Lecture 19. The H_2 and CO Molecules

1. Introduction
2. The H_2 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)

1. Introduction

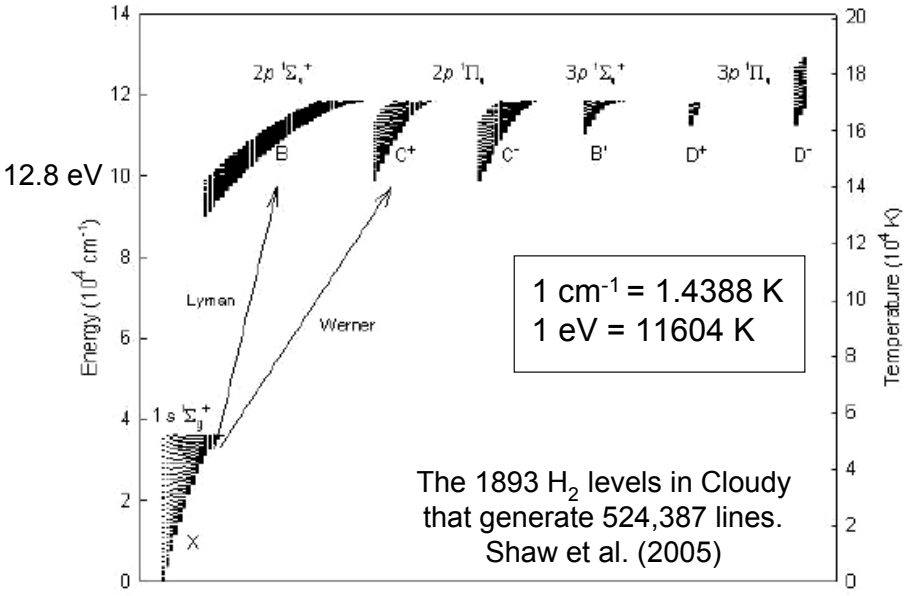
- The CNM HI is located in a thin disk.
- Young stars are found within an even thinner disk.
- The study of the dense ISM also reveals that:

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

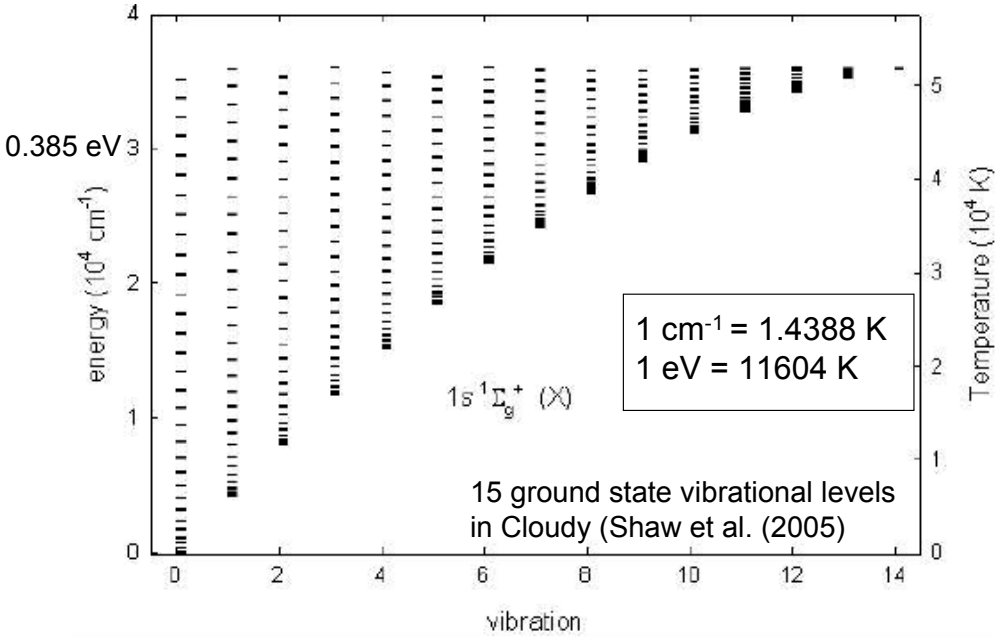
- H_2 and CO Molecules are the two most abundant of the 150 known interstellar molecules.
- They have played important roles in establishing the facts about recent star formation in the Milky Way.
- An additional reason for detailed discussion of H_2 and CO is that they are relatively simple and provide an entry to the complexities of molecular spectroscopy.

2. The H_2 Molecule

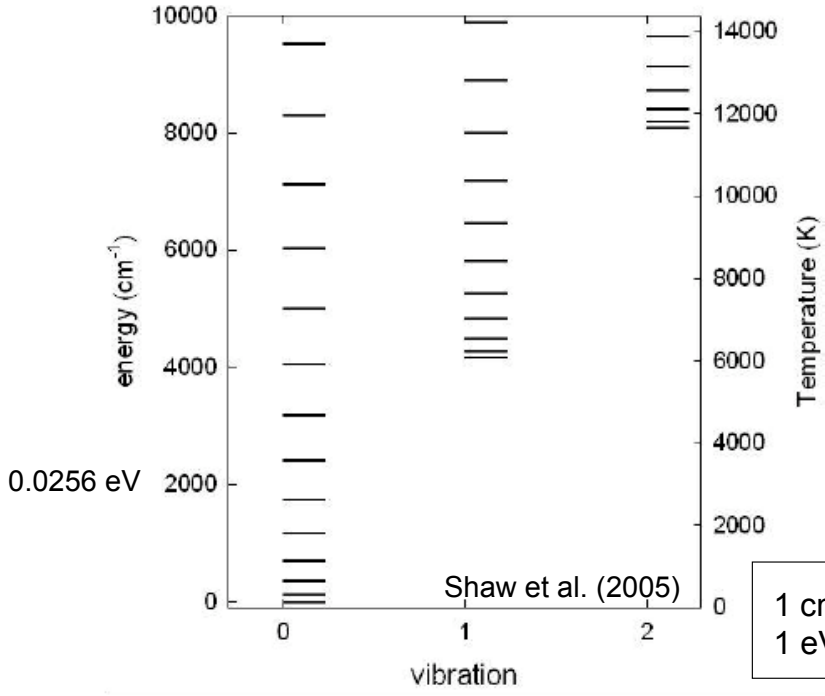
a. Electronic Transitions



b. Ground Vibrational Transitions



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



1 cm^{-1} = 1.4388 K
1 eV = 11604 K

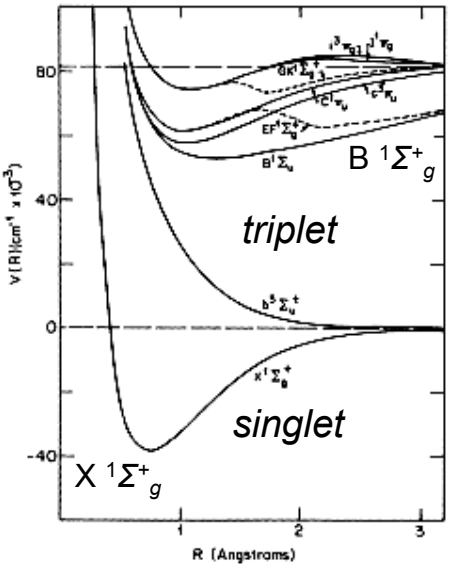
d. Symmetry Considerations
Electron Spin Exchange

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_2



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

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 $(-1)^J Y_{JM}$:

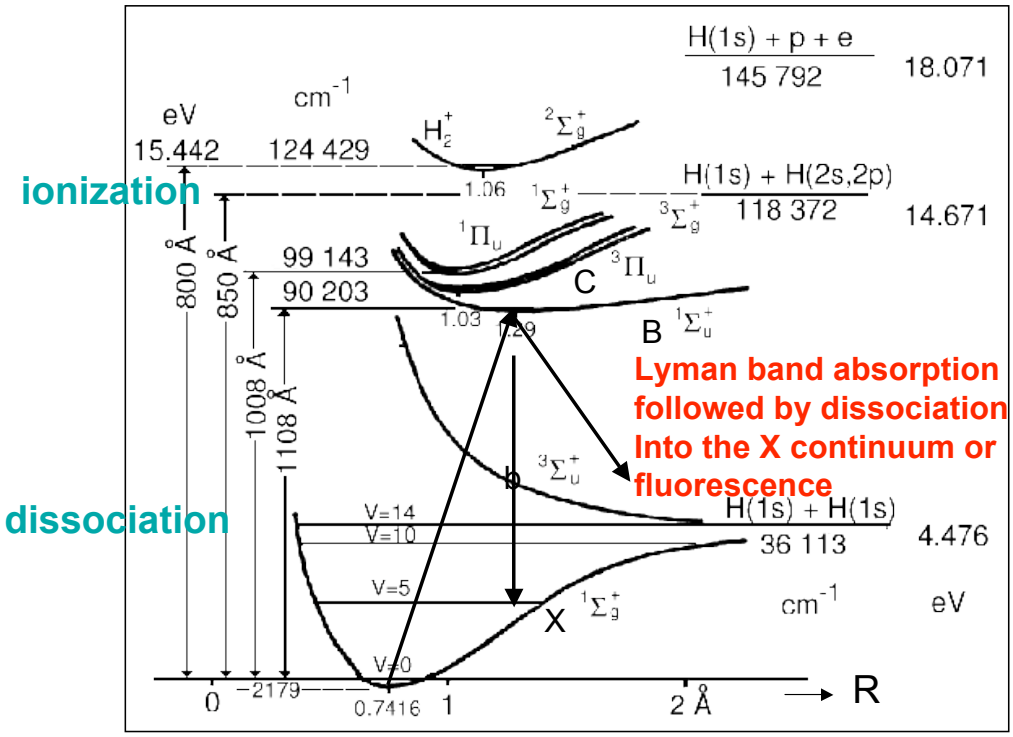
even J goes with I = 0 ("para" H_2) states
odd J goes with I = 1 ("ortho" H_2) states

para H_2 I = 0	**ortho H_2 I = 1**
J=4 ---------- 1707 K	
	J=3 ---------- 1024
J= 2 ---------- 512 K	
	J=1 ---------- 171 K
J = 0 ---------- 0 K	

f. Electronic States and Transitions

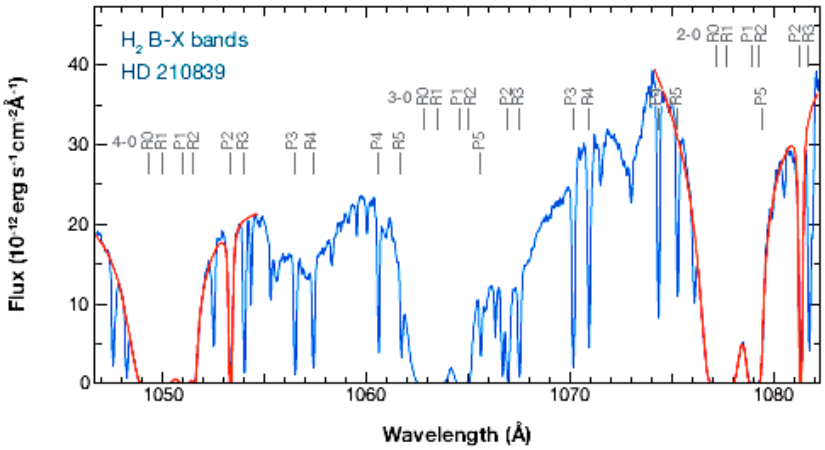
- With quantum numbers, $S = 0$, $I = 0$, $\Lambda = 0$, $J = 0$, the ground state is X $^1\Sigma^+_g$. It has 14 excited vibrational levels, each with an "infinite" number of rotational states.
- The next two singlet levels are B $^1\Sigma^+_g$ and C $^1\Pi^+_u$. Their potential curves asymptote to separated 1*s* and 2*s,p* atomic H atoms.
- Levels B & C are connected to ground by allowed electric-dipole transitions (analogs of HI Lyα). These ***Lyman and Werner bands*** start at 1108 Å and 1040 Å; they are spread more or less uniformly across the FUV band from the HI Lyman edge at 911.7 Å to the threshold at 1108 Å.
- Typical oscillator strengths are ~ 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.

Electronic Level Diagram fr H_2



minimum at 0.75 A

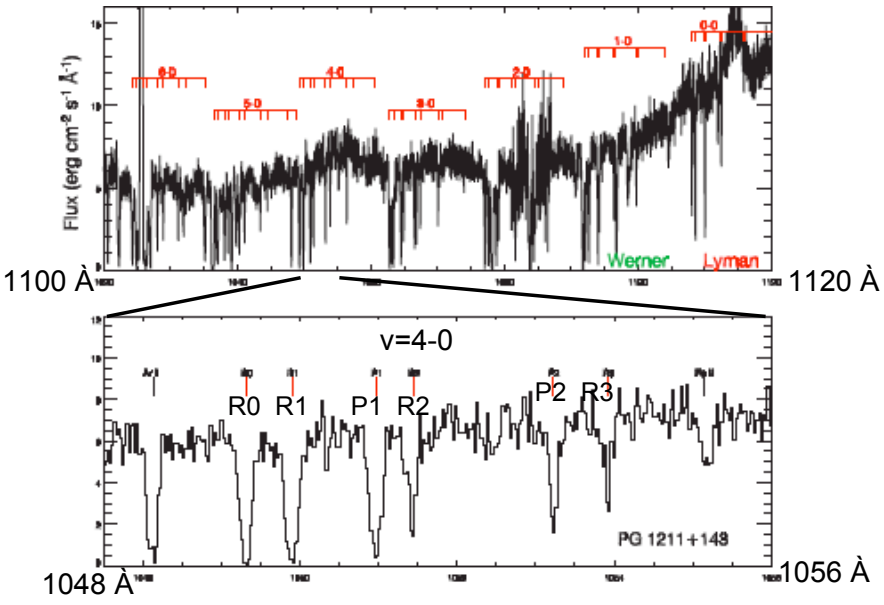
g. Observations of the Lyman Band Lines



FUSE spectrum of a bright star with interstellar absorption by the Lyman band of H_2. 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,

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

Lyman Band Absorption Towards an AGN

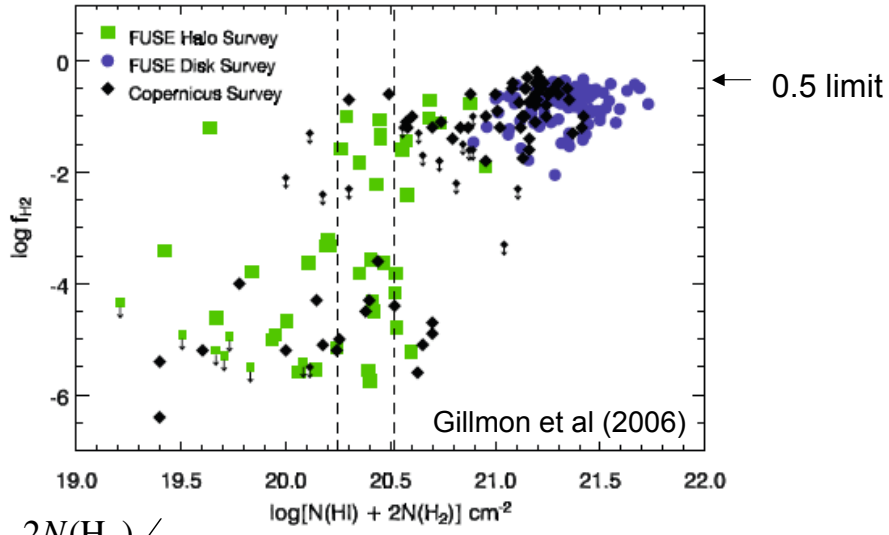


Analysis of these spectra yields H_2 column densities and excitation temperatures.

Gillmon et al., ApJ 636 891 2006 "A Fuse Survey of Interstellar H_2 towards high-latitude AGNs"

FUSE and Copernicus Survey Results

Fraction of H_2 vs. Total Hydrogen Column.



$$F = \frac{2N(\mathrm{H}_2)}{N(\mathrm{H}) + 2N(\mathrm{H}_2)} \quad \text{vs.} \quad N(\mathrm{H}) = N(\mathrm{H}) + 2N(\mathrm{H}_2)$$

The 1/2 transition position occurs near N_H = 2.4x10^{20} cm^{-2}

Lyα Pumped Fluorescence of H_2

Lyα is often a strong line covering several Å. It can overlap many Lyman band H_2 lines. The fluorescence is sensitive to *T* and the abundance of H_2. It can be used as a thermometer.

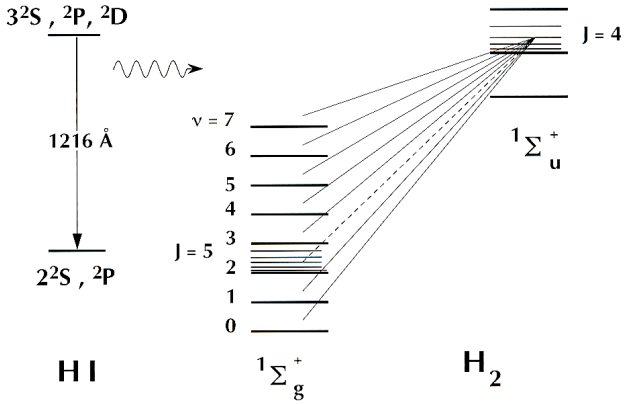
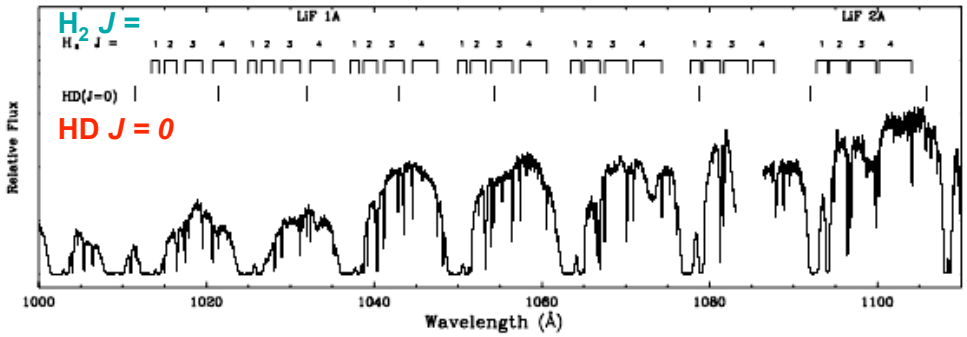


Fig. 4.10. Fluorescence of H_2 with Lyα. In order for this process to occur, the molecular hydrogen has to be both vibrationally and rotationally excited,which requires a temperature above about 1000 K

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

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 ~ 3×10^{-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_2 in this cloud.

h. Near Infrared Transitions

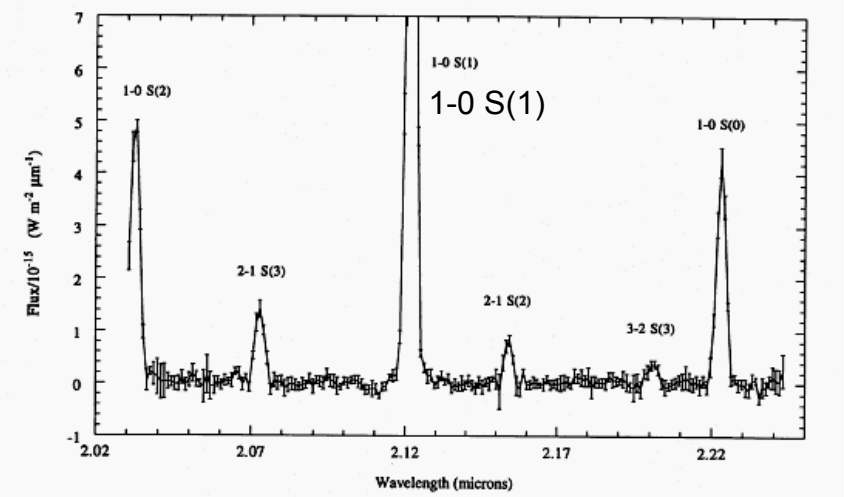
- The ground vibrational constant is $\omega \sim 4400$ cm^{-1} (6330 K); ro-vib transitions occur in the NIR near 2.2 μm.
- They are observed in warm regions, where they are collisionally excited, and in regions near a FUV source as a UV fluorescent spectrum following absorption in a Lyman or Werner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

Because H_2 has no dipole moment, these are ***weak quadrupole transitions***; a favorite is the 1-0 S(1) line at 2.12 μm, corresponding to $v'=1, J'=3 \rightarrow v''=0, J''=1$.

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

NIR H_2 Ro-Vib Lines in a Herbig-Haro Object

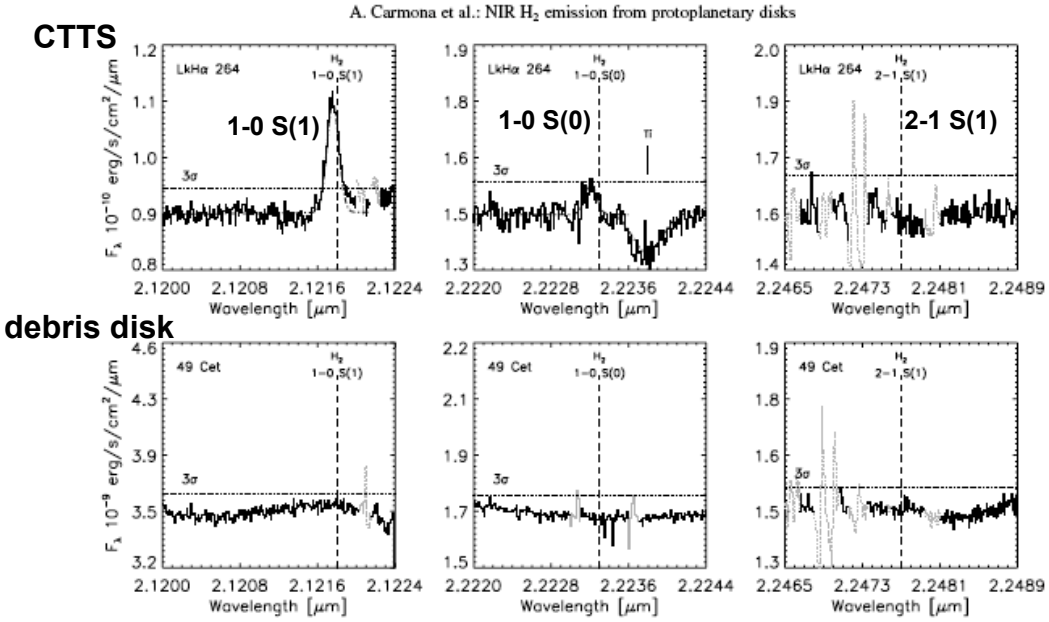
Fernandes & Brand, MNRAS 274 639 1995



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 shock appearance. Fast shocks generate UV radiation and produce fluorescence after exciting H_2.

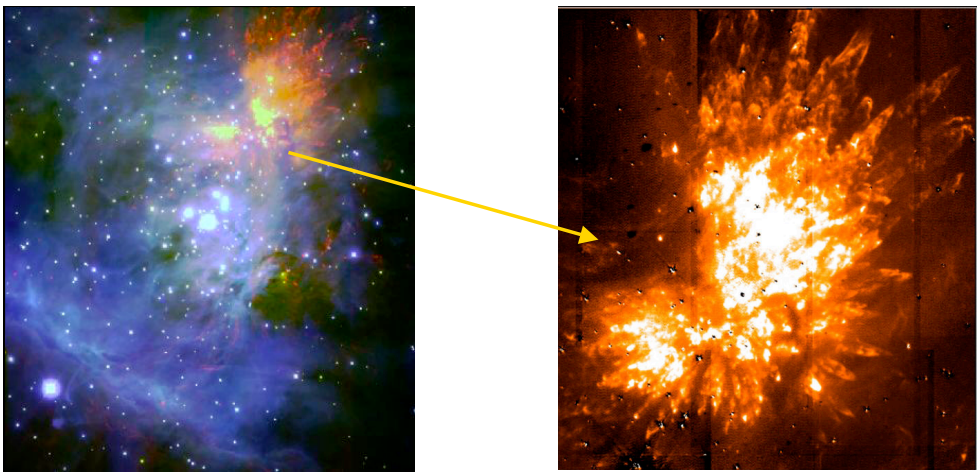
NIR H_2 Ro-vib Lines in Protoplanetary Disks

Carmona et al. A&A 476 853 2007



ESO VLT adaptive optics high resolution NIR spectrograph

Subaru Images of Orion

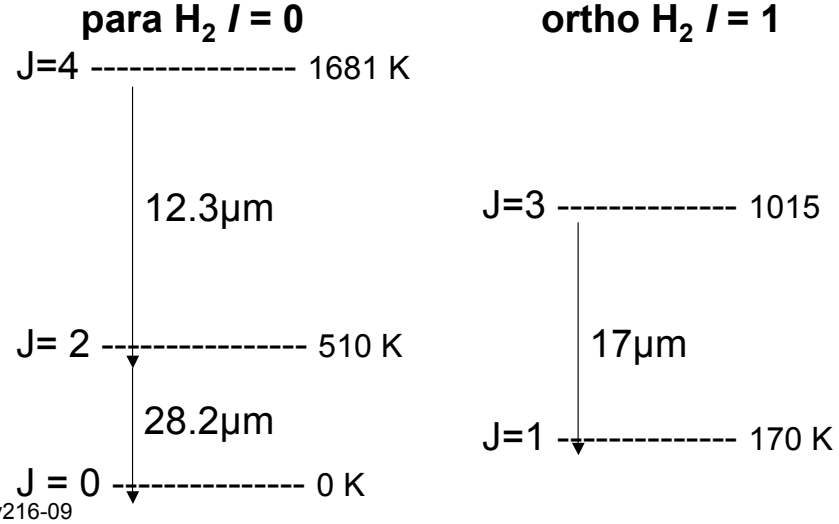


Orion Nebula Kleinman-Low Nebula

The Kleinman-Low Nebula is a region of massive star formation. The image is based on J(1.25 μm), K(2.15 μm) and $H_2$1-0 S(0). The rovib emission at 2.12 μm is presumed to arise from winds shocking the surrounding gas.

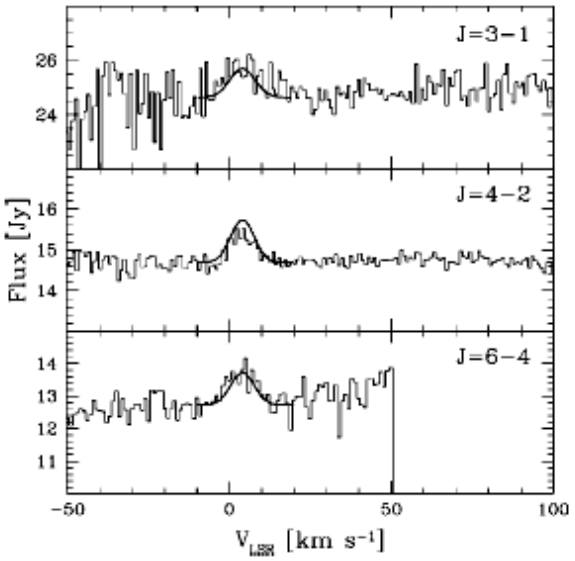
i. Mid-Infrared Transitions

- The ground rotational constant is B = 59.1 cm^{-1} (85.0 K).
- Pure rotational transitions occur in the MIR shortwards of 28 μm; they are very weak quadrupole transitions.
- Observed in lukewarm regions (T > 300 K) via collisional excitation and fluorescence near UV and X-ray sources.



H_2 Rotational Lines in a Herbig A Star AB Aur

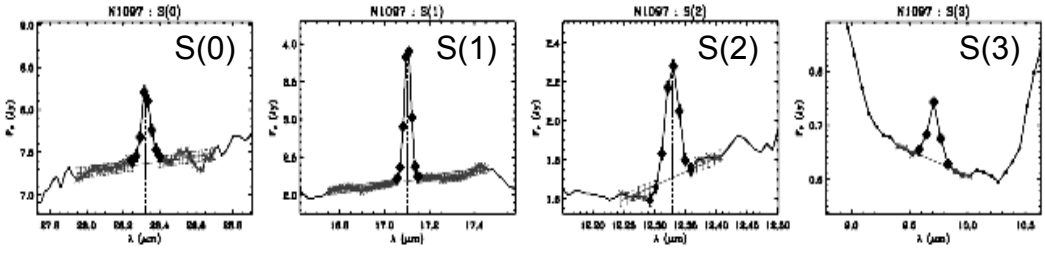
Bitner et al. ApJ 661 L69 2007



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

H_2 Rotational Line Detections in AGN

Roussel et al. ApJ 669 959 2007



OBSERVED H_2 LINES

Transition $v = 0$	Short Notation	Rest λ (μm)	Spectral Order	E_u/k (K)	A (10^{-11} 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).

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_2.
- 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(CO) = 11.09 eV compared to $D(H_2)$= 4.48 eV

- It has useful isotopes, ^{13}CO, C^{17}O, and C^{18}O.

a. Energy Levels and Transitions

Ground Level Spectroscopic Constants in cm^{-1}

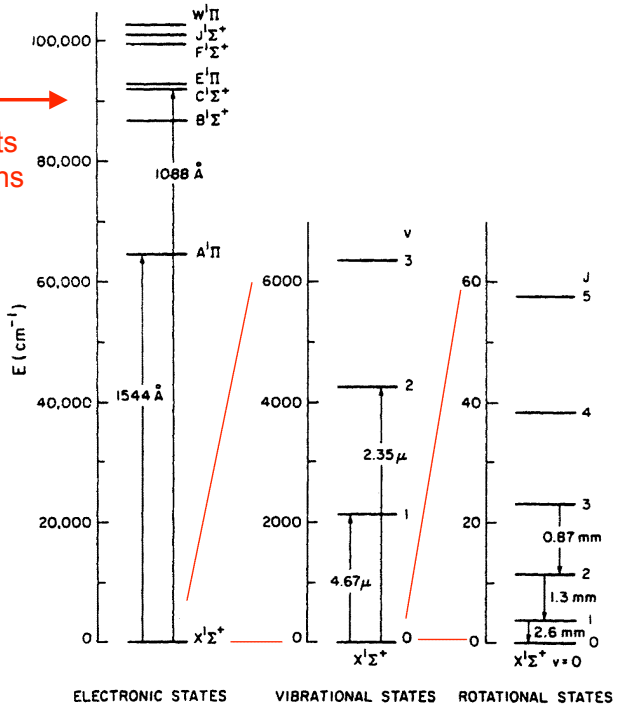
$$k = G(v) + B_v J(J+1) - D_v [J(J+1)]^2 + \cdots$$

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

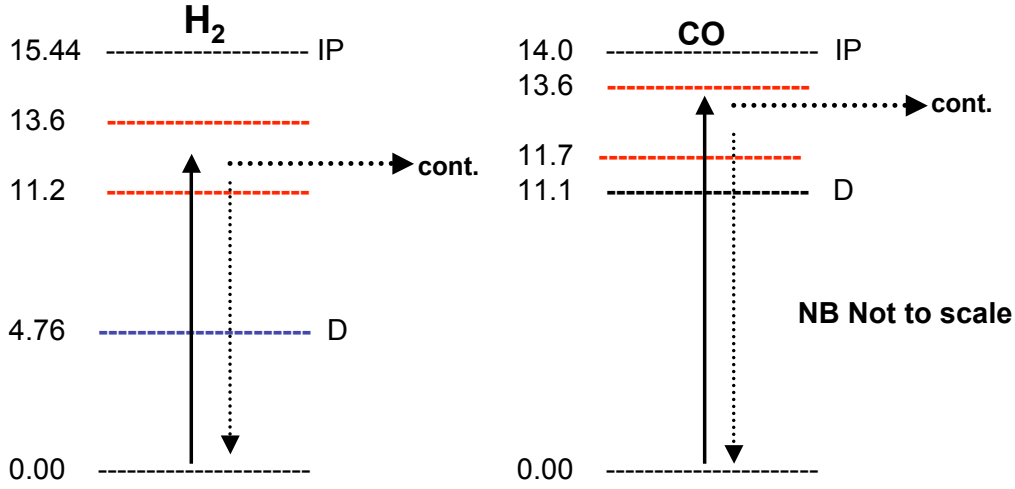
In Kelvins: B_0 = 2.766 K and $\theta_0 = (ch/k_B)$ [G(1) –G(0] = 3084 K.

Energy Levels of CO

FUV dissociation starts with electron transitions below 1108 Å



CO and H_2 Dissociation Energies



Legend: IP = Ionization Potential D = Dissociation energy

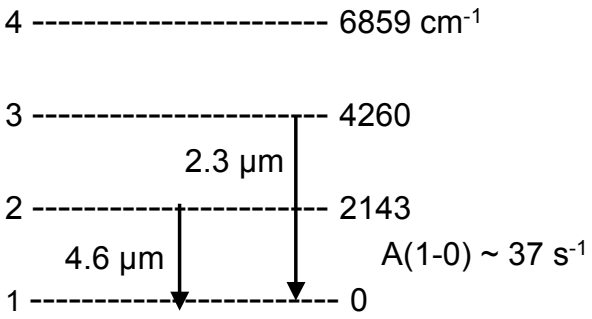
--- allowed electronic transitions in the FUV

H_2 and CO have similar electronic transitions and dissociation pathways.

b. Summary of CO Diagnostic Lines

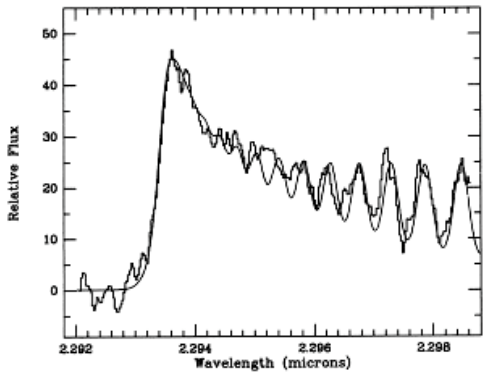
a. UV – CO is something like a heavy H_2: The UV bands occur in the far UV near 1000 Å with oscillator strengths of the same order of magnitude (10^{-2}) as for H_2. They have have been detected in absorption towards diffuse clouds where the CO maximum abundance is 10^{-5}.

b. NIR Δv = 1 transitions are the ***fundamental*** bands
Δv = 2 transitions are the ***1st overtone bands***, etc



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.

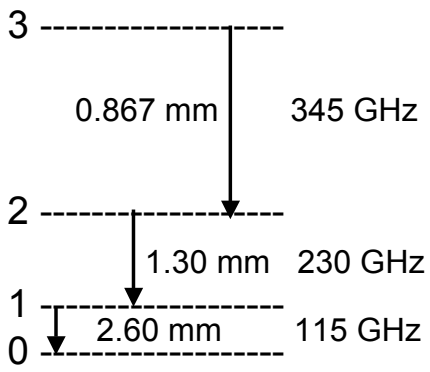
c. Pure Rotational Bands (mm-FIR)

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 cm^{-1} $2B/k_B$ = 5.532 K

CO is the ideal diagnostic and coolant for cool clouds with T ~ 10-100 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_{10} = 7.17x10^{-8} s^{-1} **$A_{J,J-1} = 3J^4/(2J+1)\ A_{10}$**

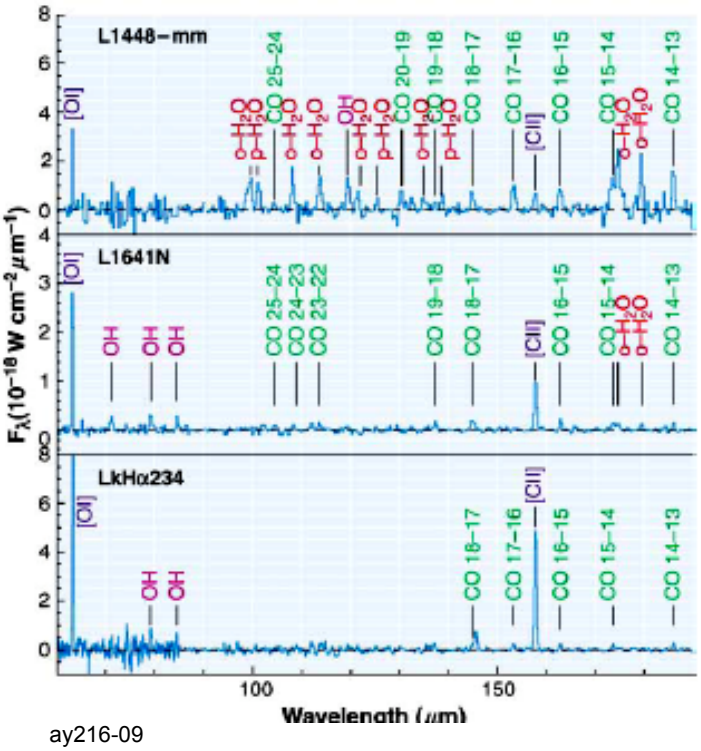
Fundamental Rotational Frequencies of CO

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
^{13}CO	110201
^{14}CO	105871
C^{17}O	112359
C^{18}O	109782
^{13}C^{17}O	107289
^{13}C^{18}O	104711

Rough ISM isotope ratios: ^{12}C:^{13}C = 70:1 ^{16}O:^{17}O:^{18}O= 1500:500:1

CO, H2O, 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_2O & MIR OH
black - 157 μm CII

4. Post-Summary

Having outlined the spectroscopy and applications of the two most abundant interstellar molecules, we are led to ask 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_2, 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.