

# Light as a messenger

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# Spectroscopic Diagnostics in Astronomy

Dr. Nadine Afram



# Contents

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- **Basics of Spectroscopy**
- **Information in Spectra**
- **Temperature and Spectral Classification**
- **Spectral Line Appearance**
- **Molecular Spectroscopy**
- **Magnetic Fields**
- **Applications in our work:**
  - **Sunspots, Starspots, Exoplanets**

# What can we learn from imaging?

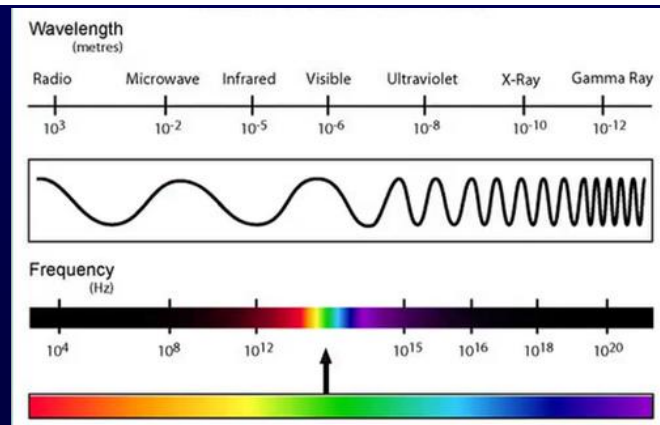
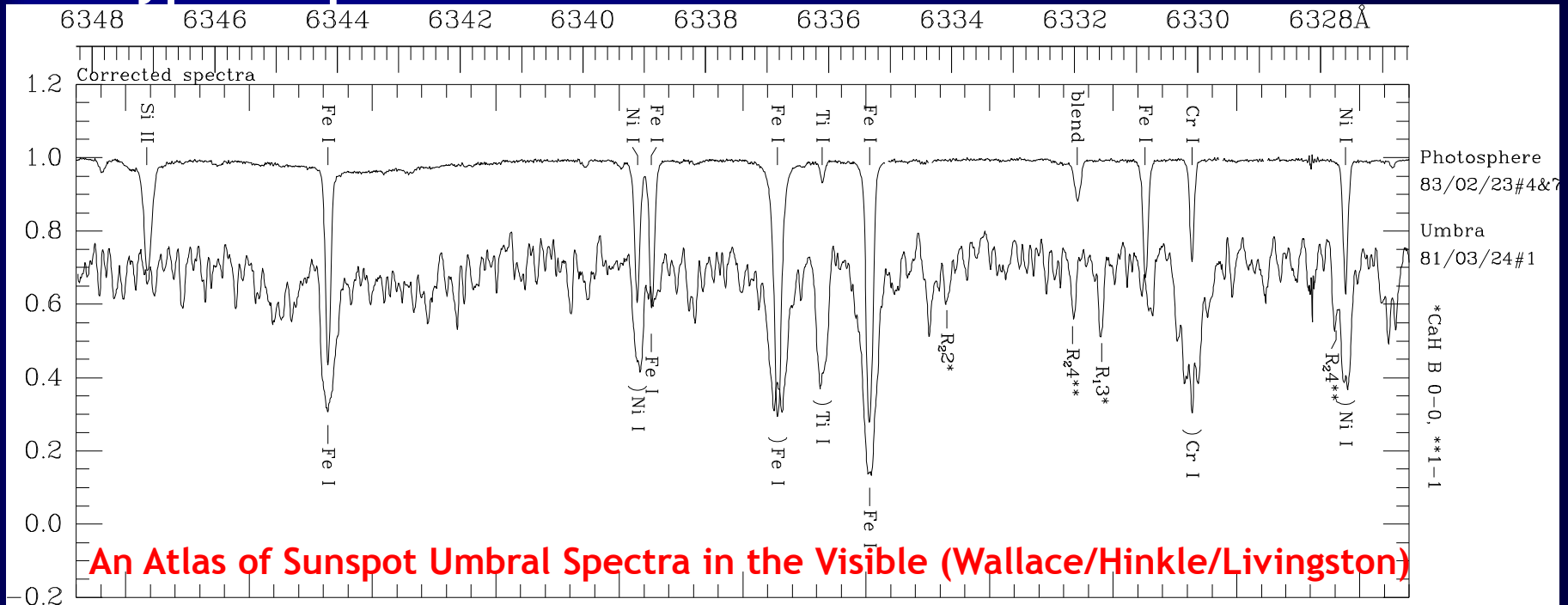


## Andromeda galaxy

- blue light: regions where hot, young stars have formed, which is mostly out on the edges (in the spiral arms)
- pink and white regions toward the center: older, cooler stars
- dark regions: giant clouds of gas and dust ring the spiral arms

# What can we learn from spectroscopy?

## A typical spectrum:

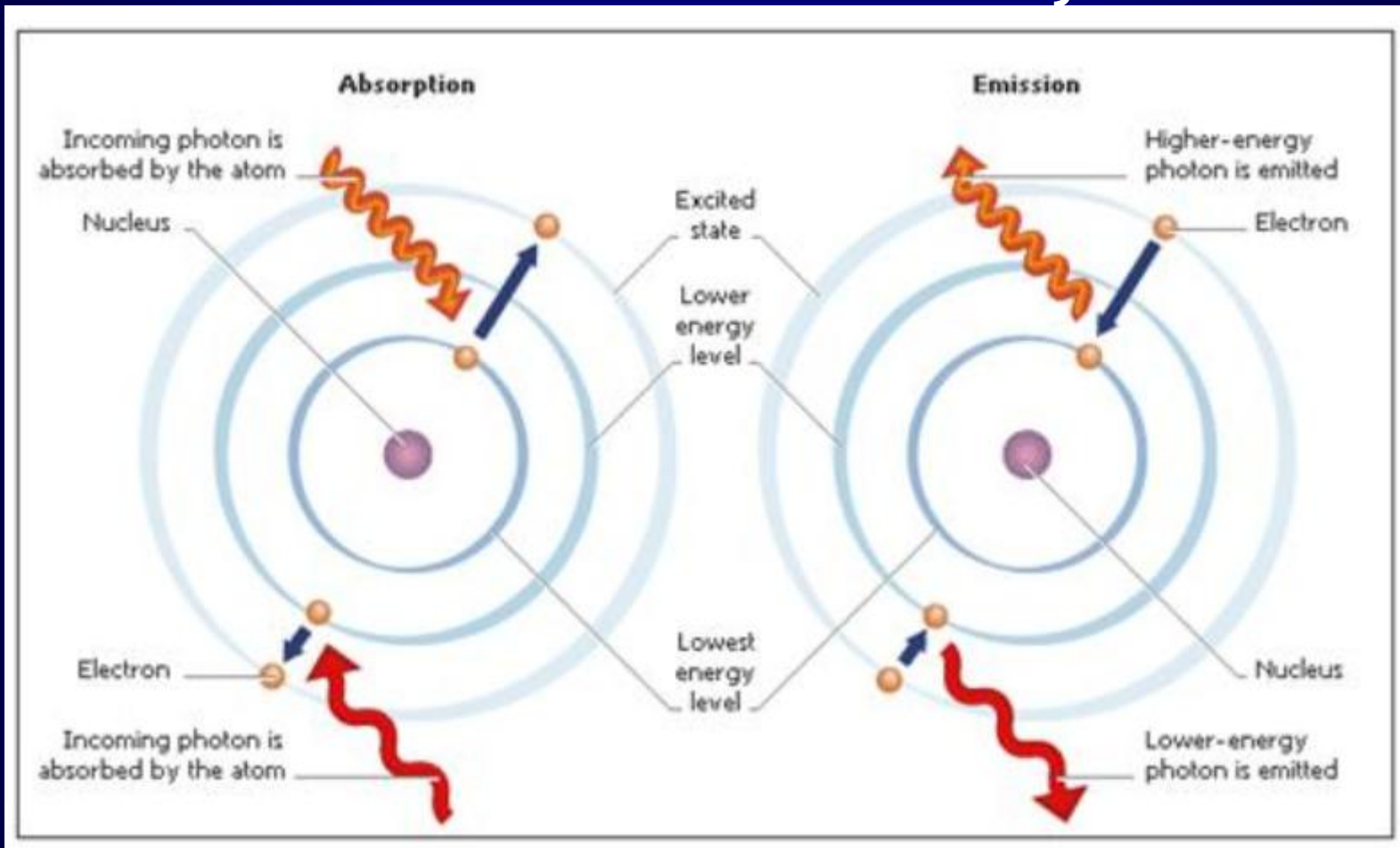


Electromagnetic spectrum

# Interaction of Light and Matter

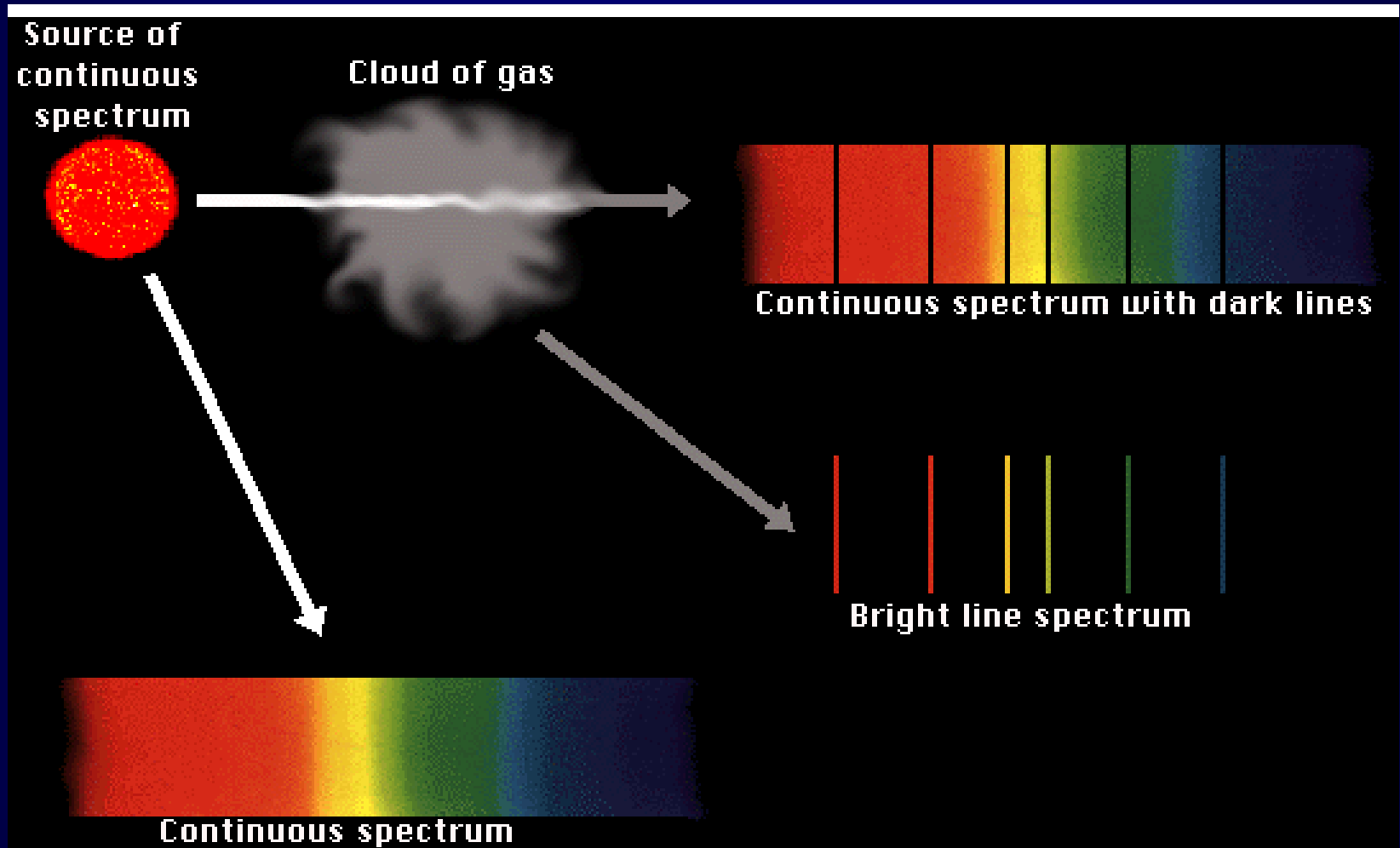
Understanding infinitesimally large

-> understand the infinitesimally small



# Atomic Spectroscopy

Different kinds of spectra:



# Different kinds of spectra

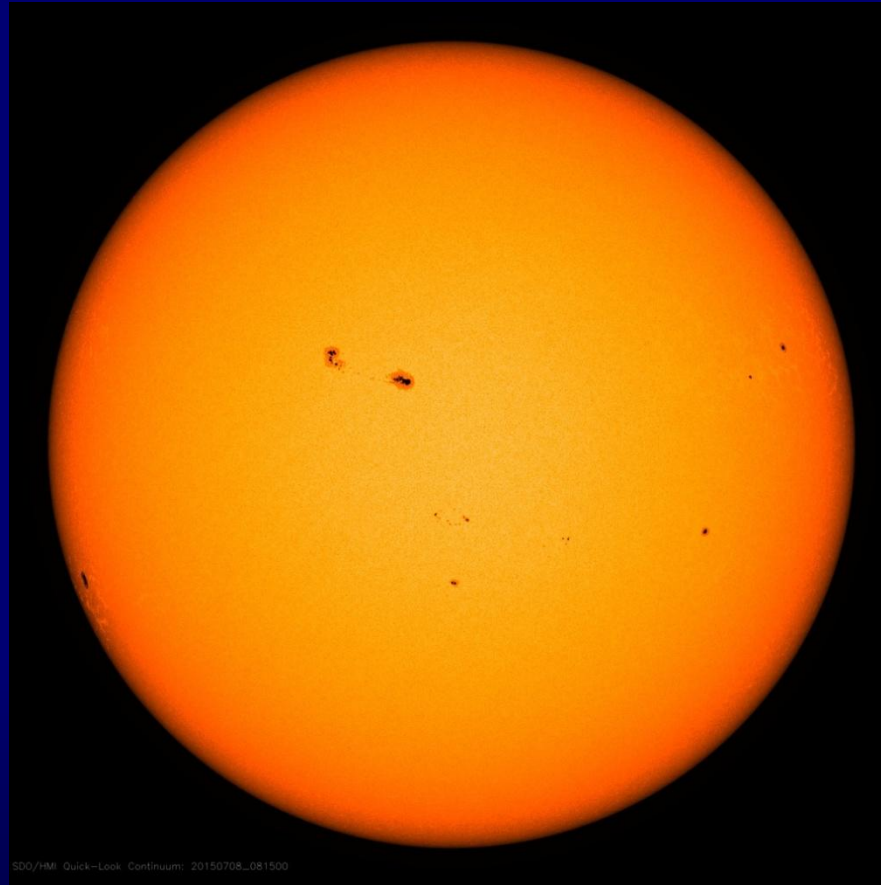
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- A hot, opaque body produces a continuous spectrum
- A hot, transparent gas produces an emission line spectrum
- A cool, transparent gas produces an absorption line spectrum

# Spectroscopy

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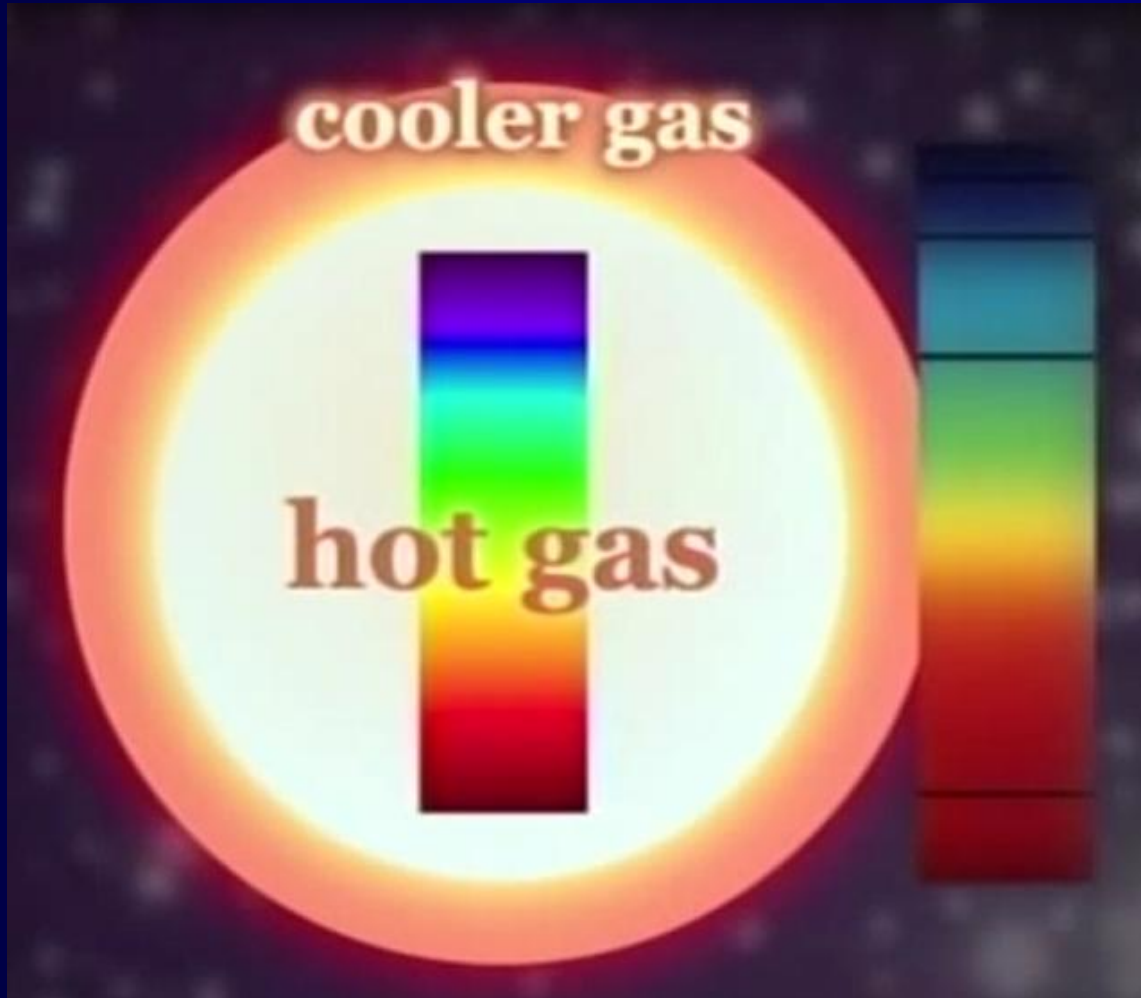
## Absorption spectrum





# Spectroscopy

## Absorption spectrum



- Surface of star cooler than gas underneath
- The light from the hot dense gas inside produces continuous spectrum
- The cooler gas above it absorbs specific wavelengths => absorption spectrum

# Spectroscopy

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- Spectral line diagnostics: deciphering a spectrum leads to information on different solar/stellar atmosphere parameters:
  - **Line width:** temperature and turbulent velocity, stellar wind speeds
  - **Line depth:** temperature and temperature gradient
  - **Wings of strong lines:** gas pressure
  - **Equivalent width:** element abundance, temperature
  - **Splitting of lines (and polarization):** magnetic field

# Spectroscopy

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- **Doppler shift of line:** (net) flows in LOS direction, rotation rates
- **Line asymmetry:** velocity gradient,  $v$ ,  $T$  inhomogeneities

=> Atmospheric temperatures, compositions of stars and planets, planet surface properties (via absorbed and emitted light), stellar ages, chemical evolution of galaxies, etc

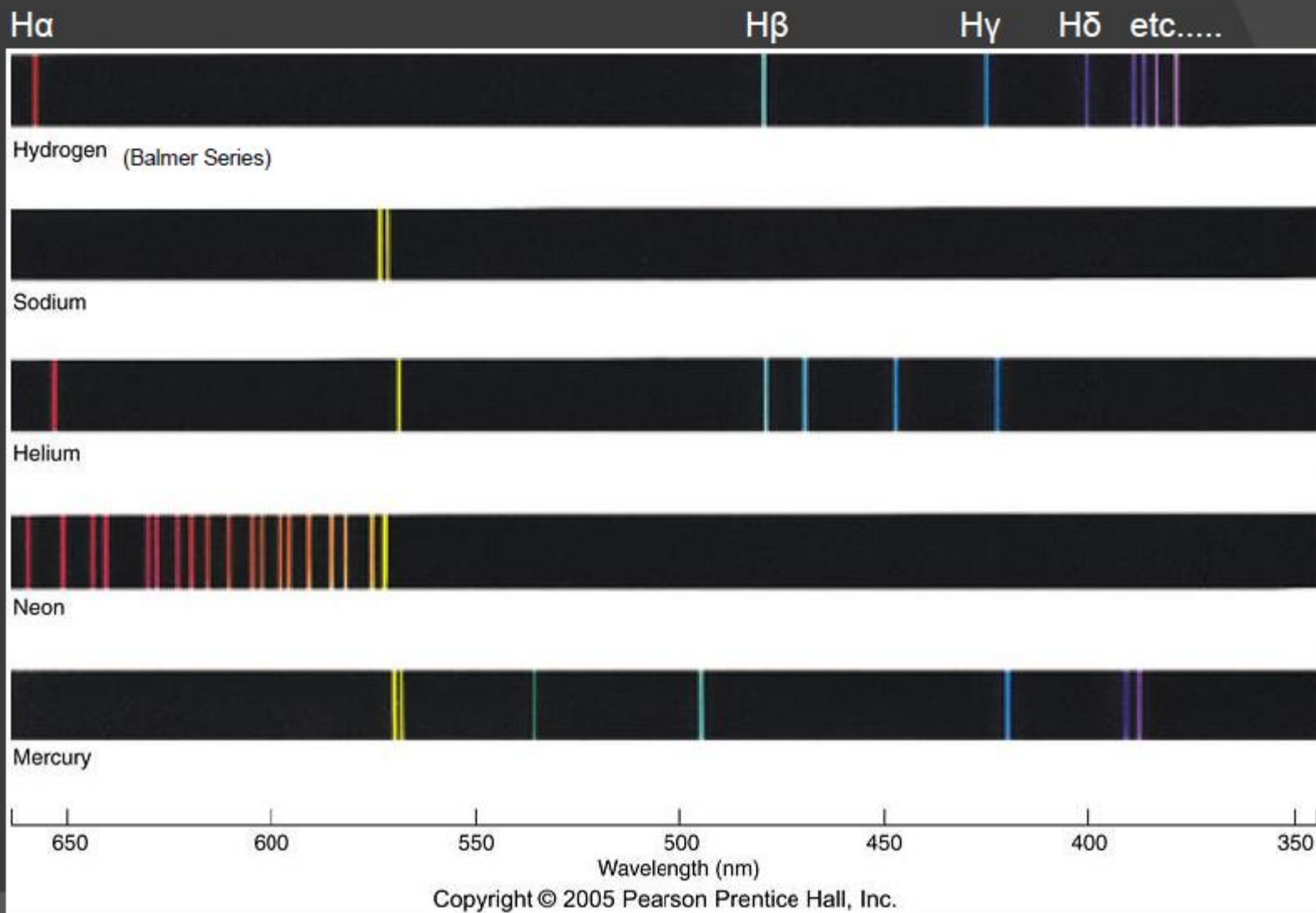
# Spectroscopy

1860s: Systematic attribution of spectra  
to chemical elements:

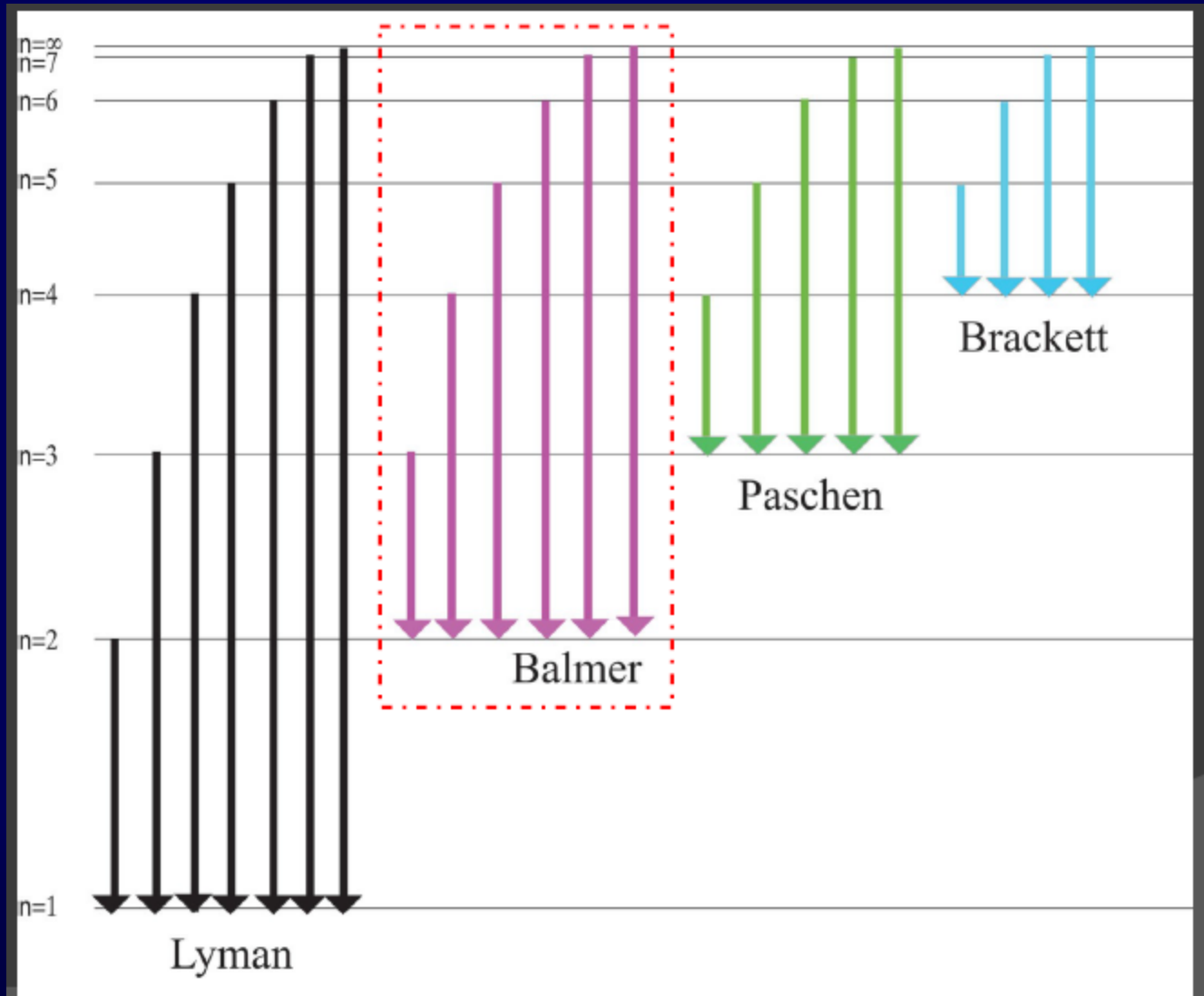
physicist Gustav Kirchhoff (left) & chemist Robert Bunsen (right)



# Spectral Fingerprints



# Energy Levels of Hydrogen



# Temperature and Spectral Classification

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- **Hydrogen: electrons in 2nd level absorb photons to produce Balmer series**
- **Temperature of gas in star affects spectrum of star**

# Temperature and Spectral Classification

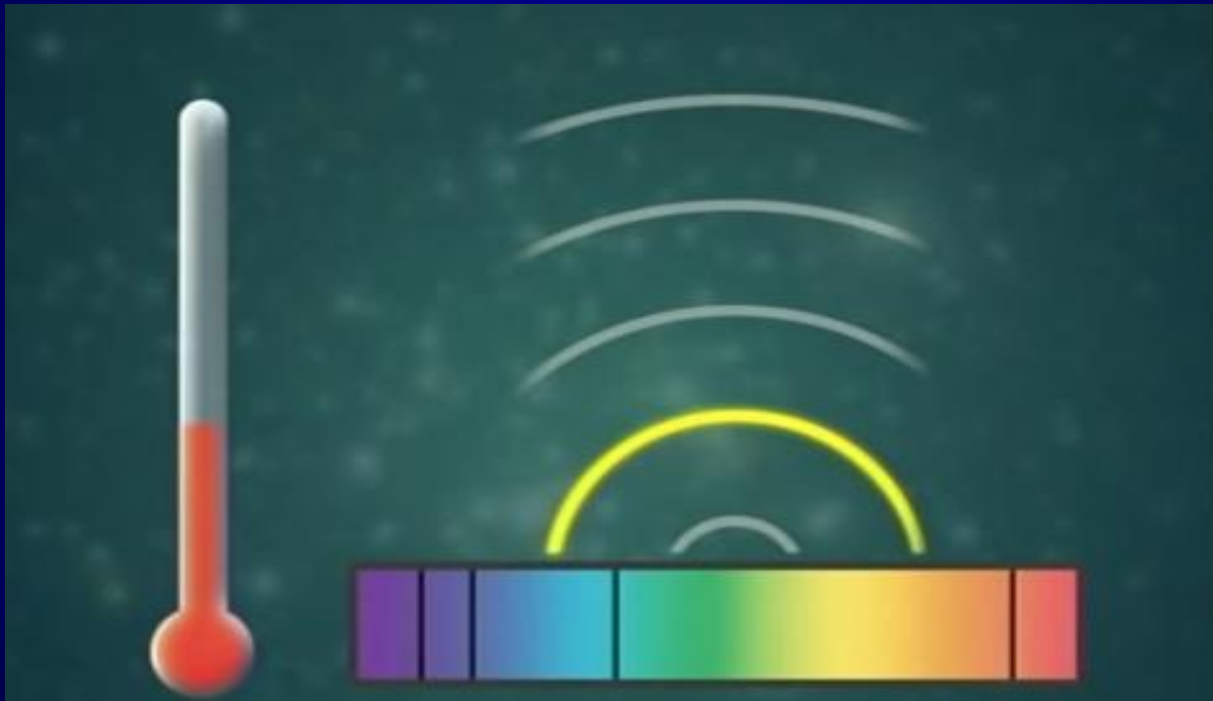
**Star of cool temperature: most electrons lower than 2nd level: weak or invisible Balmer**





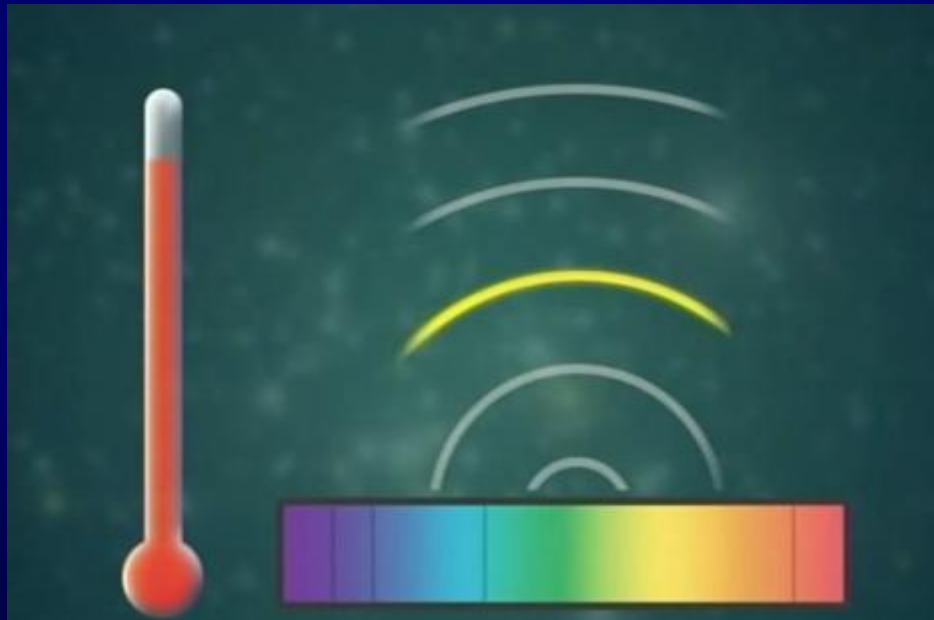
# Temperature and Spectral Classification

Star of intermediate temperature: most electrons in 2nd level: strong Balmer

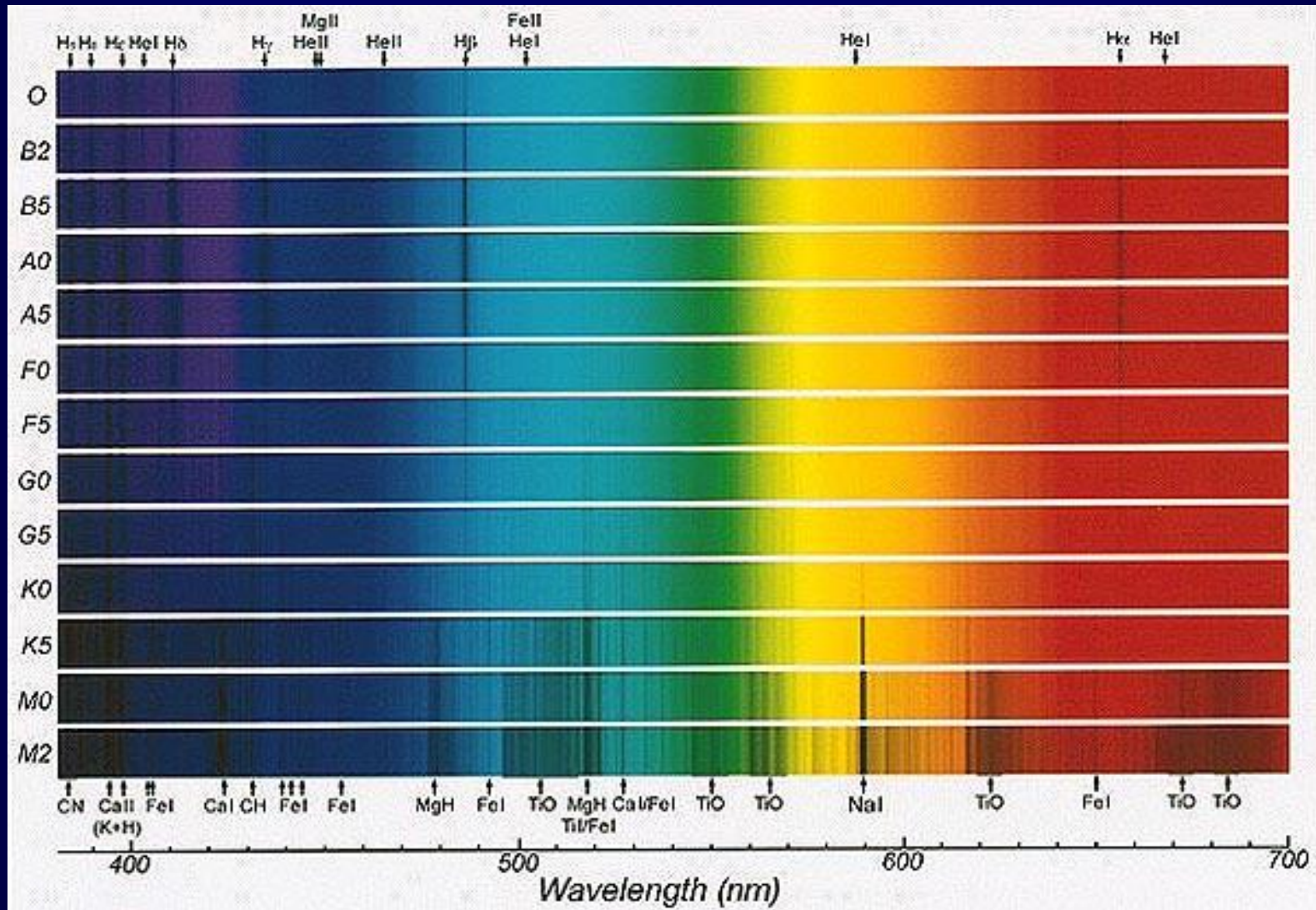


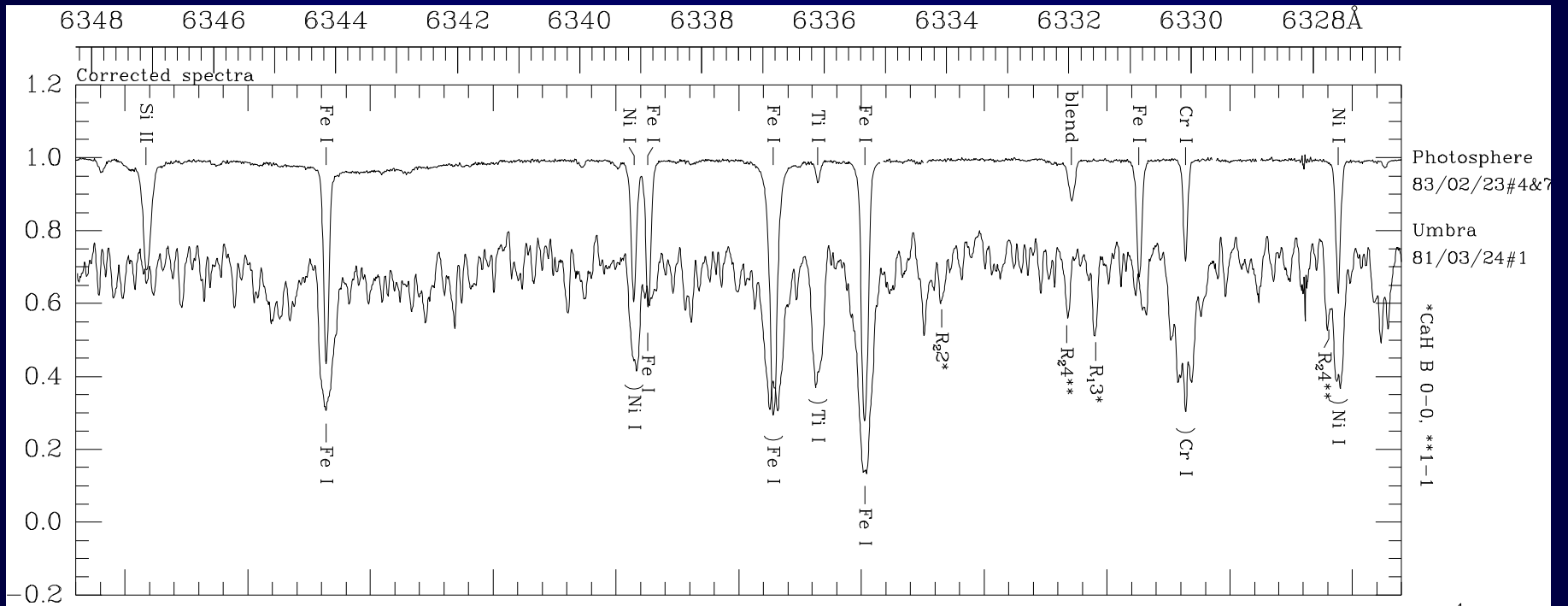
# Temperature and Spectral Classification

**Star of high temperature: most electrons excited to higher than 2nd level: weak Balmer**



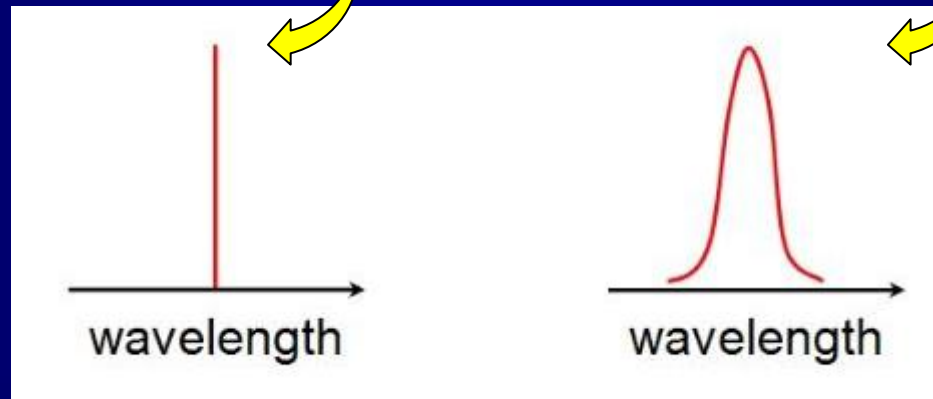
# Temperature and Spectral Classification



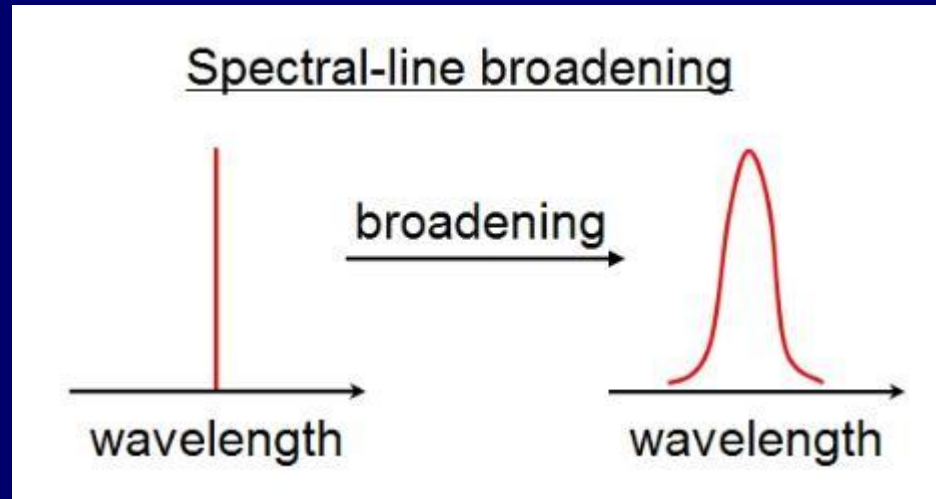


# Spectral Line Appearance

Why does a spectral line not look like this but like that ?



# Spectral Line Broadening



- Energy levels not infinitely sharp
- Atoms move relative to observer

# Doppler broadening

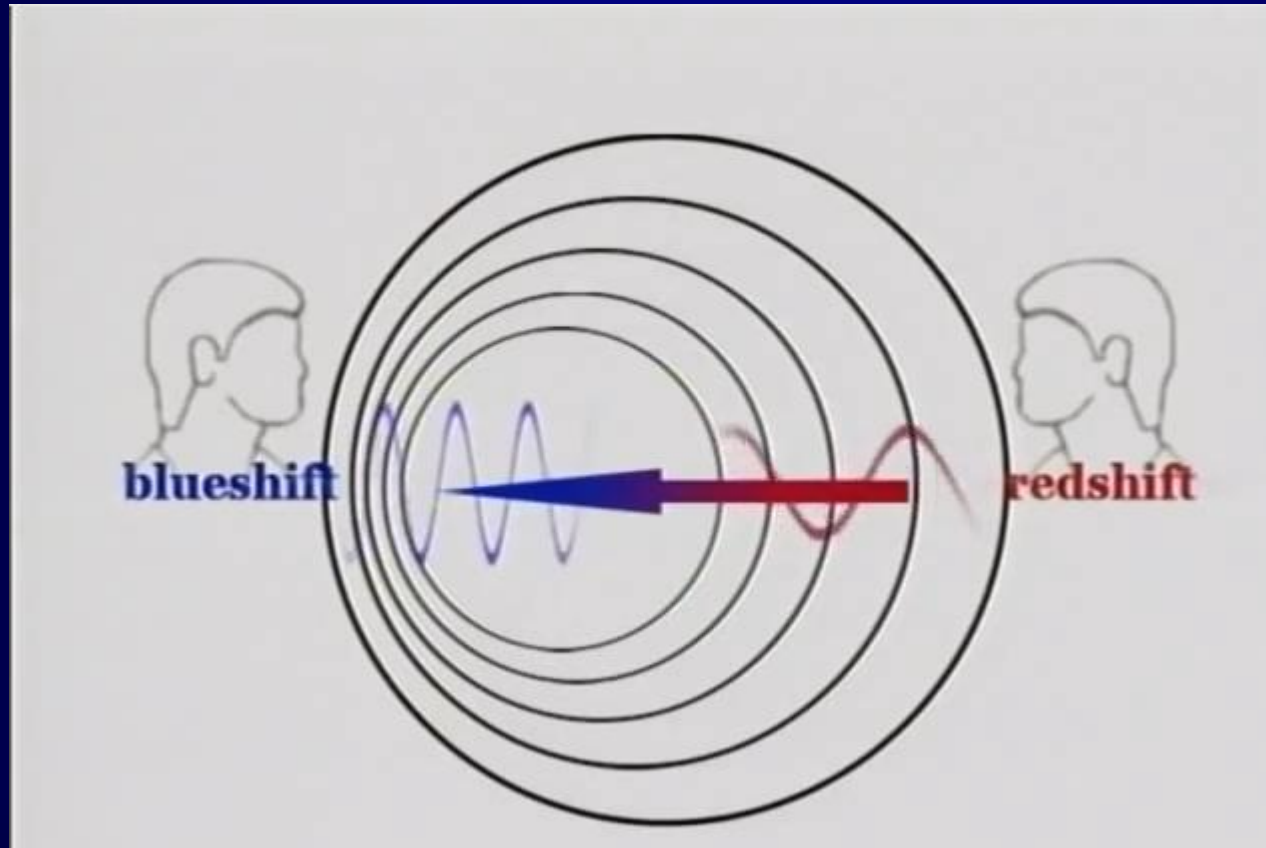
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## Light in Motion with spectroscopy

- Is the object moving away or towards us?
- Is the object spinning?
- Is the object expanding?
- Is the object orbiting another object?

# Doppler broadening

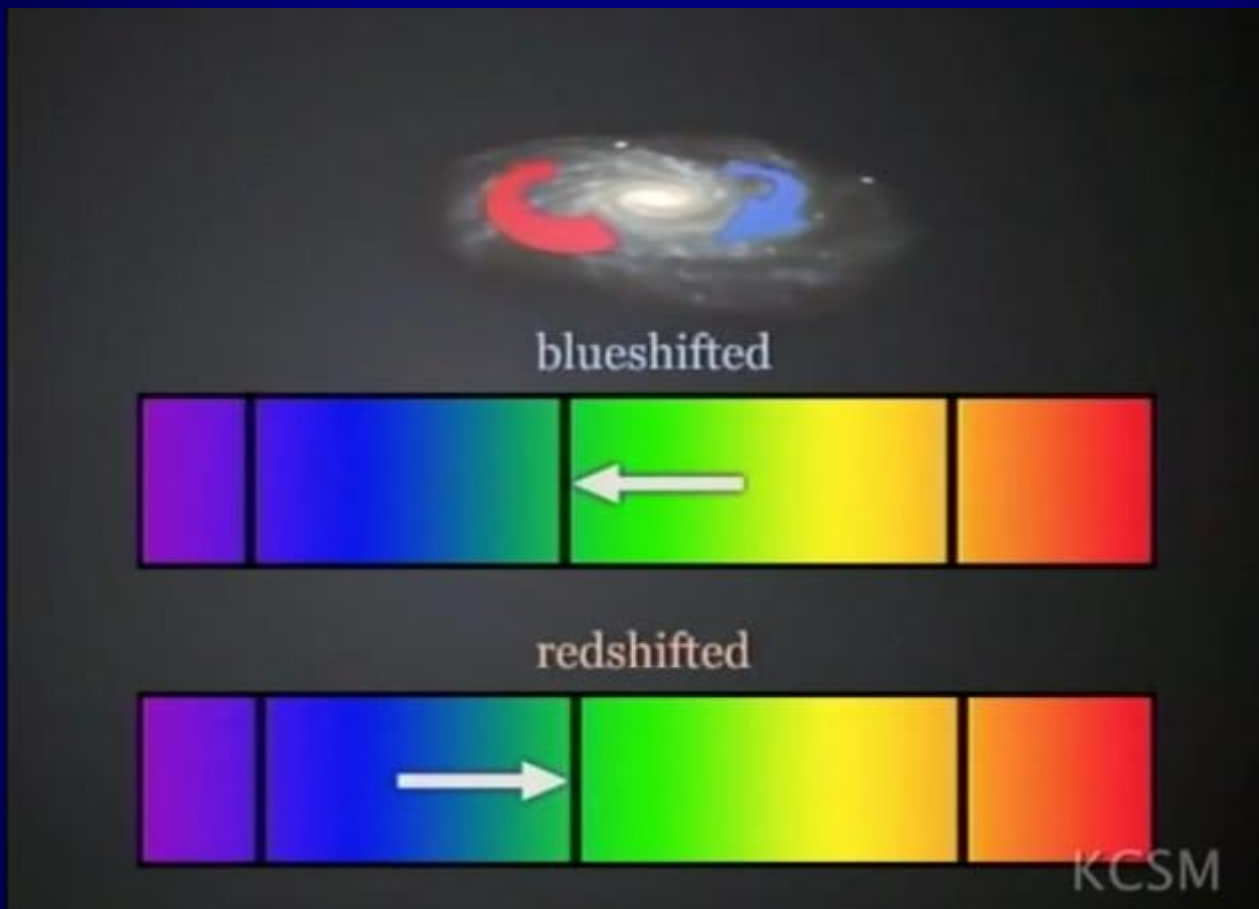
## Doppler Effect





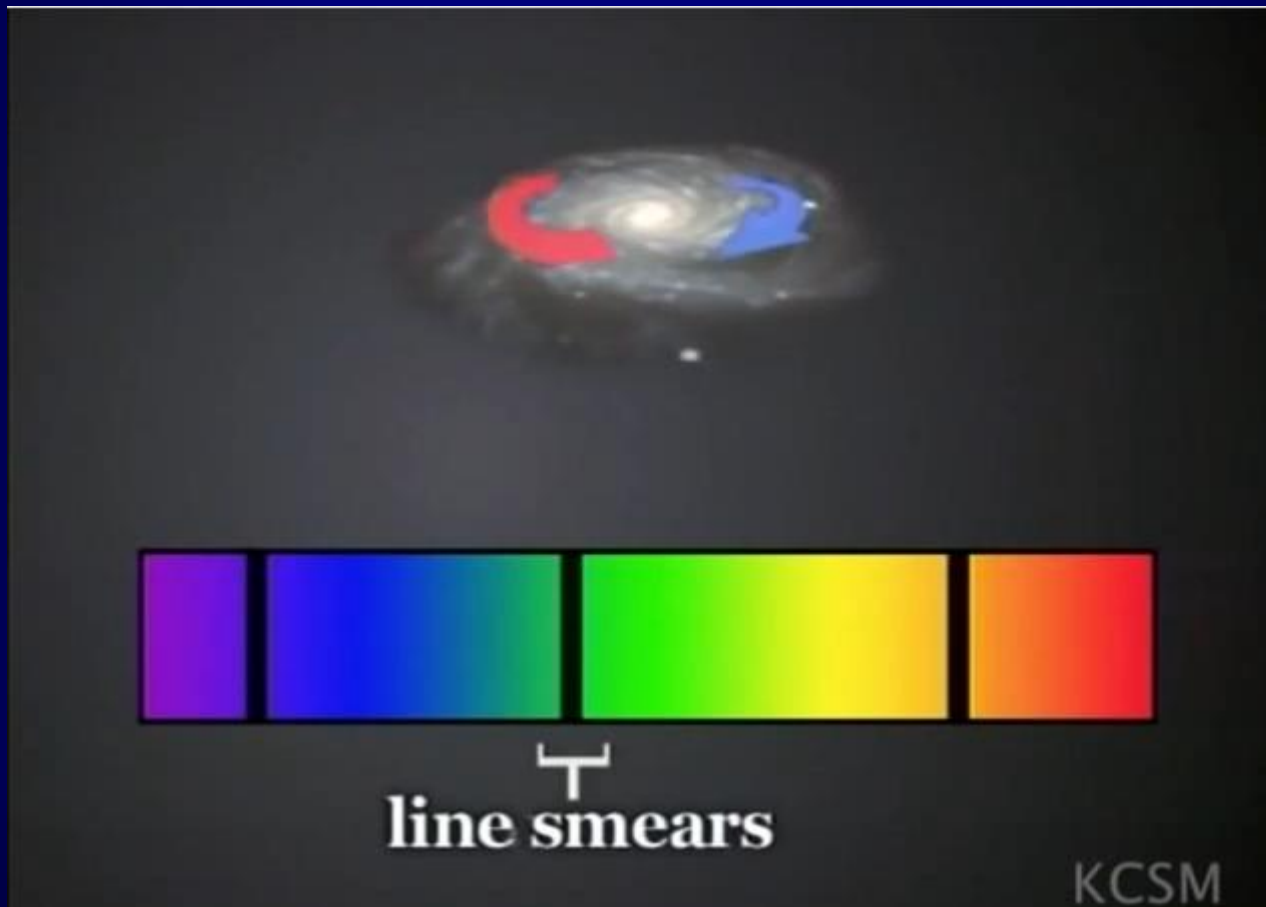
# Doppler Broadening

## Doppler Effect: Rotating object



# Doppler broadening

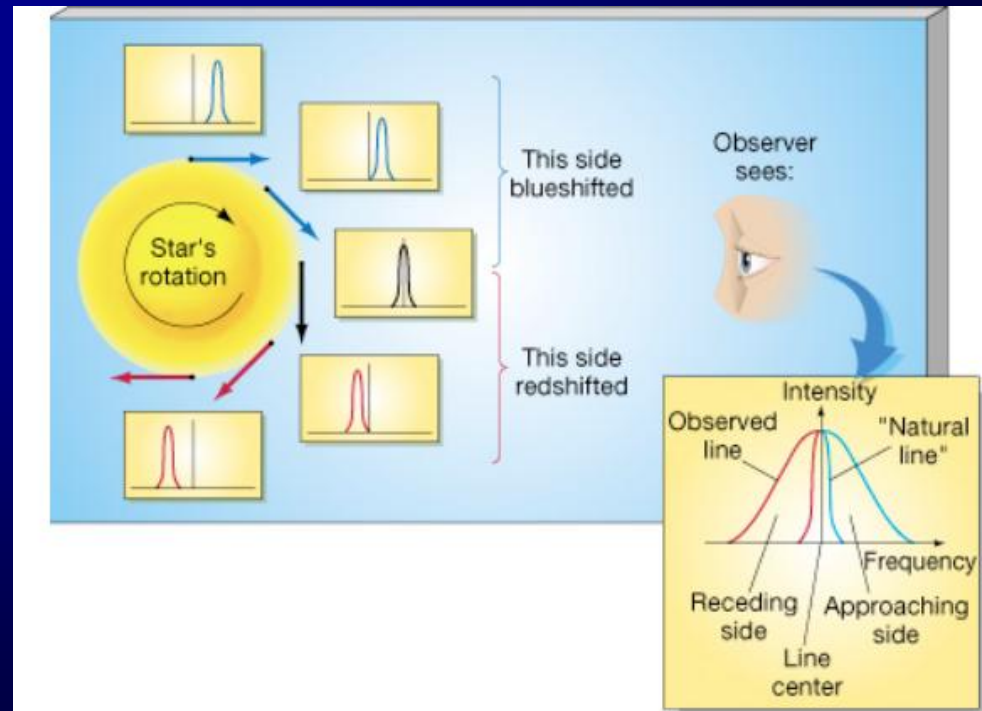
## Doppler Effect: Rotating object



# Spectral Line Broadening

Doppler broadening  
-> Doppler profile  
(Gaussian)

moving towards us: blue-shifted  
moving away: red-shifted



# Spectral Line Broadening

## Doppler broadening

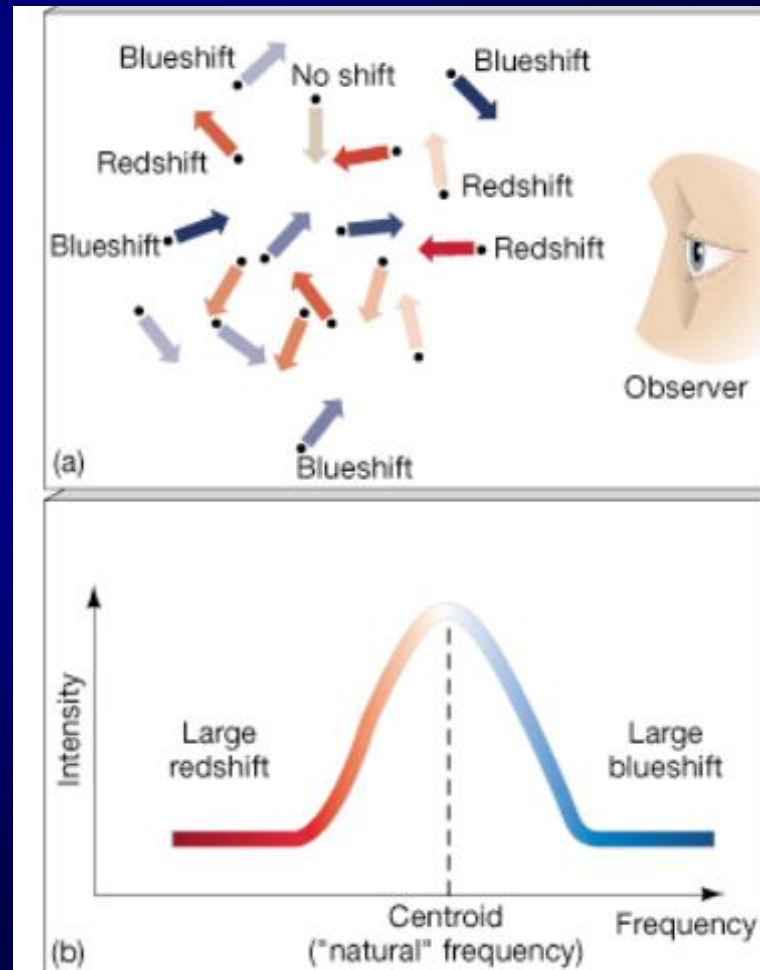
-> Doppler profile

(Gaussian)

Thermal Doppler broadening:  
atoms/molecules in random  
thermal motion

This kinetic energy is thermal:  
the hotter the gas of atoms,  
the faster they move about  
on average

=> the more the line is broadened



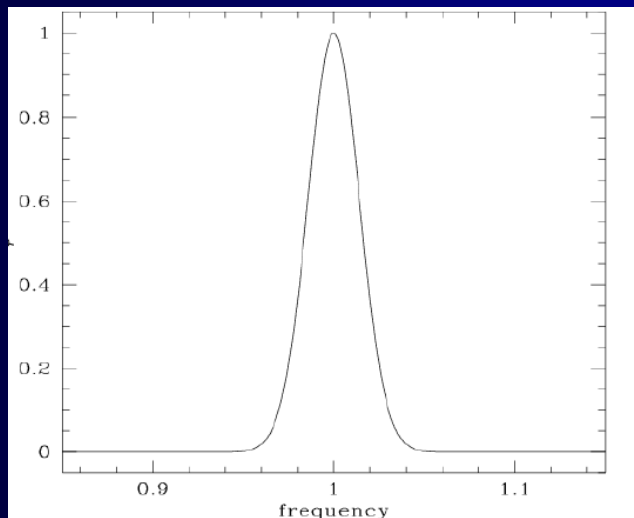
# Spectral Line Broadening

Doppler width

$$\Delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}}$$

-> Doppler profile  
(Gaussian)

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-((\nu-\nu_0)^2 / (\Delta\nu_D)^2)}$$



faster decay than  
Lorentzian

# Spectral Line Broadening

## Natural (intrinsic) broadening

### -> Lorentzian profile

Quantum-mechanical effect: the longer a state exists for, the greater the uncertainty in its energy  $\Delta E \Delta t \sim \hbar$

=> all photons emitted by an ensemble of atoms in identical excited states will not all be exactly at the same energy

=> range of possible frequencies cluster around average energy

$$\Delta \nu \sim \frac{\Delta E}{h} \sim \frac{1}{2\pi\Delta t}$$

=> naturally broadened line (in line wings, usually small effect, in low pressure environments, nebula)

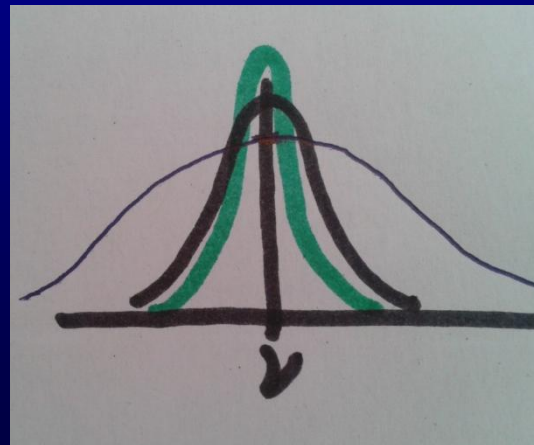
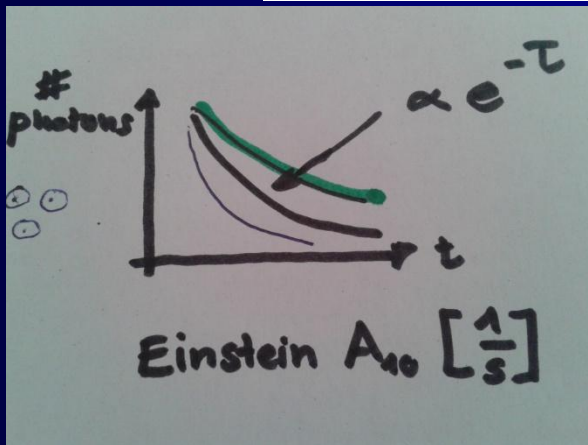
# Spectral Line Broadening

Spontaneous decay of state  $n$  to all lower energy states  $n'$

$$\gamma = \sum_{n'} A_{nn'}$$

-> Lorentzian profile

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2}$$



# Spectral Line Broadening

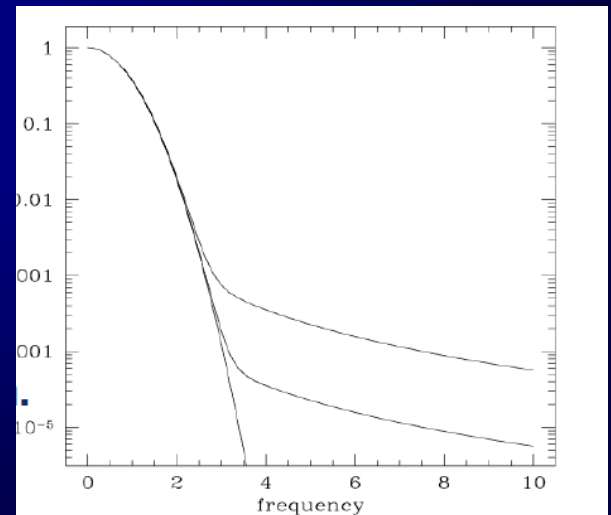
Convolution of Lorentzian (natural/collisional) and Doppler (thermal) broadening

-> Voigt profile (no analytic form)

Curves show the profile as the natural (or collisional) linewidth is increased.

Lorentz profile falls off slower than Doppler

-> core Gaussian, wings Lorentzian





# Spectral Line Broadening

## Collisional broadening

## Collisional (pressure) broadening

Collisions of atoms => exchange of energy  
(particularly in plasma)

=> change of energy of electrons in excited atoms

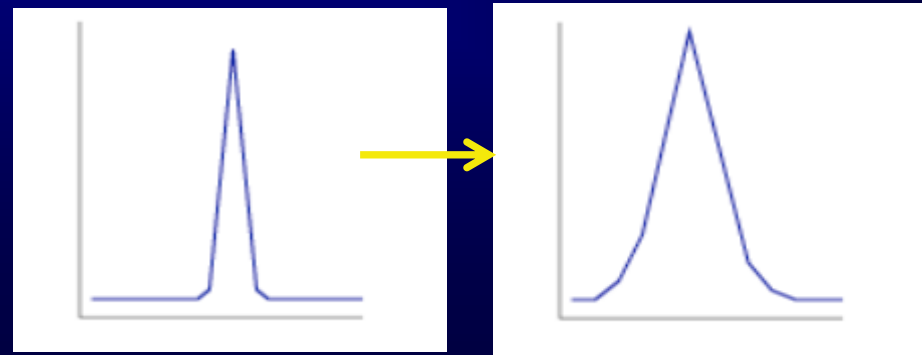
=> increase in spread of energies of emitted photons

more collisions when atoms/molecules closer, i.e.

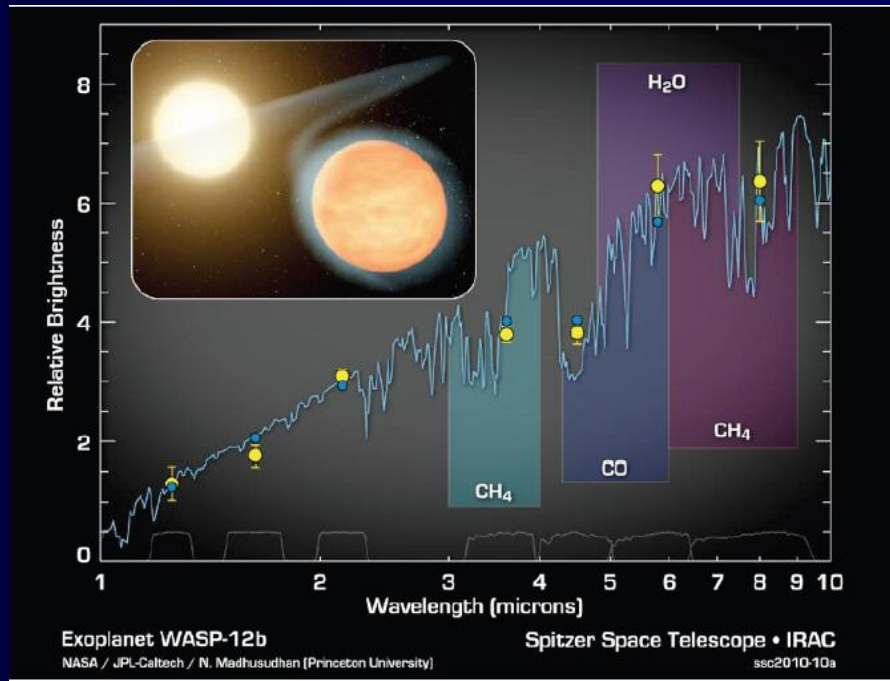
when pressure higher, collision reduce effective  
lifetime of an energy state

=> “pressure broadening”

still Lorentz, but wider  
dominate in high density  
(dwarfs)



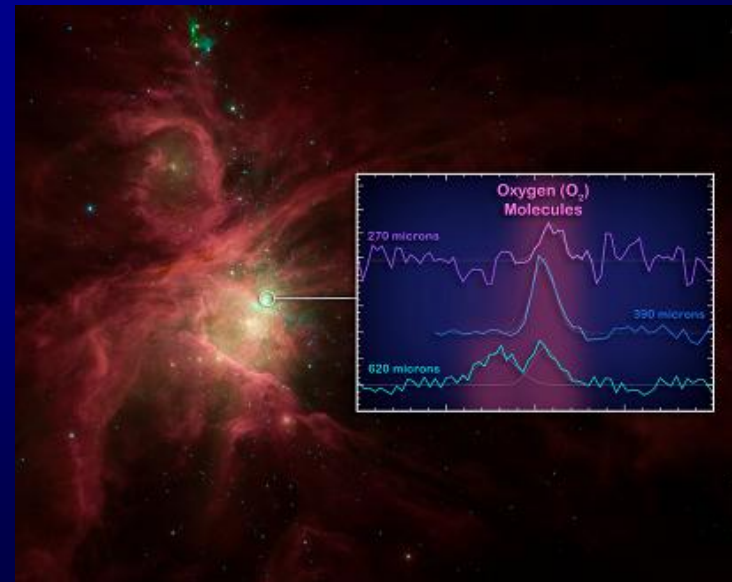
# Molecular astrophysics - fields of study



NASA Spitzer Space Telescope, molecules in the planet WASP-12b - a super-hot gas giant that orbits tightly around its star.  
CO, CH<sub>4</sub>



In Eagle Nebula, cool molecular hydrogen gas, HST



Orion nebula, O<sub>2</sub>, ESA Herschel

# Why molecules?

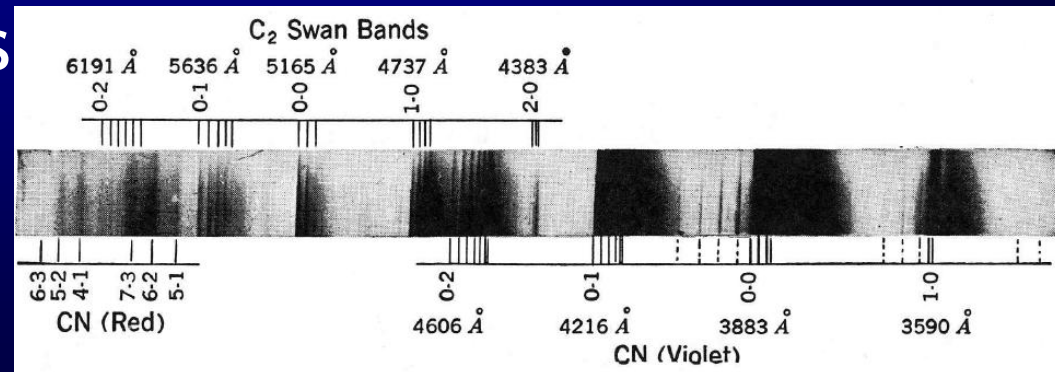
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- **Why study molecules in Astrophysics?**
  - molecules are ubiquitous
  - universe as laboratory for molecular physics
- **Why study molecules in cool stars?**
  - dominating species
  - large number of transitions
  - high temperature and pressure sensitivity
  - molecular spectra as diagnostics:
    - thermodynamic structure of cool stars
    - chemical composition
    - isotopic composition
    - stellar magnetic fields

# Molecular Spectroscopy

- In addition to the continuous and line spectra, spectra with entirely different structure: without single sharp lines but broad wavelength feature (bands): **band spectra: sources are molecules**
- Bands result from large number of blended individual molecular lines
- Molecular spectroscopy: study of the absorption, emission, and scattering of electromagnetic radiation by molecules

$C_2$  and CN  
(from Herzberg 1950)



# Molecular Spectroscopy

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Bohr postulates:

- a molecule can exist only in states of definite energies, in the stationary states; as long as the molecule is in one of these states, it does not emit or absorb light;
- light absorption or light emission is possible only as a result of a transition between two stationary states.

For the interpretation of a spectrum: establish  
the terms/energy  
levels of the stationary states

# Molecular Spectroscopy (vs. Atomic spectroscopy)

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- Much more complex because of greater complexity of internal motion in molecules
- In addition to motion of **electrons**, **vibrational** motion of the nuclei about equilibrium positions and **rotational** motion of the molecule as a whole
- Three types of energy levels and three types of spectra - electronic, vibrational, and rotational - correspond to these three types of motion
- $m_{\text{electron}}/M_{\text{nucleus}} \simeq 10^{-3}-10^{-5}$  : rates of motion of nuclei small compared to the velocities of the electrons => dynamics of nuclei and electrons largely independent

# Molecular Spectroscopy

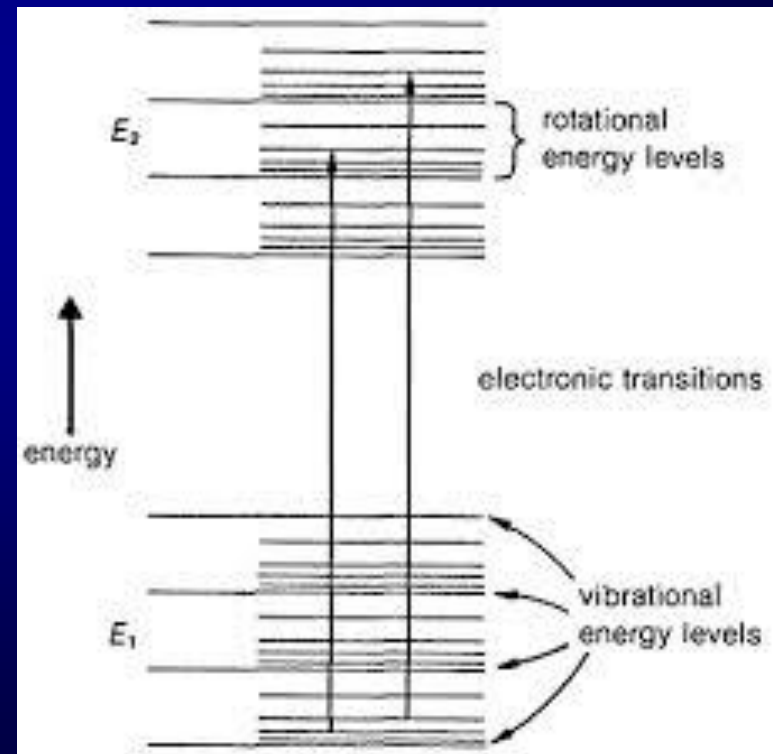
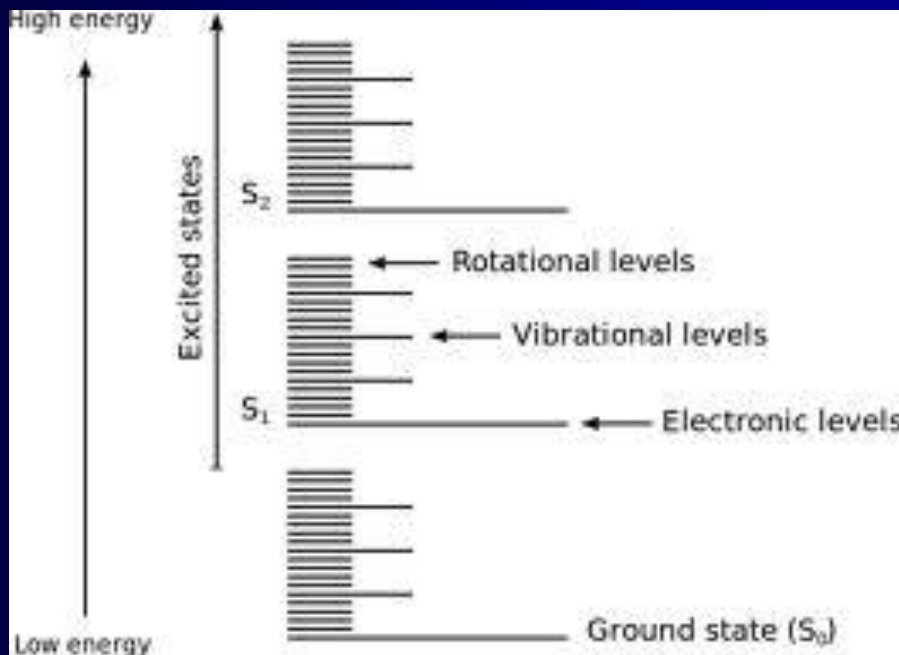
- Atoms/Molecules interact with electromagnetic-radiation to transition between energy levels
- Study transitions between energy levels
- Different transitions
  - Electronic: UV-visible
  - Vibrational: IR
  - Rotational: microwave





# Molecular Spectroscopy

- Depending on which radiation, the molecule will induce a transition corresponding to the wavelength of the radiation





# Molecular Spectroscopy (diatomic molecules)

- Total energy of molecule (without spin and magnetic interactions):

$$E = E_e + E_v + E_r + \Delta E_{ev} + \Delta E_{er} + \Delta E_{vr}$$

$E_e$ : electronic energy,

$E_v$ : vibrational energy,

$E_r$ : rotational energy,

$\Delta E_{ev}$ : electronic-vibrational interaction,

$\Delta E_{er}$ : electronic-rotational interaction,

$\Delta E_{vr}$ : vibrational-rotational interaction.

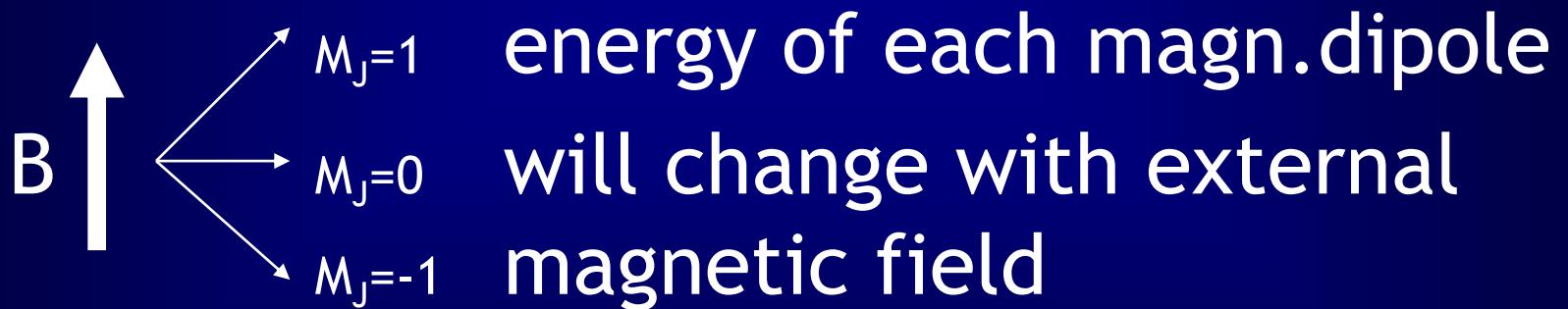
$$E_e \gg E_v \gg E_r.$$

=> changes in electronic configuration around nuclei give rise to the band systems

- the bands within the band systems come from transitions between different vibrational states of the nuclei
- the transitions between the different rotational states give rise to the lines within the bands.

# Magnetic Fields and Molecular Spectra

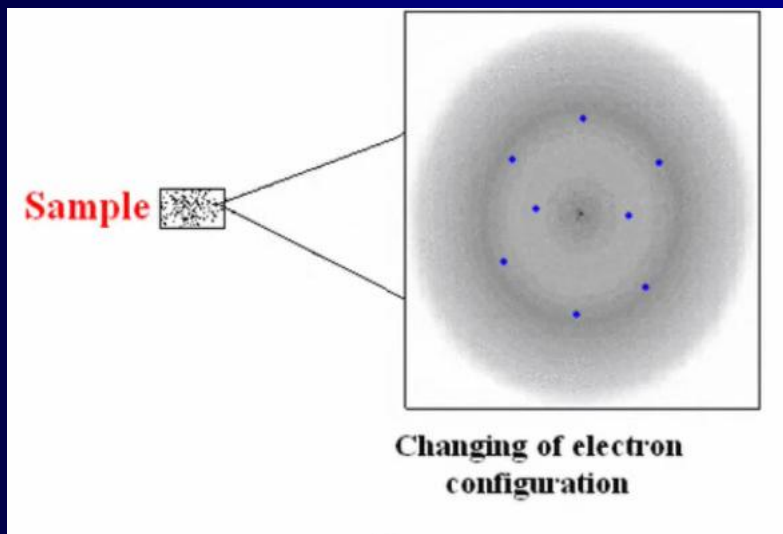
- Spinning electrons induce magnetic fields
- Magnetic dipoles
- Magnetic dipoles interact with external magnetic field to split electronic energy levels that are normally degenerate



**Zeeman effect: splitting of energy levels in presence of magnetic field**

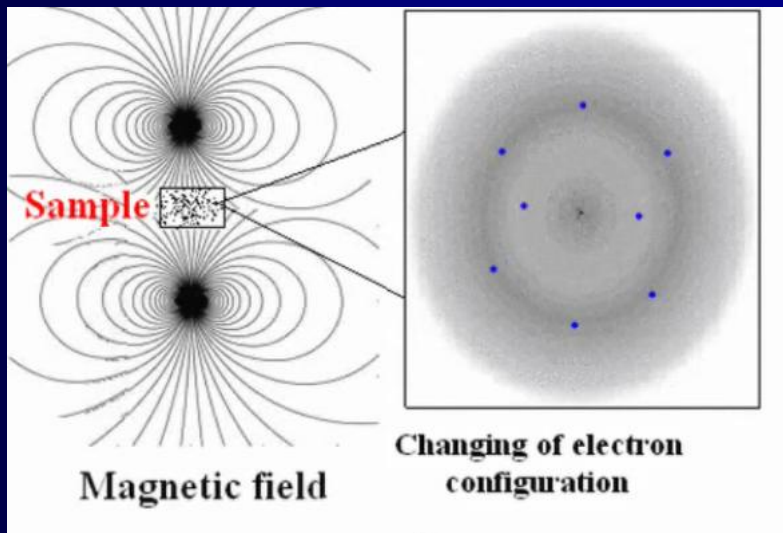
# Zeeman Effect in Molecular Spectra

- Change of electron configuration in presence of magnetic field:



# Zeeman Effect in Molecular Spectra

- Change of electron configuration in presence of magnetic field:



# Zeeman Diagnostics

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Direct magnetic field measurement with Zeeman effect:

- Observation of magnetically induced splitting (change of shape of spectral line)
- Measurement of polarization important for measuring solar magnetic fields

# Magnetic Fields

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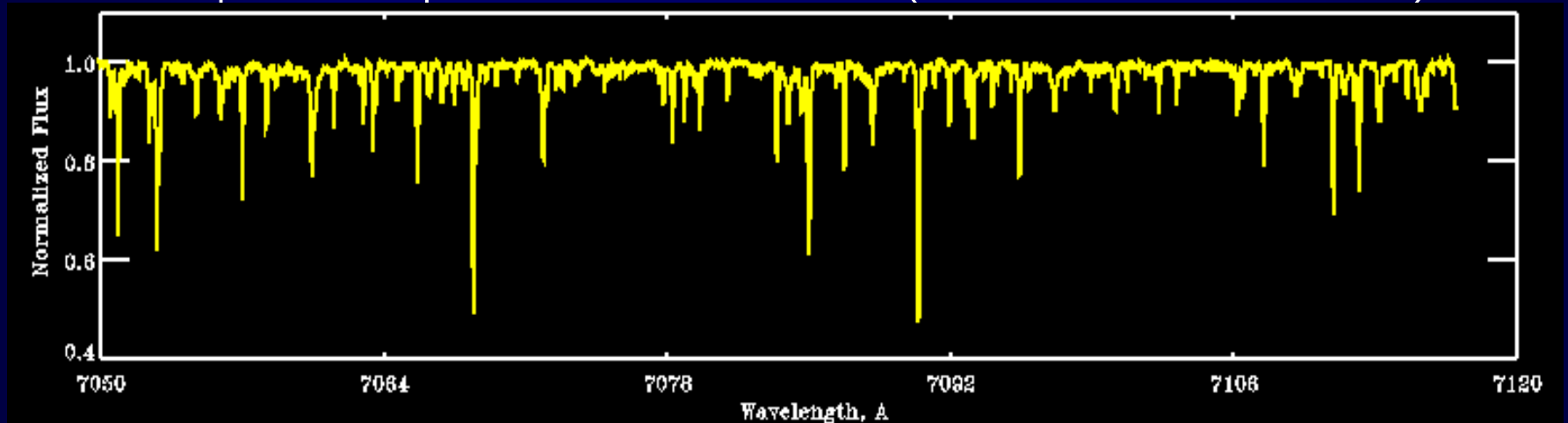
- Importance of magnetic fields
  - Solar magnetic field: variety of magnetic phenomena, laboratory, dynamo theories, Sun as star, source of activity, evolution
  - M-dwarfs: transition from stars with an outer convection zone to fully convective stars, where solar type dynamo is replaced by alternative mechanism to amplify magnetic fields
  - Exoplanets: magnetospheres as protective shields -> habitability



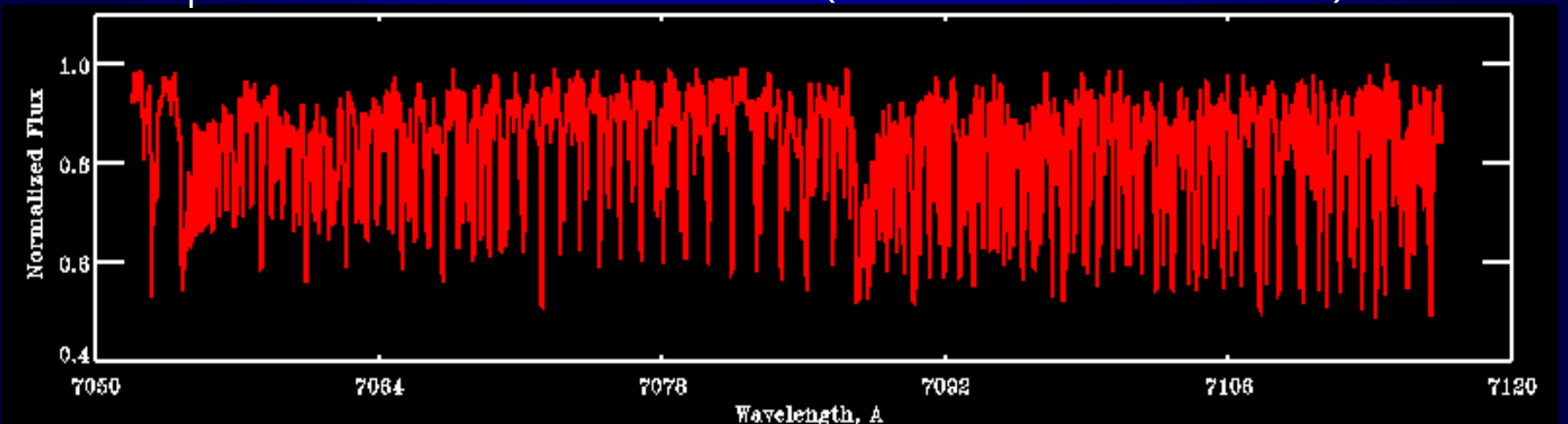


# Molecules in Sunspots

- Solar photosphere = G stars ( $5000\text{K} < T < 6000\text{K}$ )



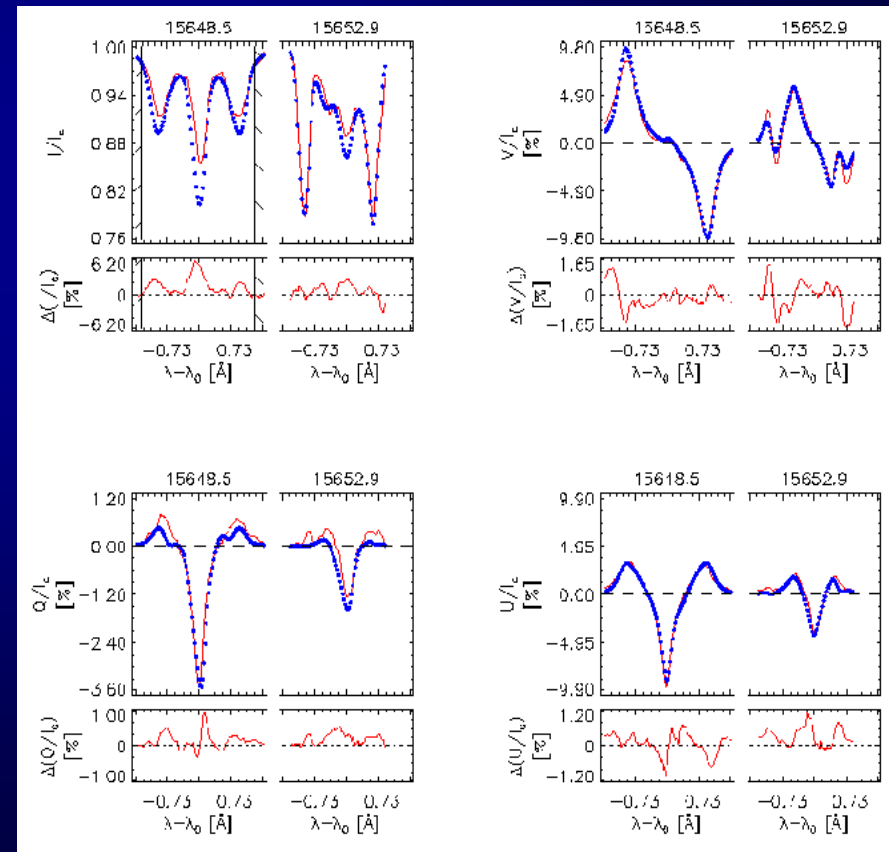
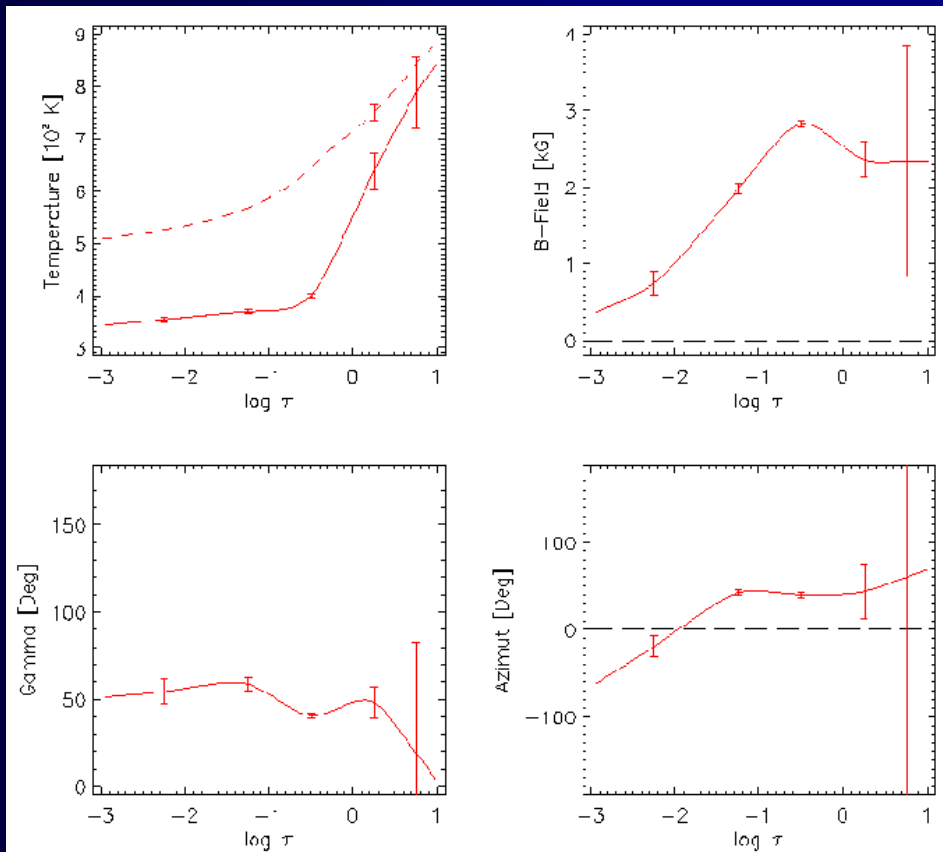
- Sunspot umbra = M stars ( $2000\text{K} < T < 4000\text{K}$ )





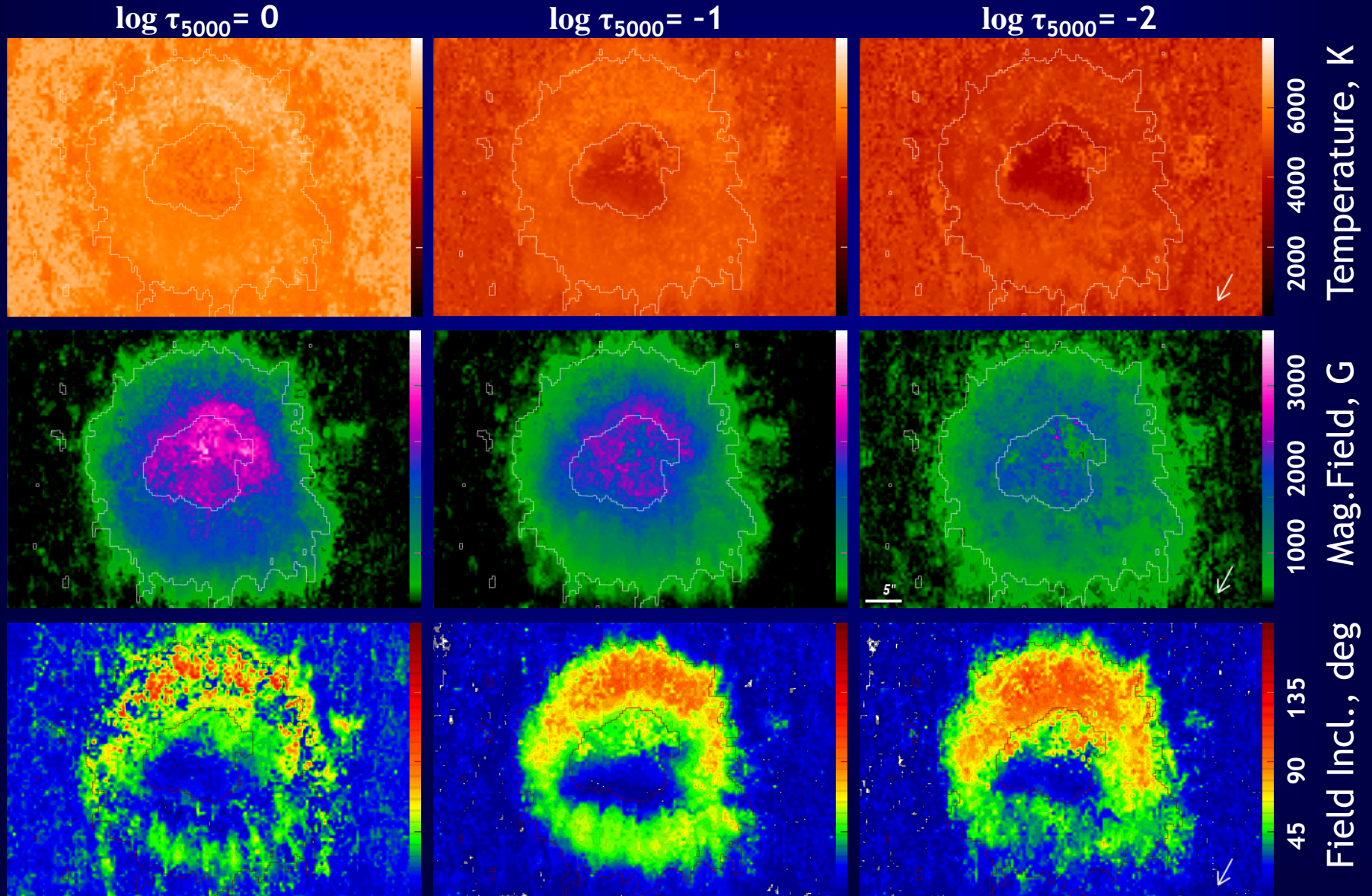
# Interiors of Sunspots - Inversions

- The nonmagnetic component becomes as hot as the photosphere
- The field strength of the magnetic component drops towards higher layers
- The field direction corresponds well to the observed position of the sunspot on the solar disk



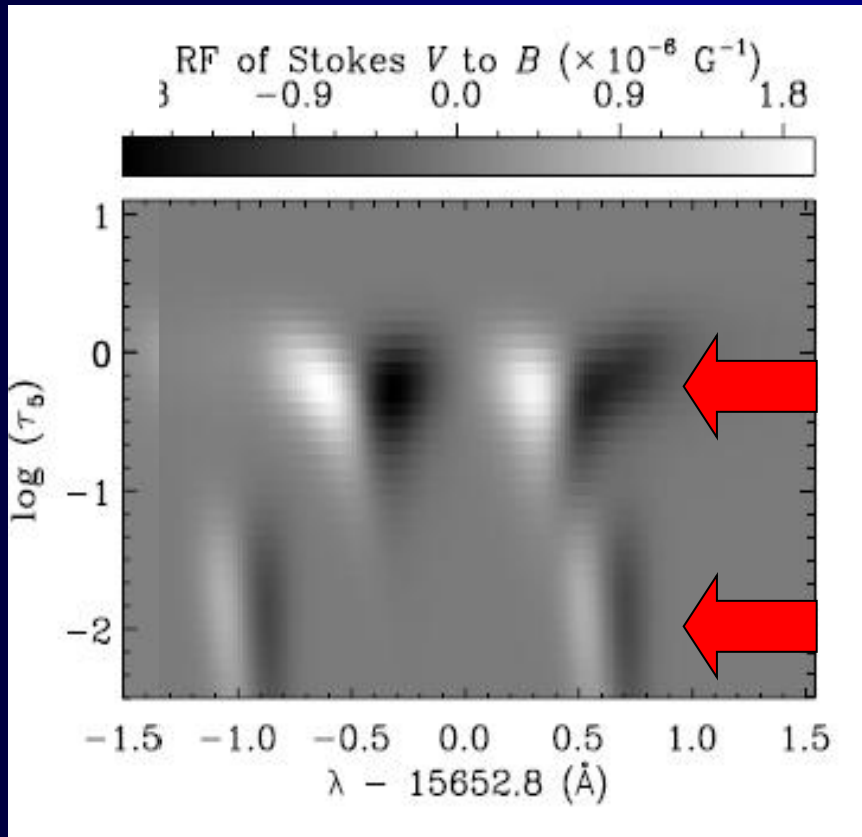
# Interiors of Sunspots

(Mathew et al. 2002)

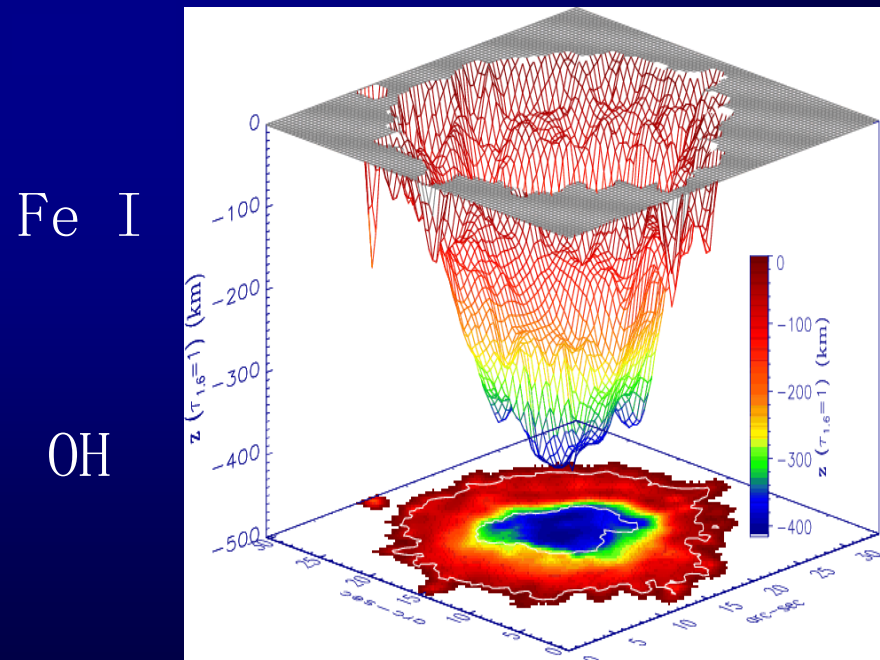


# Sunspots - 3D structure

- Simultaneous inversion of atomic and molecular lines

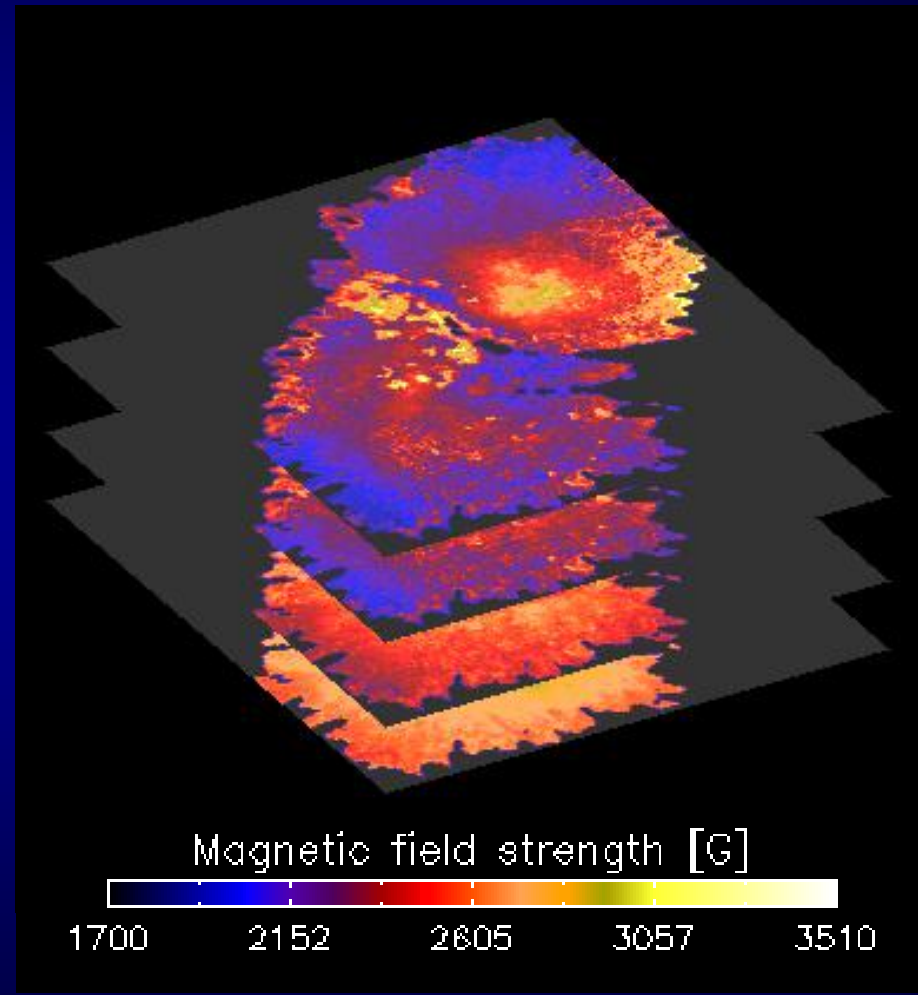
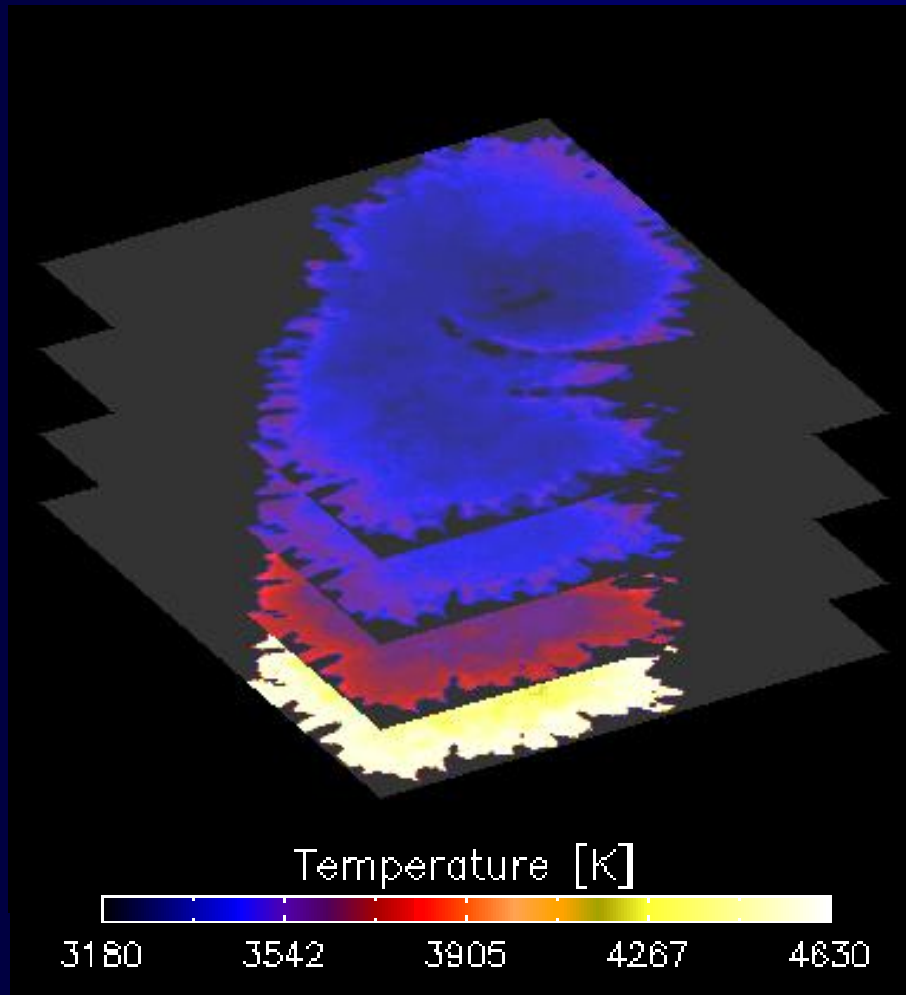


*Mathew et al. (2003)*



*Mathew et al. (2004)*

# Sunspots - 3D structure



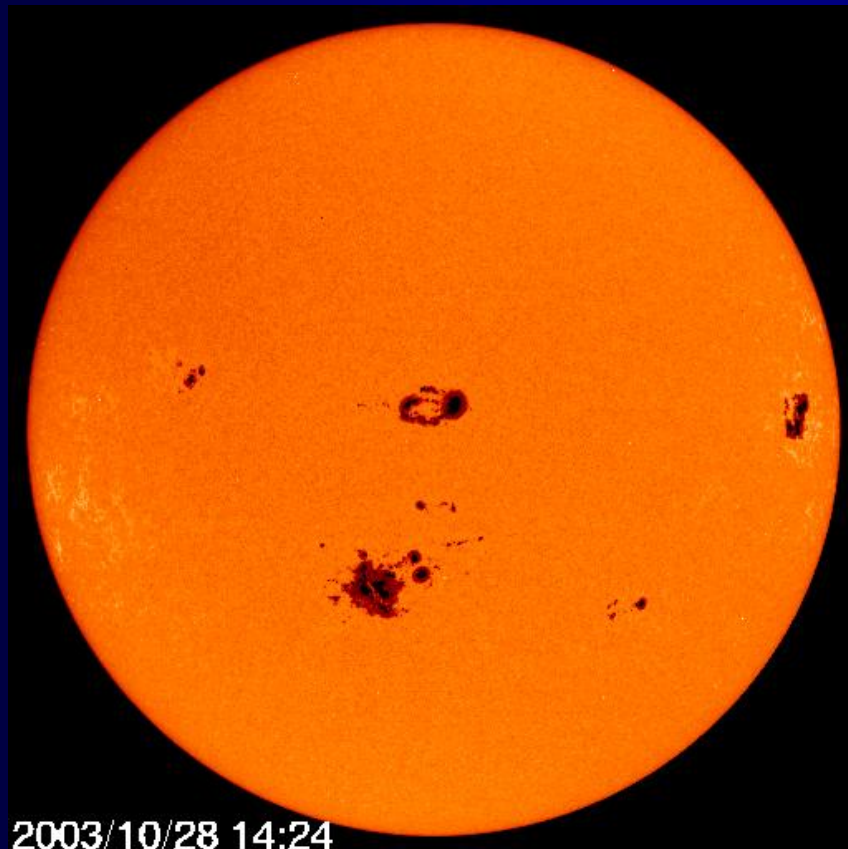
$\log \tau = 0, -1, -2, -3$

*Berdyugina et al. (in prep)*



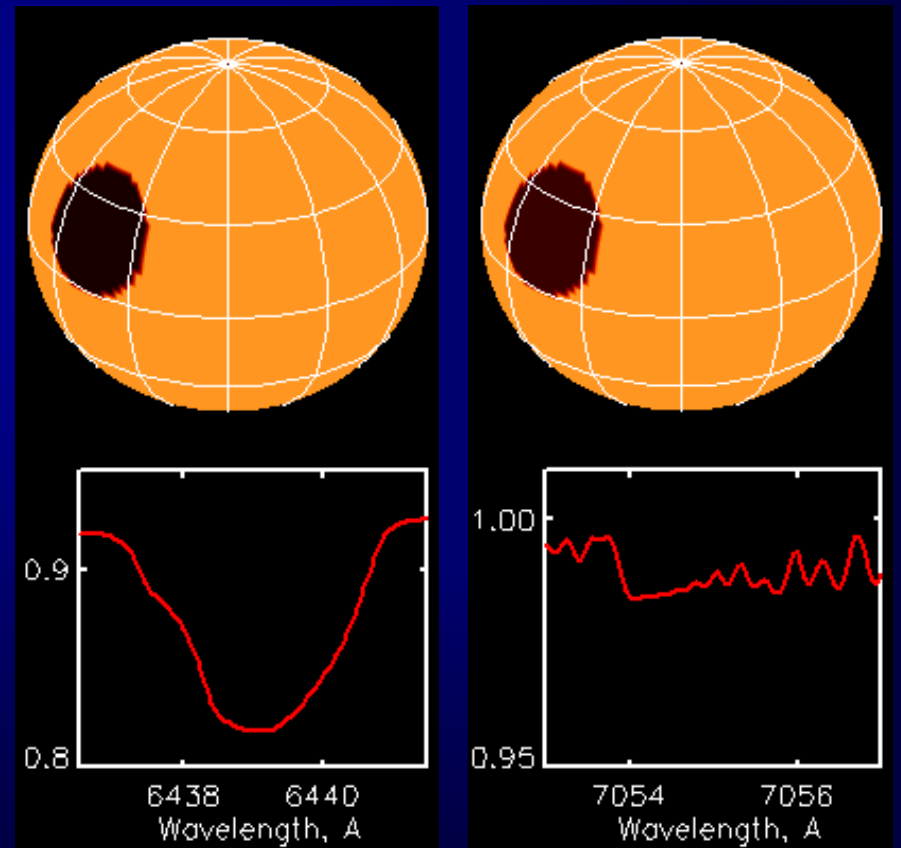
# Starspots

- Direct Imaging

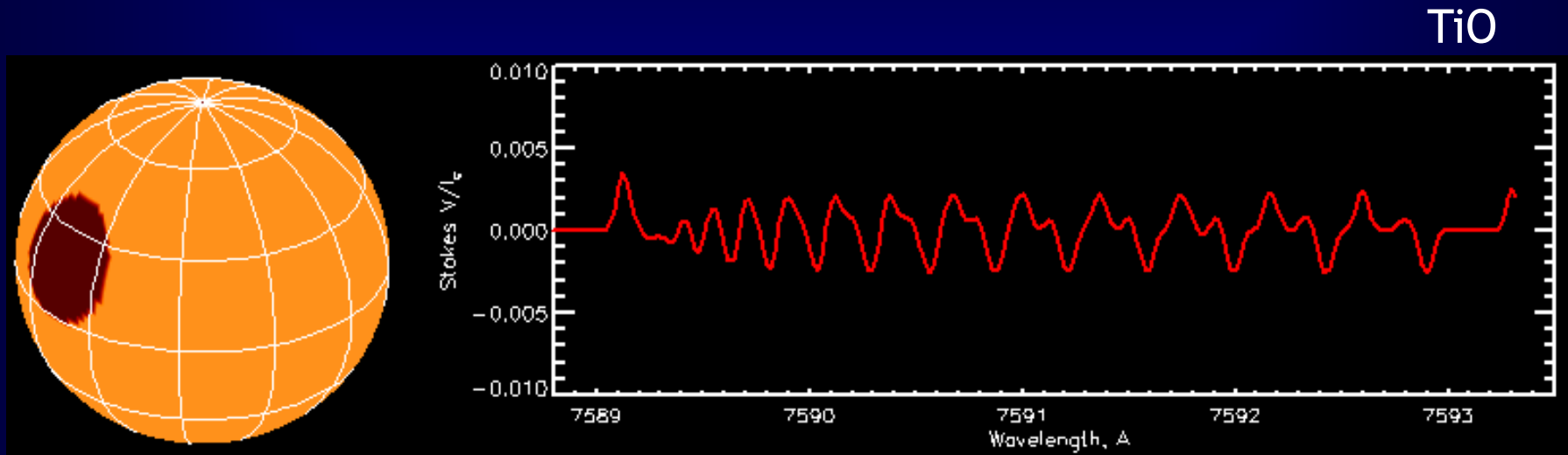


SOHO/MD

- Doppler Imaging



# Molecular Polarization in Starspots

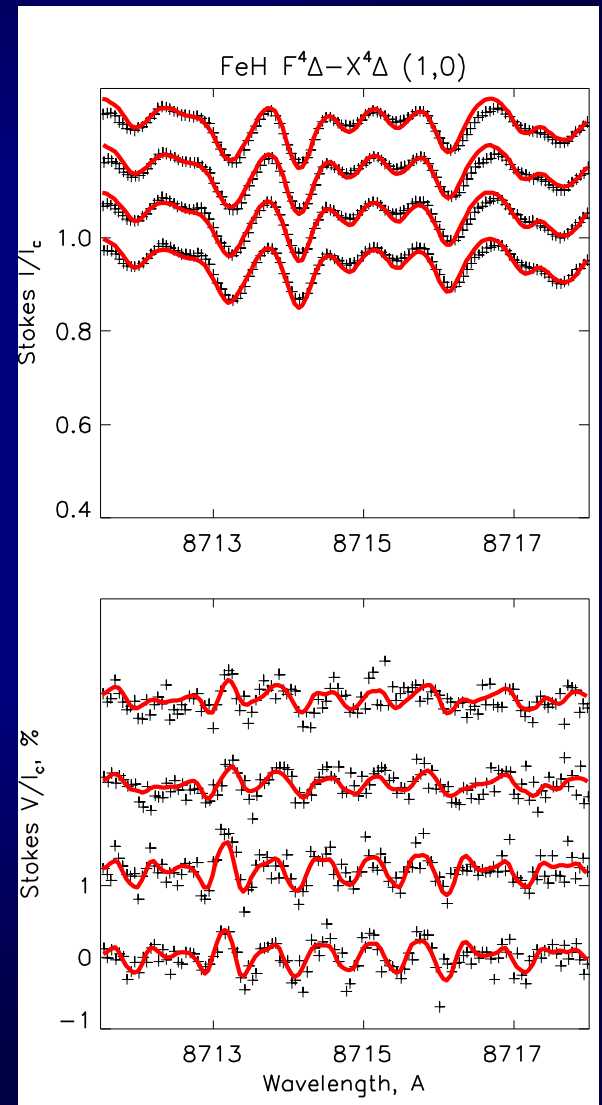
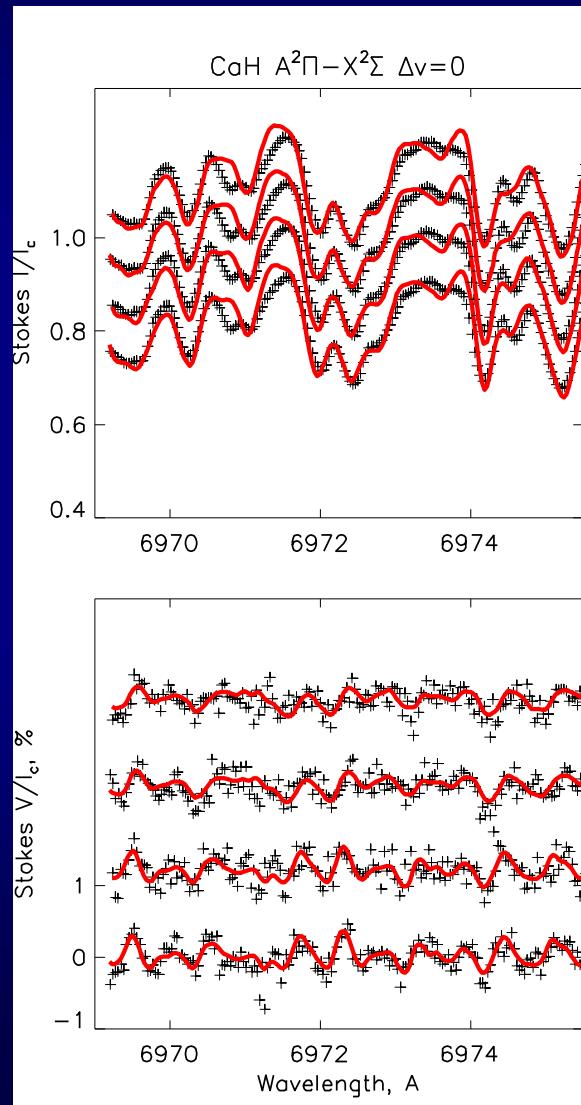
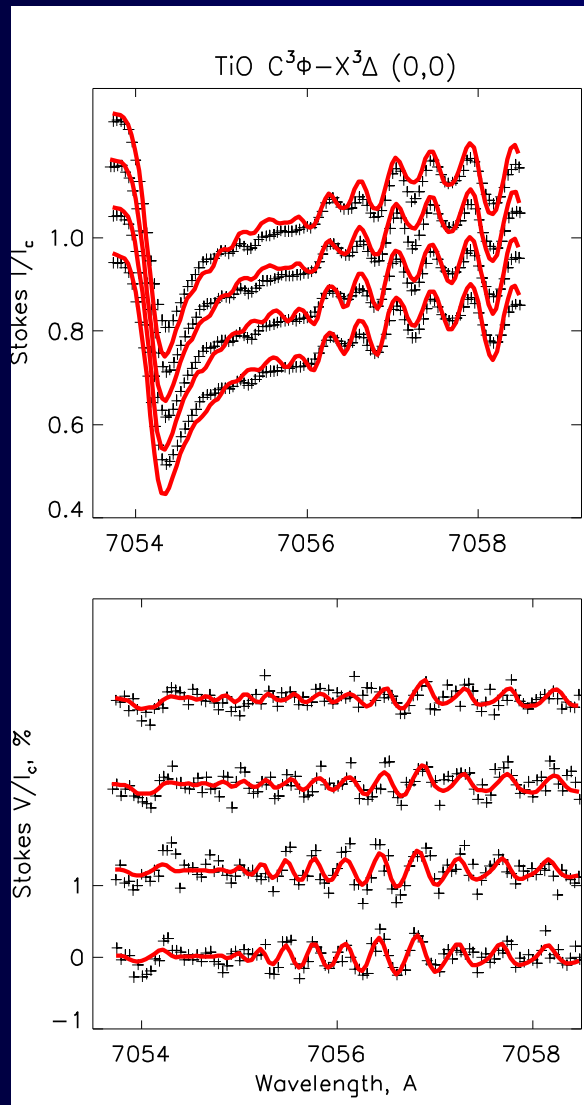


## Observations:

- 2005-2007, CFHT, ESPaDOnS
- Noise in  $V/I_c \sim 10^{-3}$ ,  $R \sim 67' \ 000$
- $\text{Max}(V/I_c) \sim 1\%$
- First detections: TiO, CaH, FeH, MgH

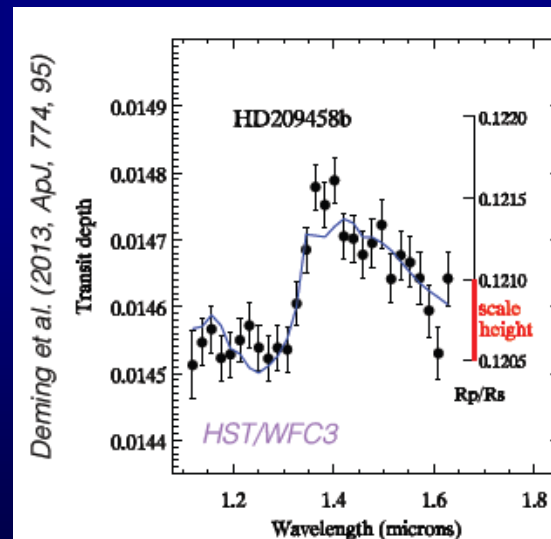
*Berdyugina et al. (2006,2008)*

# Starspots - Molecular Lines



# Exoplanet spectra

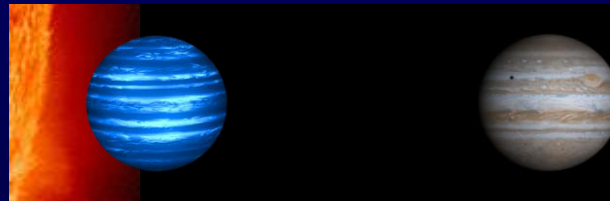
- Search for bio-signatures in exoplanetary spectra
- Water features (HD209458b)
- Cloudy atmospheres





# Molecules as probes of exoplanet atmospheres

- Clouds important in exoplanetary atmosphere (main opacity source)
- Formation and evolution of clouds not understood
- => Modeling of cloudy atmosphere in Hot Jupiters and Brown Dwarfs
- Hot Jupiters: exoplanet similar to Jupiter, higher surface temperatures (closer orbit)



- Brown dwarf: form similar to star, but not massive enough for Hydrogen fusion

# Method

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- model molecular (reflectance) spectra ( $\text{H}_2\text{O}$ ,  $\text{TiO}$ ,  $\text{FeH}$ ) with/out clouds
- vary cloud parameters (dust density, dust size, cloud position, cloud extension)
- study changes in molecular signal due to cloud parameter change, as molecules are formed at different depths => info about cloud

# Literature

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- **Tennyson** ,Astronomical Spectroscopy‘
- **Herzberg** ,Molecular Spectra and Molecular Structure: Spectra of Diatomic Molecules‘
- **Haken/Wolf** ,Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory‘
- **Khristenko** ,Molecules and their Spectroscopic Properties‘