Hydrides in (dense) PDRs

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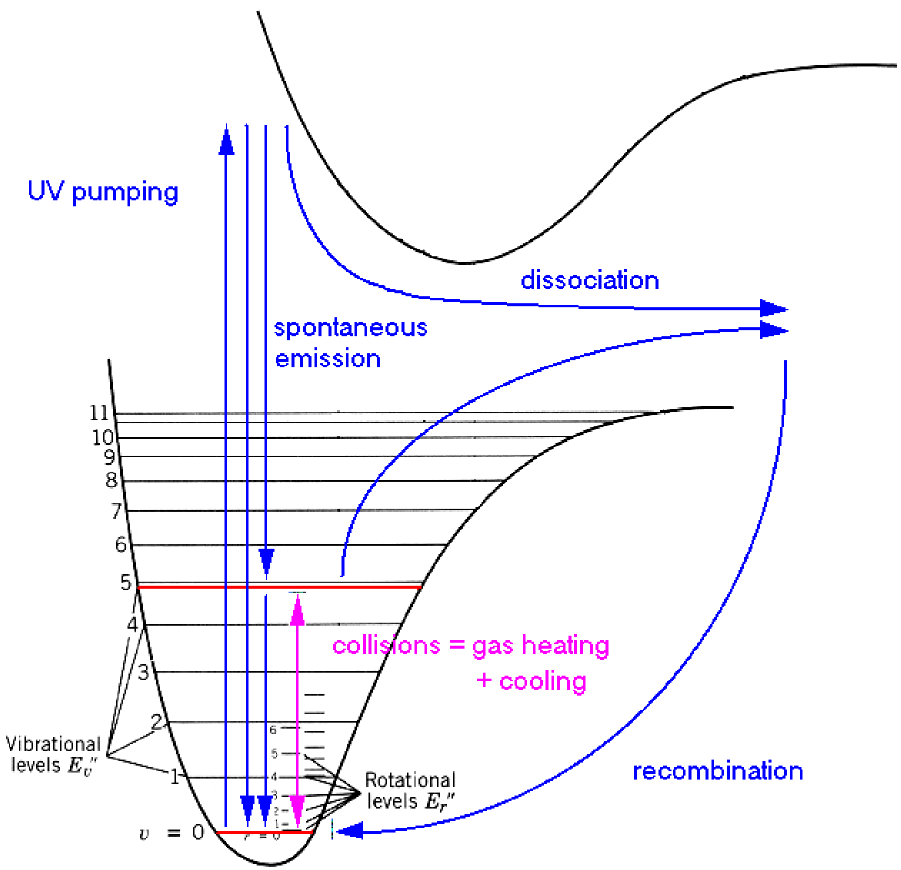
Formation of many hydrides in ISM "forbidden" by endothermicity and/or reaction barriers

Element	Ionization Potential (eV)	Endothermicity (Kelvin equivalent = $\Delta E/k_B$) for			Driver
		$X + H_2 \rightarrow XH + H$	$X^+ + H_2 \rightarrow XH^+ + H$	$X + H_3^+ \rightarrow XH^+ + H_2$	
He	24.587	No reaction	Exothermic, but primary channel is to $He + H + H^+$	29000	
C	11.260	11000	4300 ✓		Warm gas
N	14.534	15000	230	10000	Cosmic rays
O	13.618	920 ✓	✓	✓	Warm gas or cosmic rays
F	17.423	✓		10000	None needed
Ne	21.564	No reaction	Exothermic, but primary channel is to $Ne + H + H^+$	27000	
Si	8.152	17000	15000		Warm gas
P	10.487	19000	13000		Warm gas
S	10.360	10000	10000 ✓		Warm gas
Cl	12.968	515	✓		UV with $h\nu > 12.97$ eV
Ar	15.760	No reaction	✓	6400	Cosmic rays

Gerin et al. (2016)

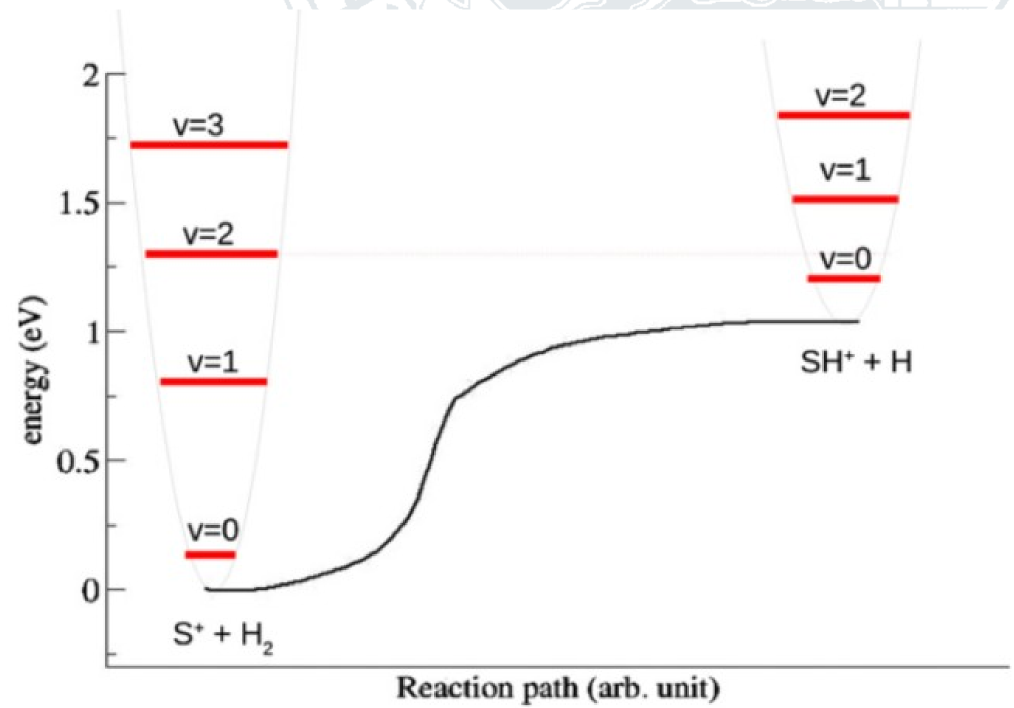
Use energy from UV- excited vibrations

- H_2 vibrational excitation:



$S^+ + H_2 \rightarrow SH^+ + H$

- Endothermic by 9860K
- Exothermic if H_2 is in v ≥ 2



Zanchet et al. (2013)

PDRs (photon-dominated regions/photodissociation regions):

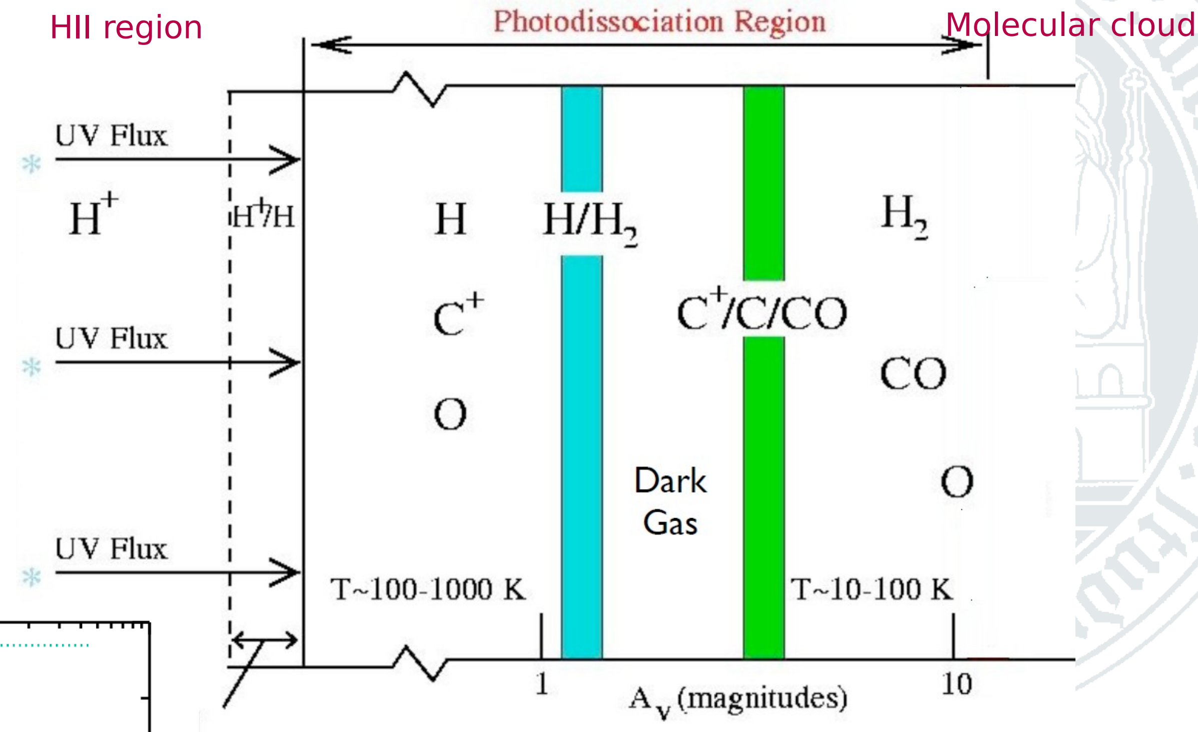
- Energy balance dominated by UV photons 5eV < hν < 13.6eV

- Prototype: Orion Bar
- Edge-on geometry
- Exposed to UV field $\chi \approx 4 \cdot 10^4 \chi_0$ from Θ^1Ori C

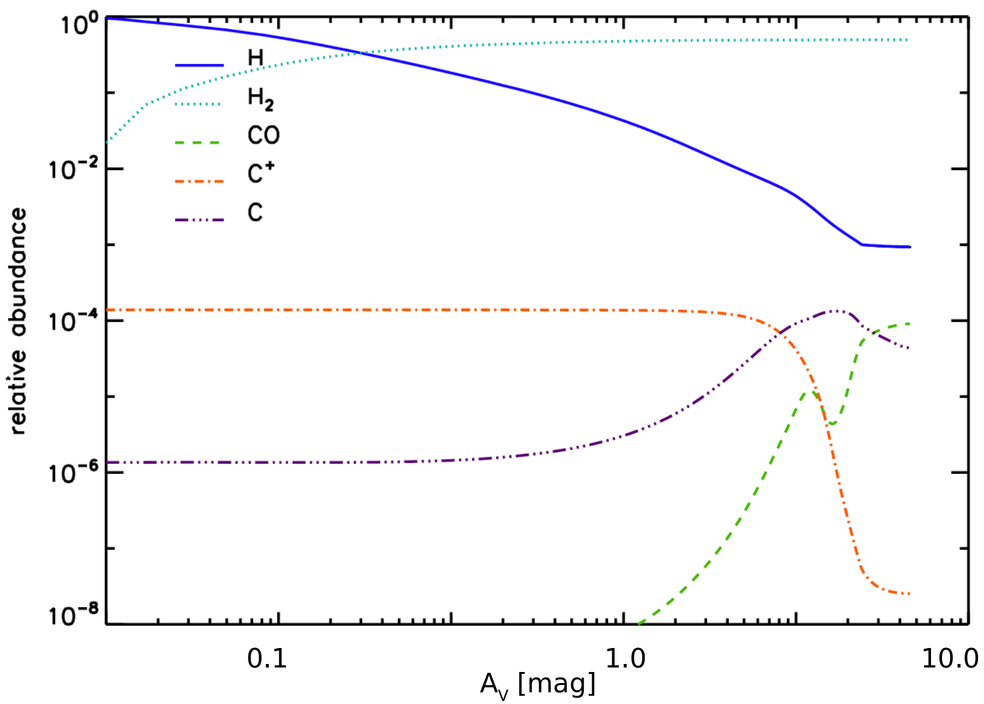
Spitzer/IRAC

Stratified structure

- Layering of chemical transitions and temperatures
- Molecules dissociated at the cloud surfaces.
- Complex molecules only in the dense cores.



Based on Hollenbach & Tielens (1999)



Resulting abundance profiles

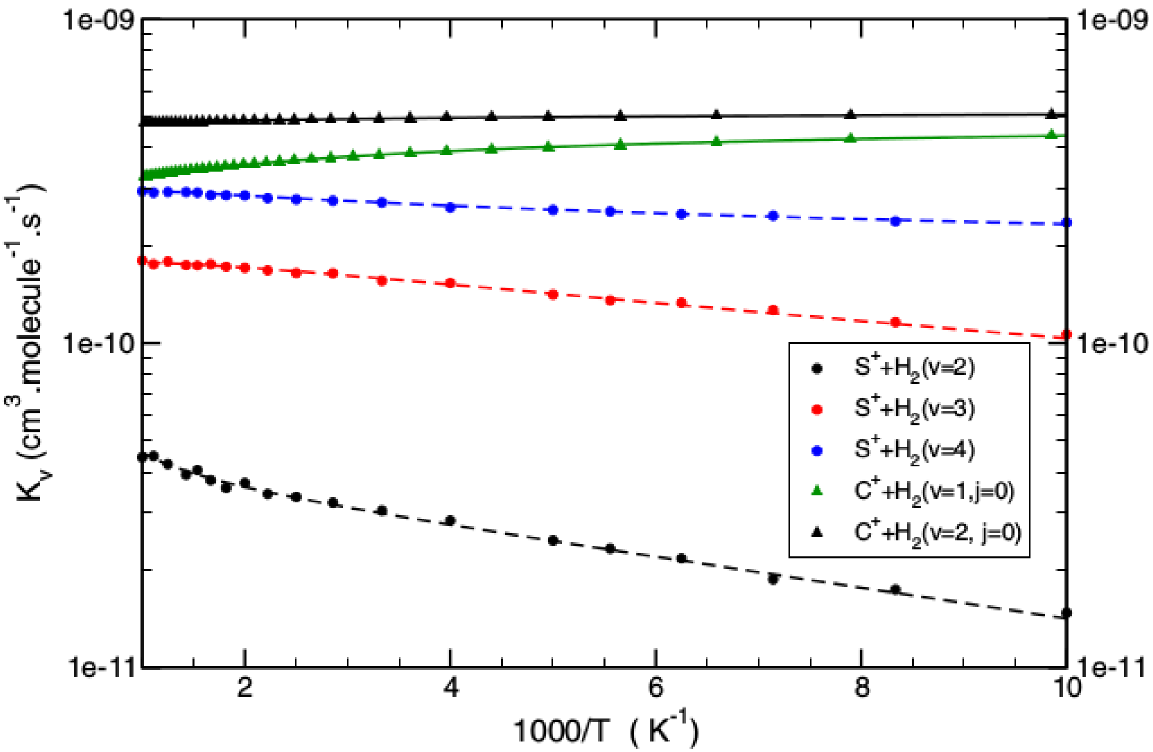
(KOSMA-τ PDR model: Röllig et al. 2006)

Chemical network

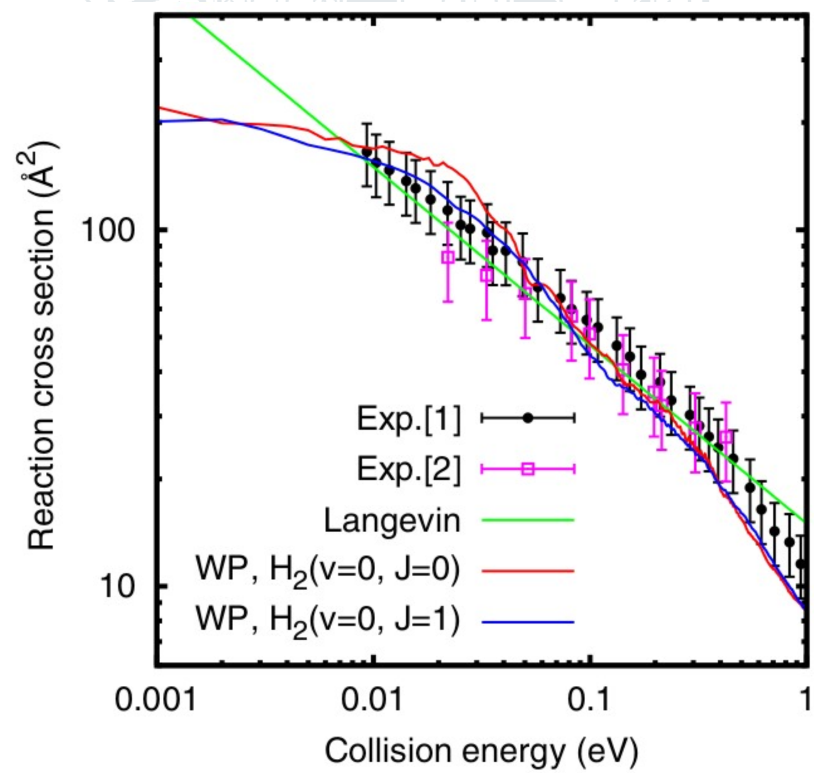
- Requires state-dependent reaction rates
  - Full state-to-state rates for excitation problem
  - *v*-dependence: $C^+ + H_2$, $S^+ + H_2$

→ Talk: E Roueff
see Grozdanov et al. (2016)

- *J*-dependence: $O^+ + H_2$



Zanchet et al. (2013)



Gómez-Carrasco et al. (2014)

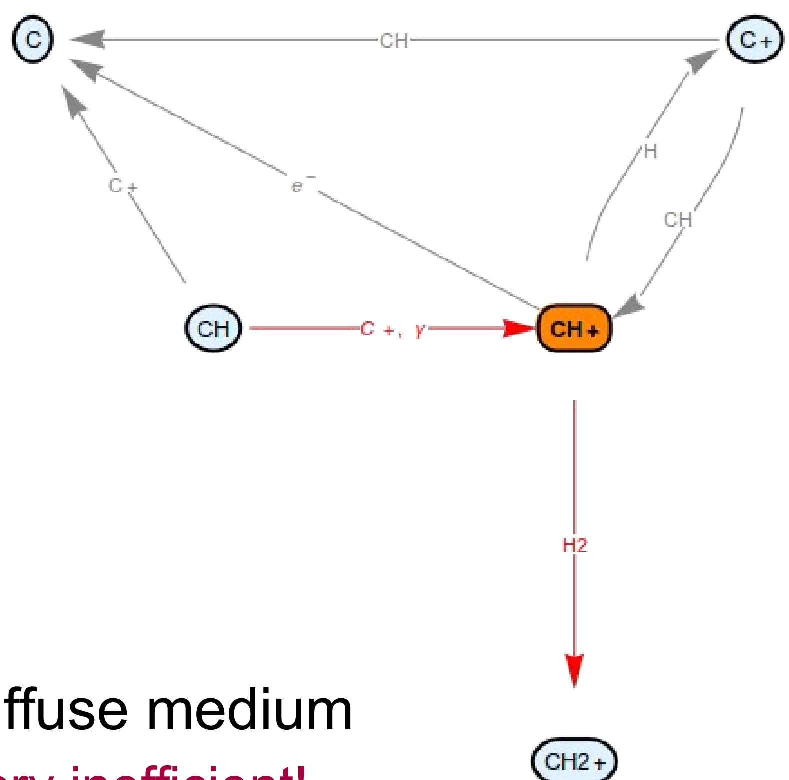
Example CH^+, SH^+

- Similar endothermic reaction paths

$C^+ + H_2 \rightarrow CH^+ + H$ • Endothermic by 4280K

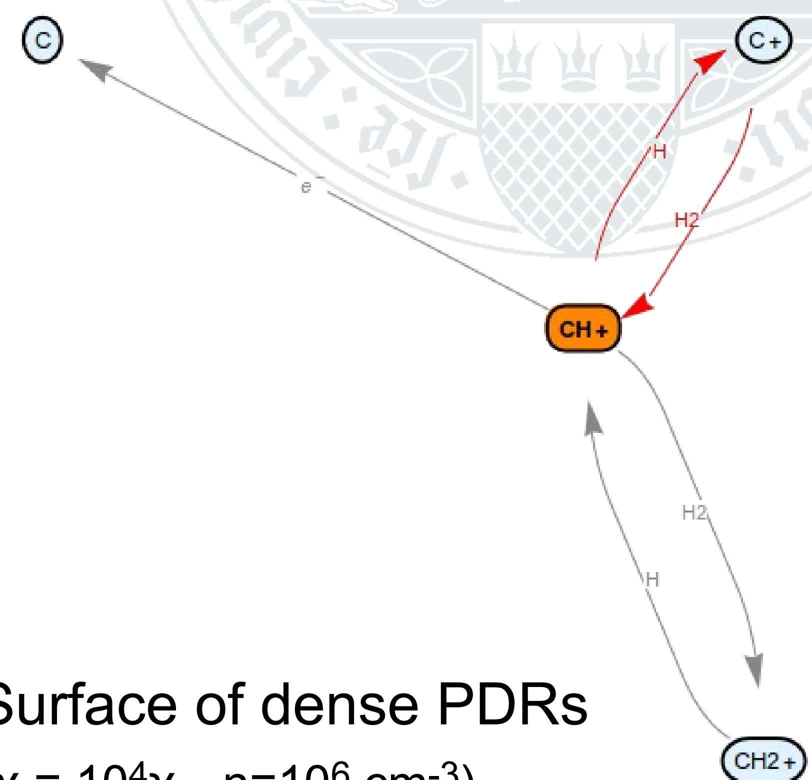
$S^+ + H_2 \rightarrow SH^+ + H$ • Endothermic by 9860K

$Si^+ + H_2 \rightarrow SiH^+ + H$ • Endothermic by 8240K



Diffuse medium

Very inefficient!



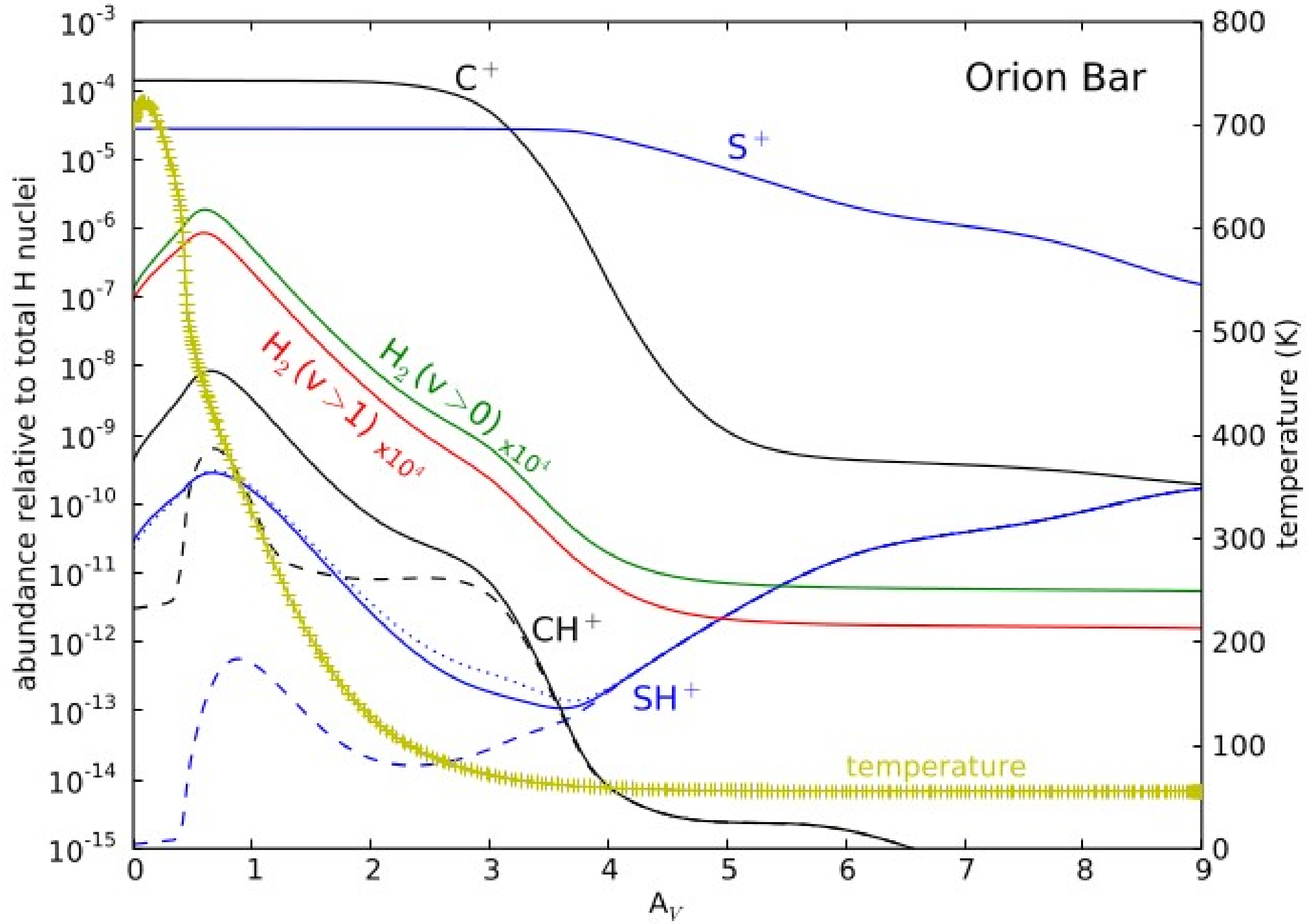
Surface of dense PDRs

($\chi = 10^4\chi_0$, $n=10^6$ cm^{-3})

Example CH^+, SH^+

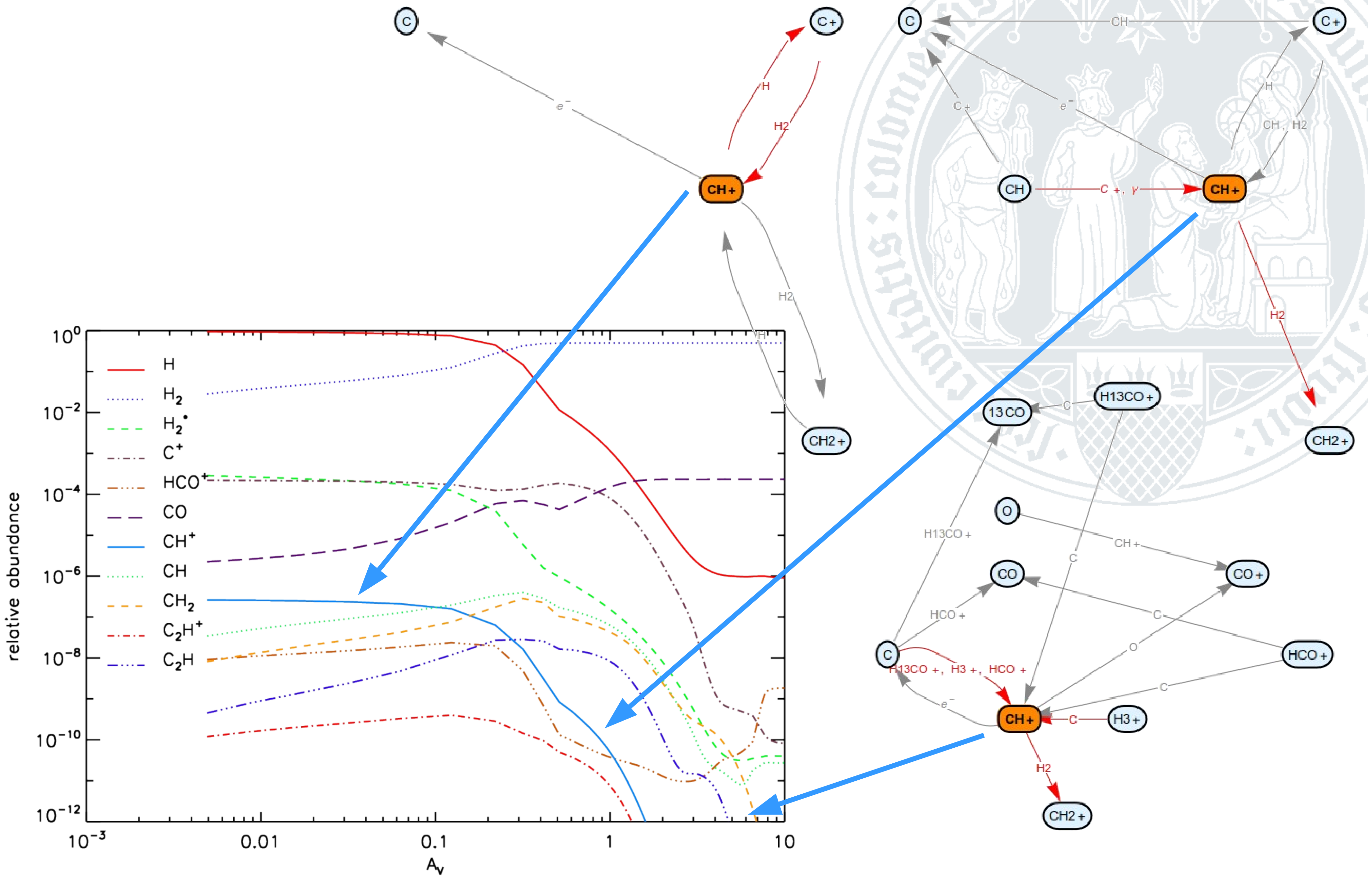
- At PDR surface
  - CH^+ enhanced by 10 – 100
  - SH^+ enhanced by 10^3 - 10^4

compared to diffuse medium conditions

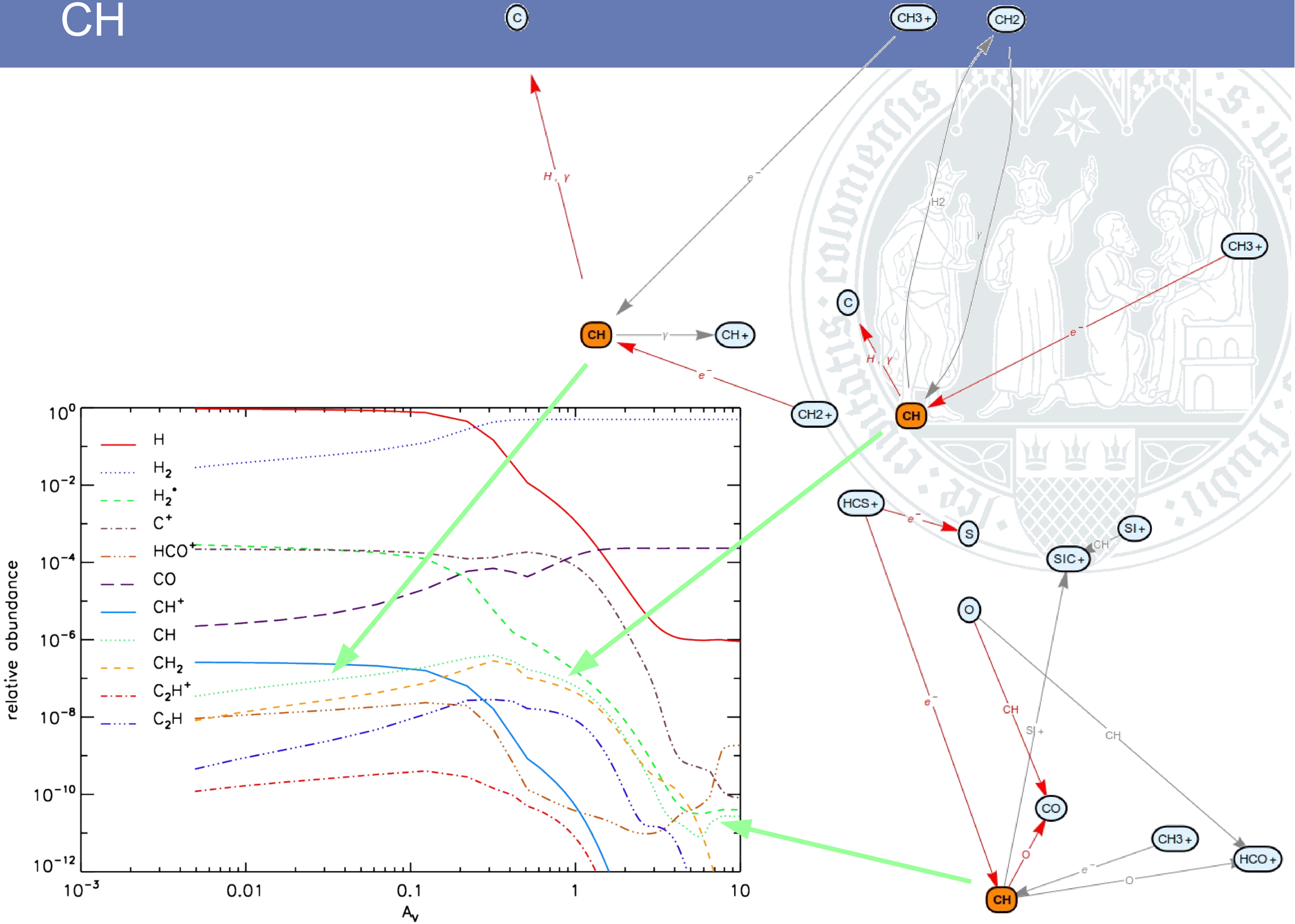


Zanchet et al. (2013)

Detailed chemistry: CH^+

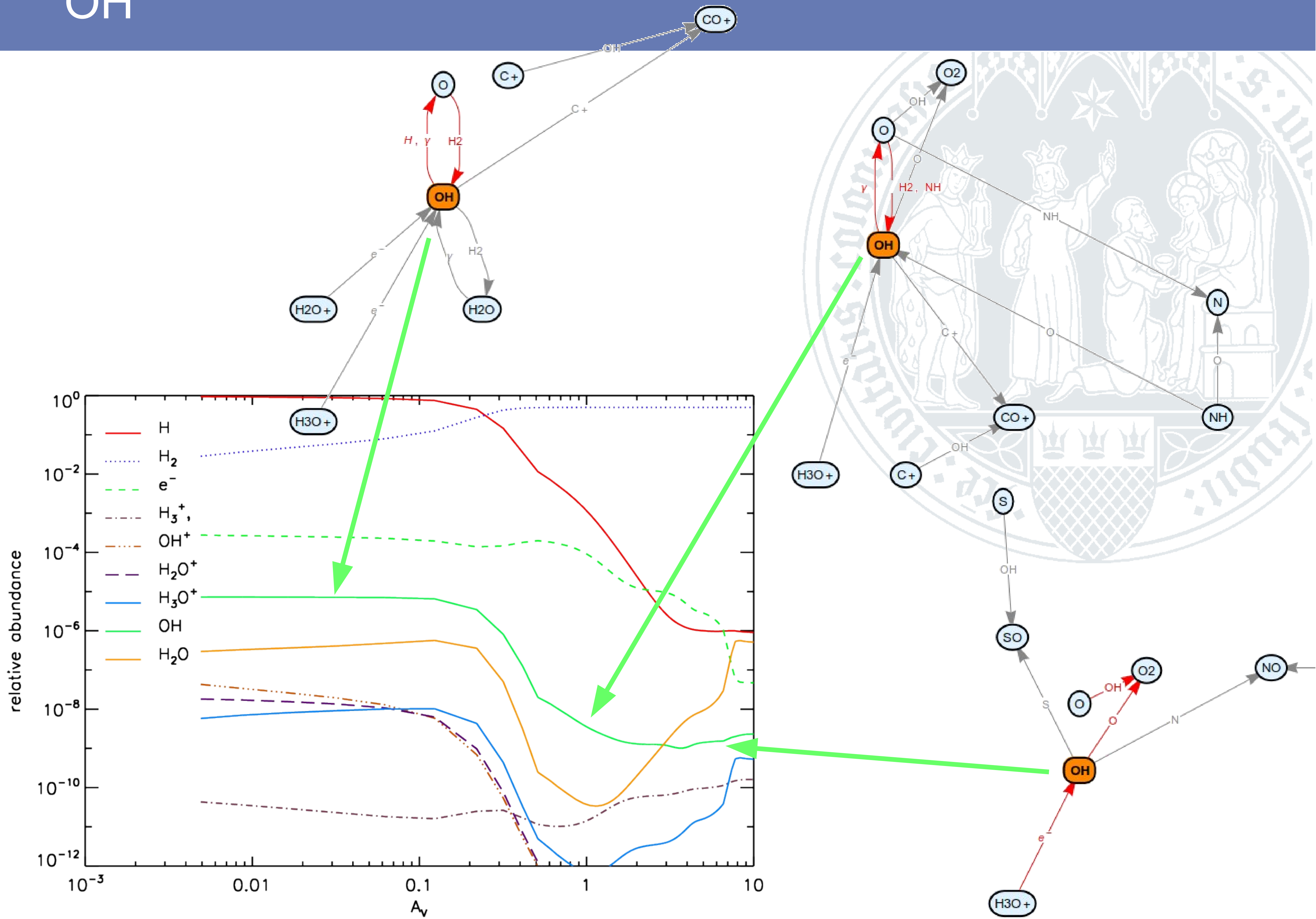


CH



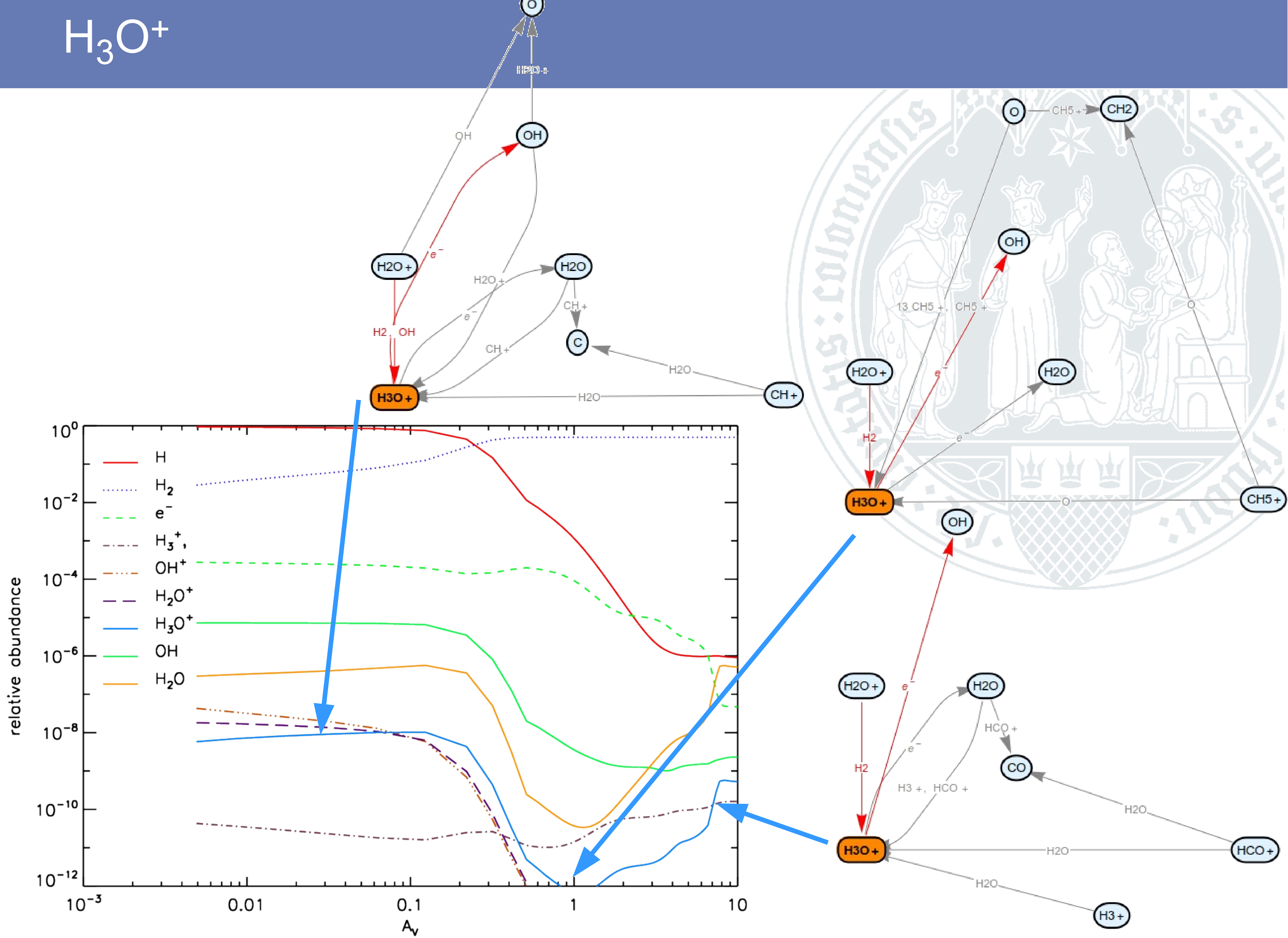
C
CH3+
CH2
H , γ
e⁻
H2
γ
CH3+
C
CH
CH+
e⁻
CH2+
CH
H , γ
e⁻
HCS+
S
SI+
CH
SIC+
O
e⁻
CH
Si+
CH
CO
O
CH3+
e⁻
O
HCO+
CH
H
H_2
H_2^*
C^+
HCO^+
CO
CH^+
CH
CH_2
C_2H^+
C_2H
relative abundance
A_V
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-3}
0.01
0.1
1
10

OH



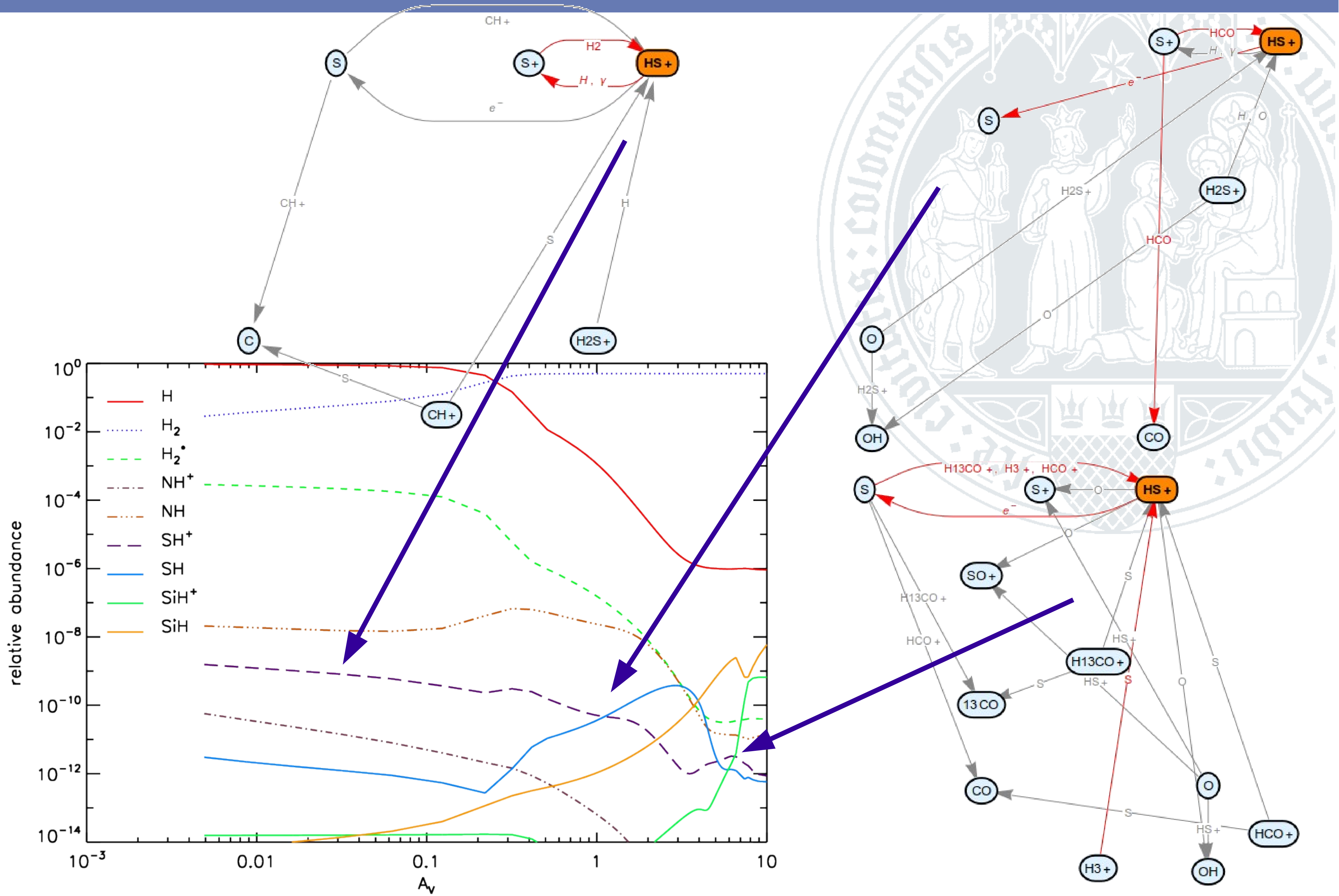
CO+
C+
OH
C+
O
H, γ
H2
OH
e−
γ
H2
H2O+
H2O
H3O+
O2
O
γ
H2, NH
NH
OH
e−
C+
O
N
O
CO+
NH
H3O+
C+
S
OH
SO
O2
O
OH
NO
S
O
N
OH
e−
H3O+
H
H_2
e^-
H_3^+,
OH^+
H_2O^+
H_3O^+
OH
H_2O
relative abundance
A_V
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-3}
0.01
0.1
1
10

H_3O^+



O
HPO+
OH
OH
H2O+
e−
H2O
H2O+
e−
CH+
C
H2, OH
CH+
H2O
CH+
H3O+
H2O
O
CH5+
CH2
OH
13 CH5+, CH5+
O
H2O+
H2O
e−
H2
e−
H3O+
O
CH5+
OH
e−
H2O+
H2O
HCO+
e−
CO
H2
H3+, HCO+
H2O
H3O+
H2O
HCO+
H2O
H3+
H
H_2
e^-
H_3^+,
OH^+
H_2O^+
H_3O^+
OH
H_2O
relative abundance
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-3}
0.01
0.1
1
10
A_V

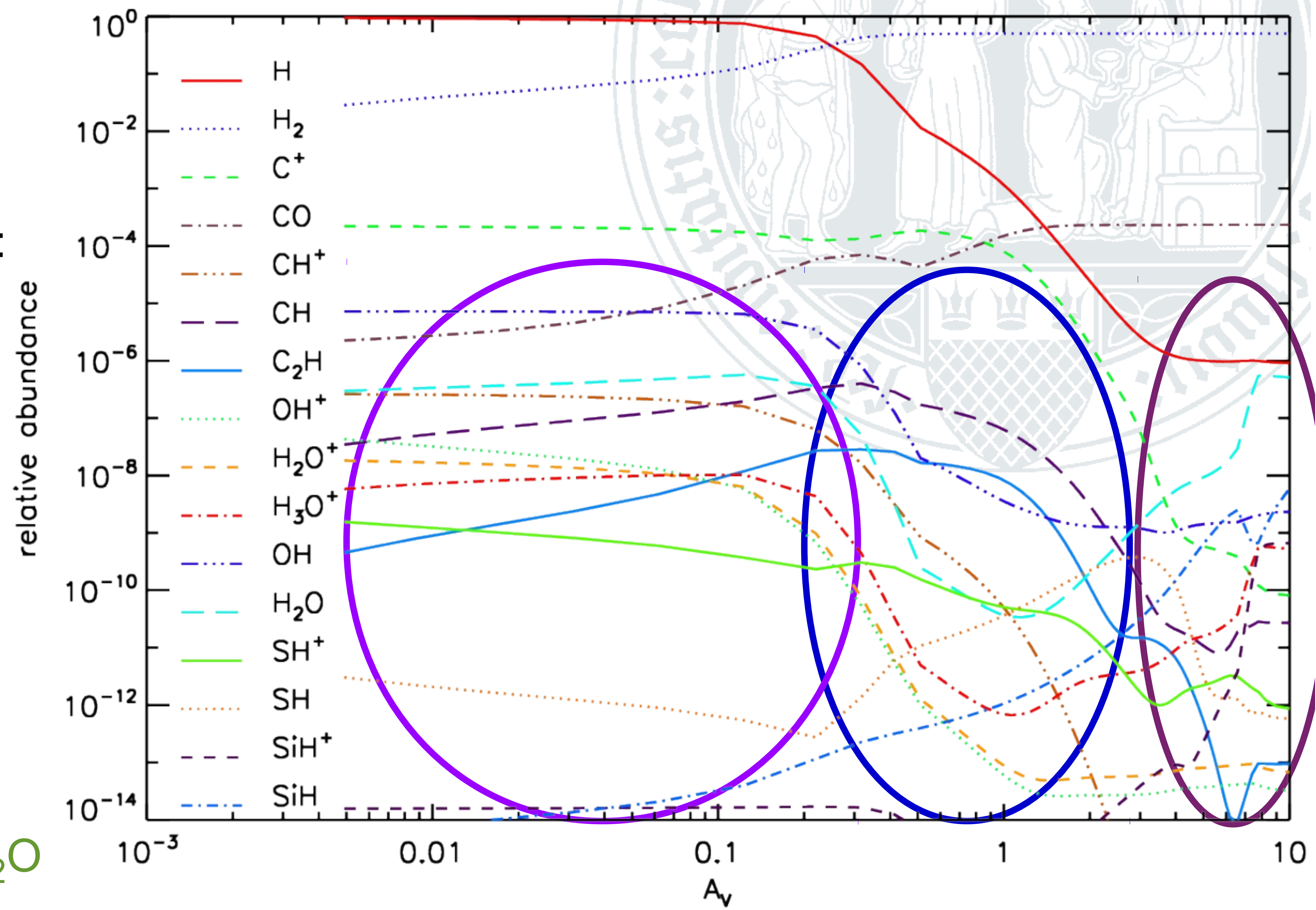
SH^+



CH +
H2
H , γ
e⁻
CH +
S
H
HS +
S +
S
C
H2S +
CH +
relative abundance
A_V
H
H2
H2*
NH+
NH
SH+
SH
SiH+
SiH
HCO
H , γ
H , O
H2S +
HCO
O
H2S +
OH
CO
H13CO +, H3 +, HCO +
S +
O
HS +
SO +
H13CO +
HCO +
H13CO +
HS +
13 CO
HS +
CO
O
HS +
HCO +
H3 +
OH

Comparison of hydrides

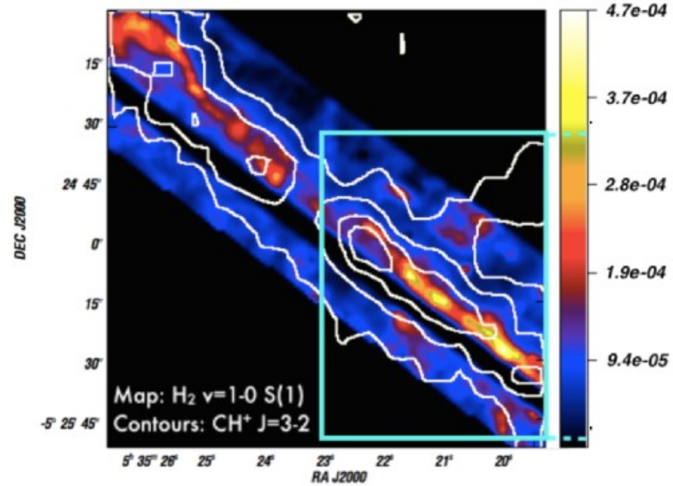
- Groups of molecules:
  - Atomic gas only:
    - CH^+, OH^+, H_2O^+, OH
  - CO-dark mol. gas:
    - SH
  - MC only:
    - SiH^+, SiH
  - Atomic + CO-dark mol. gas:
    - CH, C_2H, SH^+
  - Atomic gas + MC:
    - HCO^+, H_3O^+, H_2O

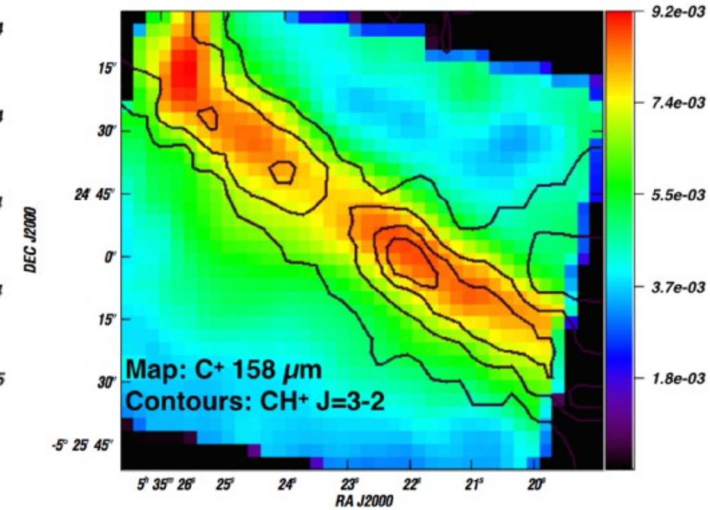


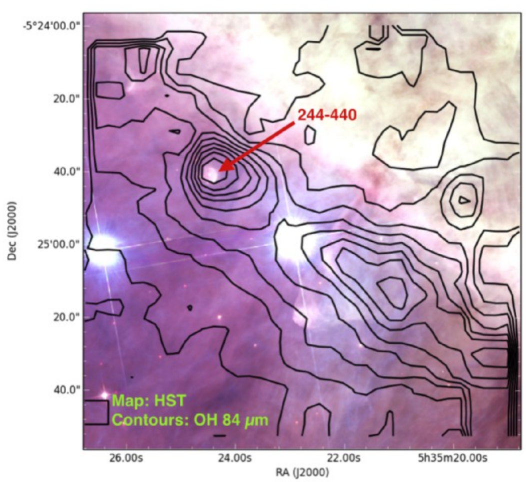
KOSMA-τ result for $\chi = 10^4\chi_0$, $n=10^6$ cm^{-3}

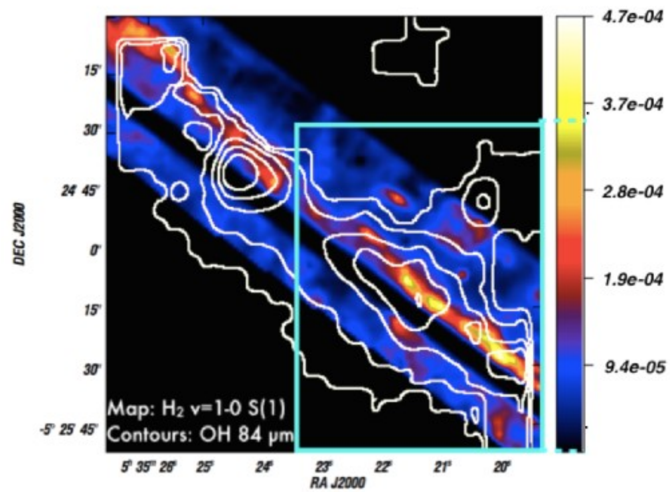
Morphology

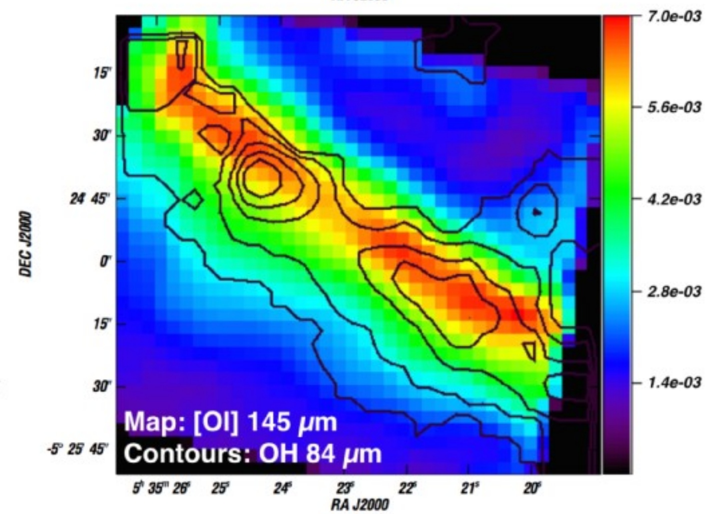
- OH ↔ CH^+
  - Good correlation
    CH^+ ↔ C^+, H_2^*, high-J CO
    OH ↔ H_2O











Parikka et al. (2016),
Goicoechea et al. (2011)

- Layering CH^+, OH stronger than predicted
- OH rather at higher densities, combined UV-density tracer

→ Talk Parikka

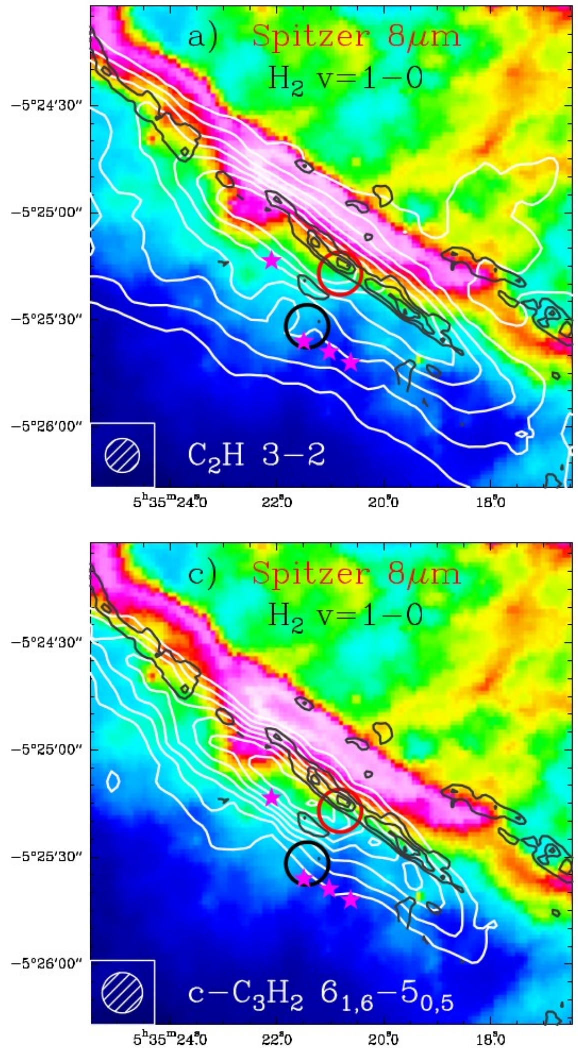
Example C_nH, C_nH_2

- Pronounced stratification

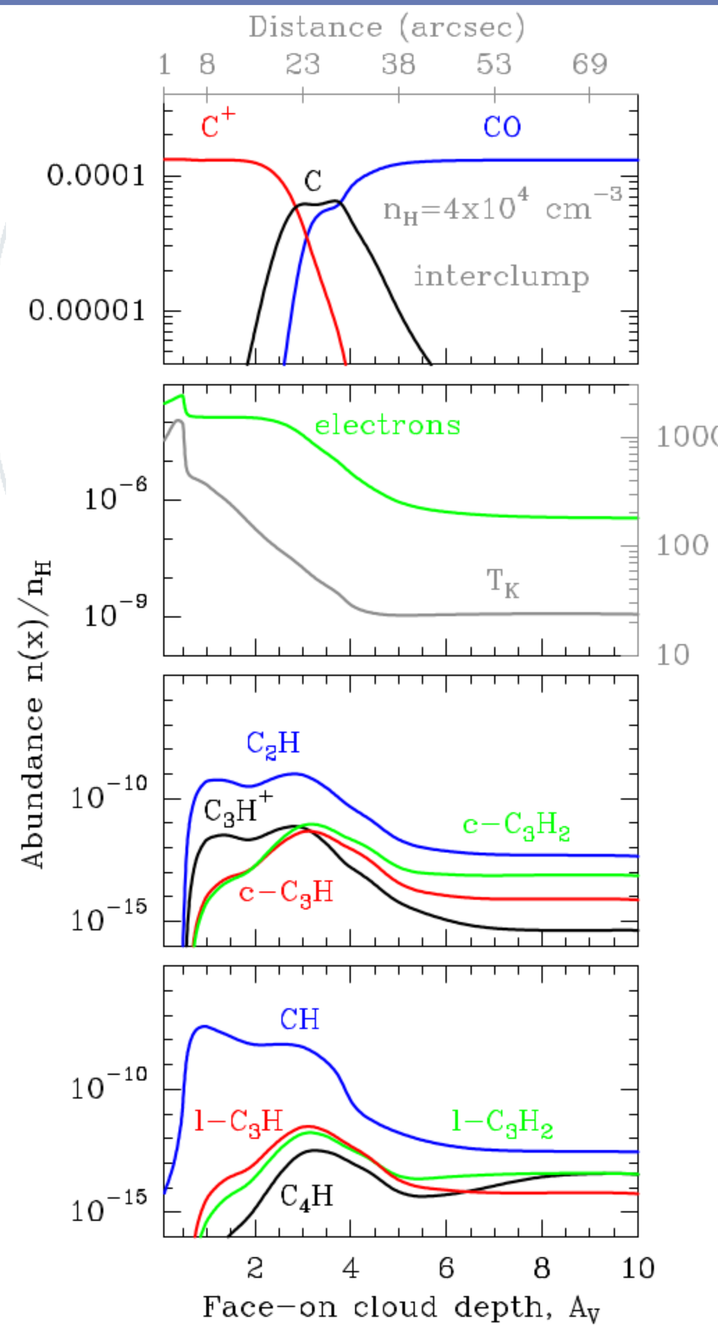
- C_2H does not follow PAHs

  → PAH destruction not main production

  → instead $C^+ + H_2$



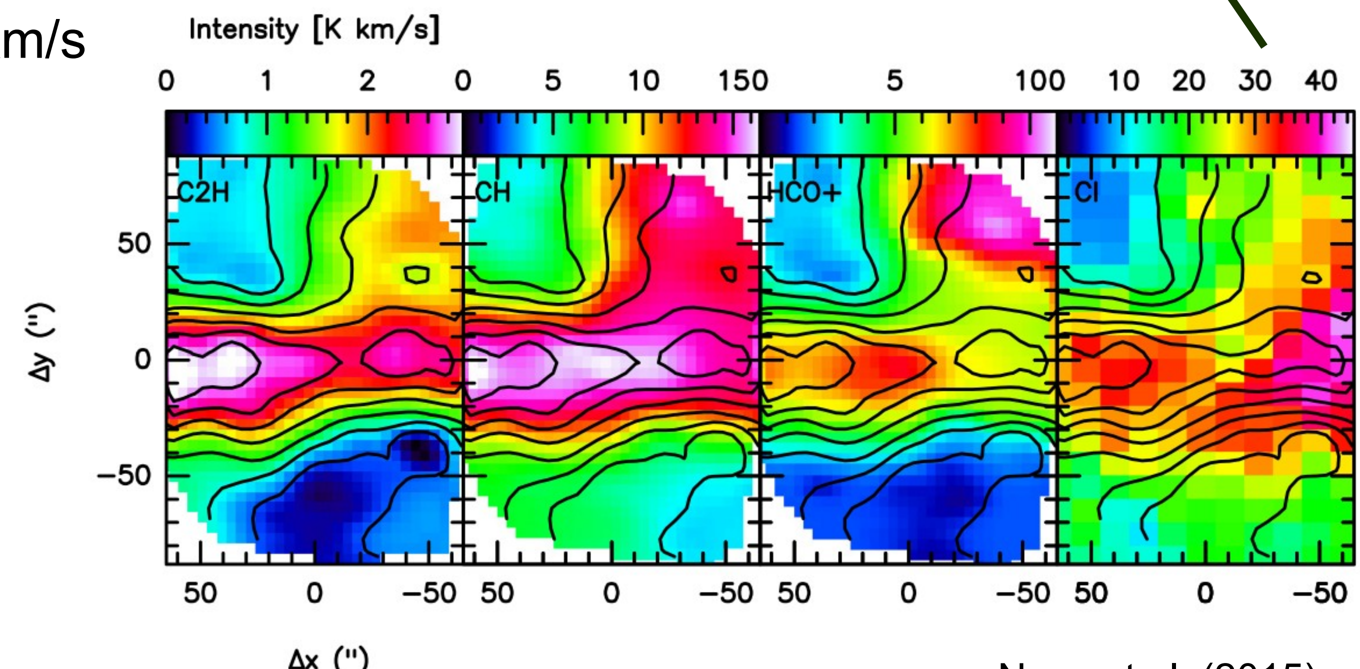
Cuadrado et al. (2015)



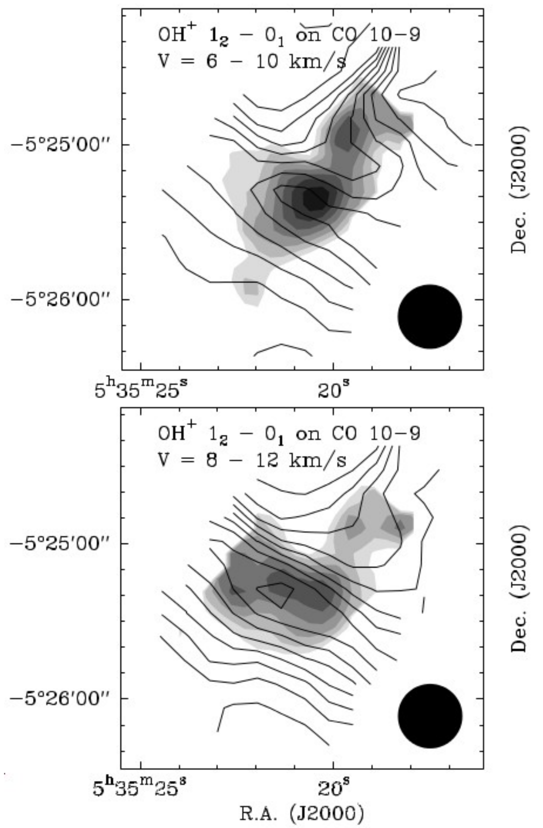
- Qualitatively in agreement with model
- Displacements wider than predicted

CH, CCH, OH^+, HCO^+

- Good spatial correlation
  - No significant stratification
- Pick-up from different gas at different velocities
  - Orion Ridge at 8km/s



Nagy et al. (2015)

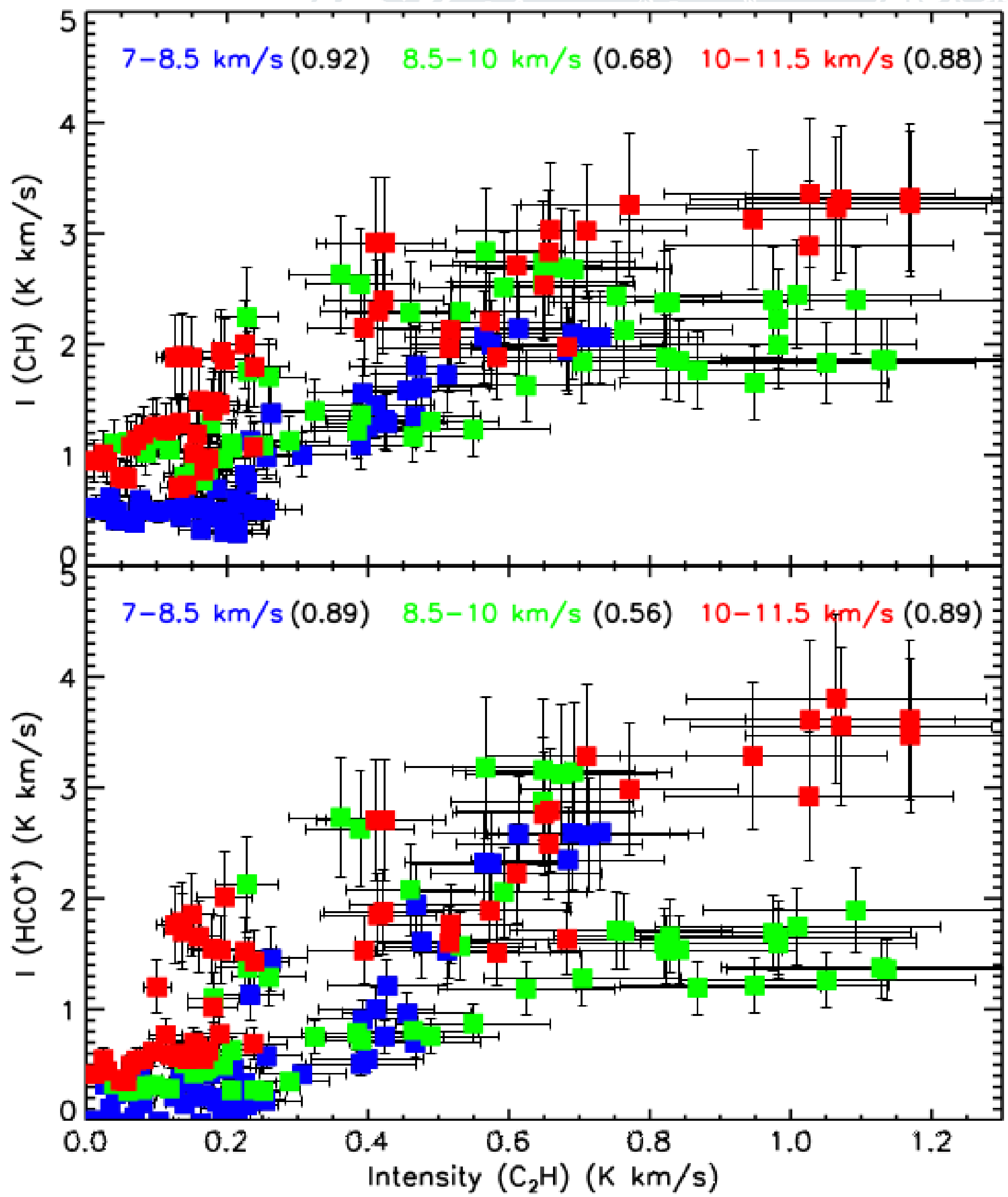


Van der Tak et al. (2013)

- Collisions with e^- main destruction and excitation of OH^+

CH, CCH, OH^+, HCO^+

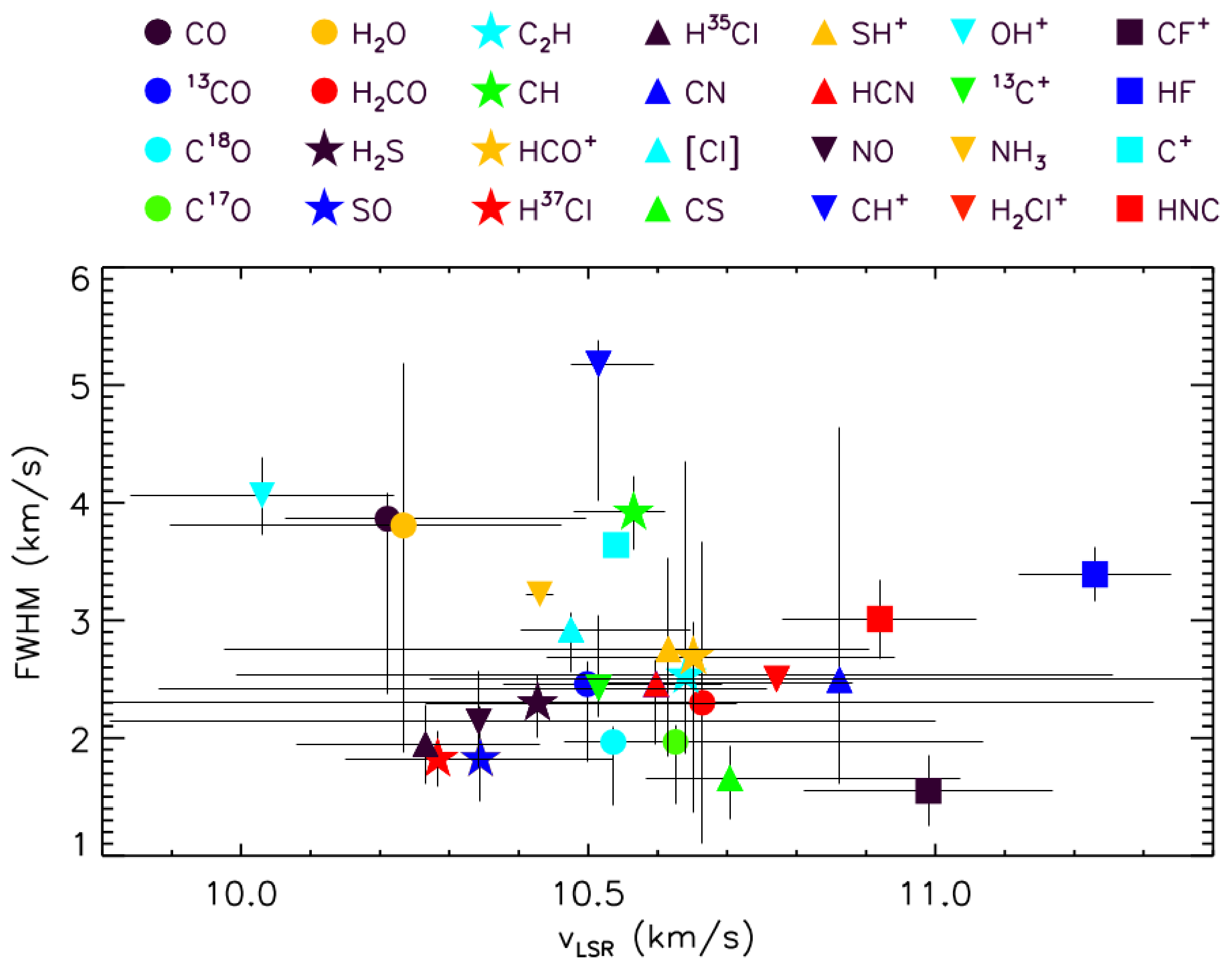
- Different correlations in different velocity components
  - Worst for main Orion Bar component
  - CI not correlated with hydrides
  - CCH requires multiple component PDR model



Nagy et al. (2015)

HIFI spectral scan in Orion Bar

- Matching line profiles for most species
- Outliers:
  - HF, CF^+
    - Veil velocities
  - CO, OH^+, H_2O
    - Orion Ridge velocities
  - CH+, CH, C^+
    - Wide lines with Bar velocities
- Does not match theoretical scheme!

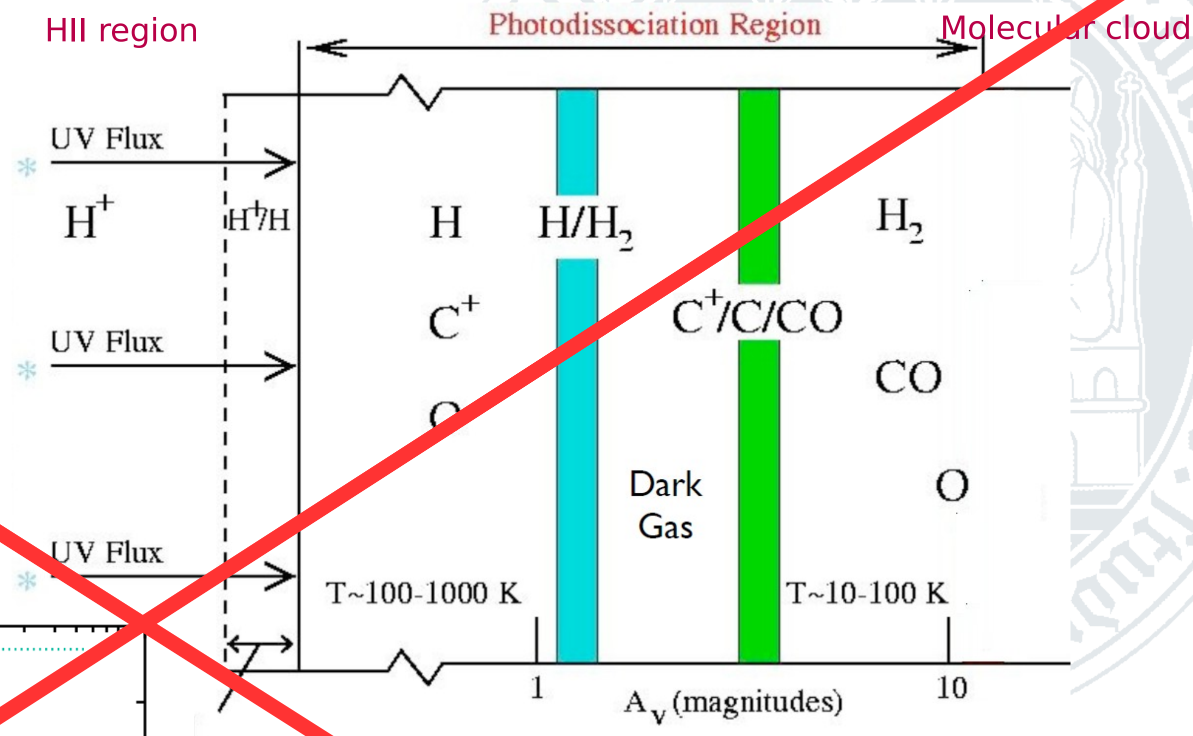


Nagy et al. (2016)

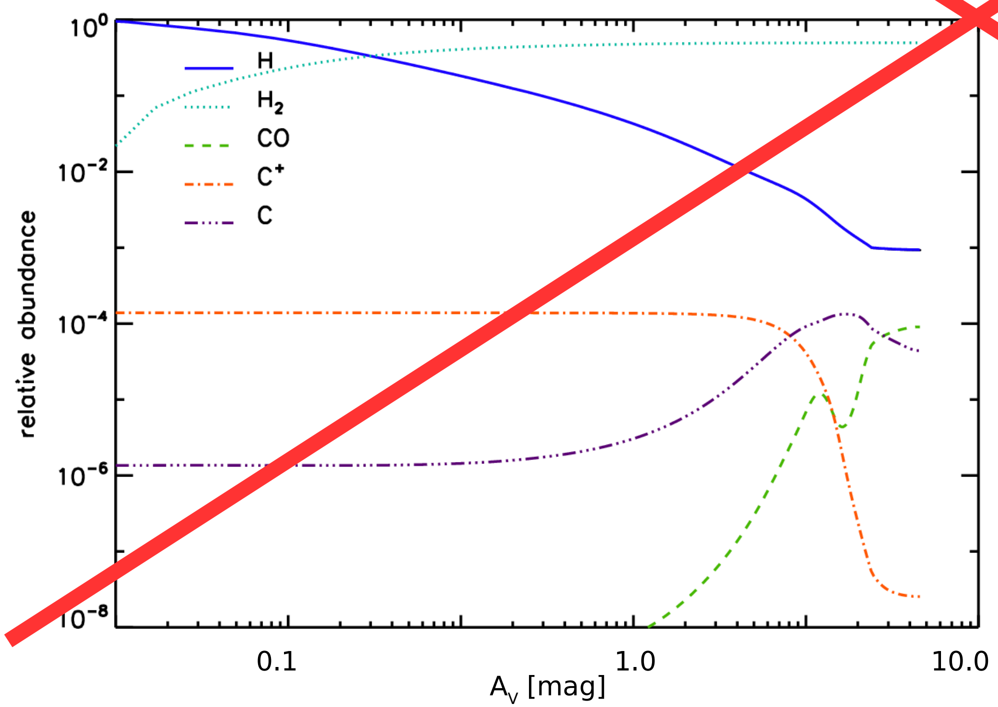
→ Poster 12

Stratified structure

- Layering of chemical transitions and temperatures
- Molecules dissociated at the cloud surfaces.
- Complex molecules only in the dense cores.



Based on Hollenbach & Tielens (1999)

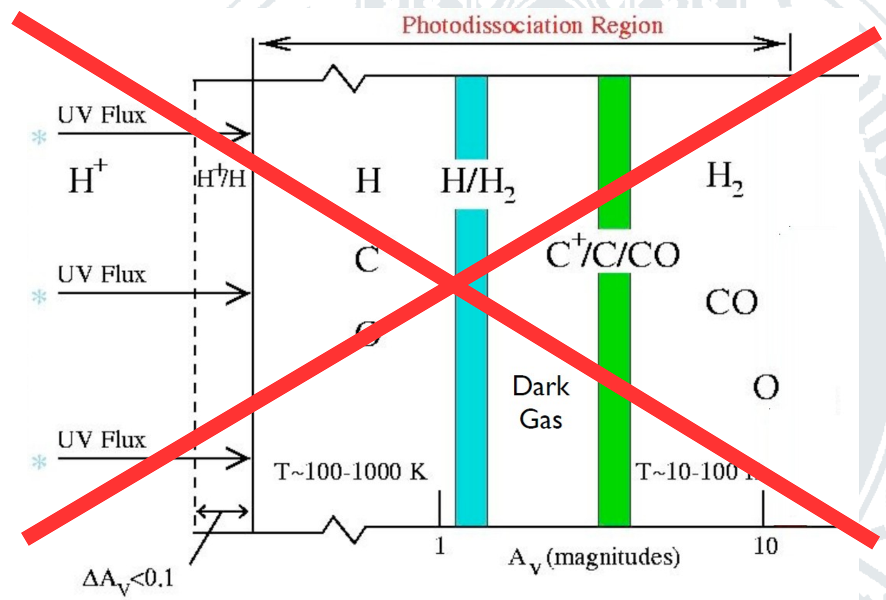


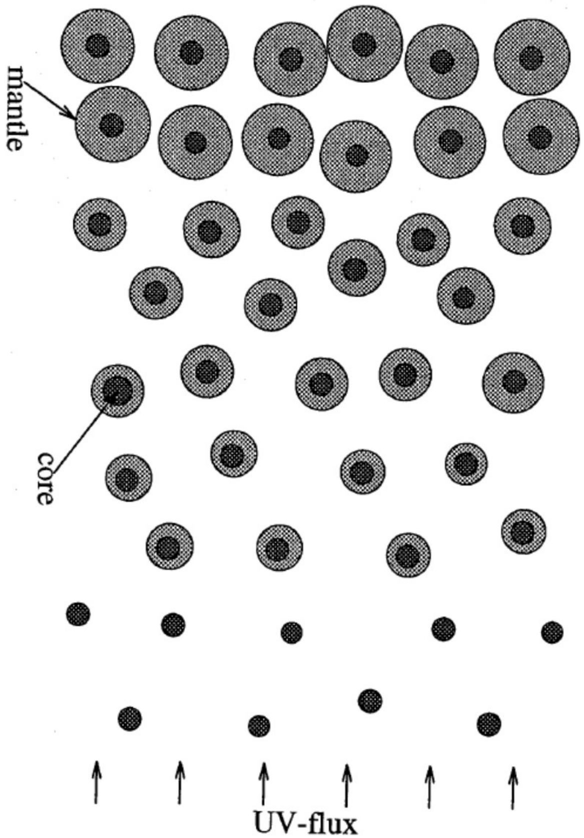
Resulting abundance profiles

(KOSMA-τ PDR model: Röllig et al. 2006)

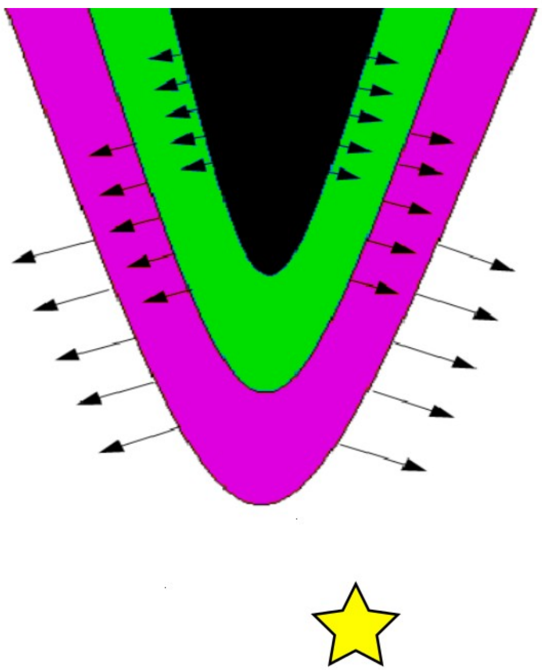
Photo-evaporation / photo-ablation

- Permanent feed of low-density envelope from dense clumps

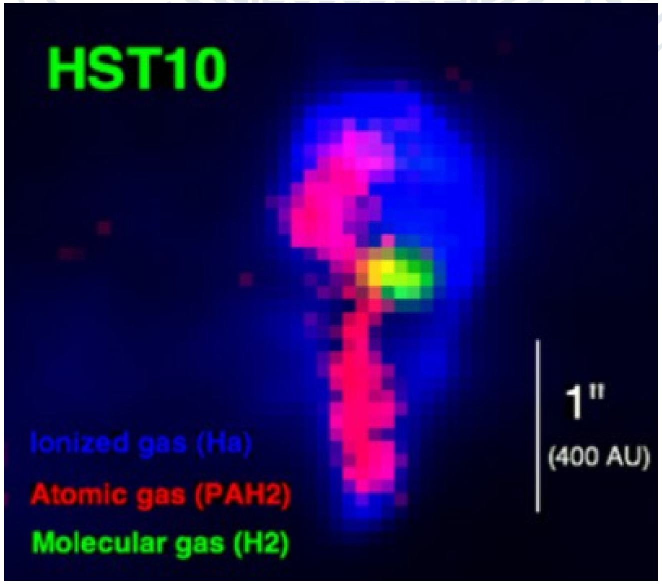




Hogerheijde et al. (1995)



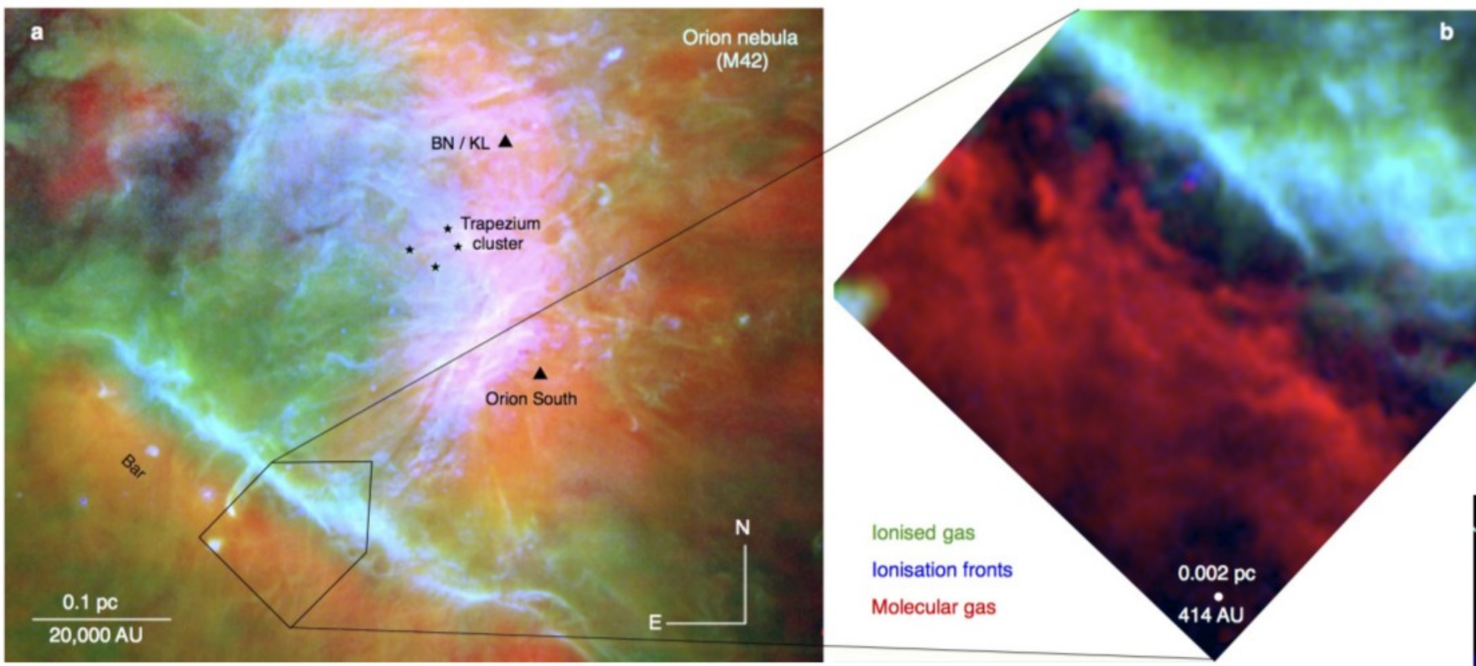
Berné et al. (2014)



Vicente et al. (2013)

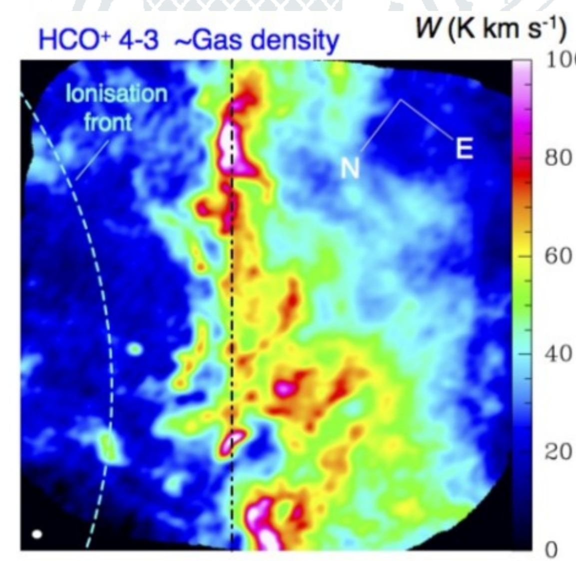
Observational evidence

ALMA mapping (Goicoechea et al. 2016):



Clumpy and filamentary structure seen in SII (6731Å, green), OI (6300Å, blue), HCO^+ (J=4-3, red), atomic gas is dark

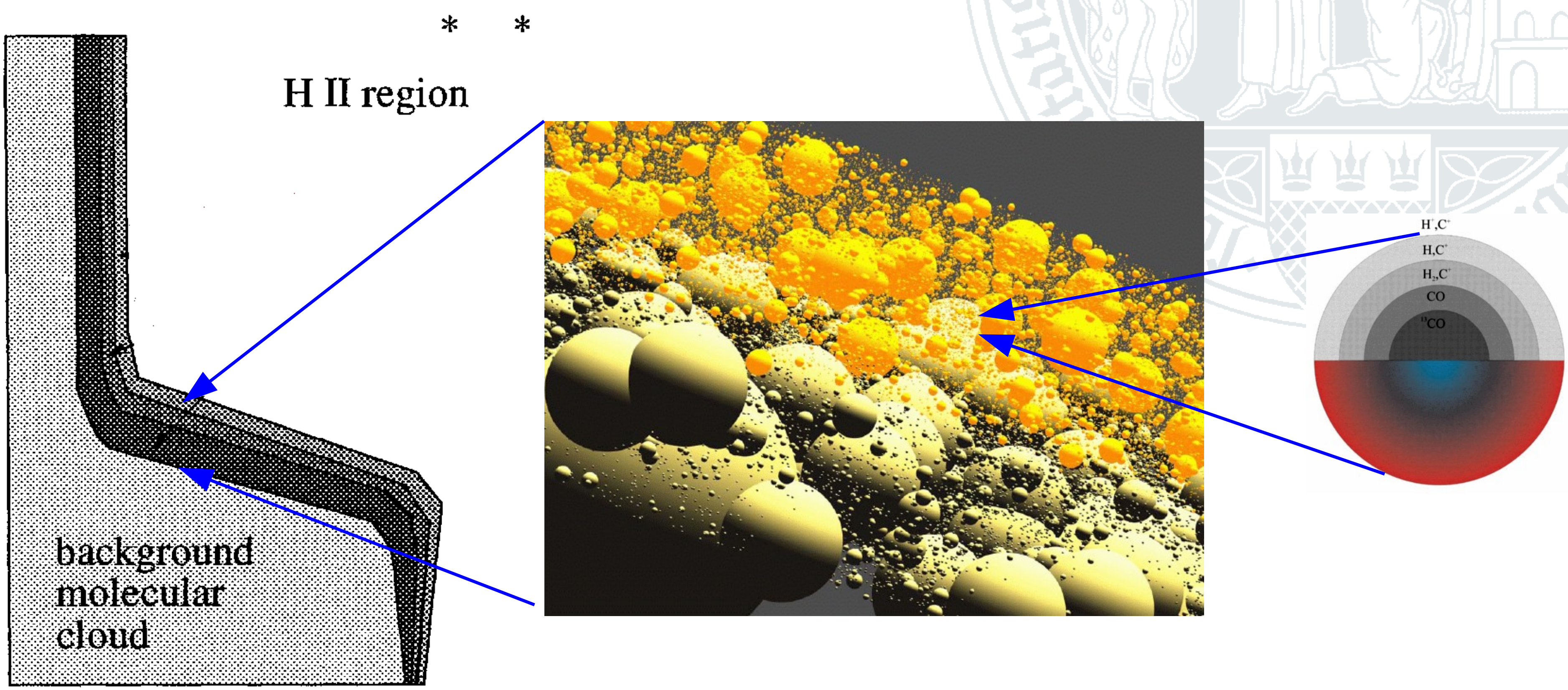
- Allows deeper penetration of UV radiation
- Every PDR has photo-evaporating low-density gas



Goicoechea et al. (2016)

KOSMA-τ-3D

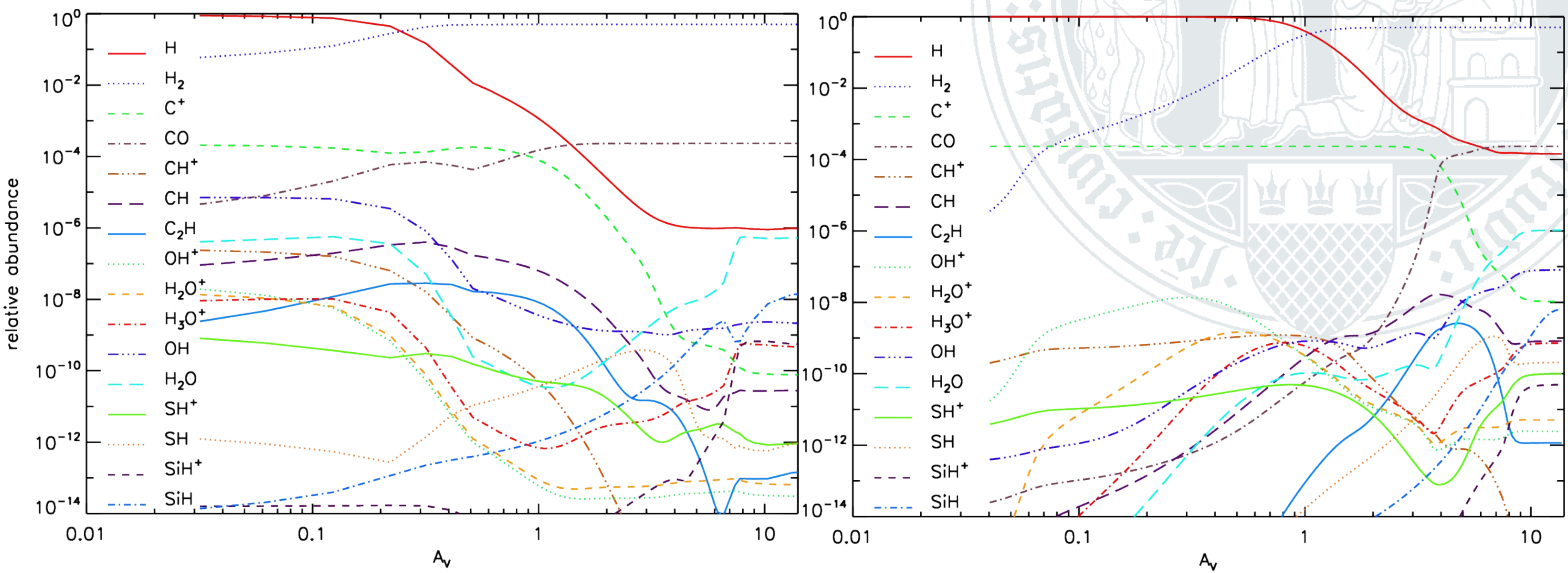
- PDR composed of mixture of clumps and interclump medium (Andree-Labsch et al. 2016)



Hogerheijde et al. (1995) Andree-Labsch et al. (2016) Röllig et al. (2006)

Significantly different chemistry

- Higher columns of CH, CCH, OH, SH, SiH and SH+ compared to high-density model

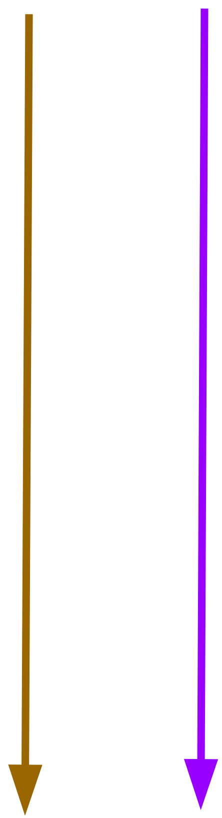


KOSMA-τ result for $\chi = 10^4\chi_0$: $n=10^6$ cm^{-3} $n=10^3$ cm^{-3}

- Exchange of material between the two phases expected

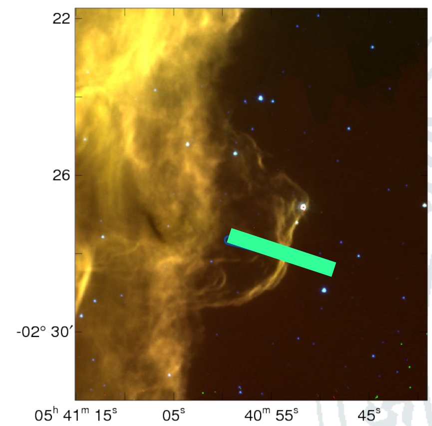
WADI:

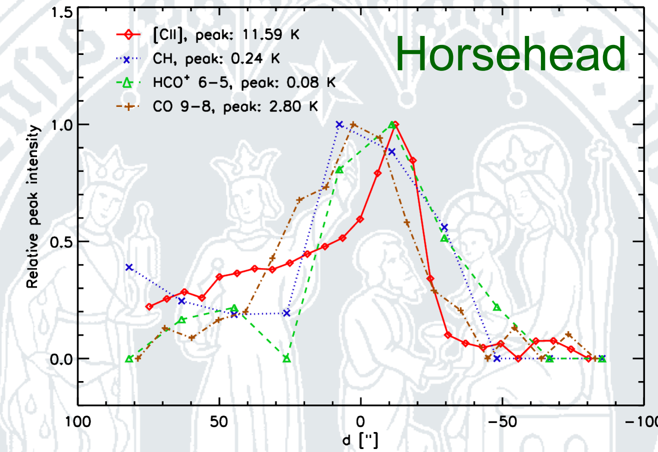
- Profiles across PDR interfaces
  - Extended CH, OH
  - Differential stratification
  - Many "puzzles" for high UV sources
  - Structures always more complex

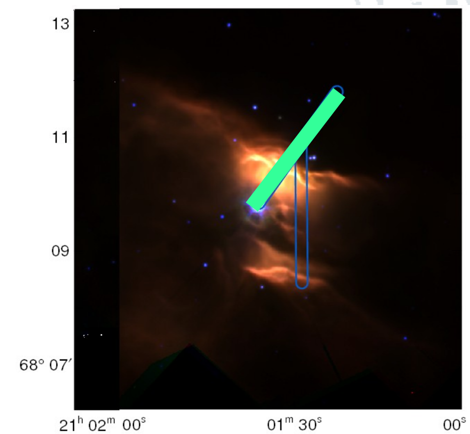


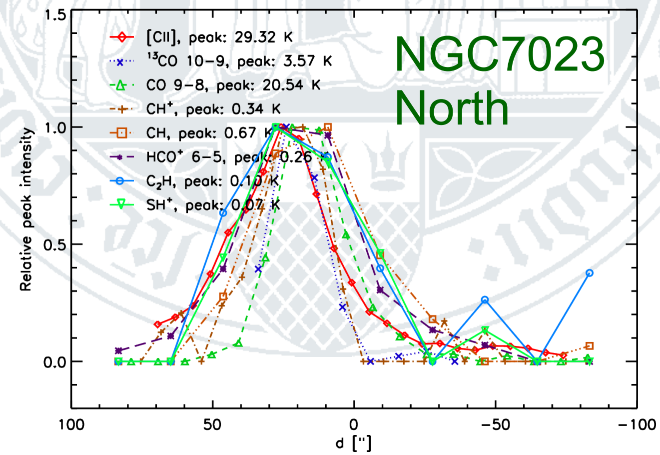
complexity UV

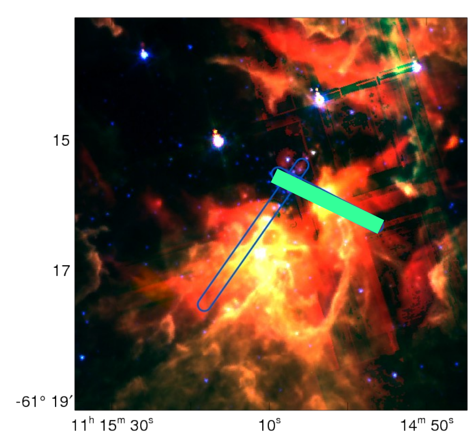
Ossenkopf-Okada et al., in prep.

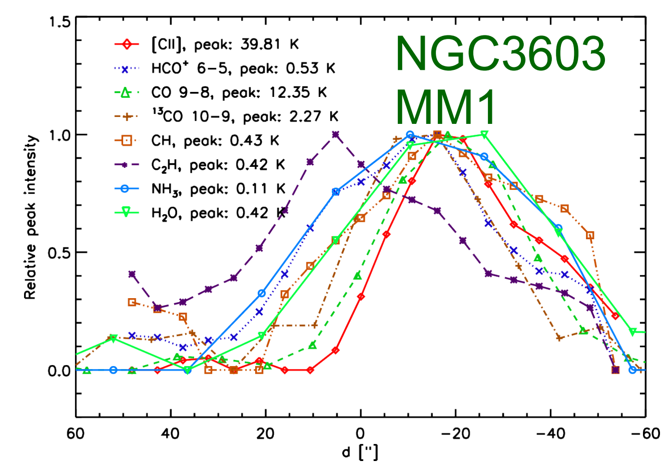




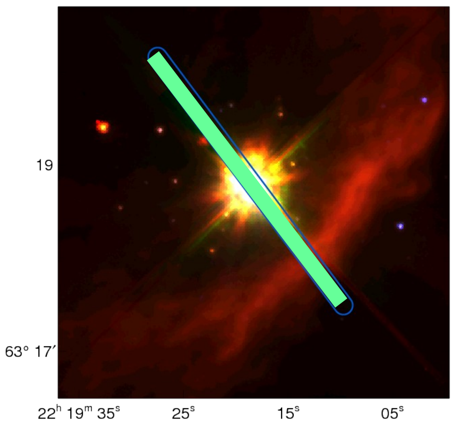


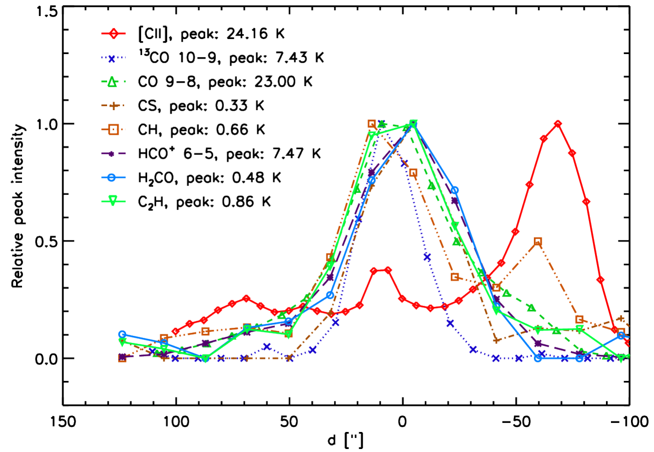




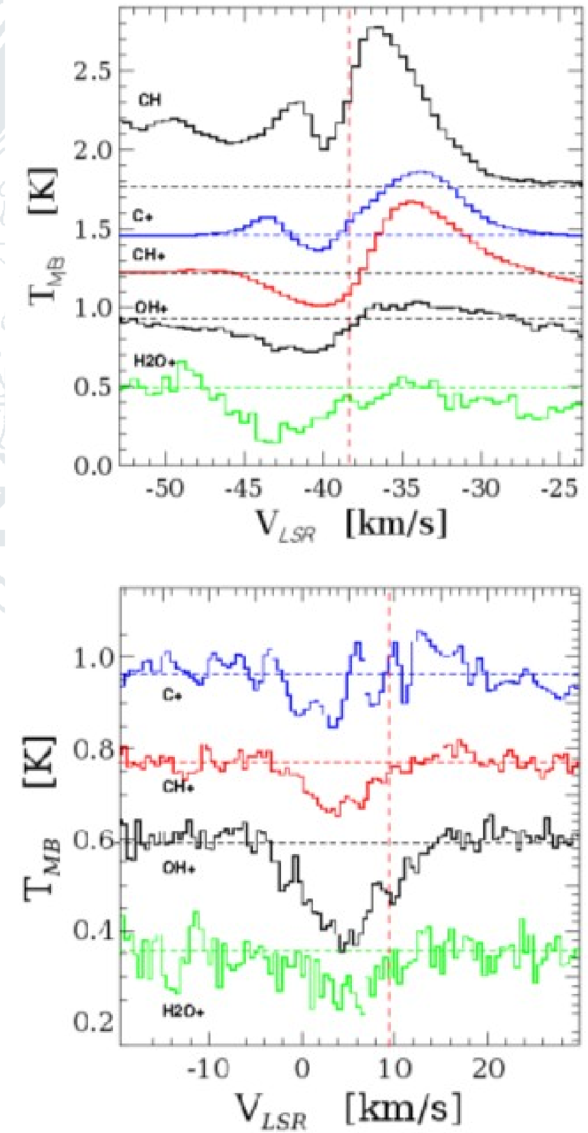


PDRs with YSOs / YSO-PDRs





S140: Ossenkopf-Okada et al., in prep.



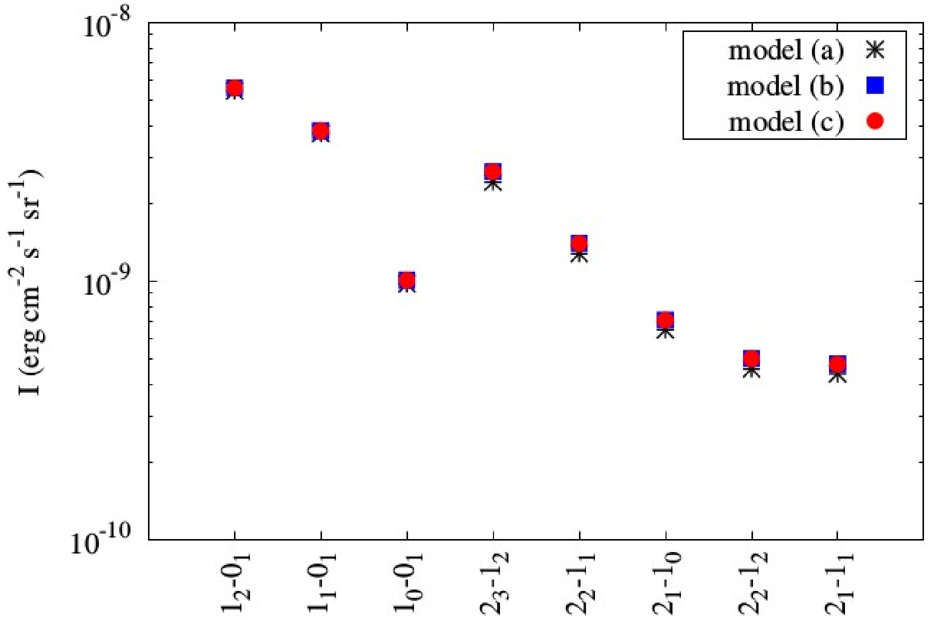
- Different correlations for many velocity components
  - Indicate different origins: outflows, envelope, irradiated cavity walls
  - CH^+ and OH^+ as UV tracer
  - H_2O^+ as X-ray tracer
- Every YSO contains multiple PDRs → Talk A. Benz

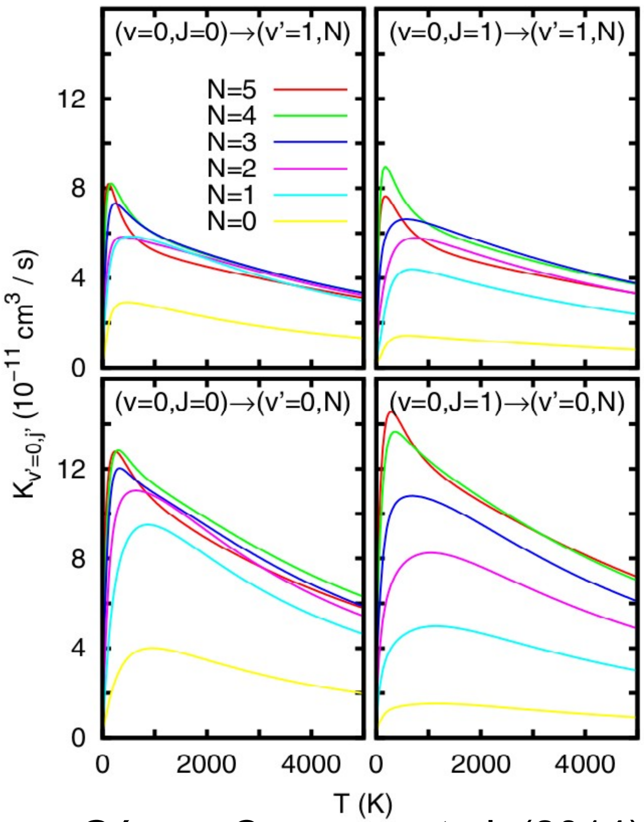
W3 IRS5: Benz et al. (2016)

Excitation

- Formation pumping can be essential
  - Requires state-to-state reaction rates
- OH^+ (Gómez-Carrasco et al. 2014)
  - Strong *J*-dependence of formation rate
  - Effect small for Orion Bar conditions

→ Talks: A. Faure, F. Lique, J. Schneider



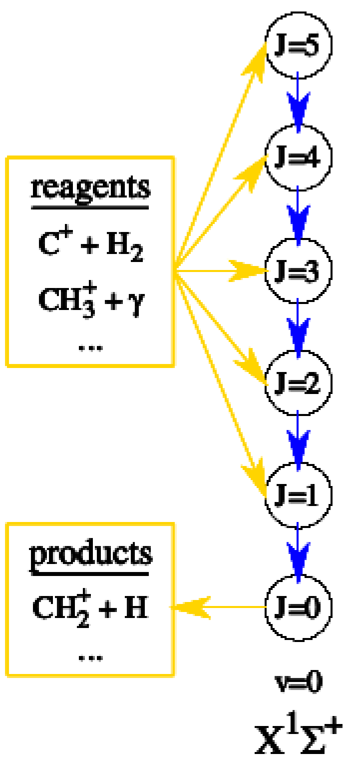


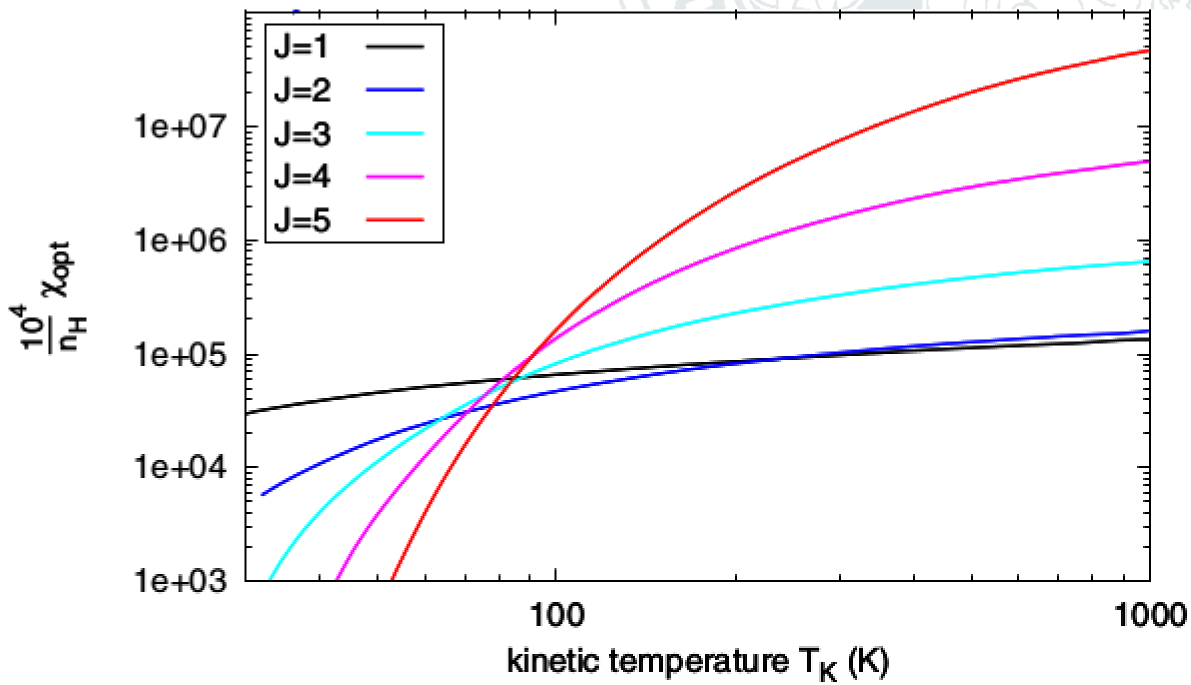
Gómez-Carrasco et al. (2014)

OH^+ intensities: (a) excitation by nonreactive collisions, (b) including chemical pumping assuming Boltzmann (T=2000K), (c) adopting branching ratios from quantum calculations

Excitation

- CH^+ (Godard & Cernicharo 2013)
  - Collisions – reactive + non-reactive dominant for Orion Bar conditions
  - High-*J* mainly populated by reactive collisions (chemical pumping)





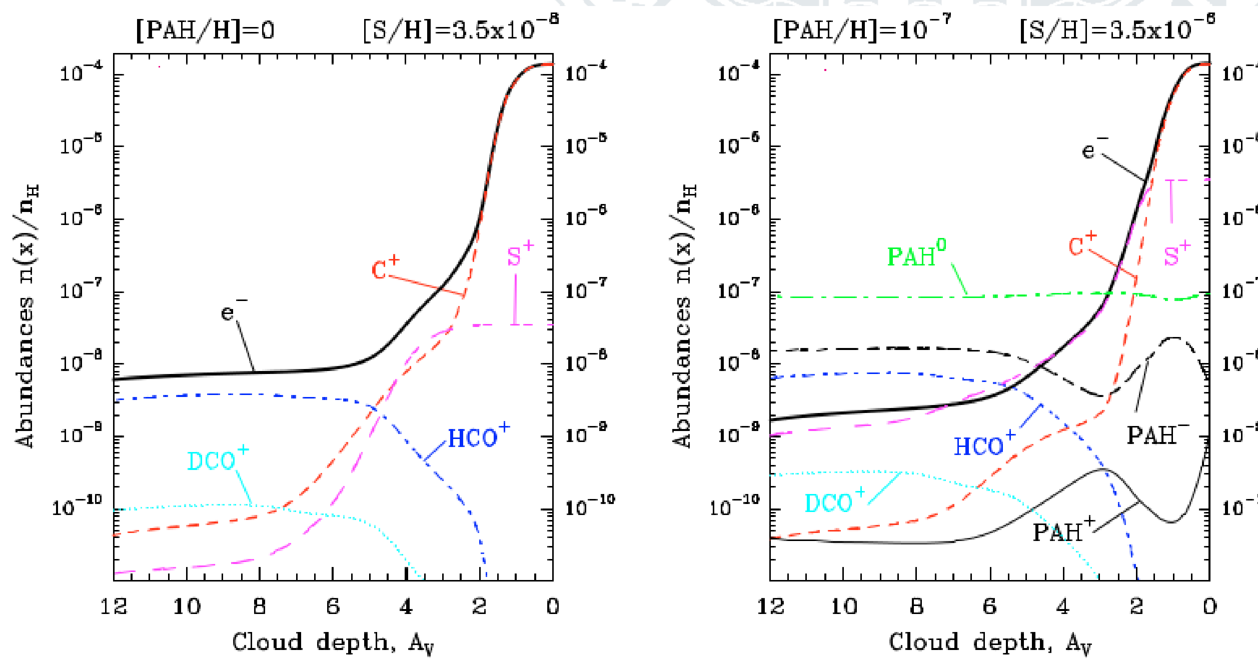
Critical UV/density ratio for dominant collisional population of different CH^+ levels (Godard & Cernicharo 2013)

Lab/Theory:

- Collision rate coefficients still missing for many species
- State-to-state reaction coefficients for many species
- Dissociation spectra – in particular for isotopologues (e.g. $H_2{}^{18}O$)
- Mechanisms and rates of surface chemistry

Codes:

- Full time-dependence at good spatial resolution
- Initial and boundary conditions
- Self-consistent inclusion of PAH temperature and charge distribution

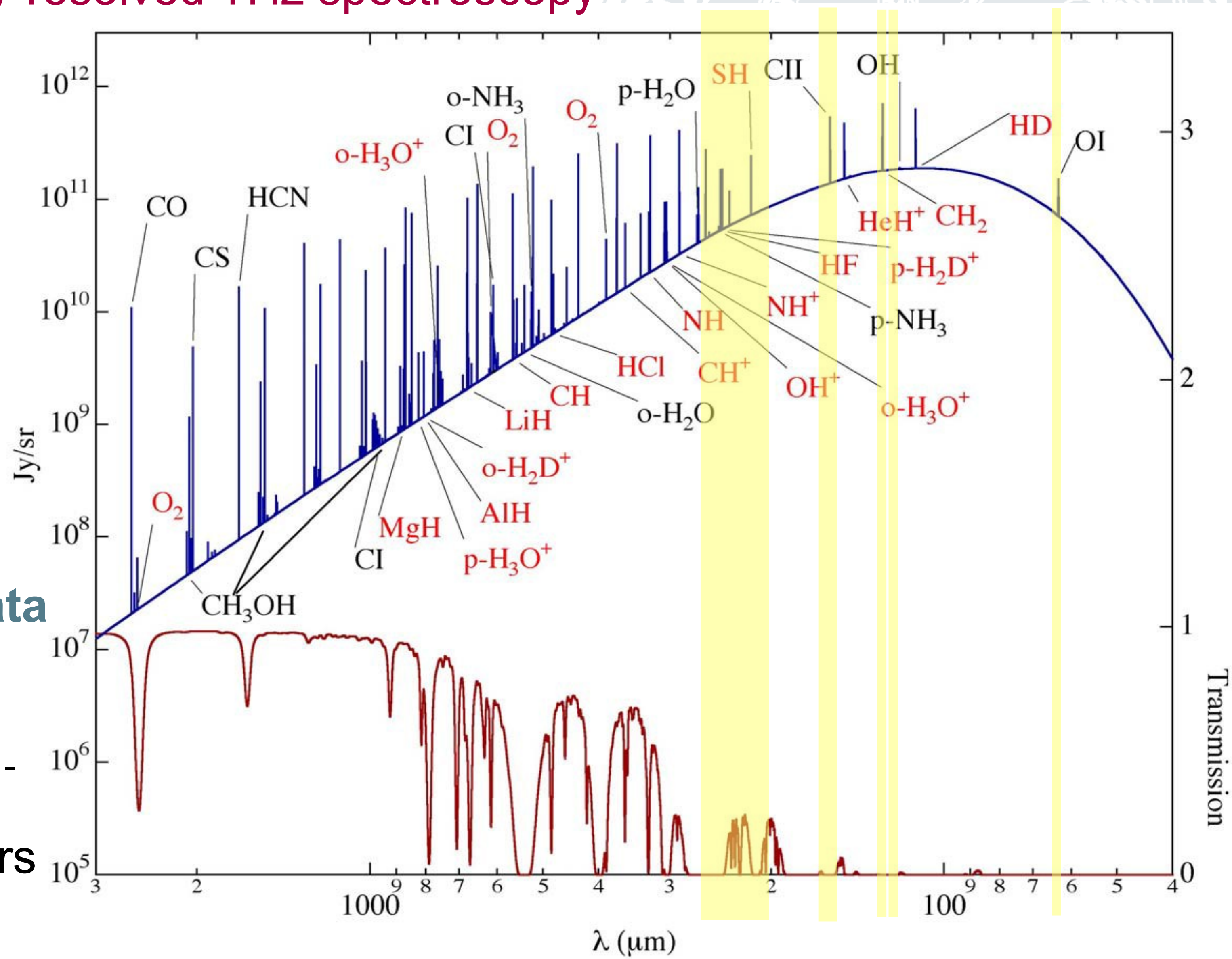


Goicoechea et al. (2009)

More systematic observations

Hydrides

- Requires velocity-resolved THz spectroscopy
- Breakthrough from HIFI
- GREAT@SOFIA needed
  - 4GREAT
  - More LOs



Complementary data

- CII, NII
- PAH, PAH^+, PAH^-
- Dense-gas tracers

Many answers, more questions

- There is no "typical PDR chemistry"
  - Comparison "diffuse clouds" ↔ PDRs does not make sense
  - Significant variation with optical depth and density
- PDRs are neither static nor have a simple geometry
    - Forget single component models
    - Forget pressure balance models
  - There is no PDR without low density gas!
    - Always produced by photo-evaporation
  - Simple hydrides (CH, OH, SH, NH, SiH) most abundant in the low density gas
  - Time dependence is essential
- Hydrides provide essential information on the photo-evaporating material