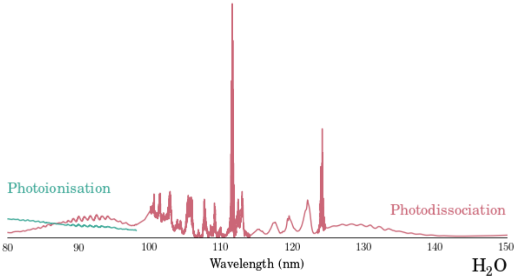
An updated list of photodissociation and ionisation rates in stellar and cosmic-ray induced radiation fields



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Objective

Update and extend the Leiden database

- Astrochemically relevant molecules, ions, and radicals
  – Some new additions
  – Recent lab./theor. studies included

- Photodissociation and ionisation rates
  - Interstellar
  - Circumstellar
  - Cosmic-ray induced radiation field

  – Detailed treatment of wavelength dependence

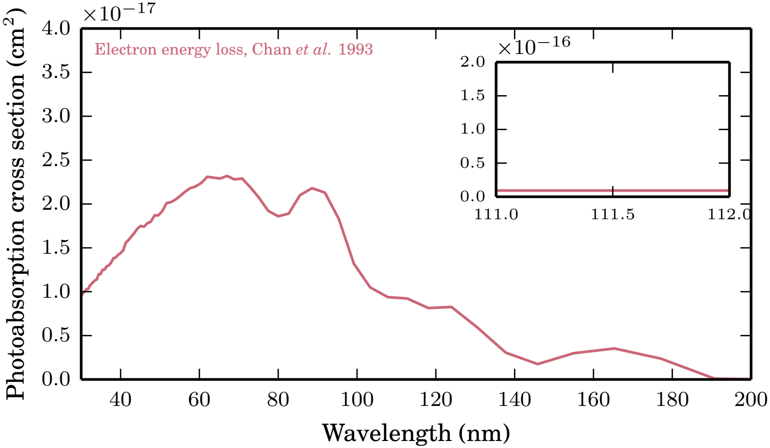
- Depth-dependent shielding
  – Detailed data for N_2

- Simple rates and parameterisations for input to astrochemical models

Sources of astrochemical photo rates

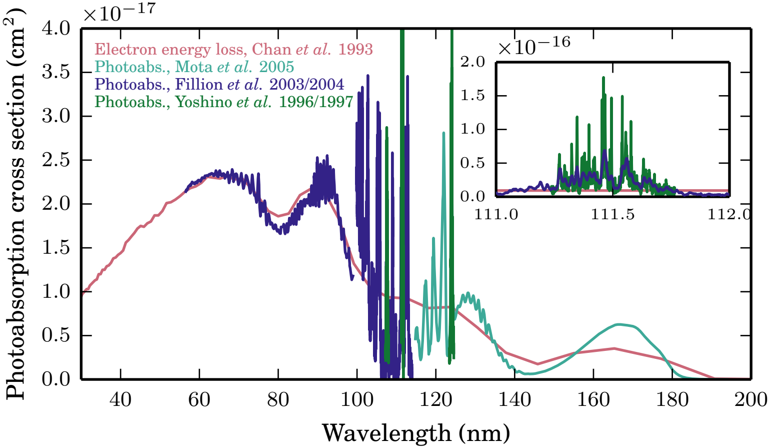
- Leiden database
  - Rates, depth-dependence
- PHIDRATES
  - Huebner et al. 1992, 2015
  - Rates and product branching
  - Solar and planetary focus
- Cosmic ray photodissociation
  - Gredel et al. 1987, 1989
- Diatomic molecules
  - H_2 e.g., Abgrall et al., Sternberg et al. 2014
  - CO e.g., Visser et al. 2009
  - N_2 e.g., Li et al. 2013, Heays et al. 2014
- Astrochemistry databases
  - UMIST / UDFA / RATE2012
  - KIDA (+OSU)
  - VAMDC virtual database

Experimental cross sections – H_2O



Often broadband low-resolution measurements.

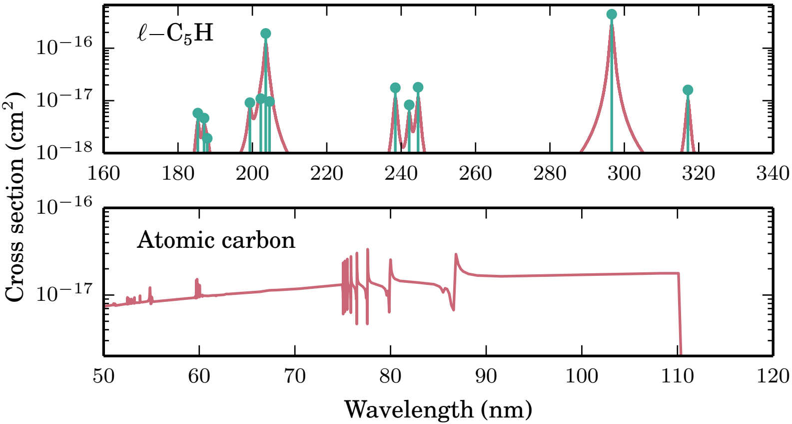
Experimental cross sections – H_2O



Often broadband low-resolution measurements.

Complemented by higher-resolutions.

Calculated cross sections



Sources:

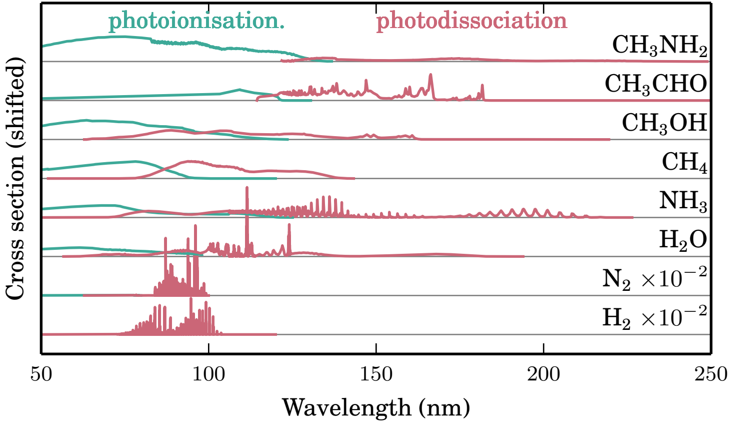
ℓ-C_5H – Hemert and Dishoeck 2008

Carbon – TOPBASE

Sources of atomic/molecular cross section

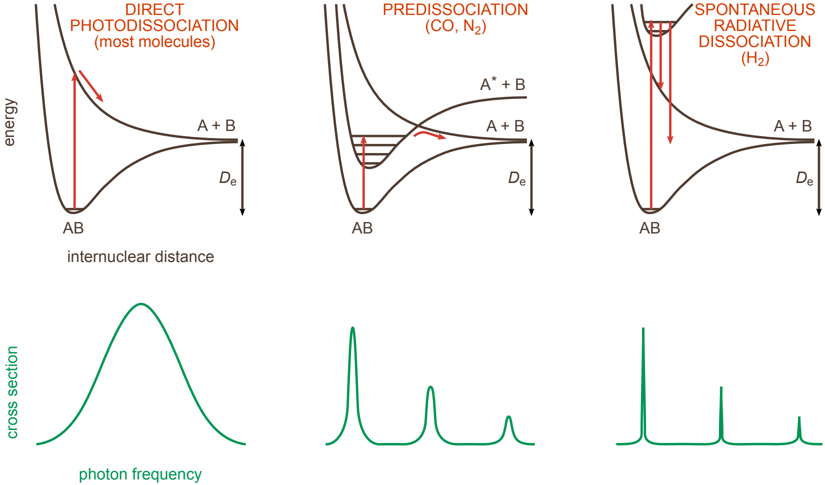
- MPI-Mainz UV/VIS spectral atlas
- Leiden database
- PHIDRATES
- MOLAT Paris Observatory
- Harvard CfA molecular database
- The opacity project (atoms/ions)
- General literature

Example cross sections



Widely varying thresholds and peak ranges

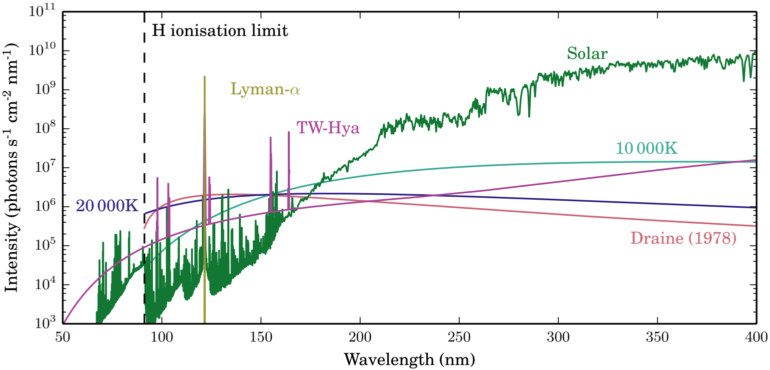
Qualitative photodissociation regimes



Larger molecules tend to be unstructured.

Photoionisation usually continuous with wavelength.

Radiation fields

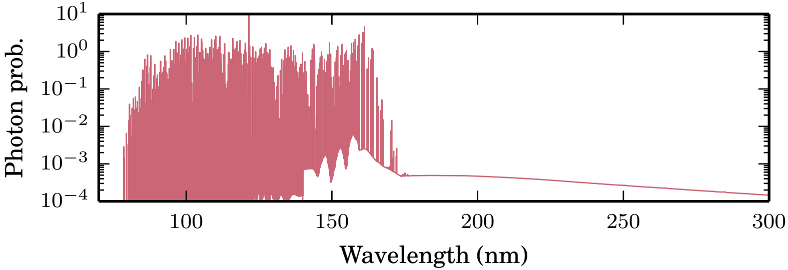


$$\text{photo rate} = \int \text{intensity} \times \text{cross section } d\lambda$$

Here we consider structured radiation fields and wavelength shorter than 91.2 nm.

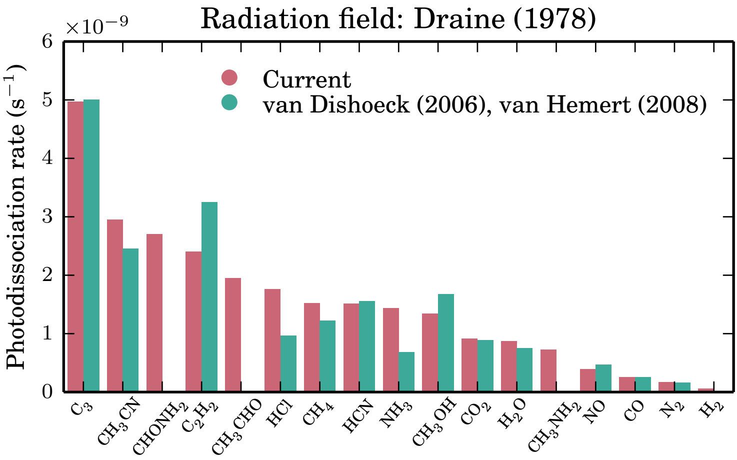
Cosmic-ray induced radiation

$$p^+ + H_2 \longrightarrow {H_2}^+ + e^-$$
$$e^- + H_2 \longrightarrow H_2^* \longrightarrow H_2 + \text{photon}$$



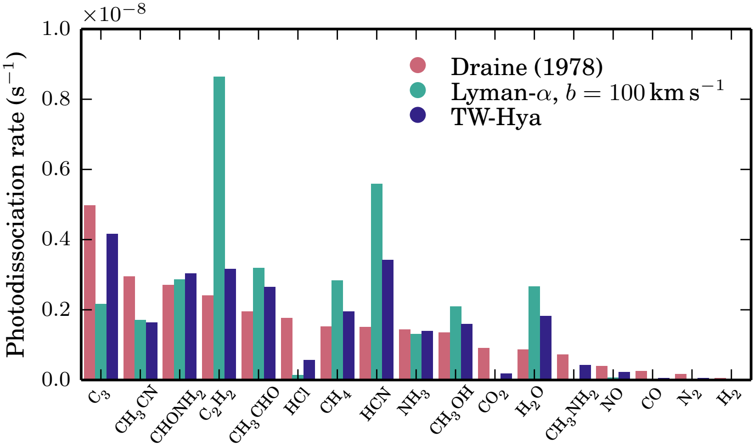
Critically dependent on high-resolution cross sections for structured molecules.

Photodissociation rates



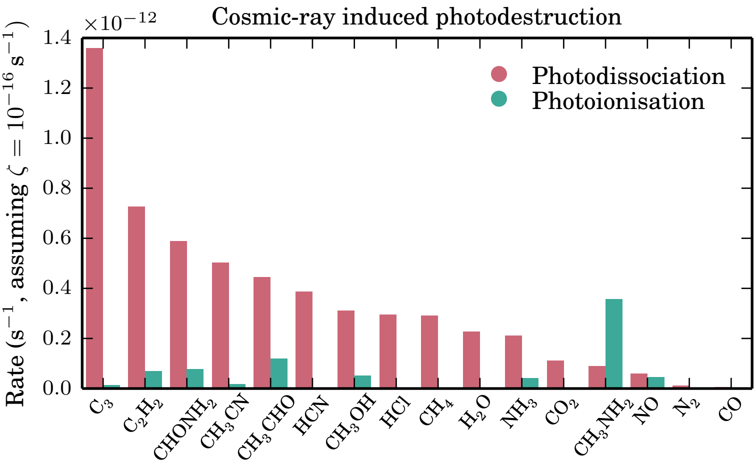
ISRF photodissociation rates not much changed

Photodissociation rates



Significant dependence on radiation field

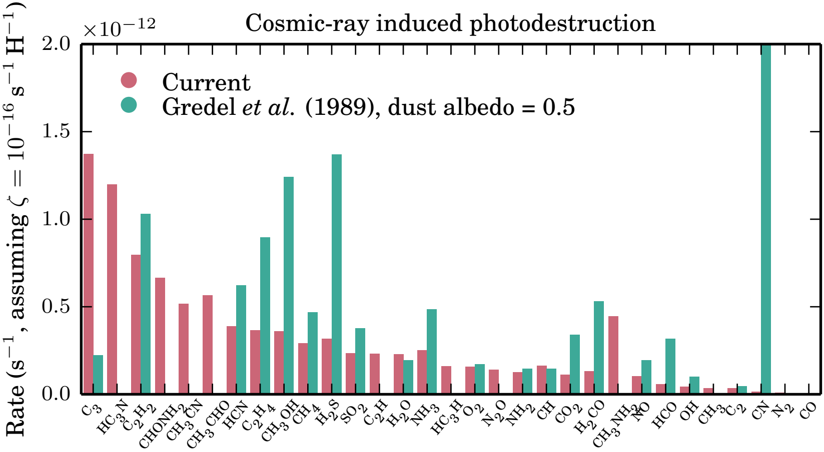
Photodissociation and ionisation due to cosmic rays



ζ = ionisation rate of H_2 due to cosmic rays.

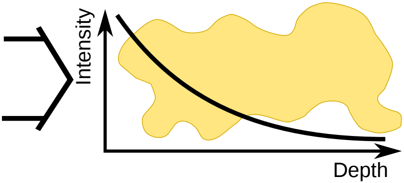
Rates are $\times 10^{-4}$ of those in the standard ISRF.

Photodissociation and ionisation due to cosmic rays



Well worth the update

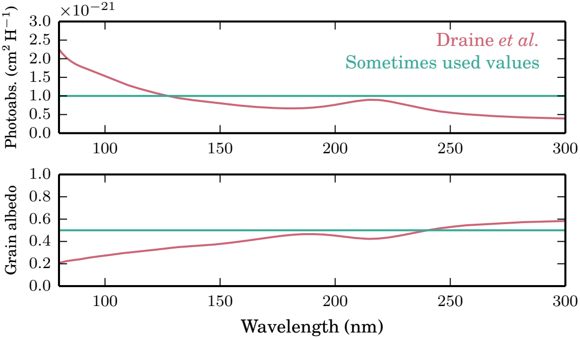
Radiation shielding



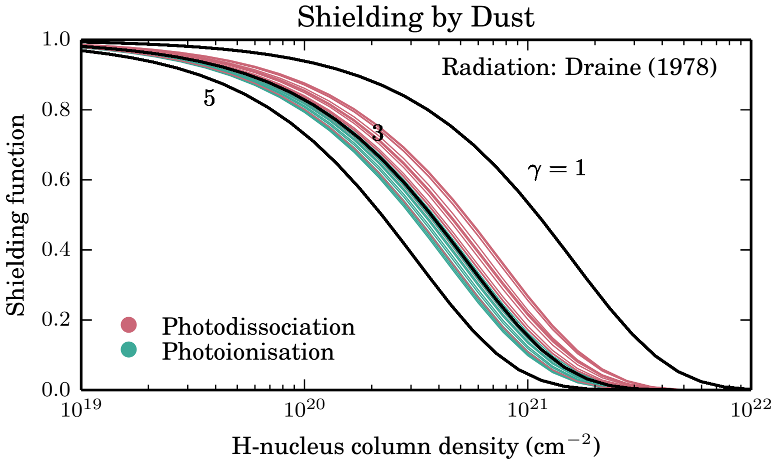
Considering: Dust, H_2, H, self-shielding

Simple model: Single-sided illumination

Dust optical properties – Draine *et al.*



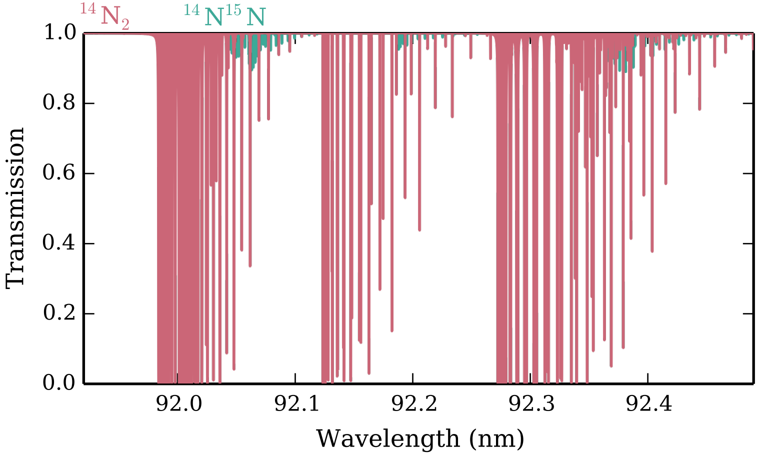
Shielding by dust – 14 molecules



1 = unshielded, 0 = no photons

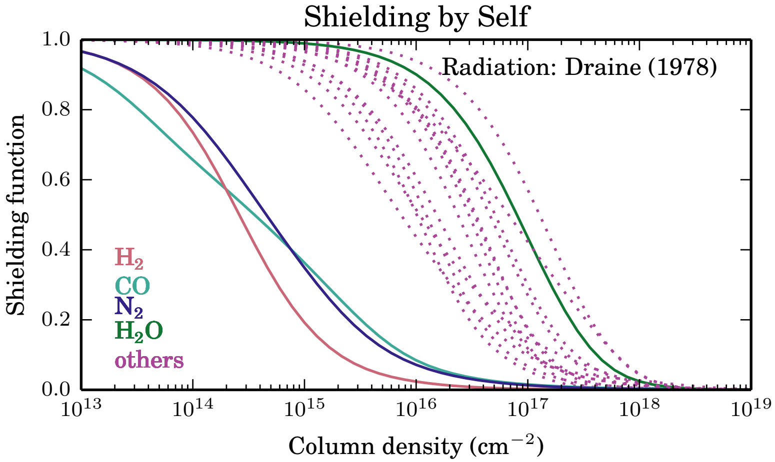
γ = A_V enhancement,

Self-shielding – N_2



- Sharply peaked $^{14}N_2$ lines quickly saturate
- $^{14}N^{15}N$ is unaffected by a saturated $^{14}N_2$ column

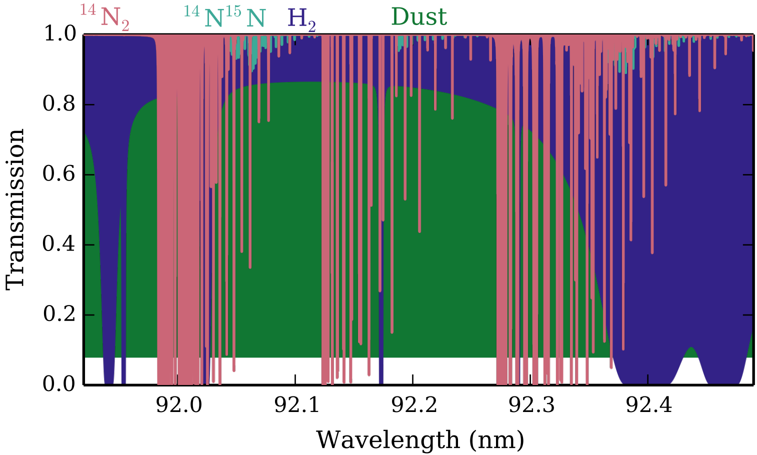
Self shielding in the ISRF – 14 molecules



1 = unshielded, 0 = no photons

Important for small and abundant molecules

More realistic shielding



In the case of N_2 and CO, comparable effects from dust, H_2, and self-shielding.

Summary

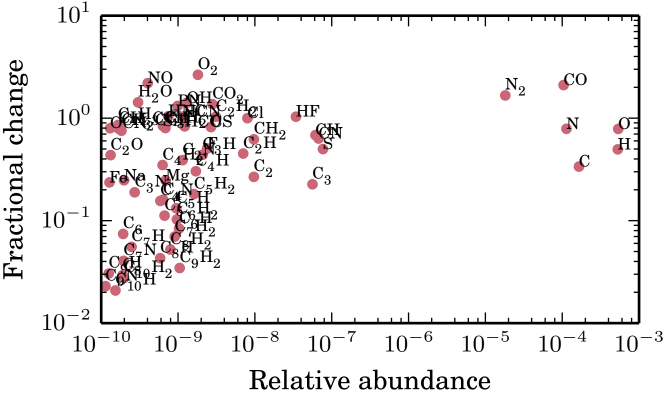
- A review of cross sections, rates, and shielding functions for astrochemically-important molecules
- Full wavelength dependence of cross sections and radiation fields
- Publication on the internet
  `home.strw.leidenuniv.nl/~ewine/photo`

Continuing problems

- In astrochemistry:
  - Characterisation of the remote radiation fields
  - Variable optical properties of dust grains
- In chemical physics:
  - Calculation of absolute cross section for radical species
  - Variation of molecular cross sections with temperature and isotopologue
  - Photofragment branching of neutral species

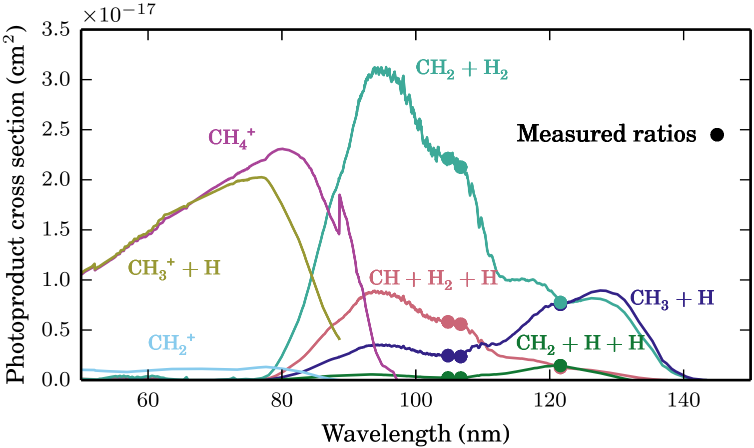
Effect new photodissociation rates on a simple astrochemical model

ISRF / 10 000 K blackbody



Single-point model: $T = 100\,\mathrm{K}$, $A_V = 1\,\mathrm{mag.}$, $n = 10^5\,\mathrm{cm}^{-3}$

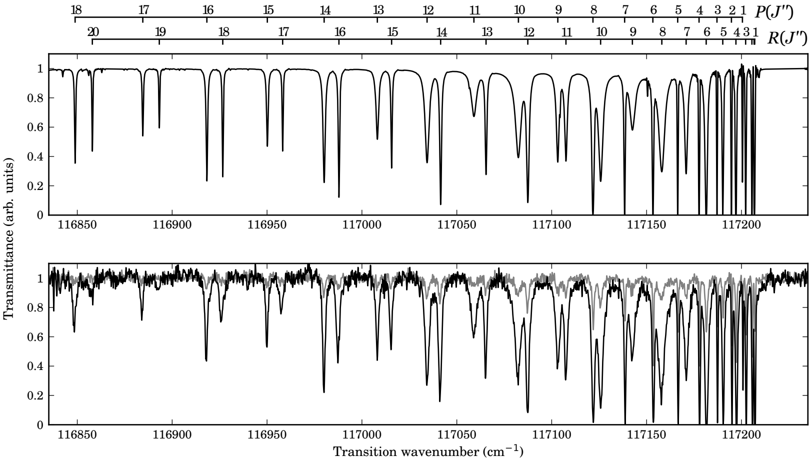
Photofragment branching – CH_4



Very few neutral branching ratios measured.
Dissociative-ionisation branching not so bad.

Modelled N_2 spectrum

$b'\,^1\Sigma_u^+(v'=20) \leftarrow X\,^1\Sigma_g^+(v''=0)$

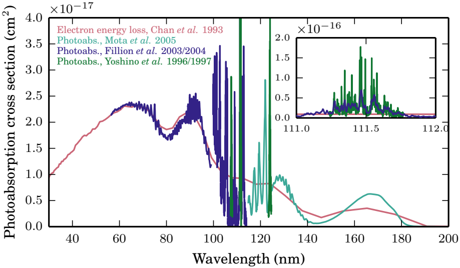


- *Upper*: Model spectrum.
- *Lower*: Laboratory spectrum (Fourier transform spectroscopy, synchrotron SOLEIL).

Less sensitive – H_2O

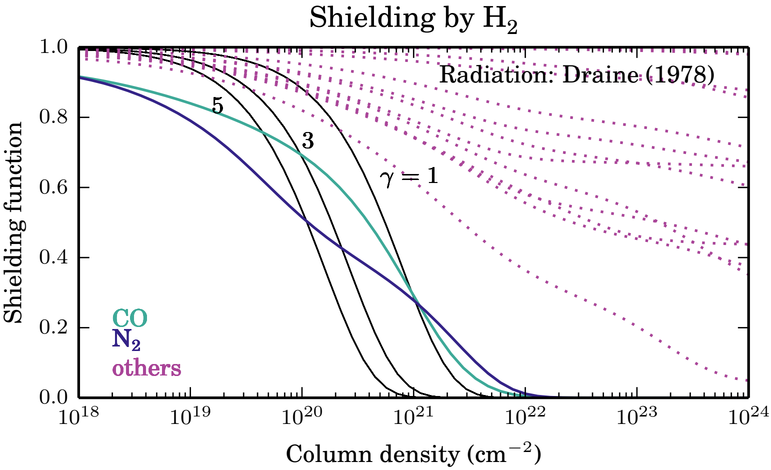
ISRF photodissociation rate

Highest – lowest resolution data = $7.4 - 8.3 \times 10^{-10}\,\mathrm{s}^{-1}$



Cosmic-ray induced photodissociation rate ($\times 10^{-16}\,\mathrm{s}^{-1}$)		
Shielded by...	Highest res.	Lowest res.
Dust	2094	2250
Dust, H_2	1914	1918
Dust, H_2, H, self, etc.	1890	1896

Shielding by H_2 - 14 molecules



1 = unshielded, 0 = no photons