



HAL
open science

Radiative transfer: molecular physics

Benjamin Godard

► **To cite this version:**

| Benjamin Godard. Radiative transfer: molecular physics. Doctoral. France. 2023. hal-04645959

HAL Id: hal-04645959

<https://hal.science/hal-04645959v1>

Submitted on 12 Jul 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

(diatomic) Molecular physics

International Research Track

2023

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

1. Introduction

2. Energy structure

Born-Oppenheimer

Vibration / rotation

Additional couplings

3. Molecular lines

Dipole transitions

Quadrupole transitions

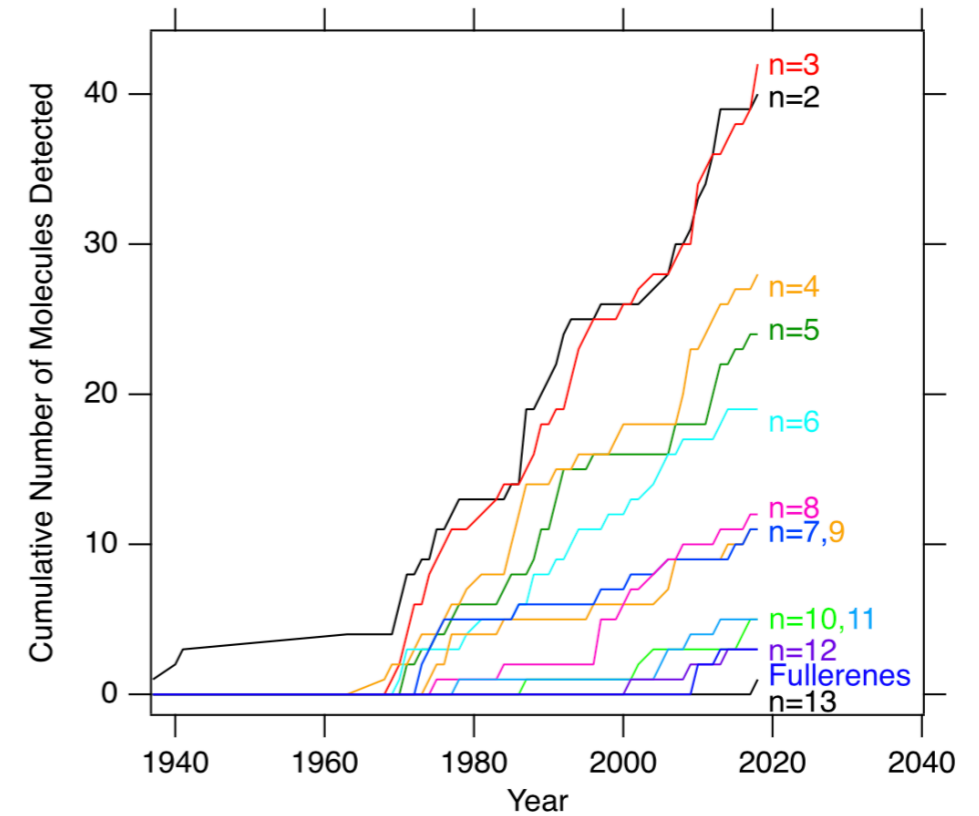
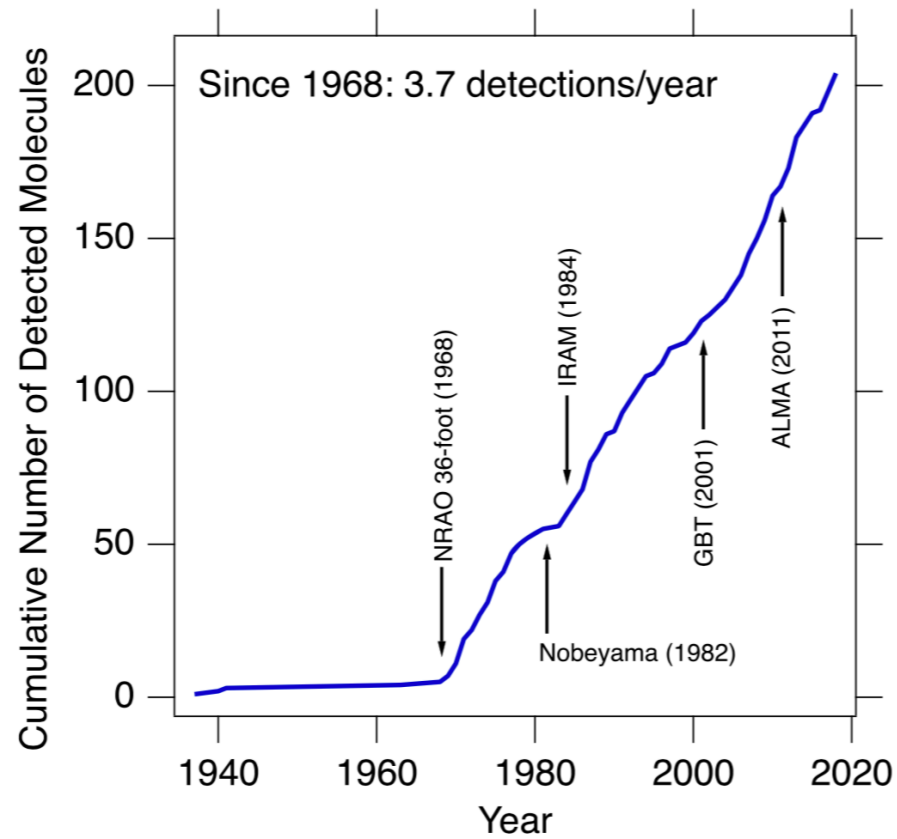
4. Photo-processes

5. Conclusions

Molecules are ubiquitous in astrophysics

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



B. McGuire (2018)

In summary, in 2018

- 204 individual molecular species
- comprised of 16 different elements
- composed of 2 to 70 atoms
- detected from tens-cm wavelength to ultraviolet

Molecules are ubiquitous in astrophysics

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Table 2
List of Detected Interstellar Molecules with Two to Seven Atoms, Categorized by Number of Atoms, and Vertically Ordered by Detection Year

2 Atoms		3 Atoms		4 Atoms	5 Atoms	6 Atoms	7 Atoms
CH	CP	H ₂ O	N ₂ O	NH ₃	HC ₃ N	CH ₃ OH	CH ₃ CHO
CN	NH	HCO ⁺	MgCN	H ₂ CO	HCOOH	CH ₃ CN	CH ₃ CCH
CH ⁺	SIN	HCN	H ₃ ⁺	HNCO	CH ₂ NH	NH ₂ CHO	CH ₃ NH ₂
OH	SO ⁺	OCS	SiCN	H ₂ CS	NH ₂ CN	CH ₃ SH	CH ₂ CHCN
CO	CO ⁺	HNC	AlNC	C ₂ H ₂	H ₂ CCO	C ₂ H ₄	HC ₅ N
H ₂	HF	H ₂ S	SiNC	C ₃ N	C ₄ H	C ₅ H	C ₆ H
SiO	N ₂	N ₂ H ⁺	HCP	HNCS	SiH ₄	CH ₃ CN	c-C ₂ H ₄ O
CS	CF ⁺	C ₂ H	CCP	HOCO ⁺	c-C ₃ H ₂	HC ₂ CHO	CH ₂ CHOH
SO	PO	SO ₂	AlOH	C ₃ O	CH ₂ CN	H ₂ C ₆	C ₆ H ⁻
SiS	O ₂	HCO	H ₂ O ⁺	l-C ₃ H	C ₅	C ₅ S	CH ₃ NCO
NS	AlO	HNO	H ₂ Cl ⁺	HCNH ⁺	SiC ₄	HC ₃ NH ⁺	HC ₅ O
C ₂	CN ⁻	HCS ⁺	KCN	H ₃ O ⁺	H ₂ CCC	C ₅ N	
NO	OH ⁺	HOC ⁺	FeCN	C ₃ S	CH ₄	HC ₄ H	
HCl	SH ⁺	SiC ₂	HO ₂	c-C ₃ H	HCCNC	HC ₄ N	
NaCl	HCl ⁺	C ₂ S	TiO ₂	HC ₂ N	HNCCC	c-H ₂ C ₃ O	
AlCl	SH	C ₃	CCN	H ₂ CN	H ₂ COH ⁺	CH ₂ CNH	
KCl	TiO	CO ₂	SiCSi	SiC ₃	C ₄ H ⁻	C ₅ N ⁻	
AlF	ArH ⁺	CH ₂	S ₂ H	CH ₃	CNCHO	HNCHCN	
PN	NS ⁺	C ₂ O	HCS	C ₃ N ⁻	HNCNH	SiH ₃ CN	
SiC		MgNC	HSC	PH ₃	CH ₃ O		
		NH ₂	NCO	HCNO	NH ₃ D ⁺		
		NaCN		HOCN	H ₂ NCO ⁺		
				HSCN	NCCNH ⁺		
				HOOH	CH ₃ Cl		
				l-C ₃ H ⁺			
				HMgNC			
				HCCO			
				CNCN			

Table 3
List of Detected Interstellar Molecules with Eight or More Atoms, Categorized by Number of Atoms, and Vertically Ordered by Detection Year

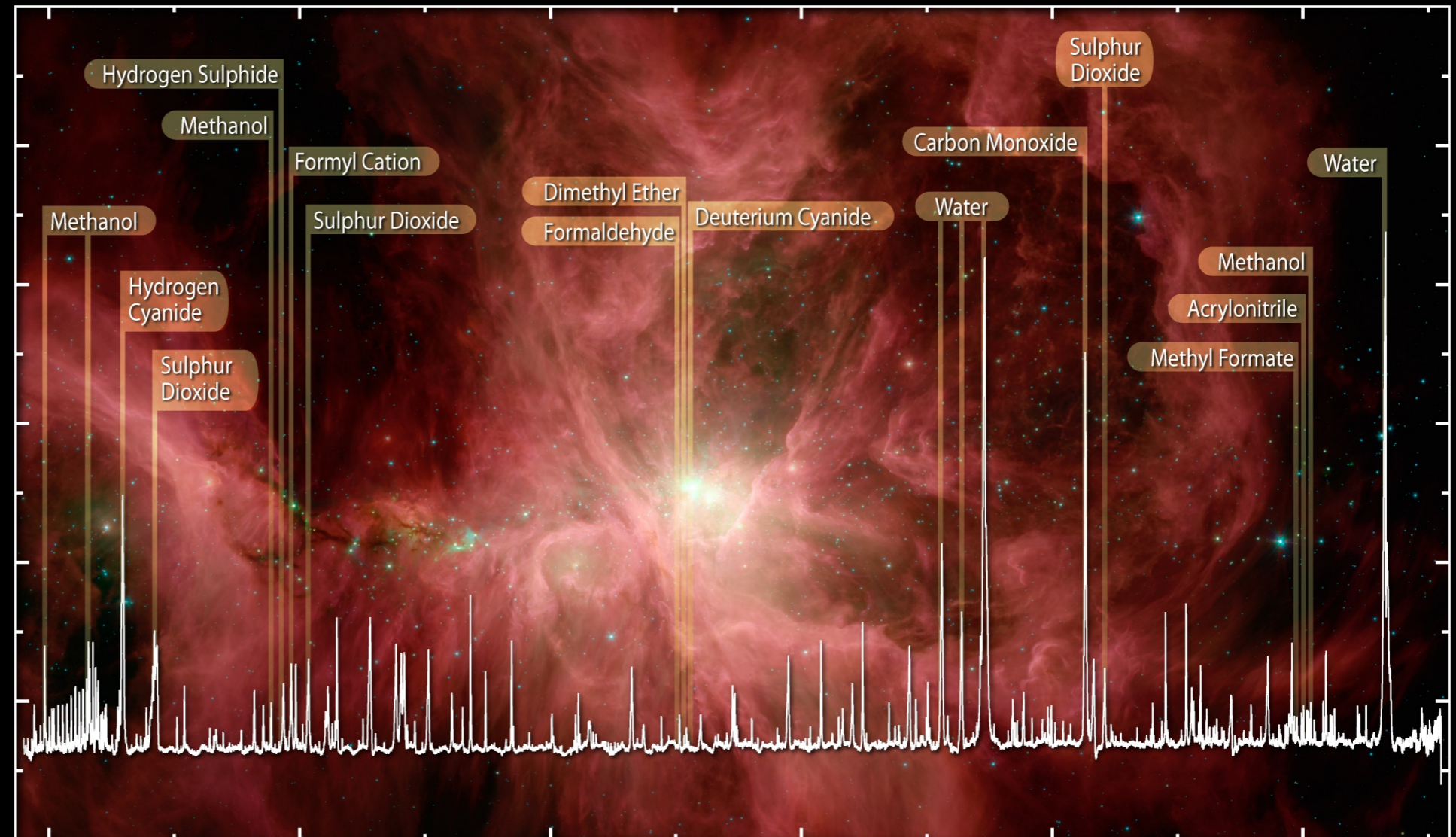
8 Atoms	9 Atoms	10 Atoms	11 Atoms	12 Atoms	13 Atoms	Fullerenes
HCOOCH ₃	CH ₃ OCH ₃	(CH ₃) ₂ CO	HC ₉ N	C ₆ H ₆	c-C ₆ H ₅ CN	C ₆₀
CH ₃ C ₃ N	CH ₃ CH ₂ OH	HO(CH ₂) ₂ OH	CH ₃ C ₆ H	n-C ₃ H ₇ CN		C ₆₀ ⁺
C ₇ H	CH ₃ CH ₂ CN	CH ₂ CH ₂ CHO	CH ₃ CH ₂ OCHO	i-C ₃ H ₇ CN		C ₇₀
CH ₃ COOH	HC ₇ N	CH ₃ C ₅ N	CH ₃ COOCH ₃			
H ₂ C ₆	CH ₃ C ₄ H	CH ₃ CHCH ₂ O				
CH ₂ OHCHO	C ₈ H	CH ₃ OCH ₂ OH				
HC ₆ H	CH ₃ CONH ₂					
CH ₂ CHCHO	C ₈ H ⁻					
CH ₂ CCHCN	CH ₂ CHCH ₃					
NH ₂ CH ₂ CN	CH ₃ CH ₂ SH					
CH ₃ CHNH	HC ₇ O					
CH ₃ SiH ₃						

B. McGuire (2018)

Molecules are ubiquitous in astrophysics

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



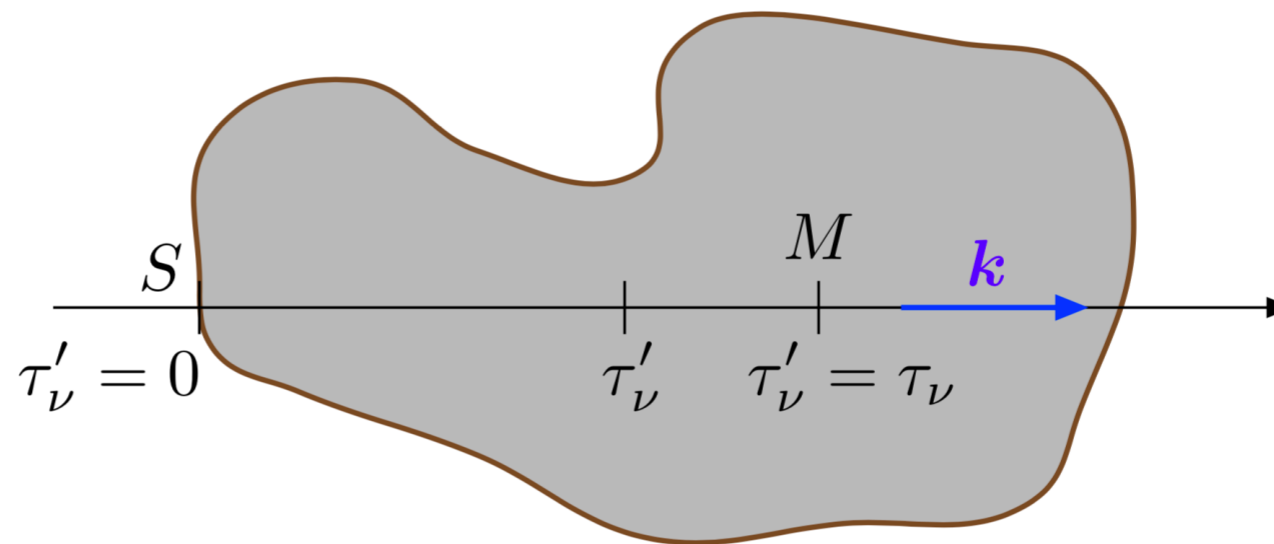
HIFI Spectrum of Water and
Organics in the Orion Nebula

© ESA, HEXOS and the HIFI consortium
E. Bergin

Radiative transfer equation

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



F. Levrier - radiative transfer lecture

$$\frac{dI_\nu}{dl} = -[\alpha_\nu + \sigma_\nu] I_\nu + j_\nu + \frac{1}{4\pi} \int_{\Omega'} \tilde{\sigma}_\nu(\mathbf{k}' \rightarrow \mathbf{k}) I_\nu(\mathbf{k}') d\Omega'$$

- absorption coefficient $\alpha_\nu = \sum_a n_a s_{\nu,a}$ cm^{-1}
- diffusion coefficient $\sigma_\nu = \sum_d n_d s_{\nu,d}$ cm^{-1}
- emissivity j_ν $\text{erg s}^{-1} \text{cm}^{-3} \text{Hz}^{-1} \text{sr}^{-1}$
- opacity $d\tau_\nu = [\alpha_\nu + \sigma_\nu] dl$
- source function S_ν $\text{erg s}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1}$

Questions related to molecules in radiative transfer

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

through which processes do molecules interact with light ?

- absorption / emission
- polarization
- dissociation / ionization / fluorescence

what are the properties of the microphysical processes ?

- transitions (energy structure / selection rules)
- interaction cross sections
- products of ionization and dissociation

how to implement these processes in radiative transfer codes ?

- what data are required ?
- couplings expected ?
- analytical considerations & numerical methods

Outline

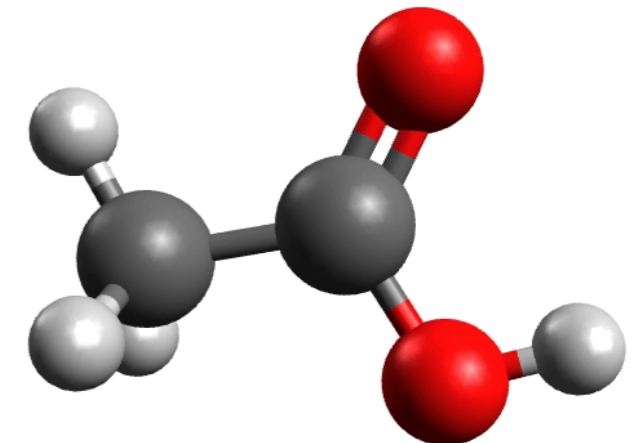
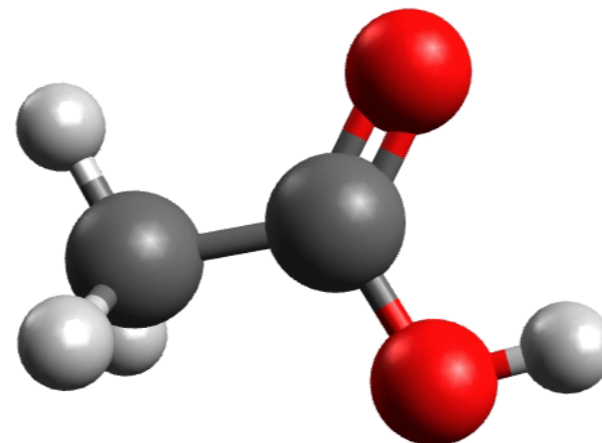
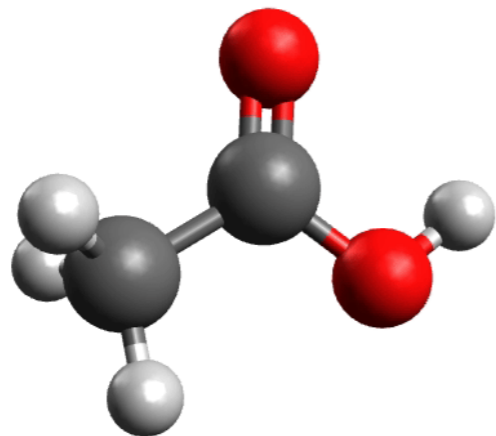
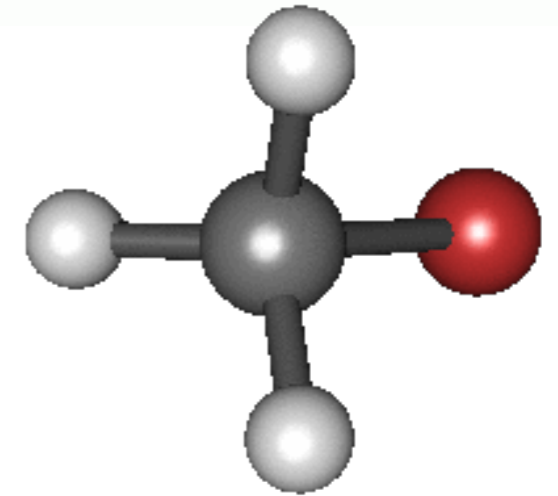
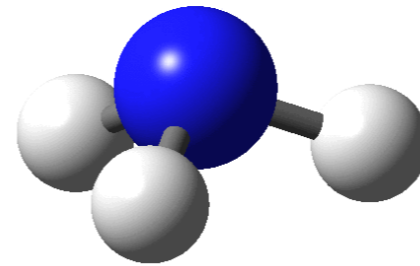
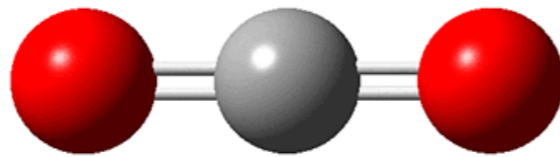
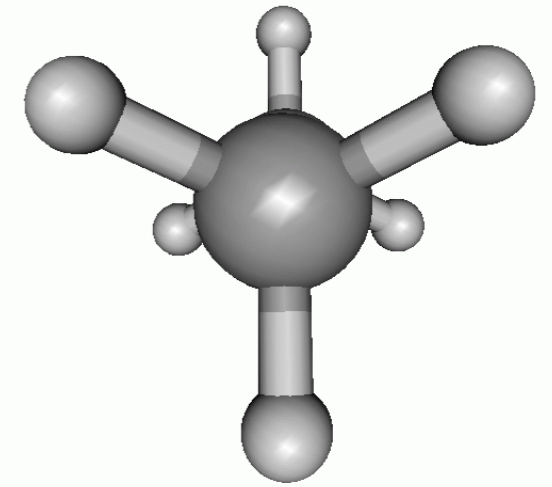
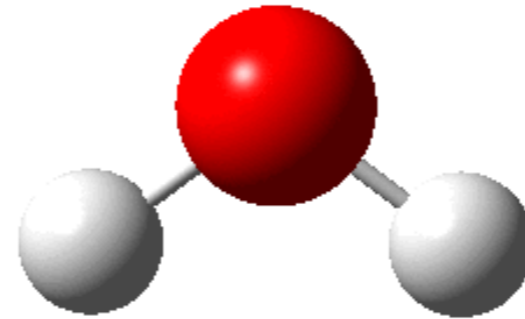
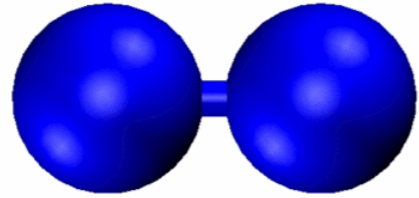
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Energy structure of molecules

Complexity of the task

Outline

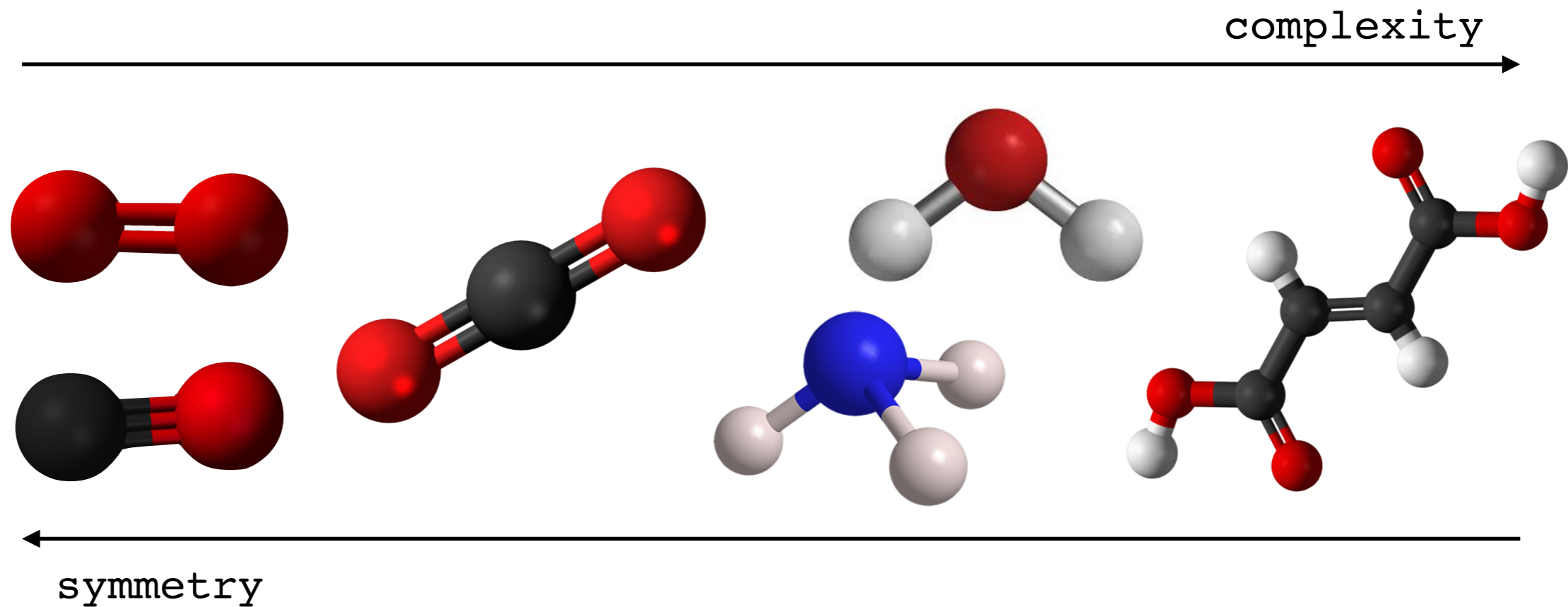
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



Complexity of the task

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



Compared to atomic energy structure

- less symmetry, complicated electronic wavefunctions
- nuclei move, additional freedom, rotational and vibrational motions

Focus on diatomic (homonuclear or heteronuclear)

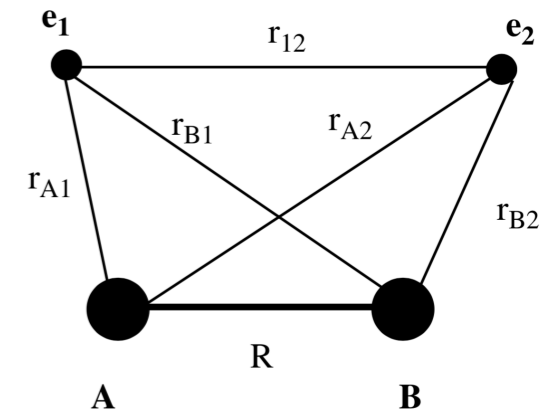
- gives a strong foothold to understand molecular spectra

Stationary states and usual hypothesis

Stationary Schrödinger equation for diatomic molecules

$$\left(-\frac{\hbar^2}{2M_A} \nabla_A^2 - \frac{\hbar^2}{2M_B} \nabla_B^2 - \frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + V_e - E \right) \psi(\mathbf{R}_A, \mathbf{R}_B, \mathbf{r}_i) = 0$$

$$V_e = \frac{e^2}{4\pi\epsilon_0} \left(-\sum_{i=1}^N \frac{Z_A}{r_{Ai}} - \sum_{i=1}^N \frac{Z_B}{r_{Bi}} + \sum_{i=2}^N \sum_{j=1}^{i-1} \frac{1}{r_{ij}} + \frac{Z_A Z_B}{R} \right)$$



Usual simplifications & hypothesis

→ Born-Oppenheimer

$$\psi(\mathbf{R}_A, \mathbf{R}_B, \mathbf{r}_i) = \psi_e(\mathbf{r}_i) \psi_n(\mathbf{R}_A, \mathbf{R}_B)$$



→ center of mass frame

$$\psi_n(\mathbf{R}_A, \mathbf{R}_B) \rightarrow \psi_n(\mathbf{R})$$



→ separation vibration - rotation $\psi_n(\mathbf{R}) = \psi_v(R) \psi_r(\theta, \phi)$



Outline

• introduction

• energy structure

• molecular lines

• photo-processes

• conclusion

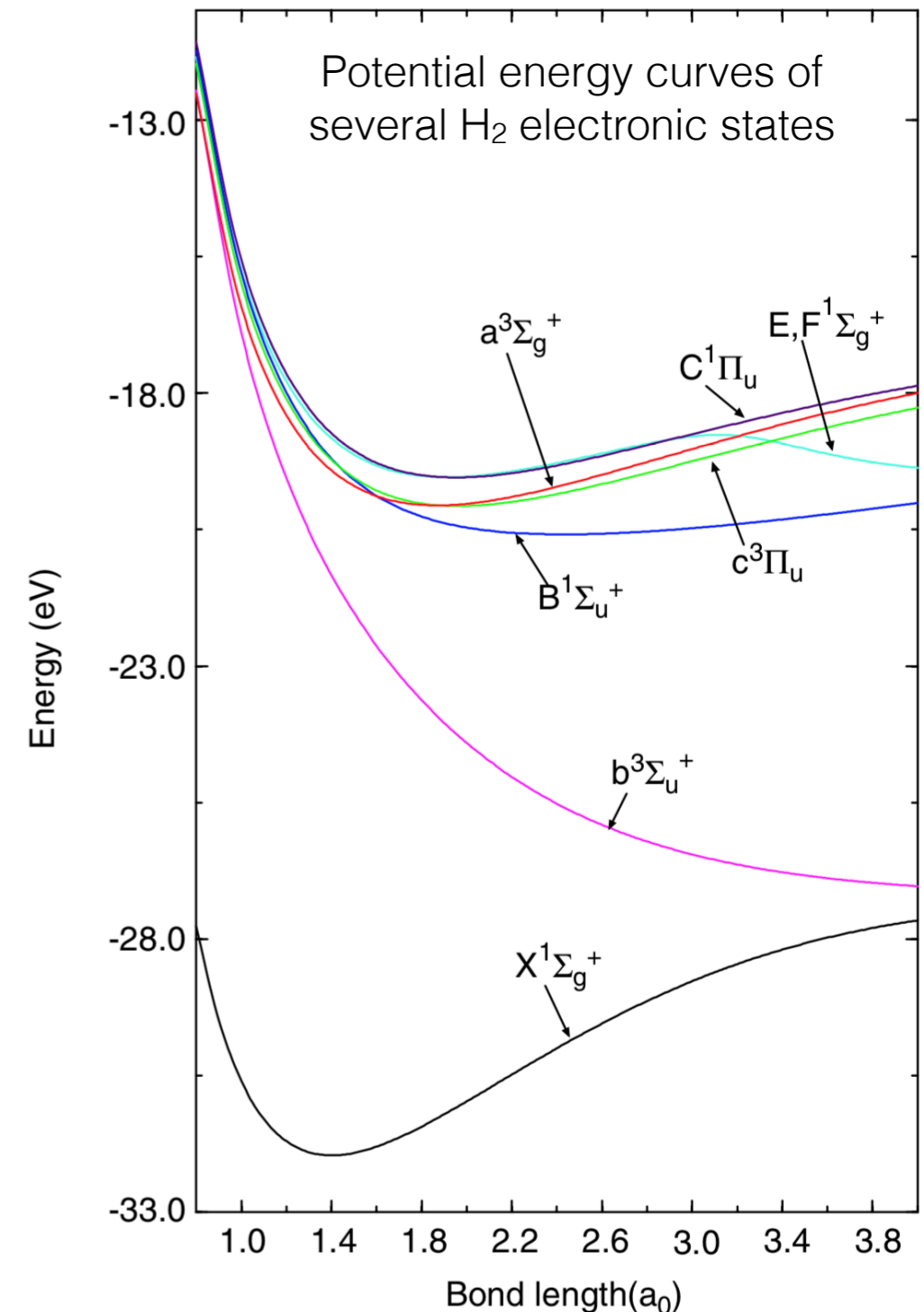
Electronic structure

Stationary Schrödinger equation for electronic wavefunction

$$\left(-\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + V_e - E_e \right) \psi_e(\mathbf{r}_i) = 0$$

- solve at each internuclear separation R
- gives eigenvalue $E_e(R)$
- gives Ψ_e & quantum numbers without couplings
 $S, \Lambda, g/u, +/ -$
- gives potential $V(R)$ seen by nuclei
- gives equilibrium radius & dissociation energy

J. Tennyson (2005)



Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Electronic structure

$$\text{letter}^{(2S+1)} \Lambda_{g/u}^{+/-}$$

Labelling of electronic states

$$\longrightarrow S = \sum_i s_i$$

total electronic spin
(careful with paired e⁻ in closed shells)

$$\longrightarrow \Lambda = \left(L = \sum_i l_i \right) |z$$

total angular momentum projected on z

Λ	0	1	2	3	4	...
states	Σ	Π	Δ	Φ	Γ	...

$$\longrightarrow g/u \text{ (gerade/ungerade)}$$

parity upon nuclei swap
(for homonuclear only)

$$\longrightarrow +/ - \text{ (parity)}$$

parity upon reflexion through nuclei plane
(for Σ states only)

$$\longrightarrow \text{letter}$$

label states of same quantum numbers

X = ground electronic state (GES)

A, B, ... = same spin multiplicity as GES

a,b, ... = diff spin multiplicity than GES

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Vibrational structure

Stationary Schrödinger equation for nuclei vibration

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + V(R) - E_v \right) \psi_v(R) = 0$$

→ for $V(R)$ approx by a parabolic potential $V_{\text{HO}}(R) = V_0 + \frac{1}{2}k(R - R_{\text{eq}})^2$

quantum harmonic oscillator

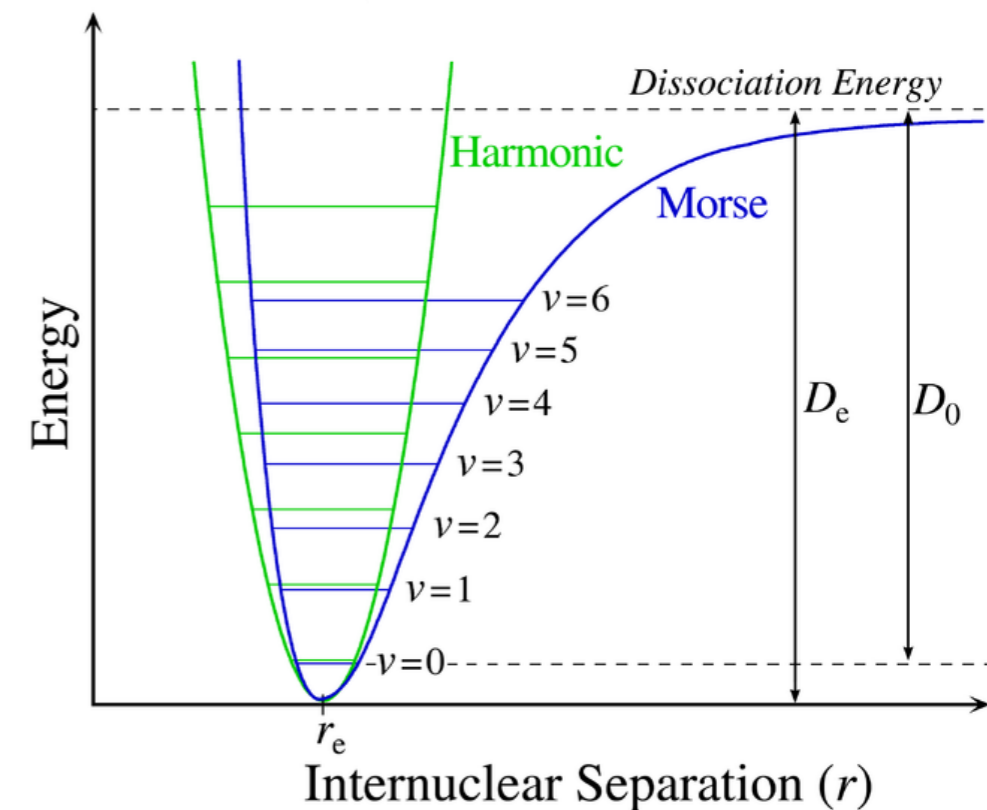
$$E_v = V_0 + \hbar \left(\frac{k}{\mu} \right)^{\frac{1}{2}} \left(v + \frac{1}{2} \right)$$

wavefunction derived from

Hermite polynomials

→ zero point energy

$$\text{zpe} = \frac{1}{2} \hbar \left(\frac{k}{\mu} \right)^{\frac{1}{2}}$$



wikipedia - Morse potential

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Rotational structure

Stationary Schrödinger equation for nuclei rotation

$$\left(-\frac{\hbar^2}{2\mu R^2} \left[\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d}{d\theta} \right) + \frac{1}{\sin^2\theta} \frac{d}{d\phi} \right] - E_r \right) \psi_r(\theta, \phi) = 0$$

→ spherical harmonics solution $\psi_r(\theta, \phi) = Y_{J, M_J}(\theta, \phi)$

Y_{J, M_J} → already seen for H atom

J → rotational angular momentum

M_J → projection of J onto molecular axis

μ → reduced mass

→ rotational eigenvalues $E_r = \frac{\hbar^2}{2\mu R^2} J(J + 1)$

→ if rotation as rigid body $E_r = B_0 J(J + 1)$

→ degeneracy of rotational levels $g_r = 2J + 1$

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Fine structure / hyperfine structure

Couplings between angular momenta

- electron angular momentum and spin, nuclei rotational motion and spin
- coupling schemes known as Hund's cases - (a) and (b) most common
- R = rotational angular momentum

Hund's case (a)	Hund's case (b)
1 - $\Lambda = L_{ z}, \Sigma = S_{ z}$	1 - $\Lambda = L_{ z}$
2 - $\Lambda + \Sigma \rightarrow \Omega$	2 - $\Lambda + R \rightarrow N$
3 - $\Omega + R \rightarrow J$	3 - $N + S \rightarrow J$

- hyperfine coupling
coupling with nuclear spin I
 $J + I \rightarrow F$

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Detailed electronic / vibrational / rotational structure

In reality, anharmonic & non rigid rotation with rot / vib couplings

- corrections terms (used in a polynomial expansion)
- derived from spectroscopic measurements of molecular lines
- anharmonic correction, centrifugal distortion, correction of rot constant

example for CH⁺

$$\begin{aligned}
 E(\Lambda, v, J) = & T_e(\Lambda) + \omega_e(\Lambda) \left(v + \frac{1}{2} \right) - \omega_e x_e(\Lambda) \left(v + \frac{1}{2} \right)^2 + \omega_e y_e(\Lambda) \left(v + \frac{1}{2} \right)^3 \\
 & + \left[B_e(\Lambda) - \alpha_e(\Lambda) \left(v + \frac{1}{2} \right) + \gamma_e(\Lambda) \left(v + \frac{1}{2} \right)^2 + \varepsilon_e(\Lambda) \left(v + \frac{1}{2} \right)^3 \right] \\
 & \times \left(J(J+1) - \Lambda^2 \right) - \left[D_e(\Lambda) + \beta_e(\Lambda) \left(v + \frac{1}{2} \right) + \delta_e(\Lambda) \left(v + \frac{1}{2} \right)^2 \right] \\
 & \times \left(J(J+1) - \Lambda^2 \right)^2 + \left[H_e(\Lambda) - \alpha_{H_e}(\Lambda) \left(v + \frac{1}{2} \right) \right] \left(J(J+1) - \Lambda^2 \right)^3 \\
 & \pm \frac{1}{2} \left[q_e(\Lambda) + \alpha_{q_e}(\Lambda) \left(v + \frac{1}{2} \right) \right] (J(J+1)) \\
 & \pm \frac{1}{2} q_{D_e}(\Lambda) (J(J+1))^2, \tag{1}
 \end{aligned}$$

constant	$X^1\Sigma^+$		$A^1\Pi$	
T_e			2.41187262	(+4)
ω_e	2.8575609	(+3)	1.864402	(+3)
$\omega_e x_e$	5.93179	(+1)	1.158317	(+2)
$\omega_e y_e$	2.2534	(-1)	2.6301	
B_e	1.41774612	(+1)	1.1886774	(+1)
α_e	4.94739	(-1)	9.1629	(-1)
γ_e	2.4904	(-3)	-2.292	(-2)
ε_e			4.952	(-3)
D_e	1.38914	(-3)	1.929606	(-3)
β_e	-2.66	(-5)	1.07331	(-4)
δ_e			-1.3123	(-5)
H_e	1.2036	(-7)		
α_{H_e}	2.079	(-8)		
q_e			4.1018	(-2)
α_{q_e}			-3.135	(-3)
q_{D_e}			-2.2	(-5)

Hakalla et al. (2006)

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

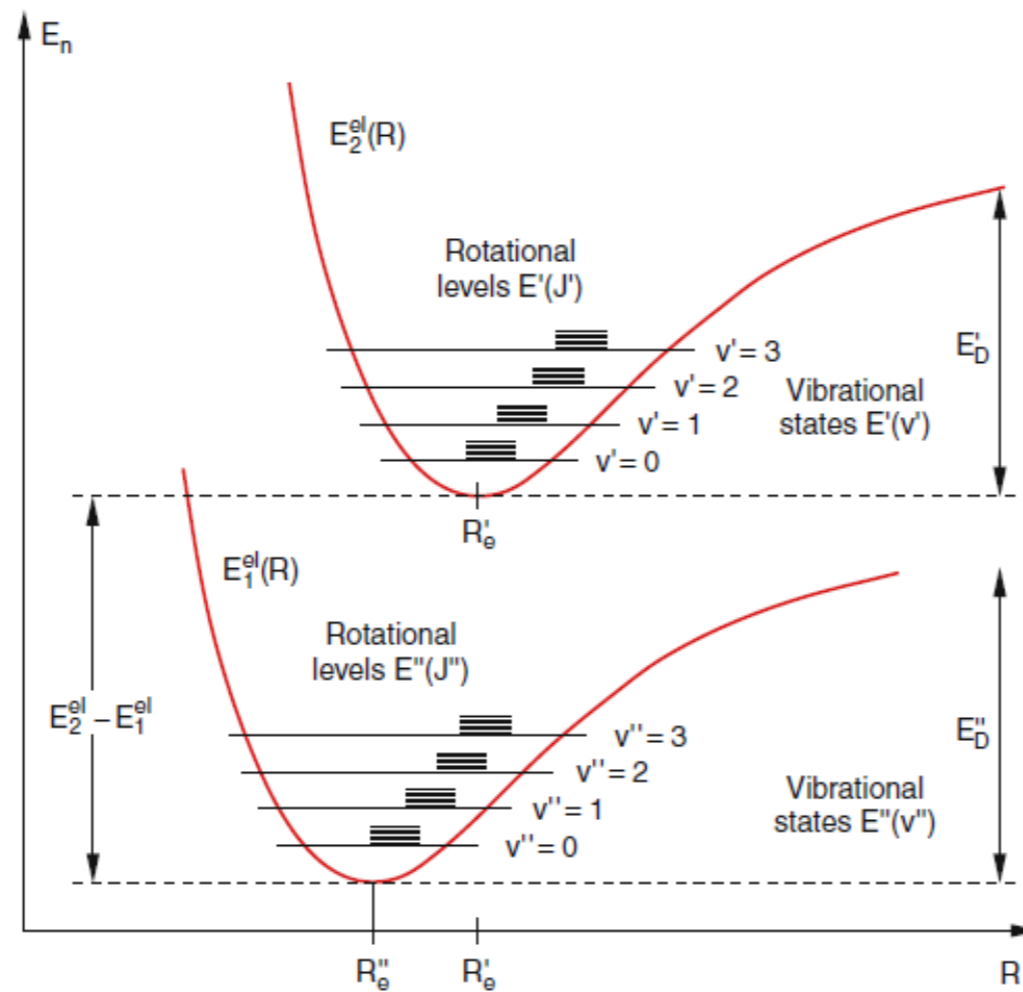
- conclusion

Detailed electronic / vibrational / rotational structure

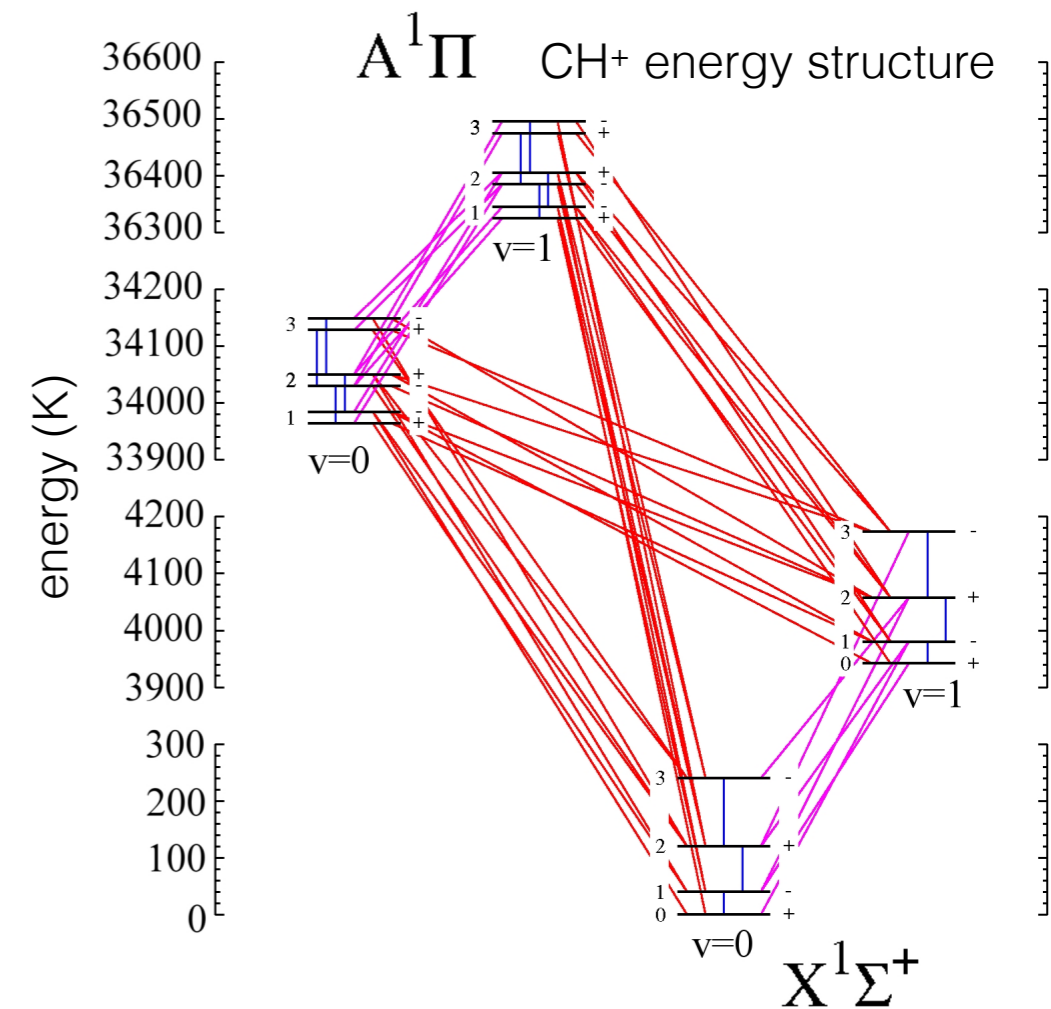
Hierarchical energy structure

→ rule of thumb $E_e > E_v > E_r$

→ ladders are not separated but superimposed



Mihály Benedict



Godard et al. (2013)

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Molecular spectra

Electric dipole transitions

Interaction of a molecule with EM field

- electric dipole, magnetic dipole, electric quadrupole, ...
- electric dipole terms $\sim 10^5 - 10^6$ times larger than the others
- electric dipole transition probability from Ψ'' to Ψ'

$$P \propto |\mathbf{M}|^2 \quad \text{with} \quad \mathbf{M} = \int \psi'^* \boldsymbol{\mu} \psi'' d\mathbf{r}$$

\mathbf{M} electric dipole moment integral

$\boldsymbol{\mu}$ dipole moment operator

- symmetry properties of Ψ', Ψ'' and $\boldsymbol{\mu}$ give the selection rules

$$\Delta S, \Delta \Lambda, \Delta v, \Delta J, \dots$$

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Selection rules on electronic quantum numbers

for allowed electric dipole transitions

→ $\Delta S = 0$ spin conserving selection rule

→ $\Delta \Lambda = 0, \pm 1$ projection of orbital momentum

→ $\Sigma^+ \leftrightarrow \Sigma^+$ for Σ states only

$\Sigma^- \leftrightarrow \Sigma^-$

→ $g \leftrightarrow u$ for homonuclear diatomic molecules

⇒ no *dipole allowed* vibration-rotation transition

within an electronic state for homonuclear species

Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Selection rules on vibrational quantum number

Outline

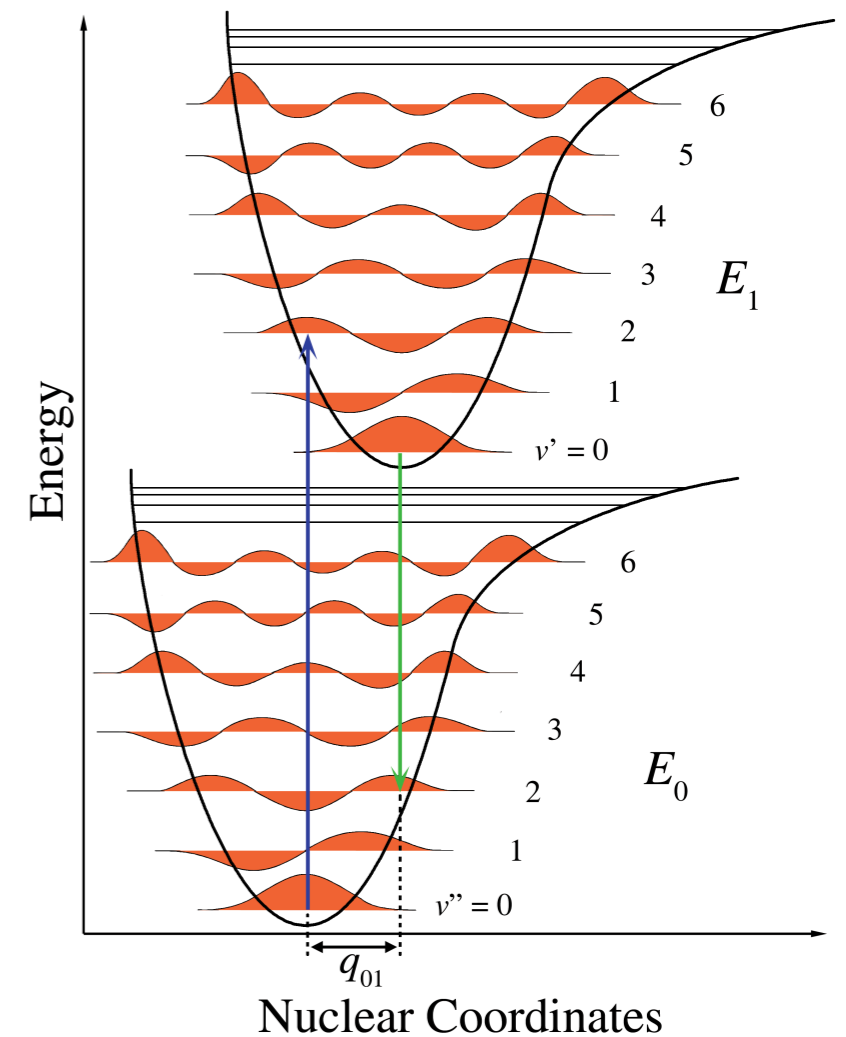
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

transitions from two different electronic states

- Franck-Condon principle
nuclei static during elec transition
transition probability proportional to
wavefunctions overlap

$$\left| \int \psi'_v(v')^* \psi''_v(v'') d\mathbf{r} \right|^2$$

- $\Delta v = \text{any}$ no selection rule



transition within the same electronic state

- $\Delta v = \text{any}$ for anharmonic oscillators
stronger transitions for $\Delta v = \pm 1$ (HO)

Selection rules on rotational quantum number

for allowed electric dipole transitions

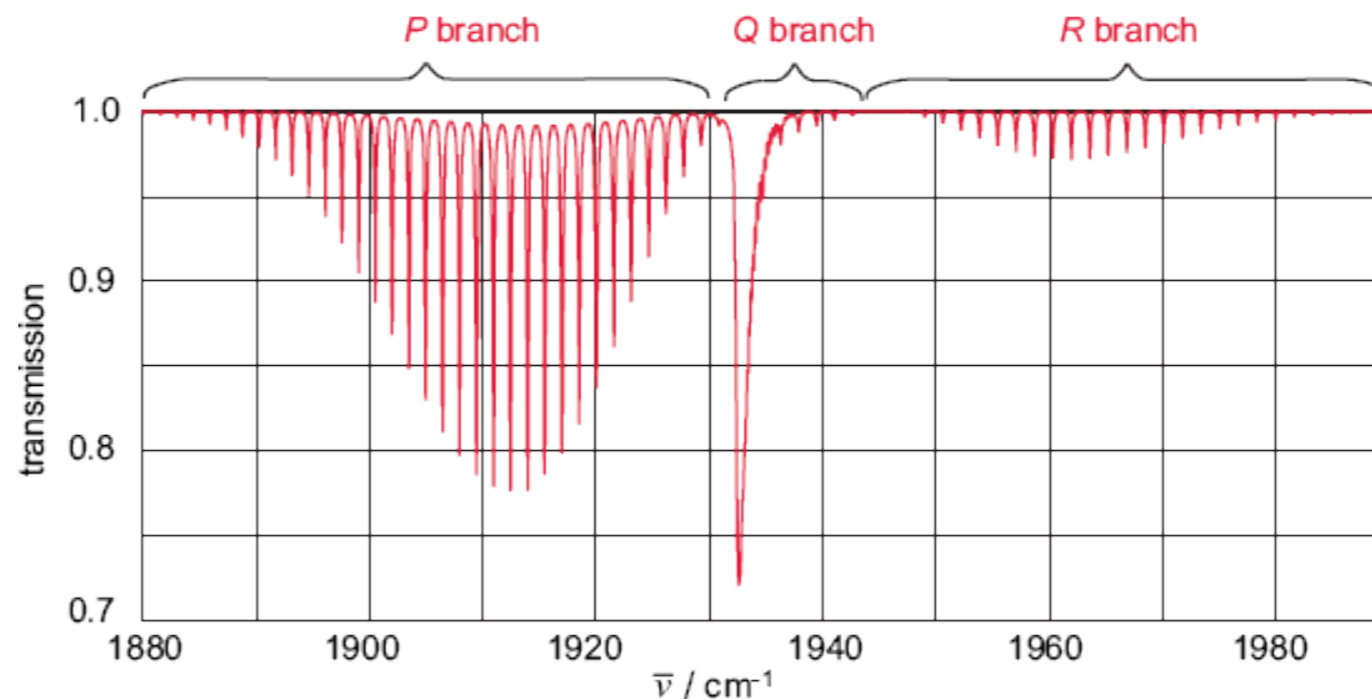
→ $\Delta J = \pm 1$ for $\Lambda = 0 - 0$ transitions

$\Delta J = 0, \pm 1$ ($0 \leftrightarrow 0$) for other $\Delta \Lambda$

→ labelling: J' (J'') associated with the upper (lower) energy level

name	$R(J'')$	$Q(J'')$	$P(J'')$
$\Delta J = J' - J''$	+1	0	-1

→ for transition within the same electronic state → regular structure



CO₂ simulated spectrum Hertel & Schultz

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Oscillator strength and Einstein coefficients

for allowed electric dipole transitions

→ the Einstein coefficient

$$A_{\Lambda'v'J'\Lambda''v''J''} = \frac{8\pi^2\nu^2e^2}{m_e c^3} \frac{2J'' + 1}{2J' + 1} f_{\Lambda'v'J'\Lambda''v''J''}$$

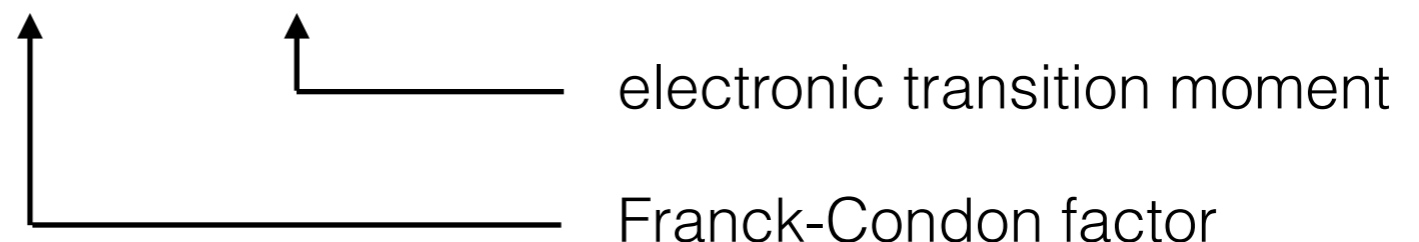
→ with the oscillator strength

$$f_{\Lambda'v'J'\Lambda''v''J''} = \frac{8\pi^2m_e\nu}{3he^2} M_{\Lambda'v'\Lambda''v''}^2 \frac{S_{\Lambda''J''}^{\Lambda'J'}}{2J'' + 1}$$

$S_{\Lambda''J''}^{\Lambda'J'}$ Hönl-London factor, dependence on nuclear angular momentum

→ under the Born-Oppenheimer and the r-centroid approximations

$$M_{\Lambda'v'\Lambda''v''}^2 = q_{\Lambda'v'\Lambda''v''} R_e^2(\bar{r}_{v'v''})$$



Outline

- introduction

- energy structure

- molecular lines

- photo-processes

- conclusion

Pure vibration-rotation of homonuclear diatomic molecules

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

electric dipole transitions forbidden within an electronic state of homonuclear diatomic molecules (e.g. H₂, C₂, N₂, ...)

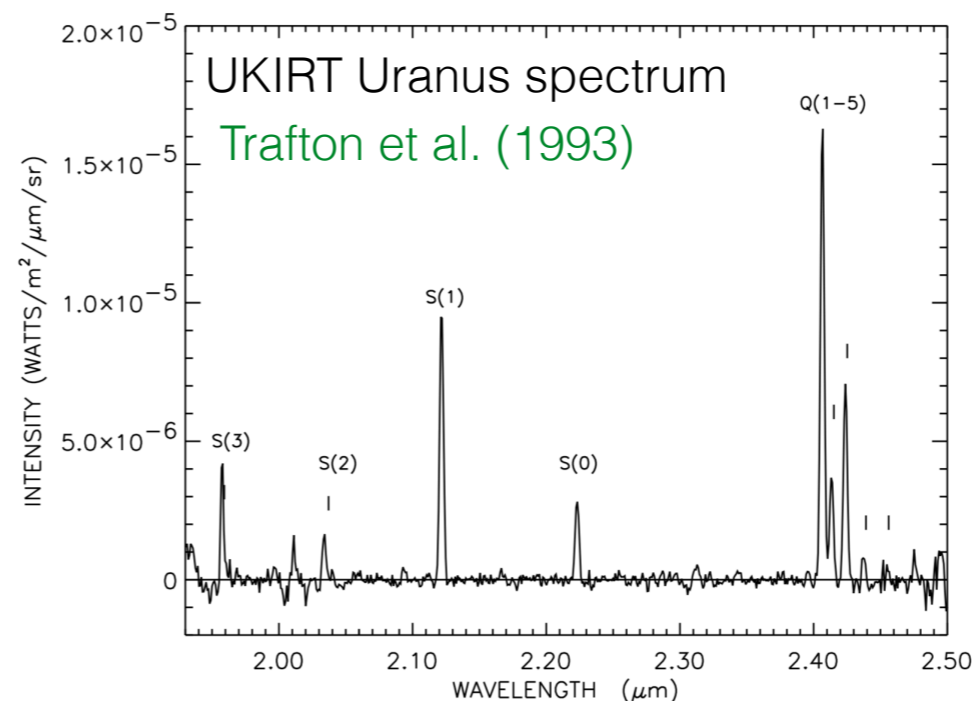
→ dipole magnetic and quadrupole electric transitions

→ example : H₂ - quadrupole electric transitions

selection rule for pure vibration-rotation $\Delta J = 0, \pm 2$ ($0 \leftrightarrow 0$)

labelling: J' (J'') associated with the upper (lower) energy level

name	$S(J'')$	$Q(J'')$	$O(J'')$
$\Delta J = J' - J''$	+2	0	-2



Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Ionization / dissociation / fluorescence

Principles of photo-processes

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

photoionization and photodissociation processes are fundamental

- to compute radiative transfer in molecular environments
- to compute chemical composition of diffuse & dense ISM, PDRs, protoplanetary disks, cometary & exoplanetary atmosphere, ...

microphysical process

- 1 - excitation of any (bound or not) electronic state



$$k = \int_{\lambda} \sigma(\lambda) N_{\lambda} d\lambda$$

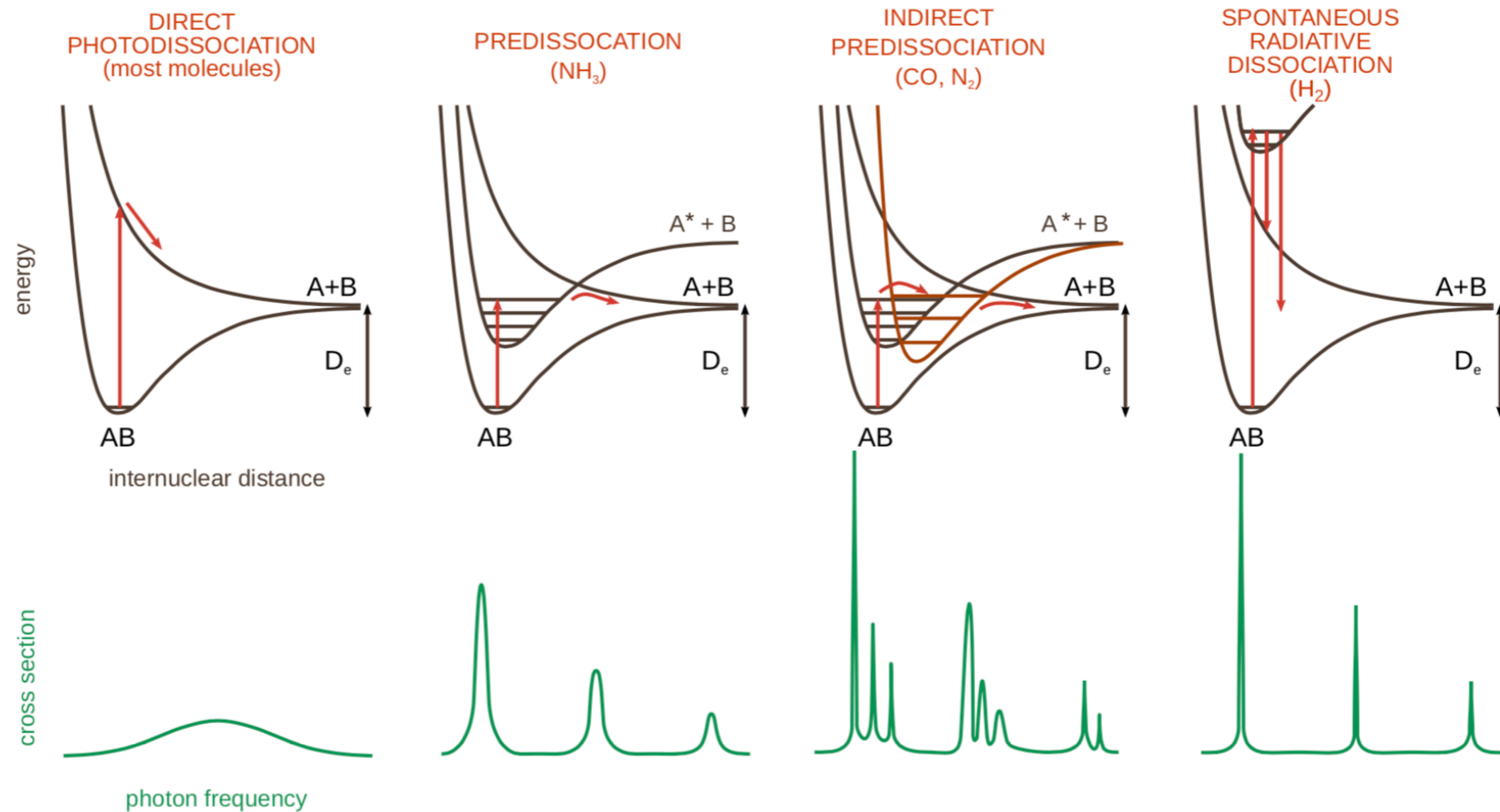
- 2 - relaxation towards a lower state branching ratios



Continuous or discret absorption

Several pathways to photodissociation

Heays et al. (2017)



- photodissociation may be a line or a continuum mechanism
- cross sections must account for all possible process
- line processes favor self-shielding

Outline

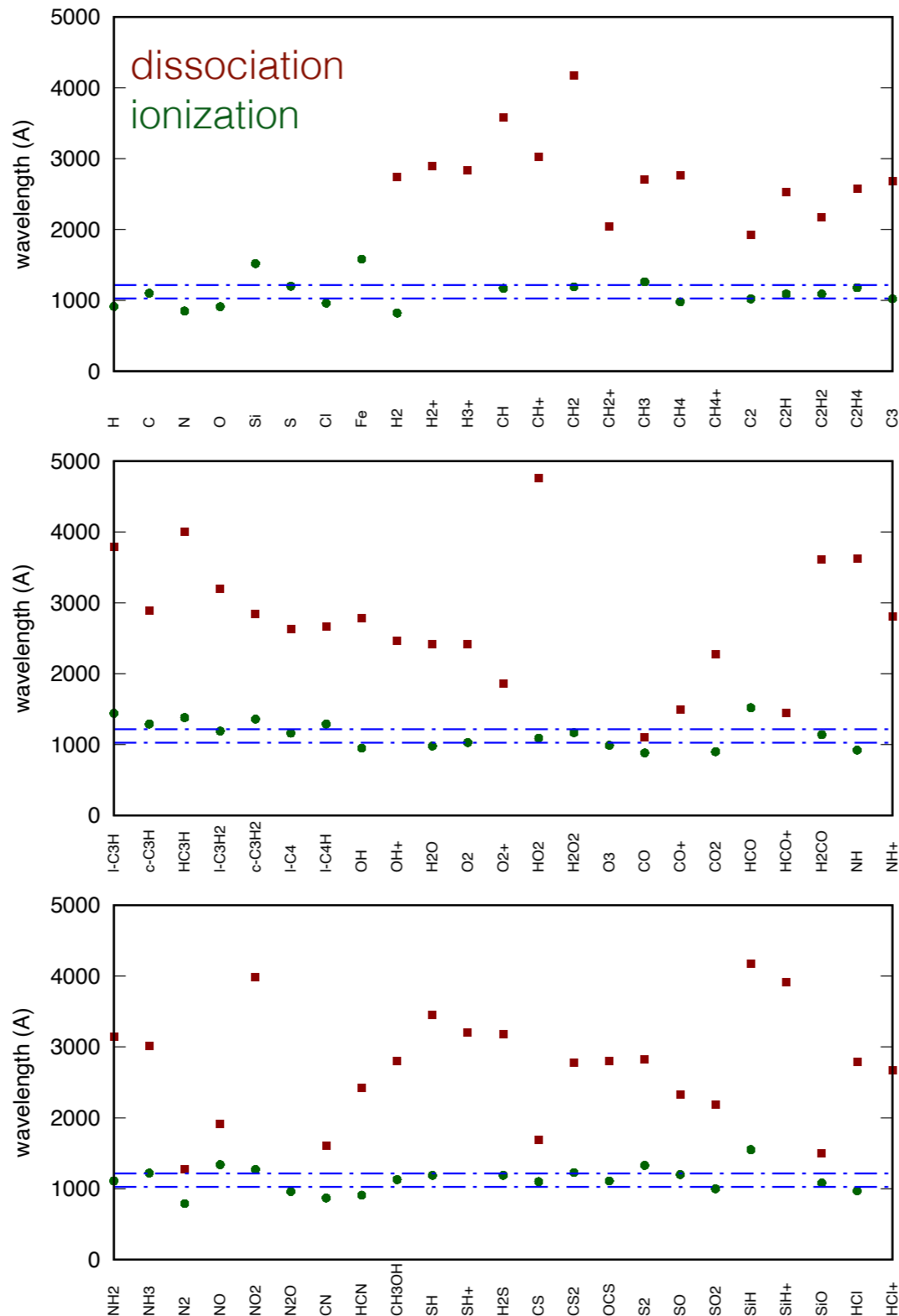
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Threshold and cross sections

Outline

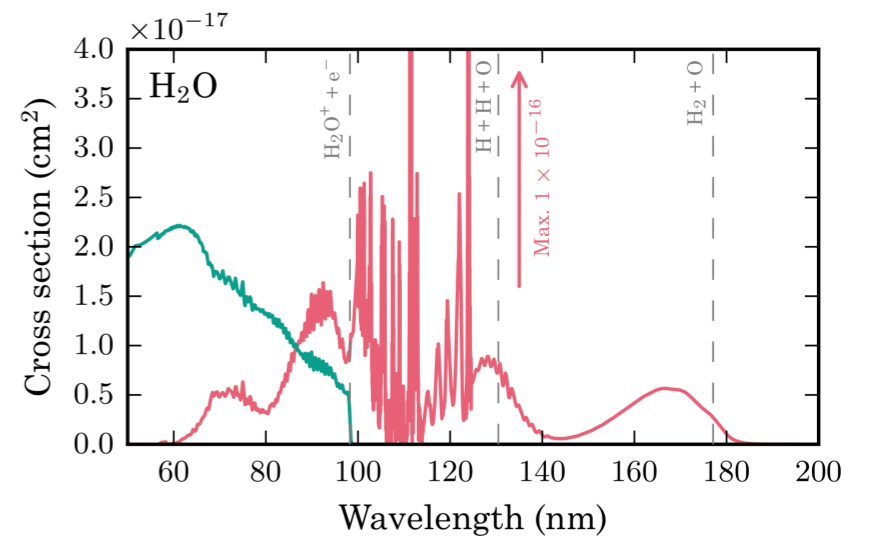
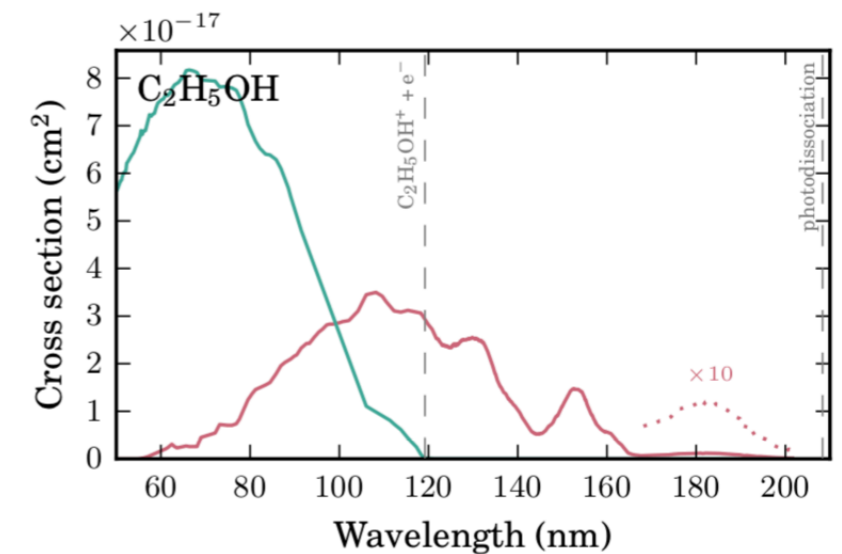
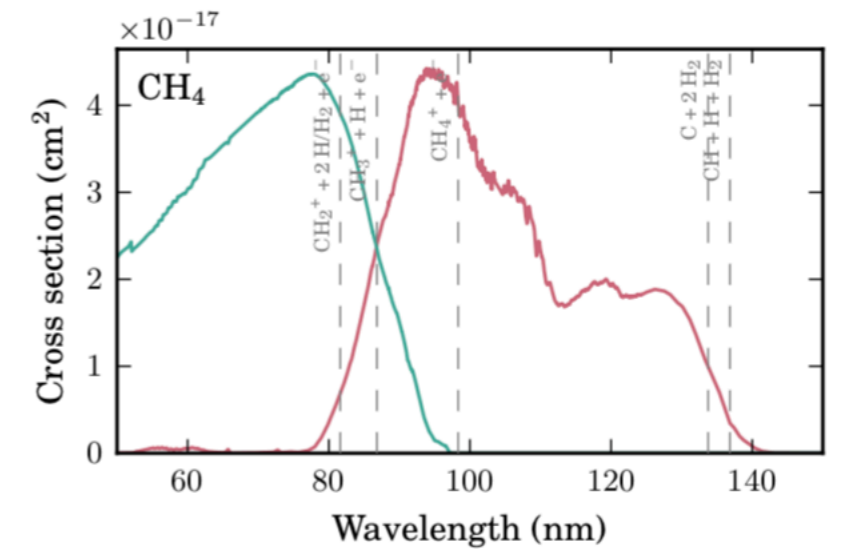
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

photo-processes threshold



derived from Heays et al. (2017)

examples of cross sections

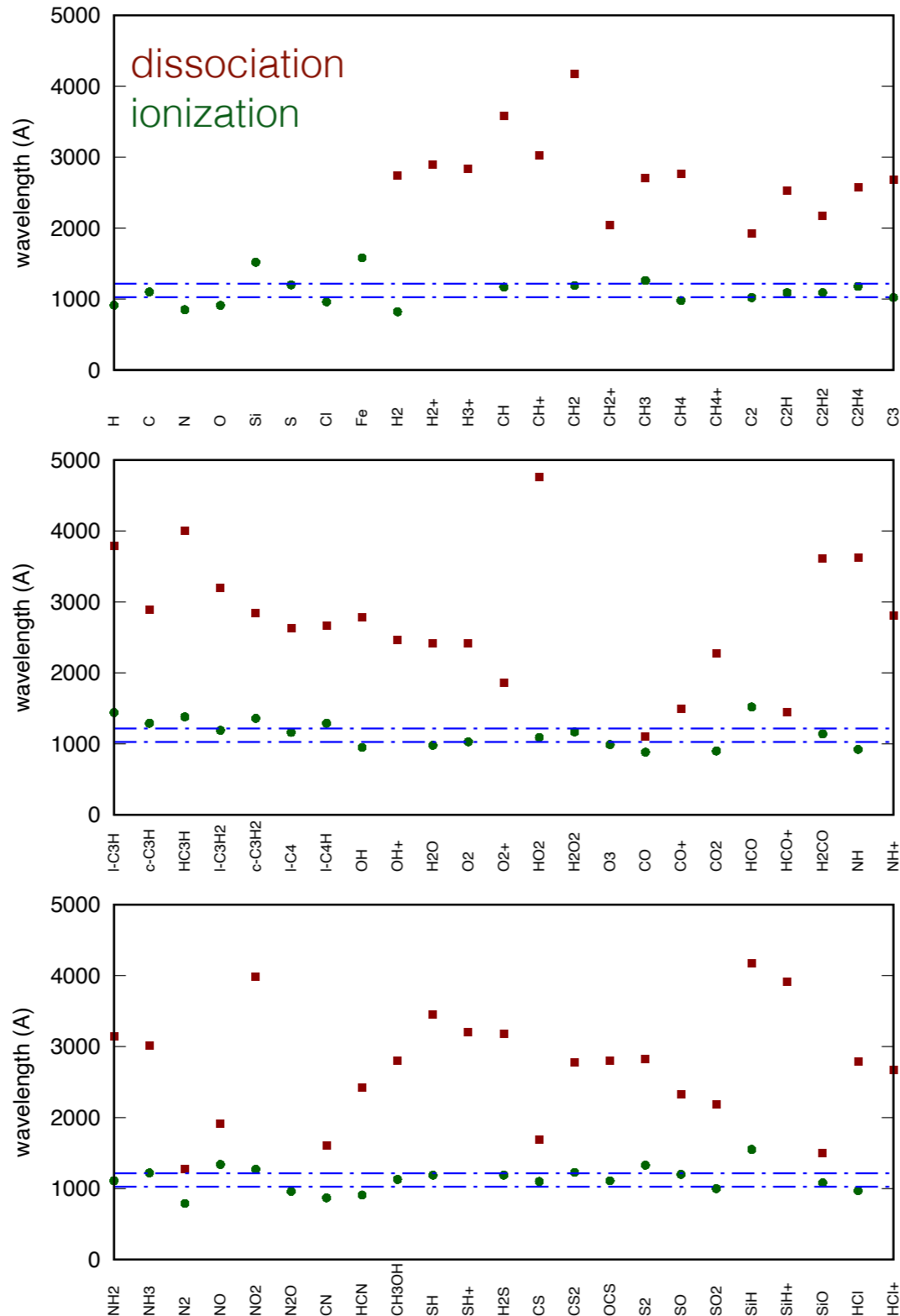


Threshold and cross sections

Outline

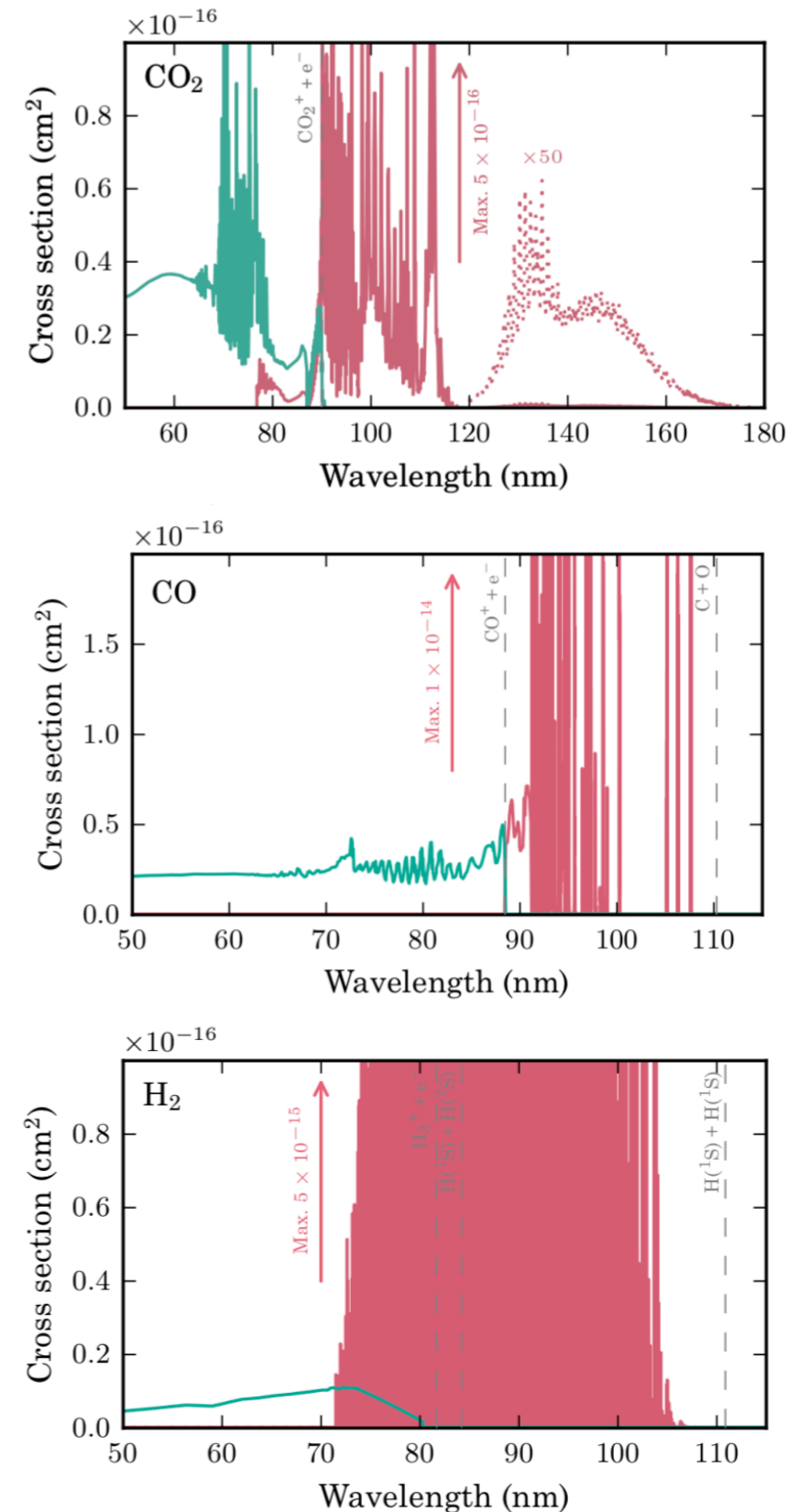
- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

photo processes threshold



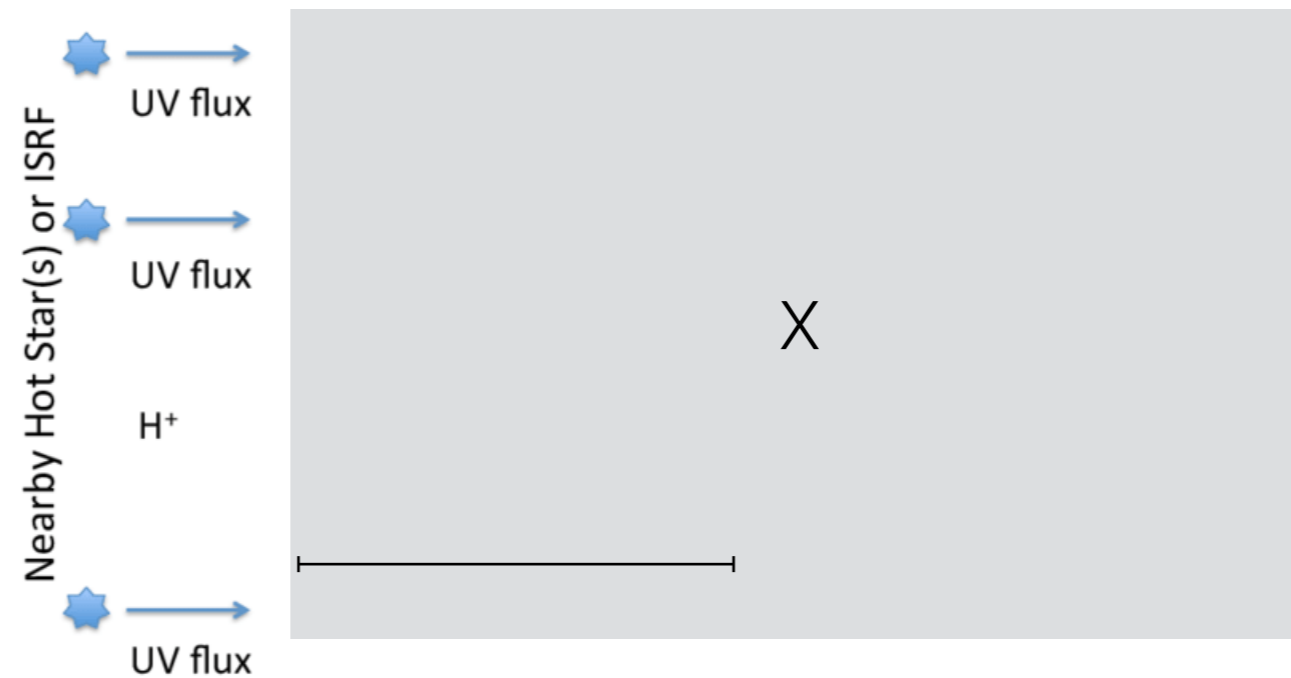
derived from Heays et al. (2017)

examples of cross sections



Self-shielding process

Consider a cloud illuminated by energetic photons

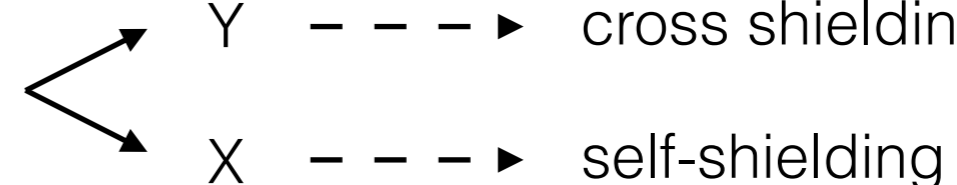


the abundance of X at any point depends on photo-processes

- intensity of the radiation field at specific wavelength
- absorption processes from the border of the cloud

by dust grains - - - - - → dust shielding

by atoms and molecules Y - - - → cross shielding

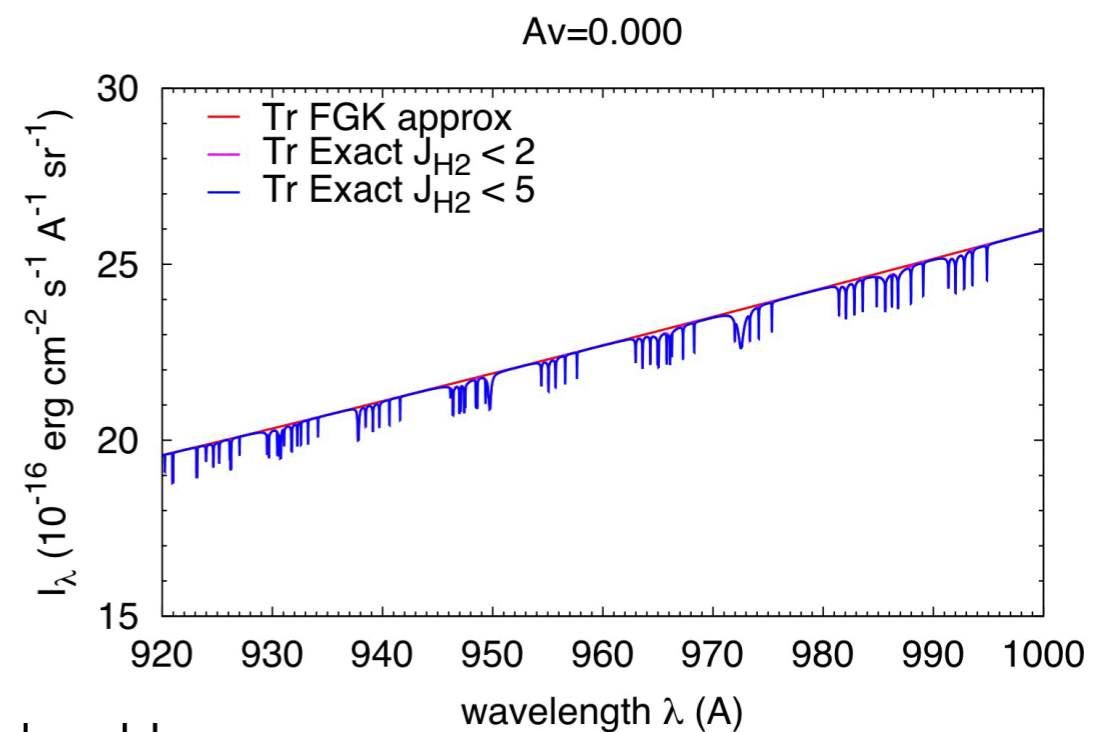
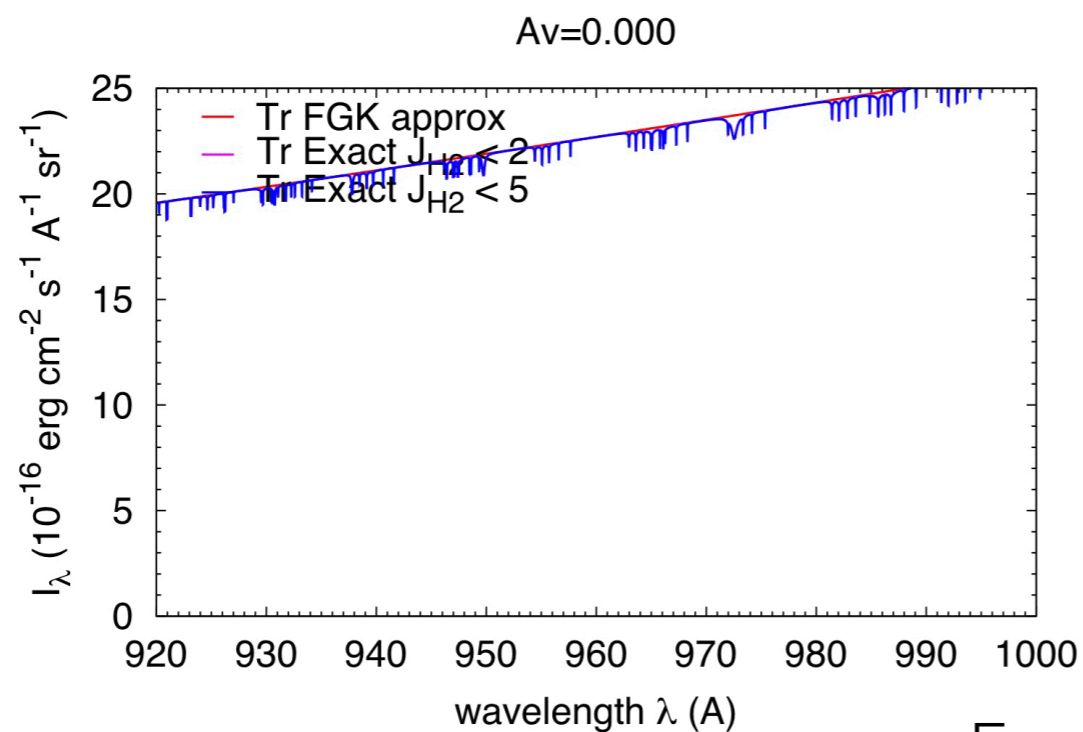
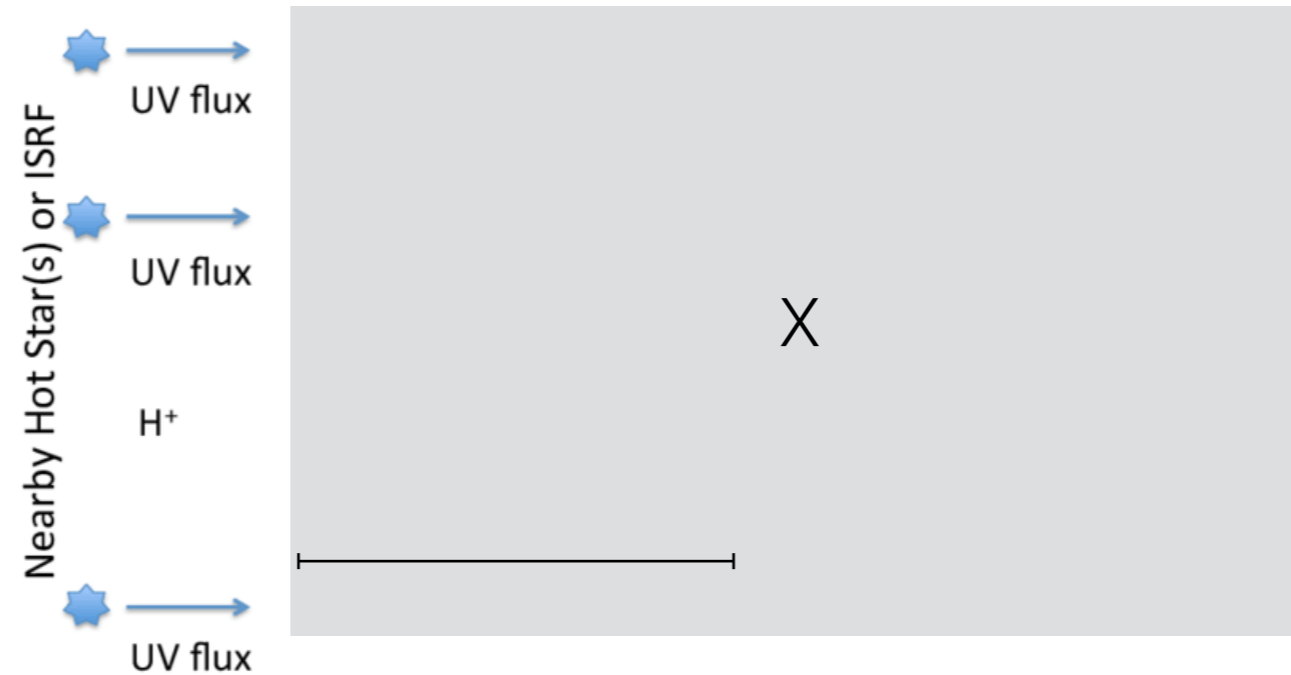


X - - - → self-shielding

- Outline
- introduction
 - energy structure
 - molecular lines
 - photo-processes
 - conclusion

Self-shielding process

Consider a cloud illuminated by energetic photons



Example : H₂

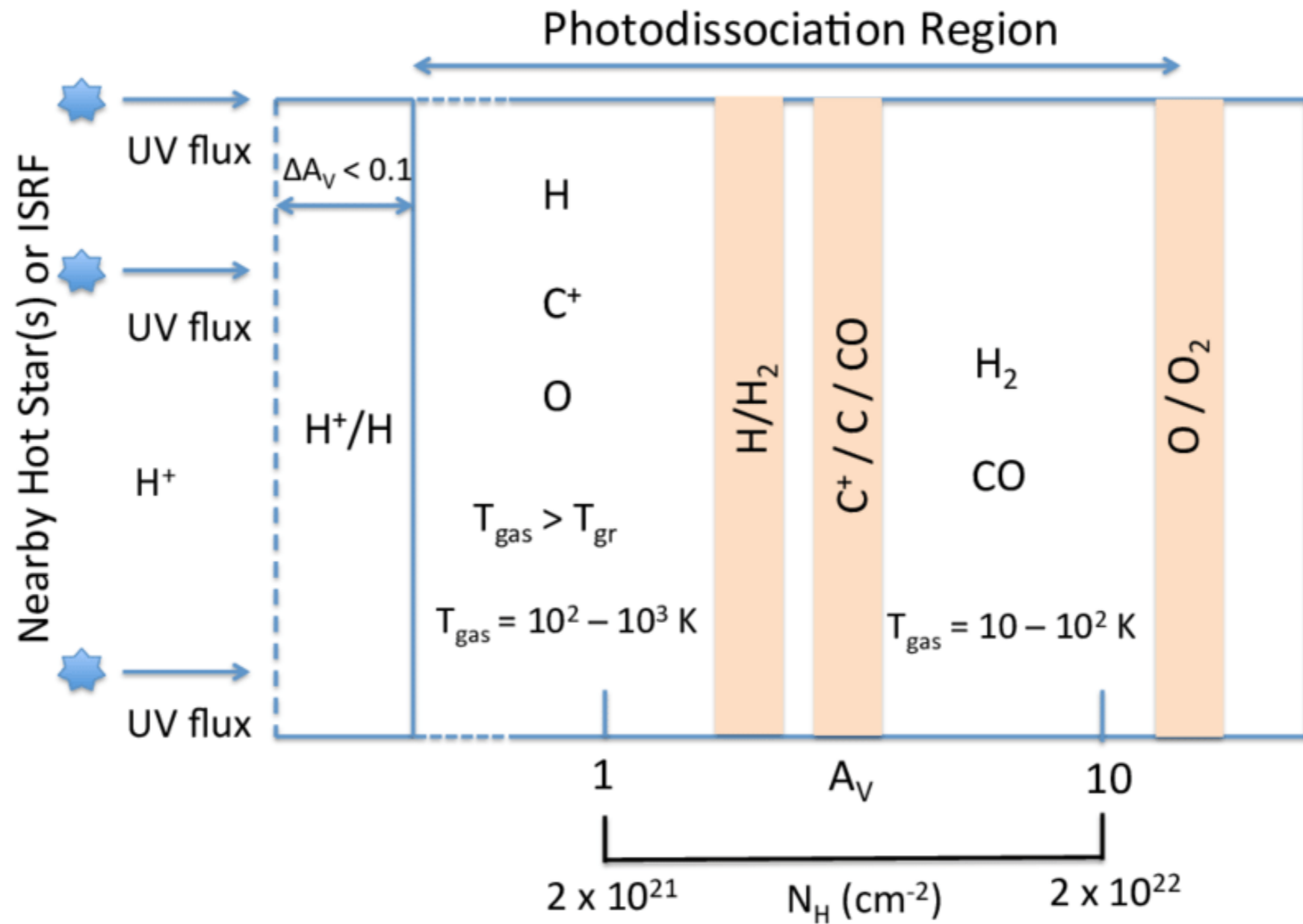
Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion

Self-shielding process

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion



Hollenbach & Tielens (1999)

Molecular structure and spectroscopy

- simplifications gives strong insight on molecular structure
Born-Oppenheimer → elec orbitals & quantum numbers
separation vibration / rotation → vib oscillator & rotational orbitals
additional couplings → fine & hyperfine structure
- electric dipole transitions obey to stringent transition rules
molecular spectra highly structured (band, branches, fine / hyperfine)
- homonuclear diatomic molecules radiate through quadrupole transitions

Interactions with radiation field

- ionization / dissociation / fluorescence originate from mol transitions
- non linear coupling between transfer and composition (e.g. self-shielding)

Outline

- introduction
- energy structure
- molecular lines
- photo-processes
- conclusion