Photodissociation and ionisation of molecules due to stellar and cosmic-ray-induced radiation

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Objective

Update and extend the Leiden database

- Astrochemically relevant molecules, ions, and radicals
- Interstellar photodissociation/ionisation rates
- Circumstellar photodissociation/ionisation rates
- Rates in the cosmic ray ionisation field
- Depth-dependent shielding
- One less thing for astrochemical modellers to worry about

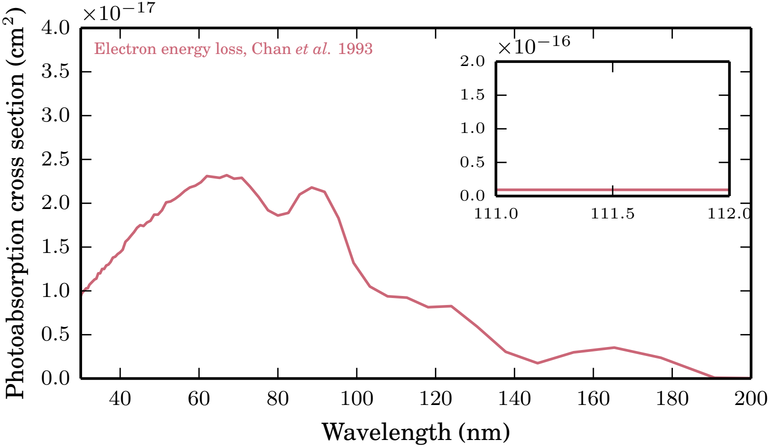
Astrochemistry data sources

- The current Leiden database
  - Rates, depth-dependence
  - Detailed CO and N_2 shielding
  - Lee 1984, van Dishoeck 1988, van Dishoeck 2006, van Hemert and van Dishoeck 2008
- Diatomic molecules:
  - H_2 e.g., Abgrall *et al.*, Sternberg 2014
  - CO e.g., Visser 2009
  - N_2 e.g., Lewis 2005, Li 2013, Heays 2014
- PHIDRATES
  - Huebner 2015, 1992
  - Rates and product branching
  - Solar and planetary focus
- Cosmic ray photodissociation
  - Gredel 1987, 1989
- Subsidiary databases
  - UMIST / UDFA / RATE2012
  - KIDA (+OSU)
  - VAMDC virtual database

Cross section data sources

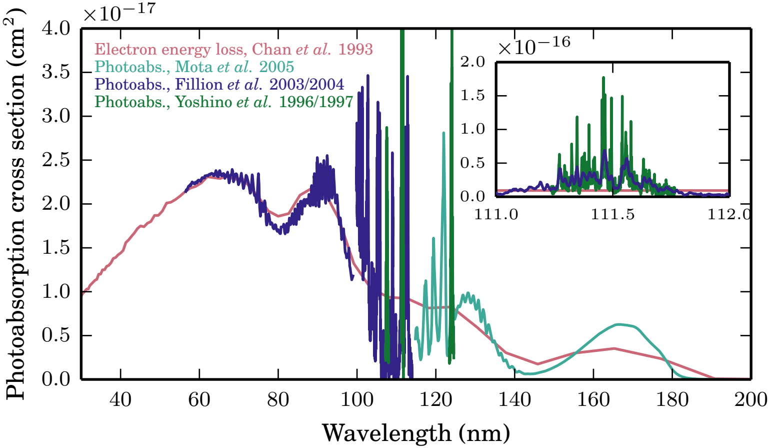
- MPI-Mainz UV/VIS spectral atlas
  - Comprehensive measured cross sections
- Leiden database
- PHIDRATES
- MOLAT Paris Observatory
- Harvard CfA molecular database
- The literature

Cross sections – H_2O



Often broadband low-resolution measurements.

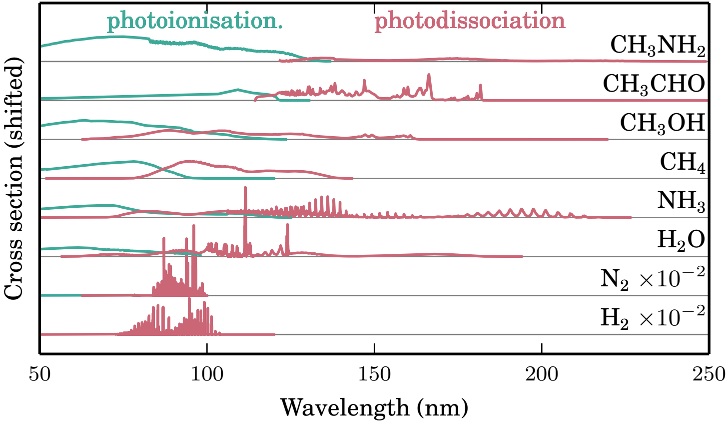
Cross sections – H_2O



Often broadband low-resolution measurements.

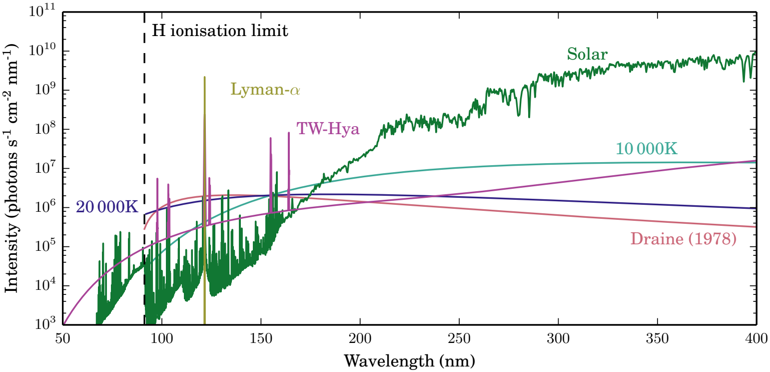
Complemented by higher-resolutions.

Example cross sections



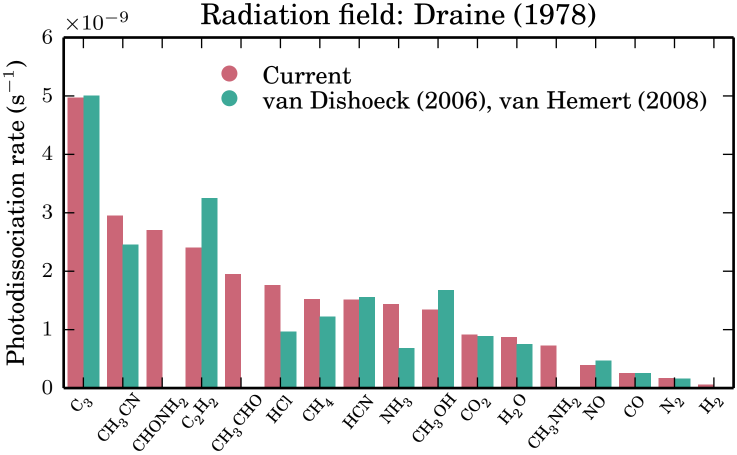
Widely varying thresholds and peak ranges

Radiation fields



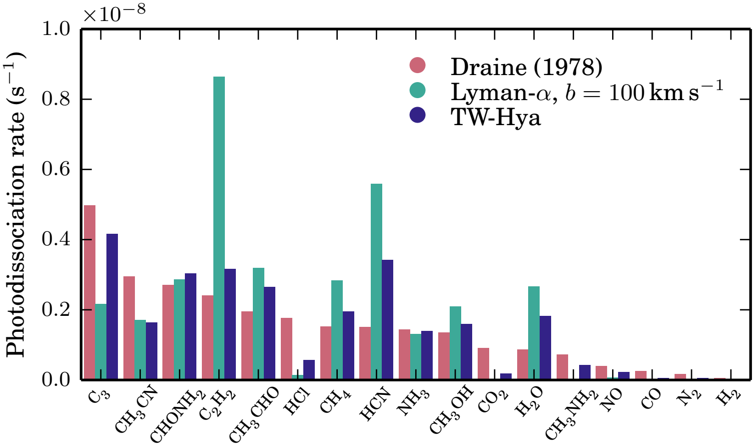
$$\text{photo rate} = \int \text{intensity} \times \text{cross section}\ d\lambda$$

Photodissociation rates



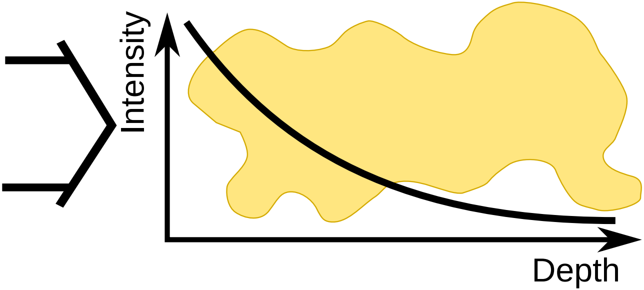
ISRF photodissociation rates not much changed

Photodissociation rates



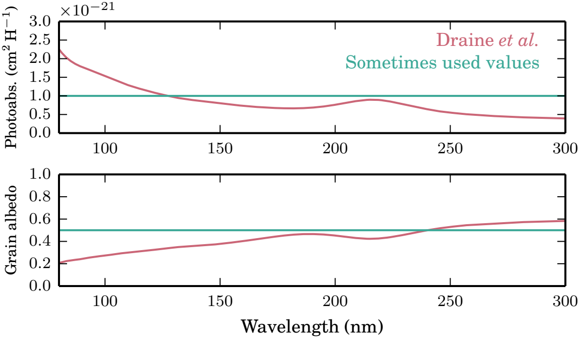
Significant dependence on radiation field

Radiation shielding



Considering: Dust, H_2, H, self-shielding
Simple model: Single-sided illumination

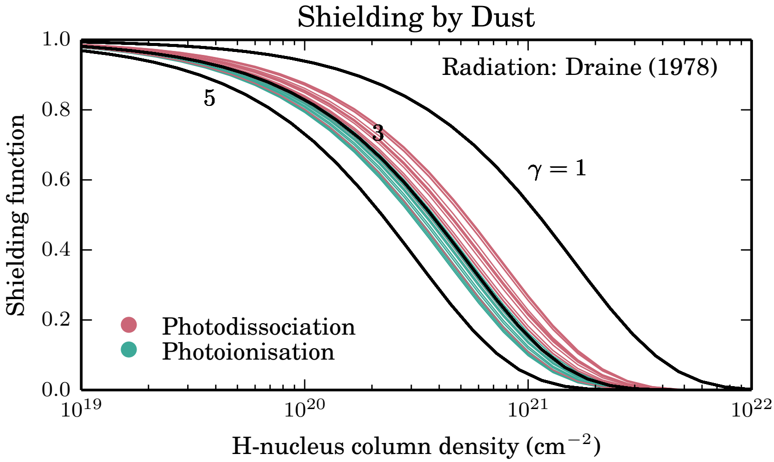
Dust grain optical properties



Draine *et al.* dust model

- Mixed carbonaceous and silicate grains according to Draine 2003, Weingartner & Draine 1992, Li & Draine 2001
- Gas:dust mass ratio of 123:1

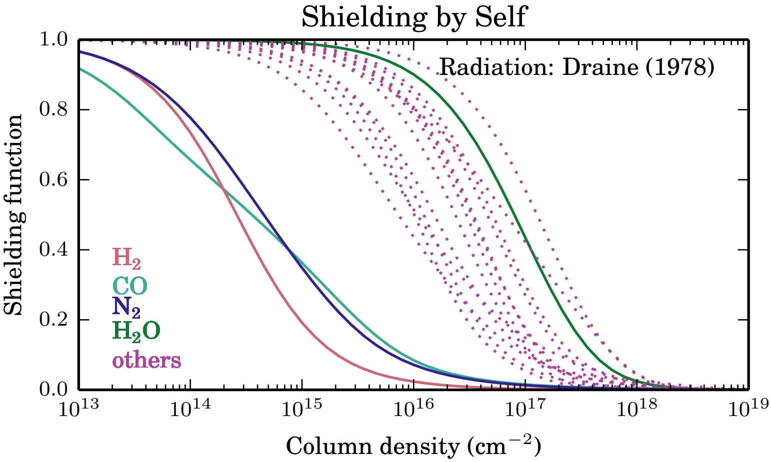
Shielding by dust – 14 molecules



1 = unshielded, 0 = no photons

γ = A_V enhancement,

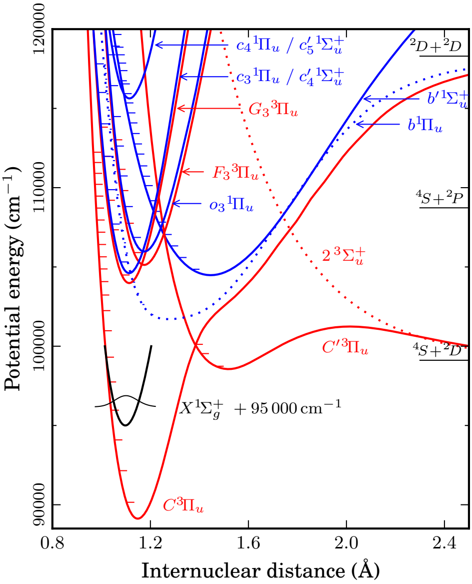
Self shielding in the ISRF – 14 molecules



1 = unshielded, 0 = no photons

Important for small and abundant molecules

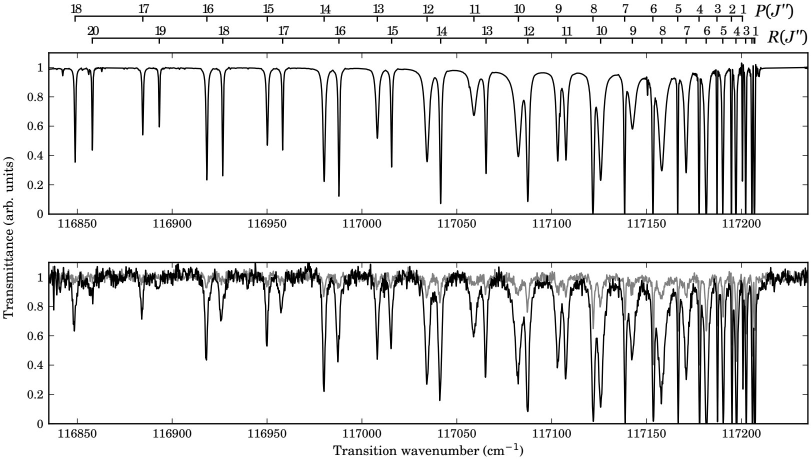
N_2 model – potential-energy curves



- ${}^1\Pi_u$ and ${}^1\Sigma_u^+$ states absorb and emit photons
- ${}^3\Pi_u$ and ${}^3\Sigma_u^+$ states have an open dissociation channel
- Spin-orbit coupling leads to predissociation of ${}^1\Pi_u$ and ${}^1\Sigma_u^+$ states

Modelled N_2 spectrum

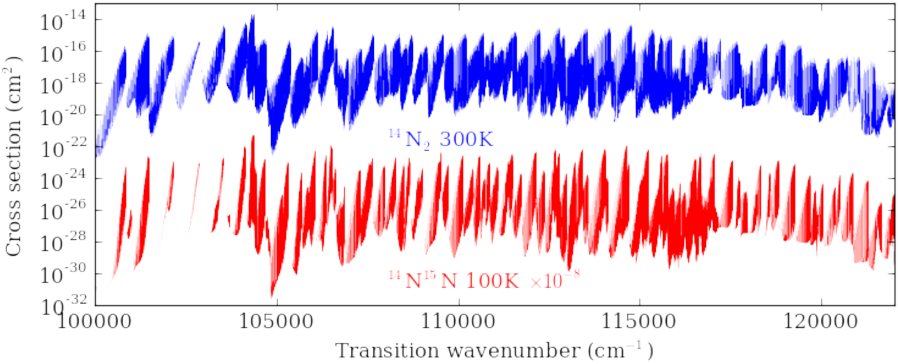
$b'\,^1\Sigma_u^+(v' = 20) \leftarrow X\,^1\Sigma_g^+(v'' = 0)$



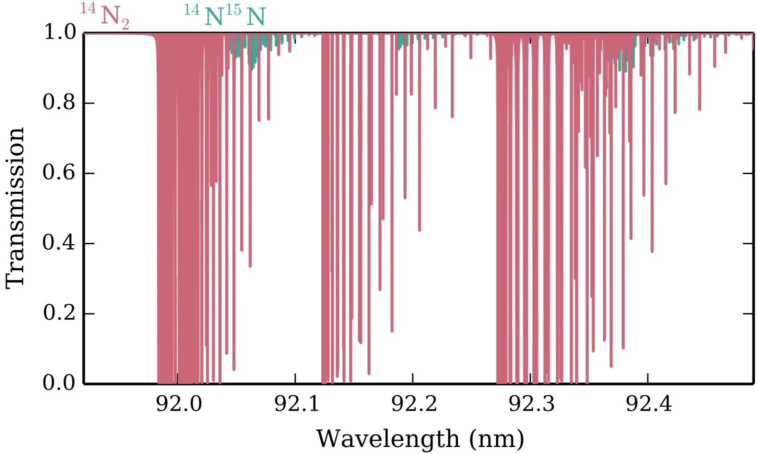
- *Upper*: Model spectrum.
- *Lower*: Laboratory spectrum (Fourier transform spectroscopy, synchrotron SOLEIL).

Modelled N_2 spectrum

Photoabsorption cross section from $X(v'' = 0)$

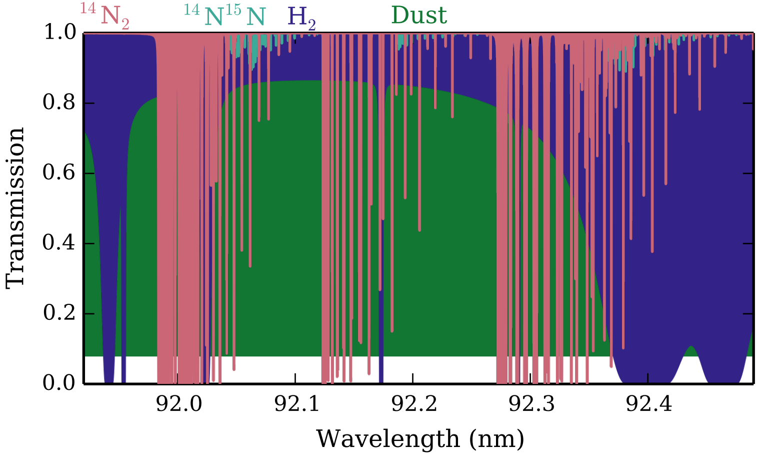


Self-shielding – N_2



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

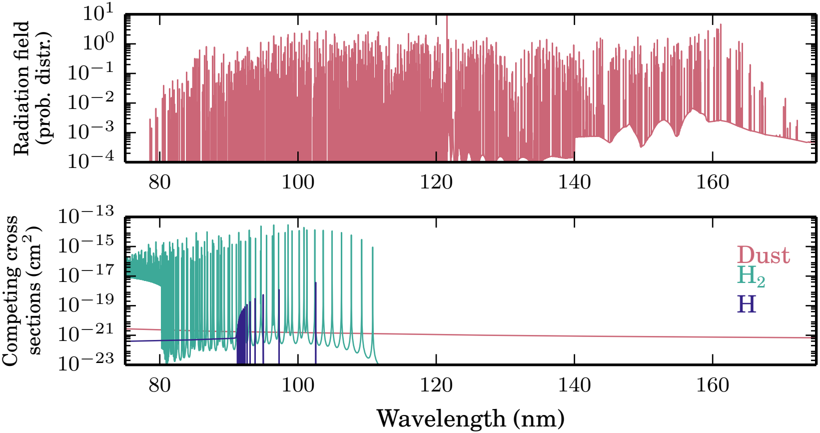
Self-shielding – N_2



- Sharply peaked $^{14}N_2$ lines quickly saturate
- $^{14}N^{15}N$ is unaffected by a saturated $^{14}N_2$ column
- Comparable or more important effect than shielding by H_2 and dust

Cosmic-ray induced radiation

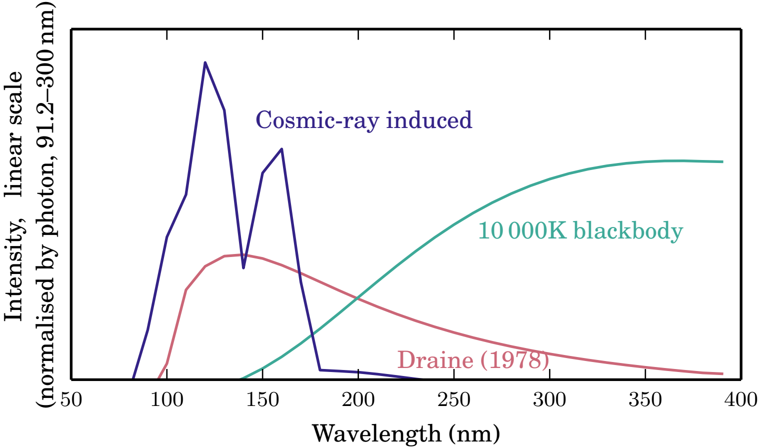
Model by Gredel *et al.*



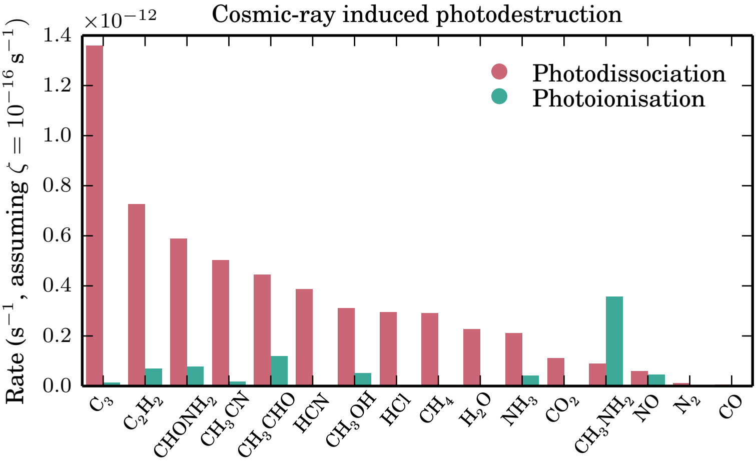
Weak continuum continues to 300 nm.

$$\text{Rate} = \int \text{intensity} \times \frac{\text{cross section}}{\text{competing absorption}}\, d\lambda$$

Cosmic-ray induced radiation



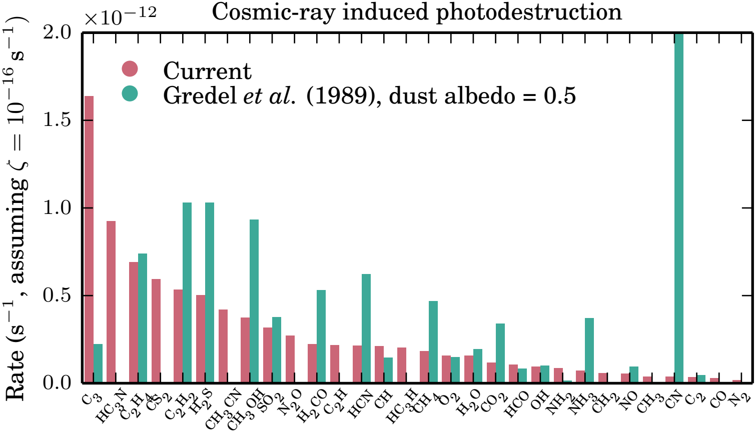
Photodissociation and ionisation due to cosmic rays



ζ = ionisation rate of H_2 due to cosmic rays.

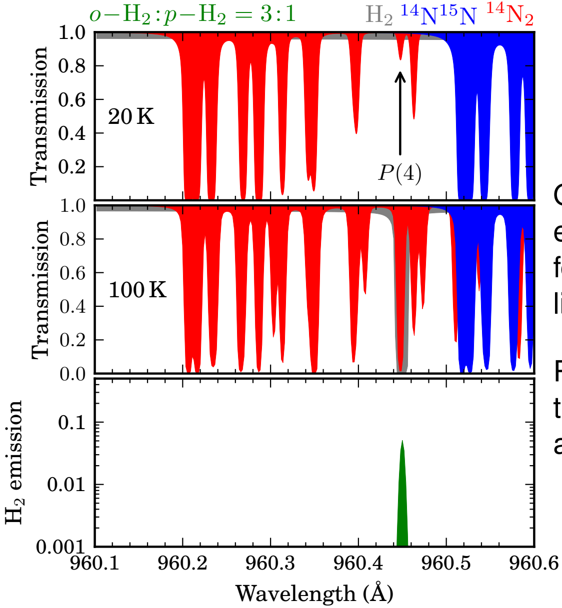
Rates are $\times 10^{-4}$ of those in the standard ISRF.

Photodissociation and ionisation due to cosmic rays



Well worth the update

Cosmic-ray induced photodissociation – N_2



Only a handful of H_2 emission lines overlap for species with line-like spectra.

Resulting sensitivity to ortho/para ratio and temperature.

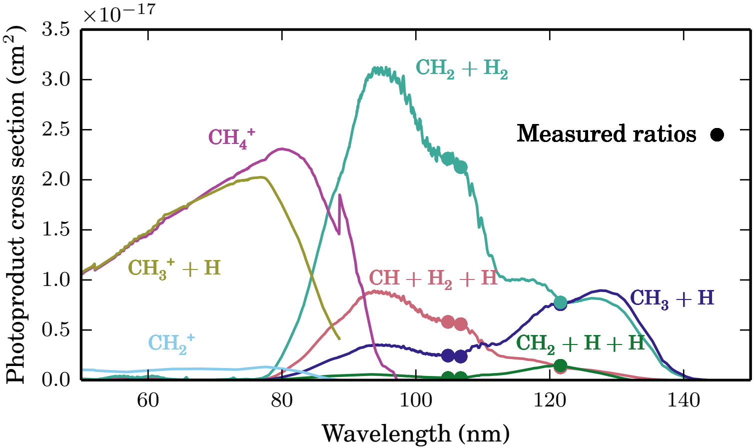
Summary

- 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 (soon)
  `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

Photofragment branching – CH_4

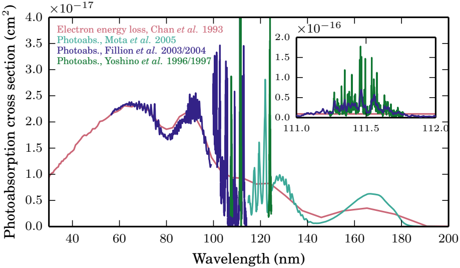


Very few neutral branching ratios measured.
Dissociative-ionisation branching not so bad.

Less sensitive – H_2O

ISRF photodissociation rate

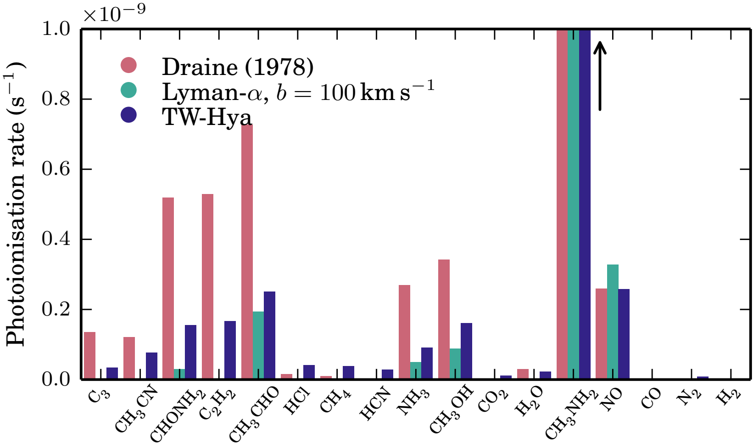
Highest – lowest resolution data = $7.4 - 8.3 \times 10^{-10}\,\mathrm{s}^{-1}$



Cosmic-ray induced photodissociation rate ($\times 10^{-16}\,\mathrm{s}^{-1}$)

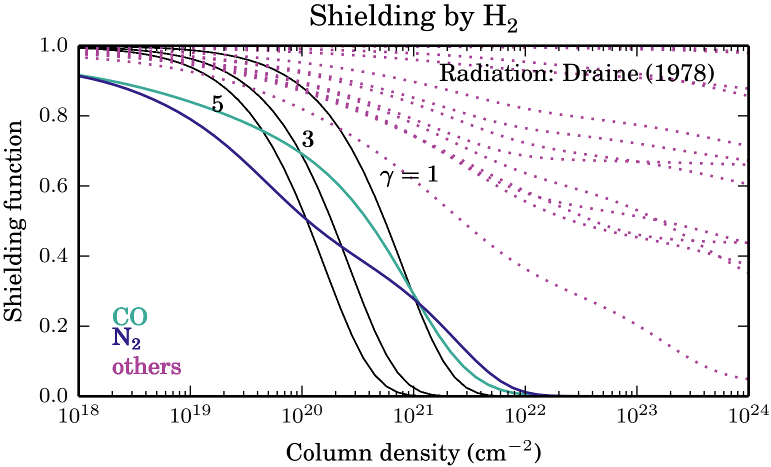
Shielded by...	Highest res.	Lowest res.
Dust	2094	2250
Dust, H_2	1914	1918
Dust, H_2, H, self, etc.	1890	1896

Photoionisation rates



Significant dependence on radiation field

Shielding by H_2 - 14 molecules



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