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Collision rates and the determination of atmospheric parameters

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Collision rates and the determination of atmospheric parameters

Outline

- Context
- Calculation of accurate collisional rates: Mg+H
- Comparison with approximate formulae: Drawin, Kaulakys
- Preliminary consequences on non-LTE modelling

Non-LTE calculations

Context

Non-LTE modeling implies that collisions compete with radiative processes for statistical equilibrium of level populations :

- 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 six orders of magnitude

This implies :

- new calculations of H collisional cross sections and rates

Collisional rates

Two steps for calculations of excitation rates by H atoms

- Determination of interaction potentials and coupling terms between the studied species and H:
  quantum chemistry increasingly difficult for high excited levels

- Dynamics in these potentials
  classical or quantum mechanical approach

Already done: Li+H, Na+H
Under way: Mg+H, O+H
In the future: Ca+H, CaII+H and possibly Fe+H(?)

Mg + H interaction potentials

Potential energy curves and coupling terms for Mg+H

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

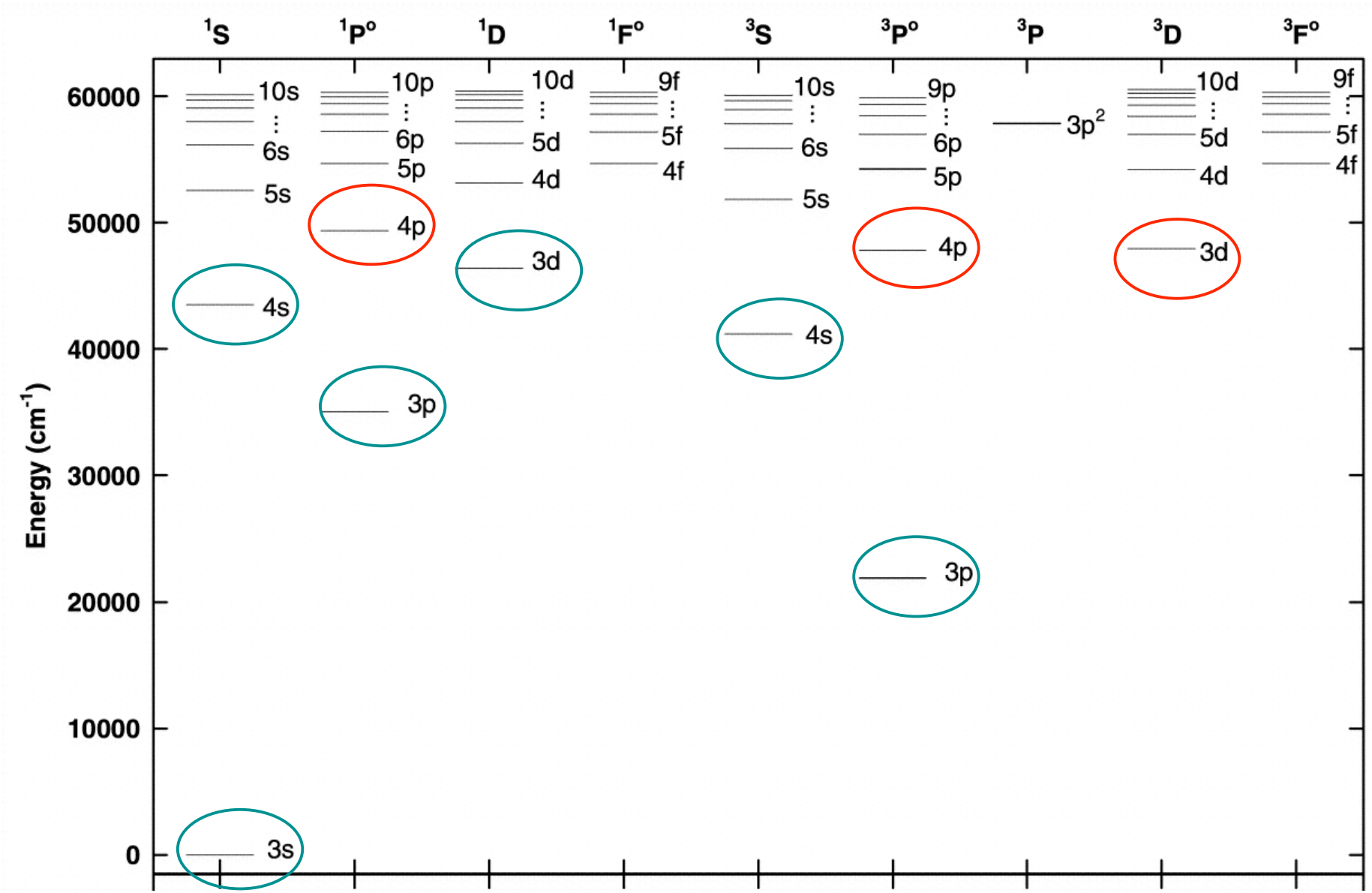
6 Mg levels considered: E< 6eV

$3s^2$ (^1S), 3s3p (^3P), 3s3p (^1P), 3s4s (^3S),
3s4s (^1S), 3s3d (^1D)

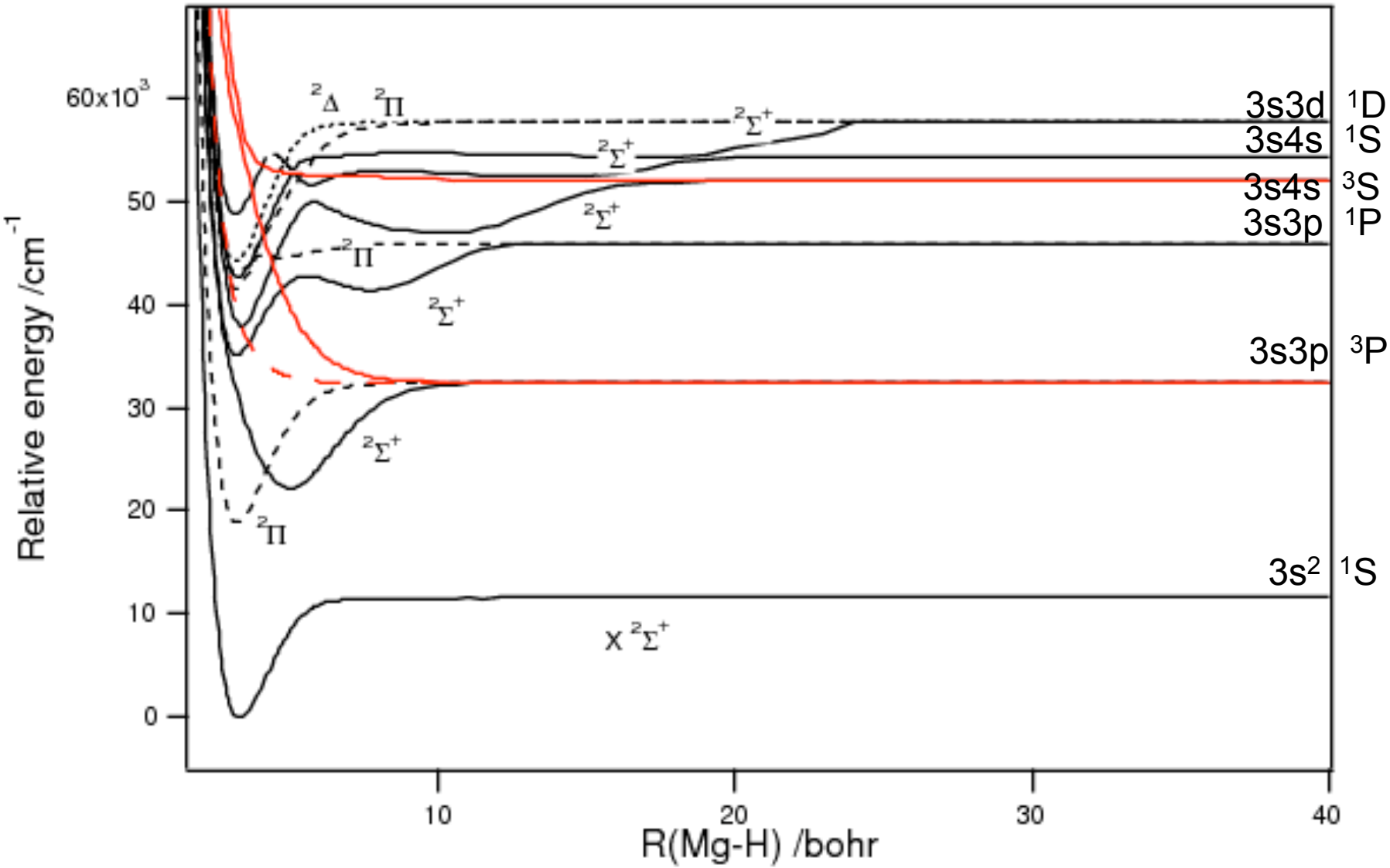
Mg+H Molecular states (quasi molecules):

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

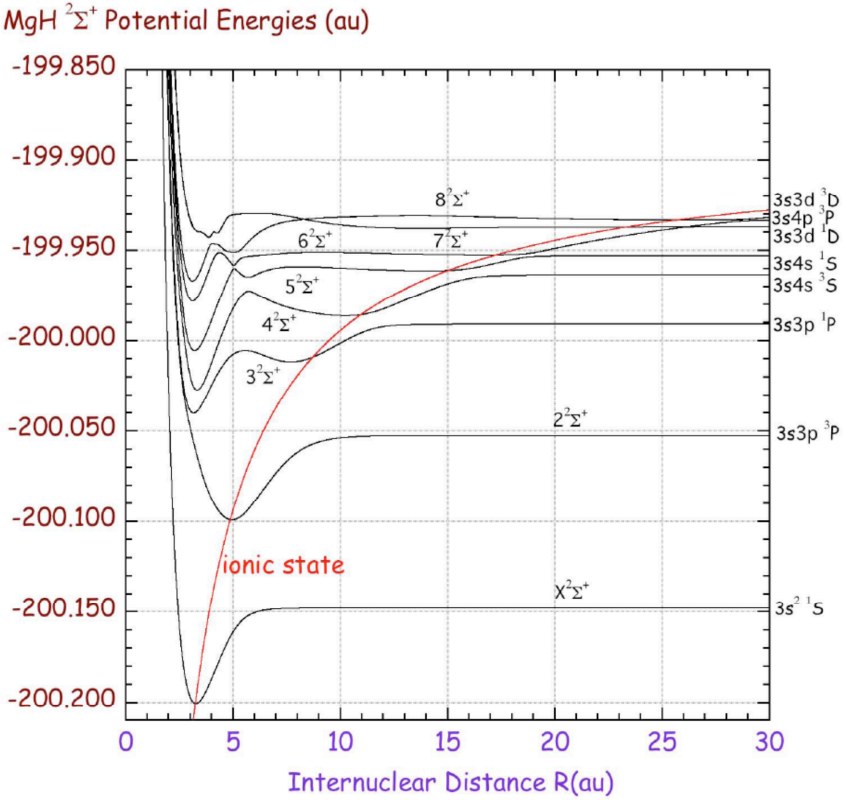
➔ 8 $^2\Sigma^+$; 5 $^2\Pi$; 2 $^2\Delta$; 2 $^4\Sigma^+$; 1 $^4\Pi$ calculated states: potential energy curves and related couplings which induce collisional transitions

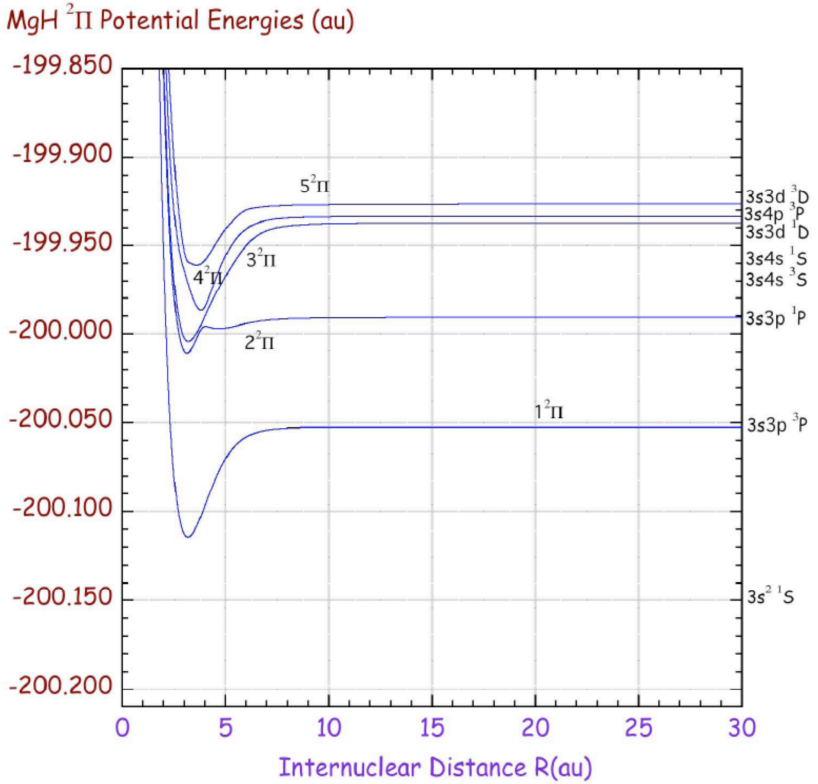

^{1}S
^{1}P°
^{1}D
^{1}F°
^{3}S
^{3}P°
^{3}P
^{3}D
^{3}F°
Energy (cm^{-1})
60000
50000
40000
30000
20000
10000
0
10s
6s
5s
4s
3s
10p
6p
5p
4p
3p
10d
5d
4d
3d
9f
5f
4f
10s
6s
5s
4s
9p
6p
5p
4p
3p
3p^2
10d
5d
4d
3d
9f
5f
4f

Mg + H potentials



Mg + H potentials

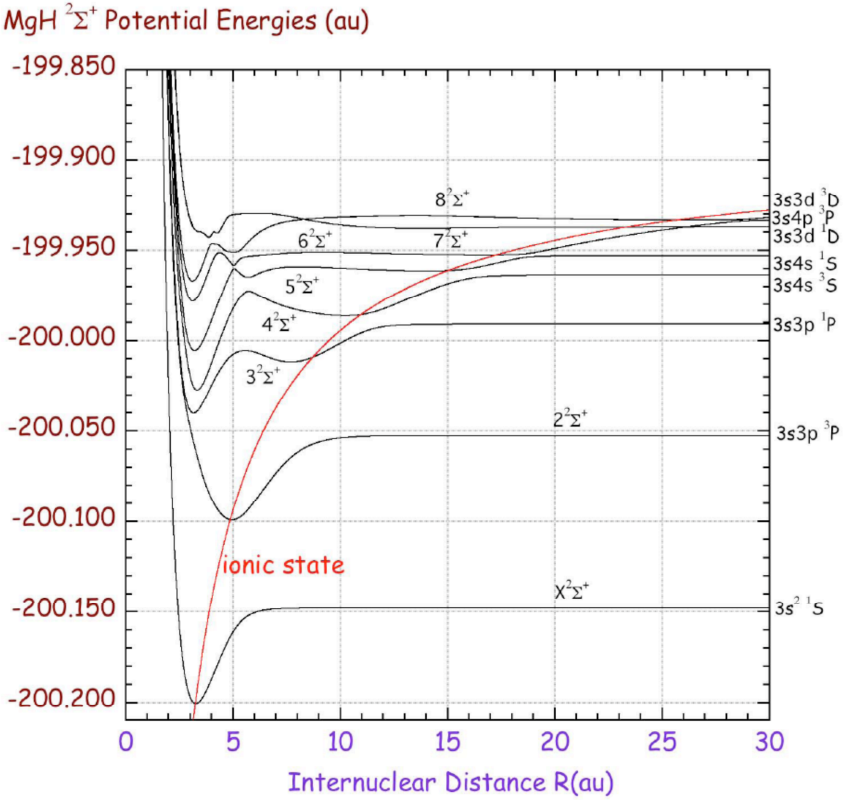




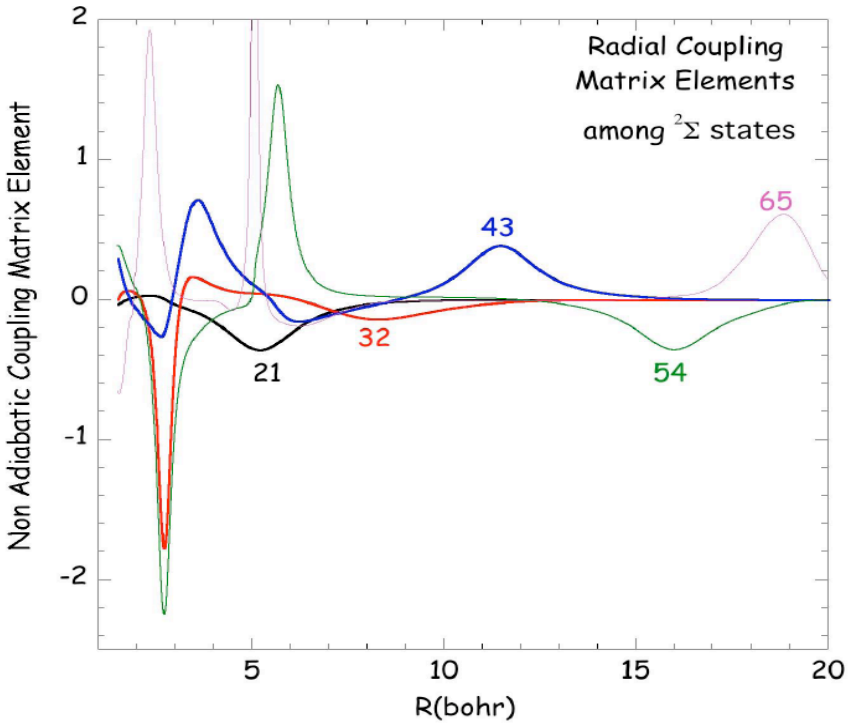
All $^2\Sigma^+$ states are highly perturbed by the Mg^+-H^- ionic state leading to ionisation/mutual neutralisation reaction: Mg+H <--> Mg^++H^-

Mg + H potentials and coupling terms

$^2\Sigma^+$ Potentials



$^2\Sigma^+$ Coupling terms



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

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	2.26e-12	1.84e-13
4s ^{3}S	5.26e-14	2.67e-10	4.52e-10		1.38e-10	4.11e-11	9.14e-12
4s ^{1}S	1.46e-13	4.83e-10	4.75e-10	9.56e-10		1.81e-09	8.64e-10
3d ^{1}D	3.72e-14	8.79e-11	1.18e-10	2.48e-10	1.57e-09		1.73e-10
ionic	1.10e-13	1.10e-10	3.57e-10	2.04e-09	2.78e-08	6.42e-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

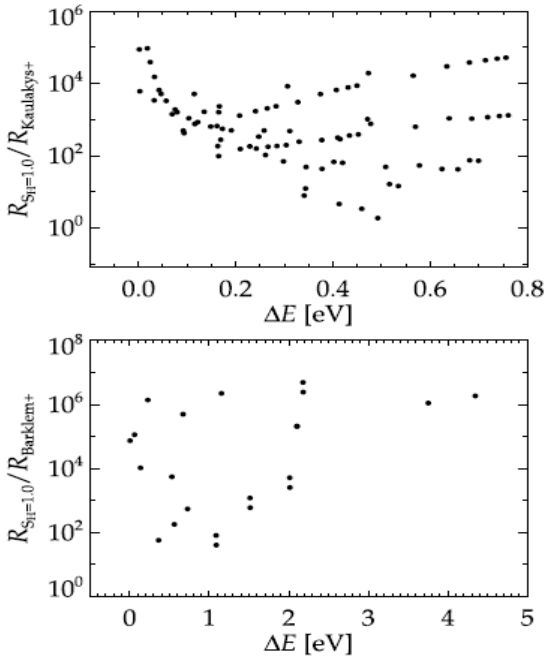
Guitou, Belyaev, Barklem, Spielfiedel, Feautrier, 2011

Comparison with approximative formulae

Drawin formula: extension of the classical formula for ionisation of atoms by electron impact, commonly used for allowed transitions
➔Gives collision rates proportional to the oscillator strength of the transition

Kaulakys formula: free electron model applicable to Rydberg atoms

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



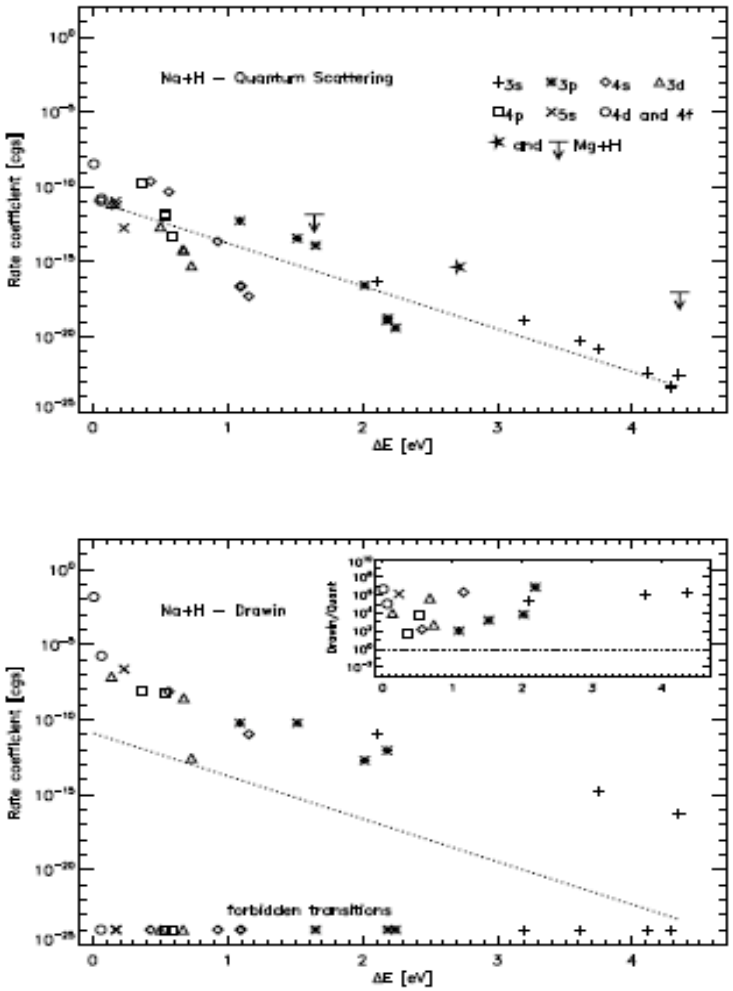
Lind et al. A&A 528, A103, 2011

➔ $R_{Drawin}/R_{Kaulakys}$

➔$R_{Drawin}/R_{quantum}$

The Drawin formula overestimates the rate coefficients by several orders of magnitude

Comparison with Drawin formula



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
- For forbidden transitions: the Drawin formula Is inapplicable
- Same trends found for Li+H and Mg+H collisions

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)

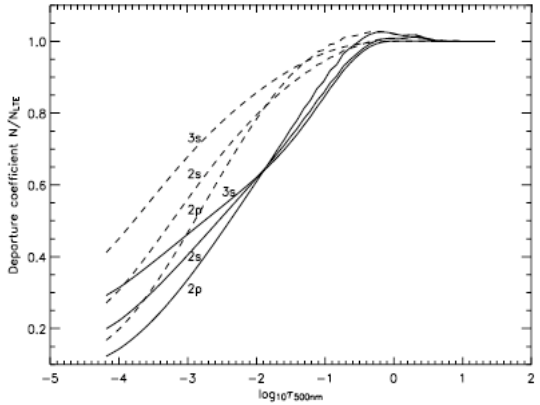
Li I line formation (code MULTI)

- 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

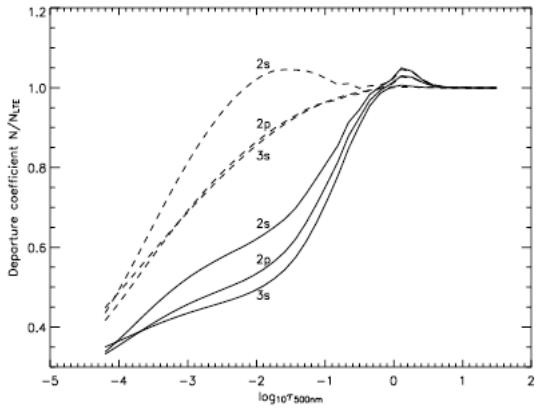
The analysis of the results show:

- 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

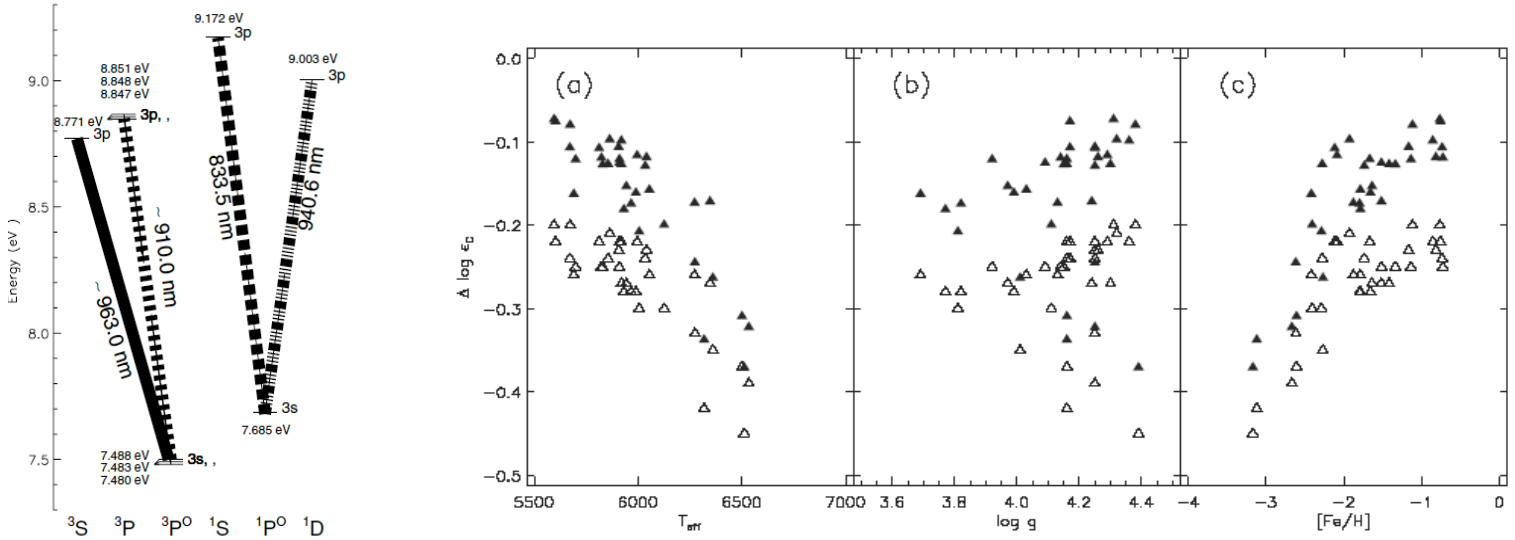
- For this resonance line, H-collisions have small effects for the Sun but larger effects for metal-poor stars due to ionisation/mutual neutralisation reaction
- Importance of 3D modelling versus 1D

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

Consequences on non-LTE modelling (5)

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 collisional non-LTE effect for this line between two excited states

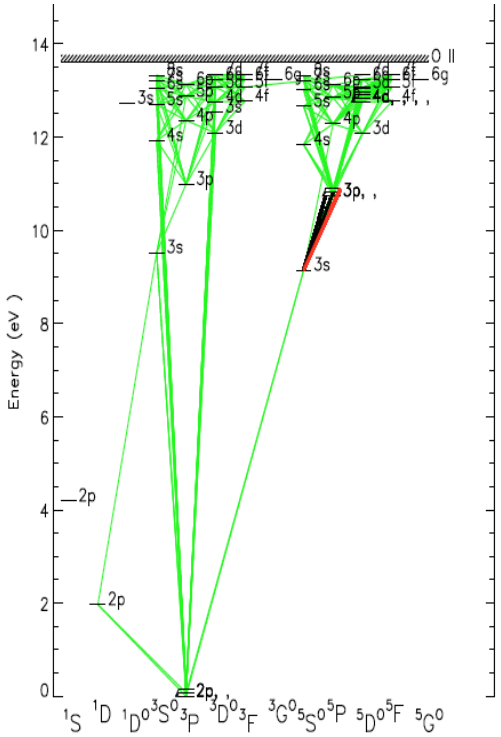
Fabbian, Asplund, Carlsson, Kiselman, A&A, 458, 899 (2006)

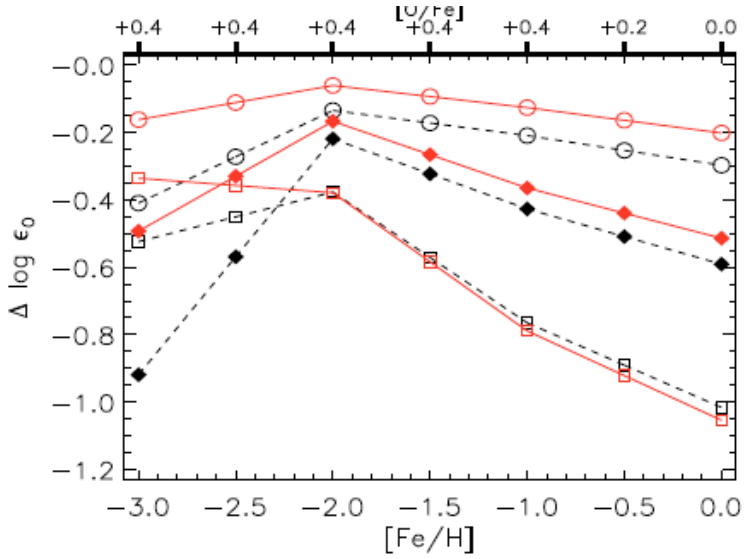
Consequences on non-LTE modelling (6)

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:
Circles: Teff=5780K, log g=4.44; triangles: 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)

Concluding remarks

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

• importance of 1D/3D modelling

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

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

• 1D/3D modelling for Mg in progress (F. Thévenin, L. Bigot)

Acknowledgments

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