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New method for fast and easy computation of radiative accelerations in stars

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ABSTRACT

Accurate determination of radiative accelerations of the elements is critical when studying atomic diffusion in stars. However, the computing time necessary to calculate these accelerations can become prohibitive because large atomic and opacity data bases are required. Parametric equations of radiative accelerations due to both bound–bound and bound–free transitions, valid at large optical depths, are presented for the following trace elements: C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca and Fe. These equations can easily be implemented in existing astrophysical applications without requiring large computing resources.

Key words: diffusion – stars: abundances – stars: chemically peculiar.

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1 INTRODUCTION

Precise determination of radiative accelerations ($g_{\rm rad}$) of the elements caused by momentum transfer following photoexcitation or photoionization is an essential ingredient in the study of elemental diffusion in stars. These accelerations depend primarily on the capacity of the ions to absorb photons from the radiative flux.

In certain stars (especially chemically peculiar stars) there exist stellar regions that are hydrodynamically stable enough so that diffusion of the elements can occur (Michaud 1970). The elements can then be stratified with depth and this stratification can affect the structure and evolution of these stars (e.g. Turcotte, Richer & Michaud 1998). In certain stars, diffusion can be important in the atmosphere and can even modify its physical structure (Dreizler & Wolff 1999; Hui-Bon-Hoa, LeBlanc & Hauschildt 2000; LeBlanc 2003).

This paper is the third of a series that aims to simplify the calculation of $g_{\rm rad}$ as compared to other methods such as opacity sampling (Seaton 1997; Richer et al. 1998; LeBlanc, Michaud & Richer 2000) or the so-called GLAM method (Gonzalez et al. 1995). In the first paper (Alecian & LeBlanc 2000, hereafter Paper I) of the series, the behaviour of $g_{\rm rad}$ was studied in order to better understand its properties and to guide us in the development of new approximate formulae of $g_{\rm rad}$ which are written in a parametric form. These formulae, published in Alecian & LeBlanc (2002, hereafter Paper II), and which are valid for trace elements at large optical depths, were improvements of the bound–bound formula of Alecian (1985) and Alecian & Artru (1990) and those due the bound–free transitions of Alecian (1994). The improvements stemmed from the use of detailed monochromatic opacities instead of Rosseland mean opacities. These new formulae depend on a number of parameters that will be calculated for the elements which the atomic data are provided by the Opacity Project (Seaton et al. 1992) through TOPBase (Cunto et al. 1993). These elements are C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca and Fe. Some of the parameters are calculated with the atomic data (see the discussion about the single-valued parameter (SVP) approximation in Paper II) while others are obtained by fitting our $g_{\rm rad}$ to those of Seaton (1997).

The aim of this paper is to furnish the values of the parameters which are found in the new approximate formulae for each ion of the elements considered here. This will enable users to easily include $g_{\rm rad}$ in their astrophysical applications, such as evolutionary models. We will first briefly describe the theory behind these new formulae. We will then explain the method used to obtain the values of the parameters found in these formulae and show results of our $g_{\rm rad}$ compared to those of Seaton (1997). We will also give the values of these parameters for Fe in a $T_{\rm eff} = 10\,000$ K stellar model. The data for the other elements and for other stellar models will be made available on the internet. A short conclusion will then be presented.

2 THEORY

In Paper II, parametric equations were developed for the bound–bound transitions by generalizing the treatment of Alecian & Artru (1990) and Alecian (1985). These equations aim to separate the terms depending explicitly on the atomic data from those depending on the concentration of the ion i under consideration. The proposed approximate formula (using the SVP approximation; see below for more details) is

$$g_{i,\rm line} = q\varphi_i^* \left(1 + \xi_i^* C_i\right) \left(1 + \frac{C_i}{b\psi_i^{*2}}\right)^{\alpha_i} \quad (1)$$

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where

$$q = 5.575 \times 10^{-5} \frac{T_{\rm eff}^4}{T} \left(\frac{R}{r}\right)^2 \frac{1}{A} \tag{2}$$

and

$$b = 9.83 \times 10^{-23} \frac{N_{\rm e} T^{-1/2}}{X_{\rm H}}. \tag{3}$$

Here, $T_{\rm eff}$ and R are the effective temperature and radius of the star, T and r are the local temperature and radius, $N_{\rm e}$ is the electronic density, $X_{\rm H}$ is the hydrogen mass fraction, A is the atomic mass in atomic units of the species under consideration and C_i is the concentration (in number) of the ion relative to hydrogen. The parameters $\varphi_i{}^*$, $\psi_i{}^*$ and $\xi_i{}^*$ are the values of φ_i, ψ_i and ξ_i (see equations 10–15 and section 3.3 of Paper II for more details) calculated where the population of ion i is close to its maximum. We will refer to this layer by its temperature $T_{\rm ion}(i)$ defined in Section 3.1. The SVP approximation (see Paper II for more details) simplifies the original equations in which all three parameters are calculated at each structure point. These parameters are obtained using the Opacity Project (Seaton et al. 1992) atomic data available through the TOPBase data base (Cunto et al. 1993). The parameter φ_i is related to the oscillator strengths of the transitions of the ion, ψ_i to their linewidths that primarily controls saturation, and ξ_i is an additional parameter introduced in Paper II that also affects saturation and appears when monochromatic opacities are considered in the development of the approximate formula for the $g_{\rm rad}$ due to bound–bound transitions. The value α_i, which is -0.5 in the case of pure Lorentzian line profiles, will be calculated by fitting our parametrized $g_{\rm rad}$ to those calculated by opacity sampling (Seaton 1997). This parameter also strongly affects saturation.

The $g_{\rm rad}$ due to bound–free transitions differ from those due to lines because the momentum acquired during photoionization is transferred to the newly ionized ion; the acceleration of the neutral species ($i = 0$) is zero while the momentum of the completely ionized ion is not. An approximate equation for the bound–free transitions based on that found by Alecian (1994) was also developed in Paper II. The main crux of this approximate formula is that it assumes that photoionization cross-sections follow a power law close to the hydrogenic case. Neglecting the momentum taken away by the electron during photoionization (e.g. Massacrier 1996), the radiative acceleration due to bound–free transitions for charged ions ($i > 0$) can be approximated by

$$g_{i,\rm cont} \approx 7.16 \times 10^{-26} \frac{N_{\rm e} T_{\rm eff}^4}{T^{3/2}} \left(\frac{R}{r}\right)^2 \frac{1}{Ai^2} \Theta_i, \tag{4}$$

where

$$\Theta_i \approx a_i \frac{N_{i-1,0} p_{i-1}}{N_{i-1} p_i g_0} \sum_k n_k g_k Q_k \tag{5}$$

and

$$Q_k \approx u_k^3 \left[\frac{u_k}{1 - {\rm e}^{-u_k}} - {\rm e}^{u_k} \ln(1 - {\rm e}^{-u_k}) \right]. \tag{6}$$

Here, $N_{i-1,0}$ is the number density of the ground level of the ion $A^{+(i-1)}$ and N_{i-1} is the number density of this ion, p_i is the partition function of A^{+i}, n_k and g_k are respectively the main quantum number and the statistical weight of energy level k of $A^{+(i-1)}$ and u_k is evaluated at the ionization threshold frequency from level k where $u = h\nu/kT$. The factor a_i has been introduced to correct possible discrepancies with respect to hydrogenic cross-sections. Its value will be determined by fitting the accelerations of the approximate formulae to those of Seaton (1997). In equation (5), Θ_i is written assuming $\overline{\kappa}_{\rm med}/\kappa_{{\rm med},k} = 1$ as prescribed by the SVP approximation and where these are opacities also defined in Paper II (see equations 1 and 2 of Paper II). This approximation renders the present equations more easily usable because the monochromatic opacities are not needed to evaluate Θ_i. Because Θ_i depends strongly on temperature, it will have to be evaluated at each structure point where needed and thus its value will not be given here. In order to simplify its calculations, the atomic levels were grouped together as described in Alecian, Michaud & Tully (1993). The atomic data of these grouped levels will be made available by the authors to future users.

The total radiative acceleration for element A is a weighted sum of the accelerations of the various ions and can be expressed as

$$g_{\rm tot} = \frac{\sum_i w_i N_i (g_{i,\rm line} + g_{i,\rm cont})}{\sum_i w_i N_i}. \tag{7}$$

The weights w_i were set equal to 1 in Paper II, but they should involve diffusion coefficients if the effect of the mobility of the ions and redistribution of momentum among the ions are to be taken into account. Generally, $w_i = 1$ is well justified in the domain of validity of the SVP approximation. More details concerning the importance of these effects on $g_{\rm rad}$ can be found in Montmerle & Michaud (1976) and Gonzalez et al. (1995).

3 APPLYING THE SVP APPROXIMATION

3.1 Calculating procedure

The SVP approximation is based on two main assumptions. The first is that the contribution of ions to the total acceleration given by equation (7) is maximum around the point where they have their maximum of population (see the definition of $T_{\rm ion}$ in Section 2 and in equation 8). The second assumption is that φ_i, ψ_i and ξ_i vary smoothly around that point (Alecian & Artru 1990). We have first tried to set $T_{\rm ion}(i)$ to be exactly the temperature of the layer where the relative population of ion i reaches its maximum. However, we have found that the following choice gives better results (the summation index l denotes the model layers):

$$\log T_{\rm ion}(i) = \frac{\sum_l N_{i,l} \log T_l}{\sum_l N_{i,l}}. \tag{8}$$

The layer which is finally chosen to compute the parameters $\varphi_i{}^*$, $\psi_i{}^*$ and $\xi_i{}^*$ is the one in which the temperature is the closest to $T_{\rm ion}(i)$ given by equation (8). This layer is generally the one where the relative population of ion i is maximum when its relative population varies with respect to $\log T$ more or less symmetrically around its maximum. However, this layer is significantly displaced when there is strong asymmetry, namely for ions adjacent to the one with noble gas configuration. We have also found that the SVP approximation gives better results if the weights of ions with noble gas configurations are increased in equation (7): the weights w_i are kept equal to 1, except for ions with noble gas configurations where they are set to 1.5. This correction is needed because when a noble gas configuration has a large ionization fraction, the ionization fraction of the neighbouring ion is not necessarily negligible. Because the values of the parameters for this neighbouring ion are calculated at its $T_{\rm ion}$, its $g_{\rm rad}$ is not precise where the noble gas configuration ion is at its maximum population.

The parameters $\varphi_i{}^*$, $\psi_i{}^*$ and $\xi_i{}^*$ involved in the approximate equation for accelerations due to bound–bound transitions were calculated for each ion considered at the temperature point nearest to

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$T_{\rm ion}(i)$ in various stellar models and assuming that elements are overabundant (by +1 dex for C, N, O and Fe, and +2 dex for the others). We chose to use the values of these parameters evaluated at these large abundances because the saturation effects are more important there and we therefore obtain better results. Even though it would be preferable to have only one set of parameters that could be used for any stellar model, more accurate results are obtained when they are calculated in a model close to the one in which the parametrized $g_{\rm rad}$ will be applied. This is mainly due to the dependence of $T_{\rm ion}(i)$ on the stellar structure, because electronic density at a given temperature is strongly dependent on the stellar model. The values of these three parameters will be made available to users.

As mentioned above, in the case of pure Lorentzian line profiles the value of α_i is -0.5 (the default value), but, as discussed in Paper I, the behaviour of real ions may be far from the ideal one. To obtain more precise $g_{\rm rad}$, the value of this parameter will be determined by fitting our approximate $g_{\rm rad}$ to those of Seaton (1997).

For the bound–free transitions, the value of Θ_i must be calculated at each point at which radiative accelerations are required. These values will not be given here. An additional parameter a_i, which is needed to calculate Θ_i, remains. This empirical parameter was included in equation (6), and therefore in equation (5), to partially correct for the approximate ionization cross-sections used. The value of a_i ($a_i = 1$ by default) will also be determined by fitting and will be given here.

3.2 Determination of α_i and correcting factors

The fitting procedure was performed in a straightforward way in which the accelerations were calculated on a grid of values of α_i and a_i. The chosen grid was such that $-0.5 \leqslant \alpha_i \leqslant -0.1$ (see figs 4, 5 and 6 in Paper I) and $0.1 \leqslant a_i \leqslant 2.0$. For the initial iteration, $g_{\rm rad}$ was calculated for the element under consideration with $\alpha_i = -0.5$ and $a_i = 1$ for all ions. New values of $g_{\rm rad}$ were then computed for each set of values of α_i and a_i for the first ion at the point in the model under consideration with temperature nearest to its $T_{\rm ion}(i)$. A pair of α_i and a_i was then chosen for this ion such that the error of $g_{\rm rad}$ of the element for a given abundance (see below) was at its minimum as compared to the $g_{\rm rad}$ given by Seaton (1997). This minimization was then repeated for each ion of the element in order to obtain their α_i and a_i values. The fit was carried out at a solar abundance for the elements C, N, O and Fe and at an abundance of +1 dex (relative to its solar value) for the other elements, because the saturation effects of the $g_{\rm rad}$ due to lines are more important at large abundances and it is thus more critical to have a proper fit there. This whole procedure was then repeated until the variation of the average error per structure point of the stellar model from one iteration to the next was less than 10^{-3} dex. This was done for each element considered here.

Although the fitted $g_{\rm rad}$ are much better than those with $\alpha_i = -0.5$ and $a_i = 1$, the fit for certain elements is still not satisfactory. This is partly due to the fact that in the approximate formula of Alecian (1994) for the acceleration due to bound–free transitions, it was supposed that it is independent of concentration. Because this supposition is not true, especially for abundant elements, an additional empirical term, which mimics saturation effects, was added to equation (4):

$$g_{i,\rm cont} \approx [g_{i,\rm cont}]_{\rm eq.\ 4} \left(\frac{\chi}{1+\chi}\right)^{b_i}. \qquad (9)$$

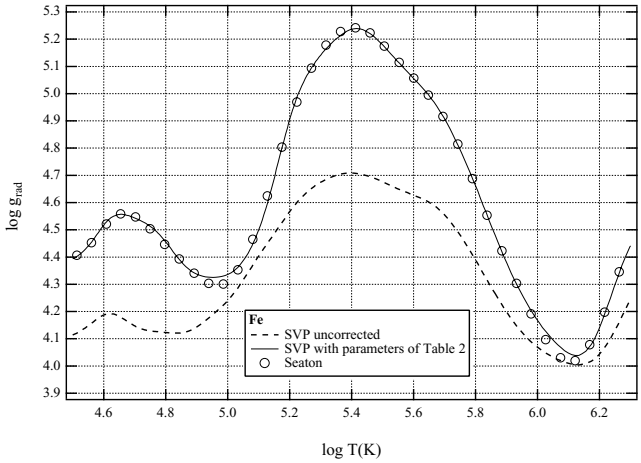

Figure 1. Comparison of Fe radiative accelerations at solar abundance in a $T_{\rm eff} = 10\,000$ K, $\log g = 4.3$ model. The logarithms of acceleration are plotted versus $\log T(K)$. Open circles represent the $g_{\rm rad}$ found by Seaton (1997), the dashed line represents the $g_{\rm rad}$ using our parametric formulae assuming $\alpha_i = -0.5$, $a_i = 1$ and $b_i = 0$ (no correction), while the solid line gives the acceleration calculated with the fitted values of α_i, a_i and b_i of Table 2, and with $w_i = 1.5$ for noble gas configurations.

Here, χ is the abundance of the element relative to its solar value in number and b_i (not to be confused with the coefficient defined by equation 3) are negative valued empirical parameters that are determined by fitting. This formula was chosen because it tends to 1 when χ is large, which is desired because the parameters α_i and a_i are determined at high abundances (i.e. $\chi = 10$). The value of b_i for each ion was obtained by fitting $g_{\rm rad}$ at abundances from -2 to +1 dex within the range $-2 \leqslant b_i \leqslant 0$ similarly to the procedure followed to obtain the values of α_i and a_i.

3.3 Results

Fig. 1 shows a comparison between $g_{\rm rad}$ before any correction and those with $w_i = 1.5$ for noble gas configuration, while using the fitted values of α_i, a_i and b_i in a $T_{\rm eff} = 10\,000$ K, $\log g = 4.3$ model from Richer & Michaud (1993). The improvement shown in Fig. 1 for iron at solar abundance is among the most spectacular, but the accelerations of all the elements are improved by this procedure. Table 1 shows the average error of the fitted $g_{\rm rad}$ on the structure

Table 1. Average error (in dex) for $g_{\rm rad}$ in a $T_{\rm eff} = 10\,000$ K, $\log g = 4.3$ model for various values of $\log \chi$.

	$\log \chi$			
Element	−2	−1	0	1
C	0.0701	0.0785	0.0657	0.2242
N	0.1036	0.0709	0.0452	0.1567
O	0.0623	0.0482	0.0238	0.1784
Ne	0.0855	0.1084	0.0470	0.0270
Na	0.1016	0.1567	0.0655	0.0519
Mg	0.1419	0.1240	0.0476	0.0365
Al	0.1085	0.1030	0.0419	0.0496
Si	0.1080	0.1132	0.0437	0.0142
S	0.0395	0.0792	0.0362	0.0211
Ar	0.0660	0.0404	0.0202	0.0085
Ca	0.1051	0.0842	0.0227	0.0147
Fe	0.0918	0.0478	0.0057	0.1066

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Table 2. Parameters for Fe in a $T_{\rm eff} = 10\,000$ K, $\log g = 4.3$ model (Fe1 corresponds to the neutral state).

Ion	$\varphi_i{}^*$	$\psi_i{}^*$	$\xi_i{}^*$	α_i	a_i	b_i
Fe1	0.00	0.00	0.00	−0.500	–	–
Fe2	0.00	0.00	0.00	−0.500	1.000	−2.000
Fe3	0.00	0.00	0.00	−0.500	1.000	−2.000
Fe4	3.73×10^{-1}	5.23	6.30	−0.350	1.200	0.000
Fe5	1.35	1.34	1.88×10^{1}	−0.325	1.450	0.000
Fe6	1.50	6.35×10^{-1}	2.08×10^{1}	−0.400	0.275	0.000
Fe7	2.14	6.51×10^{-1}	−3.10	−0.475	1.275	0.000
Fe8	1.38×10^{1}	1.71×10^{-1}	-4.59×10^{2}	−0.500	1.800	0.000
Fe9	1.90×10^{1}	1.53×10^{-1}	2.76×10^{2}	−0.300	0.100	0.000
Fe10	1.85×10^{1}	1.62×10^{-1}	1.20×10^{3}	−0.300	2.000	0.000
Fe11	1.06×10^{1}	2.33×10^{-1}	3.54×10^{3}	−0.200	0.100	0.000
Fe12	8.54	2.08×10^{-1}	4.37×10^{3}	−0.200	0.175	−0.775
Fe13	7.03	1.77×10^{-1}	8.72×10^{3}	−0.200	0.600	−0.825
Fe14	1.02×10^{1}	1.31×10^{-1}	1.45×10^{4}	−0.275	0.100	0.000
Fe15	1.08×10^{1}	4.84×10^{-2}	2.09×10^{4}	−0.350	2.000	0.000
Fe16	5.45	1.84×10^{-2}	6.26×10^{3}	−0.250	1.050	0.000
Fe17	9.97×10^{-1}	2.54×10^{-2}	4.48×10^{2}	−0.500	0.100	0.000
Fe18	7.16	1.20×10^{-2}	1.26×10^{3}	−0.400	0.300	0.000
Fe19	1.17×10^{1}	1.29×10^{-2}	3.10×10^{3}	−0.275	1.725	0.000
Fe20	1.28×10^{1}	1.36×10^{-2}	6.55×10^{3}	−0.500	0.475	0.000
Fe21	1.20×10^{1}	1.29×10^{-2}	7.13×10^{3}	−0.275	0.300	0.000
Fe22	9.94	9.78×10^{-3}	1.92×10^{4}	−0.500	0.100	0.000
Fe23	8.34	5.84×10^{-3}	2.81×10^{5}	−0.500	0.100	0.000
Fe24	4.24	2.59×10^{-3}	5.67×10^{6}	−0.500	0.100	0.000
Fe25	0.00	0.00	0.00	−0.500	1.000	0.000
Fe26	0.00	0.00	0.00	−0.500	1.000	0.000
Fe27	–	–	–	–	0.100	0.000

points of the model with $4.7 \leqslant \log T \leqslant 6.3$ as compared to those of Seaton (1997). These errors are less than 0.1 dex for most elements at most abundances within the range $-2 \leqslant \log\ \chi \leqslant 1$.

The calculated parameters $\varphi_i{}^*$, $\psi_i{}^*$ and $\xi_i{}^*$ as well as the fitted parameters α_i, a_i and b_i for Fe in the $T_{\rm eff} = 10\,000$ K model used here are found in Table 2. It should be emphasized that $\varphi_i{}^*$, $\psi_i{}^*$, $\xi_i{}^*$ and α_i are parameters that naturally appear in our $g_{\rm rad}$ equations, while a_i and b_i are correction factors added to partially correct $g_{\rm rad}$ following certain approximations made and thus produce more accurate results. Even though α_i is physically related to the line profiles, having a value of −0.5 for a pure Lorentzian profile, it was adjusted so other effects that were neglected in our equations, such as line blending, could be indirectly taken into account and so that our equations could then better reproduce the saturation of the lines.

Fig. 2 shows the accelerations obtained for all the elements considered, for several abundances, using the parameters calculated here. The value of these six parameters for other stellar models as well as the atomic data needed to calculate Θ_i can be found at http://www.umoncton.ca/leblanfn/grad. Subroutines enabling easy implementation of the $g_{\rm rad}$ equations shown here will also be made available.

4 CONCLUSION

This paper concludes the study started in Papers I and II. It provides a method and data allowing very fast computation of radiative accelerations in stars, preserving a reasonable accuracy. In addition to its numerical expediency, the SVP approximation is much easier to implement in codes because much less data are to be processed than by usual methods for computing radiative accelerations (see discussion in Paper II).

The SVP method described in Paper II has been improved in this paper by the addition of a correction factor related to the saturation of the acceleration due to photoionization and by increasing the weight of ions with noble gas configurations in equation (7). The SVP approximation consists of using equations (1), (7) and (9) with six tabulated parameters per ion. As an example, we provide these parameters for Fe in Table 2 for a $T_{\rm eff} = 10\,000$ K stellar model. This table, which is valid in the abundance range $-2 \leqslant \log\ \chi \leqslant 1$, should only be used in models with $T_{\rm eff}$ near 10 000 K. Similar tables including the other elements considered here and for other $T_{\rm eff}$ will be made available at http://www.umoncton.ca/leblanfn/grad, where we provide the complete tables in electronic form. These will be updated as soon as new atomic data or improved parameters are available.

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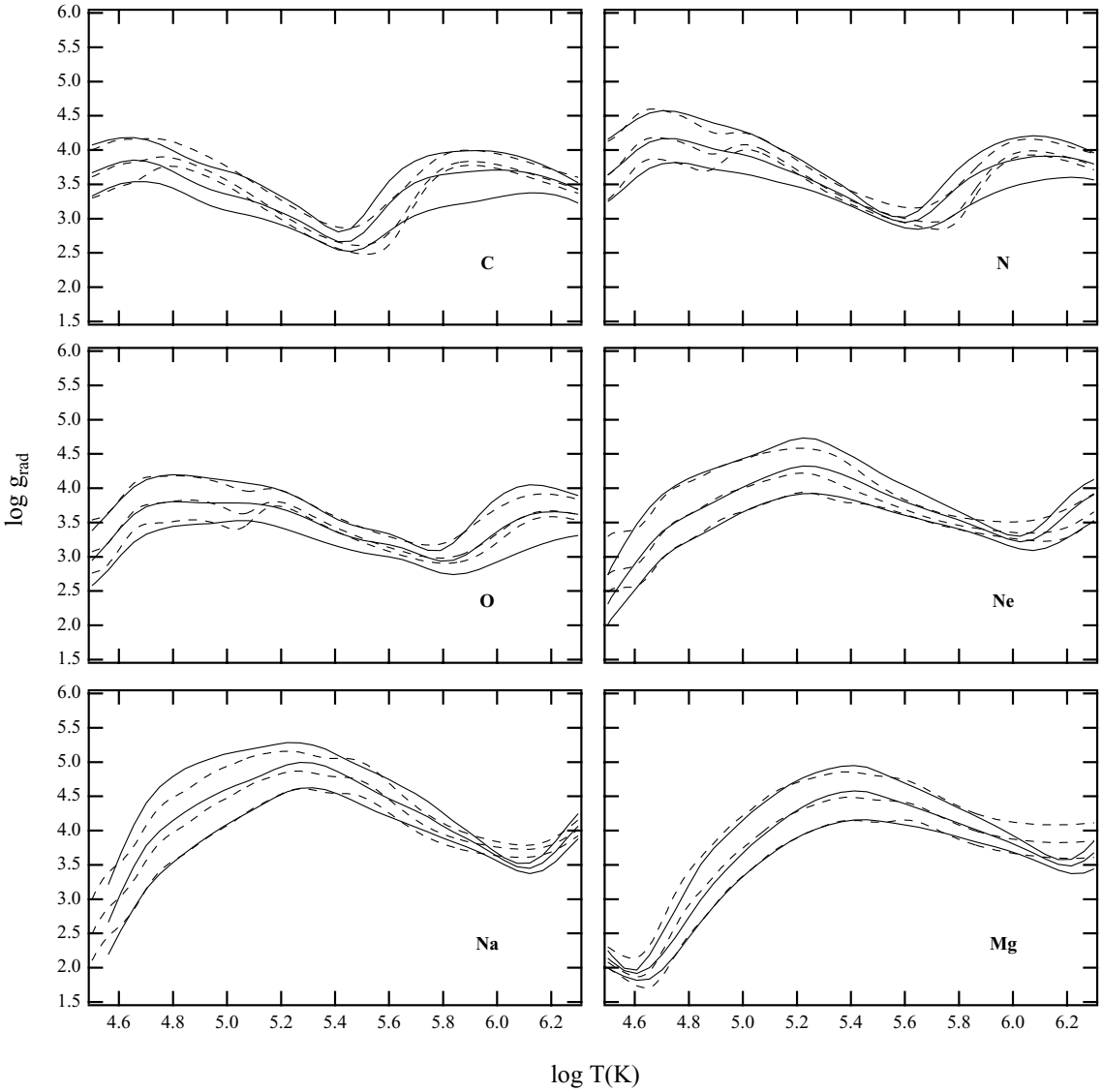

Figure 2. Radiative accelerations for all the elements considered in a $T_{\rm eff} = 10\,000$ K, $\log g = 4.3$ model. The logarithms of acceleration are plotted versus $\log T(K)$. The solid lines represent the $g_{\rm rad}$ found by Seaton (1997), the dashed lines those calculated with the fitted values of α_i, a_i and b_i, and with $w_i = 1.5$ for noble gas configurations. Three abundances are shown: $\log\ \chi = -1$, 0 and 1.

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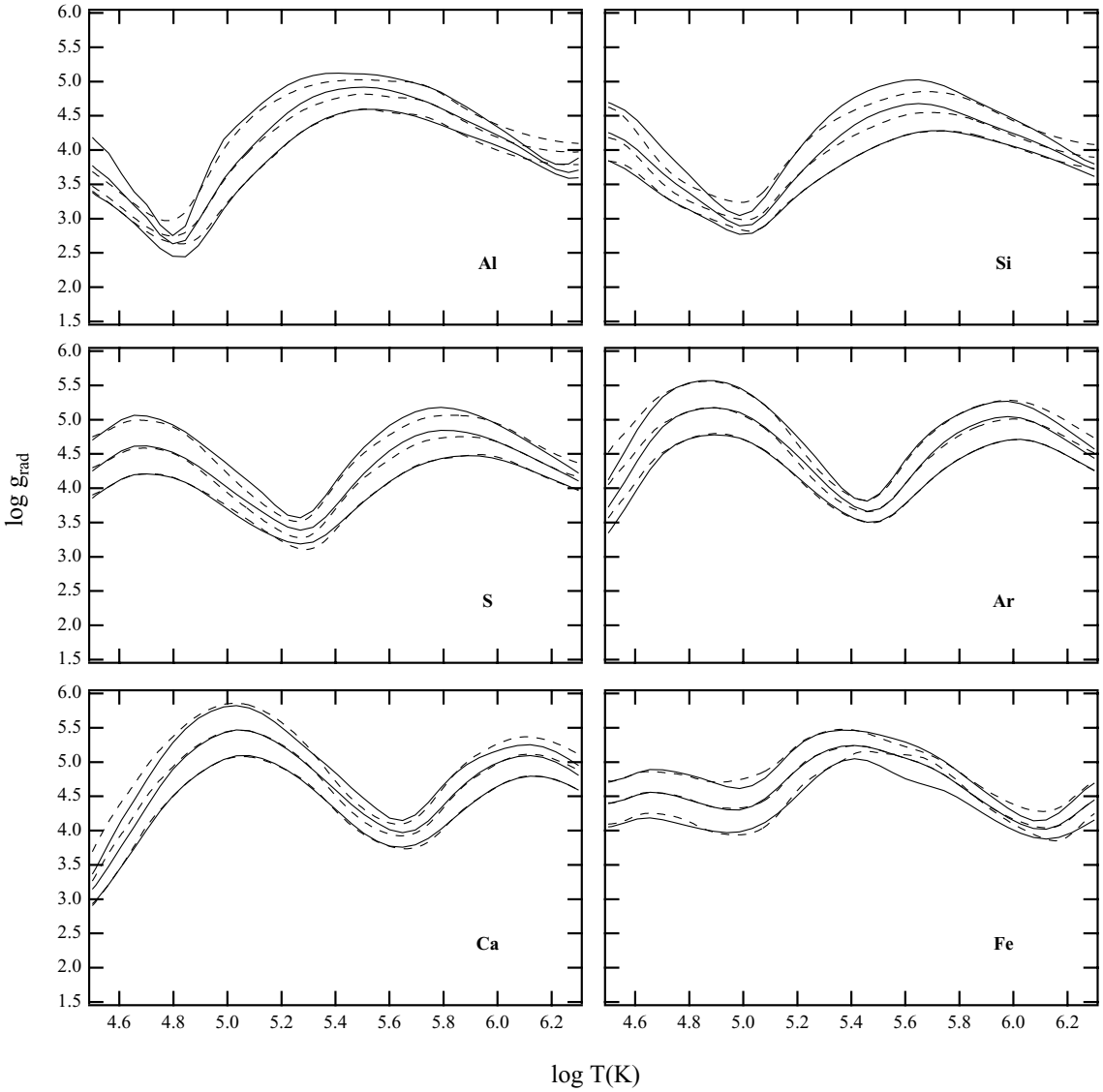

Figure 2 – *continued*

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