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S. Alba Villegas [a]; R. Freire Ferrero [b]
[a] Department of Astronomy and Astrophysics, University of Valencia, Burjassot (Valencia), Spain
[b] Observatoire Astrononmique, Strasbourg, France

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INFLUENCE OF ATOMIC DATA ON NON-LTE CHROMOSPHERIC MODELLING

S. ALBA VILLEGAS[1] and R. FREIRE FERRERO[2]

*[1] Department of Astronomy and Astrophysics, University of Valencia,
46100 Burjassot (Valencia), Spain
Observatoire Astronomique, Strasbourg, France*

The influence of various kinds of atomic parameters on computed Mg II h and k line profiles is studied. For this purpose, we have run a non-LTE code on several versions of a Mg II model atom differing from one another in the quality and source of the atomic data employed, while keeping fixed the underlying atmospheric structure. With this simple setup we show that employing good quality atomic data is a necessary condition to obtain reliable atmosphere diagnostics. This is of interest in many fields of stellar astrophysics, e. g. semi-empirical chromospheric modelling in our case, but also when modelling external velocity fields, circumstellar/interstellar absorption, etc. and so these data deserve special attention.

KEY WORDS   Stars: chromospheric modelling; lineformation: Mg II h and k lines

1   INTRODUCTION

The resonance lines of Mg II – k ($\lambda 2795.5$Å) and h ($\lambda 2802.7$Å) – are powerful, widely used diagnostics of the physical conditions existing in chromospheres of late-type stars. Proper modelling of these lines requires the use in the line-profile computations of atomic data of good quality for this ion. This potential source of uncertainty in non-local thermodynamic equilibrium (non-LTE) chromospheric modelling has not been paid much attention in the past. For Mg II simple, approximate formulae coexist in the literature with comprehensive theoretical atomic data. The computation of the latter made use of state-of-the-art quantum mechanics tools and sophisticated numerical methods. In this paper we compare several h and k line profiles computed using different Mg II atomic data to study the influence of the atomic data used. We find that the non-LTE effects affecting the line core interact with the various atomic data sets employed to produce noticeable changes in the line core shapes, while the line wings remain unaffected. We conclude that reliable atomic data should always be used in order to disentangle the effects of uncertain atomic data from those caused by true astrophysical mechanisms.

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Table 1. Mg II energy levels

i	Configuration	$E_i(cm^{-1})$	g_i
1	3s $^2S^e_{1/2}$	0.0	2.0
2	3p $^2P^0_{1/2}$	35669.31	2.0
3	3p $^2S^0_{1/2}$	35760.88	4.0
4	4s $^2S^e_{1/2}$	69804.95	2.0
5	3d $^2D^e_{5/2}$	71490.19	6.0
6	3d $^2D^e_{3/2}$	71491.06	4.0

Table 2. Radiative bound-bound transitions

Transition	$\lambda_{vac}(nm)$	f_{lu}
3p $^2P^0_{1/2}$-3s $^2S^e_{1/2}$	280.27	0.310
3p $^2S^0_{3/2}$-3s $^2S^e_{1/2}$	279.55	0.620
4s $^2S^e_{1/2}$-3p $^2S^0_{3/2}$	293.65	0.151
4s $^2S^e_{1/2}$-3p $^2P^0_{1/2}$	292.86	0.151
3d $^2D^e_{3/2}$-3p $^2P^0_{1/2}$	279.08	0.945
3d $^2D^e_{5/2}$-3p $^2S^0_{3/2}$	279.80	0.8505
3d $^2D^e_{3/2}$-3p $^2S^0_{3/2}$	279.79	0.0945

2   CALCULATIONS

Atomic model:

We have restricted ourselves to a Mg II model atom consisting of six bound levels (Table 1) and the seven allowed line transitions between them (Table 2). The influence of higher lying levels on the present results has not been explored yet, but the present model serves well our aim of illustrating the effects of varying atomic data on the resulting line profiles. The next ionization stage of magnesium is represented in our model by its ground level.

Once the number of bound levels, bound-bound transitions (lines) and bound-free transitions (continua) in the atomic model have been set, there exist several kinds of atomic data to play with: (1) for bound levels: level energies, photoionization cross-sections and collisional ionization cross-sections; (2) for bound-bound transitions: oscillator strengths, line broadening parameters and collisional excitation cross-sections. We have not paid the same attention to all of these data types. Since collisional excitation rates play a major role in non-LTE chromospheric line formation, we centred our study on them, while keeping the other atomic data types fixed through the runs (with the exception of photoionization cross-sections, see below). The data considered are thus as follows: *level energies* are from the compilation by Martin and Zalubas (1980) (Table 1). *Oscillator strengths* for the lines considered were taken from TOPBASE (Cunto and Mendoza, 1992) (Table 2).

Table 3.   Summary of MULTI runs performed

Run	Source for photoionization cross-sections	Source for electron collision cross-sections	Treatment of line formation
1	Topbase	Mendoza (1981)	CR
2	hydrogenic	Blaha (1972)	CR
3	hydrogenic	Van Regemorter (1962)	CR
4	Topbase	Mendoza (1981)	PR
5	hydrogenic	Blaha (1972)	PR
6	hydrogenic	Van Regemorter (1962)	PR

Photoionization cross-sections have little influence on the shape of the h and k line profiles. Nevertheless, for the sake of illustration two radically different approaches were followed: (1) the comprehensive quantum mechanical computations from the TOPBASE project, and (2) the simple hydrogenic approximation – (i. e. a ν^{-3} dependence) – which while being frequently used, its use is physically unjustified for Mg II. Collisional ionization rates are not found to cause noticeable changes in the line profiles, and therefore the same simple approximation (Mihalas, 1978) was used in all the runs. *Line broadening parameters* are as follows: natural line broadening was computed following Gray (1992). Stark broadening was taken from Chapelle and Sahal-Bréchot (1970) for the resonance transitions, whereas for the subordinate lines the approximate formula by Cowley (1971) was used. Broadening by H I and He I was taken into account by using the classical Unsöld formulation without enhancement factors. The *collisional excitation rates* were obtained from three sources (enumerated in order of sophistication): (1) the simple, empirical formula by Van Regemorter (1962); (2) approximate quantum mechanical calculations by Blaha (1972); and (3) comprehensive close-coupling quantum-mechanical calculations by Mendoza (1981). The uncertainty of the theoretical calculations is generally more difficult – sometimes impossible – to assess than that of experimentally measured data. Nevertheless, in the case of the data computed by Mendoza it should be quite reliable, since these collisional rates may be regarded as the most precise on physical grounds that are available.

A well-known, but otherwise irrelevant, underlying atmospheric model was used (VAL3C; Vernazza *et al.*, 1981). The magnesium abundance relative to hydrogen was taken equal to 4×10^{-5}. The program MULTI was used to perform the non-LTE calculations for the different Mg II model atoms. Two series of runs were performed: one using complete redistribution in line frequency (CR) (Carlsson, 1986) for the h and k line computations, and other using partial redistribution (PR) (Uitenbroek, 1989). Three runs within either series were performed which differed in the particular set of atomic data conforming the Mg II model atom used in the calculations, as seen in Table 3. The special coupling between photoionization data and collisional excitation rates that can be noticed in the run setup was made on purpose in order to enhance the possible differences between a precise model and
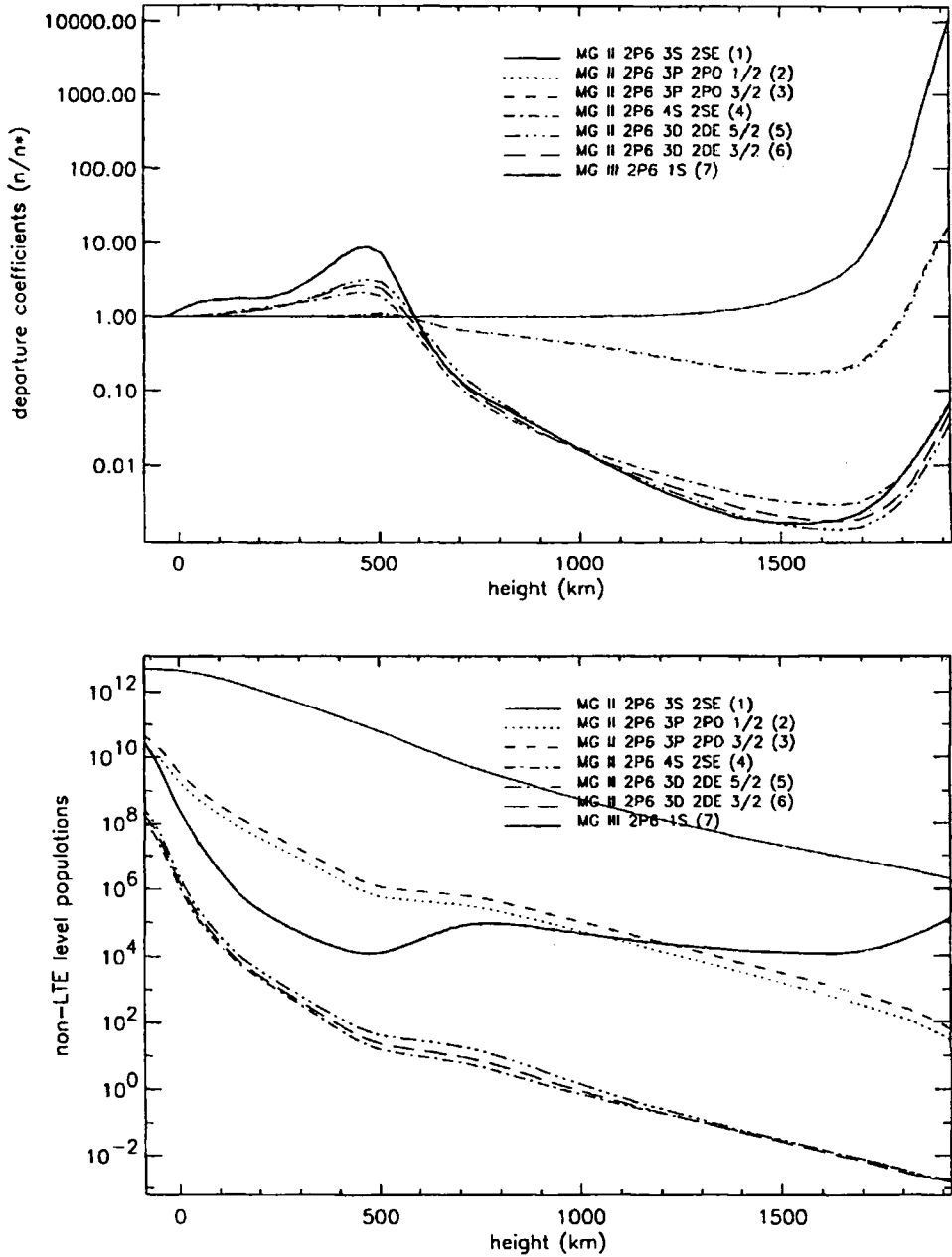
Figure 1 Atomic level populations (*bottom panel*) and departure coefficients (*top panel*) from a CR run using the collisional data from Mendoza.

a less precise one that could show up in the resulting line profiles. The subordinate lines were always treated in CR since PR effects are negligible.
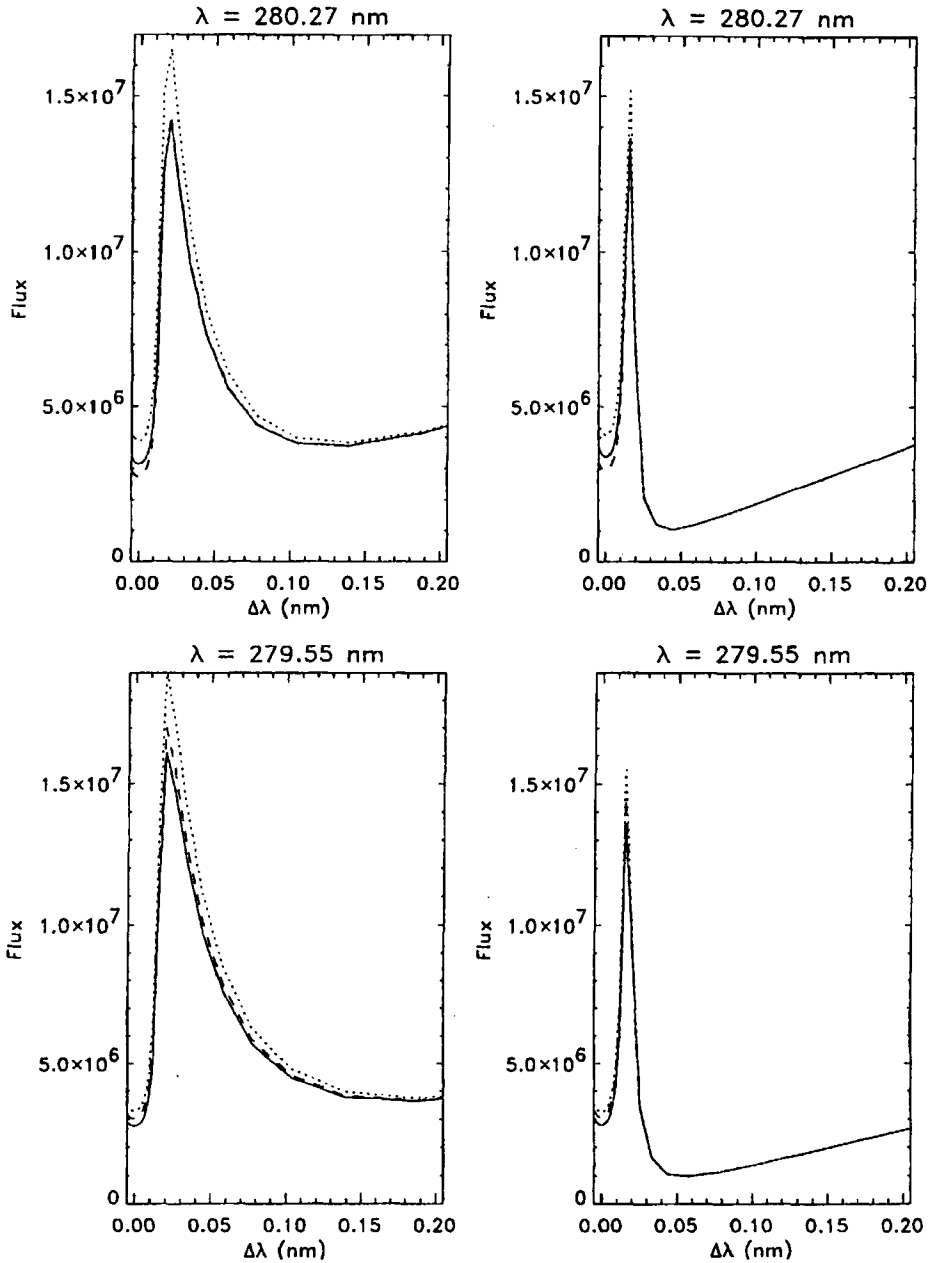
Figure 2a Computed line core flux profiles for the h (*top*) and k (*bottom*) resonance lines (*left pannels*, CR; *right pannels*, PR) using collisional data from Mendoza (*solid*), Blaha (*dots*) and van Regemorter (*dashes*).

The results of our computations are shown in Figures 1–3. Figure 1 shows the level populations and departure coefficients from LTE through the atmosphere for
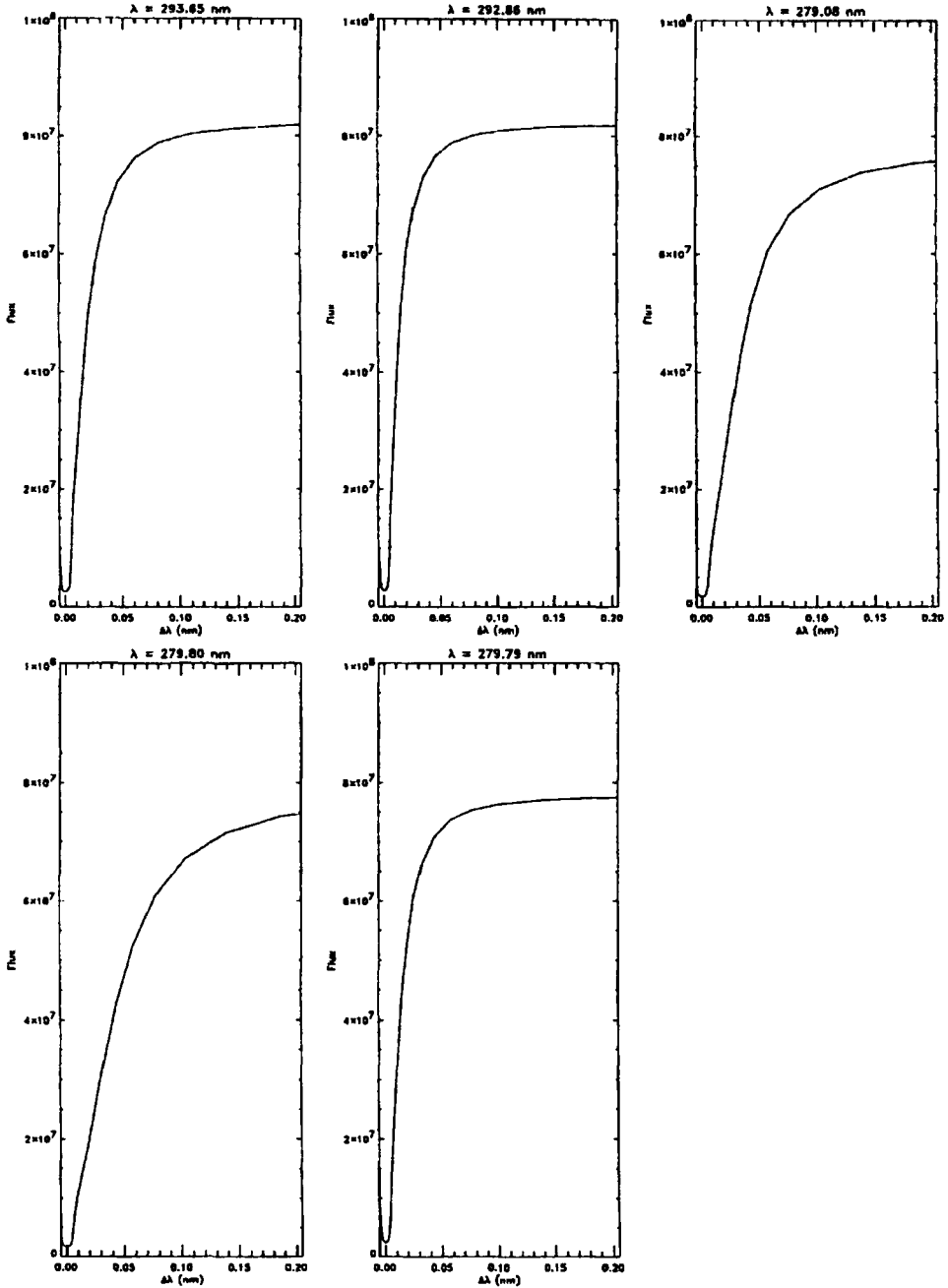
Figure 2b   Computed CR line core flux profiles for the five subordinate lines in our Mg II model. Note that all the profiles, which have been computed using collisional data from various sources (Mendoza, Blaha, Van Regemorter) appear merged together into a single profile.
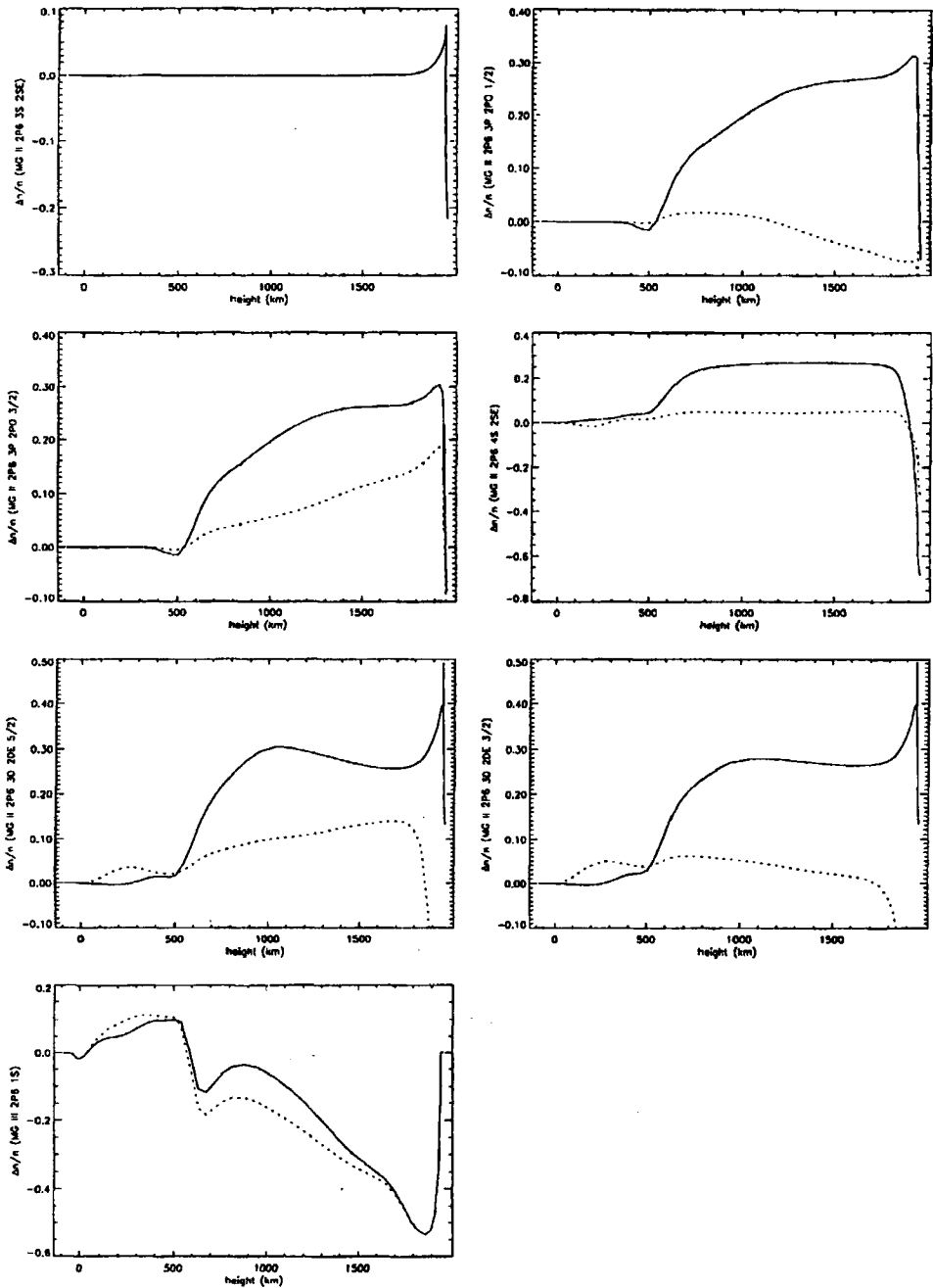
Figure 3 Differences in atomic level populations relative to those from the Mendoza run (*solid*, $\frac{n_{Blaha}-n_{Mendoza}}{n_{Mendoza}}$; *dotted*, $\frac{n_{VanReg}-n_{Mendoza}}{n_{Mendoza}}$

the Mendoza runs which we take as the reference for the intercomparisons. In Figure 2 we have plotted the h and k line profiles for all the runs. Figure 2b shows the rest of the lines which do not vary appreciably from one run to another, owing to their LTE formation in the photosphere. Figure 3 shows for each level the differences in populations for each run relative to the Mendoza run which is again taken as standard.

3 DISCUSSION

This simple study shows that there *exist* differences in the line profiles when computed using different atomic data, and gives a rough idea of the magnitude of these differences, as displayed in Figure 2. It can be seen that line profiles computed using different collisional data display different emission peak intensities as well as different line core depths. The collisional rates by Mendoza give intensities a little different from the simple formulation by Regemorter, at least for the Mg II resonance lines studied here. It can also be seen that the line profiles are influenced by the collisional data somewhat differently in the CR and PR approaches. The PR profiles change the relative height of the peak and core of the lines relatively little, whereas the CR profiles show stronger peak height variations – while the relative differences in core heights are very similar to the PR case – as well as flux enhancement widespread away from the peak which does not appear in the PR profiles.

It is we notice that, since in the case of late-type stars we have to deal necessarily with integrated light, it can be argued that the differences in line profiles found here and attributable to the use of different atomic data may well wash out owing to various effects (for example, when convolving the computed line profiles with the stellar rotation profile). Nevertheless, at least in the solar case the results of this work are still useful and can be used as a test of line formation mechanisms and chromospheric conditions through high-resolution, high detail spatial observations of the Sun.

It is striking that the application of the Van Regemorter formula – which was deduced using a very limited set of heterogeneous data for several atomic species – results in Mg II level populations that are closer to the Mendoza populations than those from the Blaha quantum-mechanical calculations (Figure 3) which, while being quantum mechanical in nature like the Mendoza data, are less sophisticated that these latter ones.

4 CONCLUSION

To conclude we point out that, owing to the differences in line profiles and level populations (to cite just two cases) arising from different atomic data, it is advisable that, in order to perform a good chromospheric diagnostic *the best available*

atomic data should be used in order to suppress as much as possible this source of uncertainty in our computations. Generally speaking, for a particular line to model in non-LTE, we are not sure *a priori* whether a highly simplified approach to the atomic data being used in the calculations will have similar effects on the computed line profile(s) as in the case of using more precise atomic data. The atomic physics community should collaborate by providing the accurate atomic data needed. Several cooperative projects (TOPBASE, OPACITY, IRON) are already underway.

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