NEW ATOMIC DATA FOR Mg I LINES

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Abstract. Theoretical oscillator strengths are reported for transitions between excited terms of the singlet and triplet S, P, D, F and G manifolds of atomic magnesium. The principal quantum numbers of the jumping electron range from $n = 4$ to 100. The calculations are based on the Coulomb approximation. Low-n results, for which other data are available previously, agree reasonably well with the sophisticated calculations of Moccia and Spizzo (1988). Data for $^{1,3}F$–$^{1,3}G$ transitions may deviate from hydrogenic values by as much as 50%.

Key words: atomic data – infrared: stars – Mg I

1. Introduction

Absorption oscillator strengths for transitions in Mg I have been calculated by many authors, *e.g.*, Froese-Fisher (1975*a*,*b*), Victor *et al.* (1976), Moccia and Spizzo (1988, hereafter MS). In these works, the principal quantum numbers of the jumping electron are smaller than 10. Over the last decade, several lines of Mg I have been discovered in the far-infrared spectrum of the sun (*e.g.*, Brault and Noyes 1983; Chang and Noyes 1983; Jefferies 1991), and their study has become an important topic in solar physics. As the recent works of Hoang-Binh (1991) and Chang *et al.* (1991) have shown, investigations on the formation of these Rydberg lines require a large body of atomic data, in particular for principal quantum numbers $n \geq 10$. We report new calculations of multiplet oscillator strengths for transitions between excited terms of Mg I, for n up to 100. These data are required to compute radiative and collisional transition rates entering the statistical equilibrium equations, and are also relevant to the study of the line broadening (Hoang-Binh *et al.* 1987).

2. Theory

The multiplet absorption oscillator strength, for a transition between a lower term i and an upper term k, is given by (Wiese *et al.* 1969):

$$f(i,k) = (303.7/g_i\lambda)S_{i,k}, \tag{1}$$

where λ is the wavelength of the transition in Å, $S_{i,k}$ is the multiplet strength in atomic units (a.u.), and g_i is the statistical weight of the lower term. The strength of a transition $3s\,nl\,^{2S+1}L$ to $3s\,n'\,l'\,^{2S+1}L'$, involving no equivalent electrons, is, for $l' = l - 1$ (Goldberg 1939),

$$S(i,k) = (2S+1)(2L+1)l(2l-1)\sigma^2, \tag{2}$$

where

$$\sigma^2 = a_0^2\, e^2/(4l^2 - 1)\, R^2, \tag{3}$$

$$R = \int_0^\infty P_{n,l}(r)\, P_{n',l'}(r)\, dr, \tag{4}$$

D. M. Rabin et al. (eds.), Infrared Solar Physics, 347–351.

and n, n' and l, l' are the principal and azimuthal quantum numbers respectively of the jumping electron; S is the total spin and L, L' the total azimuthal quantum numbers, a_0 is the Bohr radius (1 in a.u.), and $P_{n,l}(r) and P_{n',l'}(r)$ are normalized radial eigenfunctions, in atomic units, of the jumping electron in the relevant configurations.

Thus, the calculation of $f(i,k)$ reduces to that of the integral R. For $n, n' \geq 10$, it is justified to use the Coulomb approximation, for which (Hoang-Binh *et al.* 1979)

$$P_{n,l}(r) = z^{1/2} K(\nu, l) W_{\nu,l+1/2}(2\rho/\nu), \tag{5}$$

where z is the effective charge, ν is the effective quantum number, $\rho = z r$, and $W_{\nu,l+1/2}$ is the Whittaker function. The normalizing factor is (Seaton 1958)

$$K(\nu, l) = [\zeta(\nu) \nu^2 \Gamma(\nu + l + 1) \Gamma(\nu - l)]^{-1/2}. \tag{6}$$

Provided ν is not too small, $\zeta(\nu) \approx 1$; here we shall take $\zeta(\nu) = 1$ and use the analytical formula given by Hoang-Binh *et al.* (1979) to calculate R. The quantum defects have been calculated, using either the term positions of Bashkin and Stoner (1975) (for n, n' up to ≈ 8), or the extended Ritz formulae given by Risberg (1965) for larger values of n, n'. For ^1D terms, values for large n have been obtained by extrapolation of Risberg's values; $^{1,3}G$ terms are taken to be hydrogenic.

3. Results and Discussion

Calculations have been performed for transitions between the $^{1,3}S, ^{1,3}P^0, ^{1,3}D$, and $^{1,3}G$ manifolds. The principal quantum numbers of the jumping electron range from 4 or 5 to 100. Although we are mainly interested in the domain $n, n' \geq 10$, where data are generally not available, lower terms have been considered for the sake of self-consistency and for comparison with other theoretical results. The full results will be published elsewhere. Here, we show only the trends of f-values for large n and Δn. Let the principal quantum numbers of the upper and lower terms be denoted by m and n respectively; and $\Delta n = m - n$. Figure 1 displays an example of the typical behavior of the oscillator strength with respect to Δn (for n fixed), and indicates that interpolation or extrapolation are possible. An exception concerns the transitions $np\ ^1P - md\ ^1D$, for which the variation of f as a function of Δn is not monotonic for $n < 10$. In general, it is found that $f \sim 1/(\Delta n^\gamma)$, with $\gamma \approx 2.7$ in the limit of large Δn, while f is approximately linear with respect to n in the limit of large n.

To our knowledge, the most extensive body of theoretical data on Mg I has been given by MS, who considered only $n, n' \leq 9$. The agreement of our results with these sophisticated calculations is excellent in some instances, *e.g.*, for the transitions $np\ ^1P - ms\ ^1S$ (see Table 1). This is somewhat surprising, and probably fortuitous, since we do not expect the Coulomb approximation to be very good for transitions involving low n and strongly core-penetrating orbits. One the other hand, a few large discrepancies may be also noted (*e.g.*, $np\ ^1P^0 - md\ ^1D$, $\Delta n \geq 1$). On the whole, most of our low-n results agree reasonably well with those of MS. Our high-n results should be more reliable, since the radial wave function is rather well represented by the Whittaker function at large radial distances. For Mg I, Wiese

https://doi.org/10.1017/S007418090012460X Published online by Cambridge University Press

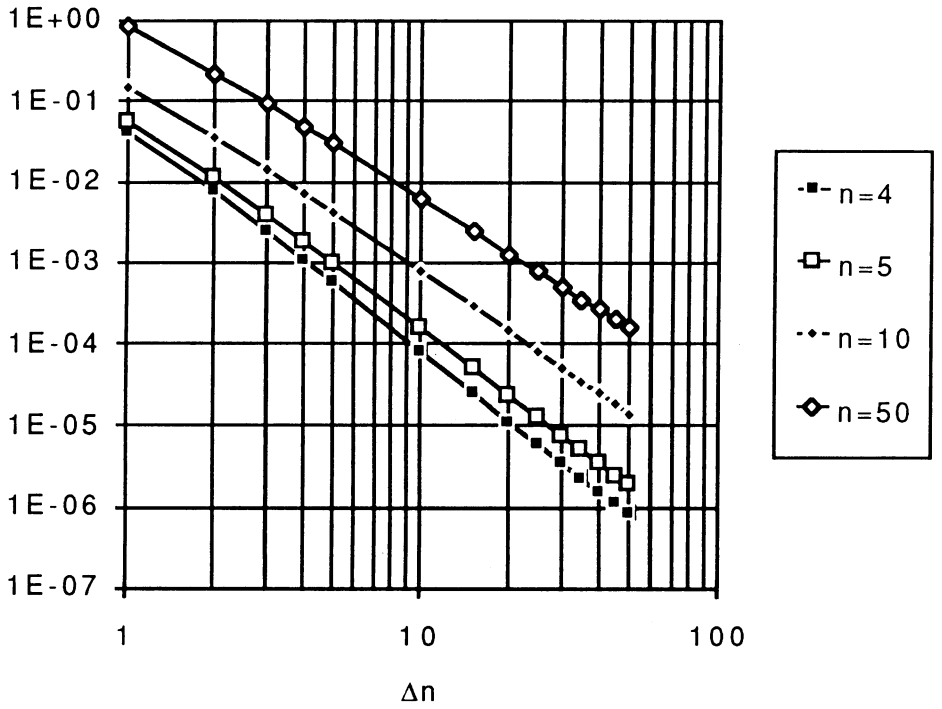

Fig. 1. $f(ns\,^1S, mp\,^1P^0)$ as a function of Δn, for selected values of n and m $(= n + \Delta n)$.

et al. (1969) estimated the uncertainty of the Coulomb approximation to be about 50%, but they felt that this was quite conservative. Our results support this view; in any case, an uncertainty of $\sim 50\%$ seems quite acceptable in many astrophysical problems. Further, they may be extrapolated to obtain threshold photoionization cross-sections for magnesium Rydberg states, as shown by Hoang-Binh (1983 and unpublished) for the case of hydrogen. In this connection, it may be noted that an efficient analytical method (also based on the Coulomb approximation), which allows one to deal easily with $n > 10$, has been proposed by Hoang-Binh and Van Regemorter (1979).

It is interesting to see how far the f-values for transitions between Mg I Rydberg states deviate from hydrogenic values. Table 2 lists f-values for $nf\,^1F^0 - mg\,^1G$ transitions in Mg I together with the corresponding hydrogenic values (quantum defects set equal to 0). It can be seen that the f-values still differ significantly from hydrogenic ones for $nf\,^1F^0 - mg\,^1G$ transitions, which involve high angular momenta $(l = 3, 4)$. This should be borne in mind when interpreting solar spectra (Jefferies 1991). Thus, it is only for transitions between $l \geq 4$ Rydberg states that

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TABLE I

Values of $f(np\,^1P^0, ms\,^1S)$. The last column shows the percentage difference between this work and the results of Moccia and Spizzo (1988).

Δn	n	This Work	MS	Difference(%)
1	4	2.97E-01	2.99E-01	-0.53
	5	4.31E-01	4.31E-01	-0.02
	6	5.65E-01	5.64E-01	+0.12
	7	6.98E-01	6.97E-01	+0.24
	8	8.32E-01	8.29E-01	+0.38
2	4	1.98E-02	1.98E-02	-0.14
	5	2.96E-02	2.97E-02	-0.36
	6	3.89E-02	3.91E-02	-0.57
	7	4.78E-02	4.79E-02	-0.11
3	4	6.11E-03	6.10E-03	+0.21
	5	9.19E-03	9.20E-03	-0.16
	6	1.20E-02	1.20E-02	+0.33

TABLE II

Values of $f(nf\,^1F^0, mg\,^1G)$

Δn	n	H	Mg I	Difference (%)
1	5	1.18E+00	1.05E+00	13.25
	10	1.08E+00	8.19E-01	31.31
	20	1.36E+00	9.48E-01	43.45
	50	2.51E+00	1.65E+00	51.80
2	5	2.29E-01	2.28E-01	0.47
	10	2.72E-01	2.34E-01	16.25
	20	3.46E-01	2.71E-01	27.70
	50	6.17E-01	4.55E-01	35.85
5	5	2.39E-02	2.61E-02	-8.74
	10	3.99E-02	3.78E-02	5.38
	20	5.28E-02	4.53E-02	16.55
	50	8.10E-02	7.17E-02	25.48

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the use of hydrogenic values is fully justified. In this connection, we note that a very efficient method for calculating exact hydrogenic radial integrals, for principal quantum numbers up to 1000, has been proposed (Hoang-Binh *et al.* 1979; Hoang-Binh 1990).

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