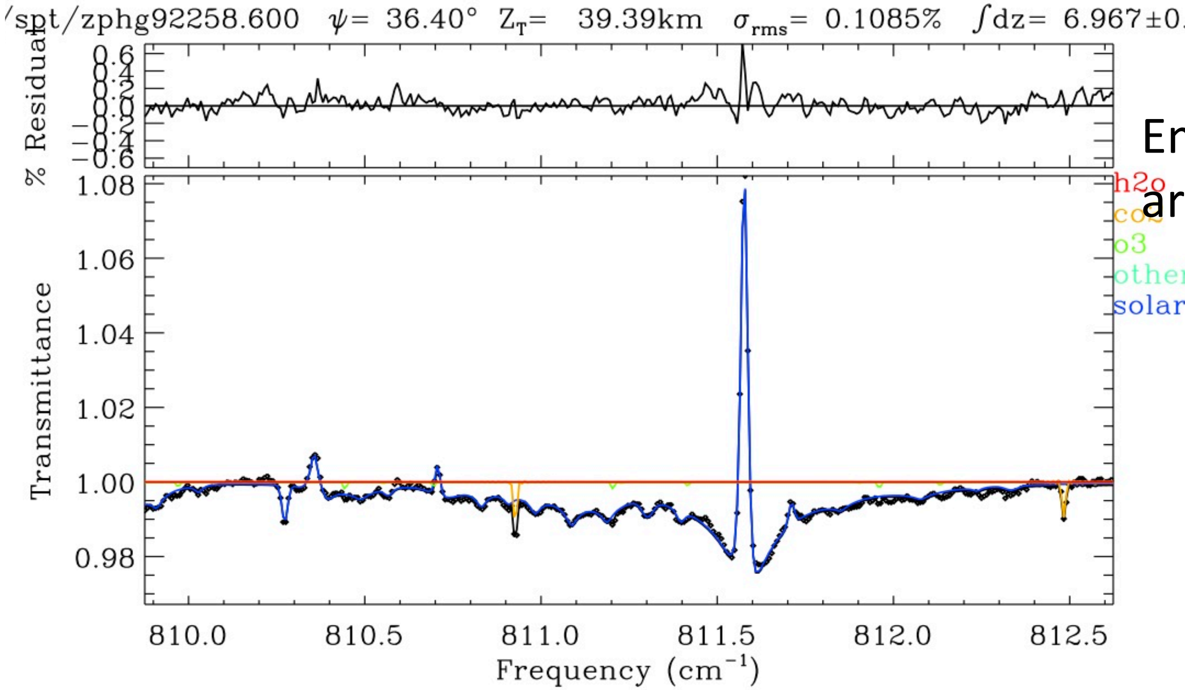


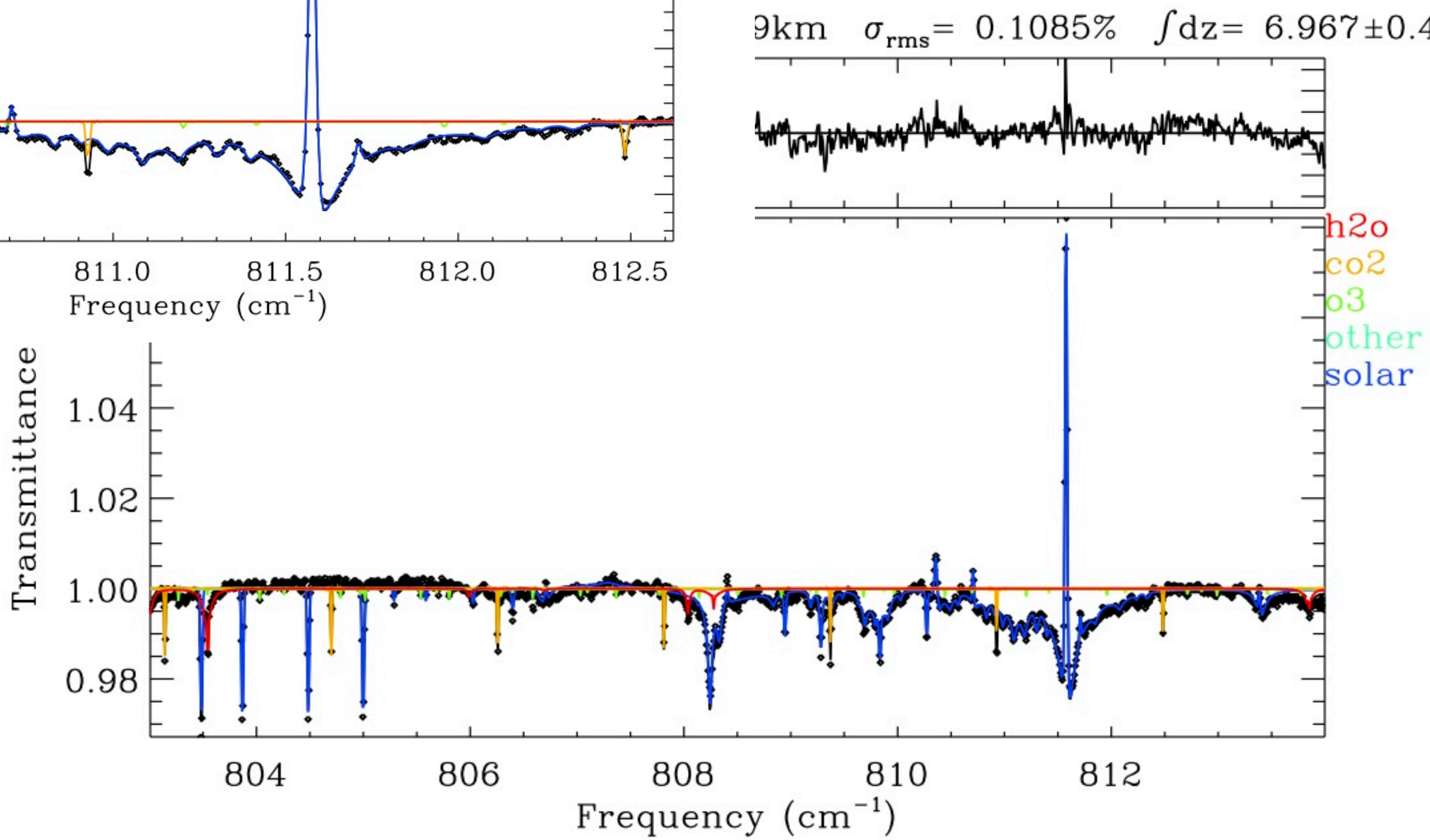
Measured Solar Line Widths



Solar Emission Lines



Emission lines (e.g., at 811.6 cm^{-1}) are not well understood



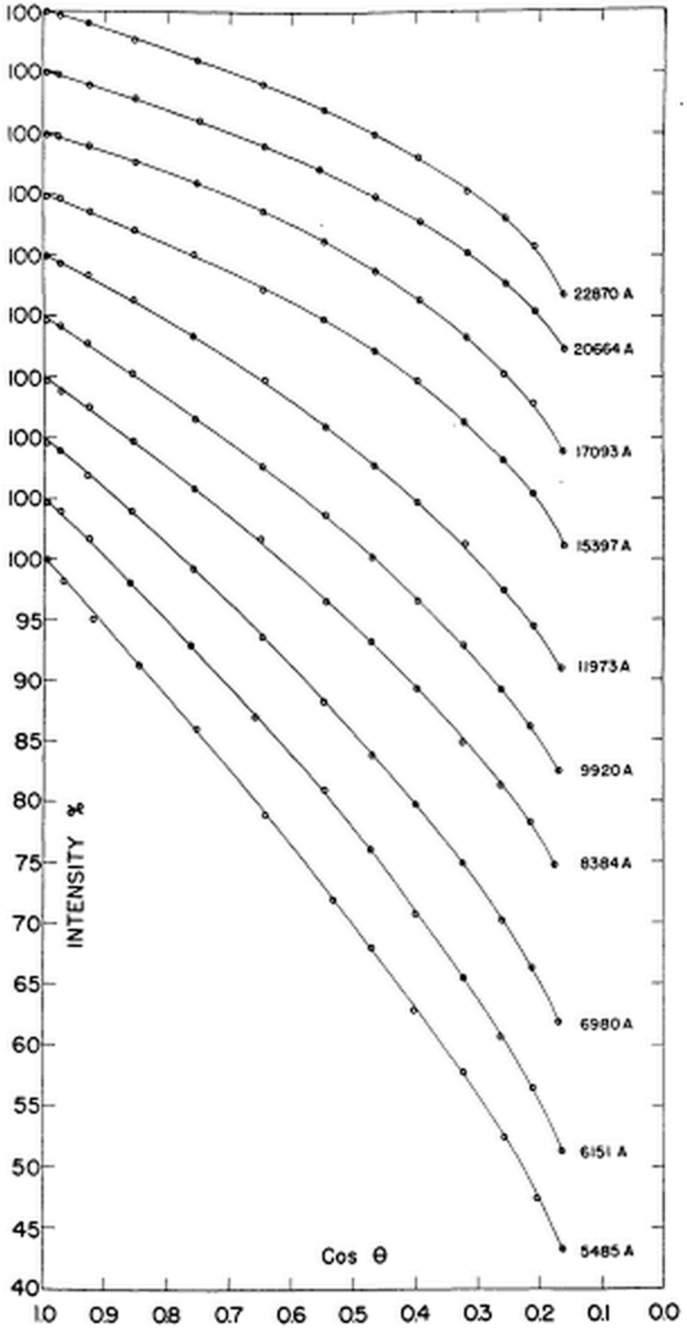


FIG. 5.—Solar limb-darkening-curves for the region 0.5–2.2 μ

OBSERVATIONS OF SOLAR LIMB DARKENING BETWEEN 0.5 AND 10.2 μ*

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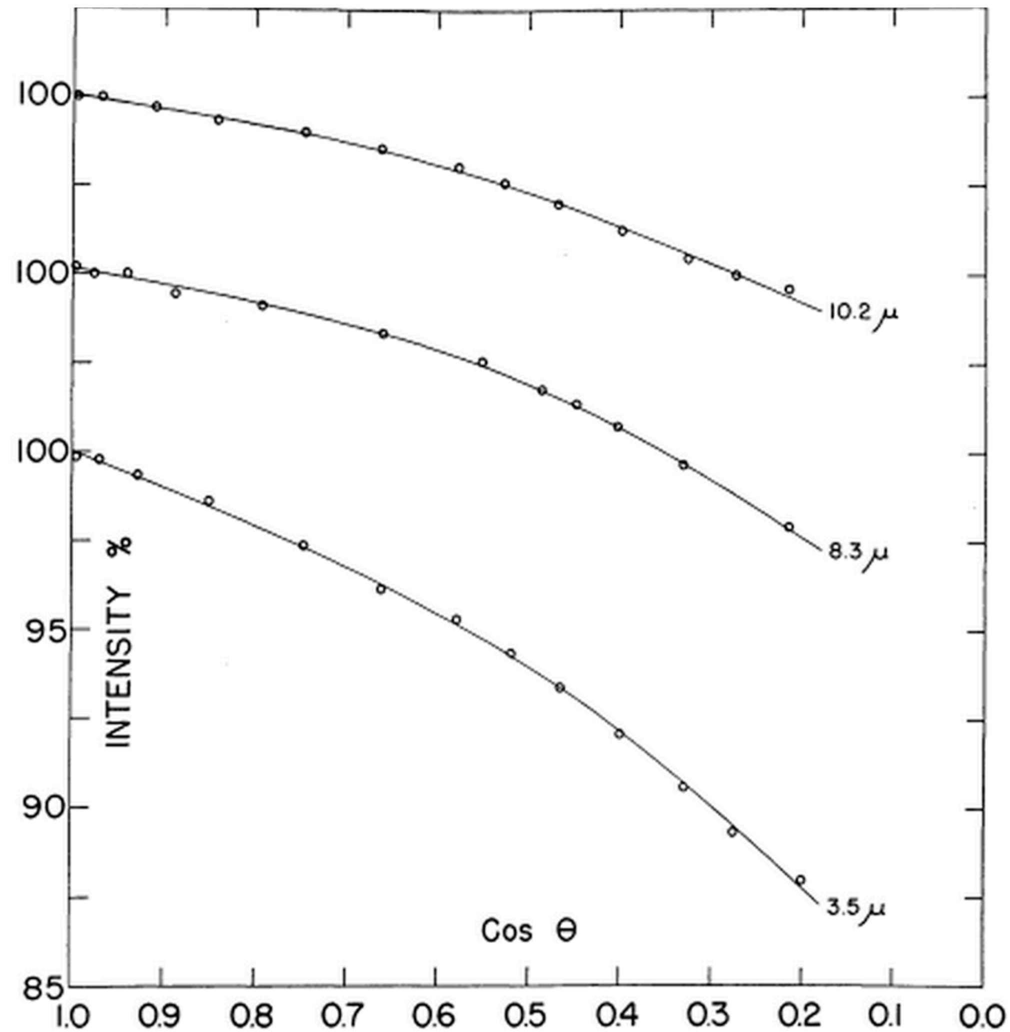

FIG. 4.—Solar limb-darkening-curves for the region 3.5–10.2 μ