Molecular Spectral Lines

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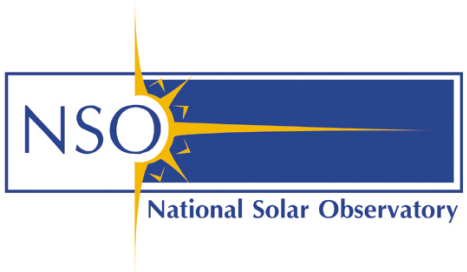
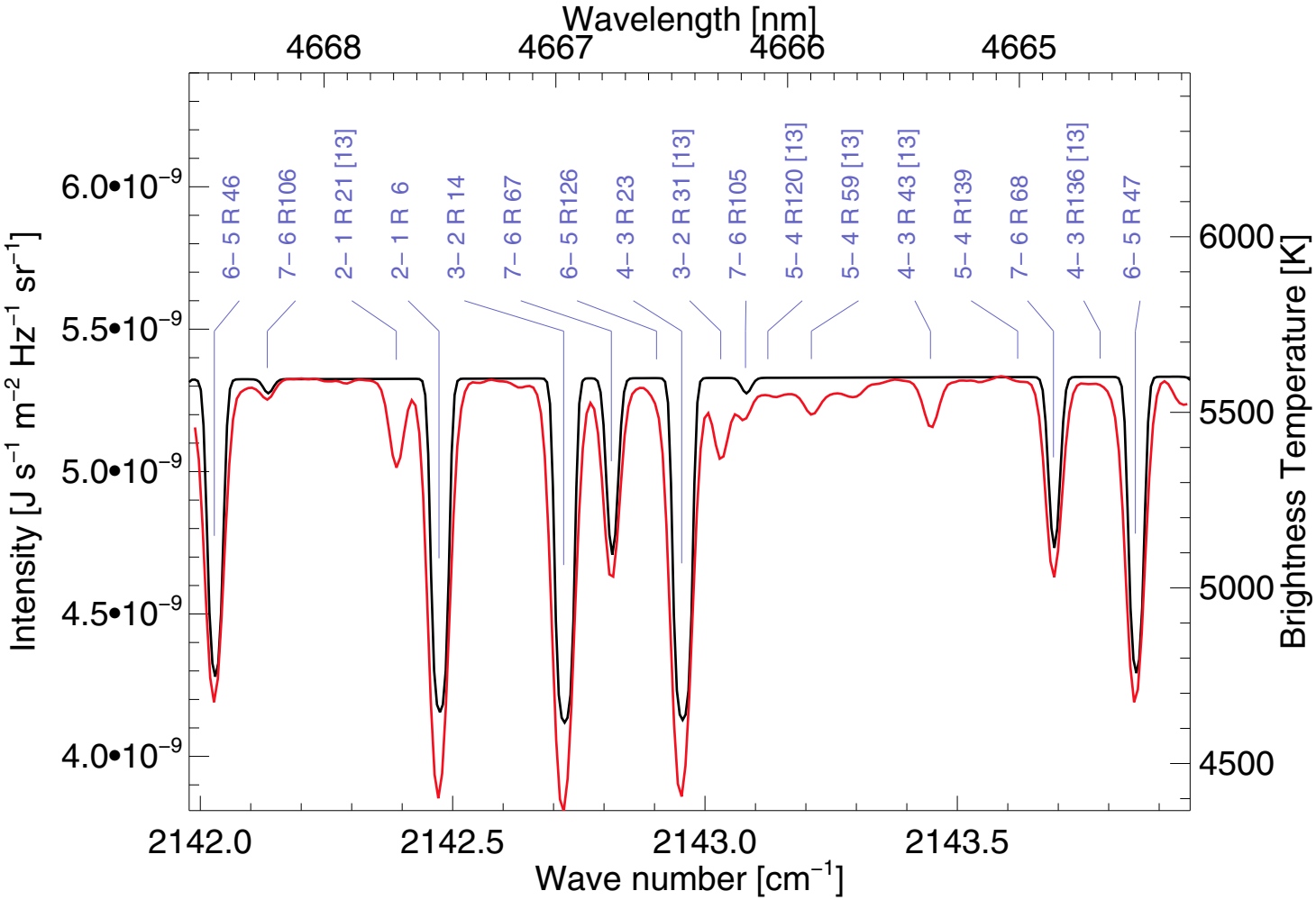


Hale COLLAGE, Boulder, Feb 23, 2016

Molecular Spectral Lines in the Solar Spectrum

- Molecules are abundant in the solar atmosphere, in particular in cooler areas like Sunspot umbrae.
- The G band is one of the most used pass bands in solar high resolution imaging. Its major source of opacity is a band of lines of the CH molecule.
- CO lines are important temperature diagnostics for the solar atmosphere.
- Molecules are sensitive to the Zeeman effect, and have much more diverse sensitivity than atomic lines. This can be used to advantage.
- In some cases molecular lines can be used for abundance determinations when spectral lines of one of the constituents are not readily observable (Fluorine).

CO Lines in the Solar Spectrum



Water Lines in Umbral Spectrum

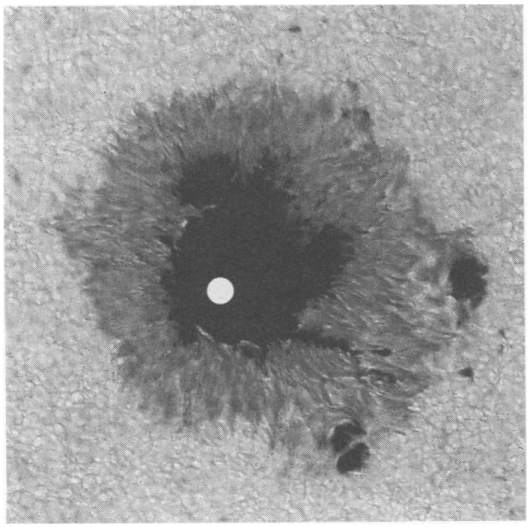


Fig. 1. A portion of the 26 July 1991 solar disk photographed in white light, which shows the 6000 K granulation field and a mature, much colder sunspot. In this reproduction, the sunspot umbra appears uniformly dark but has, in reality, brightness structure. The 7–arc sec white dot, representing the input aperture to the Fourier transform spectrometer, has been positioned in the darkest, coolest, umbral "void" (*26*) where the temperature falls to about 3500 K and the water molecule can form and exist.

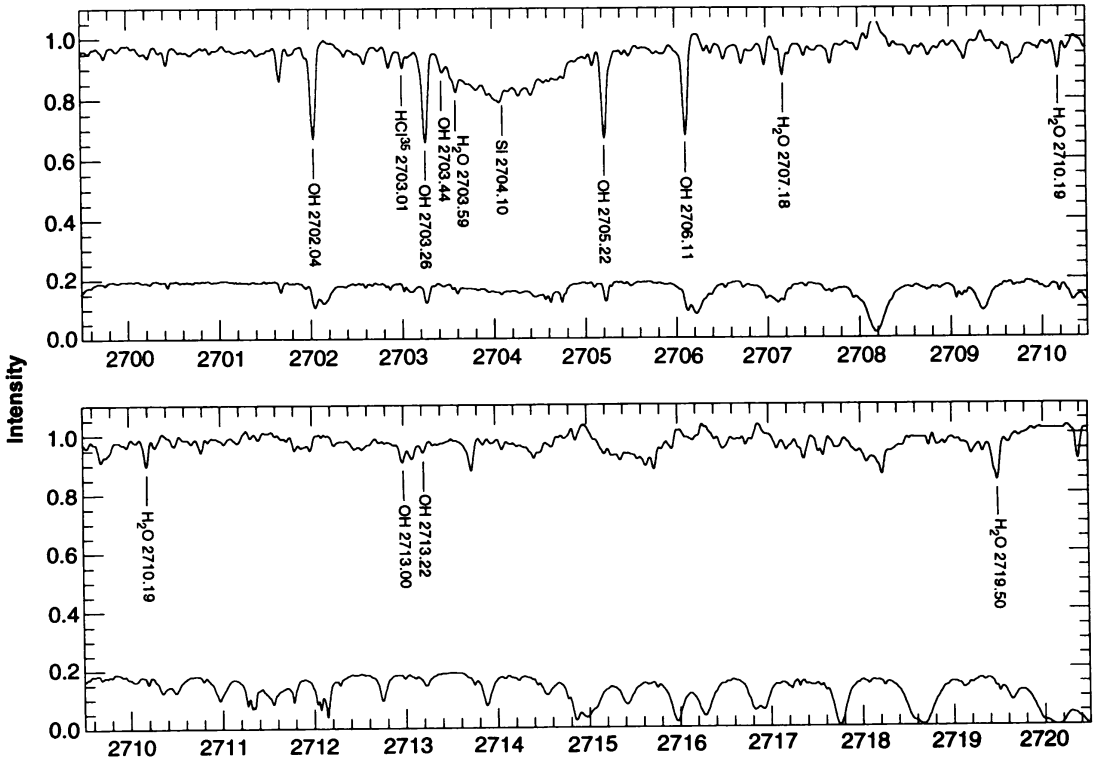
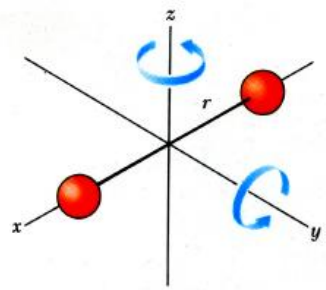
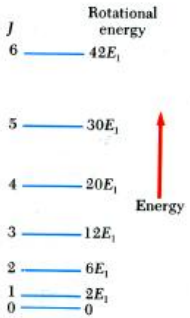
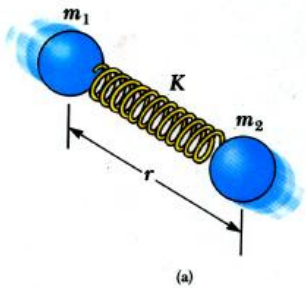


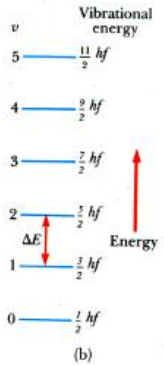
Fig. 2. A portion of the sunspot spectrum in the 3.7-μm region (*11*). The lower trace in both panels is the observed spectrum recorded at an air mass of 2.3, and the upper trace is the spectrum corrected for atmospheric absorption by extrapolation to zero air mass. The two panels form a continuous spectrum.

Degrees of Freedom and Energy Levels Diatomic Molecule









Energy Levels:

Translational energy:

$$E_{\text{trans}} = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

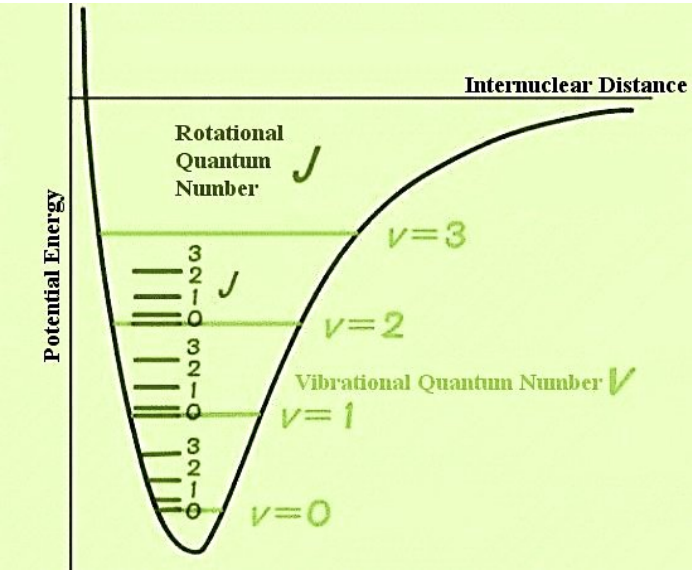
Rotational energy:

$$E_{\text{rot}} = L^2/2I$$
$$= J(J+1)\hbar^2/\mu r_0^2$$

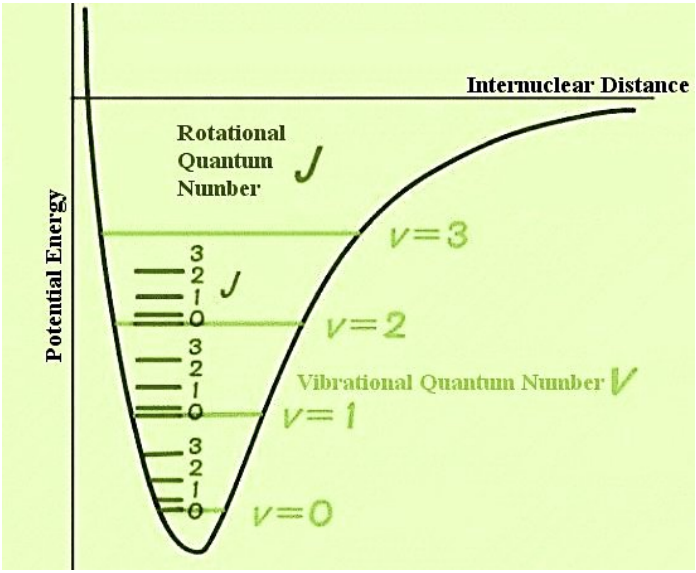
Vibrational energy:

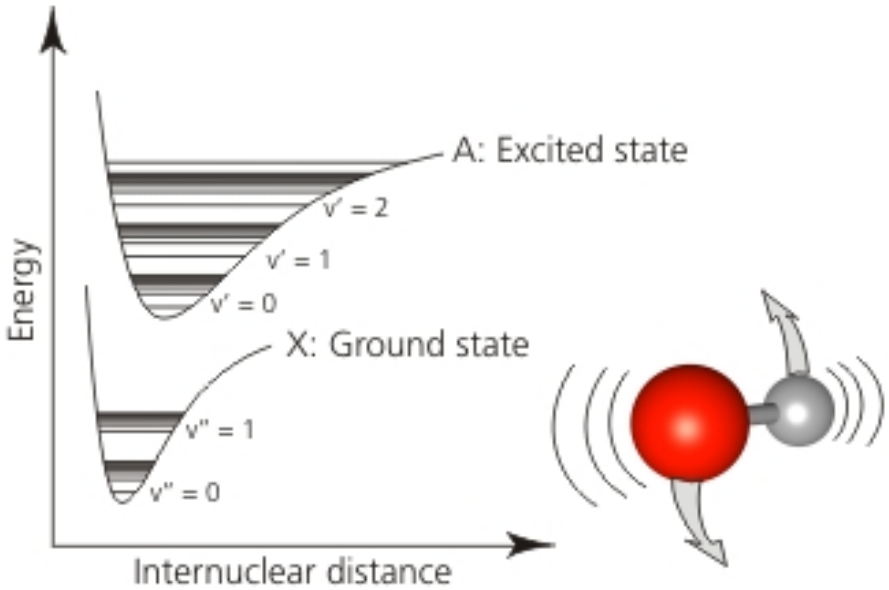
$$E_{\text{vibr}} = \left(v + \frac{1}{2}\right)\hbar\omega$$

Electronic States in Diatomic Molecule

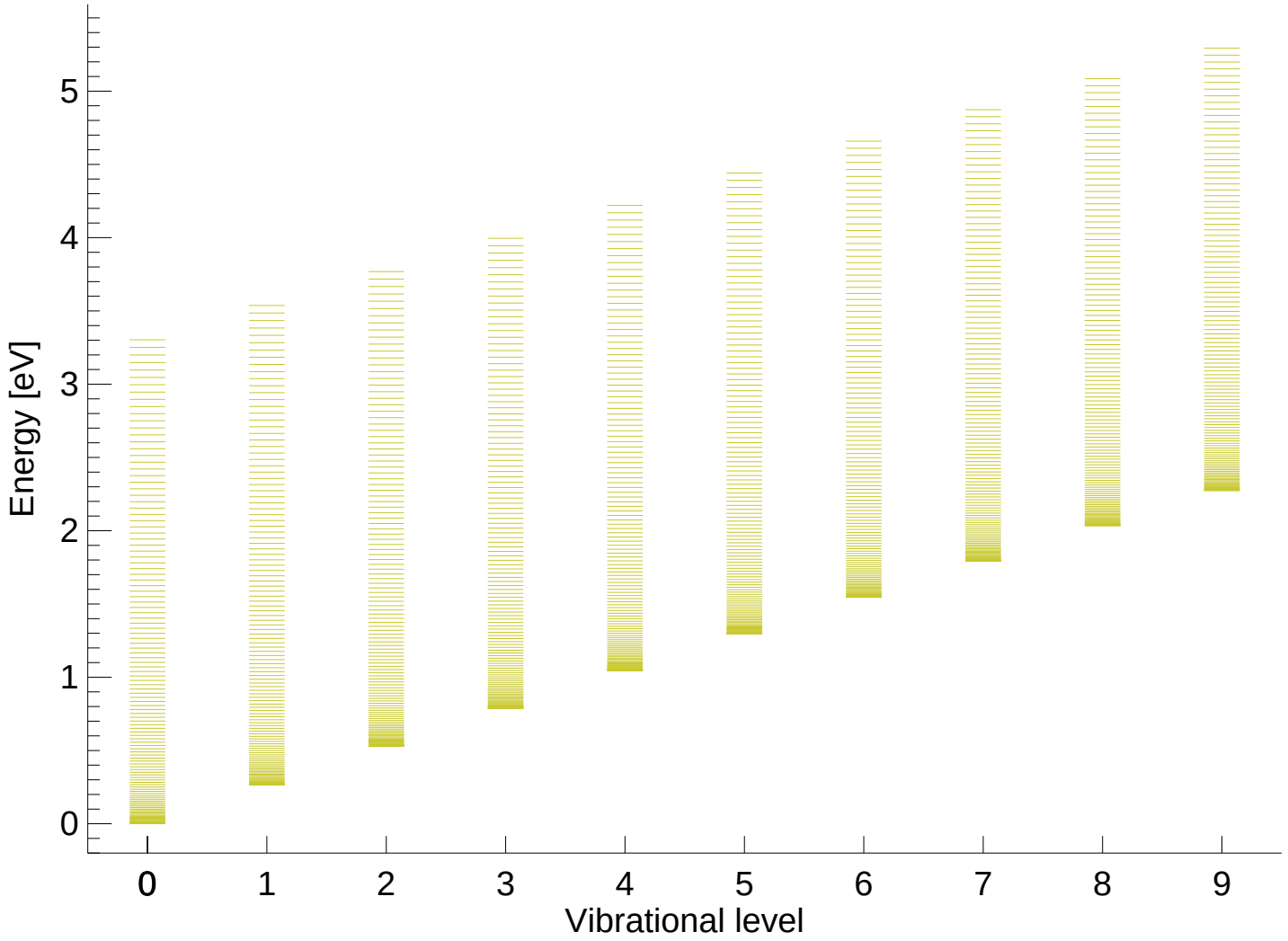


Electronic States in Diatomic Molecule

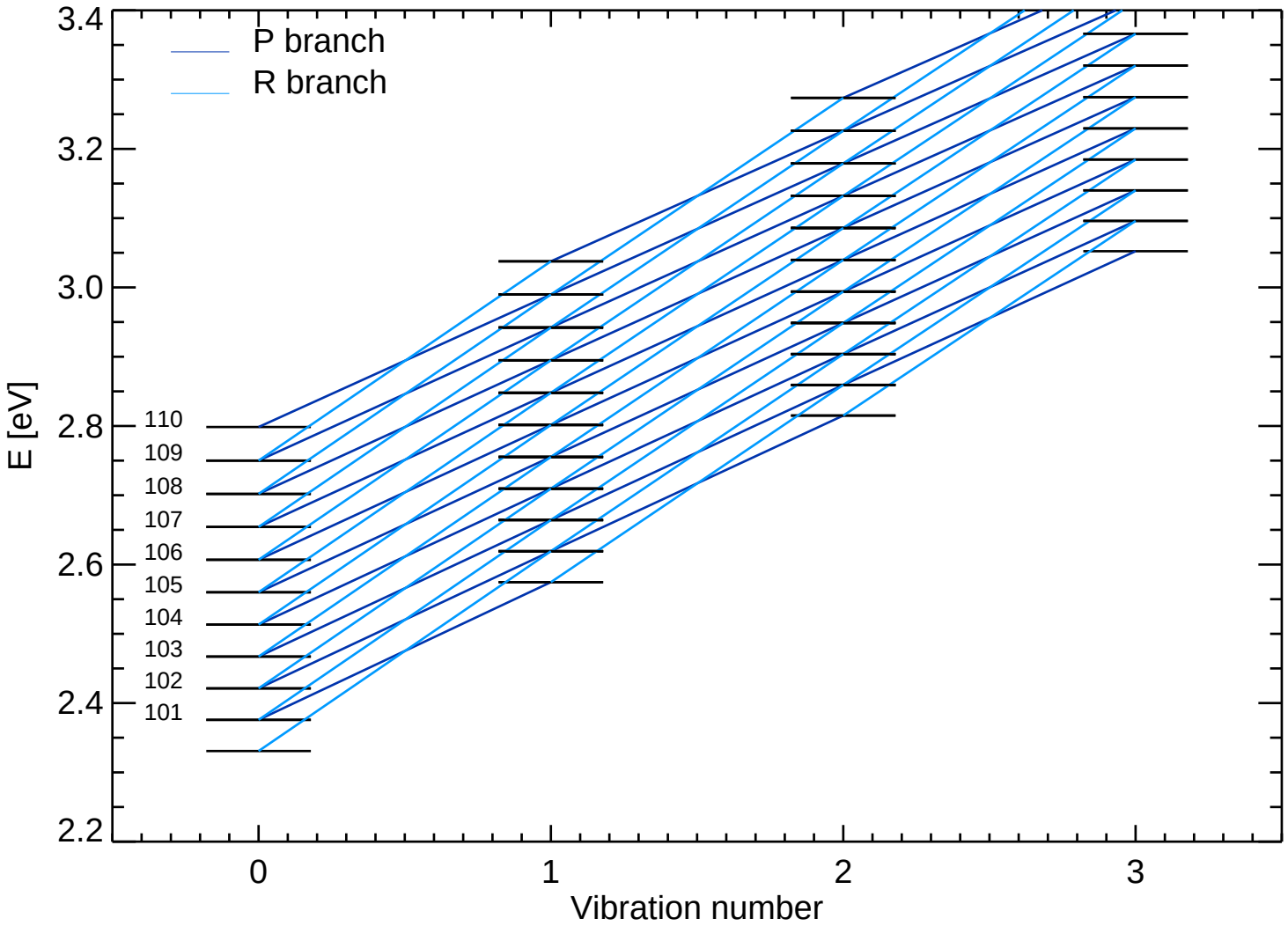




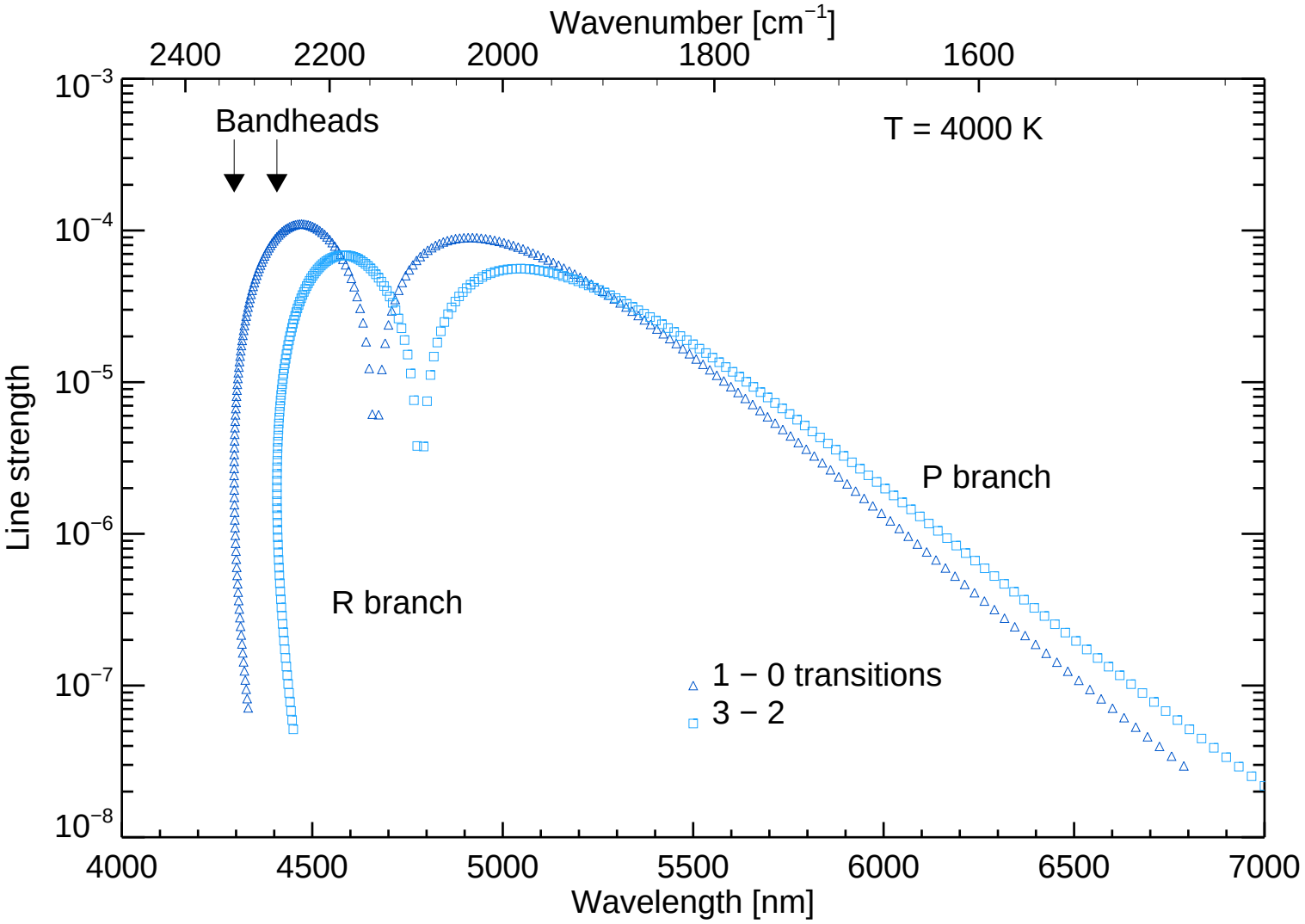
Energy Levels of the ground State (X) of the CO Molecule



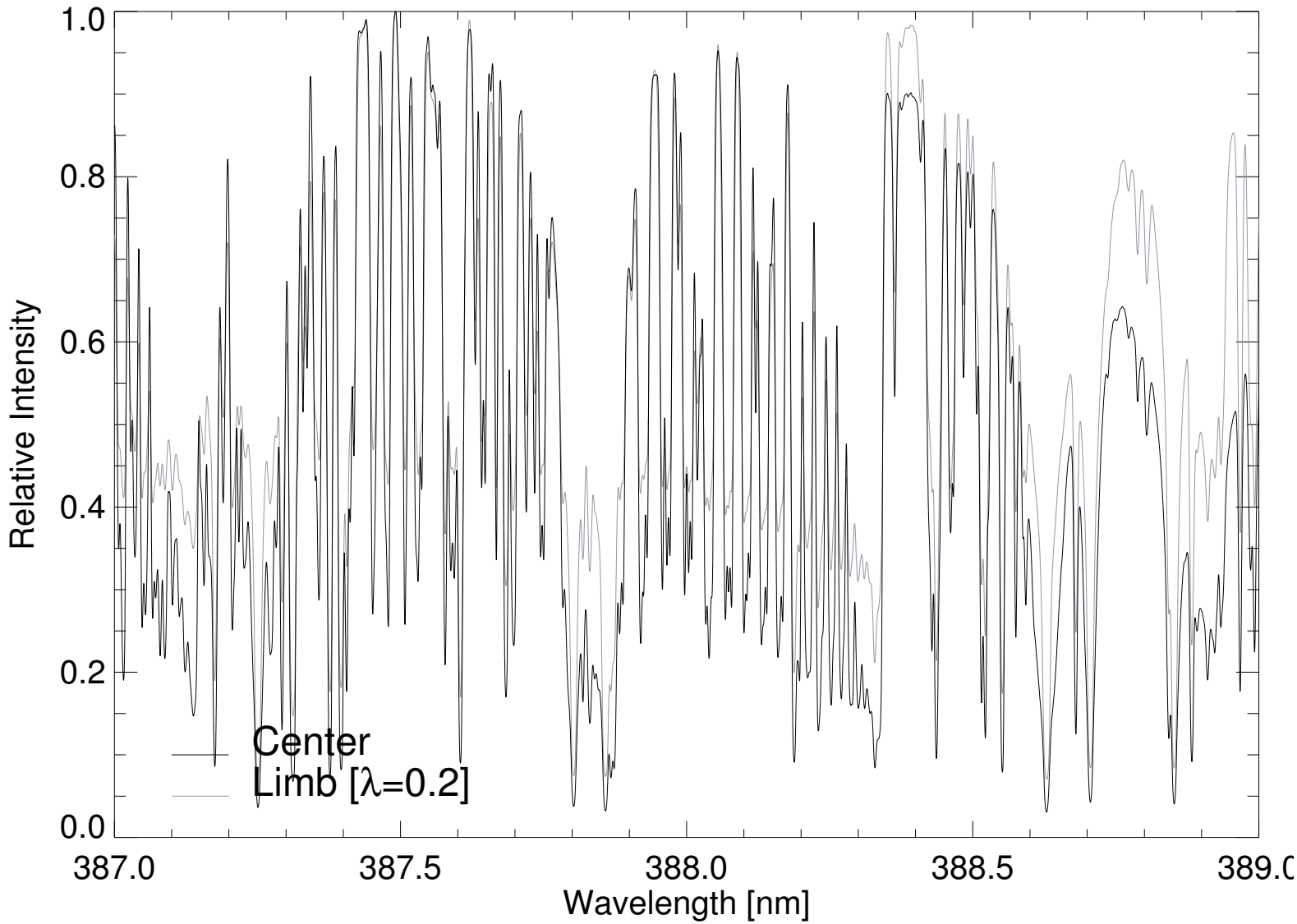
Vibration-Rotation Transitions in CO ground State



Molecular Lines are grouped in Bands



Example: CN band head at 388.3 nm



Abundance of Molecules:

Abundance of atomic Species:

$$n_A^{\mathrm{tot}} = A_A n_H$$

Chemical equilibrium:

$$\frac{n_A n_B}{n_{AB}} = \left(\frac{2\pi m_{AB} kT}{h^2}\right)^{3/2} e^{-D/kT} \left(\frac{U_A(T) U_B(T)}{Q_{AB}(T)}\right)$$

$$m_{AB} = \frac{m_A m_B}{m_A + m_B}$$

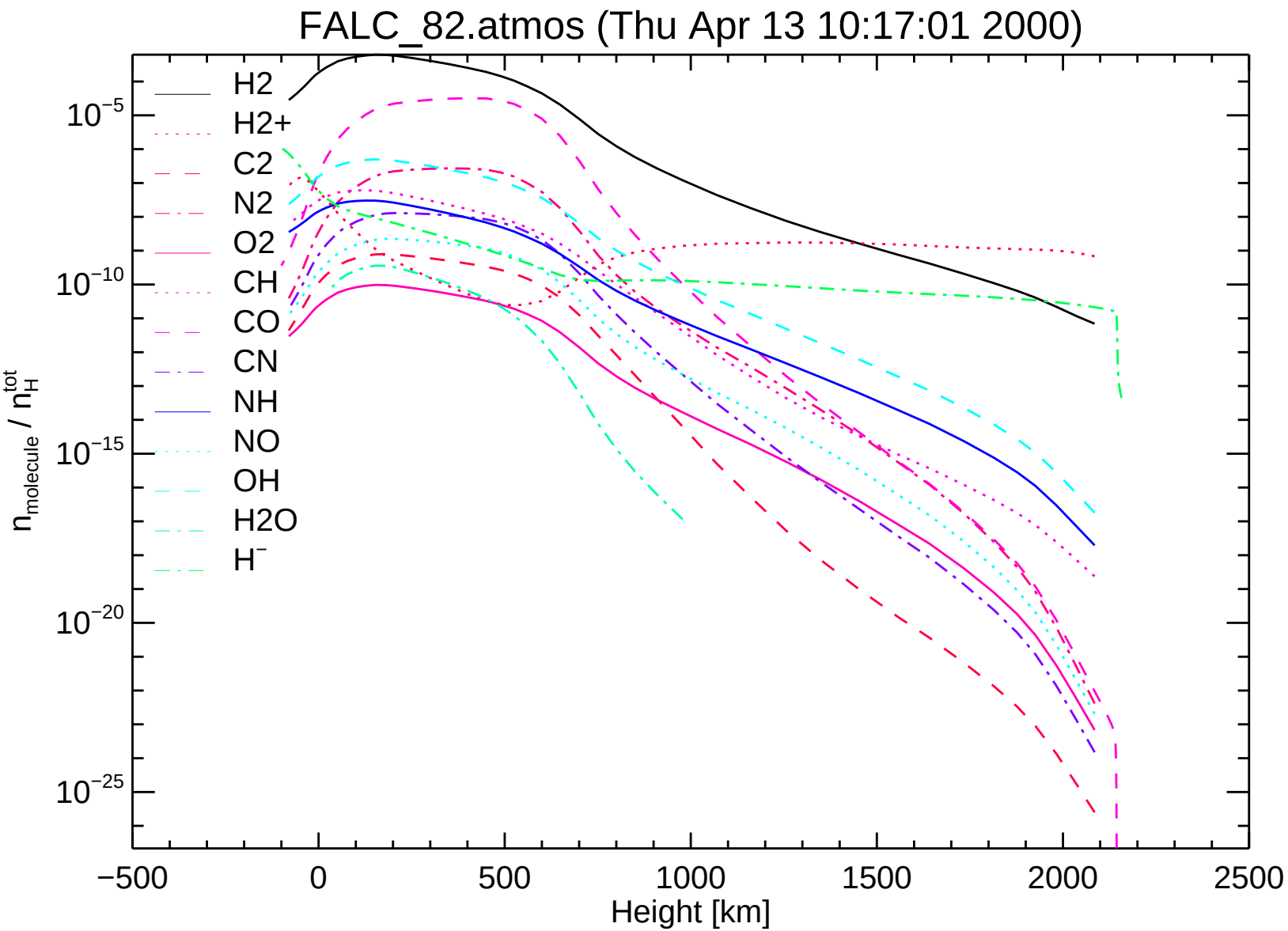
Non-linear set of coupled equations:

$$n_{AB} - n_A n_B \Phi_{AB}(T) = 0$$

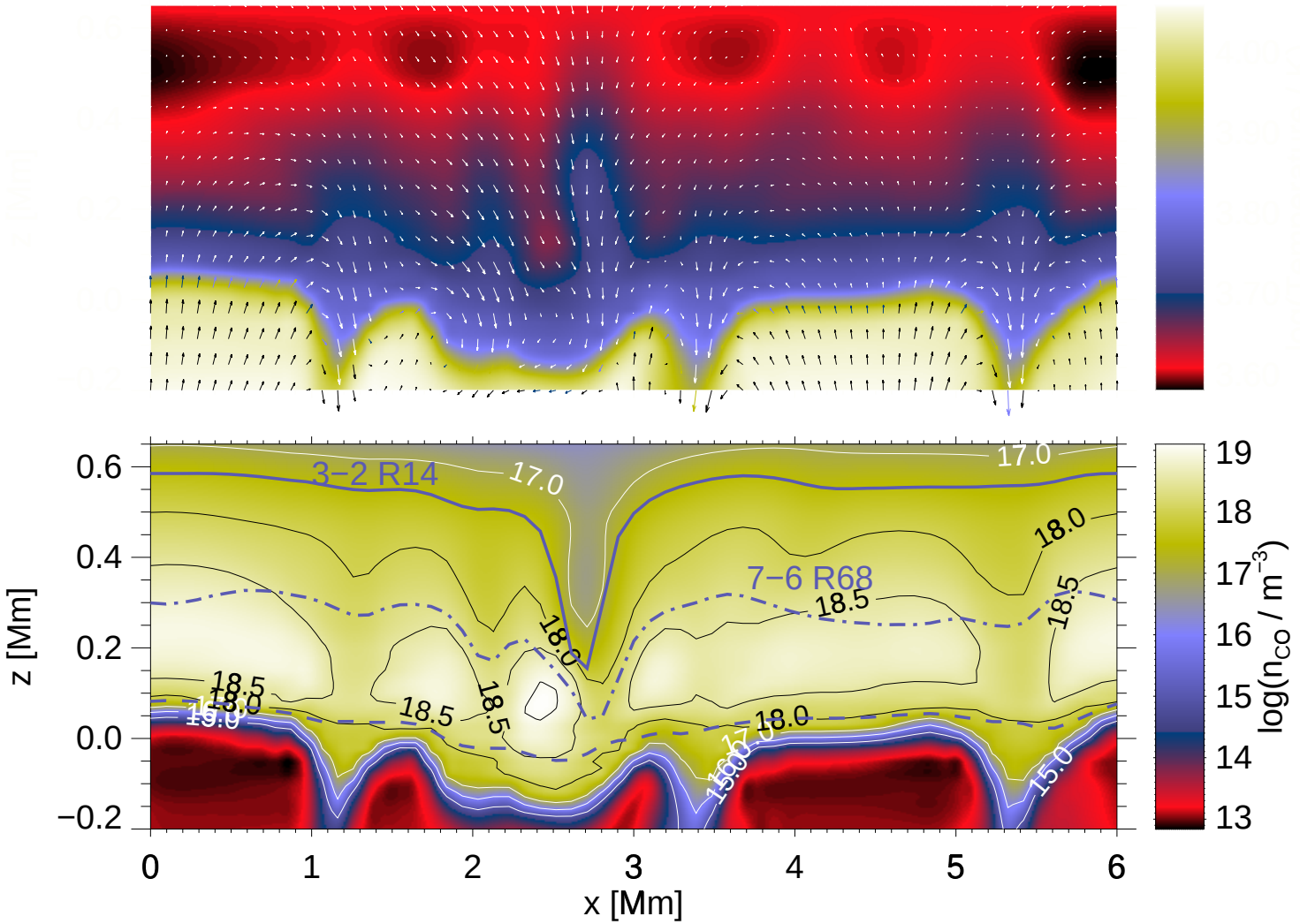
$$n_A + n_{AB} = A_A n_H$$

$$n_B + n_{AB} = A_B n_H$$

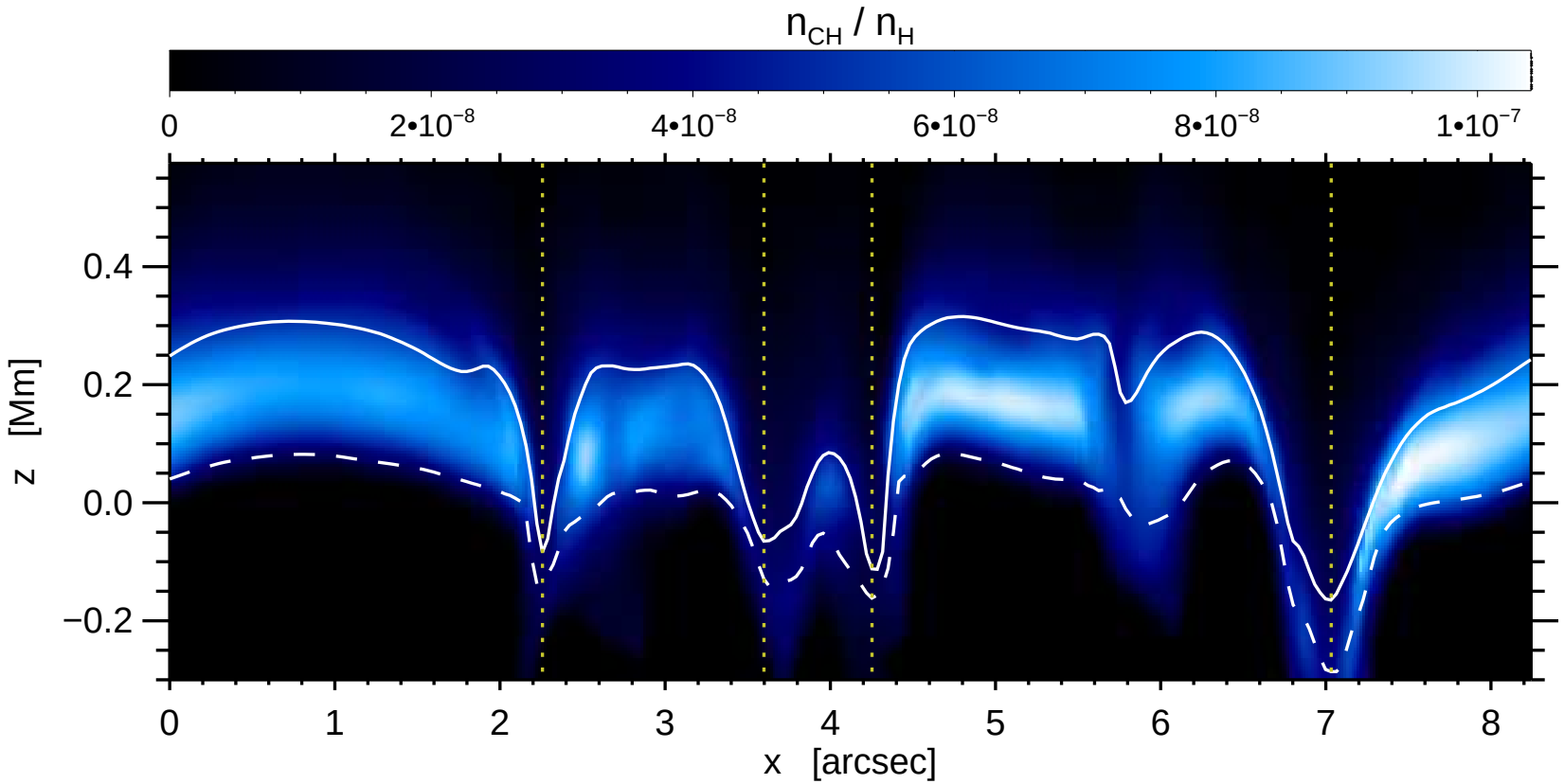
Molecular Concentrations in the Solar Atmosphere



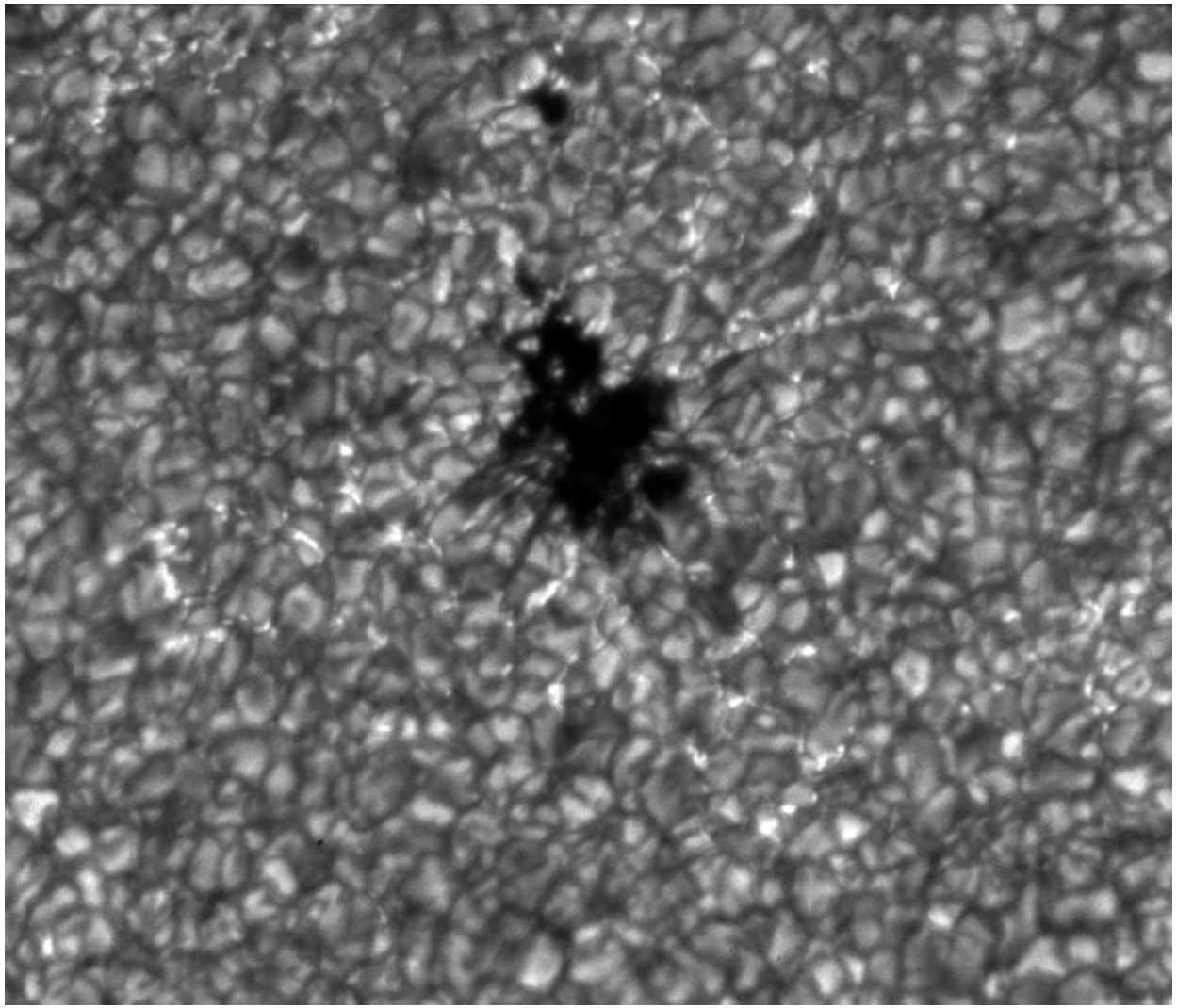
CO Concentration in Vertical Magneto-Comvection Slice



CH Concentration in Magneto-Convection Slice

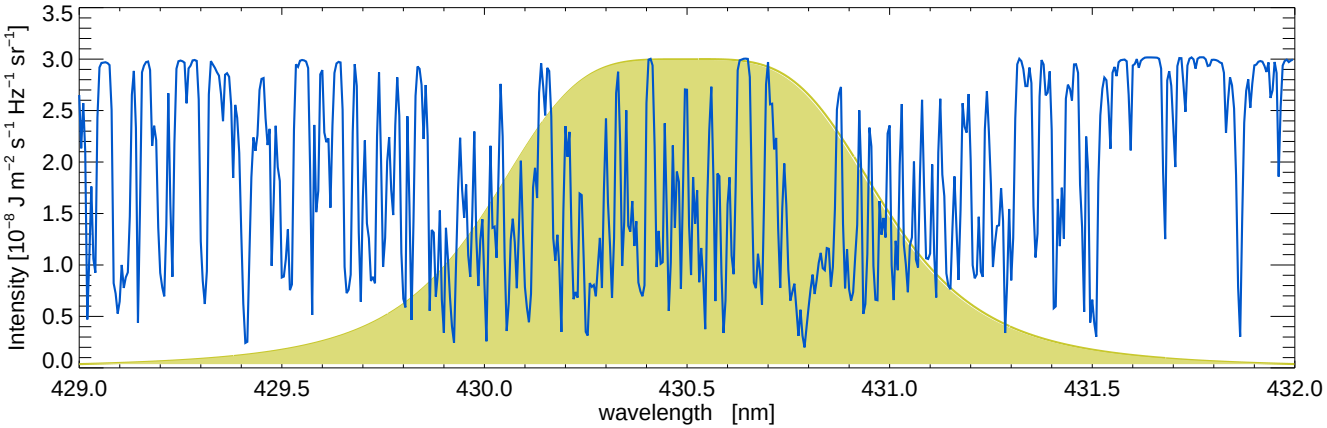


G-band Intensity as Tracer of Small-scale Magnetic Field



Courtesy: LMSAL, SVT La Palma

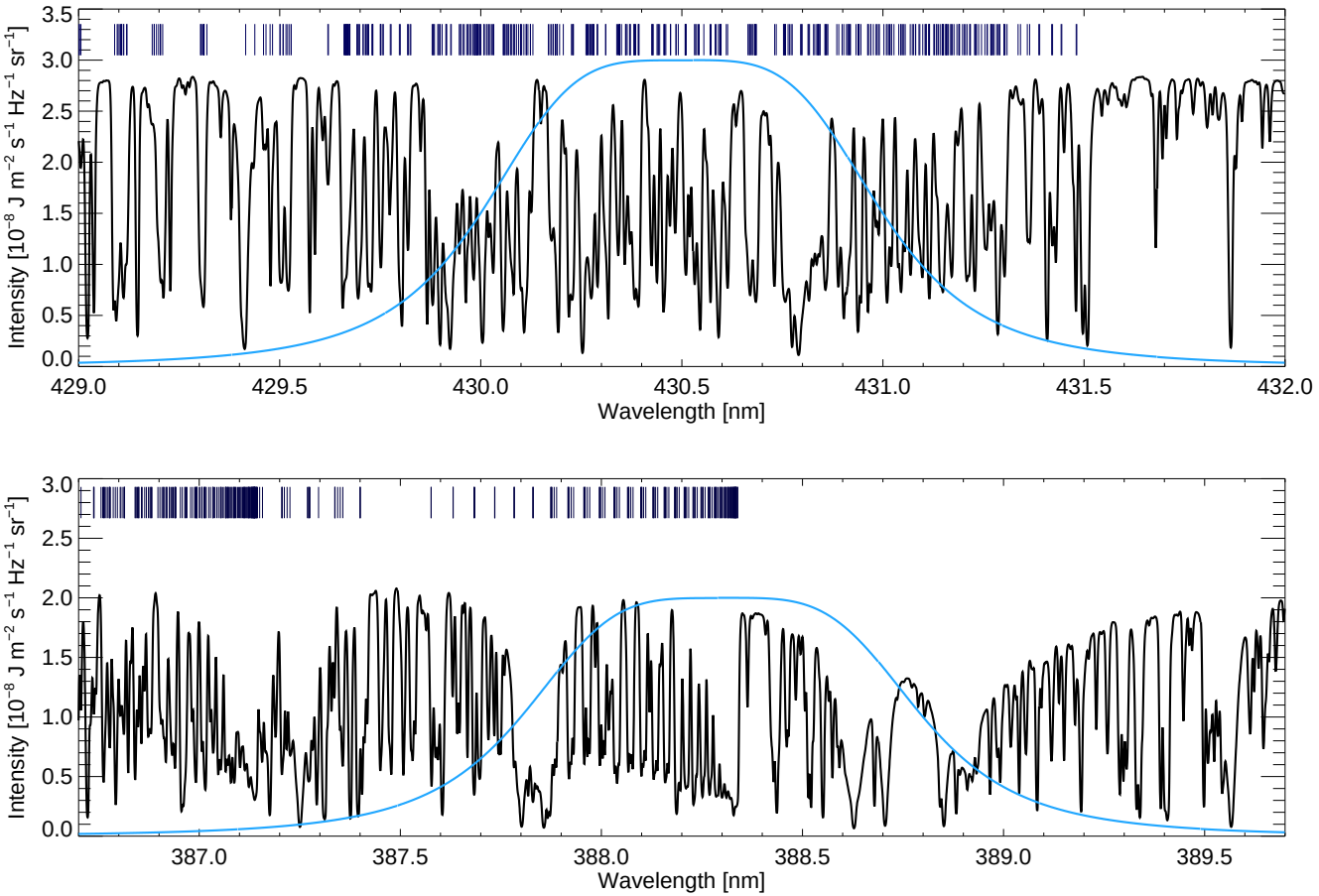
Filter Integrated Intensity



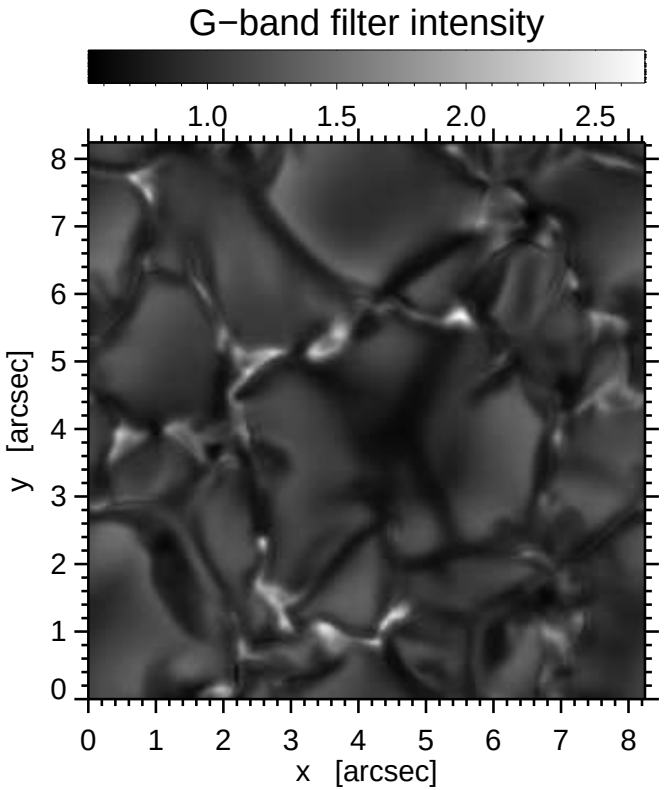
Filter signal:

$$f = \int_0^\infty I_\lambda f_\lambda d\lambda$$

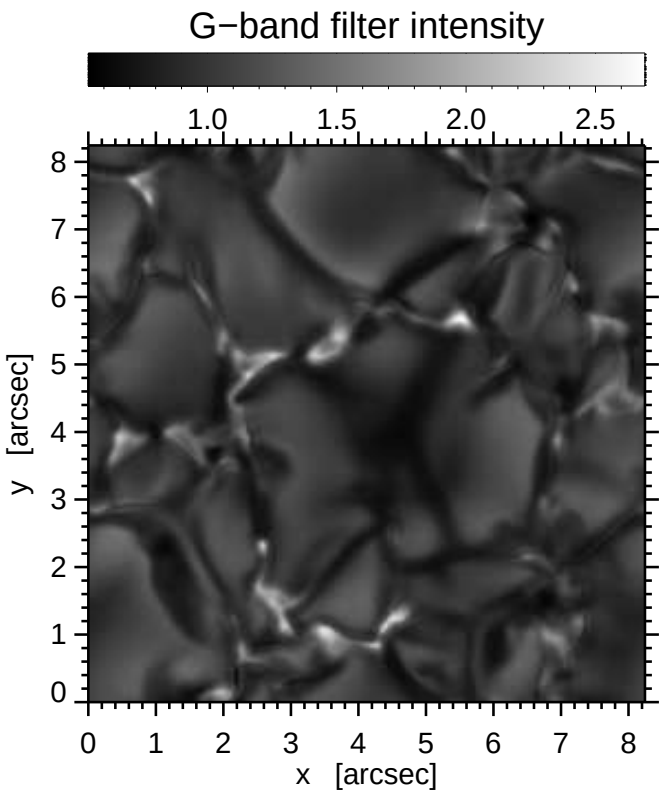
Molecular Bands in the Blue

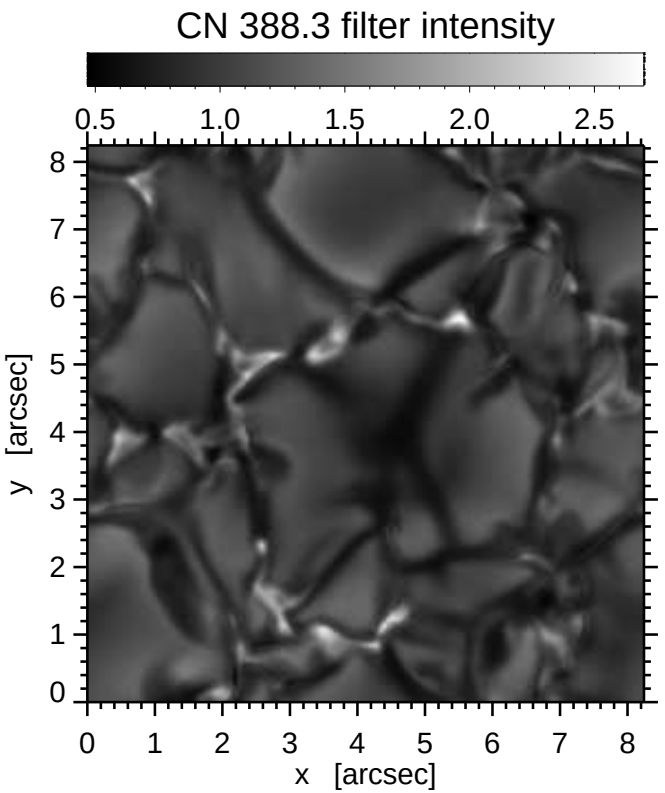


Filtergrams in CH and CN Bands

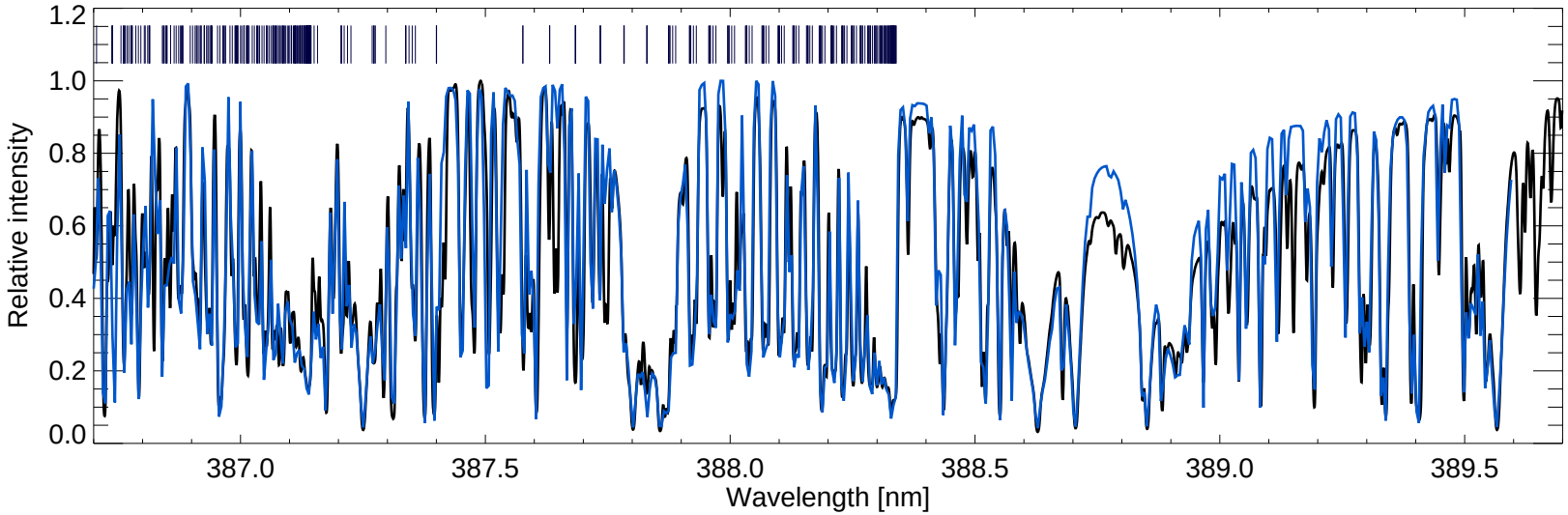


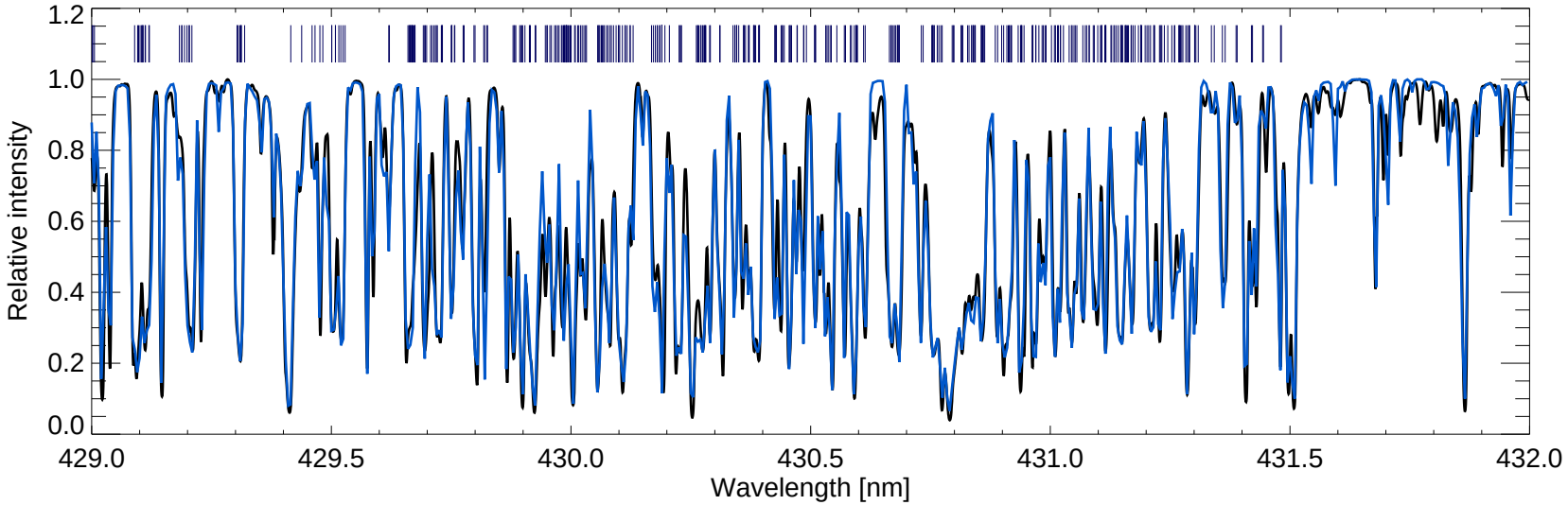
Filtergrams in CH and CN Bands



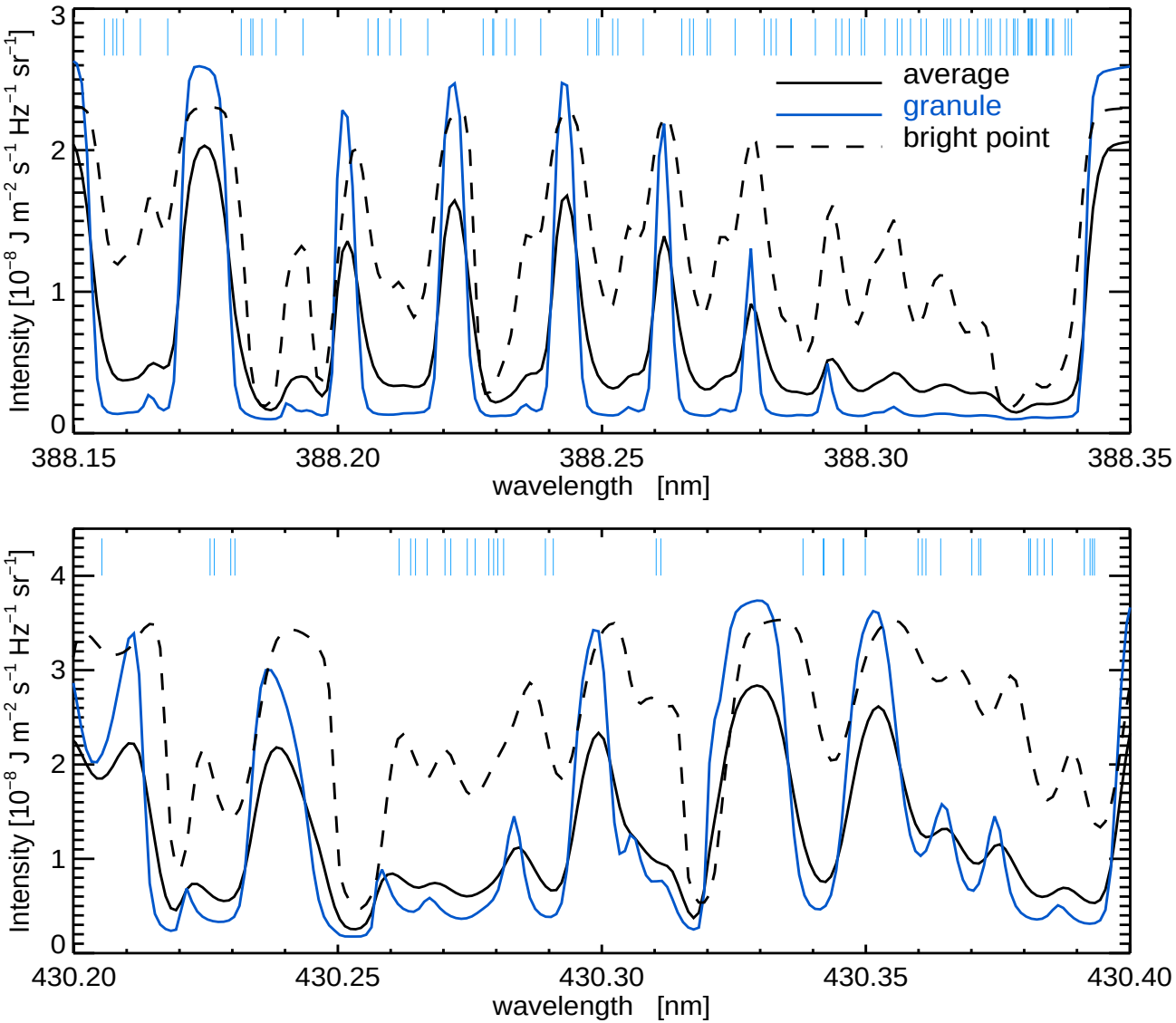


Comparison of Observed and Calculated Spectra

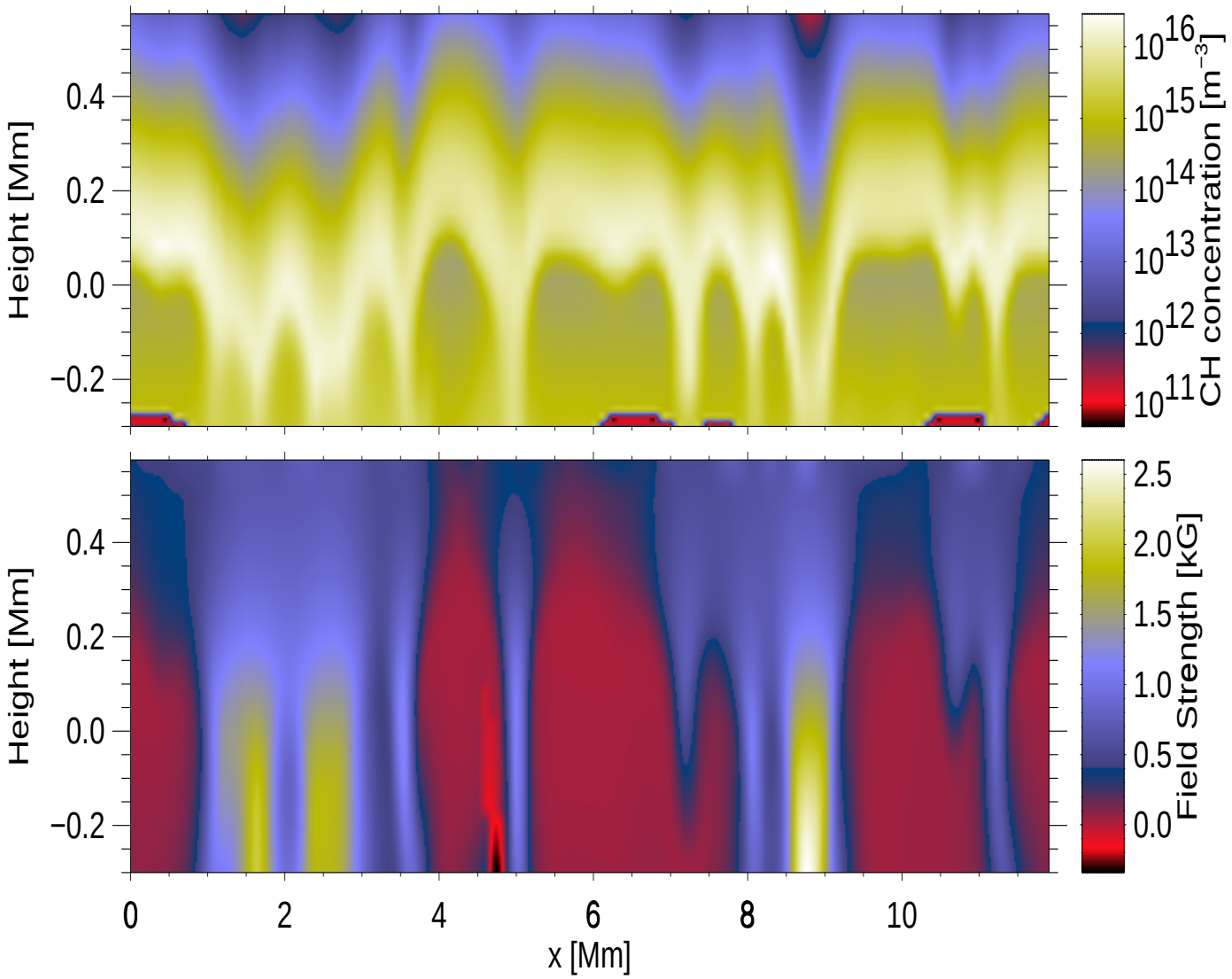




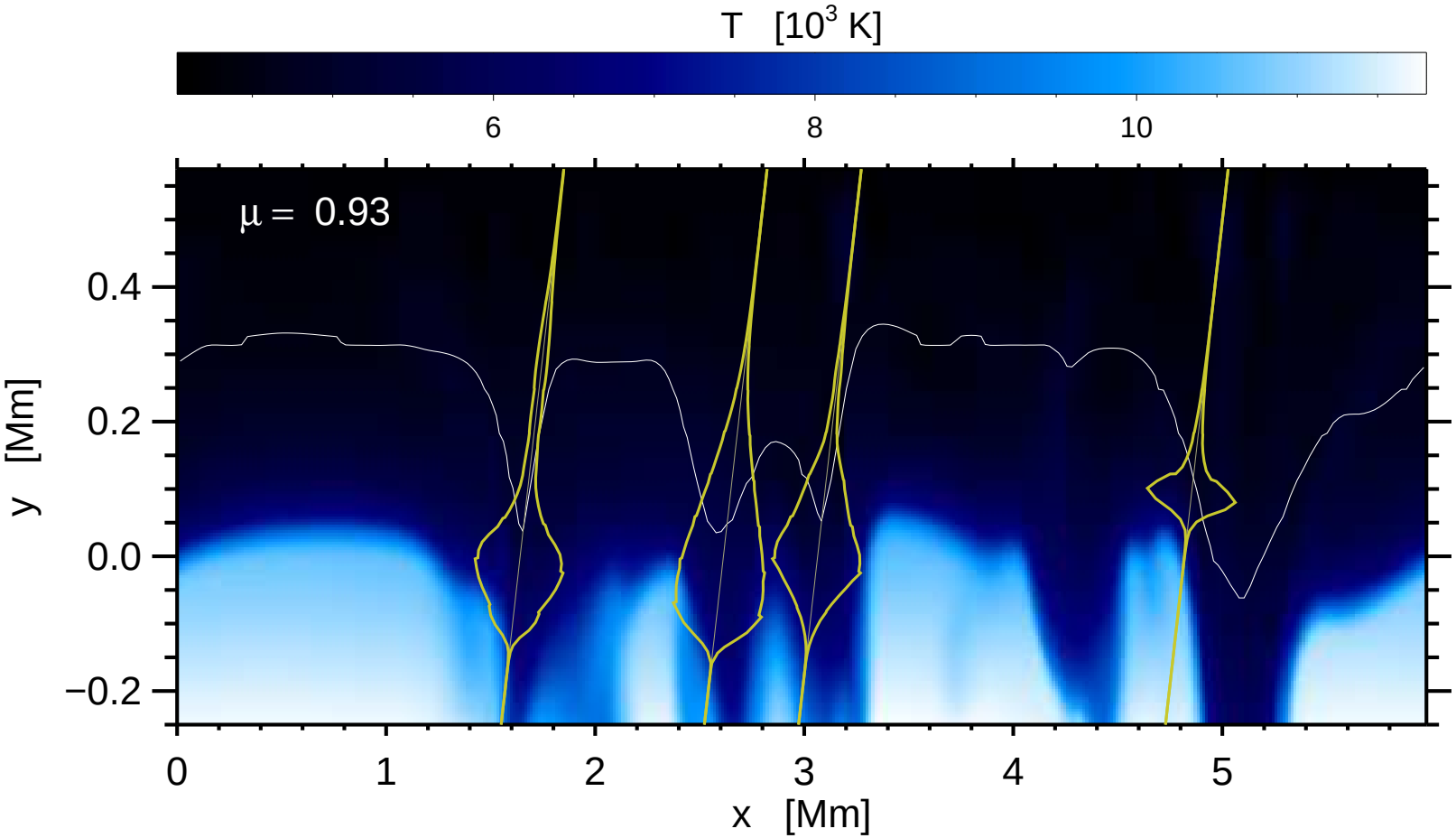
Detailed Spectra of Granule and Bright Point



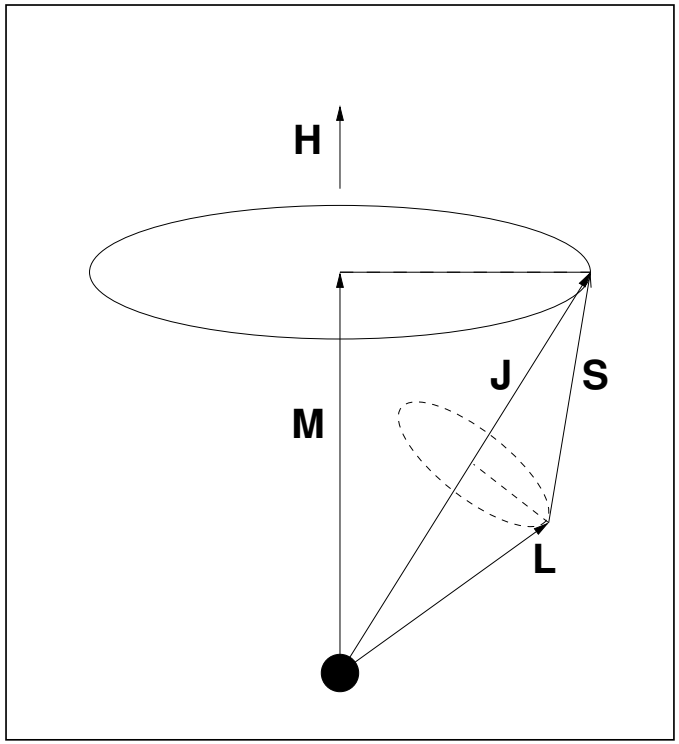
Concentration of CH Molecule and Magnetic Field



Formation Height of CH band



The Zeeman effect in atoms

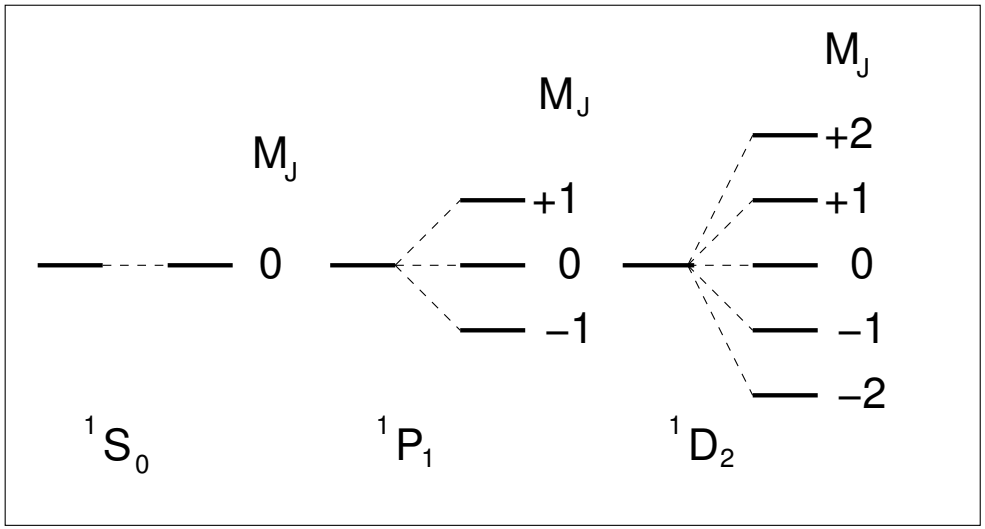


$$M_J = -J, -J+1, \ldots, J-1, J$$

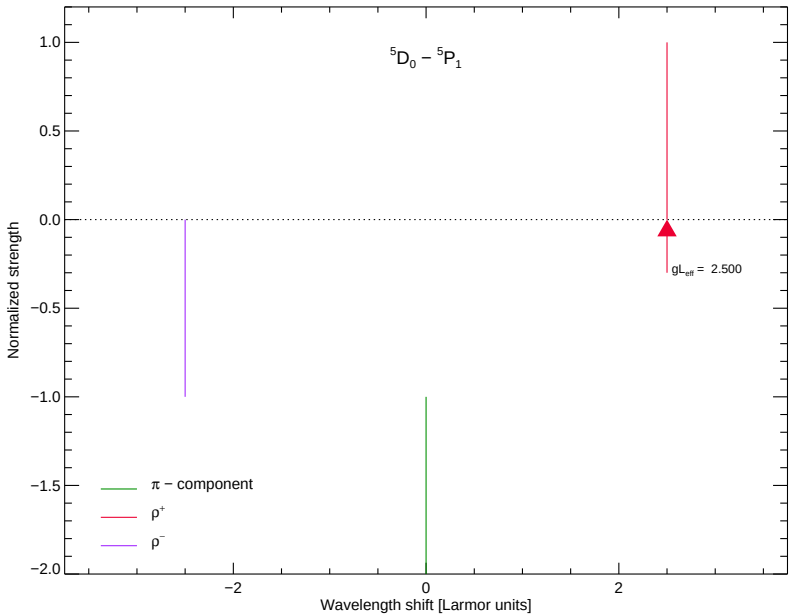
$$J_z = M_J \hbar$$

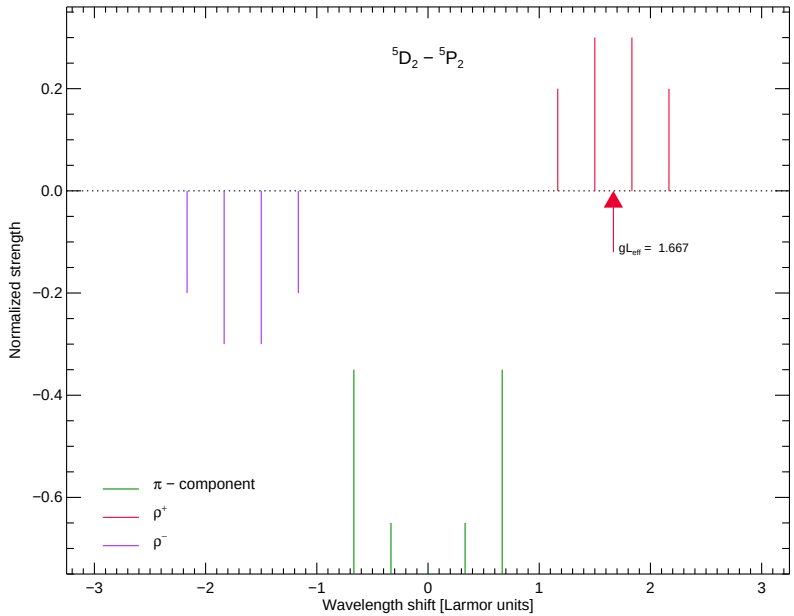
$$E = E_0 + g_{\mathrm{L}} M_J \mu_H H$$

$$g_{\mathrm{L}} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

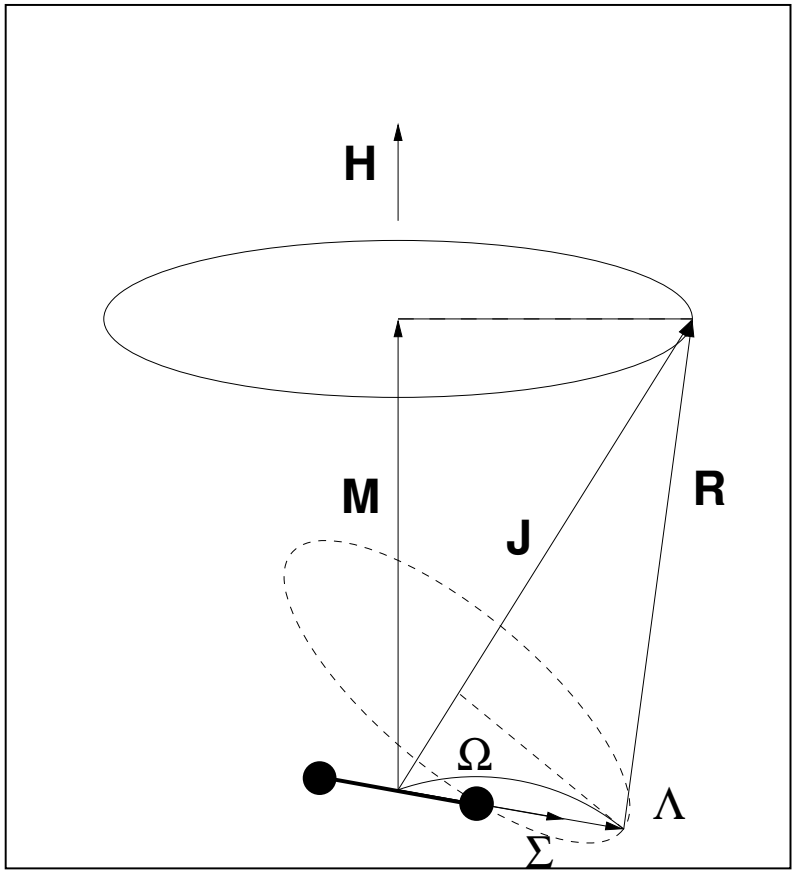


Splitting pattern for Fe I 630.25 nm and 630.15 nm

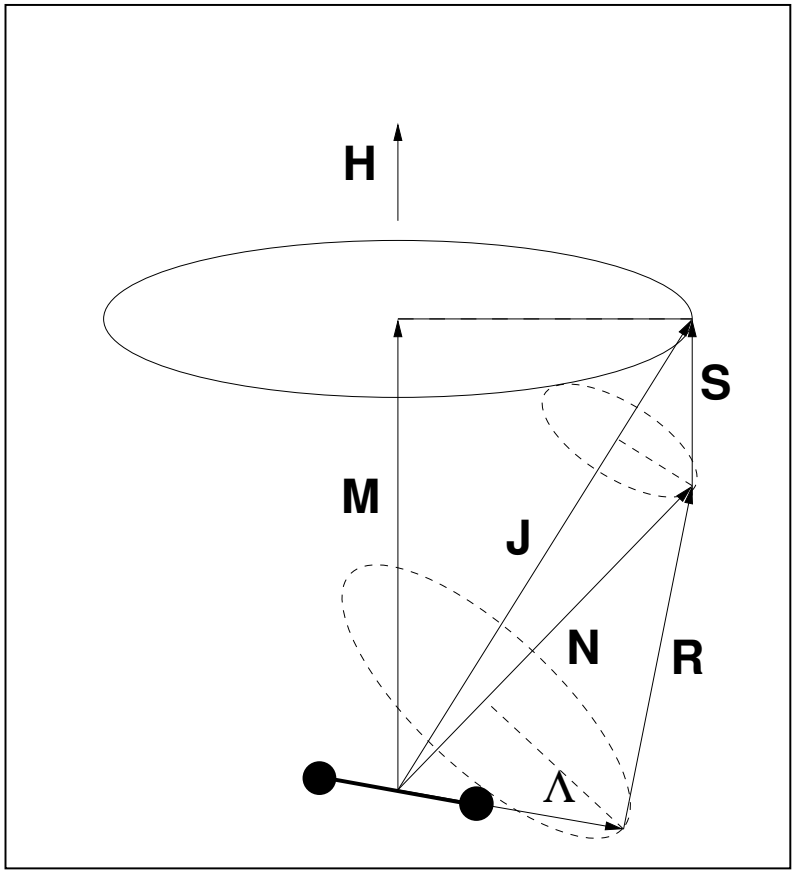




Zeeman effect in molecules: Hund's Case (a) and (b)



Hund's case (a)



Hund's case (b)

Comparison of effective Landé factors

Interaction energy:

$$E = g_{\mathrm{L}} M_J \left(e\hbar/2m_{\mathrm{e}}c\right) B$$

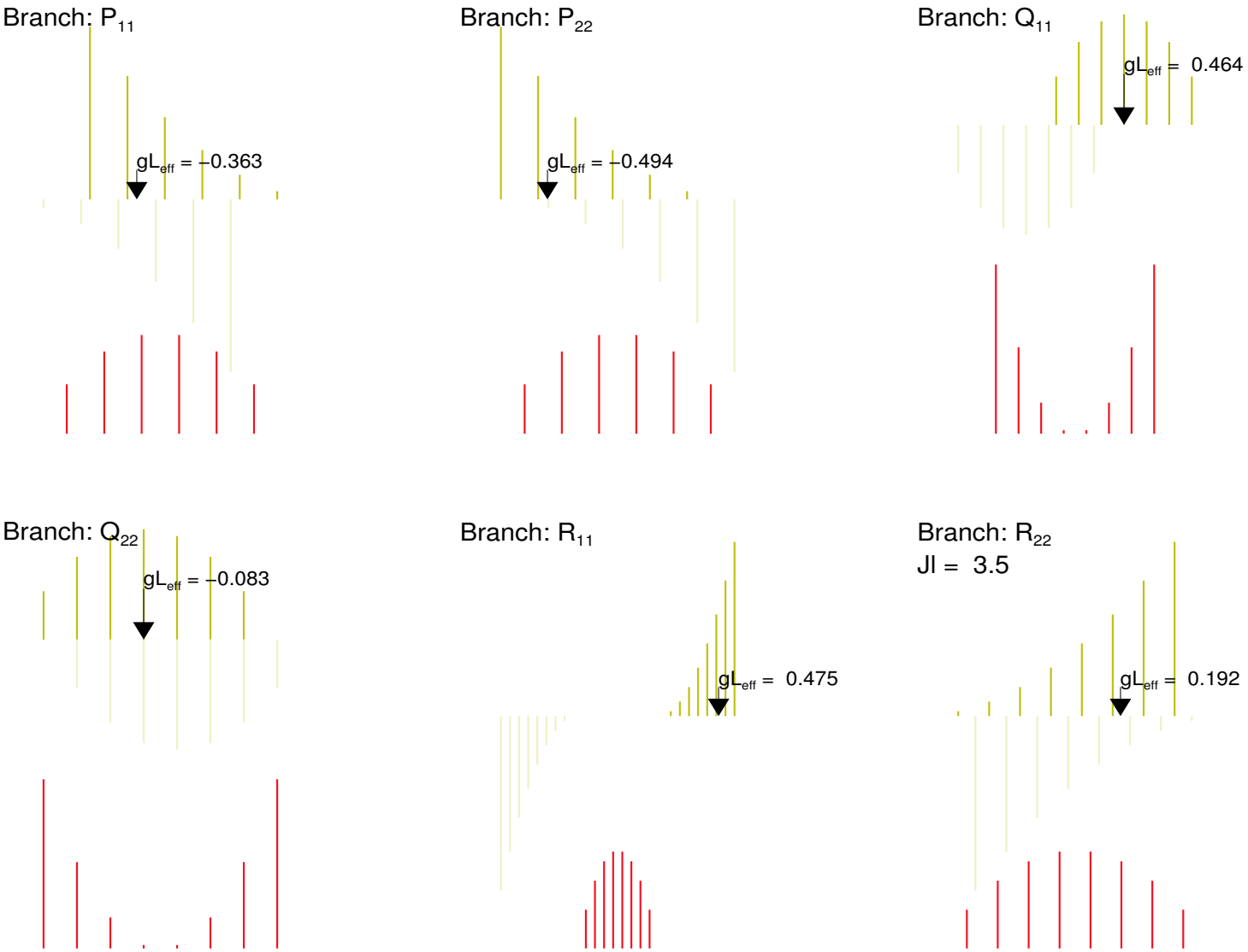
Landé factor for atomic energy level:

$$g_{\mathrm{L}} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

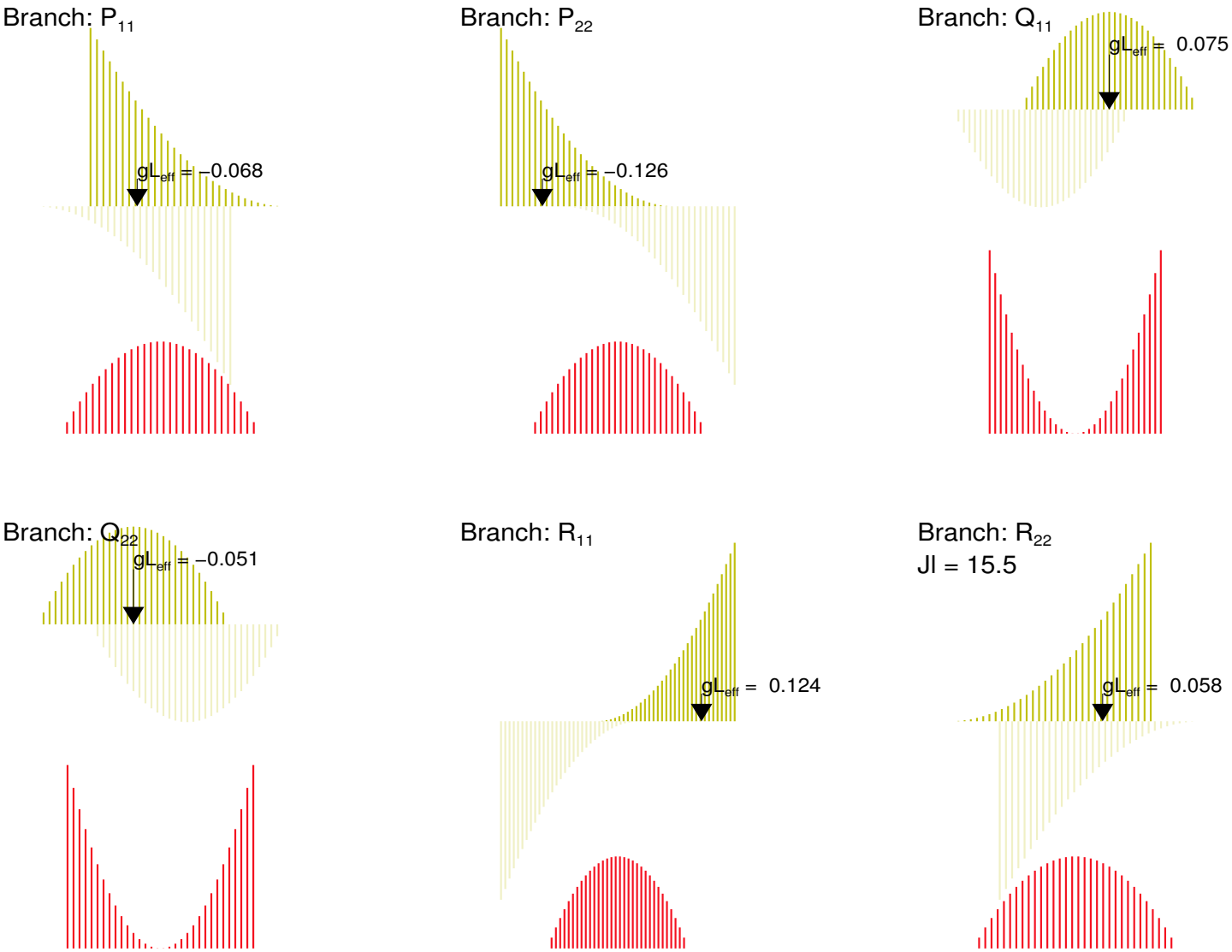
Landé factor for molecular energy level in Hund's case (b):

$$g_{\mathrm{L}} = \frac{M_J}{J(J+1)} \left\{ \frac{\Lambda^2 \left[J(J+1) + N(N+1) - S(S+1)\right]}{2N(N+1)} + \left[J(J+1) - N(N+1) + S(S+1)\right] \right\}$$

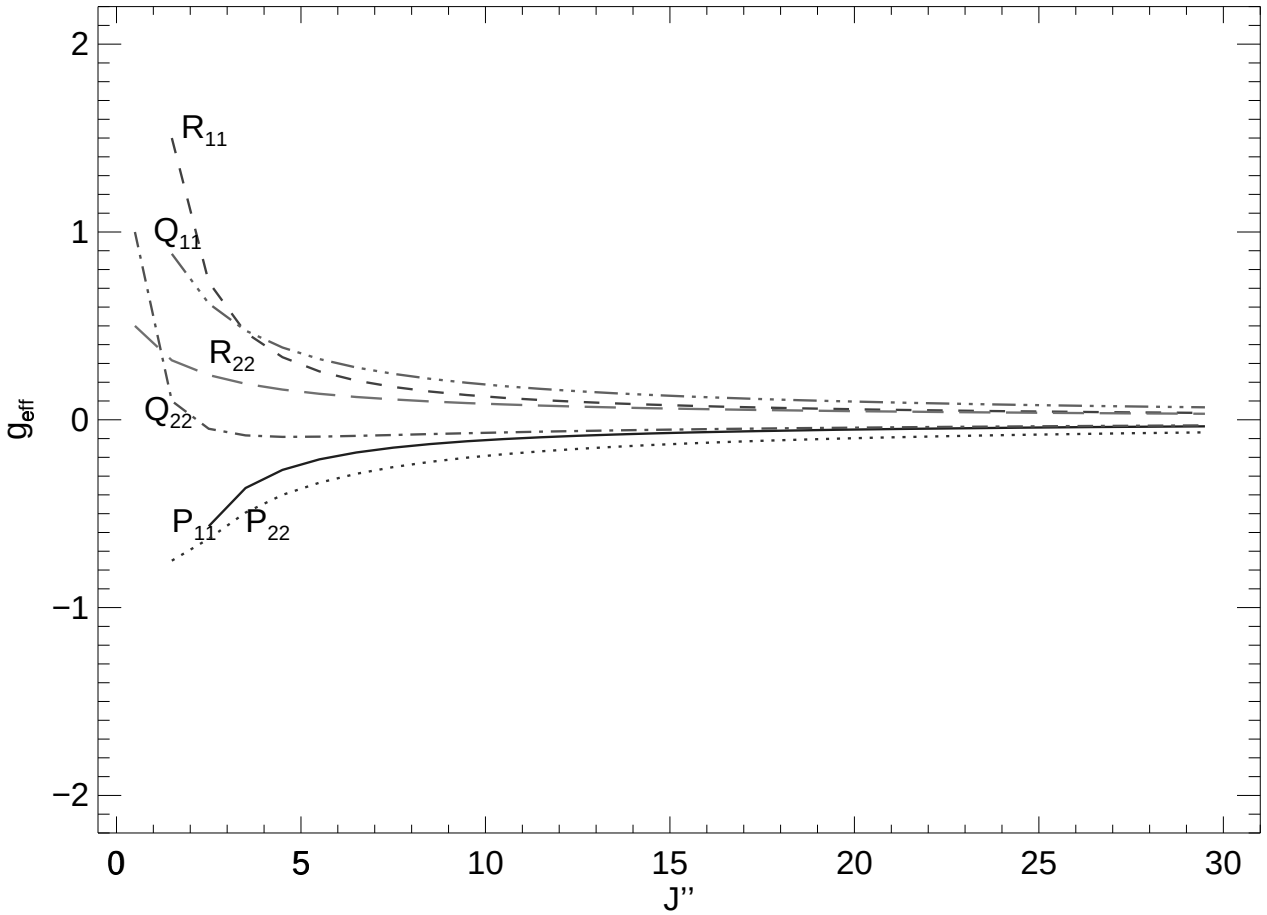
Splitting Patterns for Main Branch ($\Delta N = \Delta J$) $J'' = 3.5$



Splitting Patterns for Main Branch $J'' = 15.5$

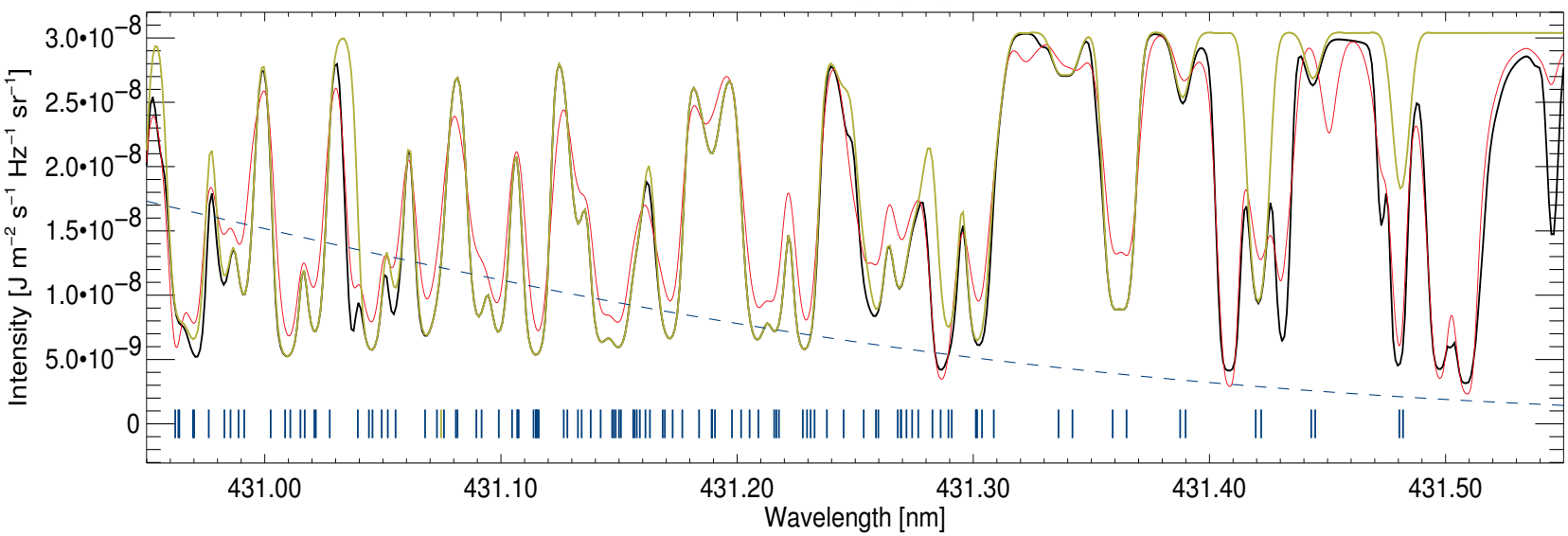


Effective Landé Factor of CH $A^2\Delta$–$X^2\Pi$ System (Main Branches)

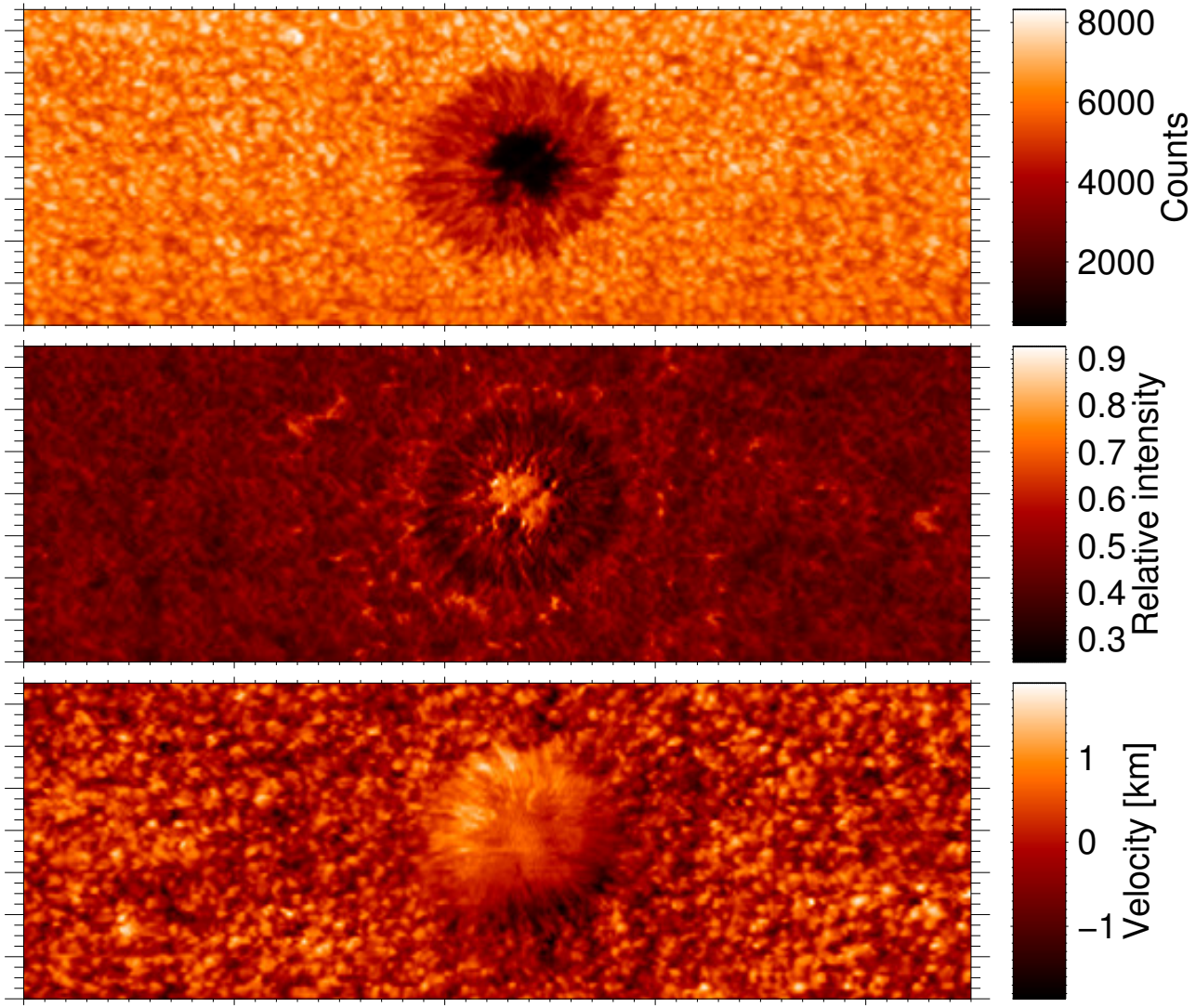


See also: Berdyugina & Solanki, 2002

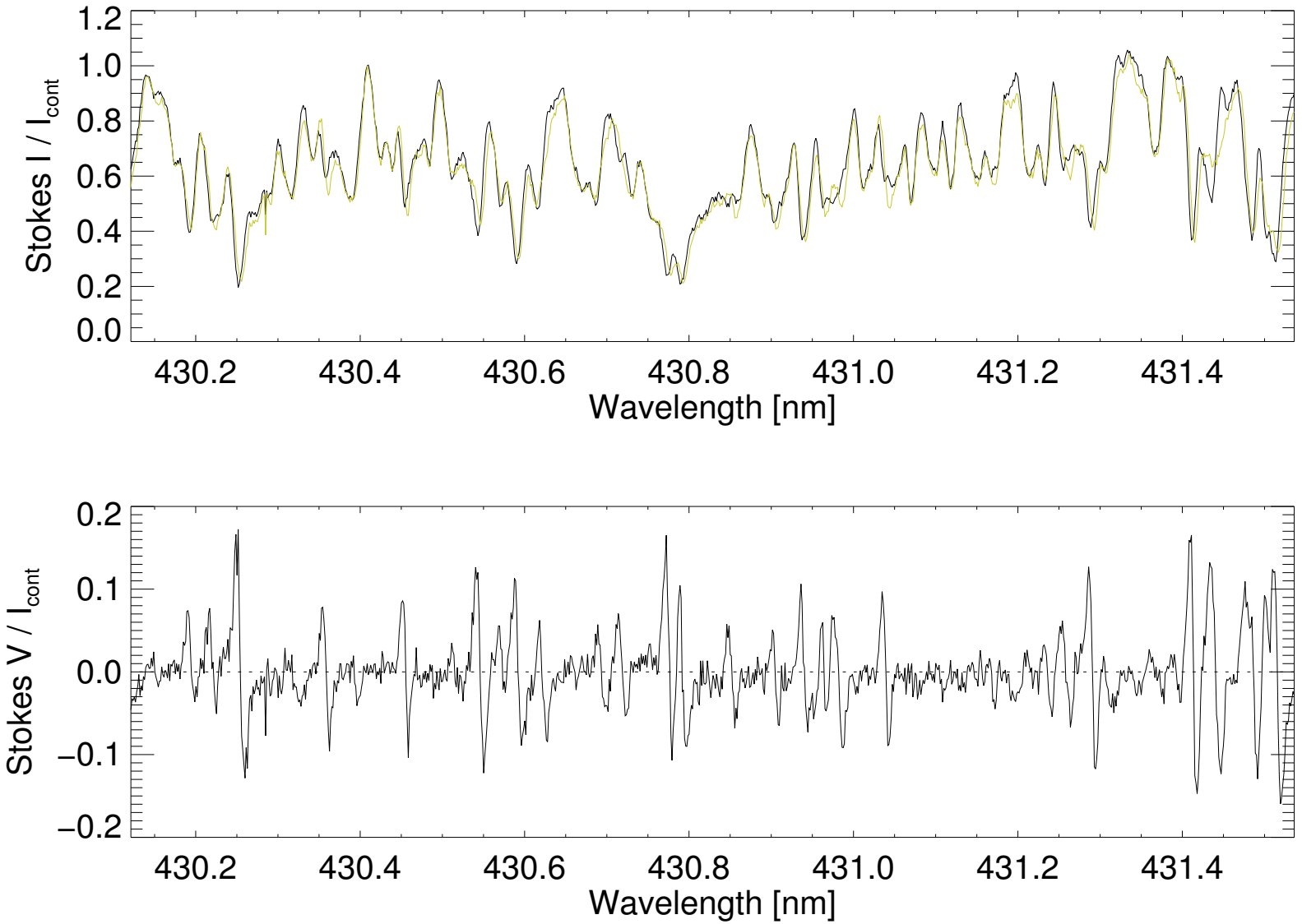
The G band Stokes V Spectrum with $B = 10^3$ G



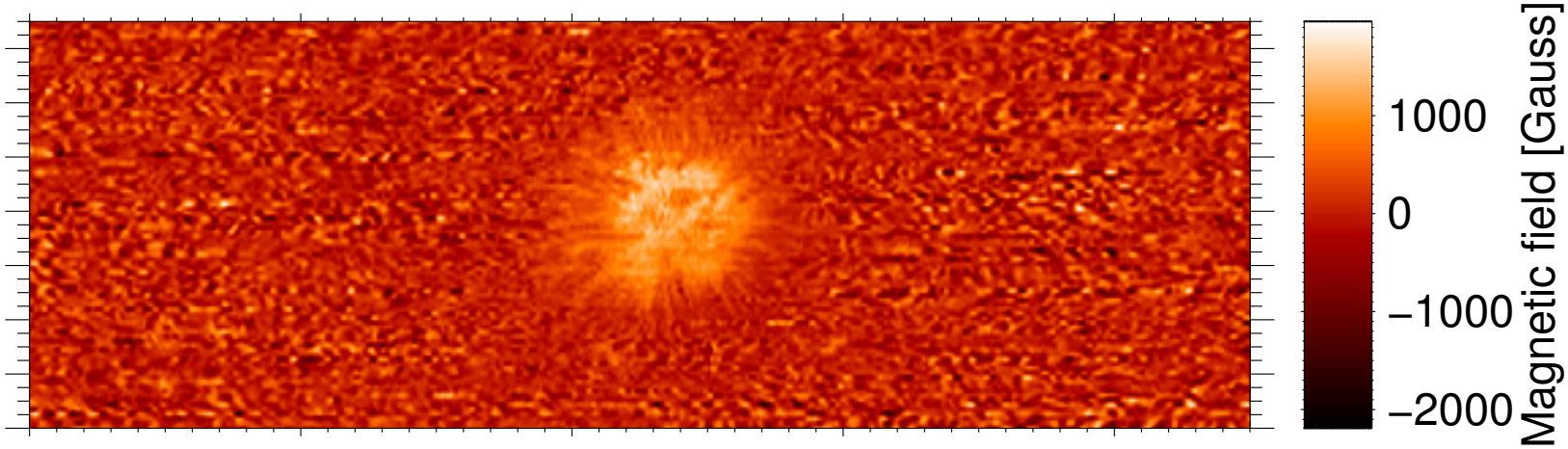
Sunspot observations in the G band



Observed Sokes V in the G band



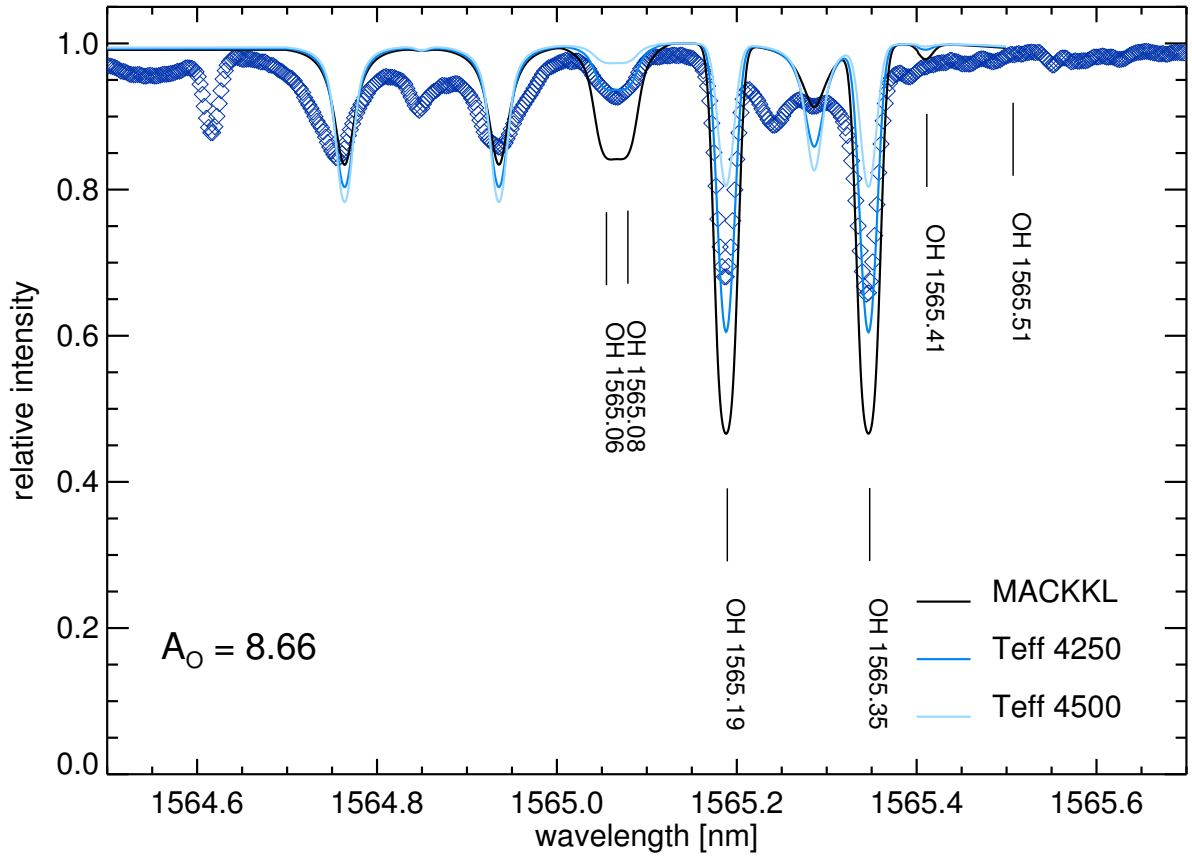
Magnetogram in CH line



Determination of Fluorine (F) Abundance

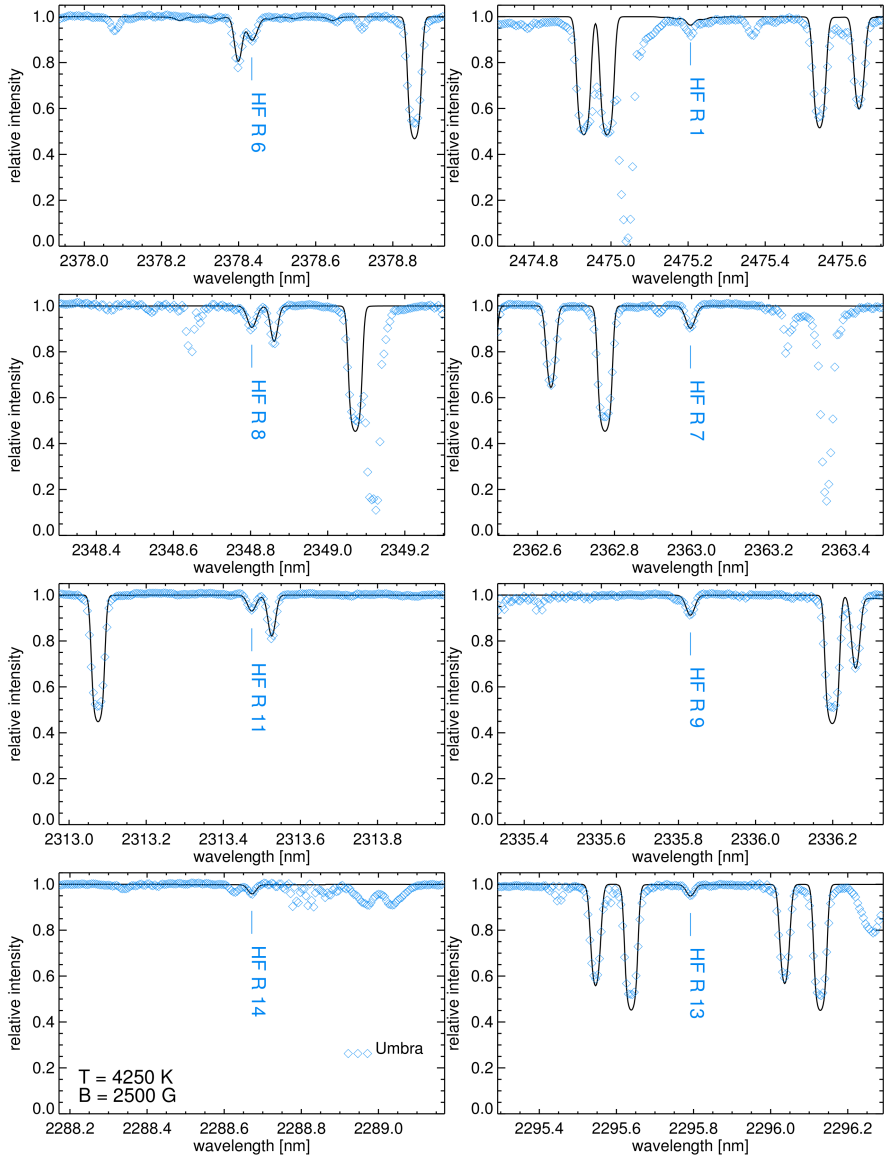
- Fluorine is an important element in tracing the mechanisms of stellar nucleosynthesis and the chemical history of the Galaxy.
- Having an almost full outer electron shell, the first excited level from the ground state lies at 102,000 cm^{-1} (12.65 eV). Almost nothing in the photosphere can excite this, so higher lying levels are almost not populated, making associated lines very weak.
- The HF molecule has line in the 2.3 micron range, but HF has a low dissociation energy (5.87 eV) and only exists in sunspot umbrae in the solar atmosphere.

Determining the effective temperature of Sunspot atlas observation



Maiorca, Uitenbroek, Uttenthaler, Randich, Busso, Magrini 2014, ApJ 788, 149

Fitting of the Fluorine lines with $A_F = 4.40$



Partition Function of Discrete System

In a closed system with discrete states $i = 1, \ldots, N$, and corresponding energy levels E_i and statistical weights g_i, the partition function $Z(T)$ is given by:

$$Z(T) = \sum_{i=1}^{N} g_i e^{-E_i/kT}$$

Back