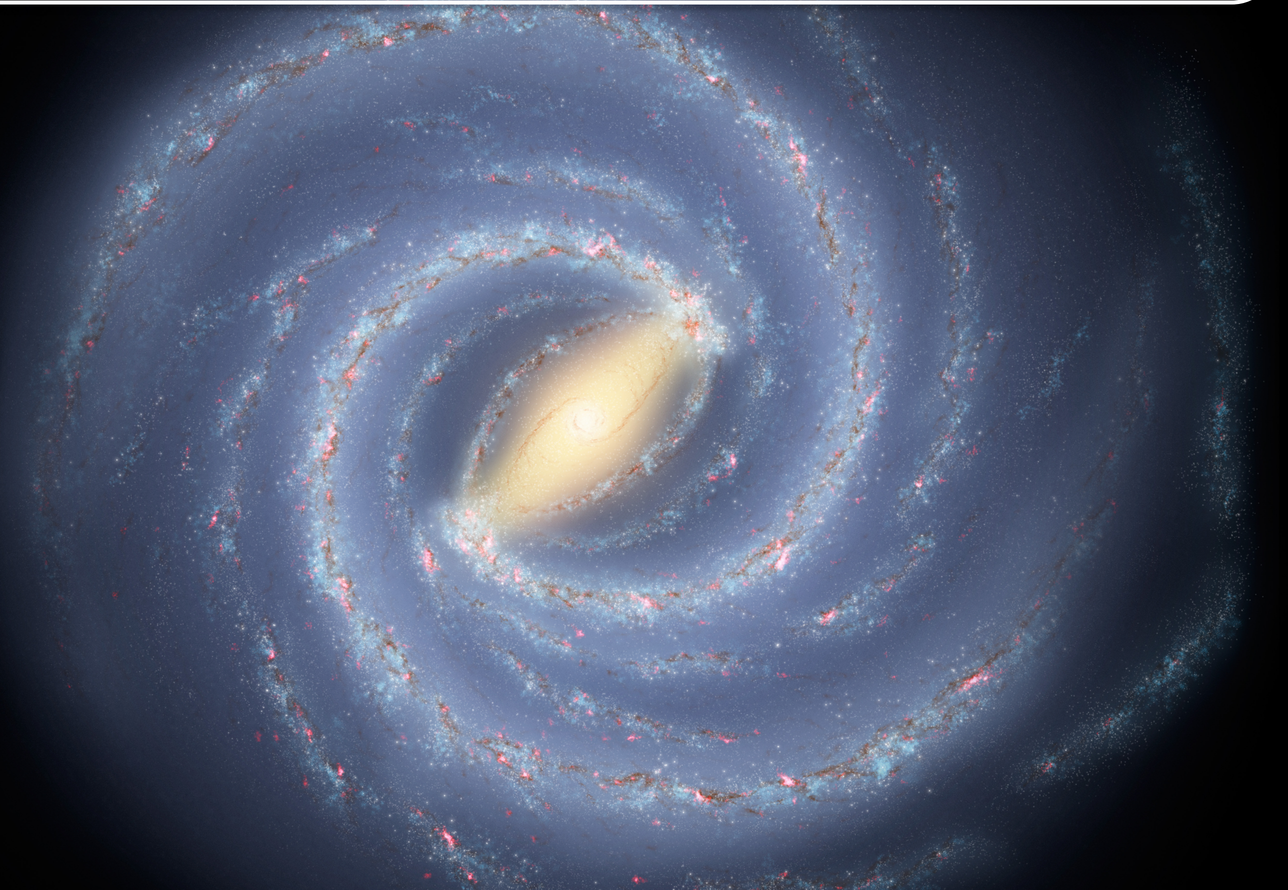
Ortho-to-para ratios of dihydride species: The interstellar NH_2 case



Romane Le Gal

Research Associate at UVa in Eric Herbst's group

Main external collaborators: Carina Persson (Chalmers, Sweden), Hua Guo (University of New Mexico)

Outline

- **Interstellar chemistry**
  - NH_2 in the interstellar medium (ISM)
  - NH_2 ortho-para ratio (OPR) observations
- **Astrochemical modeling**
  - Building chemical network
  - Results: comparison with observations

Amidogen (NH_2) in the ISM

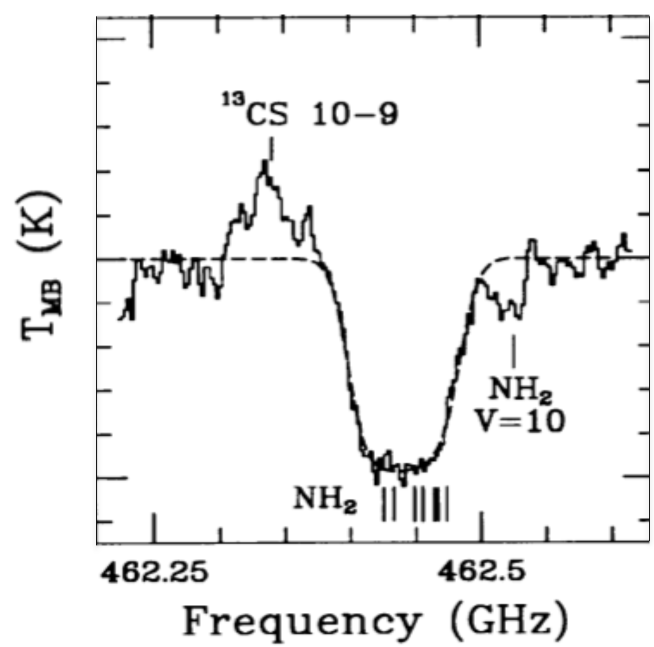
- Characteristics

- Important radical in the first steps of N-chemistry
- Chemistry closely related to NH_3

- Light asymmetrical rotor with two spin symmetry configurations:
  - ortho (H spins parallel)
  - Para (H spins anti-parallel)

- Only few observations (submm λ)

- First detection

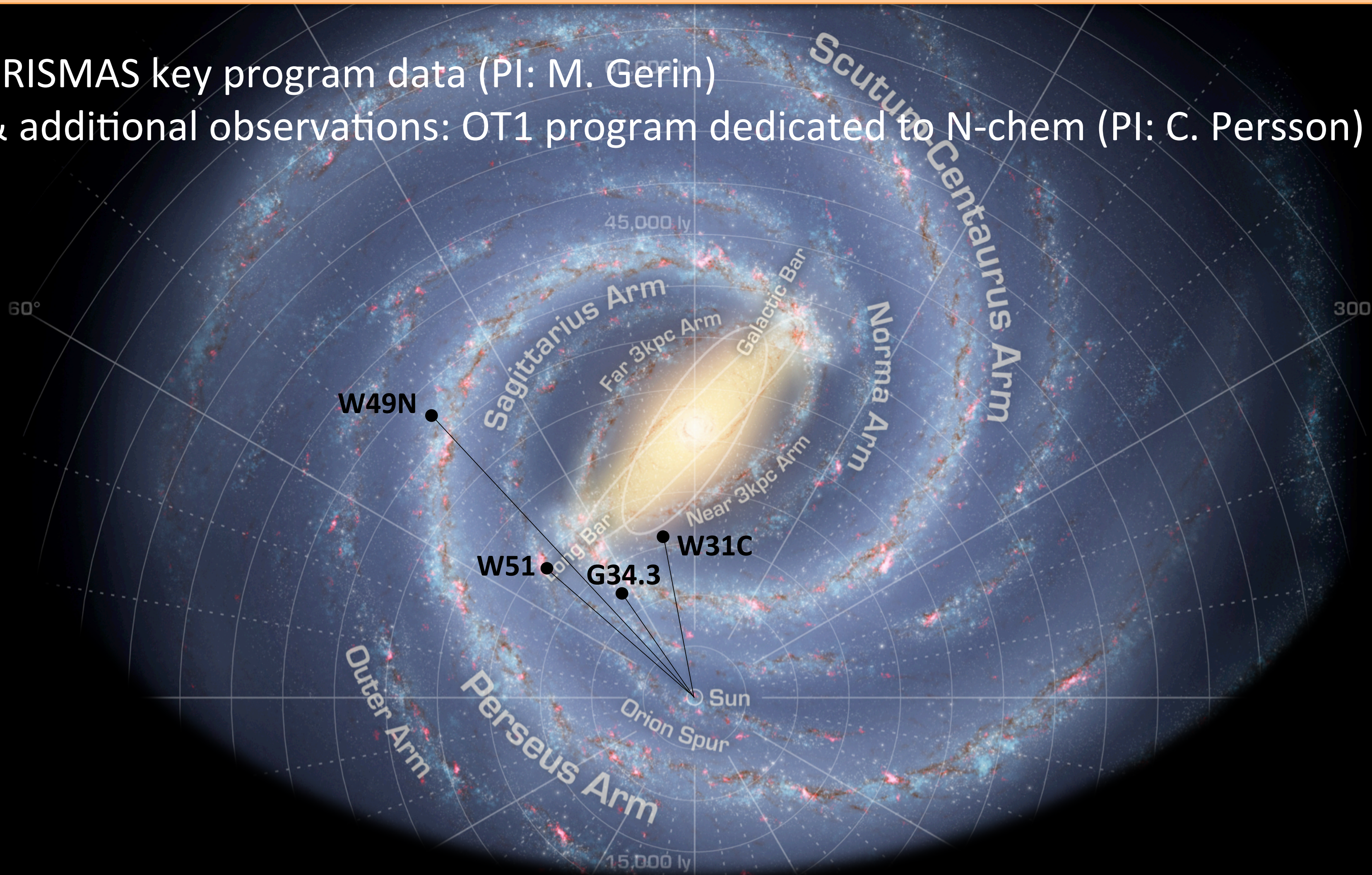


(CSO observation towards Sgr B2,

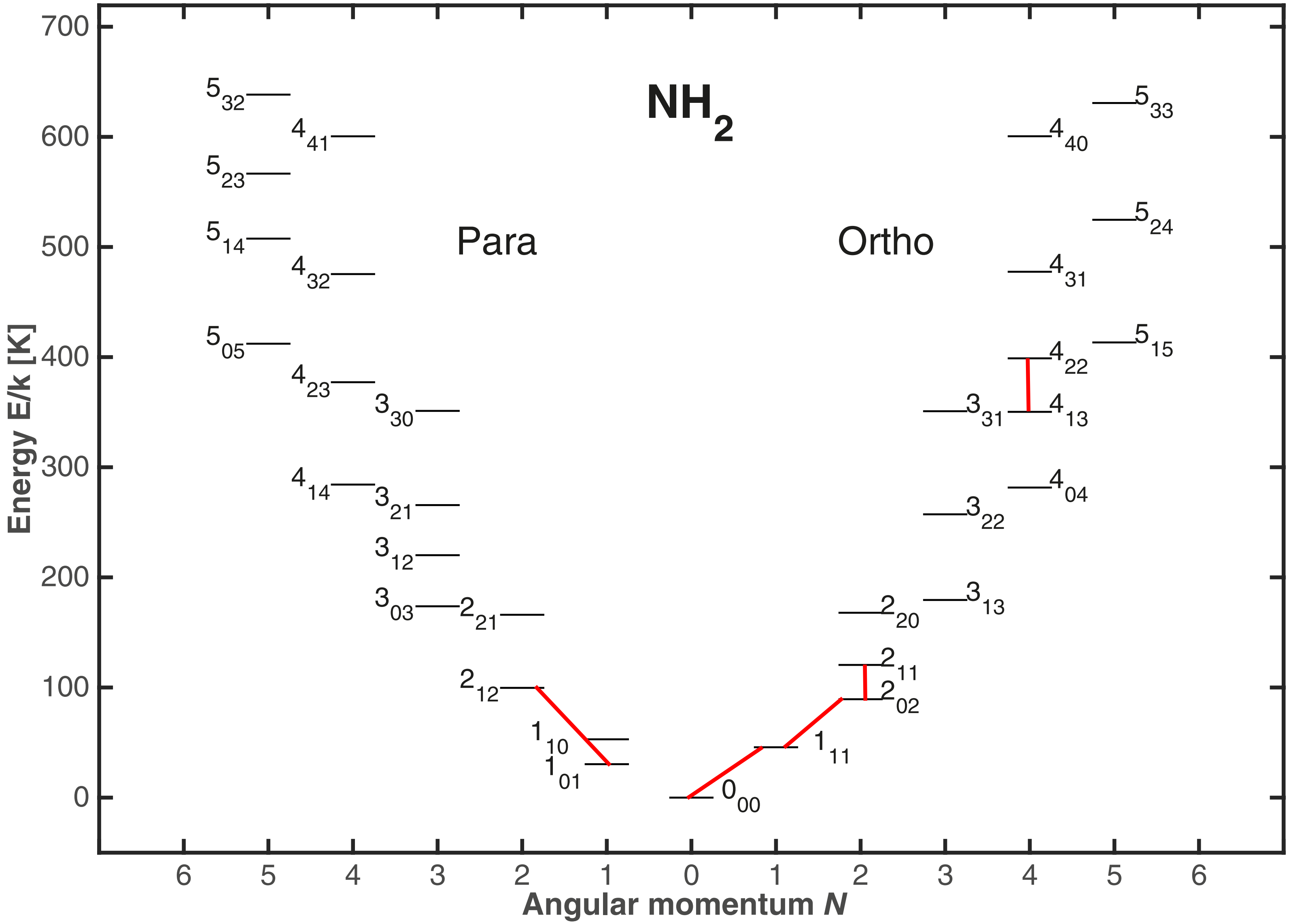
van Dishoeck et al. 1993)

NH_2 OPR observed towards high-mass star-forming regions

PRISMAS key program data (PI: M. Gerin)
& additional observations: OT1 program dedicated to N-chem (PI: C. Persson)



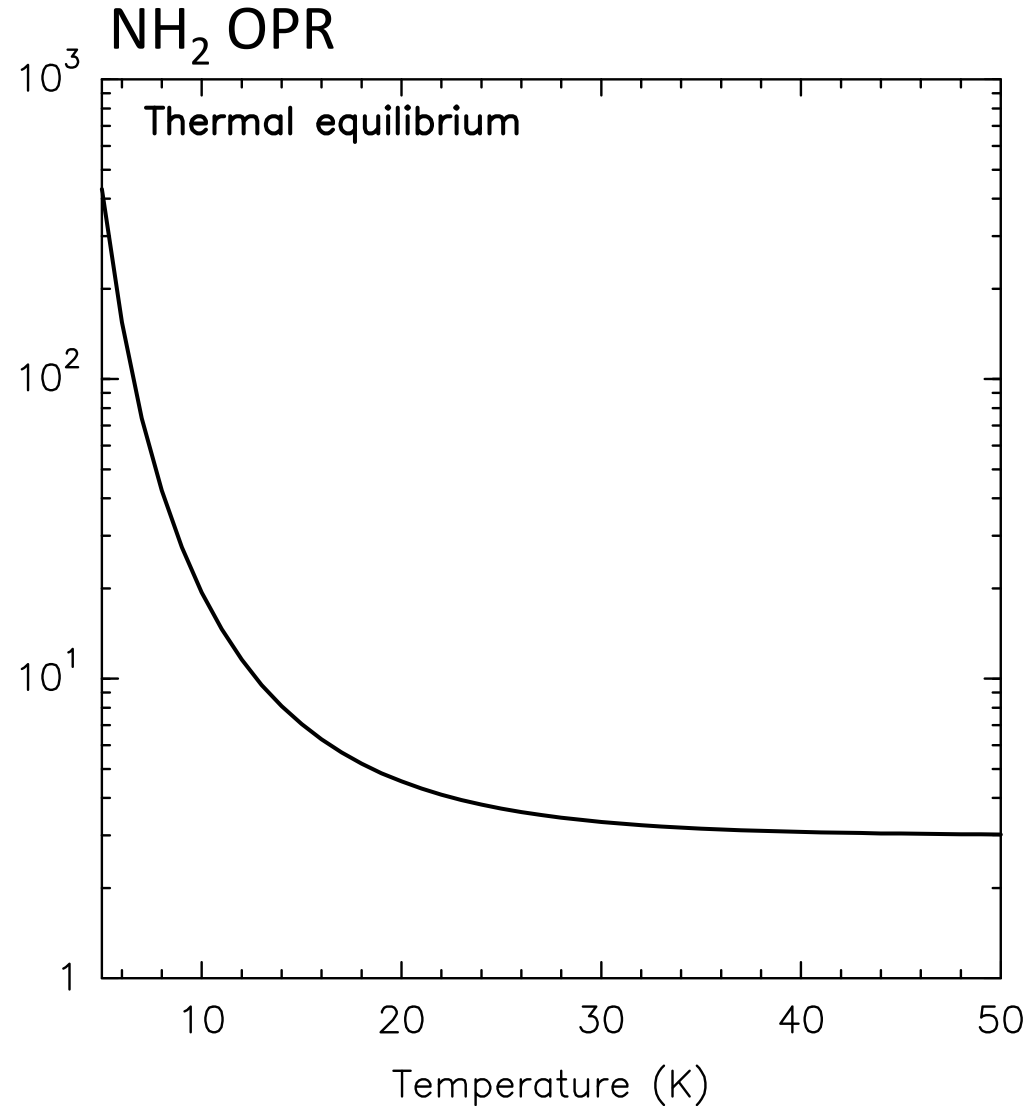
Energy level diagram of NH_2



(Persson, Olofsson, ***Le Gal*** *et al., A&A. 2016)*

NH_2 OPR thermal equilibrium with T

$$\mathrm{OPR}(T_{\mathrm{kin}}) = \frac{3\sum_J^{ortho} g_J \exp(-E_{J_{K_a,K_c}}/k_B T)}{\sum_J^{para} g_J \exp(-E_{J_{K_a,K_c}}/k_B T)}$$



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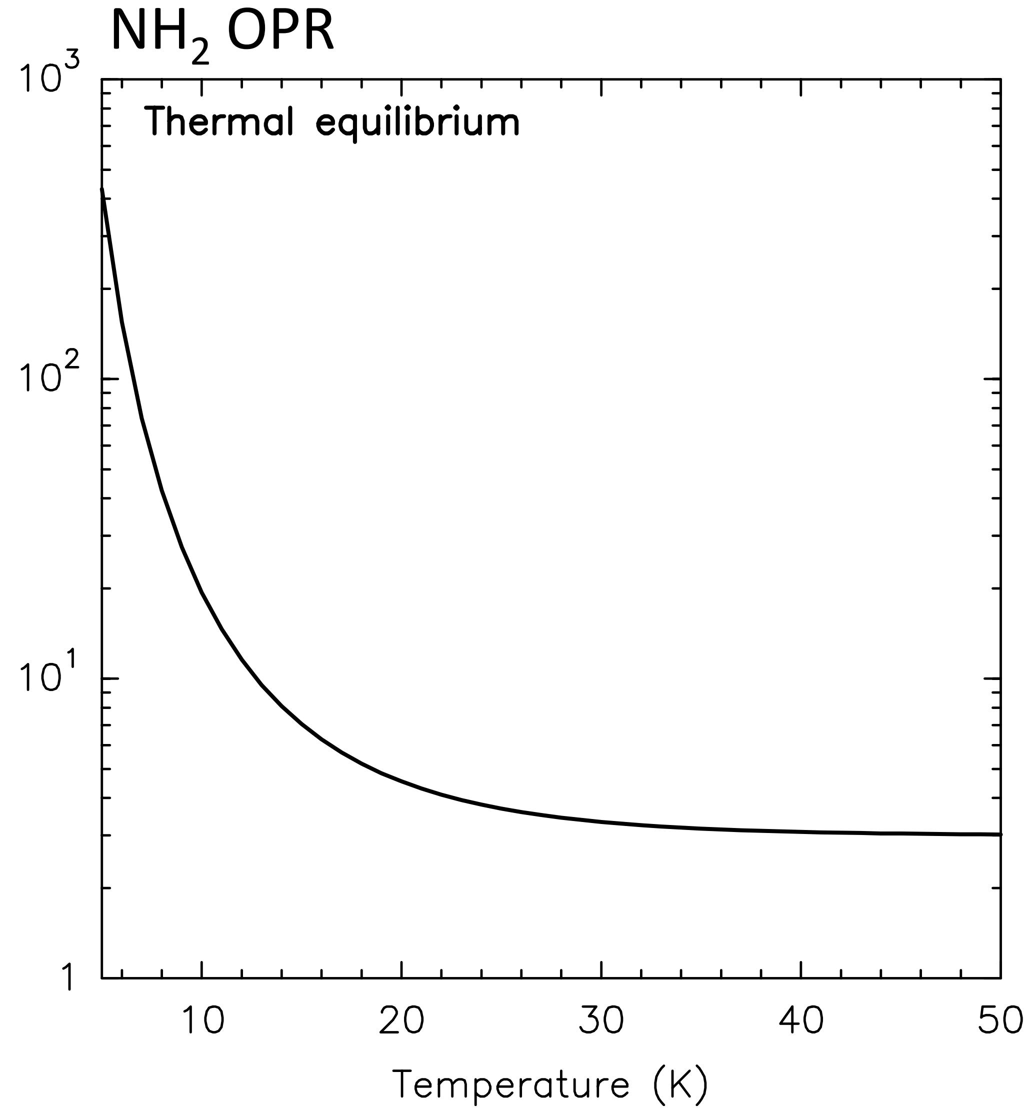
$$\mathrm{OPR}(T_{\mathrm{low}}) \approx \frac{3\, g_{J=0} \exp(-E_{0_{00}}/T_{\mathrm{kin}})}{g_{J=1} \exp(-E_{1_{01}}/T_{\mathrm{kin}})}$$

$$\mathrm{OPR}(T_{\mathrm{low}}) \approx \exp\left(\frac{-\Delta E}{T_{\mathrm{kin}}}\right) = \exp\left(\frac{30.4}{T_{\mathrm{kin}}}\right)$$



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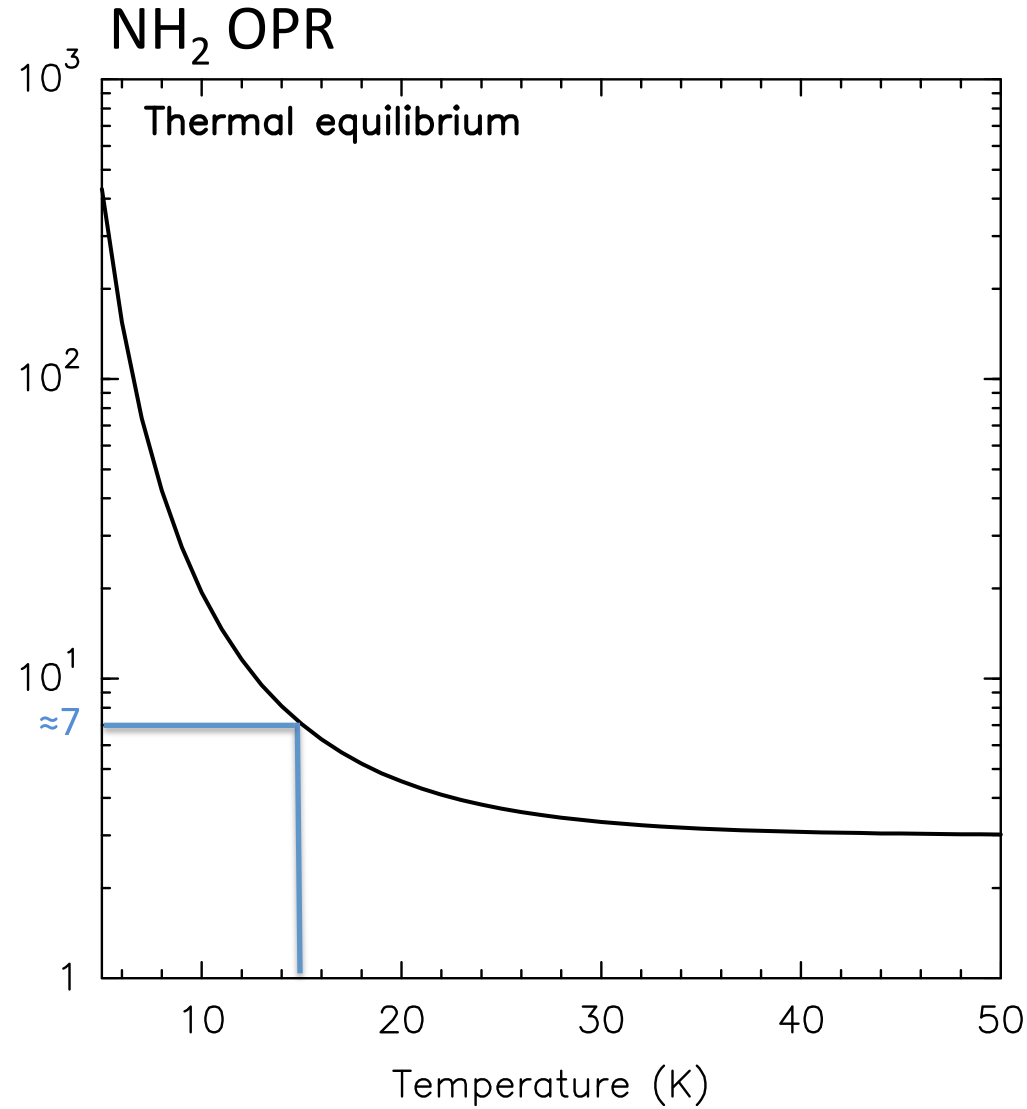

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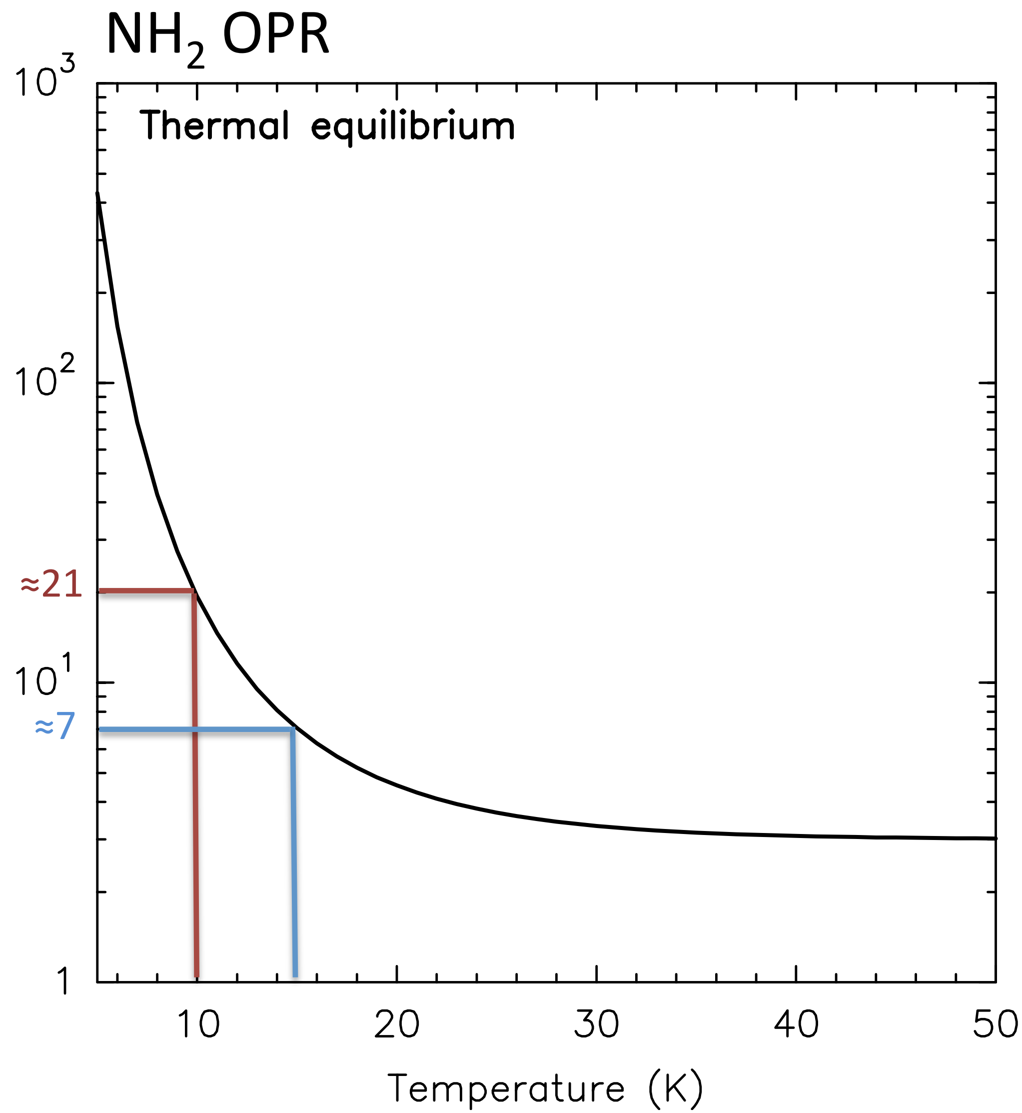
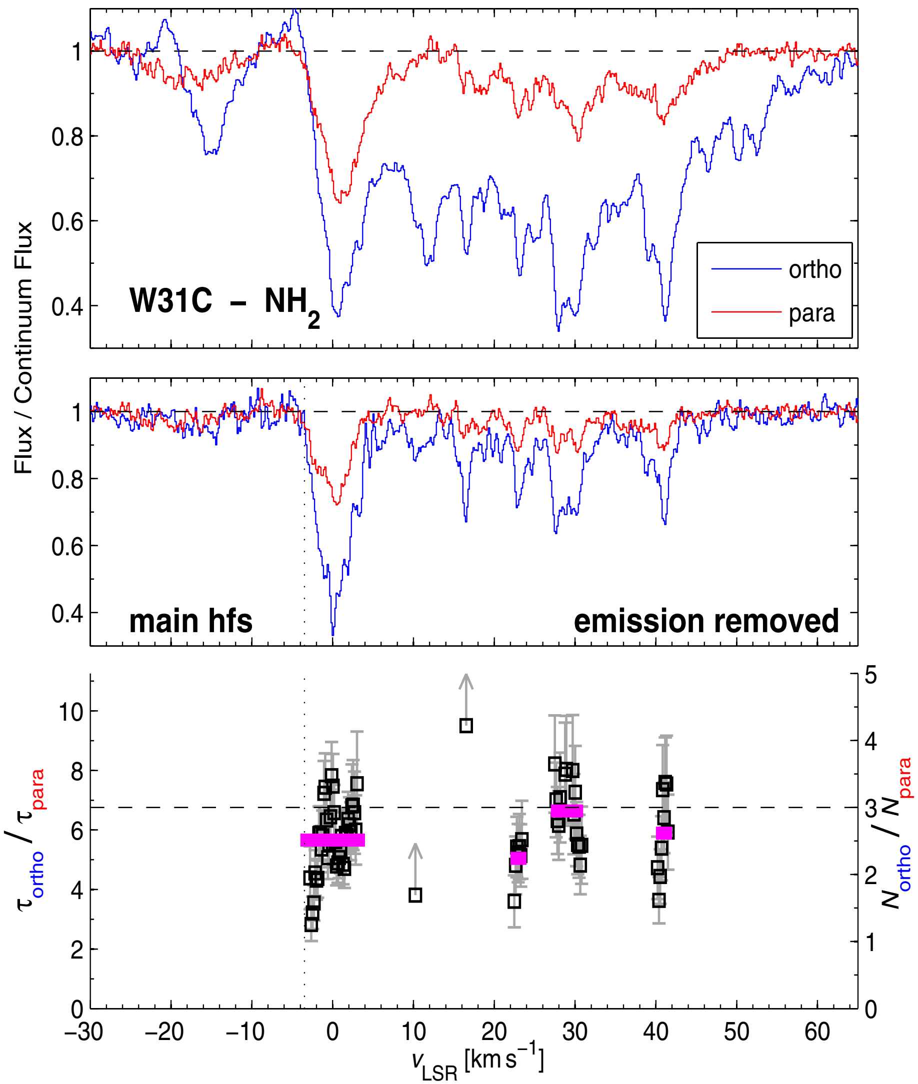
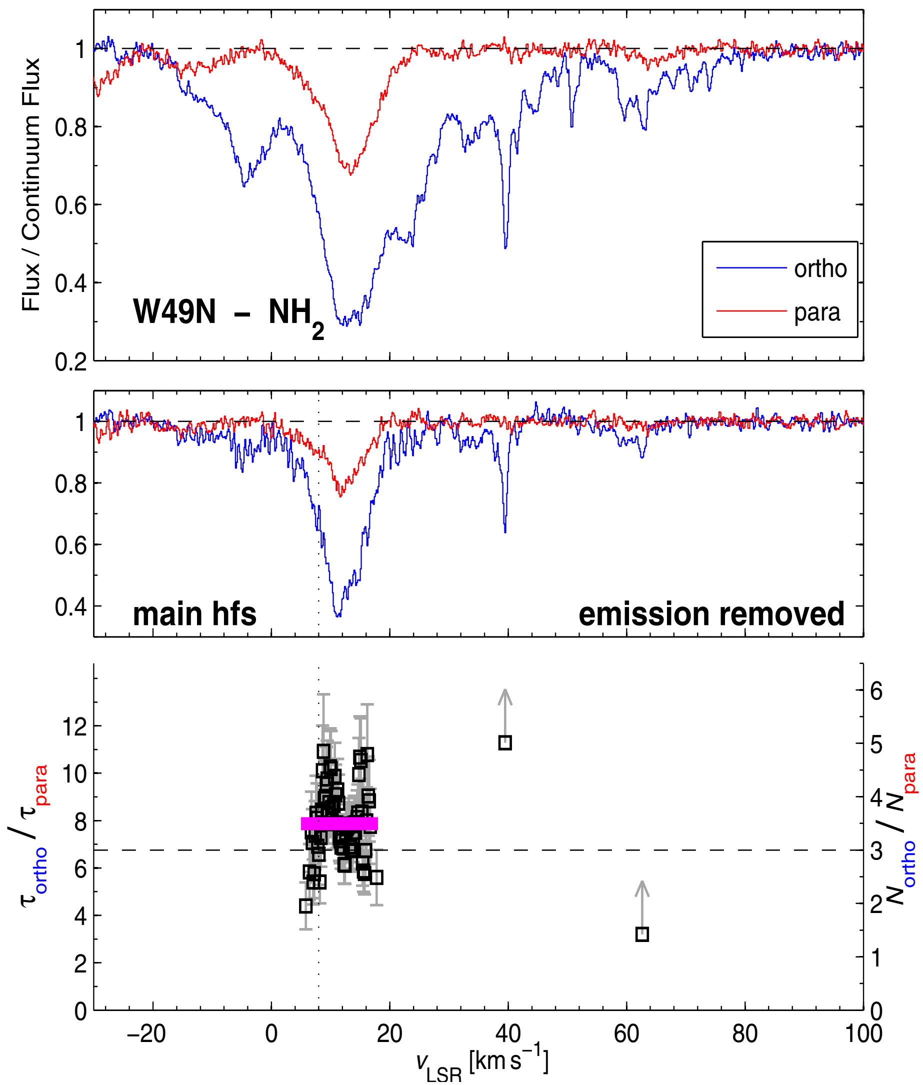


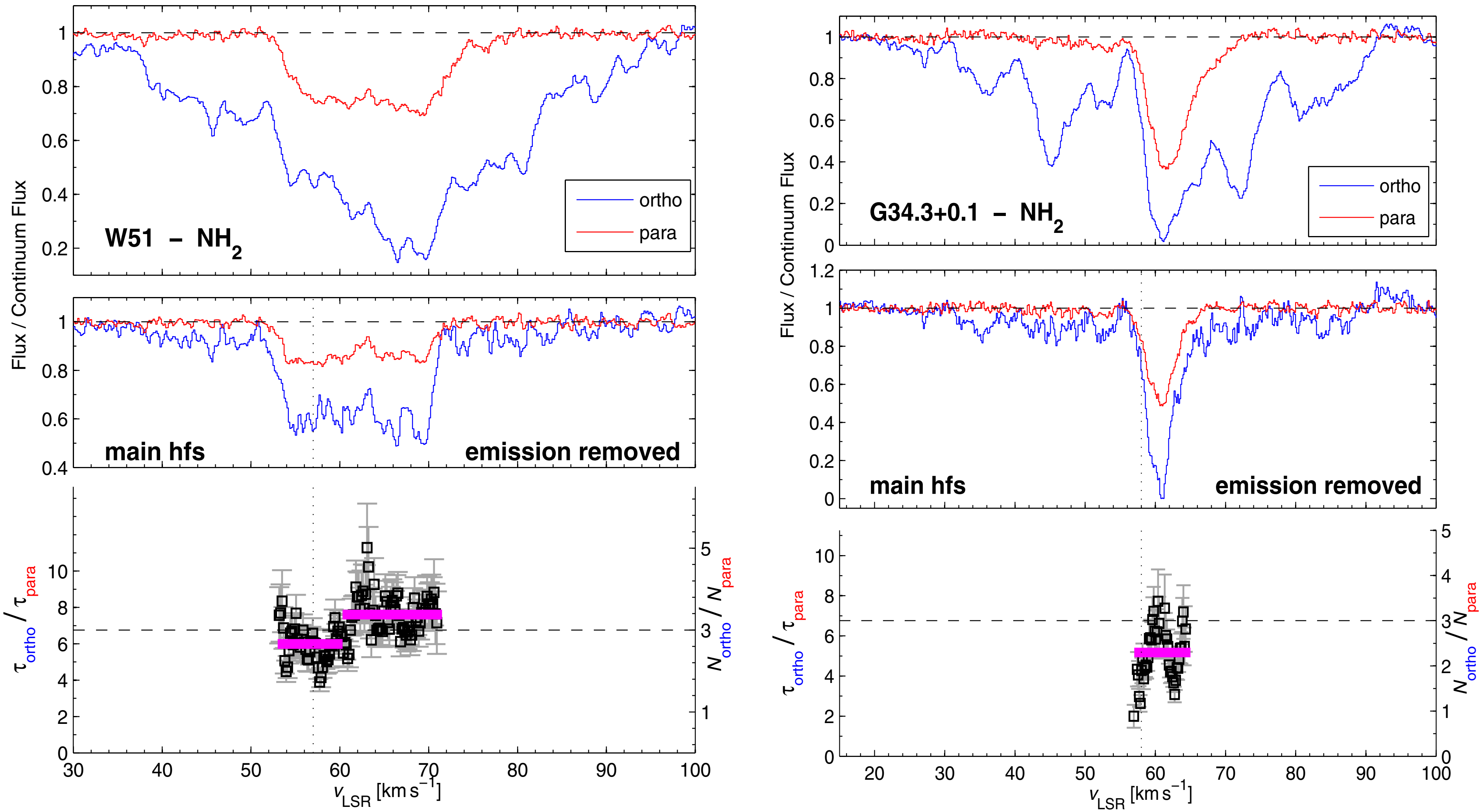
NH_2 OPR towards W31C &W49N





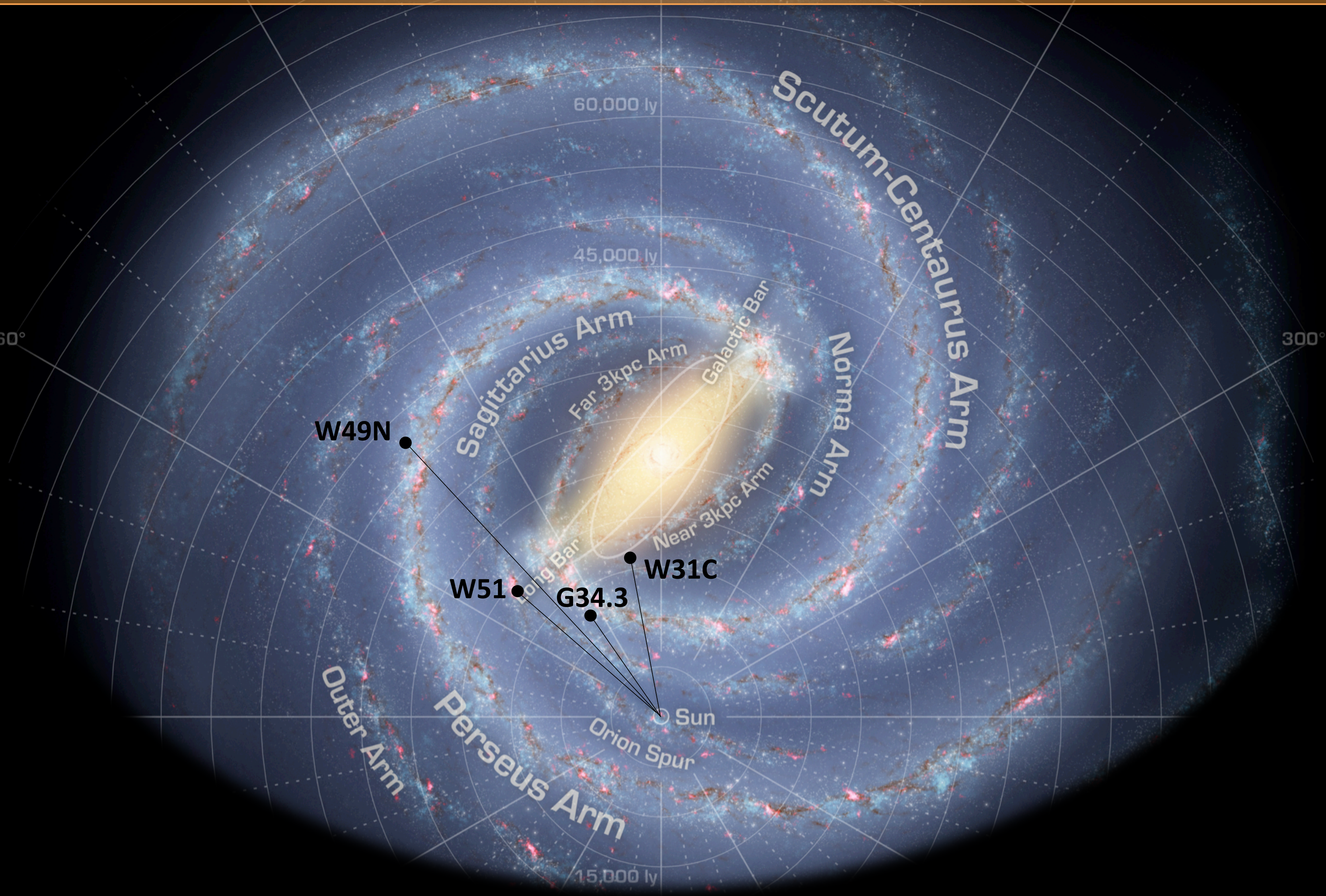
*Persson, Olofsson, **Le Gal** et al., A&A. (2016)*

NH_2 OPR towards W51 & G34.3



*Persson, Olofsson, **Le Gal** et al., A&A. (2016)*

Interpretation of the observations



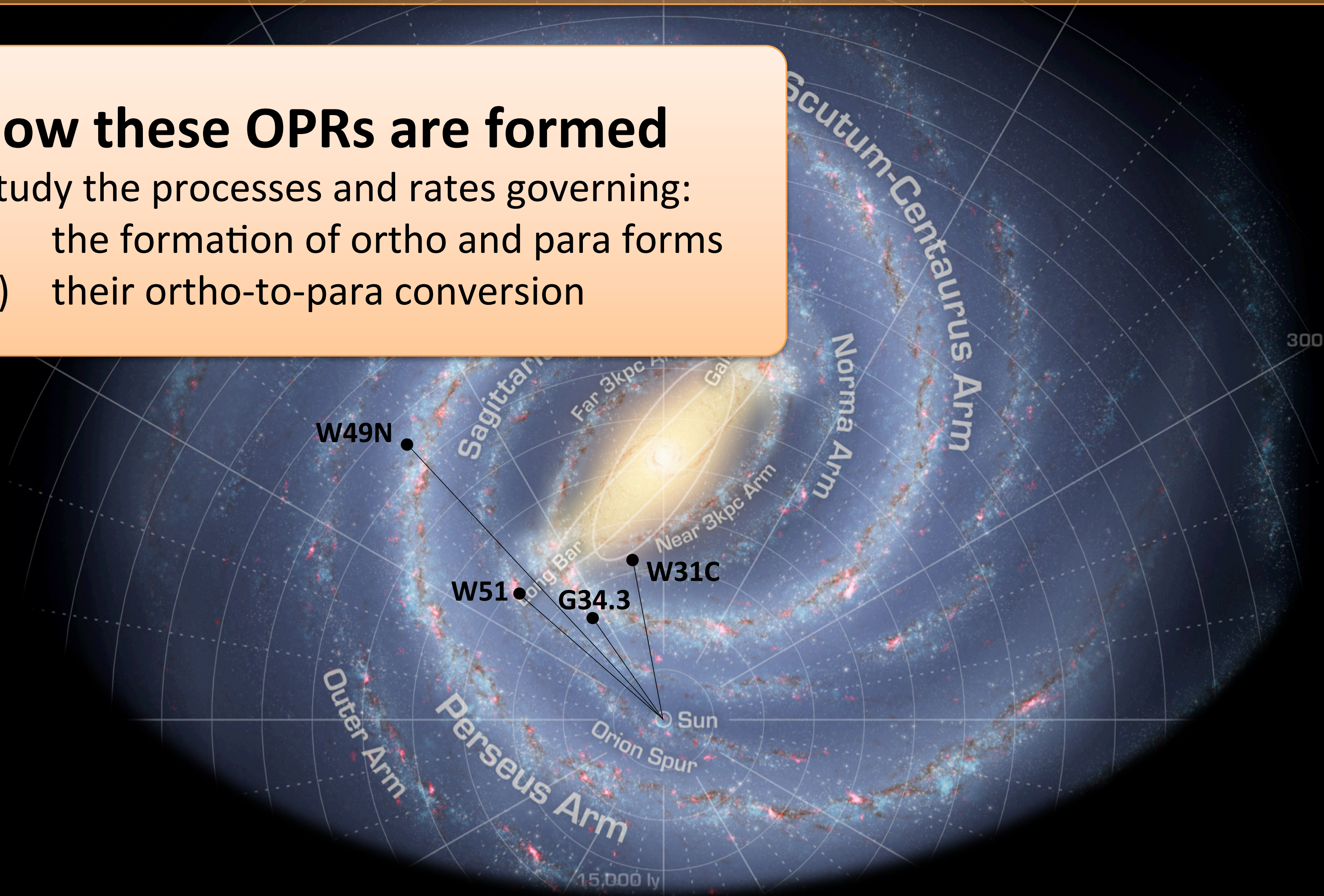
Interpretation of the observations

How these OPRs are formed

Study the processes and rates governing:

(i) the formation of ortho and para forms

(ii) their ortho-to-para conversion



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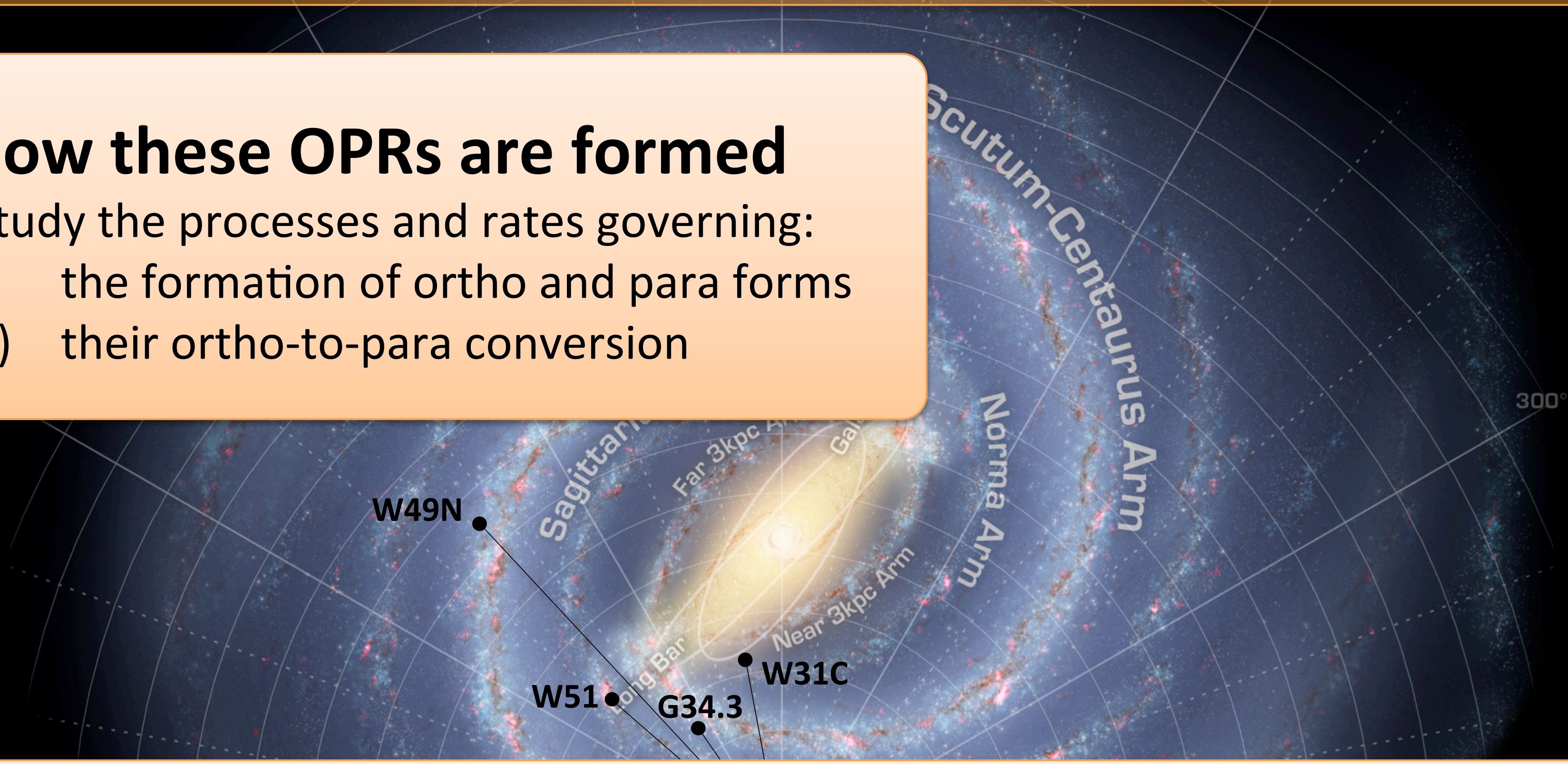


Strategy

Identifying the species and pivotal processes at stake

→ modeling the interstellar chemistry

Astrochemical modeling

- **Interstellar chemistry**
  - Hydrides in the interstellar medium (ISM)
  - NH2 Ortho-para ratio (OPR) observations
- **Astrochemical modeling**
  - Building chemical network
  - Results: comparison with observations

Building chemical network

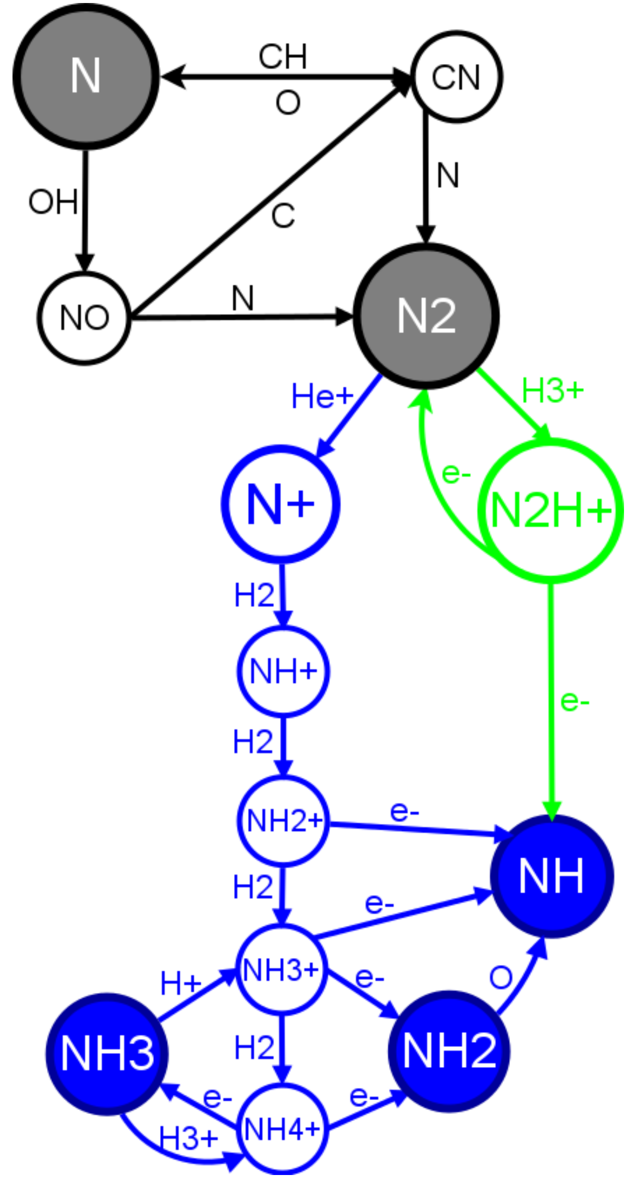
- Aims:

  - Distinguish ≠ spin configurations of H_2 and of the multi-hydrogenated N-hydrides

  ⇒ Update & upgrade of the Flower et al. 2006 network

  - Using recent experimental and theoretical work

  ⇒ Rist et al., *JPCA* 2013, Faure et al., *ApJ* 2013 & Le Gal et al., *A&A* 2014



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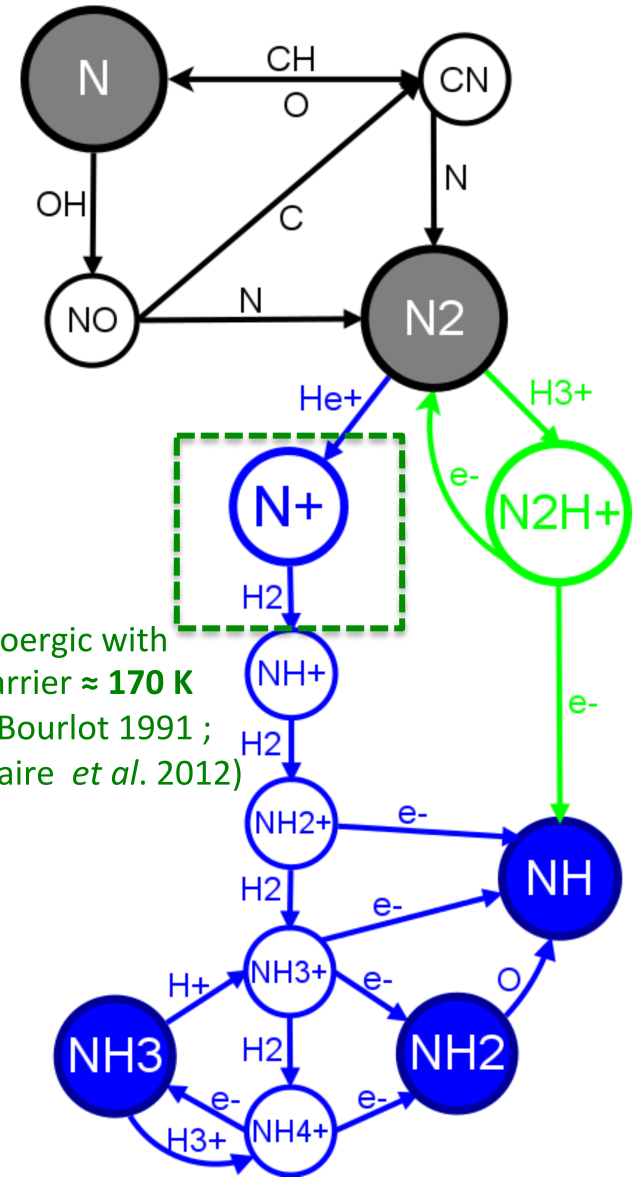
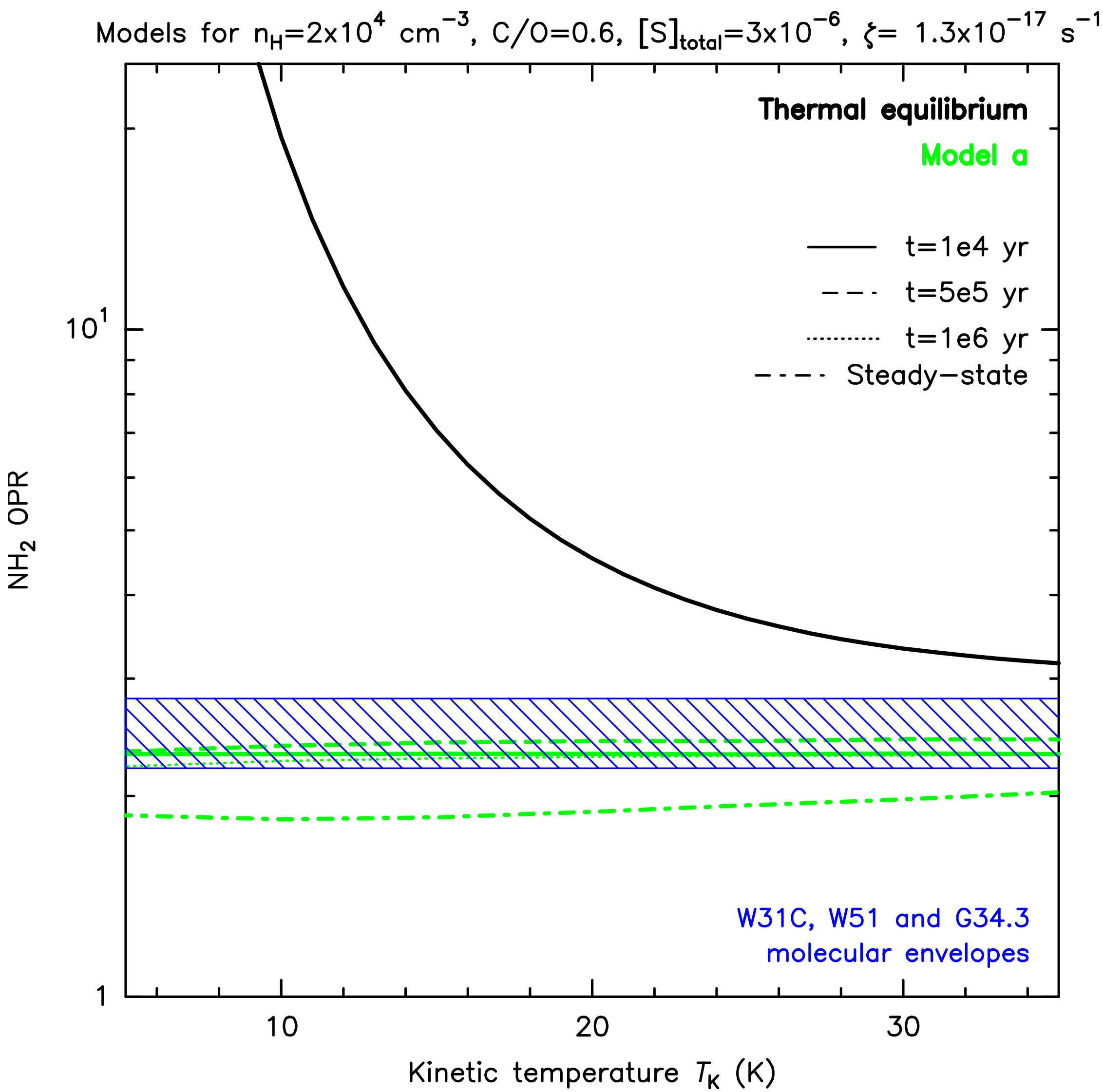


Endoergic with a barrier ≈ **170 K** (Le Bourlot 1991 ; Dislaire *et al*. 2012)

Results: NH_2 OPR with T



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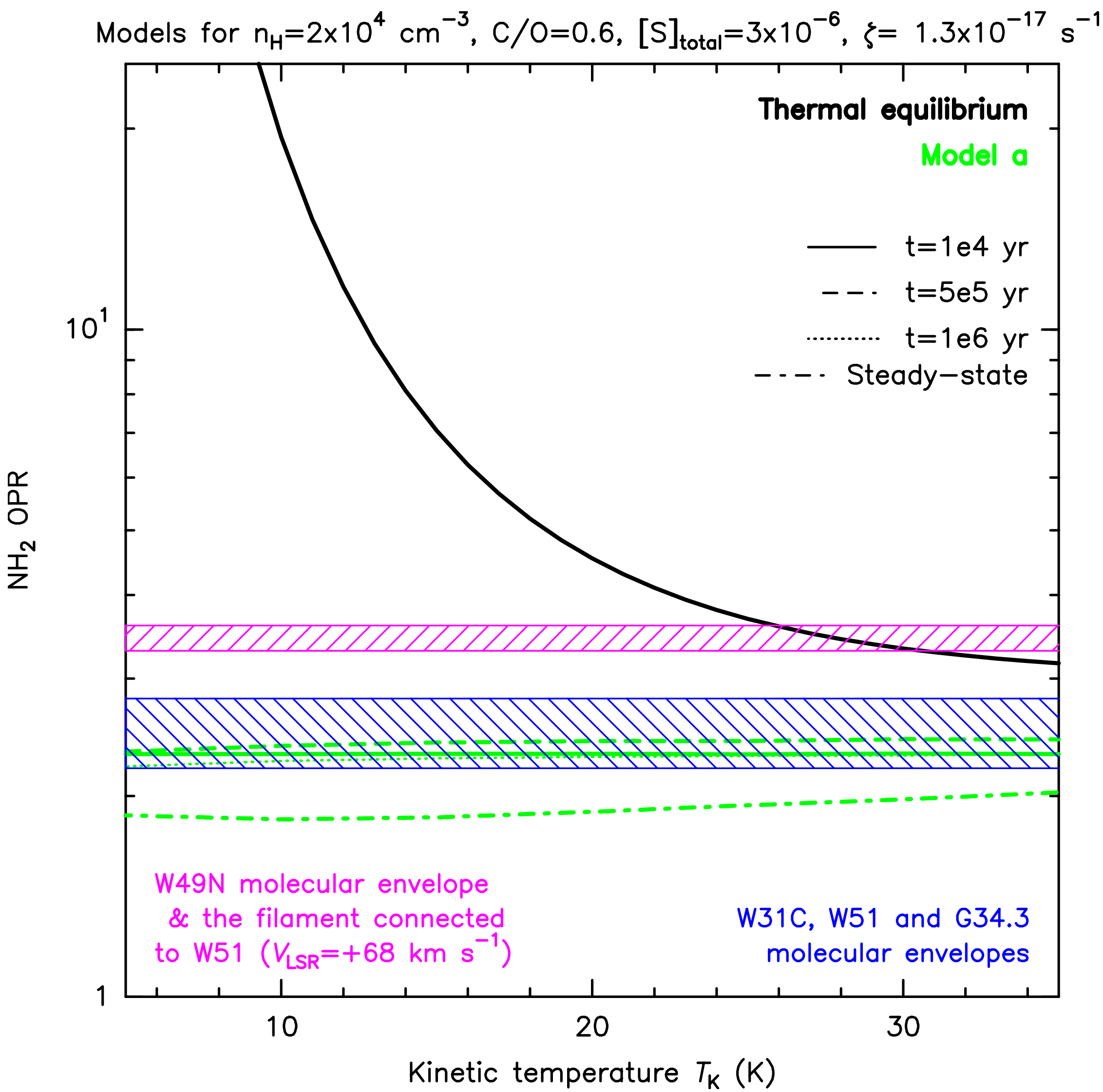

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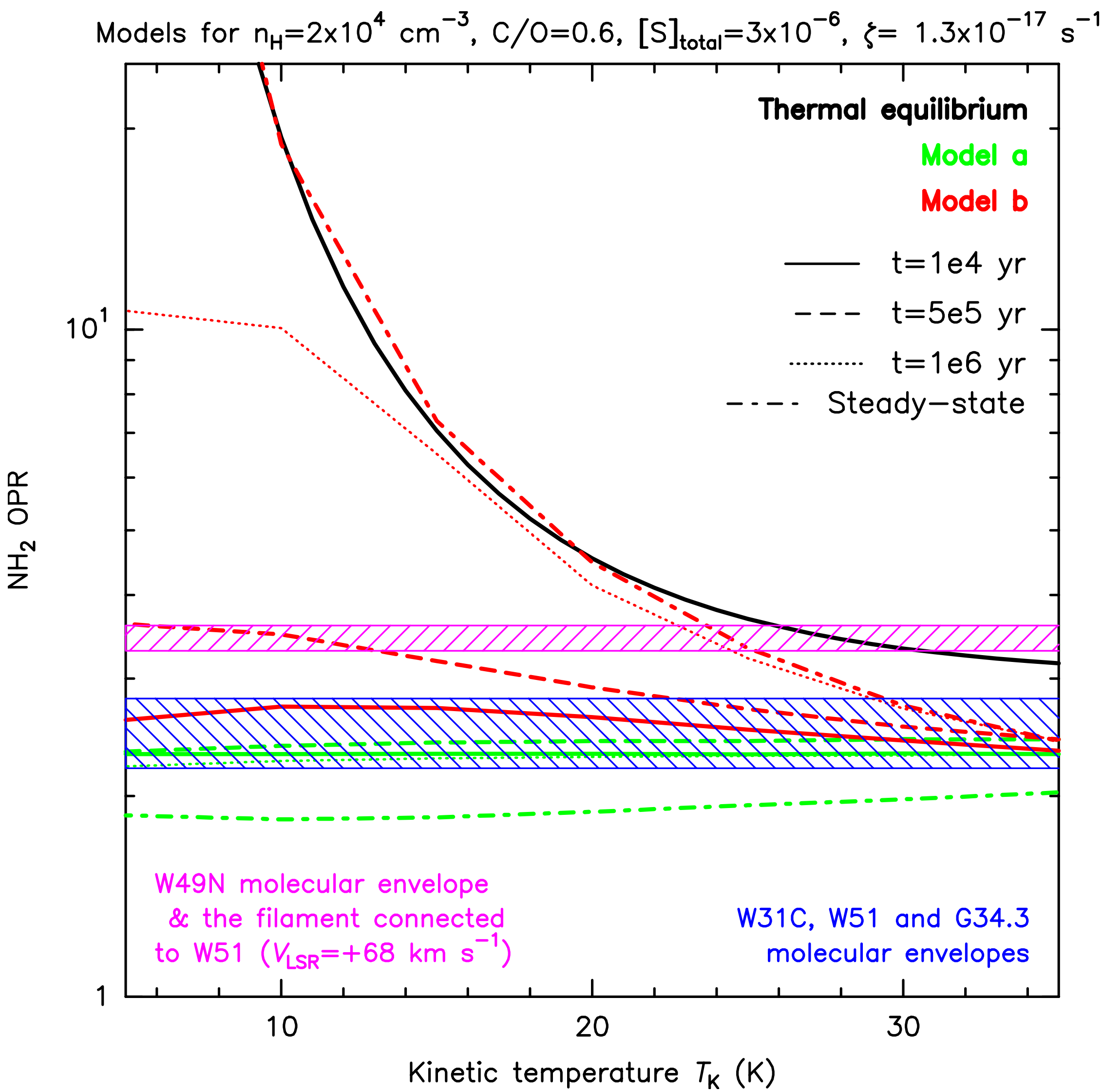


- New mechanism to allow OPR relaxation:

  $\Rightarrow$ H + NH_2 H-exchange

$$H + o{-}NH_2 \xrightarrow{k_{o\to p}} H + p{-}NH_2$$

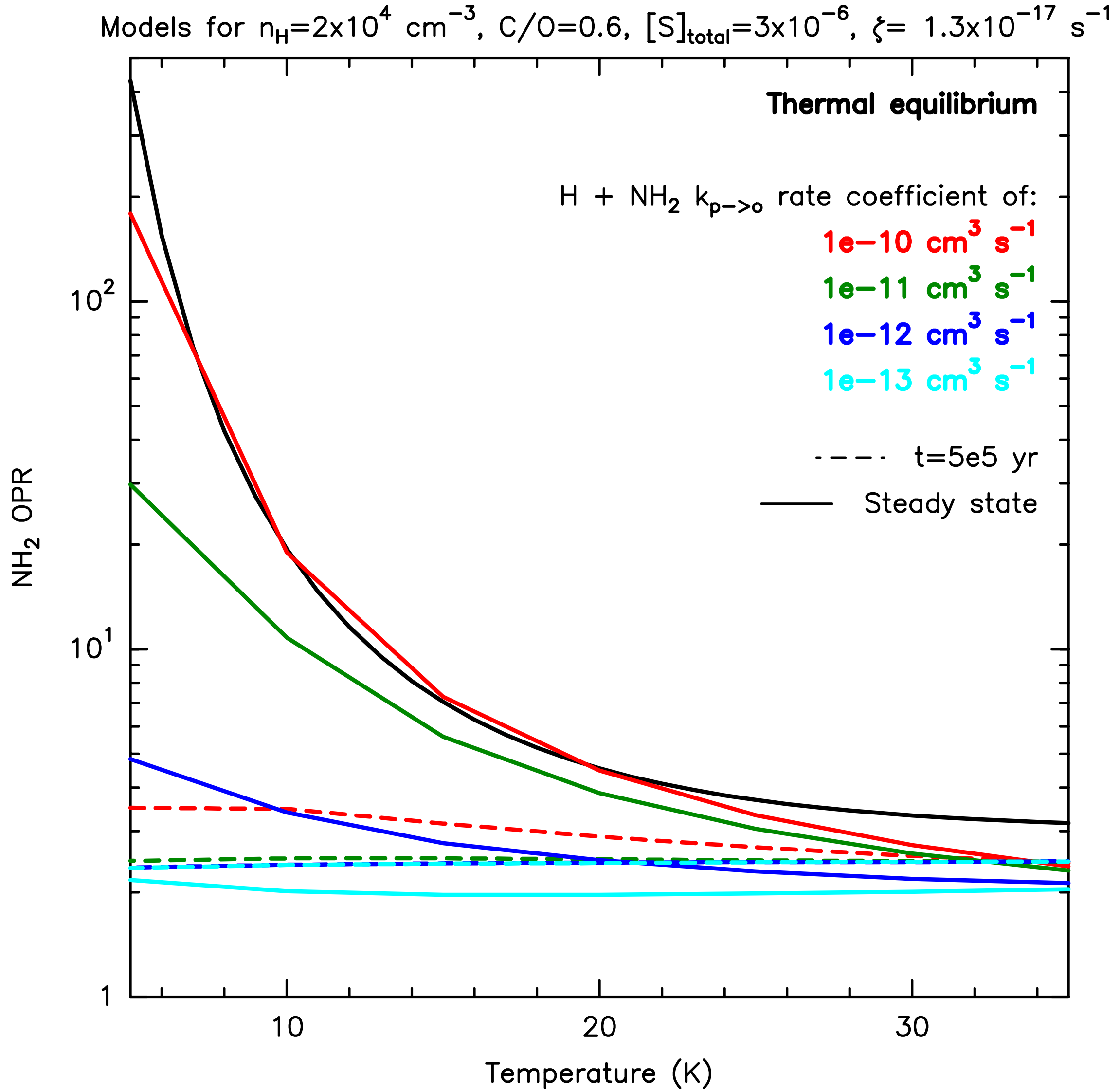
$$H + p{-}NH_2 \xrightarrow{k_{p\to o}} H + o{-}NH_2$$

$$\text{with } k_{o\to p} = k_{p\to o} \exp(-30.4/T)\,\text{cm}^3\,\text{s}^{-1}$$

$$k_{p\to o} = 1\times10^{-10}\,\text{cm}^3\,\text{s}^{-1}$$

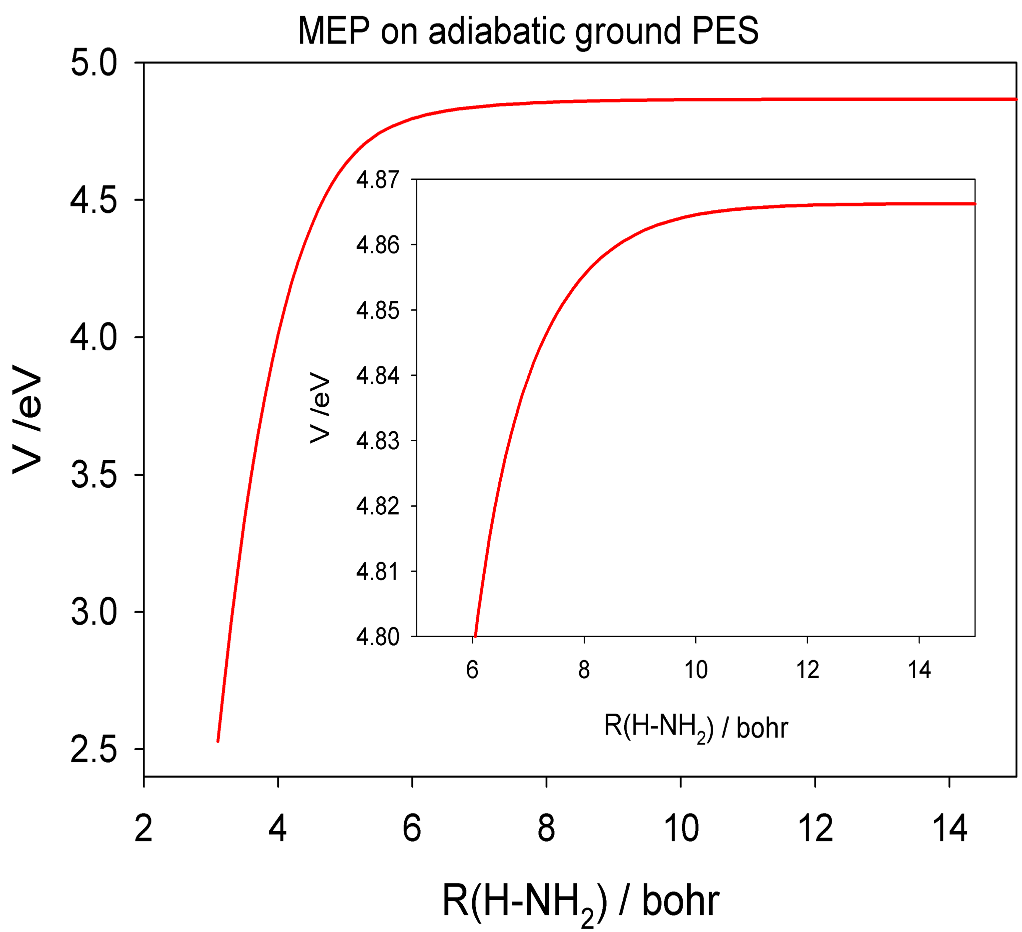
Persson, Olofsson, ***Le Gal*** *et al., A&A. (2016)*

Influence of the rate coefficient



Le Gal et al., A&A. (2016)

Results: H + NH_2 H-exchange barrierless

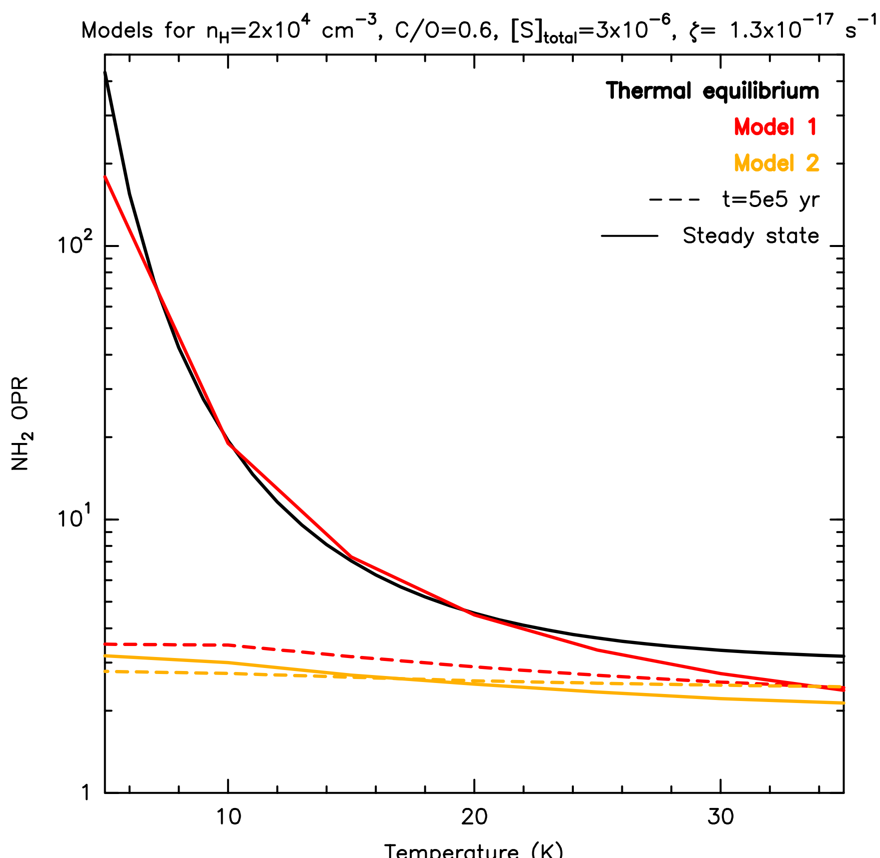


Le Gal et al., A&A. (2016)

H + NH_2 H-exchange rate coefficient of ≈10^{-10} cm^3 s^{-1} is consistent with the theoretical computations

Impact of NH_2 chemistry updates

Chemical reactions[a]						α ($cm^3\ s^{-1}$)	β	γ	References
NH_2	N	→	N_2	H	H	1.2(-10)	0.00	0.00	KIDA[b]
NH_2	O	→	NH	OH		7.0(-12)	-0.1	0.00	KIDA[c]
						3.5(-12)	0.5	0.00	Le Gal et al. (2014a)[d]
NH_2	O	→	HNO	H		6.3(-11)	-0.1	0.00	KIDA[c]



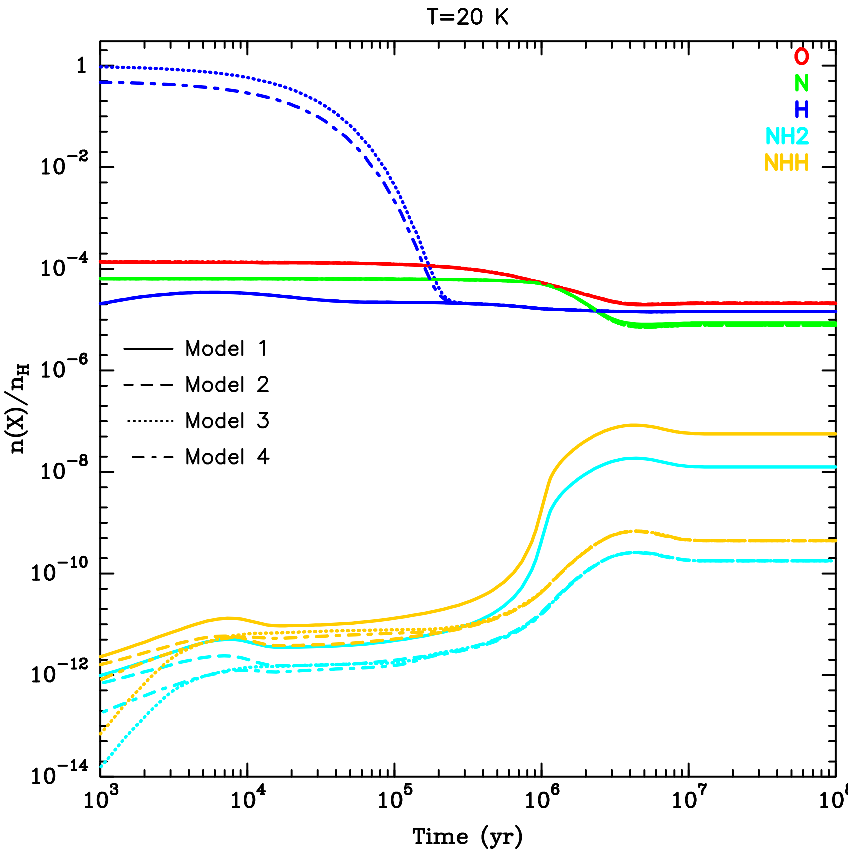
Le Gal et al., A&A. (2016)

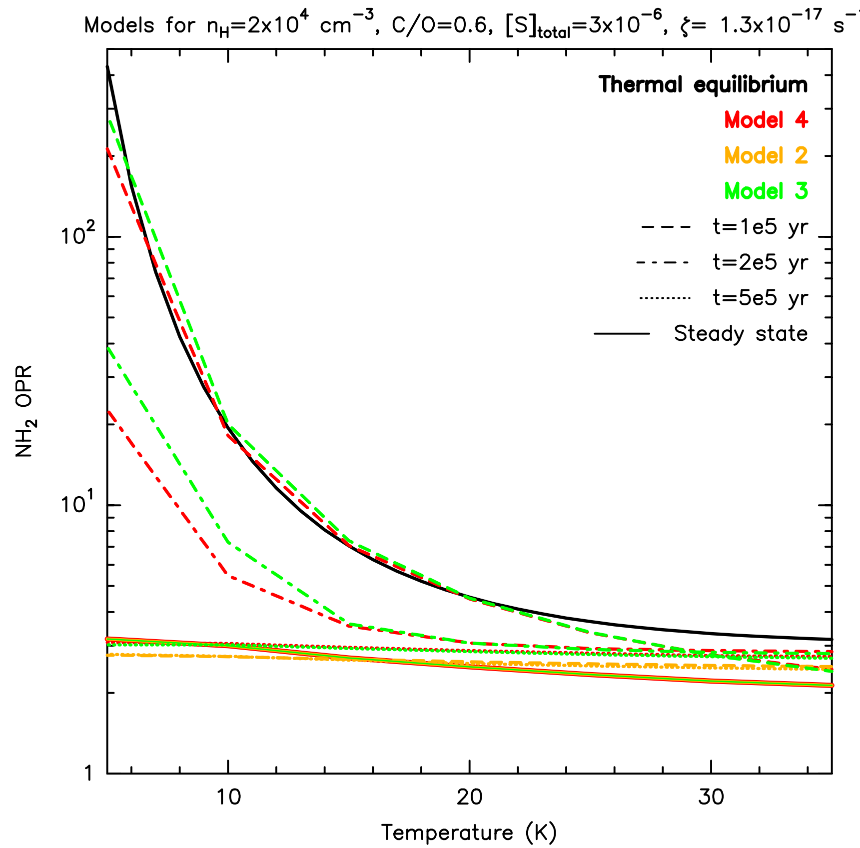
Further modeling study

Modifications \ Models	1	2	3	4	5
$H + NH_2$ H-exchange addition (reactions 5 and 6)	X	X	X	X	X
NH_2 destruction updates (see Table 2)		X	X	X	X
$[H_{tot}]_{ini} = 2 \times [H_2]$	X	X			X
$[H_{tot}]_{ini} = [H]$			X		
$[H_{tot}]_{ini} = \frac{1}{2} \times [H] + [H_2]$				X	
$\zeta = 1.3 \times 10^{-17}\ s^{-1}$	X	X	X	X	
$\zeta = 3 \times 10^{-17}\ s^{-1}$					X
$\zeta = 2 \times 10^{-16}\ s^{-1}$					
$n_H = 2 \times 10^4\ cm^{-3}$	X	X	X	X	X

Le Gal et al., A&A. (2016)

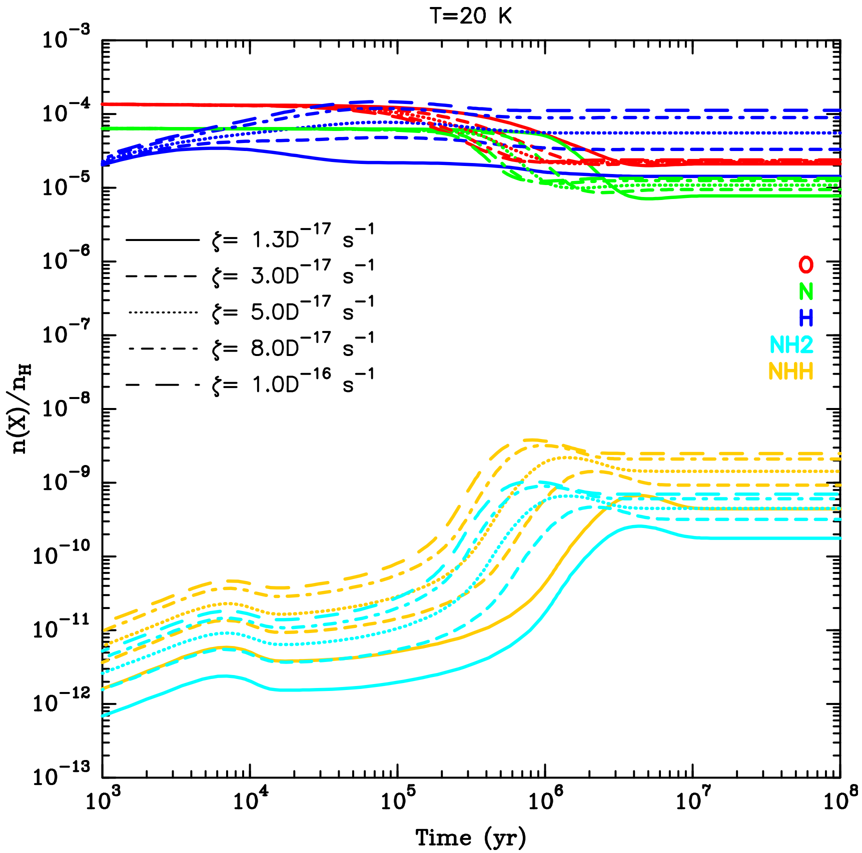
Impact of the initial form of hydrogen

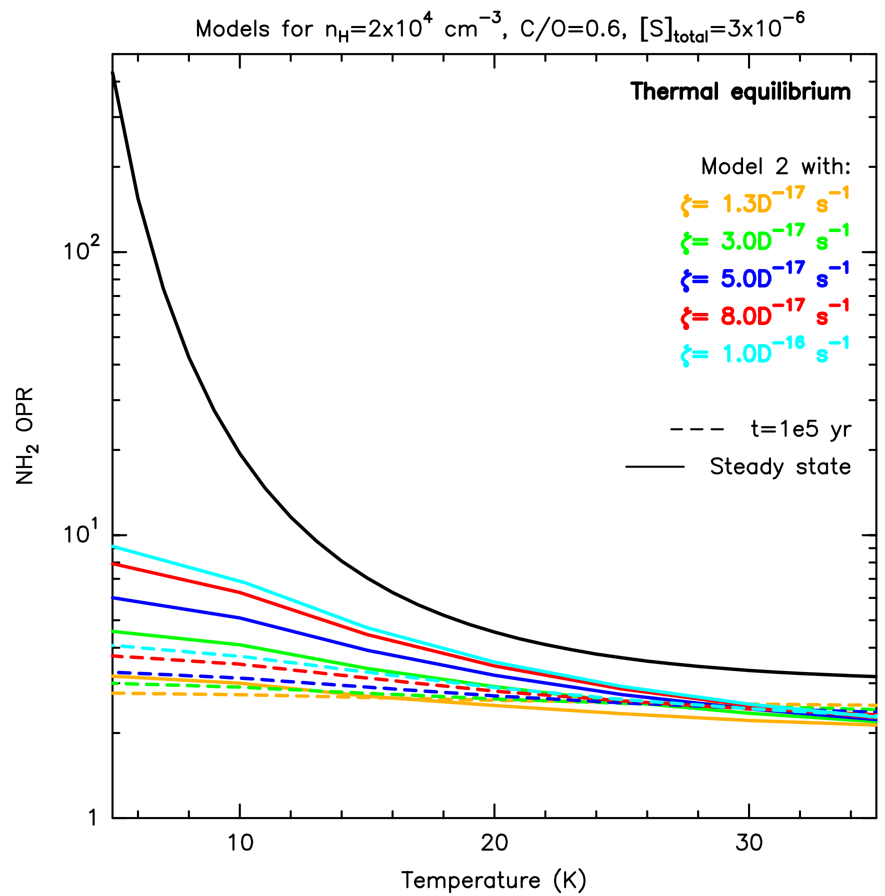




Le Gal et al., A&A. (2016)

Impact of the ionization rate





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Conclusions & future works

Conclusions:

- **Gas-phase chemistry** reproduces NH_2 OPR ratios observed in 4 high-mass star-forming regions:
  need spin chemistry for OPR < 3
  & H-exchange reaction for OPR > 3

- Models predictions:
  - **H_2 OPR ~ 10^{-3}**, consistent with NH:NH_2
  - **NH_3 OPR ≈ 0.5 – 0.7**
  - **NH_2 OPR depends on the temperature**

Future works:

- Gas-grain processes impact (adsorption, desorption, surface reactions)
- Upgrade the chemical network for more diffuse conditions

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Thanks for your attention!