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BACKGROUND

Calculation of molecular absorption spectra has historically been relegated to research-grade computer codes, available only to academic or government research programs. Designed to be embedded in complex retrieval algorithms, these codes are unwieldy as stand-alone applications. They are usually tied to specific and often archaic hardware/software configurations. Simulating even simple scenarios requires defining a host of settings, usually in unforgiving and cryptic formats.

To overcome these limitations, we introduce the GATS Spectral Calculator, an online tool that quickly and accurately computes molecular absorption and radiance spectra. The Spectral Calculator is extremely simple to use and produces research-quality spectra in just seconds. Users can select the pressure, temperature and length of a gas cell, and specify concentrations of up to six gases. Absorption or radiance is computed in any spectral interval up to 500 cm^{-1} wide in the UV, visible or IR—any molecule and spectral region covered by HITRAN 2004. The resulting spectra are displayed online, with high-resolution postscript and plain text data available for download.

The **GATS Spectral Calculator** is powered by the LINEPAK radiative transfer library. Efficient, well tested and accurate, this library is at the heart of the retrieval systems for a number of major NASA satellite remote sensing missions. With the Spectral Calculator's easy-to-use online interface, studies that used to take days to set up and analyze can now be completed in minutes, from anywhere. To guide the researcher in the analysis, we also provide a **HITRAN Browser**, which graphically displays the intensities, positions and cross-section data in the complete HITRAN 2004 dataset. These tools and further details are available at www.gats-inc.com.

HITRAN BROWSER

- Display positions of all lines in a waveband
- Plot line intensities vs wavenumber
- Select individual or all isotopologues
- Sort lines by intensity
- View cross-section spectra
- Choose linear or log axis
- Compute statistics of all lines in a waveband
- Download postscript plots for publications
- All data stored in MySQL database
- Written in javascript/PHP/perl using XmGrace

SPECTRAL CALCULATOR

- Calculate spectral transmission or radiance
- Select pressure, temperature and path length
- Compute spectra over large wavebands (up to 500 cm^{-1})
- Select individual or all isotopologues
- Include multiple gases (up to 6) with specified mixing ratios
- Plot results on log or linear axis
- Download postscript plots for publications
- ASCII data available for further analysis
- Powered by LINEPAK, tested worldwide on a host of major missions
- Works on all major browsers
- Fast (typical results displayed in less than 10 sec)

COMING SOON

- Atmospheric paths (tangent or slant paths)
- Line coupling (CO_2)
- Cross section calculations
- Continuum absorption
- Other line lists
- Blackbody source function
- Instrument functions

SUMMARY

The Online **Spectral Calculator** and **HITRAN Browser** provide powerful tools for researchers, engineers, spectroscopists and educators. With this tool you can quickly and accurately simulate absorption and emission spectra of molecular gases with the click of a button. Because it's fast—most simulations take only seconds—studies that used to take days or weeks can now be done in minutes. Sensor designers can use it to define spectral filter bandpasses. Spectroscopists can quickly identify molecular species. Atmospheric scientists can study the effects of various trace gases. Teachers and students can interactively explore the rich world of molecular spectroscopy. All this can be done at any time, from any web browser, anywhere in the world. We will continue to update and expand the features available on the **Spectral Calculator** and **HITRAN Browser**, and look forward to your suggestions for improvement at www.gats-inc.com

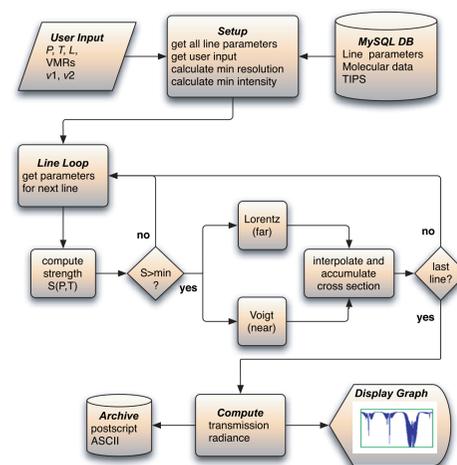


Figure 1. Spectral Calculator Architecture.

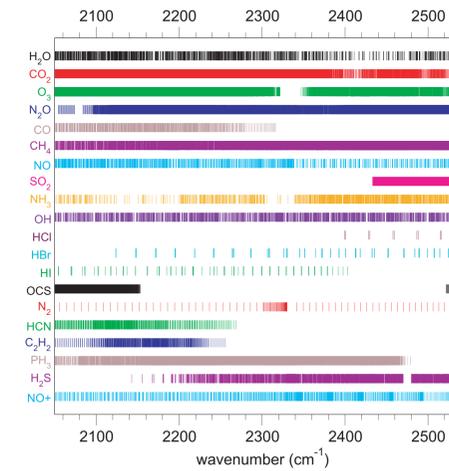


Figure 2. Line positions from the HITRAN Browser. The position of every line in the waveband is shown as a small, color-coded vertical hash mark. The species are identified on the left side, and the total number of lines are shown on the right. The waveband can be adjusted to anything from 0 to 60,000 cm^{-1} . The user can select a threshold for the line intensities to cull out the weaker lines.

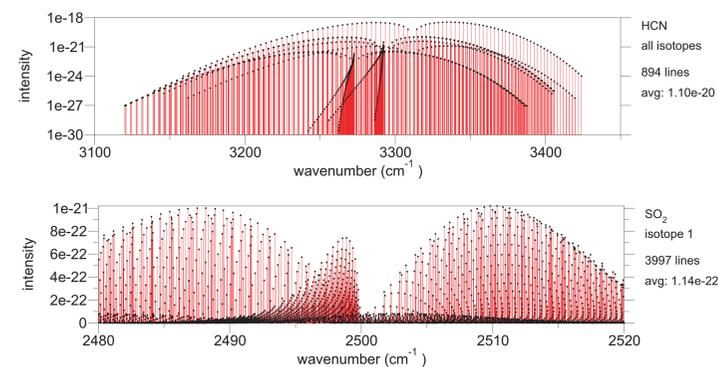


Figure 3. Line intensity plots from the HITRAN Browser. *top*) HCN (all isotopologues) on a log scale. *bottom*) SO₂ (main isotopologue only) on a linear scale. The intensities are shown as red bars with small black circles on the top.

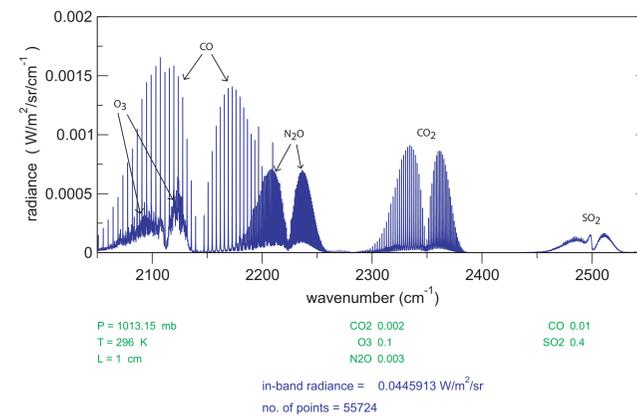


Figure 4. Radiance plot from the Spectral Calculator. This simulation shows the spectral radiance from five species. The VMR chosen for each species is listed. The user only inputs the cell pressure, temperature and length, along with the VMRs. The calculator automatically determines the required resolution and computes the radiance spectrum. This 500 cm^{-1} spectrum, requiring 55,724 points, is computed and displayed online in *less than 15 seconds*.

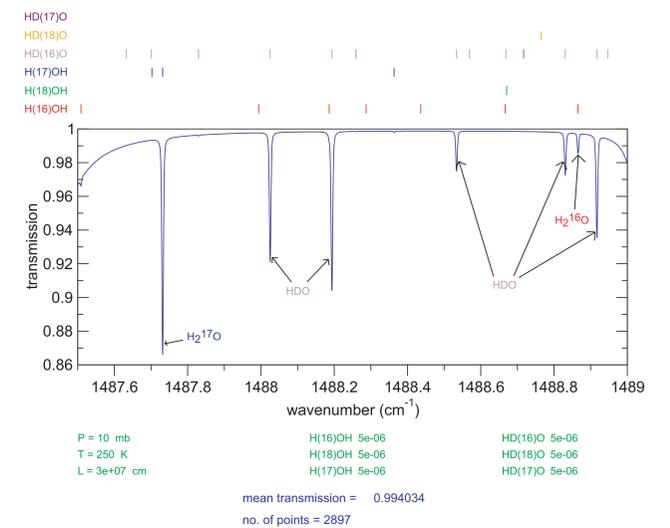


Figure 5. Transmission plot from the Spectral Calculator. This example illustrates the identification of individual water vapor isotopologues. The conditions are representative of a stratospheric limb path (300 km at 10 mbar). In this microwindow, five HDO lines, one large H₂¹⁷O line, and one small H₂¹⁶O (the main isotope) line are evident. Line positions (including inconsequential weak lines) are indicated with color-coded vertical hash marks above the graph.

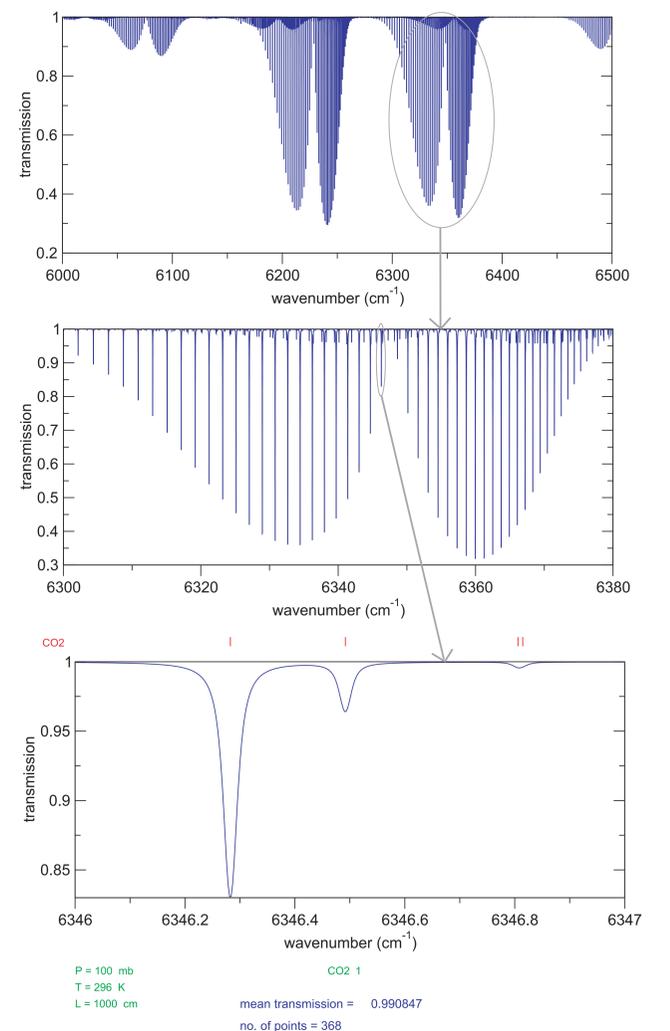


Figure 6. Spectral Calculator plots of CO₂ transmission (without line coupling). The top, middle and bottom plots show successive “zooms” of the spectra, narrowing in on a small microwindow. This set of plots takes only seconds to produce with the Spectral Calculator, and demonstrates how easily individual absorption features can be identified and modeled.