Photoprocesses under interstellar conditions.
The combined answer of gas and dust to UV radiation

✏ the general context

✏ Meudon PDR code : the 3 levels of approximation

✏ Photodissociation rates at the edge (no dust)

✏ The role of dust

✏ Impact of photodissociation approximations on model results

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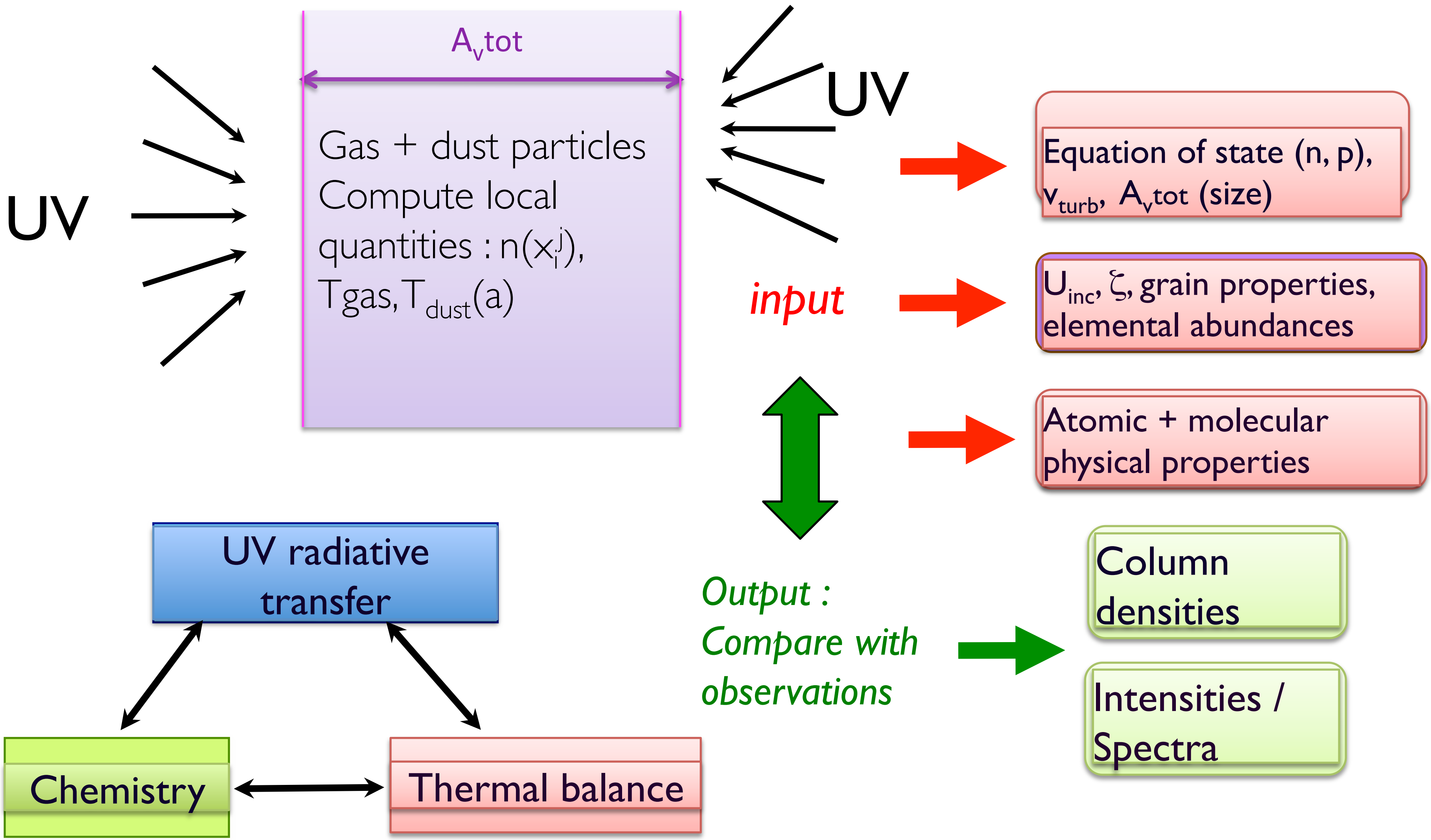
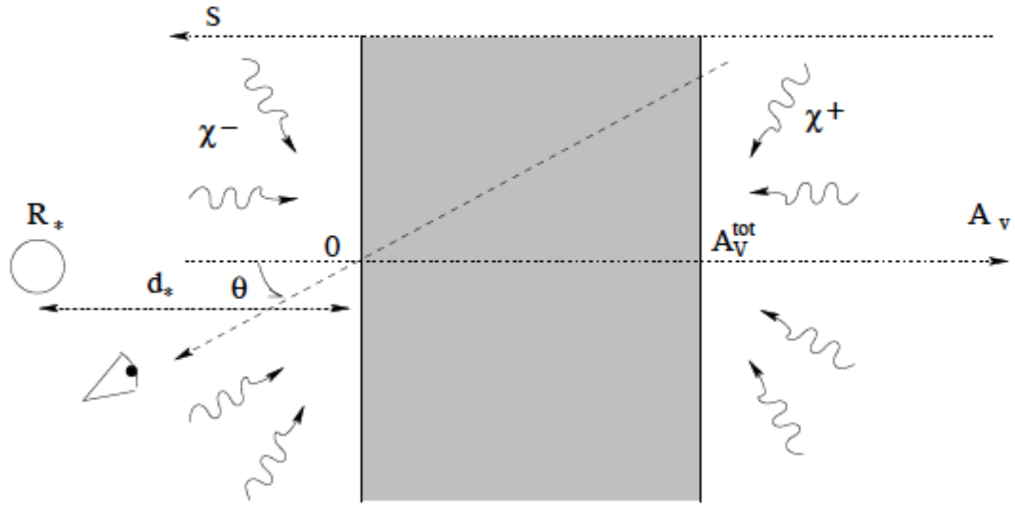
Photon Dominated Region (PDR)

Benchmark of PDR models: Röllig et al. 2007, AA 467, 187



Radiative transfer : a short summary

1D steady state (not equilibrium) irradiated slab



$$\mu \frac{\partial I(\tau,\mu)}{\partial \tau} = -I(\tau,\mu) + \frac{\omega(\tau)}{2} \int_{-1}^{+1} p(\mu,\mu')\, I(\tau,\mu')\, d\mu' + \eta(\tau)$$

$$d\tau = (\kappa + \sigma)\ ds,\ \omega = \frac{\sigma}{\kappa_{\mathrm{dust}} + \kappa_{\mathrm{gas}} + \sigma}$$

albedo (gas + dust)

Absorption
(gas + dust)

Scattering
(dust only)

Contributions to the radiation intensity

✏ Absorption κ $\kappa(a) = Q_{abs}\, 4\pi\, a^2\, f(a)\, n_{\mathrm{H}}\,;$

- ✏ dust distribution $dn = f(a)\, da$
  - size
  - composition
  - surface coating

Q_{abs} tabulated for different sizes and composition by Draine + Weingartner

- ✏ Gas composition
  - Continuum absorption (C, Si, …)
  - + lines (mostly H_2, but also CO, …)

✏ Scattering σ

$$\omega(a) = \frac{\sigma(a)}{\kappa(a) + \sigma(a)}$$

Q_{scatt} tabulated for different sizes and composition by Draine + Weingartner

- ◆ Pure dust property (tabulated by Draine & Weingartner)
- ◆ possibility of DUSTEm data base (IAS)

✏ Computations require knowledge of dielectric properties

solution

- Basics: Roberge (1983) ApJ, 275, 292
  - ✏ Spherical harmonics method (expansion on Legendre polynomials)
  - ✏ Constant dust properties with position - No gas
  - ✏ Analytical solution (used in PDR_light)
- Line contribution: Goicoechea & Le Bourlot (2007) A&A 467, 1
  - ✏ add absorption by H_2 transitions
  - ✏ self consistent solution introduced in Meudon PDR code (http://pdr.obspm.fr)
- Role of gas continuum (Rollins + Rawlings (2012) MNRAS 427, 2328
  - ✏ Stress importance of C continuum absorption

Introduction of photodissociation processes in PDR models

1. Use of analytic expression $P = A \exp(-\beta A_v)$ (s^{-1}) given in data bases (UMIST, Leiden, KIDA)

Straightforward, simple, how accurate?
We know that this is not the solution for incident isotropic radiation

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2. Add specific tabulated and precomputed shielding functions (e.g. H_2, CO, N_2, …) $P(H_2) = \chi \; P_0 \; f(H_2) \; \phi(A_v)$

   Allows to better account for physics. However precomputed values assume specific physical conditions (rad, n, T and dust properties)

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   Allows to better account for physics. However precomputed values assume specific physical conditions (rad, n, T and dust properties)

3. Integrate the appropriate cross-sections multiplied by the local radiation field intensity over the relevant wavelength integral : possibility favoured in the Meudon PDR code

   ✏ Allows to automatically account for physical conditions (gas +dust)
   ✏ Discriminate between continuum and resonance processes

In the Leiden photodissociation database, continuum cross sections are available in cm^2, whereas integrated cross-section are reported in cm^2 Å via $\sigma_I = \frac{\pi e^2}{mc^2} \lambda^2 \eta_u f_{lu}$ for resonances

On line Meudon PDR model @ pdr.obspm.fr

- coupled solution of chemistry + radiative transfer + thermal balance

- emphasis on microphysics
  - ✑ simplify geometry
  - ✑ sacrifice time evolution
  - ✑ sacrifice dynamics

- Avoid observational / empirical "laws" where possible
  - ✑ results emerge naturally from first principles
  - ✑ use as virtual world
  - ✑ use as inversion tool

- Coupling to Virtual Observatory in progress
  - ✑ a few grid and exploring tools
  - ✑ access through SVN

Different radiative transfer options of the Meudon PDR model

- running times : variable
- iterative process
  - ✏ Radiative transfer couples every point to every other
  - ✏ Sensitive to initializations
- Different levels of approximations
  - ✏ PDR_Light: rapid, analytic solution of continuum transfer + FGK* approximation for self-shielding of H_2, CO and isotopologues computed explicitly.
  - ✏ "standard" PDR including continuum absorption by gas in addition to dust continuum + FGK approximation ….
  - ✏ "exact" level (1) PDR including H_2 line overlap + full selfshielding + continuous absorption by gas
  - ✏ "exact" level (2) PDR including H_2 + CO line overlap + full self-shielding + continuous absorption by gas

FGK: Federman, Glassgold & Kwan, ApJ 277, 466, 1979

Short reminder on H_2 photodissociation

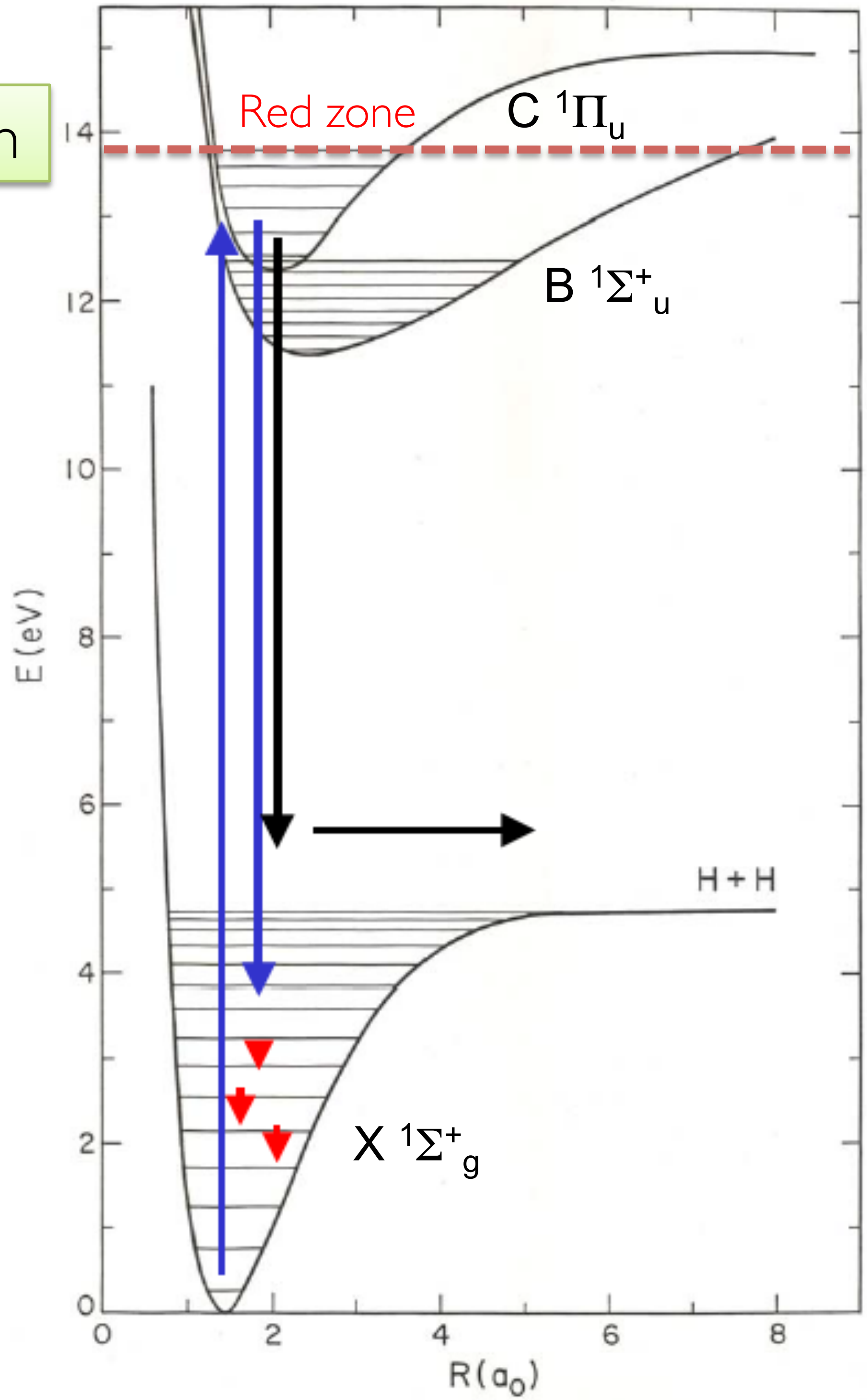
Spontaneous radiative dissociation : Solomon process mentioned in Field et al. ARAA 4, 207, 1966 : discrete absorption followed by spontaneous emission into the continuum of X ground state of H_2

➨ efficient selfshielding depending on molecular properties of H_2;

➨ dependence on v" and J"

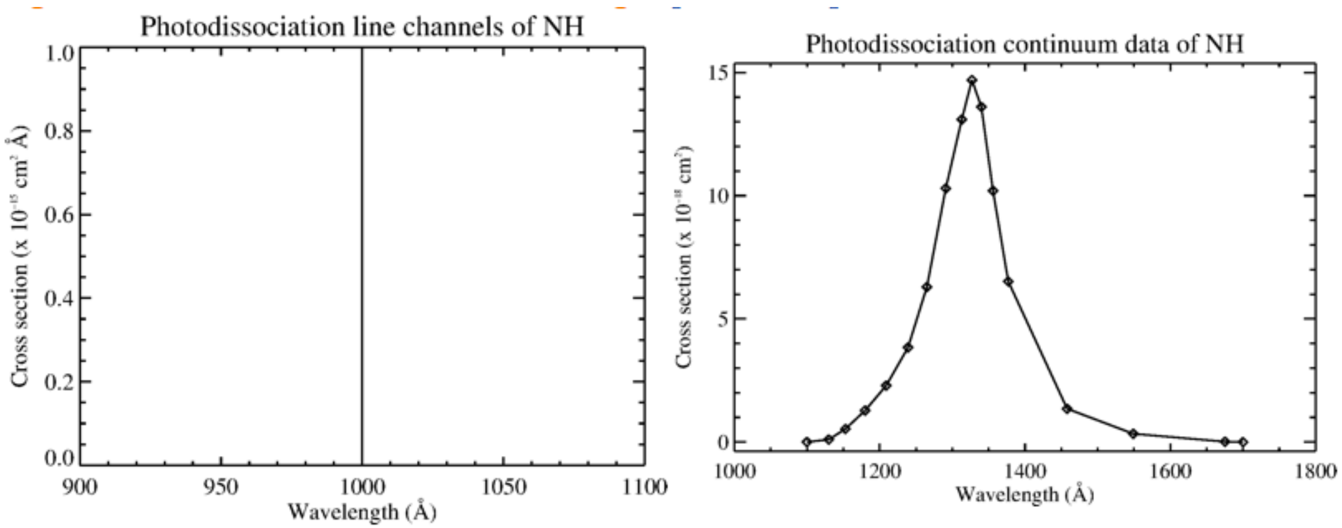
coupling with excitation and chemistry

Discrete VUV spectrum + continuum radiative probabilities computed in Abgrall et al. 1993, 1994, 2000 available in the Meudon PDR website



Use of Leiden database (http://home.strw.leidenuniv.nl/~ewine/photo/ x-sections in the Meudon PDR code

Example of NH



- For continuum case: no problem
- For discrete line mechanism, only integrated cross sections are given

  ✑ introduction of a line profile (Lorentzian) according to Breit and Wigner law (valid for isolated, non overlapping resonances)

$$\sigma = \frac{\pi e^2}{mc^2} \lambda_0^2 \eta_u f_{lu} \times \frac{2}{\pi \Delta\lambda} \times \frac{\Delta\lambda^2/4}{(\lambda - \lambda_0)^2 + \Delta\lambda^2/4}$$

  ✑ Additional assumption that all resonances have the same width

- For line + continuum: add both contributions

Check the values of photodissociation rates at the edge with the PDR_Light code (after scaling of the intensity of the radiation field):

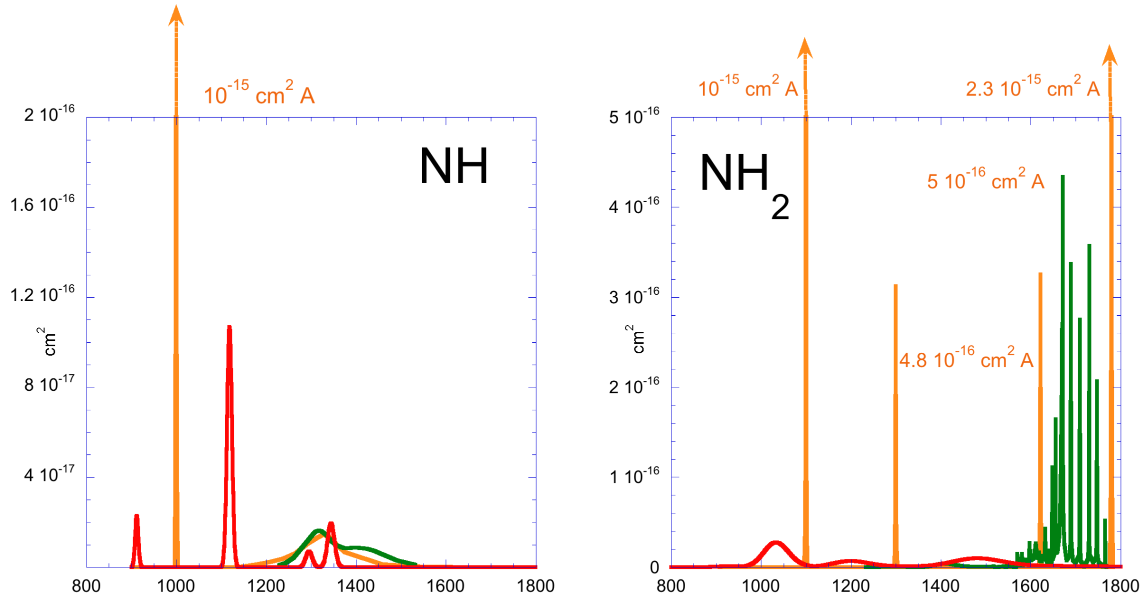
✑ *allows to test the pure gas phase results*

✑ *OK, after some adjustments in line widths for some cases with many resonances (e.g. N_2)*

Other recent available data (to be) used in the Meudon PDR code

- ✒ S and Si photoionization x-sections from opacity project (http://cdsweb.u-strasbg.fr/topbase/topbase.html)
- ✒ CN (El Qadi & Stancil, ApJ 779, 97, 2013)
- ✒ ArH^+ (Roueff et al., AA 566, A30, 2014)
- ✏ CF^+ (Dayou et al. 2015)
- ✏ NH (Loison et al. 2015)
- ✏ NH_2 (Loison et al. 2015)
- ✏ HNC photodissociation + photoionization (Loison et al. 2015)
- ✏ HCN^+, HNC^+ (Loison et al. 2015)
- ✏ C_2N (Loison et al. 2015)
- ✏ HC_2N (Loison et al. 2015)
- ✏ C_3N (Loison et al. 2015)
- ✏ HC_3N (Loison et al. 2015)
- ✏ CH_2CN (Loison et al. 2015)
- ✏ CNC^+ (Loison et al. 2015)

The example of NH / NH_2



Leiden database $\sigma_{max} = \sigma_I / \pi / \Delta\lambda(\AA)/0.5$

Loison 2015, EOM-CCSD/cc-pVTZ calculations with GAUSSIAN09 package

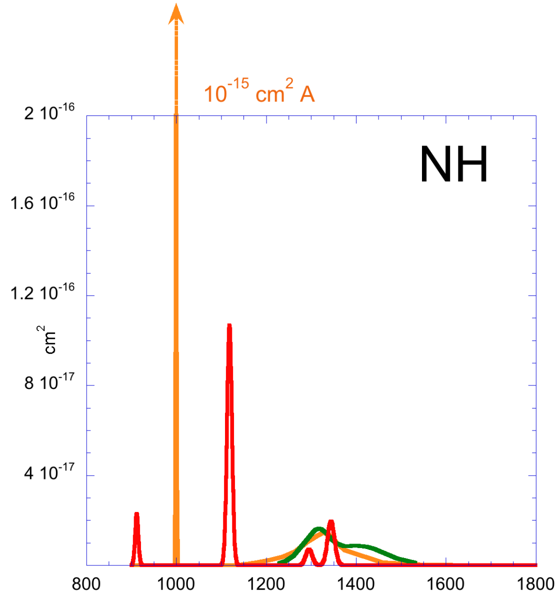
NH : digitalization of Fig. 4 of Kirby+Goldfield, JCP 94, 1271, 1991

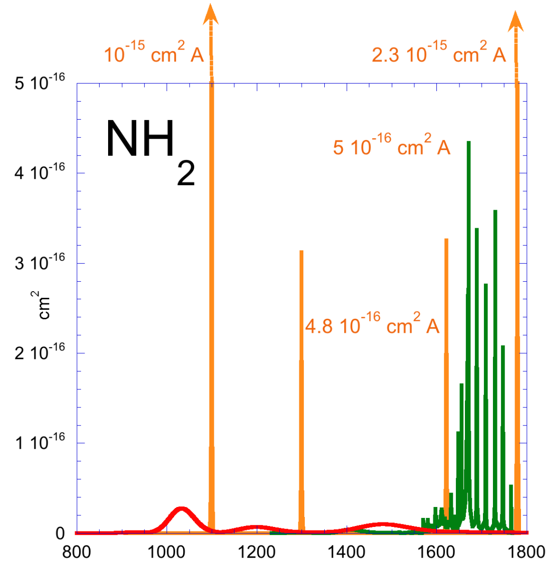
NH_2 : digitalization of Figs. 8, 11 and 12 of Koch, J. Phys. Chem. A 1997, 101, 1460 (courtesy of M. Agundez)

The example of NH / NH_2

Photorates at $\tau = 0$ (no dust) in s^{-1} computed with unit Draine ISRF (-b) stands for 10^{-b}

	NH	NH_2
Leiden DB	5.0(-10)	7.5(-10)
Loison	3.5(-10)	7.1(-10)
Agundez	4.8(-10)	8.7(-10)
FWHM=1Å	5.0(-10)	7.6(-10)





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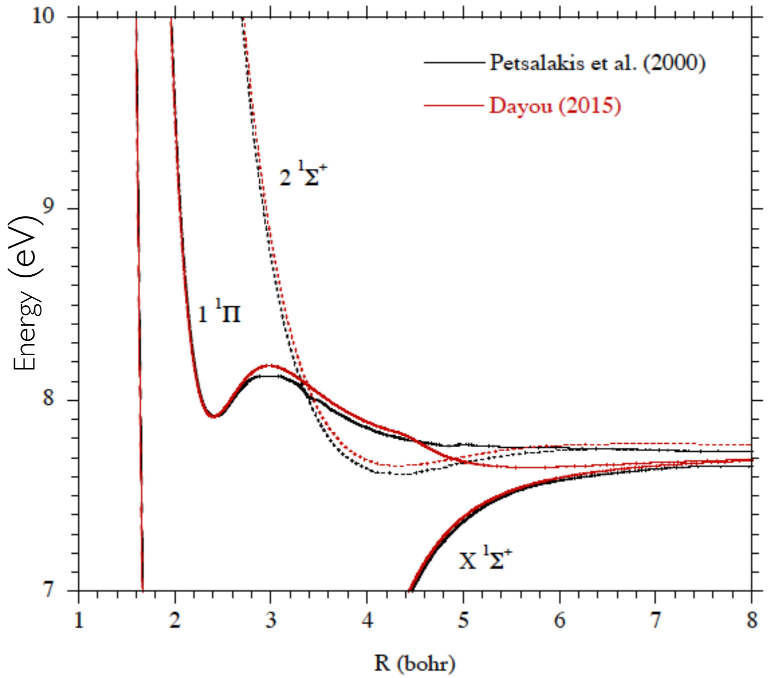
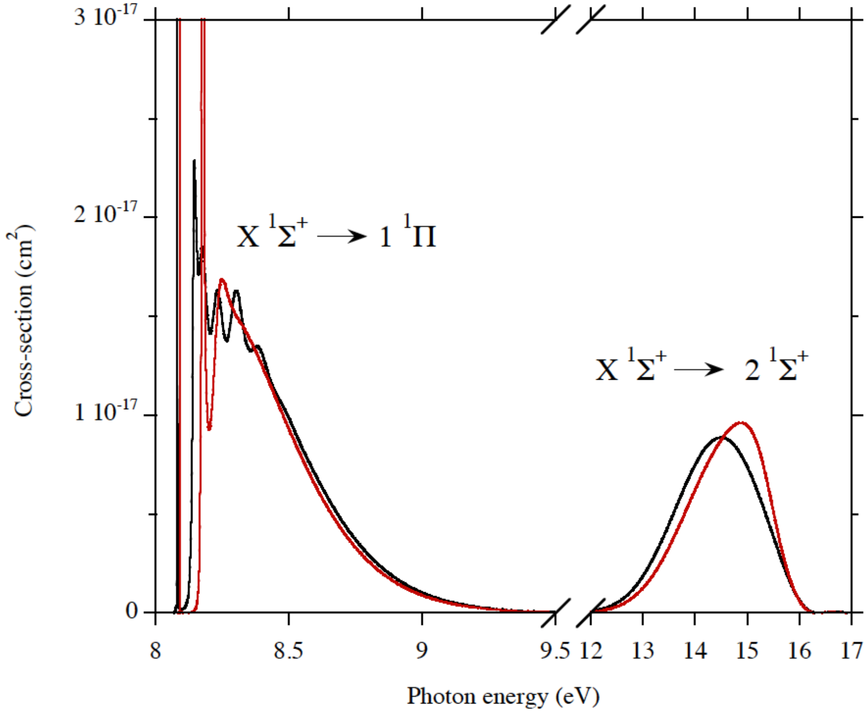
One example of new results : CF^+



Electronic potentials
Petsalakis+Theodorakopoulos CASSCF (14e-,8MO) + MRCI / aug-cc-pVTZ, Chem. Phys. 254, 181, 2000
Dayou, CASSCF (14e-,12MO) + MRCI / aug-cc-pVQZ, 2015

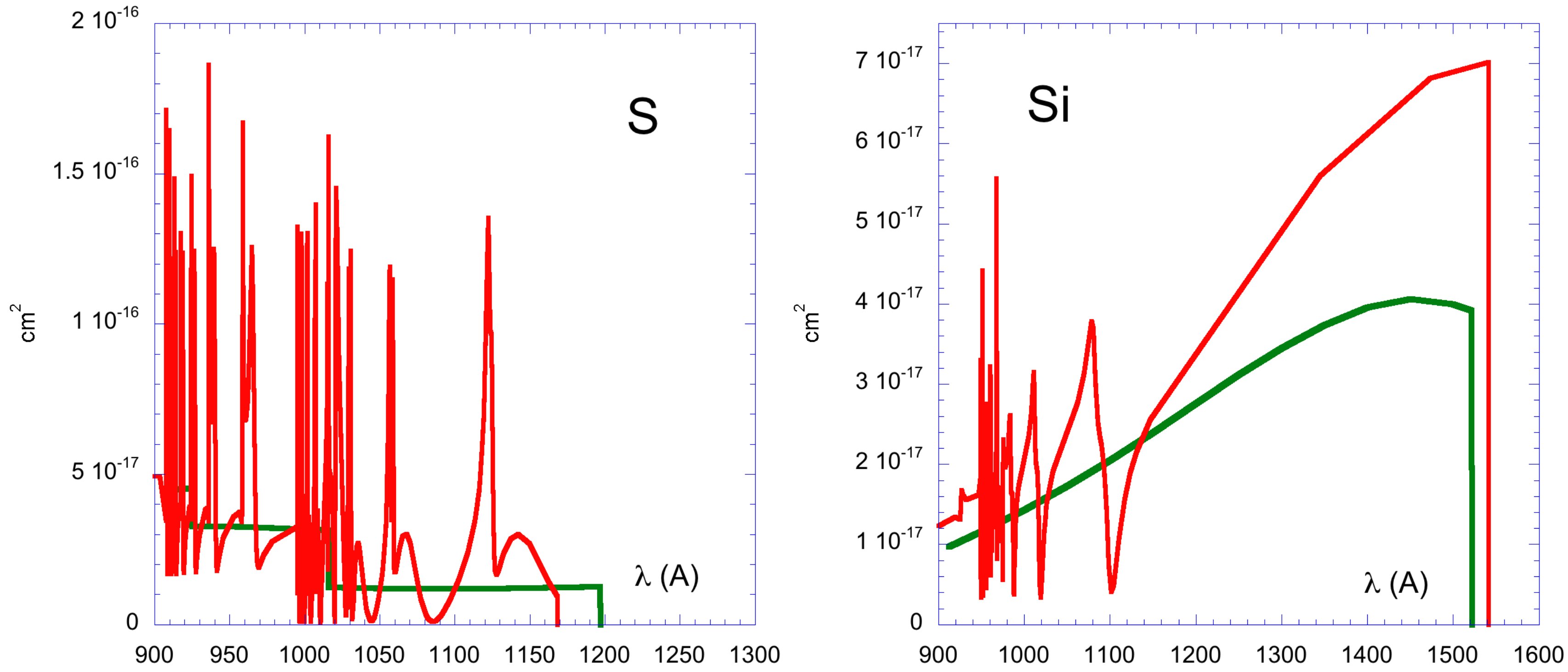
Detected in the Orion bar (Neufeld et al. 2006, Nagy et al. 2013), Horsehead PDR (Guzman et al. 2013) and in the diffuse, translucent and spiral arm clouds (Liszt et al. 2014)



x-sections computed through time dependent wave packet method (Dayou + Monnerville 2015)

P(0) = $1.9\ 10^{-10}\ s^{-1}$ with Petsalakis data
P(0) = $2.2\ 10^{-10}\ s^{-1}$ with Dayou data

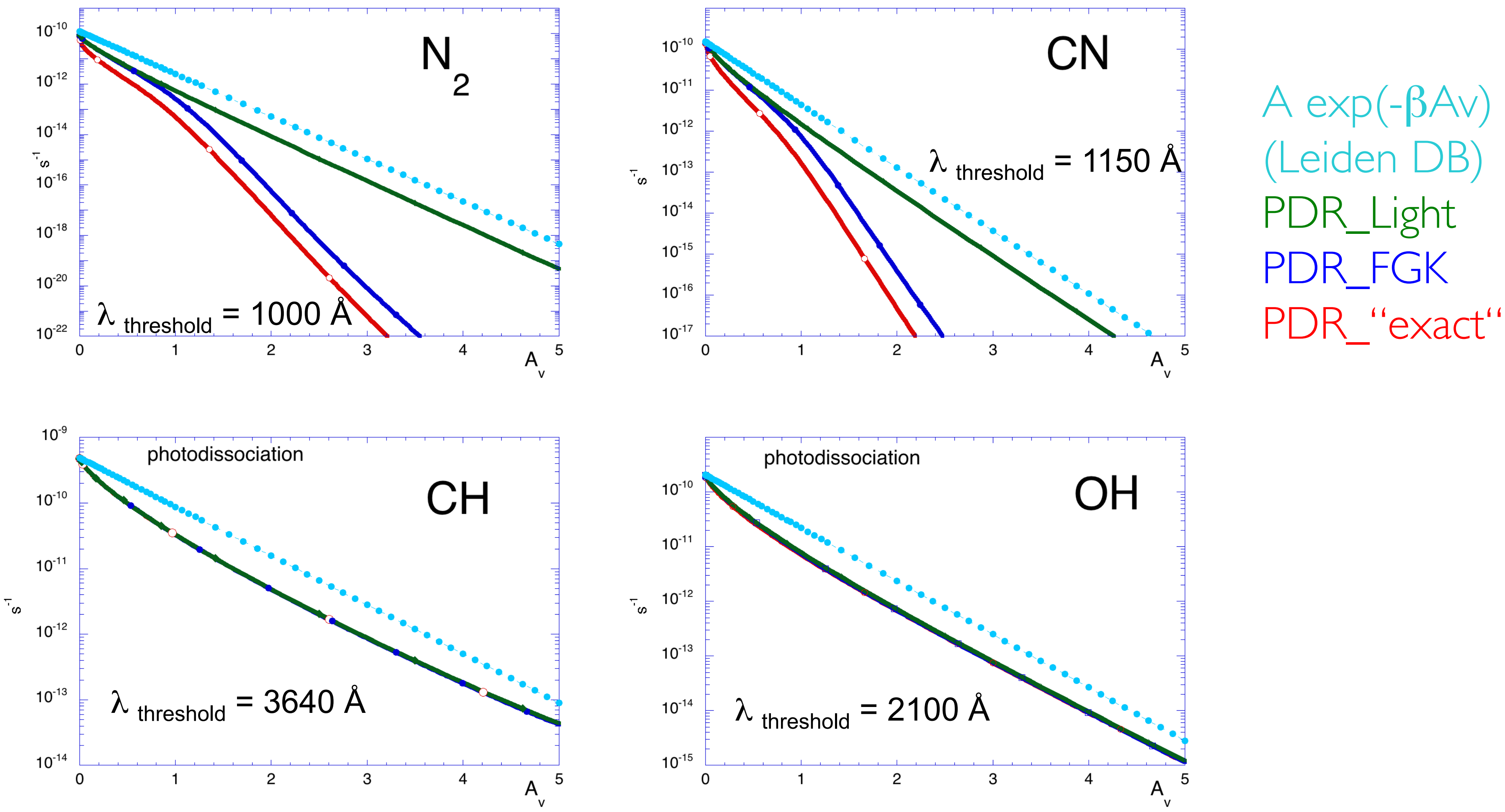
Use of Topbase photoionization cross-sections



P(0) (s^{-1})	S	Si
Leiden	6 (-10)	3.1 (-9)
With Topbase	9.9 (-10)	4.6 (-9)

Other data available at
http://phidrates.space.swri.edu

The three levels of approximation of photodissociation rates as a function of Av

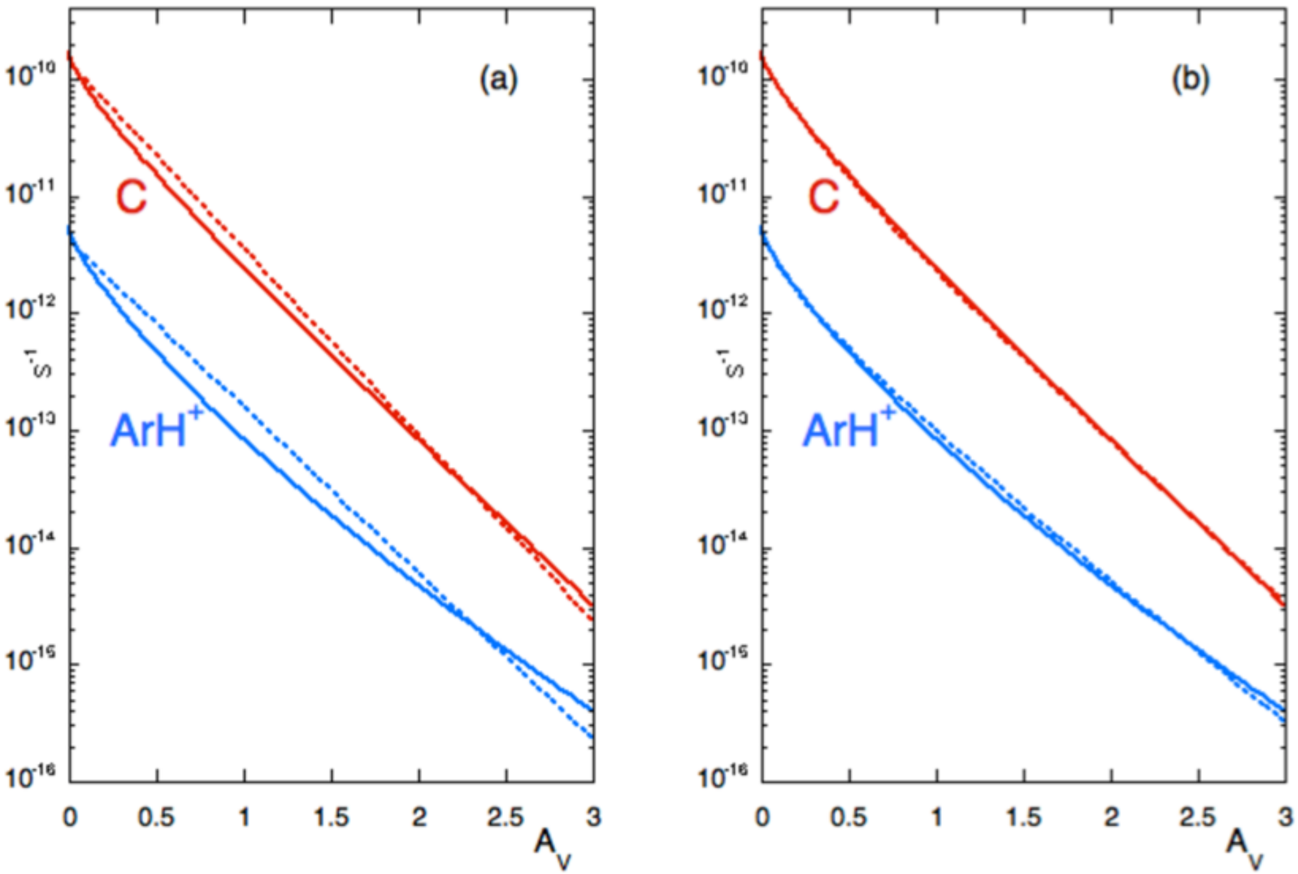


Continuous gas absorption matters for threshold wavelengths below **≈ 1150 Å**

Fitting photodissociation rates

Case of the Draine incident isotropic ISRF

$A \exp(-\beta A_V)$ $\quad$ $A' E_2(\beta' A_V)$



Exponential integral E_2 function allows to better account photodissociation probabilities for isotropic fields (cf also Neufeld & Wolfire, ApJ 706, 1594, 2009)

Roueff, Alekseyev, Le Bourlot, A&A 566, A30, 2014

Impact of radiative transfer approximations on model results (1)

Case of a diffuse cloud model: n_H = 100 cm^{-3}, T=50 K, Draine ISRF, $\zeta = 10^{-16}\ s^{-1}$,
1 side isotropic illumination, Avtot = 0.5, L≈ 3 pc;
Computed column densities in cm^2 (powers of ten between parentheses).

PDR	H	H_2	C^+	C	CO	^{13}CO	$C^{18}O$	CN	OH	C_2	CH	N_2	H_3^+	CF^+
Light	5.3 (19)	4.4 (20)	1.2 (17)	3.4 (15)	1.65 (13)	3.15 (11)	3.3 (10)	3.5 (11)	9.25 (12)	8.5 (11)	3.5 (12)	4.8 (10)	1.4 (13)	1.6 (11)
FGK	5.3 (19)	4.4 (20)	1.2 (17)	3.6 (15)	1.8 (13)	3.4 (11)	3.6 (10)	3.85 (11)	9.3 (12)	1.3 (12)	3.8 (12)	5.4 (10)	1.4 (13)	2.7 (11)
exact	3.6 (19)	4.5 (20)	1.2 (17)	5.6 (15)	3.9 (13)	8.3 (11)	7.6 (10)	7.6 (11)	9.6 (12)	1.7 (12)	4.25 (12)	2.2 (11)	1.5 (13)	2.8 (11)

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Impact of radiative transfer approximations on model results (2)

Case of a diffuse cloud model: n_H = 100 cm^{-3}, T=50 K, Draine ISRF, $\zeta = 10^{-16}$ s^{-1},
1 side isotropic illumination, Avtot = 1, L ≈ 6 pc
Computed column densities in cm^2 (powers of ten between parentheses).

PDR	H	H_2	C^+	C	CO	^{13}CO	$C^{18}O$	CN	OH	C_2	CH	N_2	H_3^+	CF^+
Light	6.3 (19)	9.0 (20)	2.2 (17)	2.5 (16)	3.4 (14)	8.2 (12)	5.1 (11)	3.3 (12)	2.9 (13)	5.2 (12)	1.2 (13)	1.6 (12)	3.2 (13)	3.7 (11)
FGK	6.3 (19)	9.0 (20)	2.2 (17)	3.1 (16)	5.2 (14)	1.3 (13)	7.6 (11)	3.9 (12)	3.2 (13)	6.5 (12)	1.2 (13)	2.6 (12)	3.3 (13)	6.0 (11)
exact	4.6 (19)	9.1 (20)	2.0 (17)	4.8 (16)	1.3 (15)	3.5 (13)	2.0 (12)	5.5 (12)	4.1 (13)	1.7 (13)	1.2 (13)	7.9 (12)	3.8 (13)	6.2 (11)

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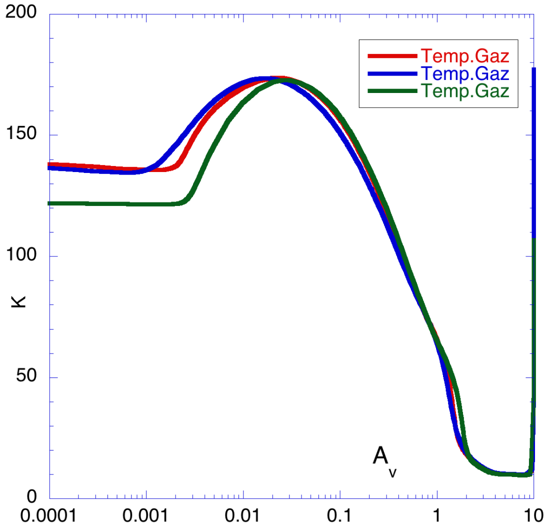
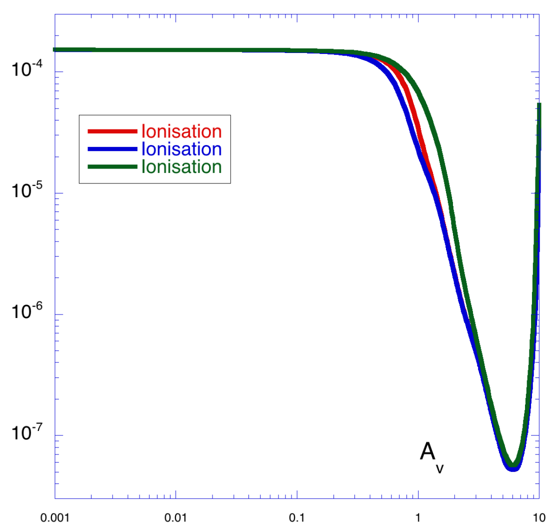
exact	4.6 (19)	9.1 (20)	2.0 (17)	4.8 (16)	1.3 (15)	3.5 (13)	2.0 (12)	5.5 (12)	4.1 (13)	1.7 (13)	1.2 (13)	7.9 (12)	3.8 (13)	6.2 (11)

Impact of radiative transfer approximations on model results (3)

Case of a dense PDR: $n_H = 2\ 10^4\ cm^{-3}$, TE, 100 × Draine ISRF on the left side, 1 × Draine ISRF on the right side, $\zeta = 10^{-16}\ s^{-1}$, Avtot = 10 ≈ 0.3 pc





PDR_Light

PDR_FGK

PDR_"exact"

Column densities (cm^2)

PDR	H	H_2	C^+	C	CO	^{13}CO	$C^{18}O$	CN	OH	C_2	CH	N_2	HF	CF^+
Light	3.9 (19)	9.3 (21)	2.4 (17)	4.8 (17)	1.7 (18)	2.7 (16)	2.3 (15)	1.6 (14)	1.3 (15)	2.3 (13)	8.2 (13)	3.4 (17)	3.1 (14)	2.2 (12)
FGK	3.8 (19)	9.3 (21)	1.8 (17)	3.6 (17)	1.9 (18)	2.9 (16)	3.1 (15)	1.3 (14)	1.5 (15)	1.4 (13)	5.1 (13)	4.1 (17)	3.3 (14)	1.9 (12)
exact	2.2 (19)	9.3 (21)	1.5 (17)	3.5 (17)	2.0 (18)	3.0 (16)	3.3 (15)	1.2 (14)	1.5 (15)	9.9 (12)	4.05 (13)	4.2 (17)	3.2 (14)	1.4 (12)

Impact of radiative transfer approximations on model results (4)

Case of a dense PDR: n_H = 2 10^4 cm^{-3}, TE, 100 x Draine ISRF on the left side, 1 x Draine ISRF on the right side, ζ = 10^{-16} s^{-1}, $A_V$tot = 10 ≈ 0.3 pc

Photodissociation of CO and isotopes include predissociation transitions up to J=30 from Eidelsberg et al. AAS 90, 231, 1991, with update of some oscillator strengths (Eidelsberg et al. AA424, 355, 2004); data available on pdr.obspm.fr

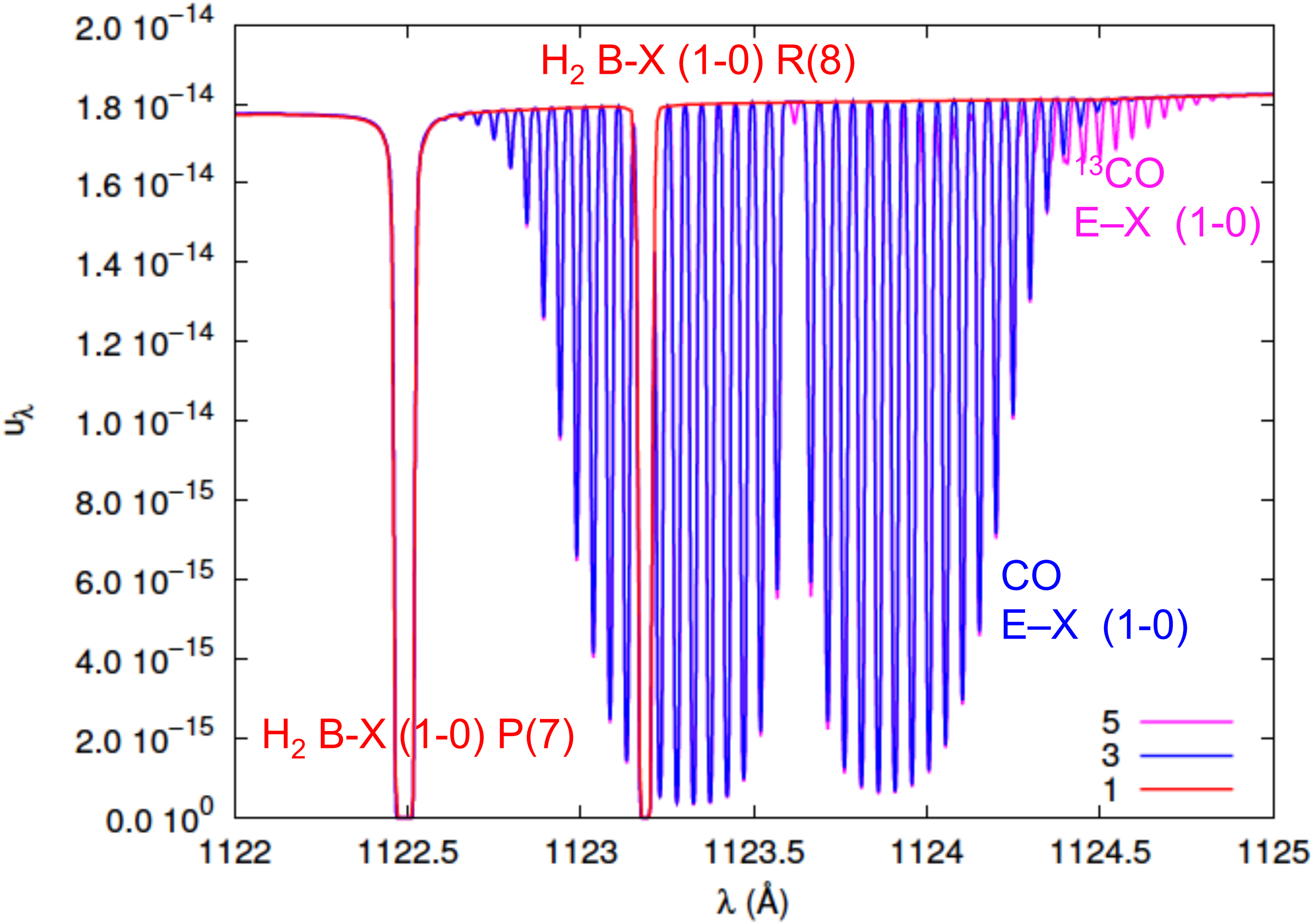
Integrated intensities (K km s^{-1})

PDR	CO				^{13}CO				$C^{18}O$			
	1=>0	2=>1	3=>2	4=>3	1=>0	2=>1	3=>2	4=>3	1=>0	2=>1	3=>2	4=>3
Light	106	104.7	80.2	45.9	22.9	24.4	10.5	1.86	2.84	2.99	0.807	0.087
FGK	123	127	102	64.0	24.5	27.2	12.7	2.57	3.74	4.30	1.38	0.197
exact	132	143	120	80.6	24.9	28.4	14.0	3.20	3.92	4.62	1.58	0.257

Orders of magnitude are obtained within simple radiative transfer model.
Mainly, chemical effects as the thermal balance leads to similar temperature profiles.

“exact transfer achievements “

1: H_2 full transfer; 10 levels ; 27107 wl
3: 1 + ^{12}CO full transfer ; 30 levels ; 58546 wl
5: 3 + ^{13}CO full transfer ; 30 levels ; 76823 wl



Isobaric model
P= 10^8 Kcm^{-3}
$A_V$tot = 5
7023 star at 0.143 pc
HD 38087extinction curve;
N_H= 1.87 10^{21} A_V cm^{-2}
+ isotropic radiation field on both sides

Message to take home

- λ dependent photodissociation/photoionization cross sections are the data requested to compute relevant photodissociation rates in different environments
  - v, J dependence asked for specific cases (H_2, CO and isotopologues, N_2 and $^{14}N^{15}N$, …); implies taking into account coupling between excitation and (photo)chemistry.
  - cross section from ground state for other species for interstellar applications (mostly subthermal excitation)

- Analytic expressions of rates may be derived **BUT** are dependent both on the actual value of the radiation field [P(0)] and on the grain properties (A_V dependence)
  - exponential decrease with A_V OK for beamed illumination (available in Leiden DB, reproduced in UMIST, KIDA)
  - $E_2(A_V)$ function better accounts for isotropic incident radiation field

wish list

- ✏ full CO and isotopologues update
    - ✏ new measurements in progress at SOLEIL synchrotron radiation source; some specific wavelengths range already studied (Eidelsberg et al. 2012, AA543, A67, Stark et al. 2014 ApJ788, 67, Eidelsberg et al. 2014, AA566, A96)
- ✏