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Laboratoire d'Étude du Rayonnement et de la Matière en Astrophysique

UNIVERSITÉ PARIS-EST Marne-la-Vallée

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Inelastic processes in low-energy collisions with H atoms: Consequences on non-LTE modeling of stellar atmospheres

A collaborative work:

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St Petersburg 2012

Collision rates with H atoms for star modeling

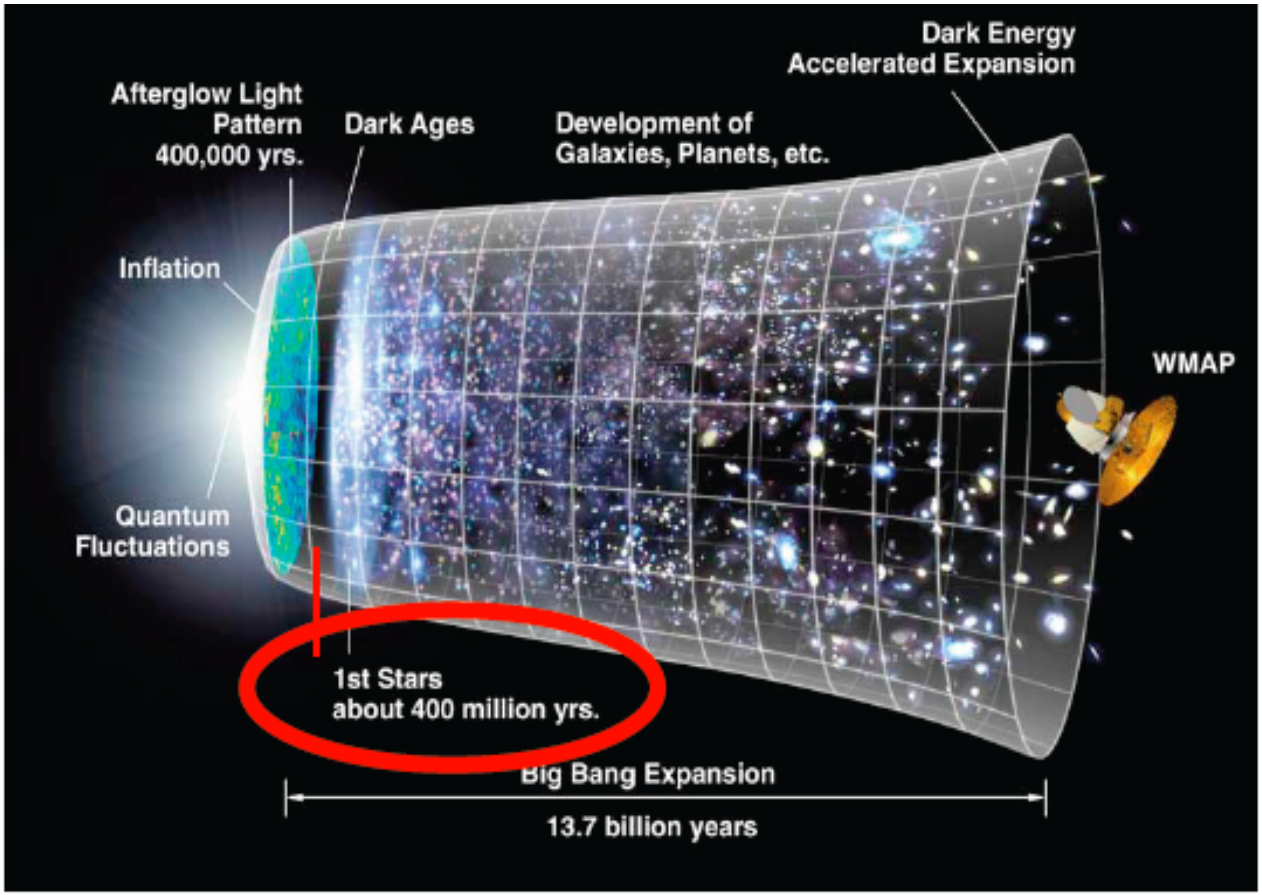
Outline

- Astrophysical context
- Calculation of accurate collisional rates: Mg+H
- Comparison with Drawin's approximate formula
- Preliminary consequences on non-LTE modeling

Astrophysical interest

- **Determination of precise and absolute stellar abundances**
- **Chemical and physical properties from spectroscopy analysis**
- **Evolution of the Galaxy**

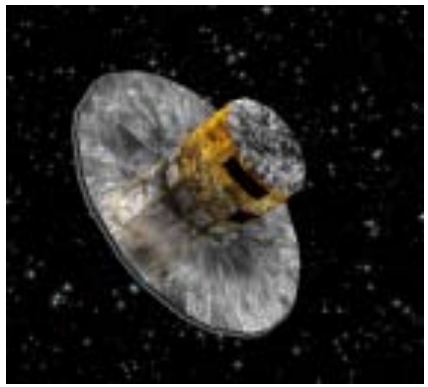
Importance of old stars



Big Bang: H, He, Li

Production of heavy elements:
C, N,O, ...Na, Mg, ...Fe, ...,Th, U

Determination of stellar atmospheric parameters: the GAIA mission



The Spatial ESA Gaia mission (2013)

Objectives:

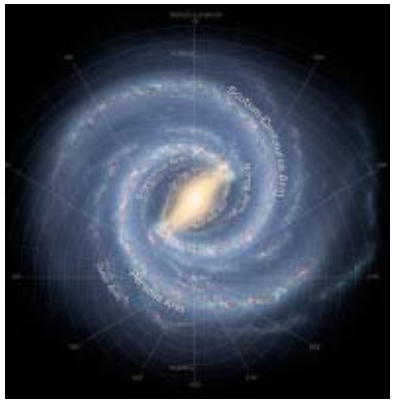
- Astrometry
- Radial velocities and spectroscopy

$$\approx 2\times10^{8}\ stars$$

Main interest:

- Astrometry: more and more distant objects
- Photometer + high resolution spectrometer➔contraints on fundamental stellar parameters

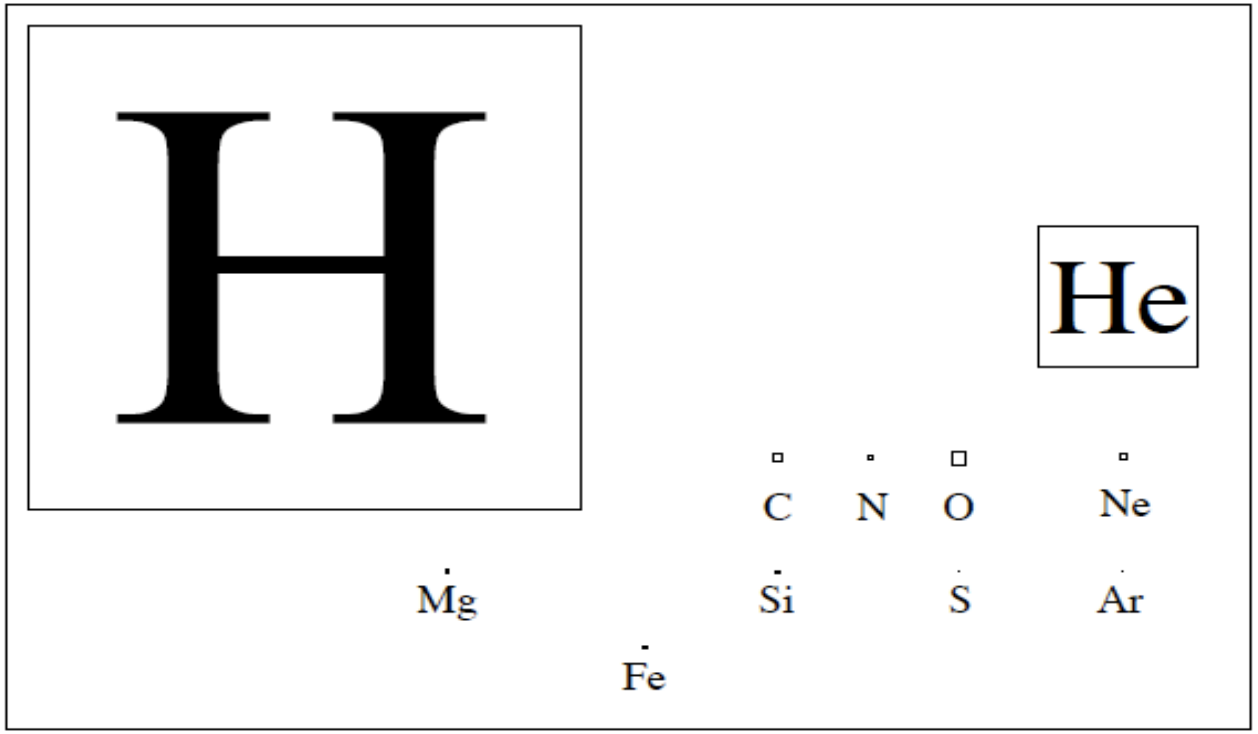
T_{eff}, gravity g, abundance of elements, metallicity [Fe/H]…



$$\left[Fe/H\right] = A^{*}_{Fe} - A^{sun}_{Fe} \quad with \quad A_{Fe} = \log\frac{n_{Fe}}{n_{H}} + 12$$

- in order to derive trends in the chemical evolution of the Galaxy

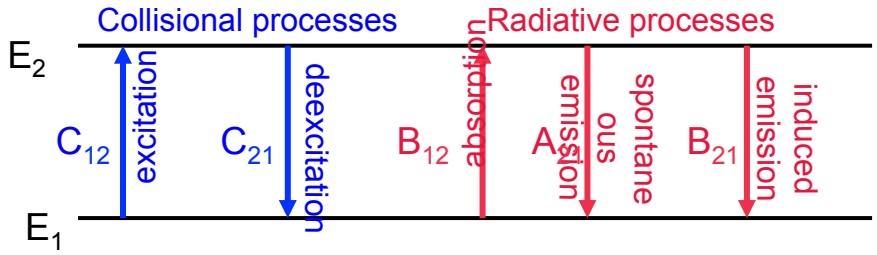
The periodic table for astronomers



- All elements apart H and He are « metals », H atoms are the most abundant atoms
- electrons are also present

Non-LTE modelling

• Non-LTE modelling implies competition between radiative and collisional processes for both excitation and ionisation



$$C_{21} = n_P \, k_{21}(T)$$

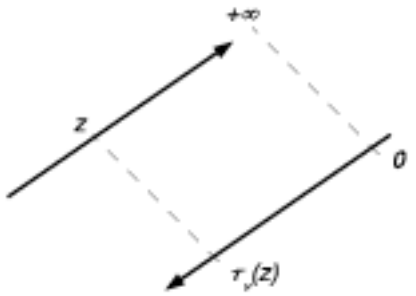
s^{-1} $cm^3 s^{-1}$

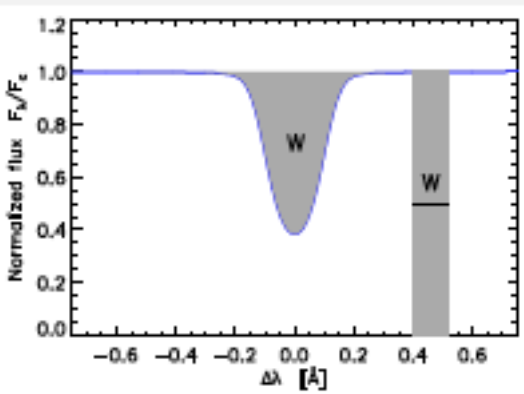
n_P: perturber density, k_{21} rate coefficient proportional to cross section $k_{21}(T) = \langle v\sigma \rangle_v$

- a priori, collisions should decrease the non-LTE effects on populations, but this is not so simple as ionisation/mutual neutralisation contribute as well.
- Don't forget radiative transfer

LTE = Local Thermodynamical Equilibrum

Radiative transfer for star atmosphere modeling: some definitions



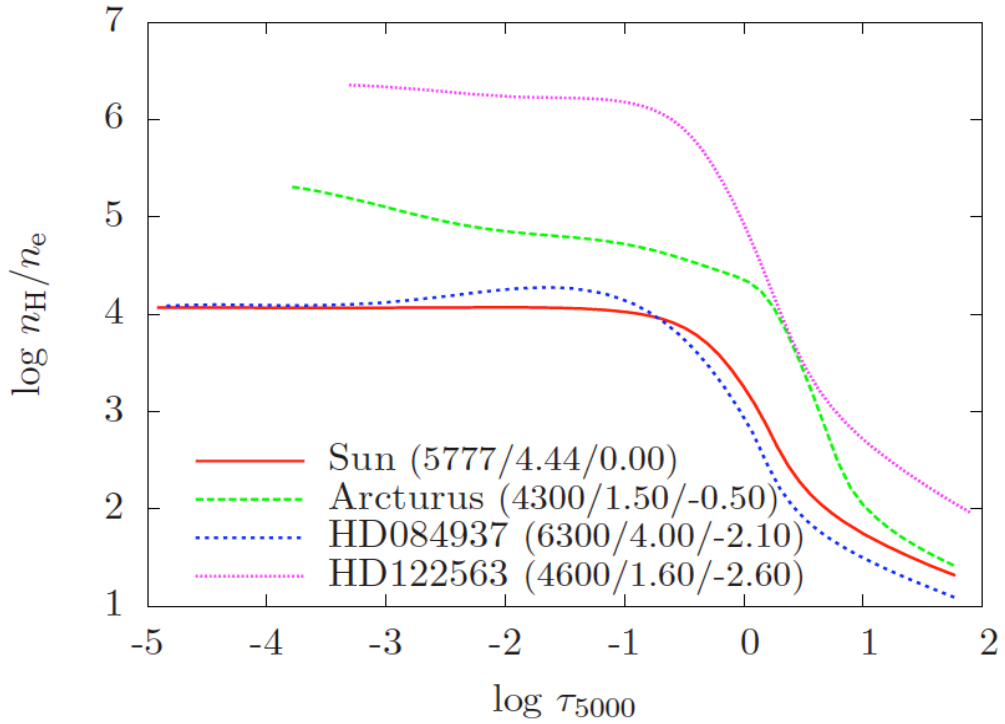


- optical depth τ: increases towards the inner atmosphere
- NLTE coefficients: b_i for level i:

$$b_i = \frac{n_i}{n_i^*};\ n_i^* \text{ population LTE}$$

- equivalent width W: depends on density, temperature, abundance, populations, perturbers, …

What are the dominant collision partners? electrons or H atoms?



atomic lines are formed for -4<log τ <0

stars with different parameters (T, log g, metallicity [Fe/H]:

H atoms are dominant for cold star atmospheres with low metallicity

Non-LTE modeling

Context

- the data for radiative processes has improved these last decades with the Opacity and Iron projects. The situation is significantly worse for collisional excitation mainly with H atoms dominant in cold stellar atmospheres.

- inelastic H collisional cross sections are usually estimated by the Drawin formula, but high accuracy measurements or quantum calculations show that the Drawin formula may overestimate the cross sections by a factor of 10 to four orders of magnitude

This implies :

- new calculations of H collisional cross sections and rates

Collisional rates

Calculations of excitation rates of X by H atoms

2 steps :

- Determination of : - interaction potentials
  - coupling terms between X and H potentials

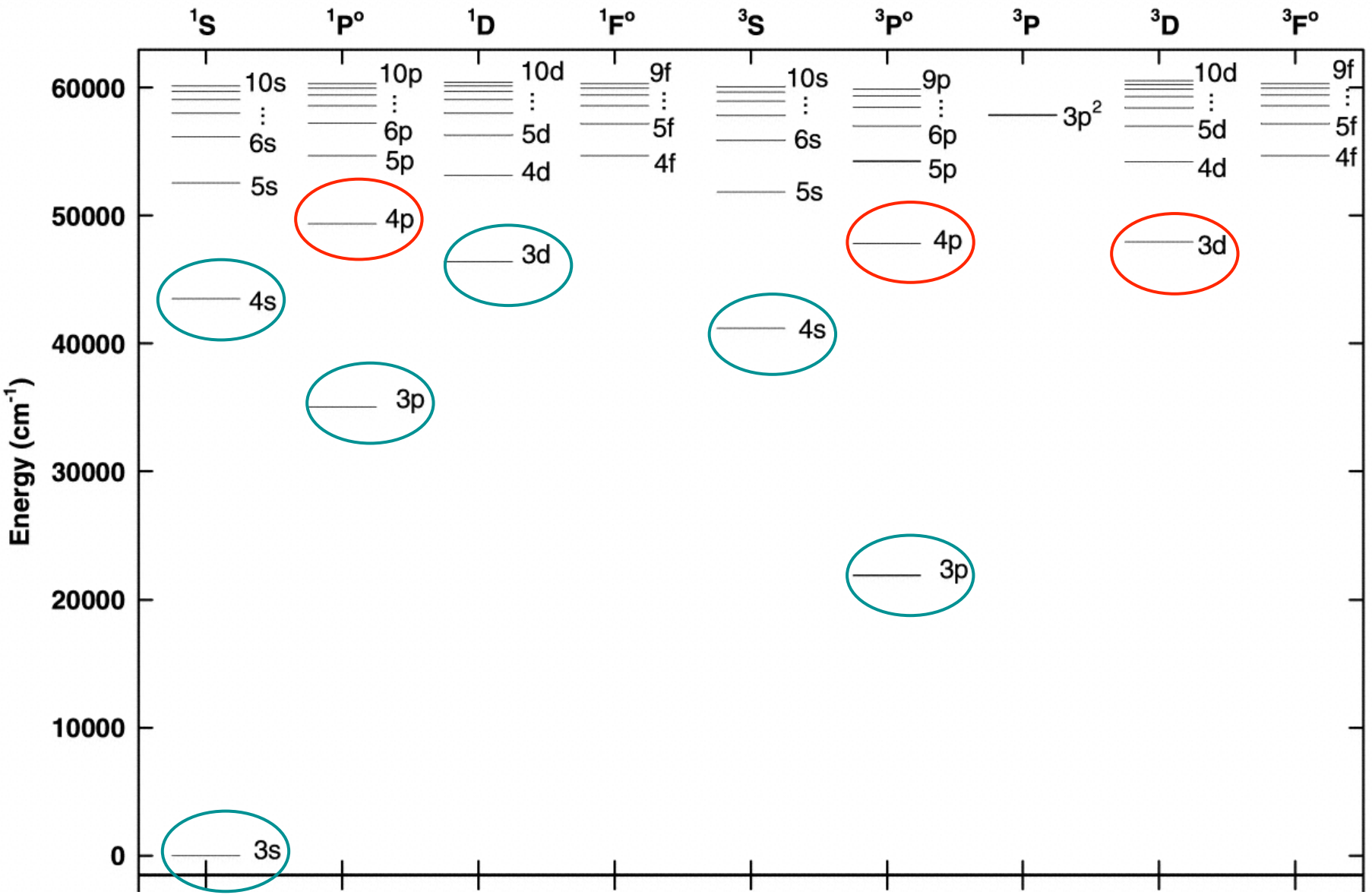
  Quantum chemistry increasingly difficult for high excited levels

- Dynamics in these potentials

Already done: Li+H, Na+H
Under way: Mg+H, O+H, Ca+H
Future: Ca^++H and possibly Fe+H (?)

Mg : Some of the strongest absorption lines in stellar spectra
Relatively easily detected even in low-quality spectra or in metal poor stars

Mg atomic levels



Mg + H interaction potentials

Potential energy curves and coupling terms for Mg+H

During the collision, the two atoms form temporarily a quasi molecule

6 to 9 Mg levels considered: E< 6eV

$3s^2$ (^1S), 3s3p (^3P), 3s3p (^1P), 3s4s (^3S),
3s4s (^1S), 3s3d (^1D) Active space 10σ, 5π, 1δ orbitals
Then 3s3d (^3D) 3s4p (^1P) 3s4p (^3P) Active space 13σ, 6π, 2δ orbitals

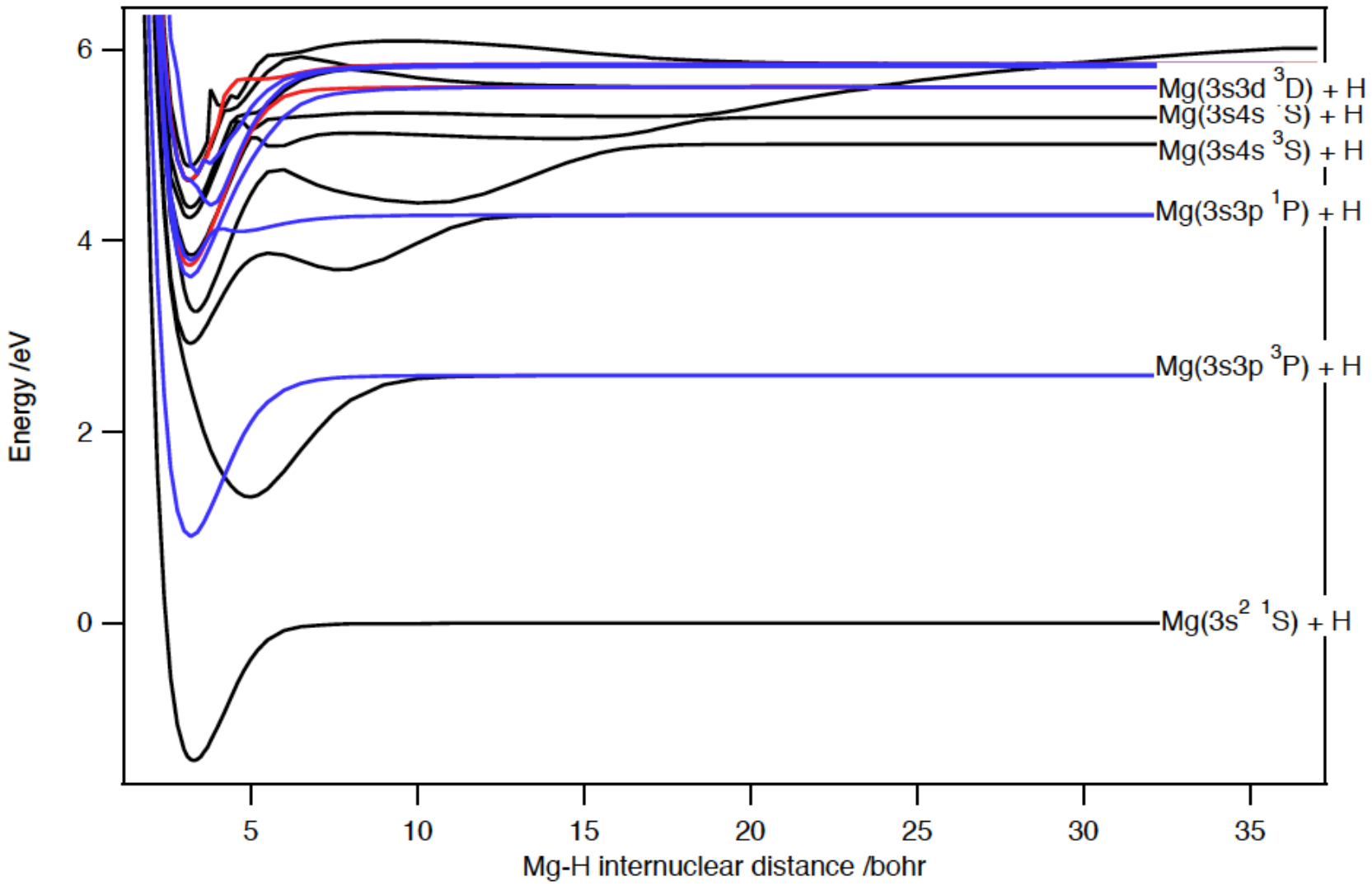
Mg+H Molecular states (quasi molecules):

Mg (^1S, ^1P, ^1D) + H (^2S) : $^2\Sigma^+$, $^2\Pi$, $^2\Delta$
Mg(^3S, ^3P, ^3D) + H (^2S) : $^2\Sigma^+$, $^2\Pi$, $^2\Delta$, $^4\Sigma^+$, $^4\Pi$, $^4\Delta$

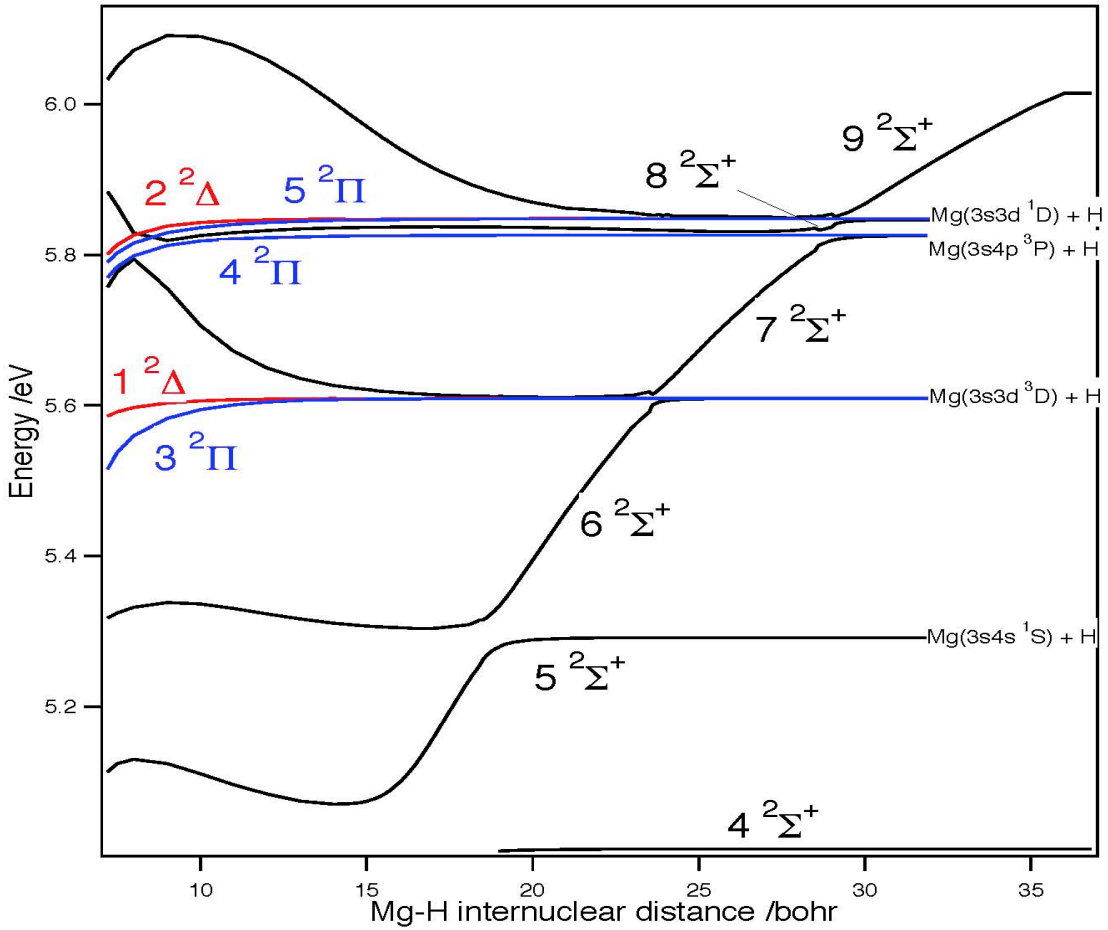
➔9 $^2\Sigma^+$; 5 $^2\Pi$; 2 $^2\Delta$; 2 $^4\Sigma^+$; 1 $^4\Pi$ calculated states: potential energy curves and related couplings which induce collisional transitions

All the calculations : MCSCF+MRCI method with Davidson correction
using the MOLPRO code version 2009.1

Mg + H doublet potentials

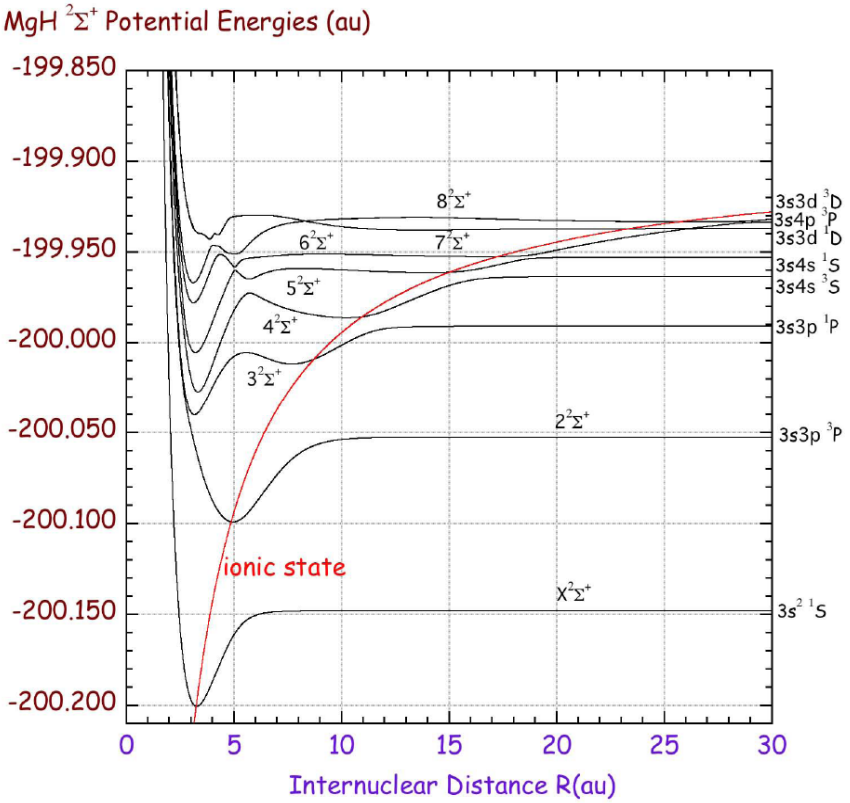


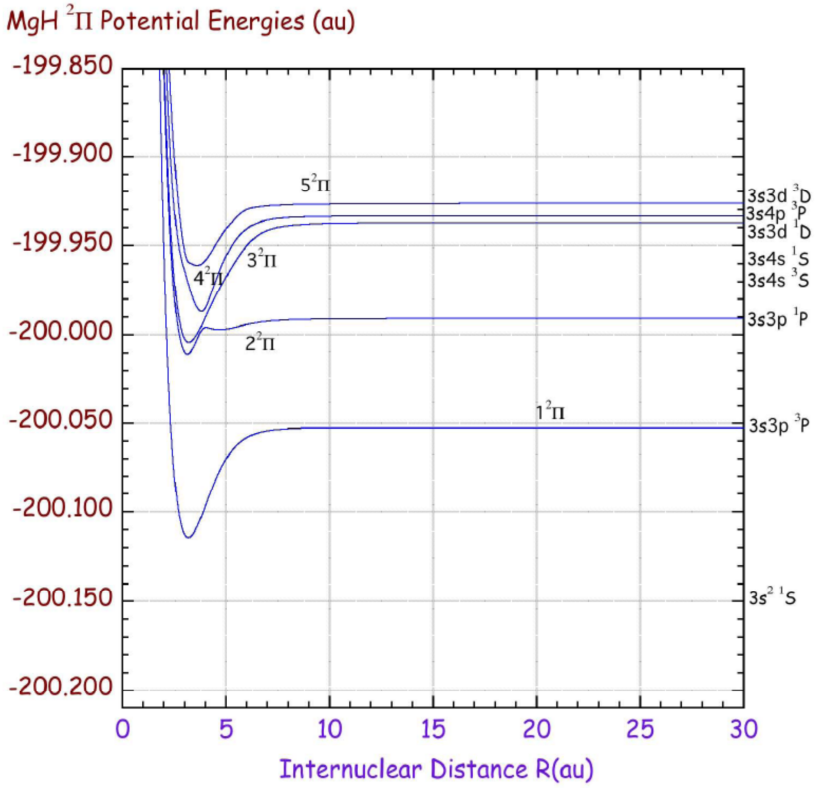
Potentials : avoided crossings at large R



new calculations with10 $^2\Sigma^+$ states

Mg + H potentials

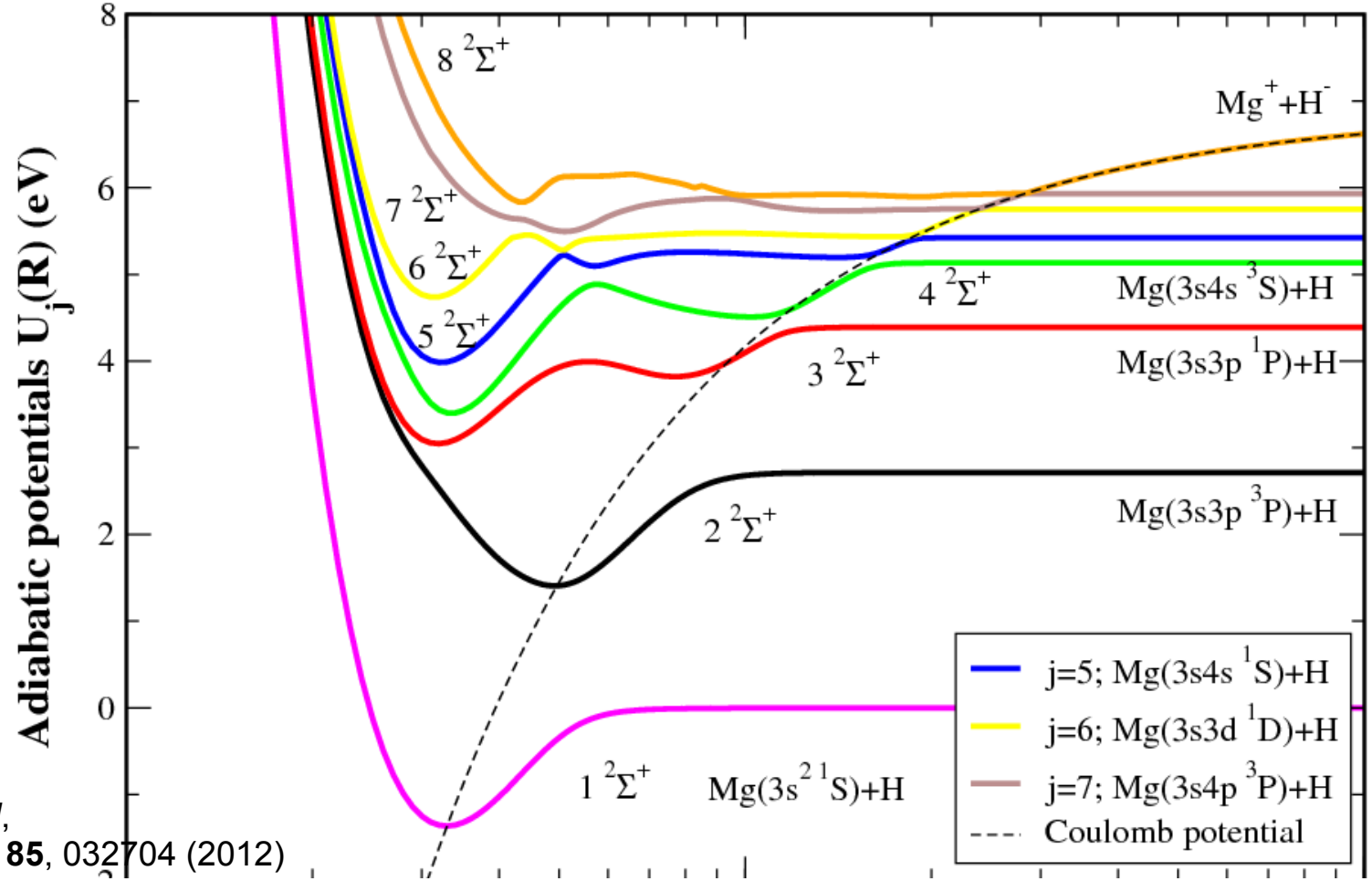




All $^2\Sigma^+$ states are highly perturbed by the Mg^+-H^- ionic state leading to ionisation/mutual neutralisation reaction: Mg+H <--> Mg^++H^-

Mg + H potentials

$$Mg + H \underset{\text{désexcitation}}{\overset{\text{excitation}}{\rightleftharpoons}} Mg^* + H \underset{\text{neutralisation}}{\overset{\text{ionisation}}{\rightleftharpoons}} Mg^+ + H^-$$



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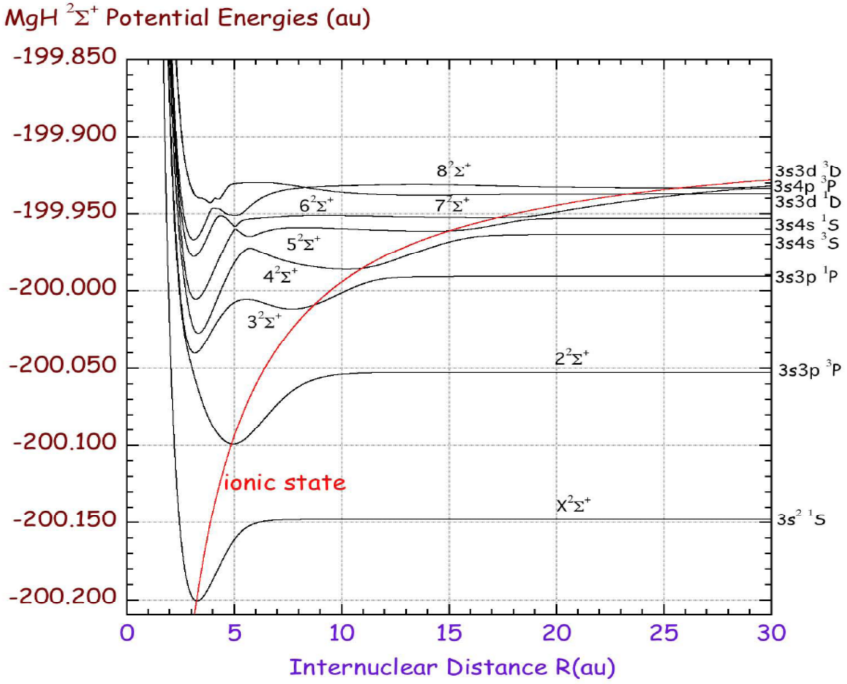
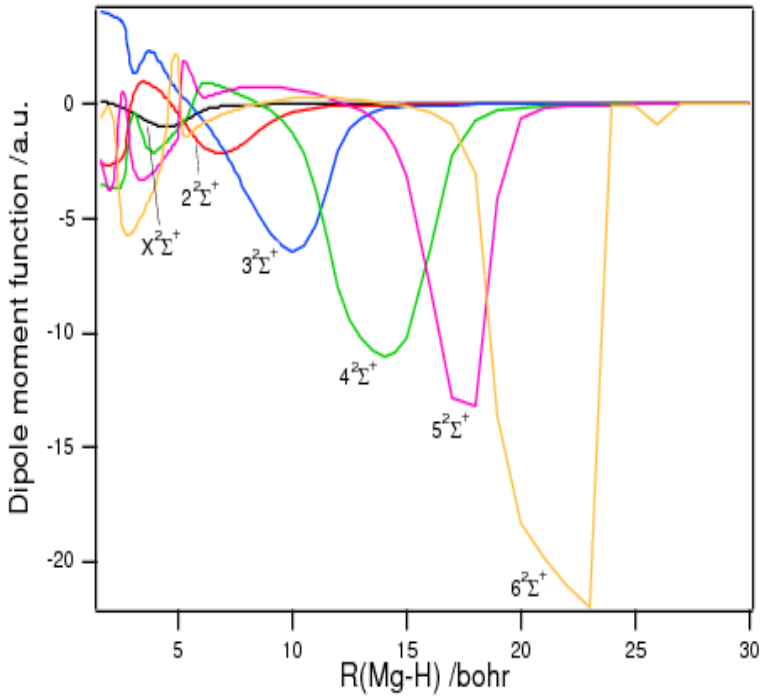
Belyaev *et al*,
Phys. Rev. A **85**, 032704 (2012)

Mg + H potentials and dipole moments

$^2\Sigma^+$ Potentials



Mg + H dipoles



In the regions with dominant ionic configuration, the dipole moment varies linearly with R

Guitou, Spielfiedel, Feautrier, Chem. Phys. Lett. 488, 145, 2010

Potentials and coupling terms

F_j wave functions for relative motion: solutions of coupled differential equations, yielding at infinity the S-matrix and cross sections

What are the coupling terms in the molecular description of the collision?

- The rotational coupling that couples j,k molecular states with $\Delta\Lambda=\pm 1$, $\Delta S=0$

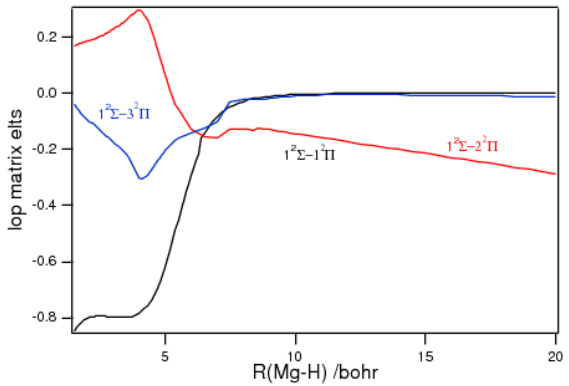
$$-i\frac{\hbar}{MR^2}\sqrt{(J\pm\Lambda+1)(J-\Lambda)}\left\langle j^2\Sigma^+\left|L_y\right|k^2\Pi\right\rangle$$

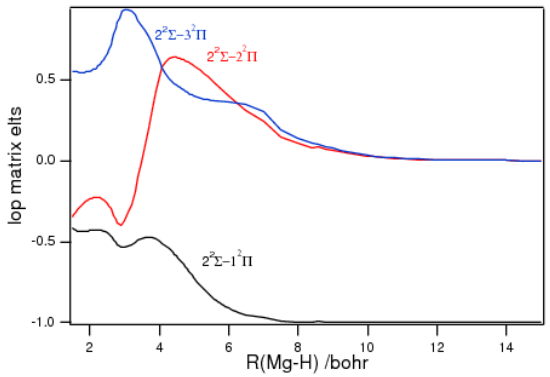
- The radial coupling between j,k states with $\Delta\Lambda=0$, $\Delta S=0$

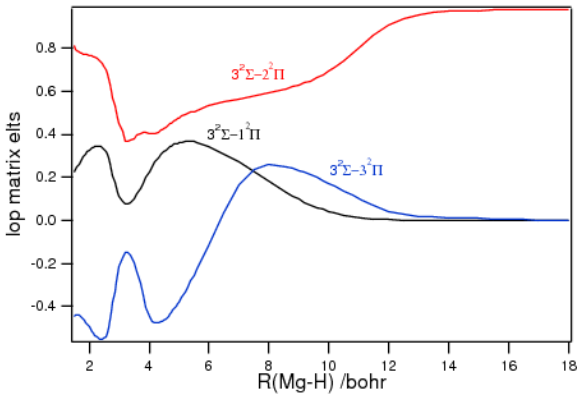
$$\frac{\hbar^2}{M}\left\langle i^2\Sigma^+\left|\frac{\partial}{\partial R}\right|j^2\Sigma^+\right\rangle\frac{dF_k}{dR}$$

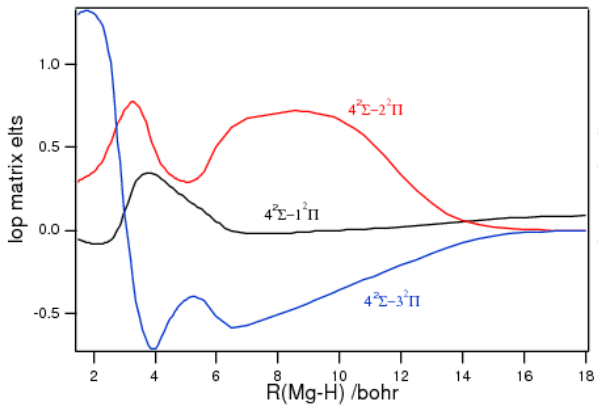
Rotational couplings

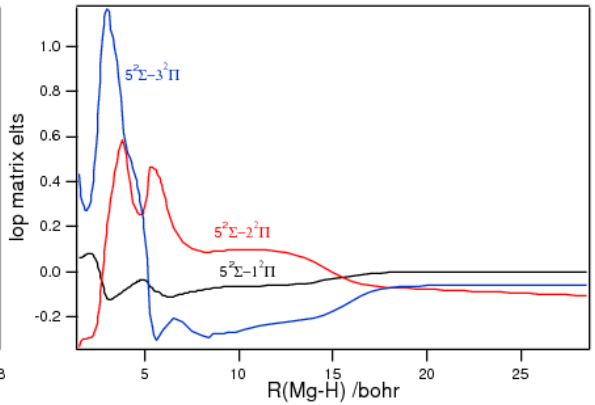
$$-i\left\langle j^2\Sigma^+ \left| L_y \right| k^2\Pi \right\rangle \quad j = 1,6;\ k = 1,3$$

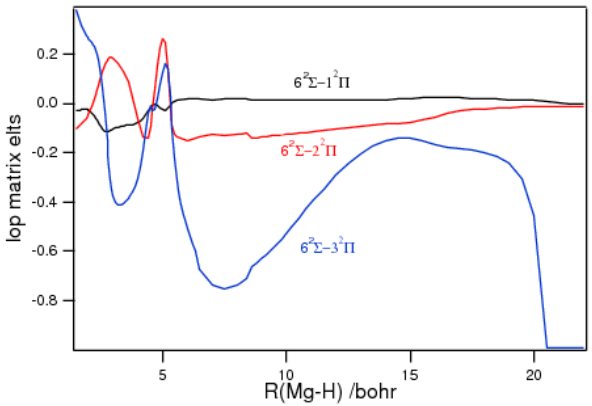








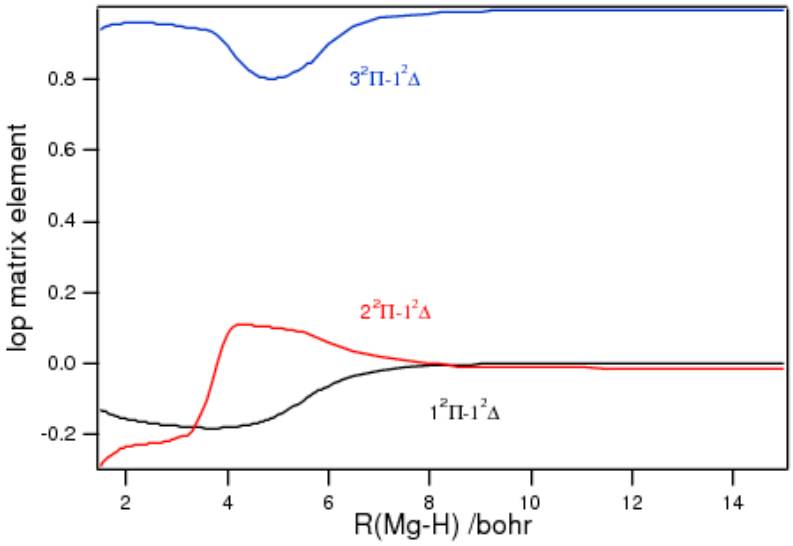


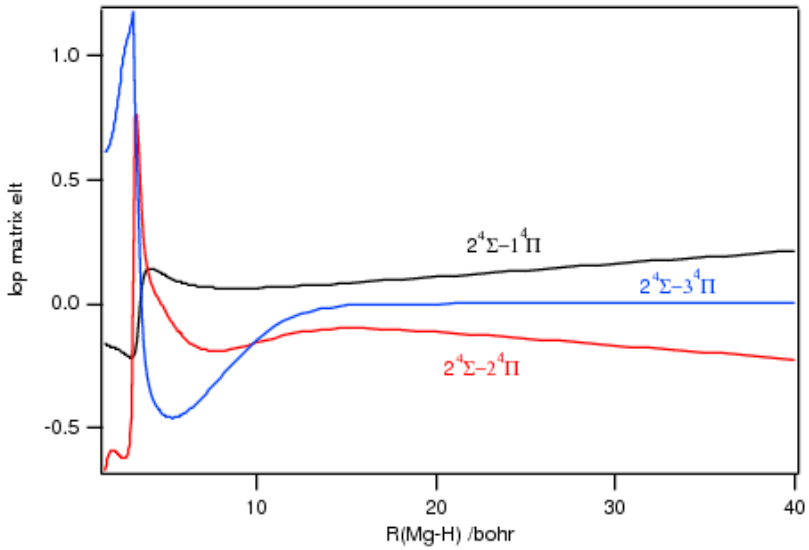


Rotational couplings

$$-i\left\langle j^2\Pi \left| L_x \right| {}^2\Delta \right\rangle \quad j = 1,3$$

$$-i\left\langle j^4\Sigma^+ \left| L_y \right| {}^4\Pi \right\rangle \quad j = 1,3$$





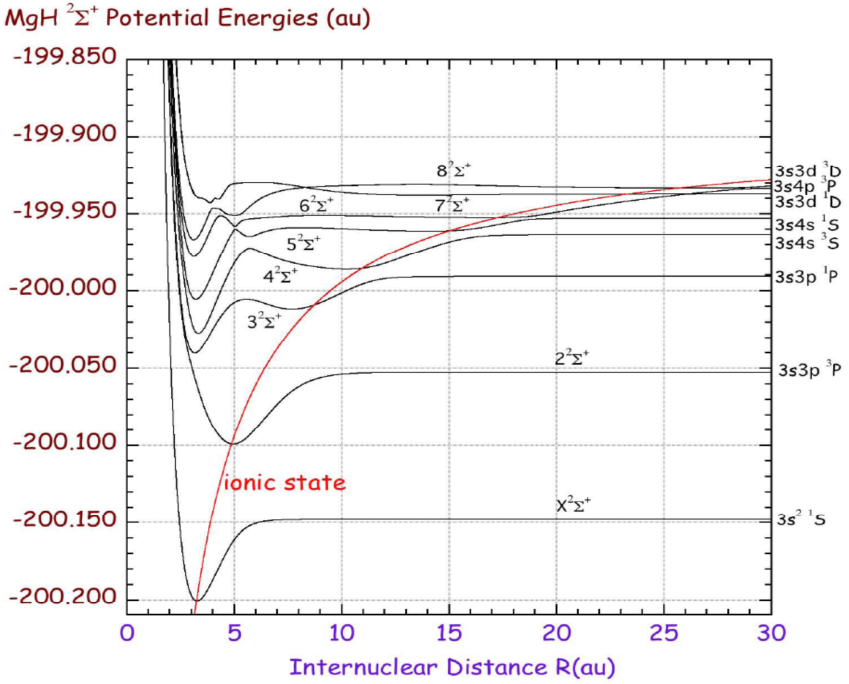
- For allowed asymptotic atomic states: L_y matrix elements do not go to zero

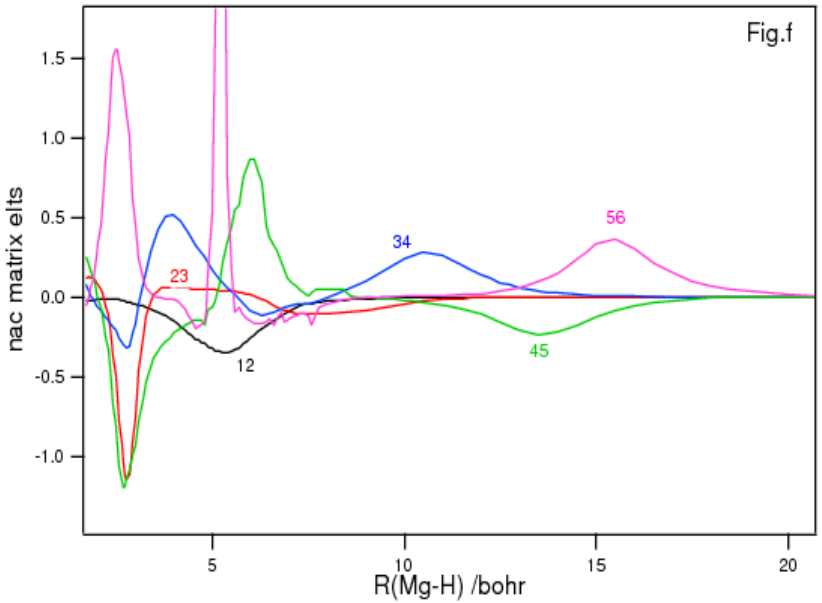
M. Guitou, A. Spielfiedel, N. Feautrier, Chemical Physics Letters **488** (2010) 145

Radial couplings between consecutive $^2\Sigma^+$ states

$^2\Sigma^+$ Potentials

$$\left\langle i^2\Sigma^+ \left| \frac{\partial}{\partial R} \right| (i+1)^2\Sigma^+ \right\rangle \quad i = 1, 5$$



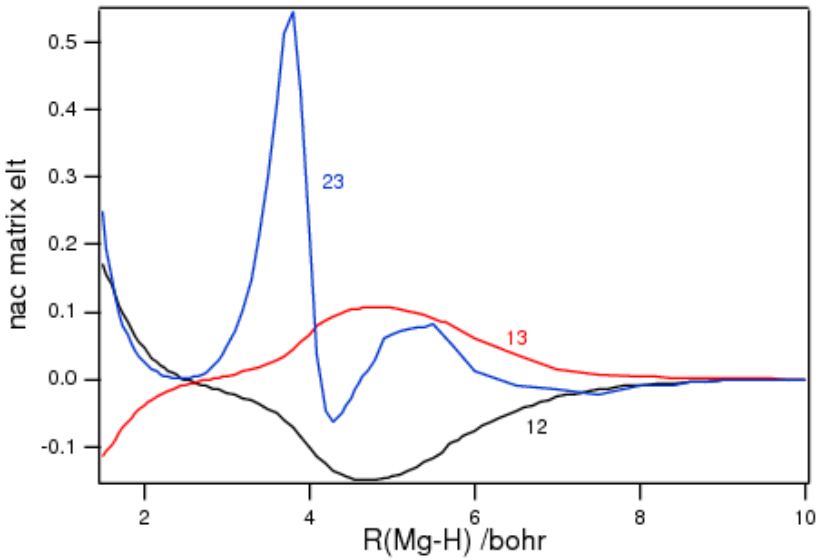


Two major regions for couplings with consequense on the collisional mechanisms:

- avoided crossings
- small R-distances

Radial couplings

$$\left\langle i^2\Pi \left| \frac{\partial}{\partial R} \right| j^2\Pi \right\rangle \quad i,j = 1,3$$

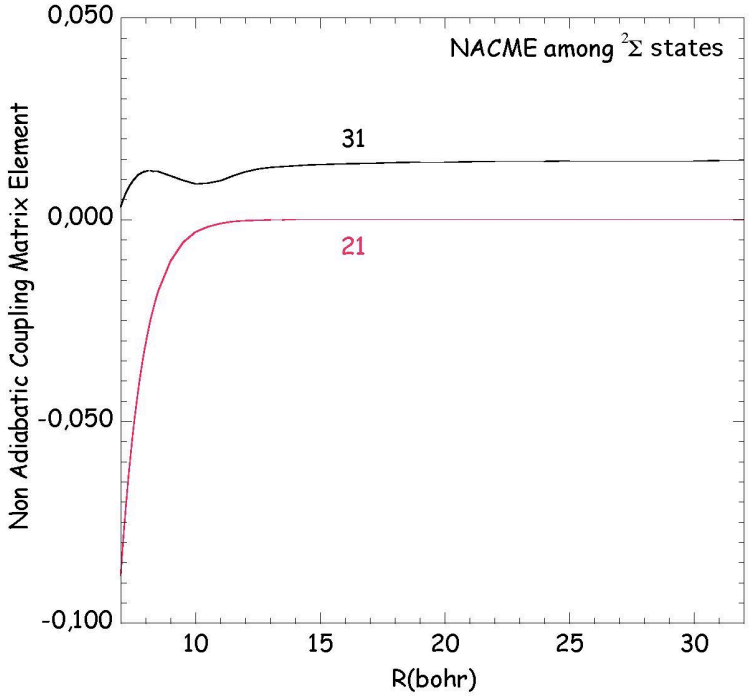


no coupling at large R values

Radial couplings

$$\left\langle i^2\Sigma^+ \left| \frac{\partial}{\partial R} \right| j^2\Sigma^+ \right\rangle \qquad i,j = 2,1 \rightarrow H + Mg(3s3p^3P)), H + Mg(3s^2\,{}^1S)$$

$$i,j = 3,1 \rightarrow H + Mg(3s3p^1P)), H + Mg(3s^2\,{}^1S)$$



The radial couplings between allowed transitions do not go to zero at large R

From molecular data to cross sections (1)

Method: usual close-coupling (CC) approach

total wave function : $\vec{r}$: electronic coordinates, $\vec{R} = (\hat{R}, R)$: relative nuclear motion

$$\Psi(\vec{r}, \vec{R}) = \sum_j \Phi_j(\vec{r}, R)\ \varphi_j(\hat{R})\ \frac{F_j(R)}{R}$$

with $\Phi_j(\vec{r}, R)$: molecular wave function for fixed R

R-matrix (➔cross sections): from the asymptotic part of the CC equations for radial F_j functions

Problem: non-zero radial coupling terms for R➔∞ (no problem for rotational couplings as divided by R^2 at large R)

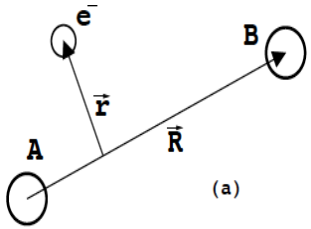
Solution: the retroprojection method[1]

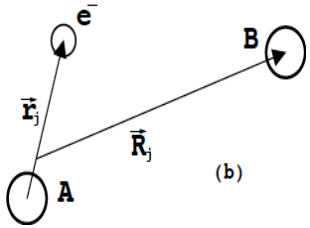
[1] Grosser,Menzel, Belyaev, PRA, 59, 1309 (1999); Belyaev, Egorova, Grosser, Menzel, PRA, 64, 052701 (2001)

From molecular data to cross sections (2)

The asymptotic problem: origin twofold

- One molecular state does not fit to one atomic state
- The Jacobi coordinate systems are not the same





- Molecular system: R refers to the center of mass of the nuclei
- Atomic system: R refers to the center of mass of the atoms

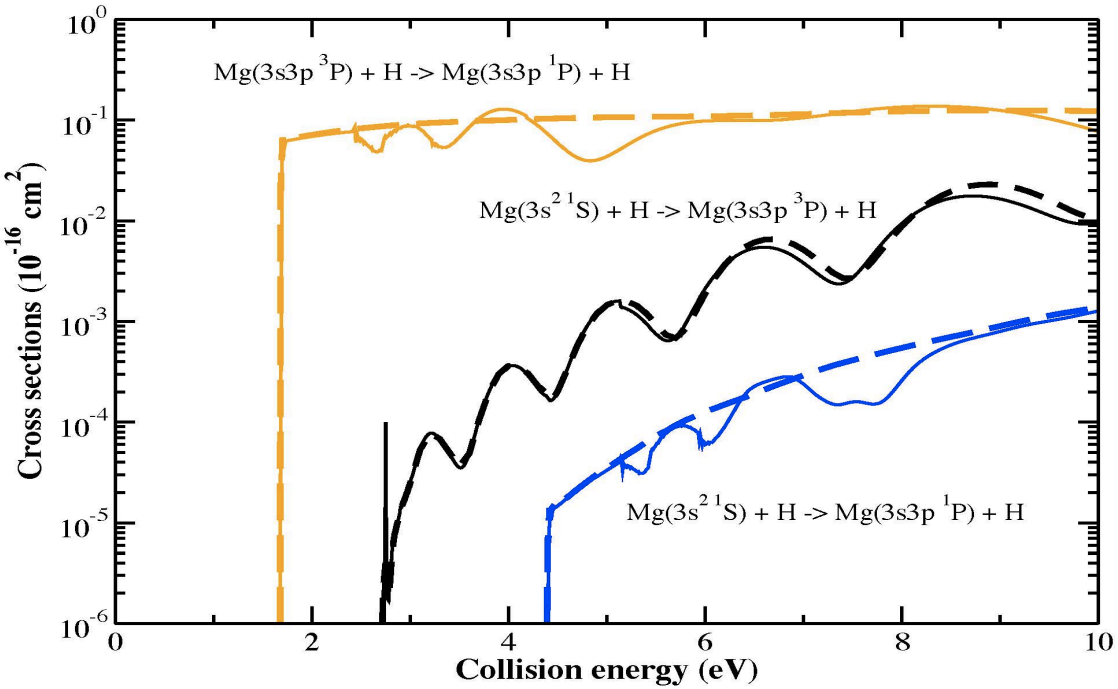
The solution (retroprojection method):

At large R: unitary transformation of the molecular R-matrix into S-matrix ➔ cross sections

Belyaev et al. Phys. Rev. A 60, 2151, (1999);Belyaev, Phys. Rev. A 82, 060701 ((2010)

Collision cross sections:

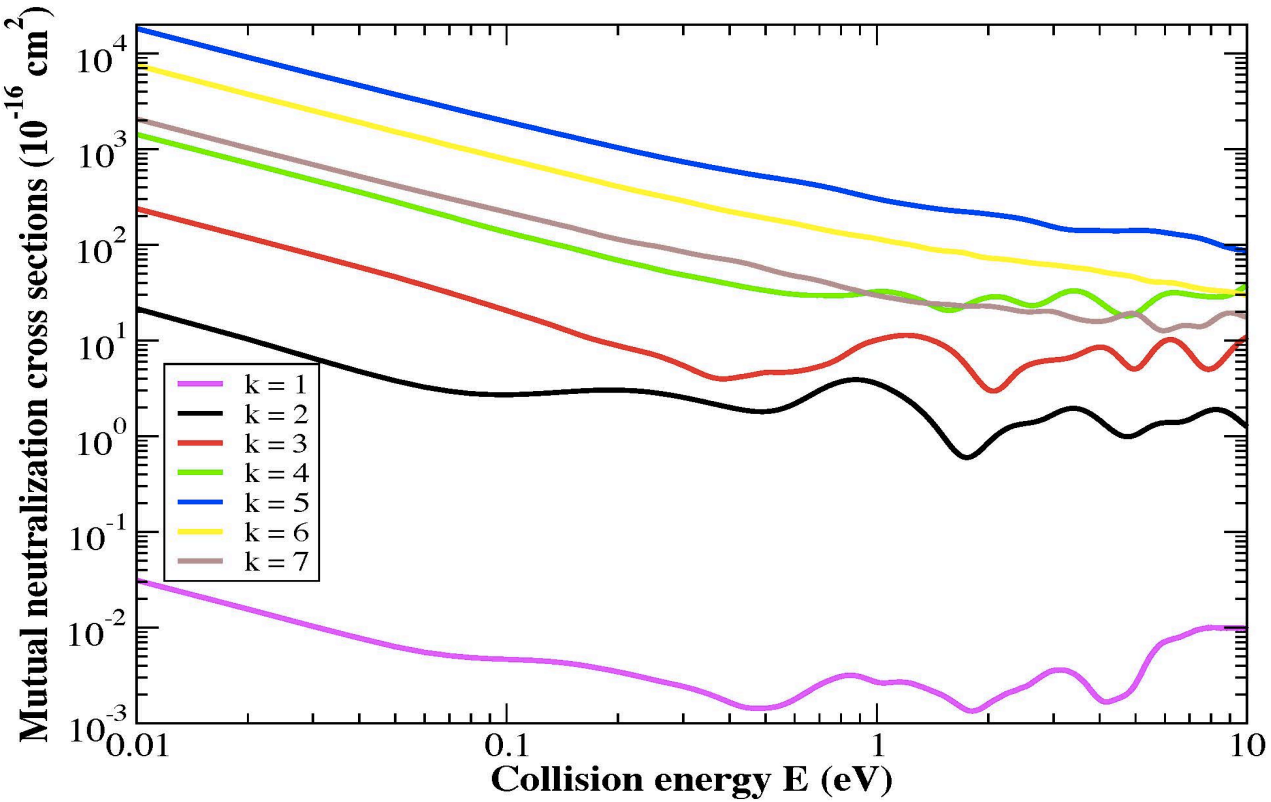
Comparison of cross sections 8 Σ^+ states vs 3 Σ^++2 Π states



- Very good agreement between both results apart from oscillations due to the presence of higher lying channels in the 8 Σ^+ calculation
- No contribution of rotational coupling

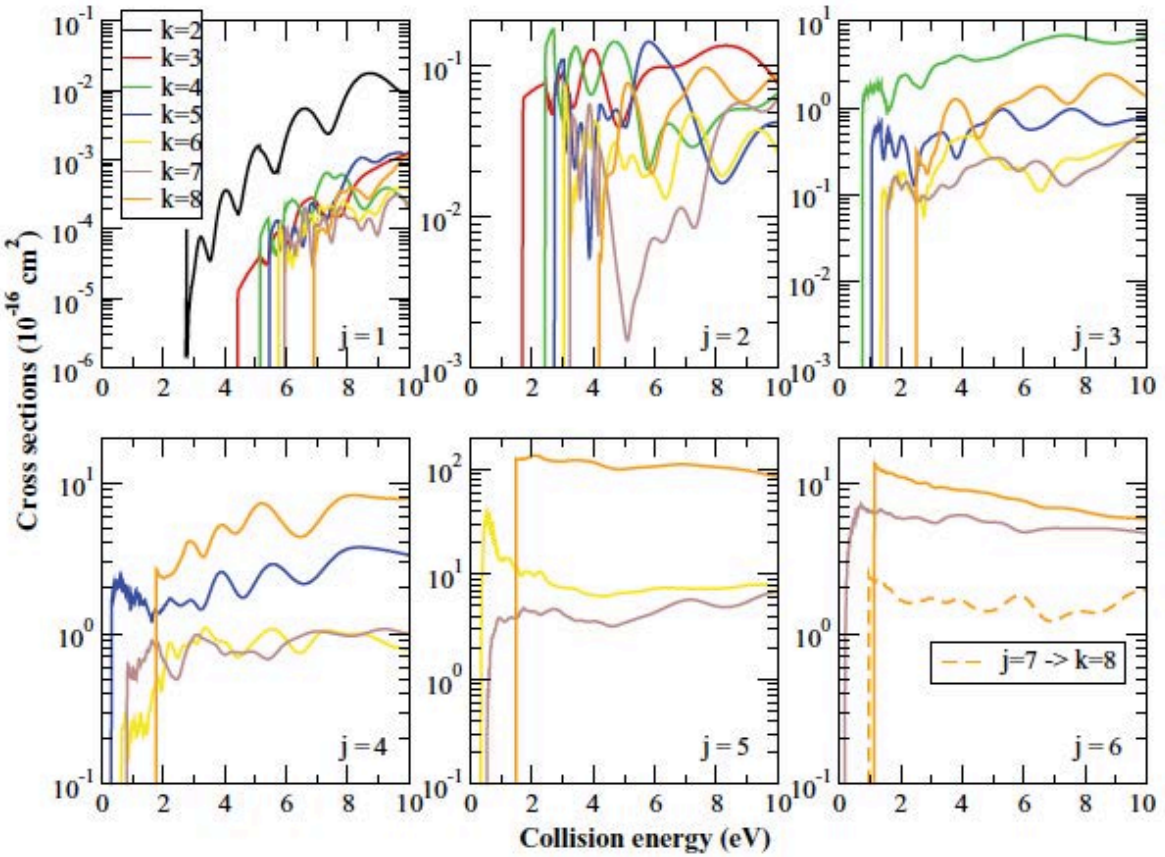
Belyaev et al. PRA 85, 032704 (2012)

Collision cross sections for mutual neutralisation in Mg^+ H^-



The largest cross section in Mg^+H^- collisions is for neutralisation into $Mg(3s4s\,^1S)+H$ state

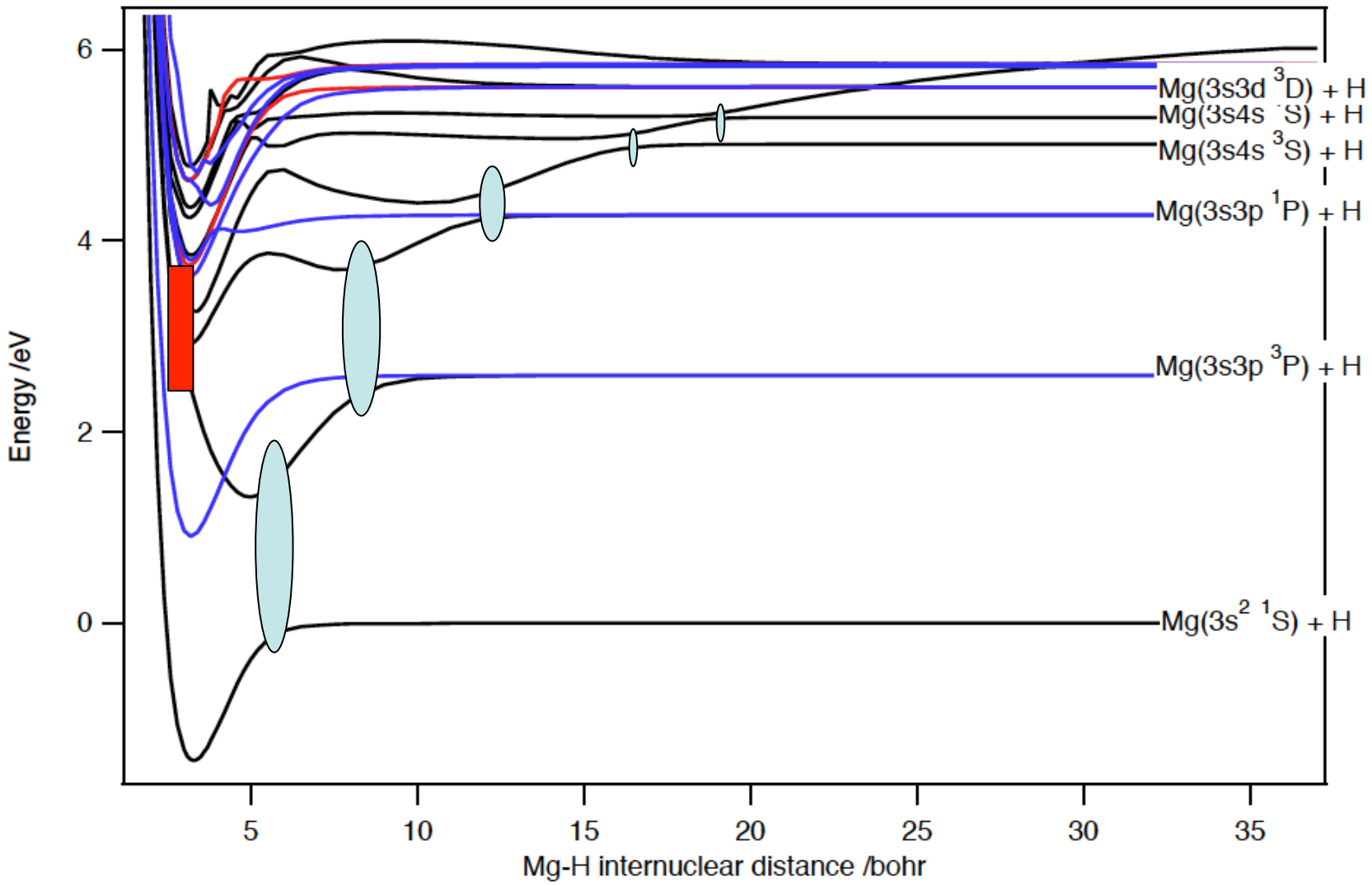
Excitation j ➔k cross sections (2)



Different mechanisms at short or large R distances explain the relative values of the cross sections

Belyaev et al. PRA 85, 032704 (2012)

Mg + H excitation mechanisms



Mg+H rate coefficients

T = 4000.00 K

initial/final states	3s ^{1}S	3p ^{3}Po	3p ^{1}Po	4s ^{3}S	4s ^{1}S	3d ^{1}D	ionic
3s ^{1}S		1.67e-17	9.32e-20	5.37e-20	2.14e-20	6.31e-21	5.05e-22
3p ^{3}Po	4.87e-15		2.76e-13	7.95e-14	2.07e-14	4.35e-15	1.47e-16
3p ^{1}Po	1.05e-14	1.07e-10		5.21e-11	7.88e-12	9.96e-13	1.84e-13
4s ^{3}S	5.26e-14	2.67e-10	4.52e-10		1.38e-10	1.18e-11	9.14e-12
4s ^{1}S	1.46e-13	4.83e-10	4.75e-10	9.56e-10		1.42e-09	8.64e-10
3d ^{1}D	2.23e-14	5.28e-11	3.12e-11	4.28e-11	7.41e-10		1.73e-10
ionic	2.42e-13	2.42e-10	7.84e-10	4.48e-09	6.10e-08	2.35e-09	

- For excitation: the dominant rate coefficient are those to the closest final state
- Large rates for transitions between excited states even for non-radiatively allowed transitions
- Important contribution of ionisation/mutual neutralisation

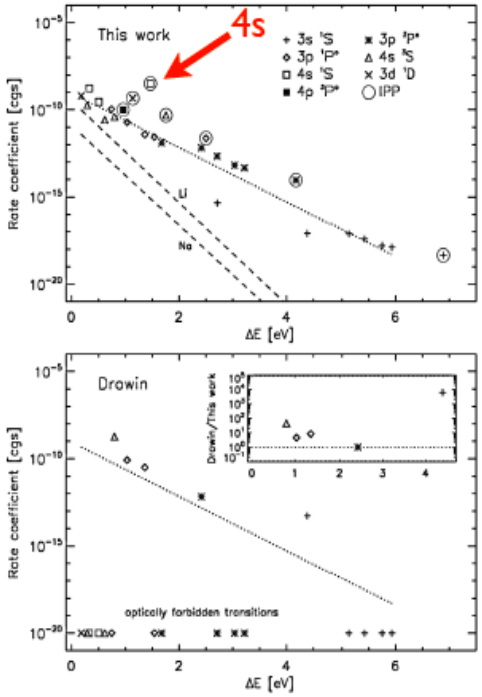
Guitou, Belyaev, Barklem, Spielfiedel, Feautrier, J. Phys. B (2011)
Barklem, Belyaev, Spielfiedel, Guitou, Feautrier, A&A (2012)

Comparison with Drawin formula

Drawin formula: extension of the classical Thomson model for ionisation of atoms by electron impact, commonly used for allowed transitions

➔Gives collision rates proportional to the oscillator strength of the transition

Mg+H rate coefficients as functions of the energy difference(ΔE) of the levels, T=6000K



←R_{drawin} vs $R_{quantum}$

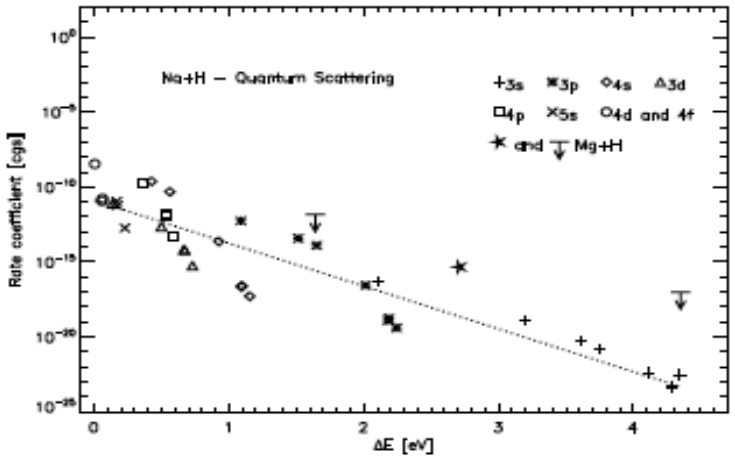
The Drawin formula

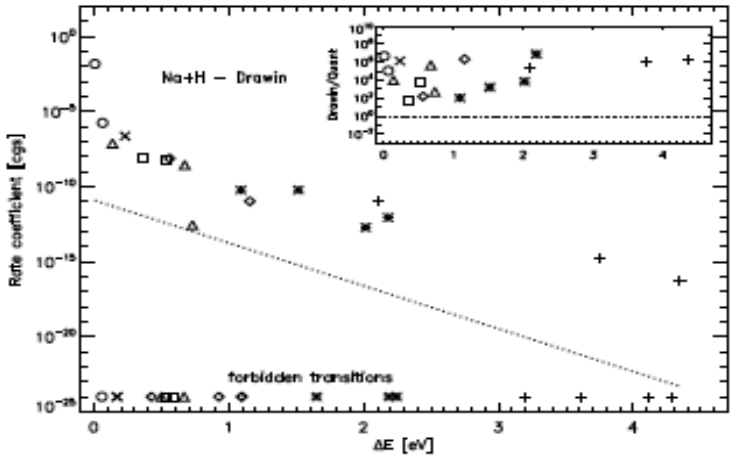
- overestimates the rate coefficients by about 4 orders of magnitude

- Cannot provide rate coefficients for optically forbidden transitions

- Same trend for other systems (Li, Na)

Comparison with Drawin formula: Na+H





Na+H rate coefficients as functions of the energy difference (ΔE) of the levels

←Quantum

- The rate coefficients decrease for increasing ΔE
- For allowed transitions: the Drawin formula overestimate the rate coefficients by several orders of magnitude

The Drawin formula cannot provide rate coefficients for optically forbidden transitions

so: in the absence of accurate data, the rate coefficients are often estimated from the Drawin formula with a corrective factor

$0 \leq S_H \leq 1$

←Drawin

Barklem, Belyaev, Guitou, Feautrier, Gadea, Spielfiedel, A&A in press, 2011

Consequences on non-LTE modelling (1)

• Non-LTE modelling implies competition between radiative and collisional processes for both excitation and ionisation

• The consequences on abundances depend non linearly on:
- the physical conditions of the star: T_{eff}, g, [Fe/H]…
- radiative transfer
- 1D or 3D non-LTE
- the number of atomic states included in the model
- the line considered for the diagnostics, …

• a priori, collisions should decrease the non-LTE effects on populations, but this is not so simple as ionisation/mutual neutralisation contribute as well.

So, to date, no general conclusion is evident, but some trends are available from a number of recent studies : Li, Na, C, O

Consequences on non-LTE modelling (2)

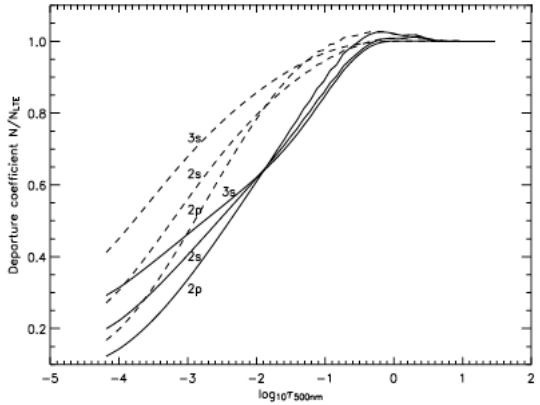
Li I line formation (code MULTI)

- departure coefficients from LTE (N/N_{LTE}) with optical depth for low lying Li levels (2s,2p,3s): full line without H collision, dashed line with H collisions

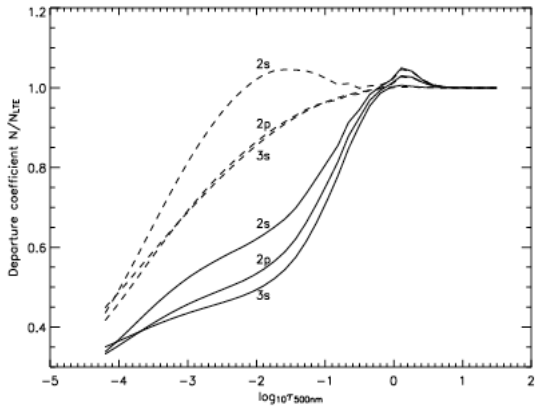
The analysis of the results show:

- due to the low collisional excitation rates for the lowest levels, the results are not very sensitive to the details of the H-collisional rates

- H-collisions push the lowest Li- states towards LTE and even superpopulation (2s) due to the Li(3s)+H <---> Li^++H^- reaction



Solar 1D model
with $\log\varepsilon_{Li}$=1.1
T_{eff} = 5777
Log g = 4.44
[Fe/H]=0.0



HD 140283 1D model
with $\log\varepsilon_{Li}$=1.8
(metal poor sub giant)
T_{eff} = 5690
Log g = 3.87
[Fe/H]=-2.5

Barklem, Belyaev, Asplund, A&A, 409, L1 (2003)

Consequences on non-LTE modelling (3)

Li I line formation (continued) : with H-collisions wH, no H-collisions nH

Predicted flux equivalent widths (in mA) for the 670.8nm line and 1D and 3D modelling

		1D			3D		
Star	[Fe/H]	W_λ(LTE)	W_λ(NLTE) nH	W_λ(NLTE) wH	W_λ(LTE)	W_λ(NLTE) nH	W_λ(NLTE) wH
Sun	0.0	0.40	0.34	0.38	0.55	0.37	0.40
HD 140283	-2.5	2.40	2.18	2.66	3.84	1.96	2.35

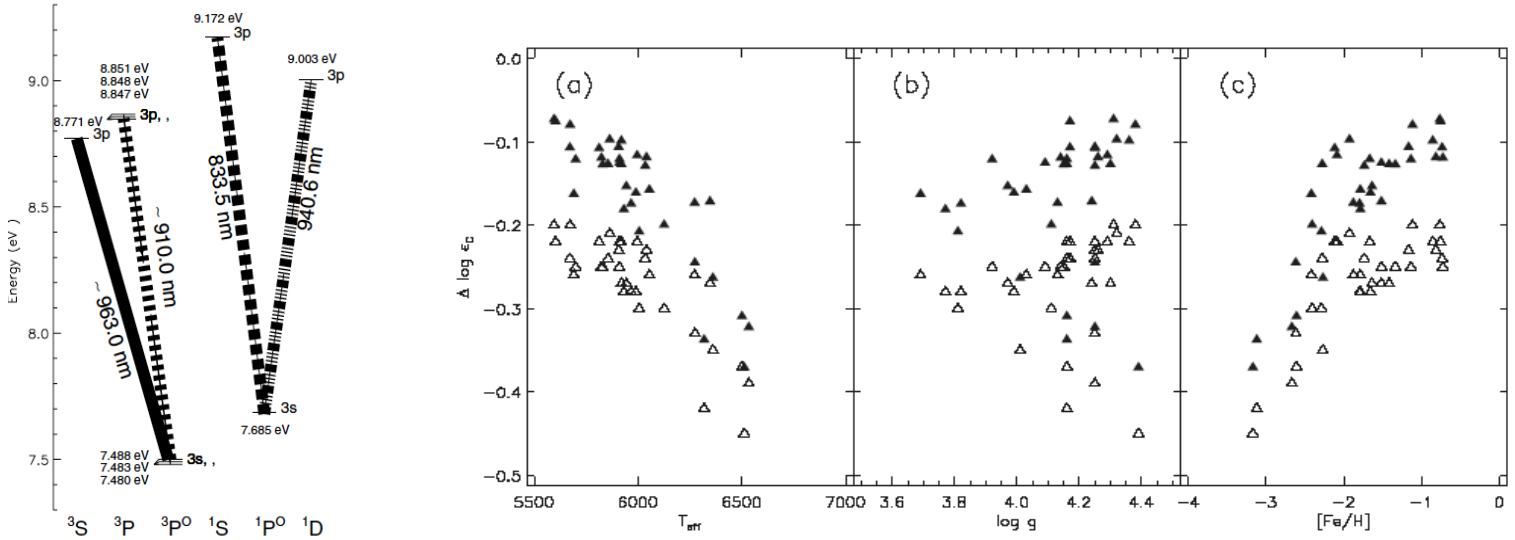
- For this resonance line, H-collisions have small effects for the Sun but larger effects for metal-poor stars due to ionisation/mutual neutralisation reaction
- Importance of 3D modelling versus 1D

Barklem, Belyaev, Asplund, A&A, 409, L1 (2003)

Consequences on non-LTE modelling (4)

C I line formation: transition $2p3s\,^3P^0$-$2p3p\,^3P$, λ=910 nm

Variation of non-LTE abundance corrections for 34 halo stars:
with (a):Teff; (b): log g; (c): [Fe/H]
empty triangles: S_H=0, filled triangles: S_H=1



➔large negative non-LTE effect for this line between two excited states
(LTE abundances are too large)

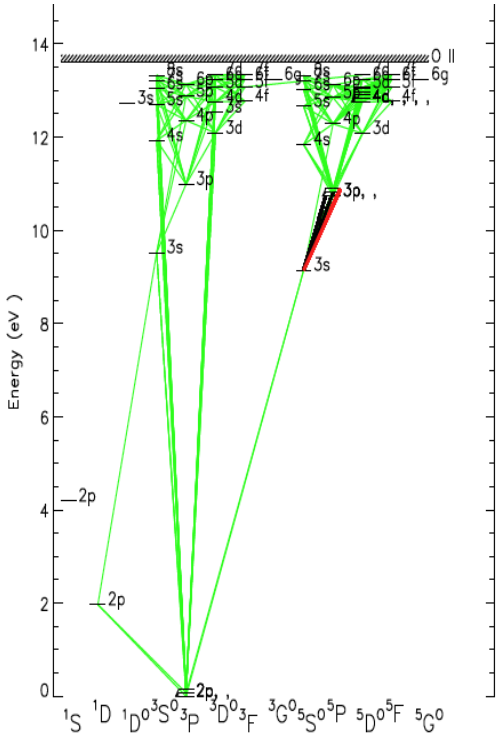
Fabbian, Asplund, Carlsson, Kiselman, A&A, 458, 899 (2006)

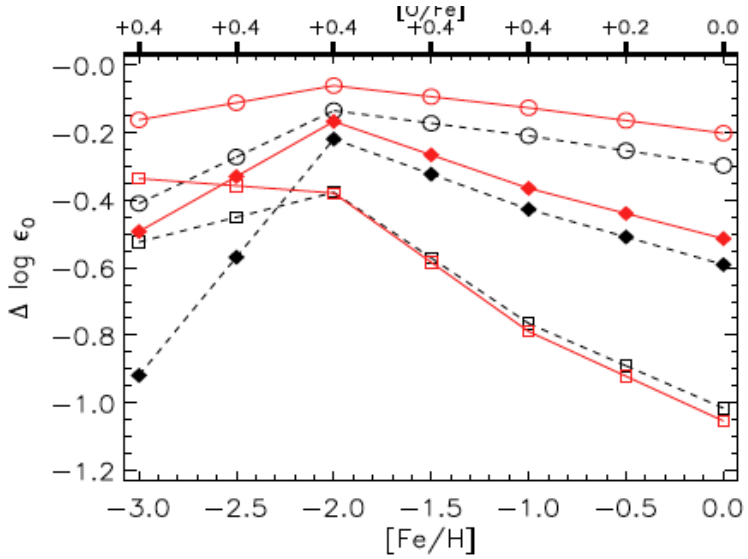
Consequences on non-LTE modelling (5)

O I IR triplet line formation: transition $2p^3 3s\ ^5S^0$-$2p^3 3p\ ^5P$, λ=777 nm

NonLTE abundance corrections versus metllicity for 3 stars:
Open circles: Teff=5780K, log g=4.44; diamonds: Teff=6500K, log g=4; squares:Teff=6500k, log g=2
Dashed lines: no collisions, solid lines: with collisions (Drawin S_H=1)

➔ At low metallicity (large H density), collisions with H atoms play a major role

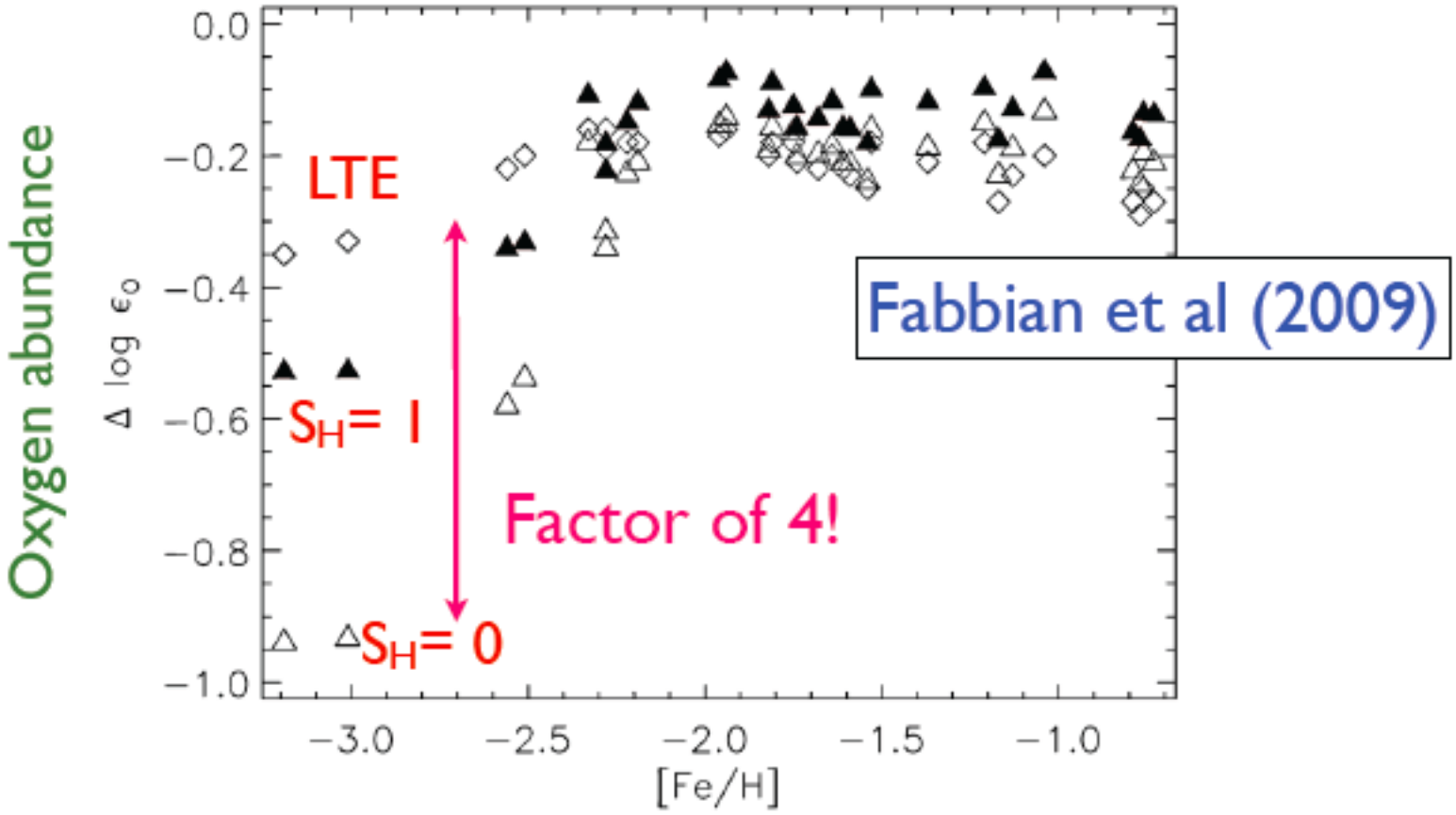




Fabbian, Asplund, Barklem, Carlsson, Kiselman, A&A, 500, 1221 (2009)

Consequences on non-LTE modelling (6)

Large uncertainties in stellar abundances due to uncertainties in collision rate coefficients



Concluding remarks

• H collisions are of particular importance for abundance determination:
- of low metallicity stars
- using lines involving excited states

• preliminary results on Li, Na and Mg show:
- a large overestimation of the rate coefficients using the Drawin formula
- importance of ionisation/mutual neutralisation

• charge transfer is the dominant process for Li and Na: Li and Na abundances overestimated by 20-60% if not included

Mg has two spin systems and both charge transfer and excitation especially between states with different spin are important

• trends to be confirmed for other atoms: calculations of H-atom collisional rates with O I and CaI are in progress, in the future Ca II

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