Theoretical transition probabilities, radiative lifetimes and Stark broadening parameters of singly ionized magnesium

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ABSTRACT

The presence of spectral lines of singly ionized magnesium (Mg II) in stellar atmospheres has been reported in different stars. Recently, the low-resolution spectrum obtained from Supernova 2014 J in M82, in which Mg II absorption lines centred on 4400 Å as well as 7600 Å stand out, has been analysed. This is the motive for the atomic data calculations in this work, which are of much interest in the astrophysical area. In this article, *ab initio* relativistic Hartree–Fock calculations in an intermediate coupling formalism using Cowan’s code allowed us to obtain the required transition probabilities to calculate the theoretical radiative lifetimes for excited nS –, nP –, nD – and nF – states of singly ionized magnesium. An asymptotic dependence of lifetime (τ_{nl}) on the effective principal quantum number (n^*) has been determined. Also, the Griem semi-empirical approach was used to obtain the theoretical Stark parameters (width and shift) of spectral lines; these data are displayed for an electron density of 10^{17} cm^{-3} and temperatures $T = 10\text{--}100 (\times 10^3 \text{ K})$. We have compared the results of lifetimes for 16 levels and Stark parameters for seven spectral lines with previously reported experiments available in the literature. Finally, we discuss the behaviour of the Stark parameters versus temperature for three relevant spectral lines (2802.70, 2797.99 and 7868.04 Å).

Key words: atomic data – atomic processes.

1 INTRODUCTION

Magnesium is one of the most abundant elements on Earth, with multiple applications. Magnesium is also present as an impurity in many industrial interest alloys, making it a good candidate for diagnosis of the properties of laser-produced plasma (LSP) from these alloys: see Moreno-Díaz (2017). LSP industrial application requires a parallel investigation of the formed plasma from a fundamental point of view: see, for example, the recent work by Moreno-Díaz et al. (2016) on a method applied to treated material in laser shock processing (LSP) processes.

Also, magnesium is an important chemical element for studying the history of α -process nucleosynthesis. This element is observed relatively easily in the spectra of stars, even in metal-poor star atmospheres, and its overabundance in extremely metal-poor stars is one of the fundamental parameters of chemical evolution models for our Galaxy (Civiš et al. 2013). Spectral lines of singly ionized magnesium (Mg II) are of importance for the investigation, diagnostics and modelling of stellar atmospheres. In the solar spectrum, the triplet of lines (2790.77, 2797.93 and 2797.99 Å) is shown along with the resonance h and k lines (2802.70 and 2975.53 Å) of Mg II, mainly in absorption and in some cases also as lines of emission; see Morrill & Korendyke (2008) and

Pereira et al. (2015). Vallely et al. (2016) analysed a time series of optical spectra of Supernova 2014 J in M82 and at early times the spectral features are dominated by Si II, S II, Mg II and Ca II. Also, the Mg II triplet lines (4481.33, 4481.15 and 4481.13 Å) and (7898.04, 7877.05 and 7896.37 Å) appeared as absorption lines. Also, this last triplet has been used by Lambert & Warner (1968) and Vennes, Kawka & Németh (2011) for the determination of the abundance of magnesium, first in the solar photosphere and also in the white dwarf GALEX J193156.8+011745. Therefore, we think that the calculation of transition probabilities, radiative lifetimes and Stark broadening parameters is necessary. For all these reasons, a theoretical study of the aforementioned atomic data of Mg II is presented in this work.

Mg II has ground configuration $1s^2 2s^2 2p^6 3s^1 S_{1/2}$ and excited states of type $1s^2 2s^2 2p^6 nL$. The energy levels and transition data can be found in Martin & Zalubas (1980), Moore (1970) and Kaufman & Martin (1991). Furthermore, Biémtot & Brault (1986) measured the spectra of Mg I and Mg II produced by a hollow-cathode discharge observed by the Fourier transform spectroscopy technique between 1800 and 9000 cm^{-1} . This observation has allowed an extension of the term systems of Mg I and Mg II, as well as the values of the relative intensities of the observed spectral lines. This extension is collected in the National Institute of Standards and Technology (NIST) database (Kramida et al. 2018).

Theoretical works on transition probabilities can found in the bibliography, but there are no experimental ones. However,

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radiative lifetimes of Mg II have been measured by several authors. In chronological order, the lifetime of the $2p^6 3p^2 P^0_{1/2}$ level was measured by Smith & Gallagher (1966) using the Hanle-effect method with optical excitation. Berry, Bromander & Buchta (1970) measured the lifetime levels $2p^6 4s^2 S_{1/2}$, $2p^6 3p^2 P^0_{1/2}$, $2p^6 3d^2 D_{3/2}$ and $2p^6 f^2 F^0_{5/2}$ by mean of the beam-foil technique. Andersen et al. (1970), using the beam-foil excitation technique, measured the $2p^6 3p^2 P^0_{1/2}$ level. The radiative lifetimes of the $3p^2 P^0 \rightarrow 3s^2 S_{1/2}$ multiplets at 2795.53 and 2802.70 Å were measured by Smith & Lyszt (1971) using a phase-shift technique. The beam-foil technique has been used to measure the radiative lifetimes of the transitions $4d^2 D \rightarrow 4p^2 P^0$, $6f^2 F^0 \rightarrow 3d^2 D$, $6f^2 F^0 \rightarrow 4d^2 D$ and $7f^2 F^0 \rightarrow 4d^2 D$ by Andersen, Mølhave & Sørensen (1972). With the same technique, Lundin et al. (1973) have determined radiative lifetimes of states $4s^2 S$, $3p^2 P^0$, $3d^2 D$, $4p^2 P^0$ and $4f^2 F^0$. Lifetime measurements for 11 levels have been made by Liljeby et al. (1980), also using the beam-foil technique.

In the case of Stark parameters of Mg II (widths and shifts), there are also some experimental values in the bibliography. Stark width parameters from lines ($3s-3p$ transition, 2802.70 Å and $3d-4f$ transition, 4481.33 Å) have been measured in an argon plasma jet by Chapelle & Sahal-Bréchet (1970). Using an electromagnetically driven shock tube and a rapid-scanning Fabry–Perot spectrometer, Jones et al. (1972) have measured Stark widths and shifts of resonance h and k lines (2802.70 and 2795.53 Å). The Stark widths and shifts of the 2795.53- and 2936.51-Å lines have been measured in an argon-welding type plasma by Fleurirer, Sahal-Bréchet & Chapelle (1977). Goldbach et al. (1982) have measured resonance lines h and k again, but with wall-stabilized arc burning in argon with a small addition of Mg vapour.

Stark widths and shifts of six Mg II spectral lines very important in astrophysical situations (2790.77, 2795.53, 2797.99, 2802.70, 2928.63 and 2936.51 Å) have been measured by Djeniže et al. (2004) with a linear low-pressure arc as a plasma source. In the same way, Bukvić, Srećković & Djeniže (2004) have measured resonance h and k spectral lines and values of the 2790.77- and 2797.99-Å lines in the $3p-3d$ transition. Djeniže, Srećković & Bukvić (2005) have again measured the Stark width and shift of the 4481.13-Å spectral line in the $3d^2 D_{5/2}-4f^2 F^0_{7/2}$ transition in nitrogen plasma generated in an optically thin linear, low-pressure, pulsed arc discharge. The Stark broadening parameter of the same line was also measured by Cvejić et al. (2013) with a laser-induced plasma.

In this article, we present theoretical values of transition probabilities for 320 spectral lines of Mg II that are shown in the NIST database and arise from configurations $2p^6 ns$ ($n = 4-10$), $2p^6 np$ ($n = 3-9$), $2p^6 nd$ ($n = 3-8$) and $2p^6 nf$ ($n = 4-10$). Lifetimes of 47 levels are also calculated and compared with experimental values available in the bibliography. These calculations have been made with *ab initio* relativistic Hartree–Fock (HFR) in an intermediate coupling (IC) formalism using Cowan’s code. In Section 2, the method and the theoretical calculations are described. Following this, Section 3 provides the results and a discussion of transition probabilities, radiative lifetimes and Stark broadening parameters, including an analysis of the different regularities of these last.

2 METHOD OF CALCULATION

In this work, HFR calculations in an IC scheme have been realized. We have used a similar procedure to that described in previous works, such as Alonso & Colón (2013), Moreno-Díaz, Alonso-Medina & Colón (2014), Alonso-Medina, Colón & Moreno-Díaz (2015) and Moreno-Díaz (2017). Wave functions and transition

probabilities were obtained by the standard method of least-squares fitting of experimental energy levels, presented by Martin and Zalubas (1970), Moore (1971) and Kaufman & Martin (1991), by means of Cowan’s computer code (Cowan 1981). For the HFR calculations, the Cowan computer code provides not only the radial parts, for determination of transition probabilities, but also an initial estimation of the parameters for the IC fittings. Our set consists of 26 configurations, $2p^6 ns$ ($n = 3-10$), $2p^6 nd$ ($n = 3-9$), $2p^6 ng$ ($n = 5-11$) and $2p^6 ni$ ($n = 7-10$), of even parity, and 20 configurations of odd parity, $2p^6 np$ ($n = 3-9$), $2p^6 nf$ ($n = 4-10$) and $2p^6 nh$ ($n = 6-11$) of Mg II. Since magnesium is a light element, core polarization effects have not been introduced. The values obtained with the HFR *ab initio* calculations were used as a starting point in the setting of energy levels. Thus, we obtained the LS composition of each level and the degree of configuration mix, considering their interactions and the experimental energy levels. Fig. S1 (available online) displays a partial Gotrian energy-level scheme of Mg II, showing the adjusted levels and spectral lines, previously mentioned, of greater astrophysical interest.

Because of the high number of parameters to adjust (which exceeds of the number of experimental levels), we have excluded a certain number of parameters from the adjustment process. The scaling factors of the Slater parameters (F^k and G^k) and configuration interaction integrals (R^k), not optimized in the least-squares fitting, were chosen to equal 0.85, as suggested by Cowan (1981). For the spin-orbit integrals ζ_{nl} , characterized by small numerical values and no adjustment in the fitting procedures, we have used the HFR *ab initio* values without scaling. The values found for the different parameters involved in the IC calculations, compared with HFR (used as a start in the fitting process), are shown in Table S1 (available online). The wave functions obtained in Cowan’s code were used in the calculations to obtain the matrix elements required.

The transition probabilities are obtained from the matrix elements by using the standard expression of Martin & Wiese (1996):

$$A_{nl} = \frac{2\pi e^2}{m_e c \epsilon_0 \lambda^2} \frac{g_l}{g_n} f_{ln} = \frac{16\pi^3}{3h \epsilon_0 \lambda^3 g_n} |\langle P_n | \mathbf{r} | P_l \rangle|^2, \quad (1)$$

where A_{nl} and f_{ln} are the transition probability and the oscillator strength, respectively, e and m_e are the electron charge and electron mass, λ is the transition wavelength, c is the light speed, h is the Planck constant, g_l and g_n are the statistical weights and $\langle P_n | \mathbf{r} | P_l \rangle$ is the calculated matrix element including the modification pointed out above. Once all the probabilities of transition are known that come from a level, also the lifetime of that level are known. Then the only possibility to compare the results of probabilities is with other theoretical works. In this article, this comparison is not realized because discrepancies can be present, in many cases due to the theoretical approach of each author. However, the calculated radiative lifetimes have been compared with the experimental values of other authors. In Tables S2–S5 (available online), the theoretical transition probabilities and radiative lifetimes of some levels of Mg II are shown. The ratio between the theoretical lifetimes of this study and the previously measured experimental lifetimes can be seen in Fig. S2 (available online).

As we have already indicated, information on the lifetimes is necessary for estimating use of the Rydberg states for practice applications. Theoretical investigations of the optical properties of Rydberg states in Mg II are of current interest. In this work we obtained approximations of lifetimes for excited nS –, nP –, nD – and nF – states, with the equation

$$\tau_{nl} = \tau_0 (n^*)^\alpha, \quad (2)$$

where n^* is the effective principal quantum number and τ_0 and α are two constants, applicable to states with principal quantum number in the range $n = 3-10$. This expression is used by several authors: see as an example Rykova & Verolainen (1994) and Glukhov et al. (2013). The constant τ_0 for different series of states, as shown in Table S6 (available online), range from $\tau_0 = 0.05$ ns of nF^- states to $\tau_0 = 0.62$ ns of nP^- states. On the other hand, the value of the exponent is around $\alpha = 3$, with a deviation in the results of less than ± 0.5 . Fig. S3 (available online) shows the representation of the lifetime of the levels versus the effective principal quantum number of each level corresponding to different series ($ns^2S_{1/2}$, $np^2P^0_{1/2}$, $nd^2D_{3/2}$, $nf^2F^0_{5/2}$). The values of the half-lives measured by Smith & Gallagher (1966), Andersen et al. (1970), Berry et al. (1970), Smith & Lyszt (1971), Lundin et al. (1973), Liljeby et al. (1980) and Andersen et al. (1970) can be seen together. It is verified that said half-lives follow expression (2) and the corresponding alpha values can be observed for each graph. These values confirm the asymptotic nature of the dependence of $\tau_{nl} \propto (n^*)^3$, indicating that, for the studied levels, the model used in this work is applicable with good precision.

On the other hand, previously determined matrix elements have also been used in the calculation of Stark broadening parameters from the semi-empirical approach suggested by Griem (1968), using his semi-empirical formulae (23) and (35). This calculation procedure is similar to those presented in recent publications by the authors Colón, Moreno-Díaz & Alonso-Medina (2013), Alonso-Medina & Colón (2014), Moreno-Díaz et al. (2014) and recently Moreno-Díaz (2017). This approach was obtained taking into account Baranger's original formulation (Baranger 1958) and the use of an effective Gaunt factor, proposed by Seaton (1962) and Van Regemorter (1962).

In Tables S7–S10 (available online), the theoretical Stark width and shift parameters for some levels of Mg II are shown. In Fig. S4 (available online), we compared the dependence on the Stark parameters for several spectral lines of Mg II with the electron temperature.

3 RESULTS AND DISCUSSION

3.1 Transition probabilities and radiative lifetimes

In Tables S2–S5 (available online), we present the results obtained in this work for transition probabilities of 320 spectral lines in the wavelength range 870–180 000 Å and lifetimes of 47 levels of Mg II. Of these last, 16 have been compared with experimental values available in the literature. In the first column, we present the transition (the upper and lower level). The second one displays the wavelength in Å (see Martin & Zalubas 1980). In the third column we show the relative intensity I_{rel} (the intensities of lines referred to the intensities of Mg I lines at 2150.353 and 5843.407 cm^{-1} , Biélmont & Brault 1986). The remaining columns present our values: the fourth column shows the transition probabilities and in the fifth our radiative lifetimes are compared with the experimental values of other authors (Smith & Gallagher 1966; Andersen et al. 1970; Berry et al. 1970; Smith & Lyszt 1971; Lundin et al. 1973; Liljeby et al. 1980; Andersen et al. 1970).

In order to facilitate the comparison, in Fig. S2 (available online) we present the ratio between experimental values of radiative lifetimes and the theoretical values obtained in this work for several levels of Mg II (τ_{exp}/τ_{this} work) versus the energy of the levels. As can be seen, our values are in good agreement with the experimental ones, with the exception of some levels. In any case, the deviations

are less than 10 per cent. Andersen et al. (1970) and Lundin et al. (1973) found that the radiative lifetime of the doublet (2802.70 and 2795.53 Å) was difficult to solve. They had to study this lifetime using line 2802.70 Å, because line 2795.53 Å is mixed with line 2790.77 Å of the transition $3p^2P^0_{1/2}-3d^2D_{3/2}$. They found an appreciable cascading in this transition that complicates the interpretation of the obtained lifetime. Also, in $4p^2P^0-4d^2D$ and $3d^2D-6f^2F^0$ transitions, Andersen et al. (1972) found cascading.

Fig. S3 (available online) shows the representation of the lifetimes of the levels $ns^2S_{1/2}$, $np^2P^0_{1/2}$, $nd^2D_{3/2}$ and $nf^2F^0_{5/2}$ studied against the effective principal quantum number of each level corresponding to each series. As can be seen, the mentioned lifetimes follow expression (2). In addition, in each graph the values of α can be appreciated and we corroborate that these values are close to 3. Values of constants τ_0 and α for all series studied are presented in Table S6 (available online).

In conclusion, regarding these calculations, we can say that the transition probabilities as well as the lifetimes of their different states can be calculated with reasonable safety using ab initio HFR. For this reason, we think that these values are a good basis for the calculations of the Stark broadening parameters presented below.

3.2 Stark width FWHM and Stark line shift

The results for the Stark line width and line shift at an electron density of 10^{17} cm^{-3} and several temperatures $T = 10-100 (\times 10^3 \text{ K})$ are displayed in Tables S7–S10 (available online). The first three columns denote the corresponding transition array, the multiplet and the wavelengths (in Å: Martin & Zalubas 1980) for each transition studied. The temperatures (in K) are shown in the fourth column. Theoretical Stark broadening line widths (in pm) are displayed in the fifth column and, where appropriate, the experimental values from the literature. The final column displays the theoretical Stark line shift (a positive shift is red) and in the same way the experimental values of other authors: see Cappelle & Sahal-Bréchet (1970), Jones et al. (1972), Fleurier et al. (1977), Goldbach et al. (1982), Bukvić et al. (2004), Djeniže et al. (2004), Djeniže et al. (2005) and Cvejić et al. (2013). Our Stark full width at half-maximum (FWHM) values are in good agreement with the experimental ones, with some exceptions. For example, in the values of the Mg II resonance doublet measured by Goldbach et al. (1982), the width was found lower by a factor of 2 than all previous experimental values, as mentioned by these authors.

The dependence of Stark parameters on electron temperature is shown in Fig. S4 (available online). In this figure we represent the values of calculated Stark width FWHM ω (pm) and Stark line shift d (pm) versus temperature for three lines.

The lines 2802.70 and 2797.99 Å are presented in comparison with the experimental values of other authors. These lines could be used in the diagnosis of plasmas. We show the line 7898.04 Å, which in addition to being used in plasma diagnosis also has great astrophysical interest and belongs to a multiplet, arising from levels with high energies of the order of $93\,000 \text{ cm}^{-1}$. As expected, the trends found coincide with those anticipated theoretically.

To conclude, using Cowan's code we have obtained the matrix elements necessary for the calculation of the Stark broadening parameters of Mg II spectral lines. We know that there are different ways to perform these calculations, but we have used Griem's semi-empirical method. This method has given us good results within the margins of experimental error.

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SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

Figure S1. Partial Gotrian diagram of Mg II energy levels (Martin & Zalubas 1980), showing several spectral lines of great astrophysical interest.

Figure S2. Ratio between experimental values of radiative lifetimes and the theoretical values obtained in this work for several levels of Mg II ($\tau_{\text{exp}}/\tau_{\text{this work}}$) versus the energy of the levels.

Figure S3. Experimental lifetimes of the $1s^2 2s^2 p^6 (ns^2 S_{1/2}, np^2 P^0_{1/2}, nd^2 D_{3/2}, nf^2 F^0_{5/2})$ series in Mg II as a function of the effective principal quantum number n^* : black filled circles – our work, red open circles – Liljeby et al. (1980), green diamonds – Berry et al. (1970), blue upwards-pointing triangles – Andersen et al. (1970), magenta downwards-pointing triangles – Lundin et al. (1973), orange left-pointing triangles – Smith & Gallagher (1966), light green right-pointing triangles – Smith & Lyszt (1971), purple x symbols – Andersen et al. (1970).

Figure S4. Calculated Stark width FWHM (ω (pm)) and shift (d (pm)) at an electron density of 10^{17} cm^{-3} versus temperature and experimental values from other authors, for 2802.70-, 2797.99- and 7898.04-Å spectral lines of Mg II.

Table S1. Parameters resulting from the least-squares fitting of the intermediate coupling calculations.

Table S2. Mg II $1s^2 2s^2 2p^6 ns$ ($n = 4-10$) relative intensity I_{rel} (the intensities of the lines are referred to the intensities of Mg I lines at 2150.353 and 5843.407 cm^{-1} : Biémont & Brault 1986), transition probabilities A_{ij} (in 10^7 s^{-1}) and radiative lifetimes τ (in ns).

Table S3. Mg II $1s^2 2s^2 2p^6 np$ ($n = 3-9$) relative intensity I_{rel} (the intensities of the lines are referred to the intensities of Mg I lines at 2150.353 and 5843.407 cm^{-1} : Biémont & Brault 1986), transition probabilities A_{ij} (in 10^7 s^{-1}) and radiative lifetimes τ (in ns).

Table S4. Mg II $1s^2 2s^2 2p^6 nd$ ($n = 3-8$) relative intensity I_{rel} (the intensities of the lines are referred to the intensities of Mg I lines at 2150.353 and 5843.407 cm^{-1} : Biémont & Brault 1986), transition probabilities A_{ij} (in 10^7 s^{-1}) and radiative lifetimes τ (in ns).

Table S5. Mg II $1s^2 2s^2 2p^6 nf$ ($n = 4-10$) relative intensity I_{rel} (the intensities of the lines are referred to the intensities of Mg I lines at 2150.353 and 5843.407 cm^{-1} : Biémont & Brault 1986), transition probabilities A_{ij} (in 10^7 s^{-1}) and radiative lifetimes τ (in ns).

Table S6. Values of constants τ_0 and α for different series of excited states of Mg II.

Table S7. Mg II $1s^2 2s^2 2p^6 ns$ ($n = 4-6$) line widths (FWHM) ω (pm) and shifts d (pm) normalized to $N_e = 10^{17} \text{ cm}^{-3}$.

Table S8. Mg II $1s^2 2s^2 2p^6 np$ ($n = 3-5$) line widths (FWHM) ω (pm) and shifts d (pm) normalized to $N_e = 10^{17} \text{ cm}^{-3}$.

Table S9. Mg II $1s^2 2s^2 2p^6 nd$ ($n = 3-5$) line widths (FWHM) ω (pm) and shifts d (pm) normalized to $N_e = 10^{17} \text{ cm}^{-3}$.

Table S10. Mg II $1s^2 2s^2 2p^6 4f$ line widths (FWHM) ω (pm) and shifts d (pm) normalized to $N_e = 10^{17} \text{ cm}^{-3}$.

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