

# Lecture 19. The H<sub>2</sub> and CO Molecules

1. Introduction
2. The H<sub>2</sub> Molecule
3. The CO Molecule
4. Summary

## References

Stahler & Palla , “The Formation of Stars”, Secs. 5.2-3  
Shull & Beckwith, ARAA 20 163 1982  
Shaw et al. ApJ, 624, 2005 (CLOUDY)

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## 1. Introduction

- The CNM HI is located in a thin disk.
- Young stars are found within an even thinner disk.
- The study of the dense ISM also reveals that:

**Molecular clouds found within the thin disk are closely associated with recent star formation**

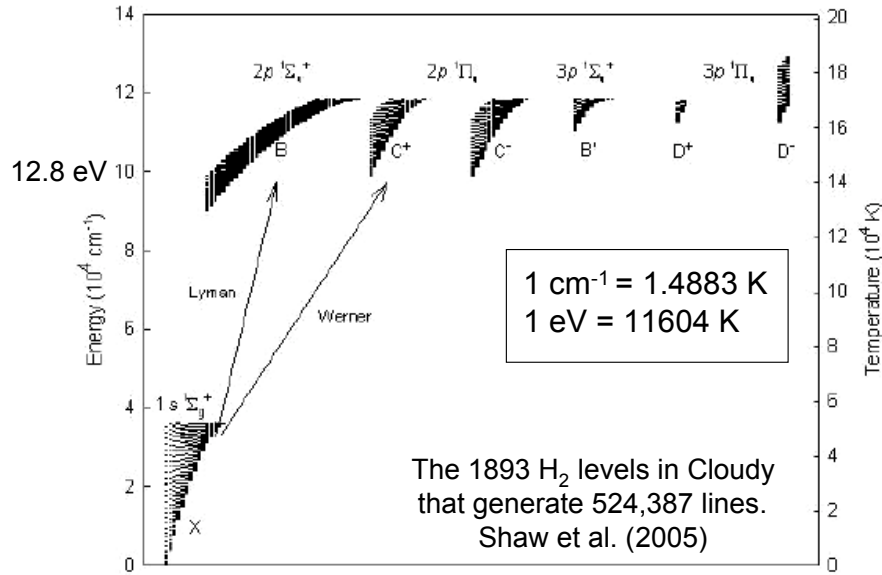
- H<sub>2</sub> and CO Molecules are the two most abundant of the 150 known interstellar molecules.
- They have played important roles in establishing the facts about recent star formation in the Milky Way.
- An additional reason for detailed discussion of H<sub>2</sub> and CO is that they are relatively simple and provide an entry to the complexities of molecular spectroscopy.

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## 2. The H<sub>2</sub> Molecule

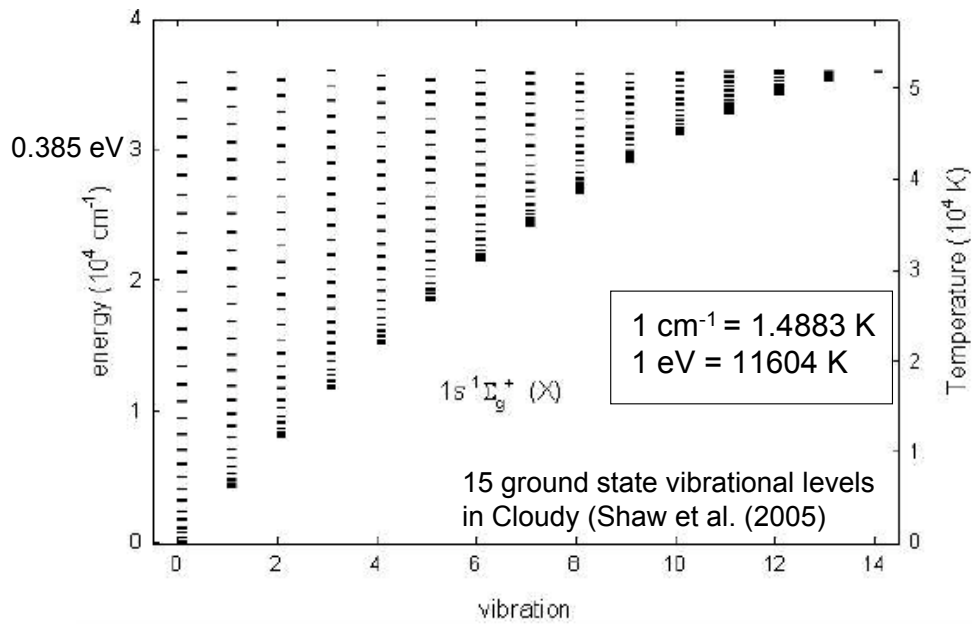
### a. Electronic Transitions



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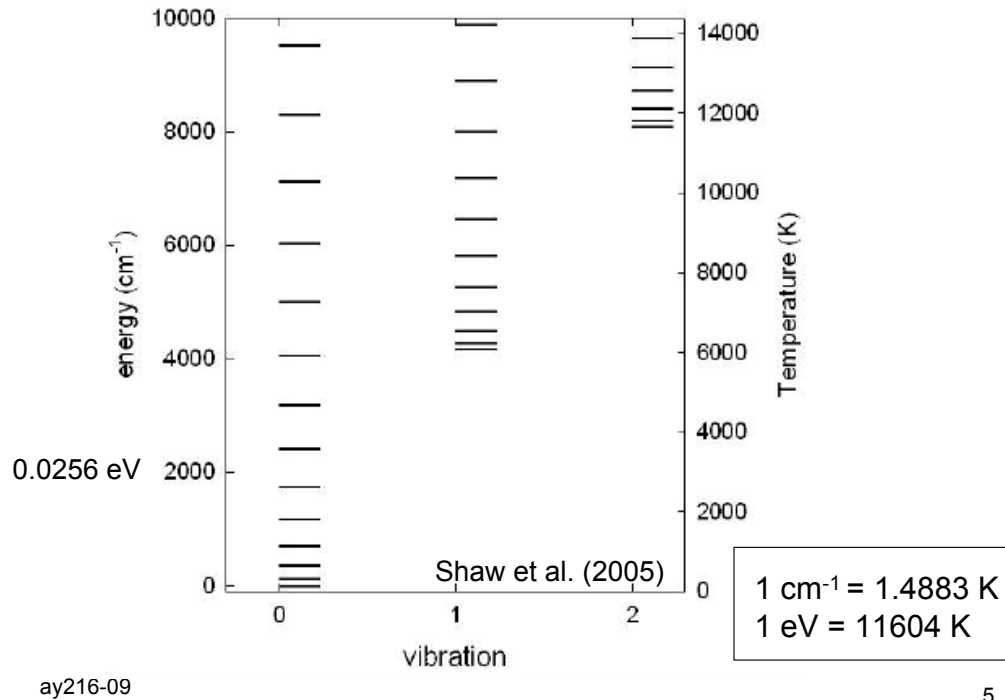
### b. Ground Vibrational Transitions



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### c. Rotational Levels for $v = 1, 2, 3$ (Cloudy)



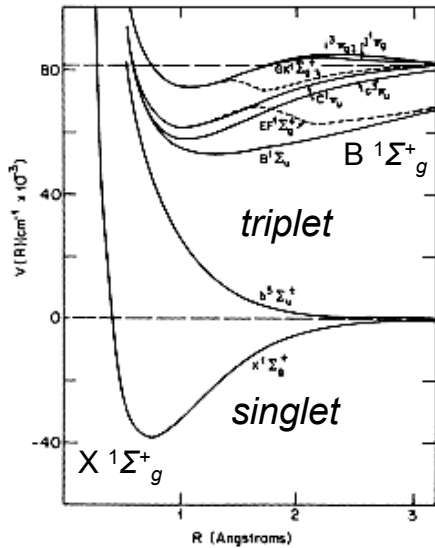
### d. Symmetry Considerations Electron Spin Exchange

The two electrons have total spin  $S = 0$  or  $1$ , which are anti-symmetric and symmetric under exchange. The Exclusion Principle requires the corresponding spatial wave functions to have the opposite symmetry.

There are two basic types of potential curves, **singlet** and **triplet**. They asymptote to two ground state H atoms, one attractive and one repulsive (next slide)

The triplet state has the higher kinetic energy and less (attractive) Coulomb energy because of its odd spatial wave function.

## Potential Energy Curves for H<sub>2</sub>



*potential energy curves that asymptote to two ground state H atoms at zero energy*

X, B, C etc. are binding curves and electron levels

Shull & Beckwith, ARAA 20 163 1982

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### e. Symmetry Considerations: Proton Exchange

The protons can have spin  $I = 0$  or  $1$ , which are anti-symmetric and symmetric under exchange. The Exclusion Principle requires overall anti-symmetry on exchange. This primarily affects the pure rotational states: For a homonuclear diatomic molecule, the rotational wave function is a familiar spherical harmonic  $Y_{JM}(\theta, \phi)$ .

On exchange, it goes into  $(-1)^J Y_{JM}$ .

**Even  $J$  states go with  $I = 0$  ("para" H<sub>2</sub>) states and odd  $J$  states with  $I = 1$  ("ortho" H<sub>2</sub>).**

**para H<sub>2</sub>  $I = 0$**   
 $J=4$  ----- 1707 K

**ortho H<sub>2</sub>  $I = 1$**

$J=3$  ----- 1024

$J=2$  ----- 512 K

$J=1$  ----- 171 K

$J=0$  ----- 0 K

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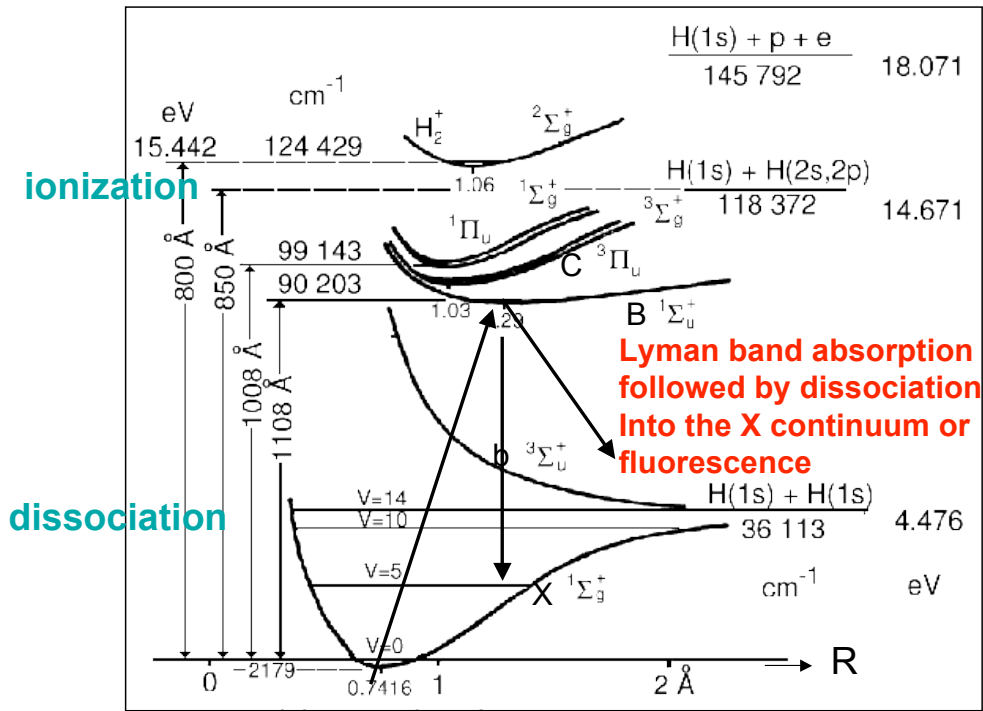
## e. Electronic States and Transitions

- With quantum numbers,  $S = 0$ ,  $l = 0$ ,  $\Lambda = 0$ ,  $J = 0$ , the ground state is  $X \ ^1\Sigma_g^+$ . It has 36 excited vibrational levels, each with an infinite number of rotational states.
- The next two singlet levels are  $B \ ^1\Sigma_g^+$  and  $C \ ^1\Pi_u$ . Their potential curves asymptote to separated  $1s$  and  $2s,p$  atomic H atoms.
- Levels B & C are connected to ground by allowed electric-dipole transitions (analogs of HI Ly- $\alpha$ ). These **Lyman and Werner bands** start at  $1108 \text{ \AA}$  and  $1040 \text{ \AA}$ ; they are spread more or less uniformly across the FUV band from the HI Lyman edge at  $911.7 \text{ \AA}$  to the threshold at  $1108 \text{ \AA}$ .
- Typical oscillator strengths are  $\sim 10^{-2}$ .
- The Lyman and Werner bands were detected in a rocket experiment by Carruthers (1970) and then extensively observed by the UV satellites *Copernicus* and FUSE.

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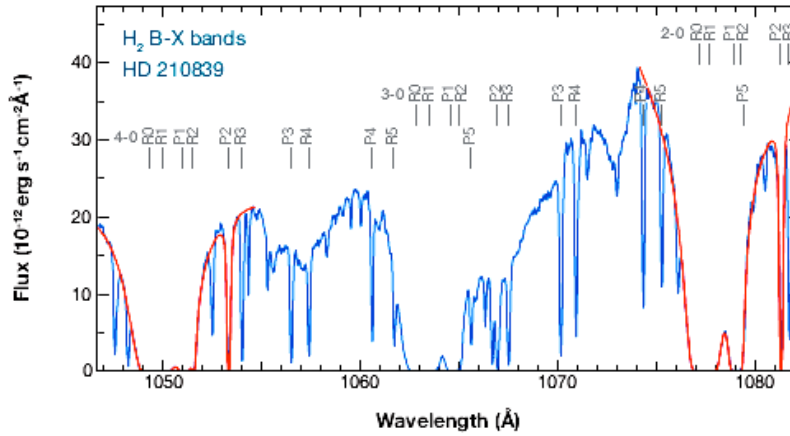
### Electronic Level Diagram for $H_2$



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## f. Observations of the Lyman Band Lines



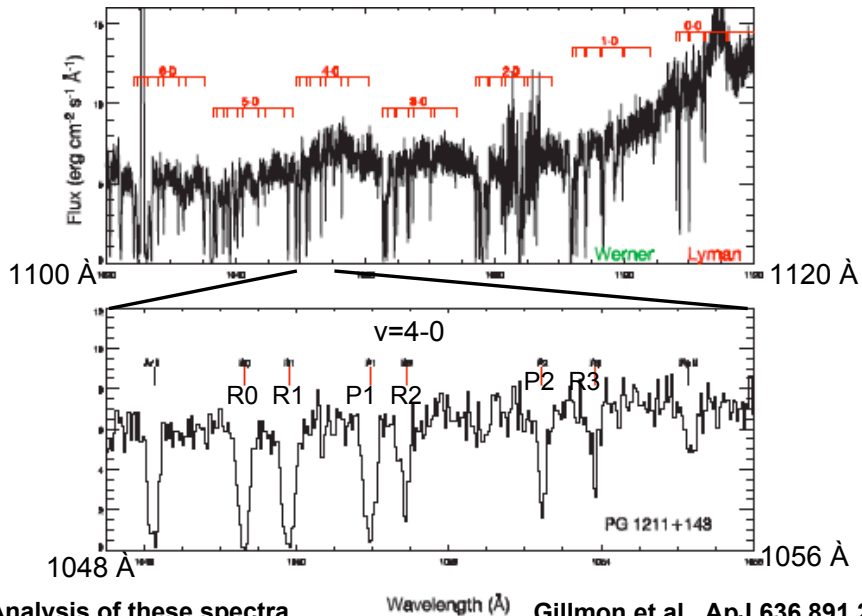
FUSE spectrum of a bright star with interstellar absorption by the Lyman band of H<sub>2</sub>. The red curve is a fit by Rachford, ApJ 577 221 2002. The objective is to determine the thickness of the interstellar cloud from the depth of the absorption

$$d\tau_\nu = f_{jk} \frac{\pi e^2}{m_e c^2} \phi(\nu - \nu_{jk}) dN_j$$

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## Lyman Band Absorption Towards an AGN



Analysis of these spectra yields H<sub>2</sub> column densities and excitation temperatures.

Wavelength (Å)

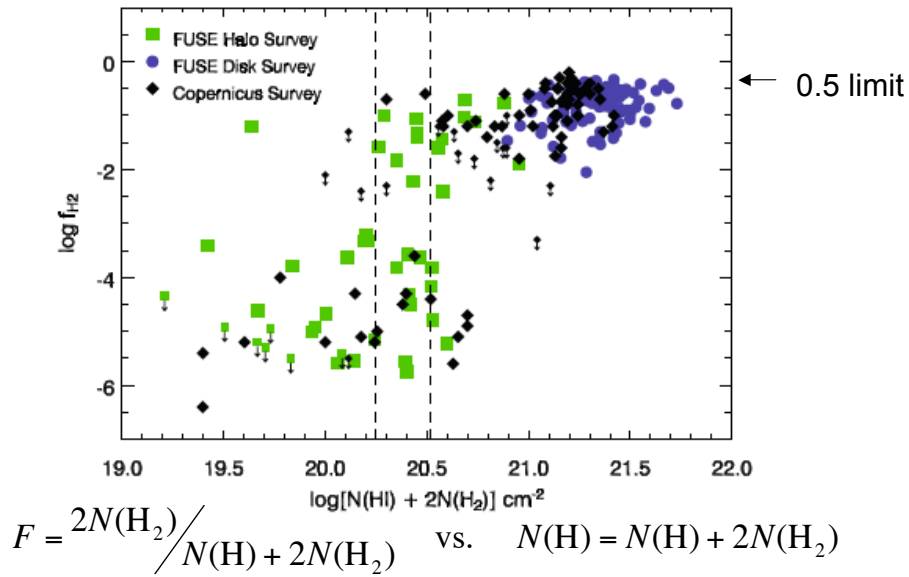
Gillmon et al., ApJ 636 891 2006  
 "A FUSE Survey of Interstellar H<sub>2</sub> towards high-latitude AGNs"

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# FUSE and Copernicus Survey Results

Gillmon et al (2006)



The 1/2 transition position occurs near  $N_{\text{H}} = 2.4 \times 10^{20} \text{ cm}^{-2}$

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## Ly $\alpha$ Pumped Fluorescence of H<sub>2</sub>

Ly $\alpha$  is often a strong line covering several Å. It can overlap many Lyman band H<sub>2</sub> lines. The fluorescence is sensitive to  $T$  and the abundance of H<sub>2</sub>. It can be used as a thermometer.

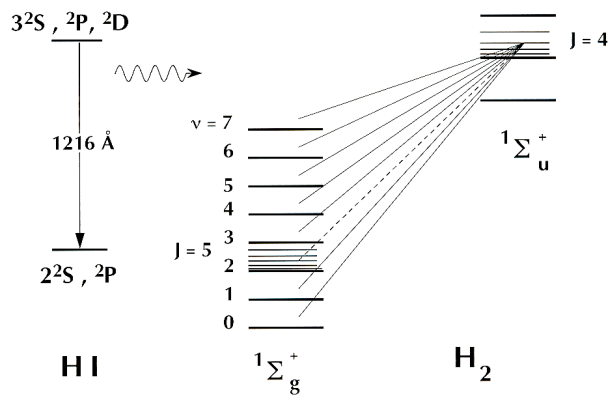


Fig. 4.10. Fluorescence of H<sub>2</sub> with Ly $\alpha$ . In order for this process to occur, the molecular hydrogen has to be both vibrationally and rotationally excited, which requires a temperature above about 1000 K

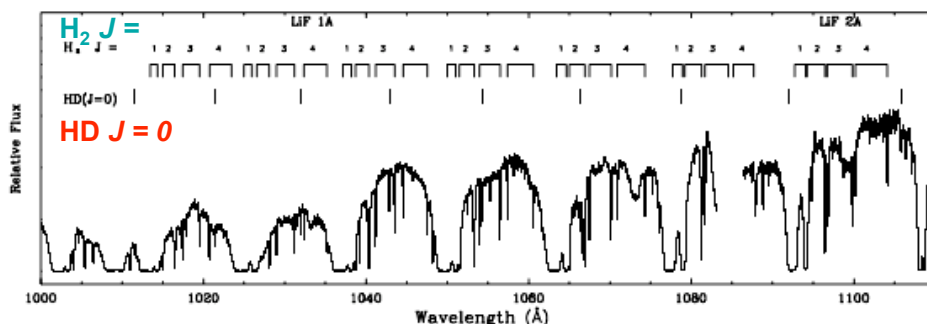
First observed in sunspot spectra by Jordan (1977), analyzed theoretically by Shull (1978) and observed in the nearby T Tauri star TW Hya (Herczeg et al. 2002).

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# FUSE Observations of HD

Lacour et al. A&A 430 967 2005



Fuse FUV absorption line spectrum of a nearby translucent cloud HD 110432 with saturated Lyman band lines [E(B-V)=0.4]. Typical derived HD abundances are  $\sim 3 \times 10^{-6}$ . Since the abundance of deuterium in the ISM is a factor of 5 or more larger, D is incompletely transformed into molecules, probably due to photodissociation. Normal hydrogen is only 55% converted into H<sub>2</sub> in this cloud.

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## g. Near Infrared Transitions

- The ground vibrational constant is  $\omega \sim 4400 \text{ cm}^{-1}$  (6330 K); ro-vib transitions occur in the NIR near 2.2  $\mu\text{m}$ .
- They are observed in warm regions, where they are collisionally excited, and in regions near a FUV source as part of the fluorescence spectrum following absorption in a Lyman or Werner band transition.
- Neutral gas near a star-forming region is a good example.

Because H<sub>2</sub> has no dipole moment, these are **weak quadrupole transitions**; a favorite is the 1-0 S(1) line at 2.12  $\mu\text{m}$ , corresponding to  $v'=1, J'=3 \rightarrow v''=0, J''=1$ .

	O	P	Q	R	S
$J' =$	$J''-2$	$J''-1$	$J''$	$J''+1$	$J''+2$

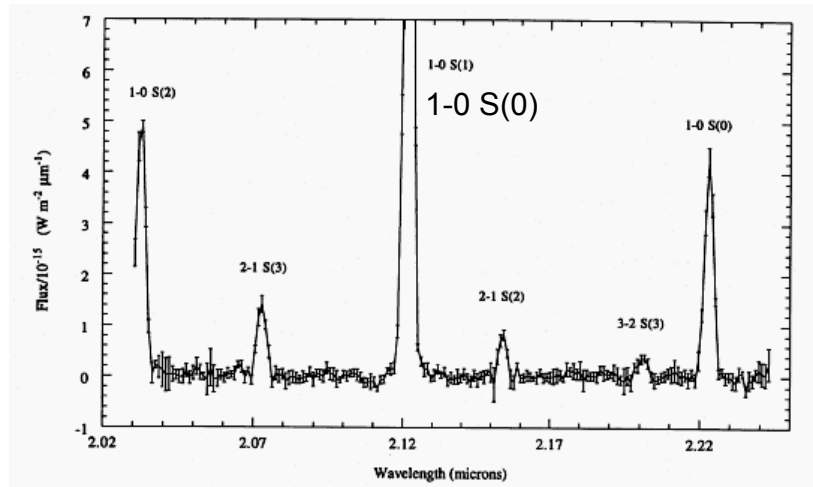
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# NIR H<sub>2</sub> Ro-Vib Lines in a Herbig-Haro Object

Fernandes & Brand, MNRAS 274 639 1995



This spectrum of HH-7 was taken with the slit pointing towards the source of the outflow from the YSO SVS13 in Perseus. HH objects occur in jets as a fast wind overtakes slower gas; they often manifest a bow-shock appearance. Fast shocks generate UV radiation and produce fluorescence after exciting H<sub>2</sub>.

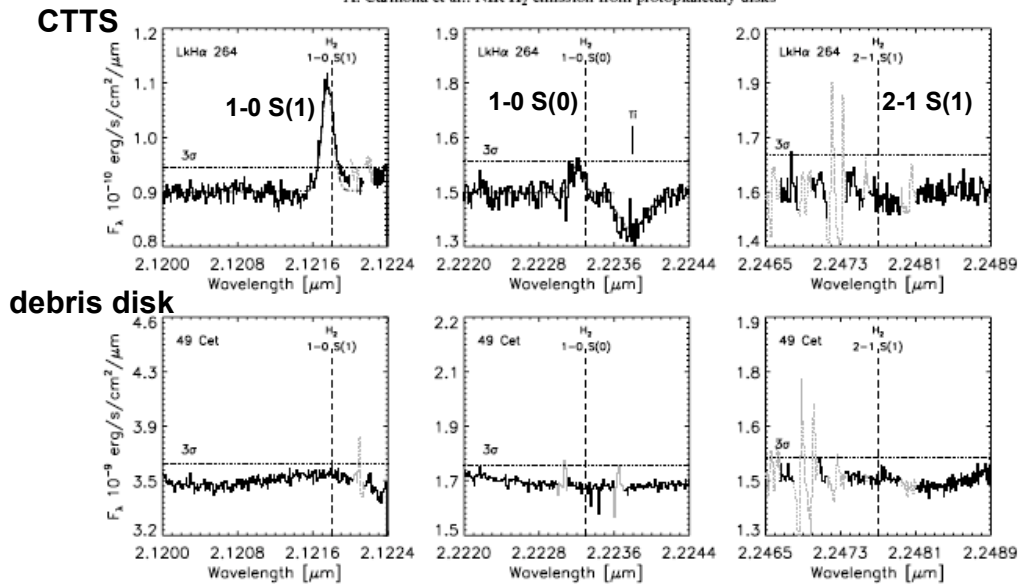
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# NIR H<sub>2</sub> Ro-vib Lines in Protoplanetary Disks

Carmona et al. A&A 476 853 2007

A. Carmona et al.: NIR H<sub>2</sub> emission from protoplanetary disks



ESO VLT adaptive optics high resolution NIR spectrograph

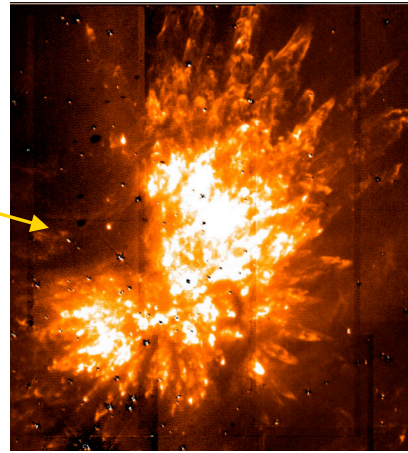
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## Subaru Images of Orion



Orion Nebula



Kleinman-Low Nebula

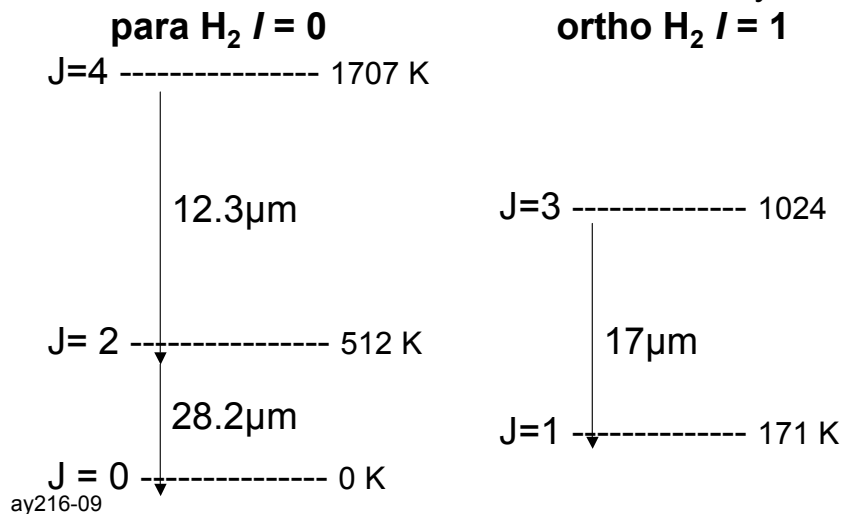
The Kleinman-Low Nebula is a region of massive star formation. The image is based on J( $1.25 \mu\text{m}$ ), K( $2.15 \mu\text{m}$ ) and H2 1-0 S(0). The rovib emission at  $2.12 \mu\text{m}$ , presumed to arise from winds shocking the surrounding gas.

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### h. Mid-Infrared Transitions

- The ground rotational constant is  $B = 60.85 \text{ cm}^{-1}$  (87.6 K).
- Pure rotational transitions occur in the MIR shortwards of  $28 \mu\text{m}$ ; they are very weak quadrupole transitions.
- Observed in lukewarm regions ( $T > 300 \text{ K}$ ) via collisional excitation and fluorescence near UV and X-ray sources.

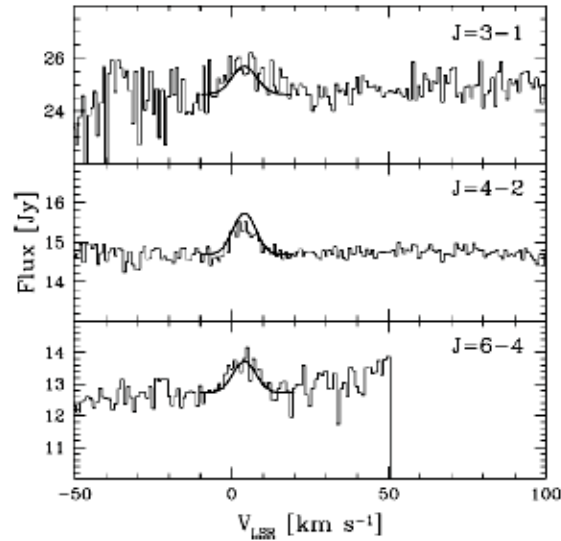


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# H<sub>2</sub> Rotational Lines in a Herbig A Star Aur

Bitner et al. ApJ 661 L69 2007



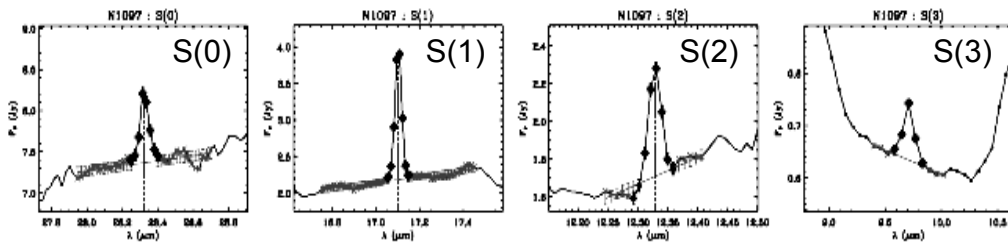
TEXES (Texas Echelon Cross Echelle Spectrograph)  
at Gemini North and NASA IRTF

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# H<sub>2</sub> Rotational Line Detections in AGN

Roussel et al. ApJ 669 959 2007



OBSERVED H<sub>2</sub> LINES

Transition $v = 0$	Short Notation	Rest $\lambda$ ( $\mu\text{m}$ )	Spectral Order	$E_u/k$ (K)	$A$ ( $10^{-11} \text{ s}^{-1}$ )
$J = 2-0$ .....	S(0)	28.219	LH 14	510	2.95
$J = 3-1$ .....	S(1)	17.035	SH 12	1015	47.6
$J = 4-2$ .....	S(2)	12.279	SH 17	1681	275.0
$J = 5-3$ .....	S(3)	9.665	SL 1	2503	980.0
$J = 6-4$ .....	S(4)	8.025	SL 1	3473	2640.0
$J = 7-5$ .....	S(5)	6.910	SL 2	4585	5880.0
$J = 8-6$ .....	S(6)	6.109	SL 2	5828	11400.0
$J = 9-7$ .....	S(7)	5.511	SL 2	7196	20000.0

NOTE.—The rotational upper level energies were computed from the molecular constants given by Huber & Herzberg (1979), and the transition probabilities are from Black & Dalgarno (1976).

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### 3. The CO Molecule

#### Some Advantages of CO

- It has a small but finite permanent dipole moment (0.110 Debye). Its pure rotational and rovib transitions are strong compared to H<sub>2</sub>.
  - Its long wavelength transitions occur in reasonably good parts of the mm and sub-mm spectrum bands.
  - Its large binding energy means it is widely distributed with roughly constant abundance, at least where hydrogen is mainly molecular.
- N.B.  $D(\text{CO}) = 11.09 \text{ eV}$  compared to  $D(\text{H}_2) = 4.48 \text{ eV}$
- It has useful isotopes, <sup>13</sup>CO, C<sup>17</sup>O, and C<sup>18</sup>O.

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#### a. Energy Levels and Transitions

##### Ground Level Spectroscopic Constants in cm<sup>-1</sup>

$$k = G(v) + B_v J(J + 1) - D_v [J(J + 1)]^2 + \dots$$

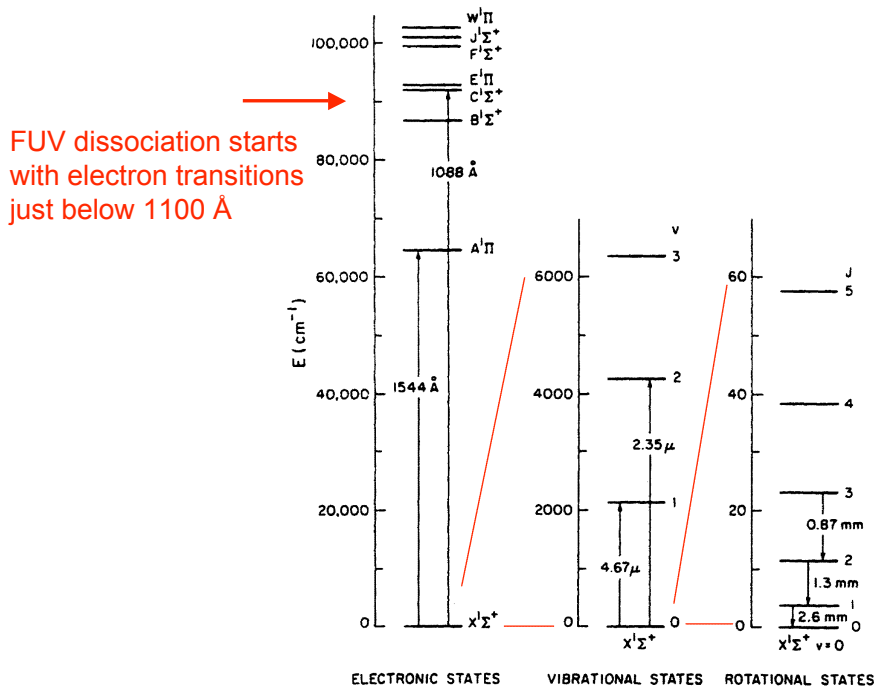
$v$	0	1	2
$B_v$	1.922529	1.905026	1.887524
$D_v \times 10^6$	6.1206	6.1203	6.120
$G(v) - G(0)$		2143.272	4260.64

In Kelvins:  $B_0 = 2.766 \text{ K}$  and  $\theta_0 = (ch/k_B) [G(1) - G(0)] = 3084 \text{ K}$ .

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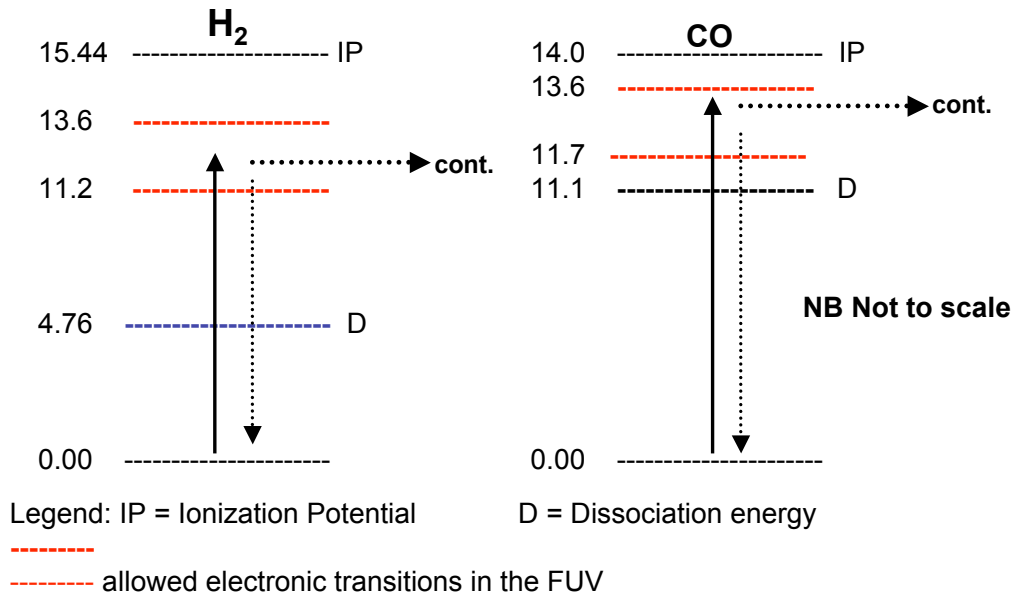
# Energy Levels of CO



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## CO and H<sub>2</sub> Dissociation Energies



**H<sub>2</sub> and CO have similar electronic transitions and dissociation pathways.**

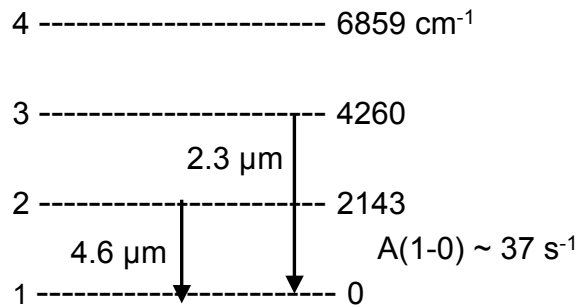
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## b. Summary of CO Diagnostic Lines

a. UV – CO is something like a heavy H<sub>2</sub>: The UV bands occur in the far UV near 1000 Å with oscillator strengths of the same order of magnitude (10<sup>-2</sup>) as for H<sub>2</sub>. They have been detected in absorption towards diffuse clouds where the CO maximum abundance is 10<sup>-5</sup>.

b. NIR  $\Delta v = 1$  transitions are the **fundamental** bands  
 $\Delta v = 2$  transitions are the **1<sup>st</sup> overtone bands**, etc

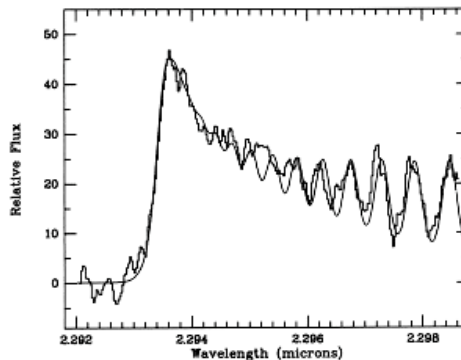


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## CO First Overtone Bandhead

Carr & Tokunaga ApJ 393 L67 1992



Bandhead of the CO  $v=2-0$  ro-vib transitions  
 observed in the YSO SVS 13 in Perseus

From Lecture 18, the bandhead arises from centrifugal stretching:  $B' < B''$ . For large enough  $J$  in the R-branch, the increasing trend of the low- $J$  rovib energy differences is reversed. The level spacing near the bandhead becomes very small, and the increased brightness makes it easy to detect CO in young stellar objects (YSOs) under the proper excitation conditions.

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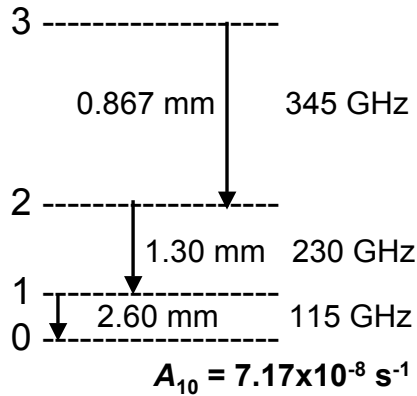
### c. Pure Rotational Bands (mm-FIR)

For the ground electronic and vibrational level and small  $J$ :

$$E_J = J(J+1)B \quad \Delta E_J = E_J - E_{J-1} = 2BJ$$

$$B = 1.922529 \text{ cm}^{-1} \quad 2B/k_B = 5.532 \text{ K}$$

CO is the ideal diagnostic and coolant for cool clouds with  $T \sim 10\text{-}100 \text{ K}$ .



CO has been detected from the ground throughout much of mm and sub-mm bands. Very dry conditions are needed at high frequencies, e.g., the Atacama desert plateau at 5525 m in N. Chile (site of ALMA). The CO 9-8 1.087 THz line was detected by Marrone et al. (2004).

$$A_{J,J-1} = 3J^4/(2J+1) A_{10}$$

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### Fundamental Rotational Frequencies of CO

CO mm Frequencies in MHz by FJ Lovas (<http://www.physics.nist.gov/PhysRefData/Micro/Html/contents.html>) rounded to 6 figures and ignoring hfs

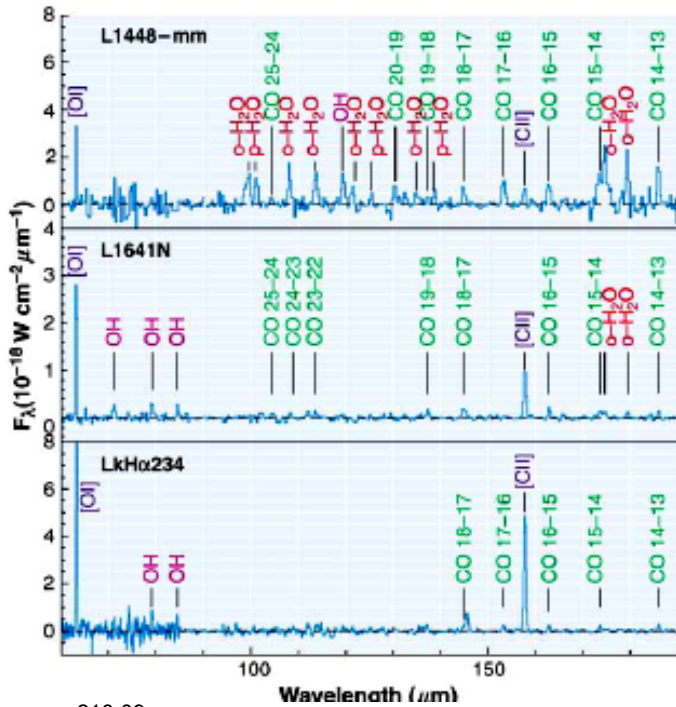
CO	115271
<sup>13</sup> CO	110201
<sup>14</sup> CO	105871
C <sup>17</sup> O	112359
C <sup>18</sup> O	109782
<sup>13</sup> C <sup>17</sup> O	107289
<sup>13</sup> C <sup>18</sup> O	104711

Rough ISM isotope ratios: <sup>12</sup>C:<sup>13</sup>C = 70:1    <sup>16</sup>O:<sup>17</sup>O:<sup>18</sup>O = 1500:500:1

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## CO, H<sub>2</sub>O, and OH FIR Lines from YSOs



ISO FIR spectra of three YSOs in a sequence of increasing age and decreasing activity.

Benedettini et al. (2003)

green - high-J CO  
red - FIR H<sub>2</sub>O & MIR OH  
black - 157  $\mu\text{m}$  CII

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## 4. Post-Summary

Having outlined the spectroscopy and applications of the two most abundant interstellar molecules, we are led to ask any additional questions, such as

1. How are interstellar molecules formed and destroyed?
2. How are they excited?
3. What role do they play in determining the physical conditions in the ISM?
4. How do the observations of H<sub>2</sub>, CO, and other molecules inform us about the evolution of interstellar clouds and the formation of stars?
5. What other molecules are important in these studies?

Some answers will be attempted in subsequent lectures.

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