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ACCURATE CALCULATION OF Mg II 3*s*–*np* OSCILLATOR STRENGTHS[1]

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ABSTRACT

A careful and accurate semiempirical calculation of transition matrix elements yielded the oscillator strengths of resonance lines for the lowest *np* configurations in Mg II. Through an extension of previous work, particular attention was given to the determination of branching ratios for the fine-structure levels in the upper states. The new *f*-values provide strong theoretical support to the recent astronomical determinations by Fitzpatrick (1997) and could settle the question of the Mg abundance in the interstellar medium. The branching ratio $f(3s\text{–}4p_{3/2})/f(3s\text{–}4p_{1/2}) = 1.78$, a value that deviates from the assumed ratio of 2 used in earlier work.

Subject headings: atomic data — ISM: abundances — ISM: atoms — ultraviolet: general

1. BACKGROUND

The observational determination of the abundance of Mg in interstellar space has been hindered for a long time by two facts: (1) the principal transitions $\lambda\lambda$2796, 2803 (3*s*–3*p*) in the near-UV are strongly saturated, and (2) the next detectable transitions $\lambda\lambda$1239, 1240 (3*s*–4*p*) in the far-UV are very weak because the transition matrix elements have an accidental cancellation (e.g., Raftopoulos 1985; Theodosiou, Curtis, & Nicolaides 1996). Specifically, the early estimates of the 3*s*–4*p* oscillator strengths were of the order of 10^{-4}, 3 full orders of magnitude lower than the $f(3s\text{–}3p)$ values. There is a bit of historical background on these two lines: when Professor Edlén started to work at Paschen's Laboratory, his first assignment was to determine whether these lines were actually absent or just very weak in the observed spectra. Through very long exposures, Edlén was able to demonstrate the existence of these lines, although they were extremely low in intensity (see Henderson et al. 1997).

The phenomenon of accidental cancellations in the atomic transition matrix elements is well established both in the continuum, in the form of a "Cooper minimum" in the photoionization cross section (Fano & Cooper 1968), and in the discrete spectrum (Curtis & Ellis 1978; Theodosiou 1980; Curtis & Ellis 1980; Curtis 1981; Raftopoulos 1985; Curtis 1991; Theodosiou et al. 1996; Henderson et al. 1997). Much of the work on the systematic study of discrete-transition matrix element cancellations was done by Curtis (1981, 1991) in the pursuit of this fascinating regular quirk of nature. The cancellation results from the complete or near cancellation between the positive and negative contributions to the integrand of the dipole (and generally any multipole) transition radial matrix element. It comes about by the gradual shift of the initial- and final-state wave function nodes as a function of the orbital filling and of electron correlations in atoms and ions as one moves within the periodic table. Raftopoulos (1985) tabulated the atoms and ions for which we expect to have a (near) cancellation of the dipole as well as monopole and quadrupole matrix elements based on the states' effective quantum numbers (i.e., energies).

The existence of a cancellation in the 3*s*–4*p* transition of Mg II was noticed in previous calculations (Black, Weisheit, & Laviana 1972; Butler, Mendoza, & Zeippen 1984; Froese Fischer 1976; Laughlin 1992) or was contained as a by-product in survey calculations of the Na isoelectronic sequence (Biémont 1978; Lindgaard & Nielsen 1977; MacEchran & Cohen 1973; Saraph 1976; Sigut & Pradhan 1995; Theodosiou et al. 1996). However, no particular attention was paid to the resulting irregular branching ratio. With the exception of the recent work of Fleming et al. (1998), neither was any particular effort made to refine the oscillator strength value, considering its small value and its sensitivity to the method of calculation.

2. METHOD OF CALCULATION

Theodosiou (1984) developed a semiempirical method to calculate accurate transition matrix elements for alkali-like and helium-like systems for which no core excitation or channel mixing is present. The method employs a self-consistent Hartree-Kohn-Sham potential to describe the atomic field and utilizes the experimental energy levels as input, supplemented by ab initio core polarizabilities. The method was very successful in predicting accurate oscillator strengths and excited-state lifetimes for a variety of atomic systems, including Li, He, Be^+, Na, K, Ca^+, Cu, Rb, Zn^+, Cd^+, Cs, Ba^+, and Fr (see, e.g., Curtis 1993; Theodosiou et al. 1996 and references therein). The general approach is refined here to account for more salient features of the transitions at hand. The almost complete cancellation of the Mg II $3s\text{–}4p_{1/2,3/2}$ transition matrix elements makes their calculation very delicate and prone to drastic changes in value, even for minor inaccuracies in the description of the atomic core, the form of the transition matrix operator, and the energy values of the relevant atomic states.

The wave functions are determined by the Coulomb approximation with a central potential core (CACP) method (Theodosiou 1984), i.e., by direct inward integration of the Schrödinger equation

$$\left[\frac{d^2}{dr^2} - V(r) - \frac{l(l+1)}{r^2} + E_{nl}\right]P_{nl}(r) = 0\ . \qquad (1)$$

[1] This paper is dedicated to the memory of Jason Cardelli, who brought this interesting problem to our attention.

The central potential

$$V(r) = V_{\rm HKS}(r) + V_{\rm pol}(r) + V_{\rm so}(r) = V_m(r) + V_{\rm so}(r) \quad (2)$$

consists of three terms: $V_{\rm HKS}(r)$, a Hartree-Kohn-Sham–type (Desclaux 1969) self-consistent field term,

$$V_{\rm pol}(r) = -\frac{1}{2}\frac{\alpha_d}{r^4}\{1 - \exp[-(r/r_c)^6]\} - \frac{1}{2}\frac{\alpha_q}{r^6}\{1 - \exp[-(r/r_c)^{10}]\}, \quad (3)$$

a core-polarization term, and

$$V_{\rm so}(r) = -\frac{1}{2}\alpha^2\left\{1 + \frac{\alpha^2}{4}[E - V(r)]\right\}^{-2}\frac{1}{r}\frac{dV_m(r)}{dr}\boldsymbol{L}\cdot\boldsymbol{S}, \quad (4)$$

a spin-orbit interaction, Pauli approximation term. Here α_d and α_q are the dipole and quadrupole polarizability of the core, r_c is a cutoff distance, and α is the fine-structure constant.

The energy levels E_{nl} are obtained from the available experimental term values, and the necessary radial matrix elements were calculated using the modified dipole operator expression similar to the one used by Norcross (1973),

$$\left\langle nlj\left| r\left[1 - \frac{\alpha_d}{r^3}\left(1 - \frac{1}{2}\{\exp[-(r/r_{cl})^3] + \exp[-(r/r_{cl'})^3]\}\right)\right]\right| n'l'j'\right\rangle. \quad (5)$$

The cutoff distances r_{cl} are taken to be equal to the values used in the polarization potential $V_{\rm pol}$ needed to reproduce the lowest experimental energy for each symmetry; they are different for each value of l. They are the only adjustable parameters in this approach.

3. RESULTS AND DISCUSSION

The following parameters were used in the calculation:

$\alpha_d = 0.4698a_0^3$,
$\alpha_q = 0.5183a_0^5$,
$r_{c0} = 0.8432a_0$, and
$r_{c1} = 0.9921a_0$.

The polarizabilities α_d and α_q were taken from the ab initio calculations of Johnson, Kolb, & Huang (1983), whereas the cutoff distances appearing in the potential and the radial matrix elements were calculated iteratively to fit the 3s and the 4p energy levels to better than $\Delta E/E = 10^{-7}$. Table 1 presents a compilation of the present results for the absorption oscillator strengths to the Mg II 3p and 4p levels and the branching ratios $f(3s - np_{3/2})/f(3s - np_{1/2})$, together with relevant previous calculations and measurements of these quantities. The uncertainties in our theoretical results are based on the sensitivity of the values to variations in the adjustable parameters. Earlier theoretical efforts assume *LS* coupling between fine-structure levels; as a result, those data do not appear in Table 1. Preliminary reports of the present oscillator strength results appeared elsewhere (Theodosiou 1995, 1998).

The first observation is the already mentioned drastic (thousandfold) reduction of the oscillator strength in moving from the 3p to the 4p levels. Its origin is traced back to the accidental cancellation in the radial matrix element $\langle 3s|r|4p\rangle$. Our prediction for the doublet value, 0.000988(7), is in excellent agreement with the empirically obtained value, 0.00096(6), of Fitzpatrick (1997). The recent theoretical value, 0.00083, by Fleming et al. (1998) also agrees well with the astronomical value but falls outside the stated error bars. The second and remarkable result of the present calculations is the finding that the branching ratio $f_{3/2}/f_{1/2}$ is, as expected, 2.00 for the 3s–3p transitions, but only 1.78 for the 3s–4p transitions. All previous calculations

TABLE 1

RESULTS AND COMPARISON WITH OBSERVATIONS AND OTHER APPROACHES

Oscillator Strength or Branching Ratio	CACP, Present	Other Theory	Observations
$f(3s_{1/2}-3p_{1/2})$	0.300(5)	...	0.304(2)[a]
$f(3s_{1/2}-3p_{3/2})$	0.601(10)	...	0.610(6)[a]
$f(3s–3p)$ doublet	0.901(11)	0.939[b], 0.92[c], 0.917(10)[d]	0.914(7)[a]
$f(3s_{1/2}-3p_{3/2})/f(3s_{1/2}-3p_{1/2})$	2.006(47)	2[c]	2.007[a]
$f(3s_{1/2}-4p_{1/2}) \times 10^4$	3.56(5)	...	3.2(2)[e], $6.25(^{+3.8}_{-1.9})$[f]
$f(3s_{1/2}-4p_{3/2}) \times 10^4$	6.32(5)	...	6.4(4)[e], $12.5(^{+7.8}_{-3.8})$[f]
$f(3s–4p) \times 10^4$ doublet	9.88(7)	4.0[b], 8.3[c], 7.4(1.0)[d]	9.6(6)[e]
	...	15[g], 2.2[h]	
	...	10[i], 4[j]	
	...	8[k], 7.2[l]	
$f(3s_{1/2}-4p_{3/2})/f(3s_{1/2}-4p_{1/2})$	1.78(3)	2[c, m]	2[m]

[a] Beam laser, Ansbacher, Li, & Pinnington 1989.
[b] SOC/CIV3, Hibbert et al. 1983.
[c] SOC/CIV3, Fleming et al. 1998.
[d] Multiconfiguration Hartree-Fock (MCHF), Godefroid & Froese Fischer 1999.
[e] *Hubble Space Telescope* (*HST*), Fitzpatrick 1997.
[f] *HST*, Sofia, Cardelli, & Savage 1994.
[g] Central potential, Black et al. 1972.
[h] SUPERSTRUCTURE, frozen core, Saraph 1976.
[i] MCHF, Froese Fischer 1976.
[j] Variational Hartree-Fock, Biémont 1978.
[k] CACP, Laughlin 1992.
[l] R-matrix + SUPERSTRUCTURE, Sigut & Pradhan 1995.
[m] Assumed.

by other authors assumed that a strict *LS* coupling scheme is applicable to Mg II, and so it was assumed by Fitzpatrick. While this assumption is found to be appropriate for the 3*s*–3*p* case, this is clearly not the case for 3*s*–4*p*.

A justification of this result can be found in the study of the behavior of the relevant radial matrix elements: one can consider the matrix elements in an abstract fashion as functions of the effective quantum number n^*, defined through the equation for the binding energy

$$E_{nlj} = -\frac{\zeta^2}{2(n^*_{nlj})^2}, \quad (6)$$

where ζ is the order of the spectrum of the states involved, using the Bates-Damgaard approximation (Bates & Damgaard 1949) to calculate the radial part

$$R\{ns(n^*_s);\ np(n^*_p)\} = \langle ns\,|\,r\,|\,n'p\rangle = \int_0^\infty P_{ns}(r) r P_{n'p}(r)\,dr, \quad (7)$$

where the reduced radial wave functions $P_{nl}(r) = rR_{nl}(r)$ are normalized to unity. Figure 1 shows the result for our case of $3s(n^*_s = 1.9025) \rightarrow np(n^*_p)$, obtained using the program CAMATREL (Theodosiou 1978). From the figure, it is obvious that the 3*s*–3*p* matrix element is relatively large and does not change much on a percentage basis between the members of the doublet. However, the 3*s*–4*p* matrix element is much smaller, practically zero, and changes faster (on a percentage basis) within the doublet. Therefore, even though the change of effective n^* is the same for the 3*p* ($n^*_{3p_{1/2}} = 2.2645$; $n^*_{3p_{3/2}} = 2.2657$) and 4*p* ($n^*_{4p_{1/2}} = 3.2861$; $n^*_{4p_{3/2}} = 3.2873$) doublets, the radial matrix elements change much faster for the transitions to 4*p*.

Although this result does not seem to affect the conclusions by Fitzpatrick (1997), we would expect that, by using the correct branching ratios in future work, analyses will yield more consistent results. As a first attempt in this direction, a curve-of-growth analysis was performed on the velocity components seen in the spectrum of ζ Oph (Savage, Cardelli, & Sofia 1992). For the warm gas near $v_{\rm helio} = -27$ km s^{-1} a *b*-value of 3.0 km s^{-1} was adopted, and for the main component at $v_{\rm helio} = -15$ km s^{-1} the *b*-value was set at 1.5 km s^{-1} (see Savage, Cardelli, & Sofia 1992). Column densities, weighted by the uncertainties in equivalent width and oscillator strength for each member of the $\lambda\lambda$1239, 1240 doublet, were obtained for each component using the oscillator strengths derived here and those of Fitzpatrick (1997).

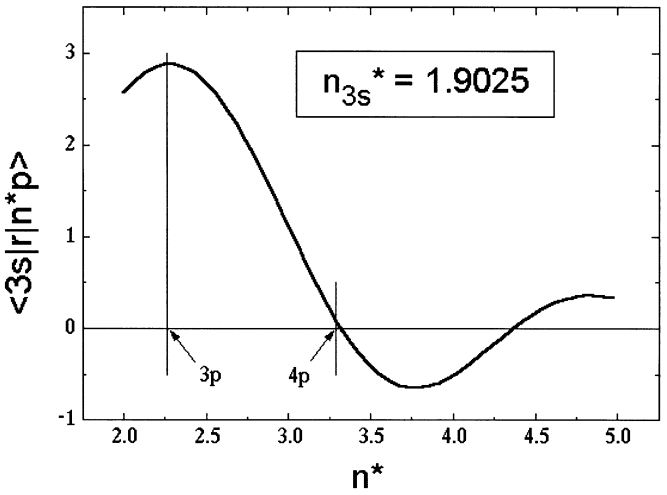

FIG. 1.—Radial matrix element vs. effective quantum number of upper state.

Table 2 displays the results of this analysis. For the warm component, where the optical depth at line center remains low ($\tau \leq 0.2$), the two results are indistinguishable because the uncertainties in measured equivalent widths are too large to prefer one set of oscillator strengths over the other. For the main component, where τ reaches $\approx$2.4, the comparison also does not lead to definitive conclusions. Here the limitation lies in the fact that, while use of Fitzpatrick's oscillator strengths and a *b*-value of 1.5 km s^{-1} yield excellent agreement for the results from the two lines, use of our oscillator strengths and a slightly larger *b*-value ($\approx$1.6–1.7 km s^{-1}) produce equally good results. In order to make a more discriminating test, (1) higher quality astronomical data are required; (2) empirical determinations from astronomical data should be limited to sight lines with relatively simple component structures; (3) only species likely to coexist in the gas should be included in the analysis; and (4) the branching ratio should be left as a free parameter in the fitting procedure. Adoption of points 2–4 would provide the basis for a more secure determination for comparison with our theoretical branching ratio.

Since circulating our results on the branching ratio, several data sets have been reanalyzed by the original authors. E. L. Fitzpatrick (1999, private communication) allowed both the sum and the ratio of the partial oscillator strengths $f(3s–4p_{3/2})$ and $f(3s–4p_{1/2})$ to vary. His new results are $f_{3/2} + f_{1/2} = 0.00095(6)$ and $f_{3/2}/f_{1/2} = 1.82(8)$, in complete agreement with our predictions. J. C. Howk (1999, private communication) has also reexamined the relevant GHRS observations of Howk, Savage, & Fabian (1999) for the gas toward μ Col. Plots of the $N_a(v)$ profiles for this doublet assuming a branching ratio of 1.75 give better agreement between the profiles obtained from each line of

TABLE 2

ASTRONOMICAL COMPARISON

Parameter	λ1239.925	λ1240.395
Warm Component		
W_λ (mÅ)	4.52 ± 0.46	1.75 ± 0.51
b-value (km s^{-1})	3.0	3.0
f(Fitzpatrick)	$(6.4 \pm 0.4) \times 10^{-4}$	$(3.2 \pm 0.2) \times 10^{-4}$
N (cm^{-2})	$(5.6 \pm 0.7) \times 10^{14}$	$(4.1 \pm 1.2) \times 10^{14}$
$N_{\rm weighted}$	$(5.2 \pm 0.6) \times 10^{14}$	...
f(this paper)	$(6.32 \pm 0.05) \times 10^{-4}$	$(3.56 \pm 0.05) \times 10^{-4}$
N (cm^{-2})	$(5.67 \pm 0.63) \times 10^{14}$	$(3.71 \pm 1.12) \times 10^{14}$
$N_{\rm weighted}$	$(5.2 \pm 0.5) \times 10^{14}$	...
Main Component		
W_λ (mÅ)	13.57 ± 0.56	8.74 ± 0.63
b-value (km s^{-1})	1.5	1.5
f(Fitzpatrick)	$(6.4 \pm 0.4) \times 10^{-4}$	$(3.2 \pm 0.2) \times 10^{-4}$
N (cm^{-2})	$(3.1 \pm 0.4) \times 10^{15}$	$(2.9 \pm 0.4) \times 10^{15}$
$N_{\rm weighted}$	$(3.0 \pm 0.3) \times 10^{15}$	...
f(this paper)	$(6.32 \pm 0.05) \times 10^{-4}$	$(3.56 \pm 0.05) \times 10^{-4}$
N (cm^{-2})	$(3.16 \pm 0.29) \times 10^{15}$[a]	$(2.59 \pm 0.28) \times 10^{15}$[a]
$N_{\rm weighted}$	$(2.87 \pm 0.20) \times 10^{15}$	...

[a] Use of $b \approx$ 1.6–1.7 km s^{-1} would produce better agreement between these results.

the doublet. Thus, available interstellar measurements tend to favor our prediction on the 3*s*–4*p* branching ratio.

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