Radiation Physics and Chemistry 130 (2017) 406–410

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Photoionization cross sections of the excited 3s3p $^3P^o$ state for atomic Mg

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ARTICLE INFO

Keywords:
Photoionization
Mg
Excited states
R-matrix method

ABSTRACT

The photoionization cross sections of the excited levels (3s3p $^3P^o_{0,1,2}$) of atomic Mg have been studied theoretically using both the nonrelativistic and fully relativistic *R*-matrix method. For the threshold cross sections, as previous nonrelativistic studies, present calculations show significant differences (a factor of 3) from former experimental values. Large discrepancies with experiment calls for additional measurements of the photoionization cross sections from the excited states of Mg.

1. Introduction

Mg is an important source of opacity for wavelengths between 251 and 207 nm (Seaton et al., 1992). So the photoionization (PI) cross section of Mg is required for models of the solar chromosphere. There have been many theoretical and experimental investigations for photoionizations of ground state ($3s^2\ ^1S$) of Mg (see our more recent work (Wang et al., 2010) and references therein). The theoretical calculations have obtained good agreement with experimental measurements. Then, Diop et al. (2013) used the Screening Constant by Unit Nuclear Charge (SCUNC) method to calculate high lying energy positions and widths of the 3pns $^{1,3}P^o$, 3pnd $^{1,3}P^o$ and 3pnd $^3D^o$ Rydberg series in Mg. Their results are in excellent agreement with our previous R-matrix calculations (Wang et al., 2010). For excited 3s3p $^3P^o$, on the other hand, many theoretical studies also been carried out. Travis and Matsushima (1968) calculated PI cross sections of Mg using the quantum defect method and hydrogenic approximations. Butler et al. (1993) calculated PI cross sections for Mg-like ions in the close-coupling approximation. Moccia and Spizzo (1988) calculated one-photon ionization cross sections of Mg using L^2 CI technique. Fang and Chang (2000) studied the photoionization from excited Mg atoms using a B-spline-based configuration interaction approach. Kim (2001) calculated photoionizations of the excited 3s3p $^{1,3}P^o$ states of Mg using an enhanced non-iterative variational *R*-matrix approach. Rescigno (1985) calculated PI cross sections for the ground and metastable $(3s3p)^3P^o$ states of Mg by the complex-basis-function expansion method. Mendoza and Zeippen (1987) calculated PI cross sections of the ground and excited states of Mg in a 8-state close-coupling approximation. It should be noted that all these theoretical calculations are performed in *LS* scheme. To our knowledge, no relativistic calculations are performed for the metastable 3s3p $^3P^o$ state of Mg. In contrast to theoretical studies the experimental measurements are very scarce. There are only two measurements in the literature. Bötticher (1958) measured the cross section near the threshold of 3p in $^3P^o$ term of Mg, but the absolute scale of the measurement relies upon the oscillator strength of the 3s3p $^3P^o \rightarrow$ 3s5s $^3S^e$ transition. Lombardi et al. (1981) measured the PI cross section of the 3p in $^3P^o$ term of Mg near threshold absolutely. In these existing studies, however, there is a difference of a factor of three between theoretical and experimental cross section in the threshold region (see Table 1). The theoretical values are less than 20 Mb, while the experimental results are lager than 40 Mb. This discrepancy is believed to be due to experimental problems by some authors (Butler et al., 1993). At the same time, in order to account for all of the opacity in the wavelength region 207–251 nm one must assumes a larger cross section of 37 Mb (Vernazza et al., 1981). In order to clarify this situation we decided to carry out further calculations using both the no relativistic and relativistic *R*-matrix method in this paper, where the relativistic calculation is carried out for the first time, to our best knowledge.

2. Theoretical methods

Very recently we (Wang et al., 2010) employed the *R*-matrix method (Burke and Berrington, 1993) for a detailed investigation of the photoionizations of the ground state of Mg. The results were in excellent agreement with the experiment. In this paper, we applied the same *R*-matrix method to calculate the PI cross sections of excited 3s3p $^3P^o$ of Mg using the programs RMATRX1 (Berrington et al., 1995) (for nonrelativistic *LS* calculation) and Ait-Tahar et al. (1996) (for relativistic calculation). We will give a brief description of the *R*-matrix

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http://dx.doi.org/10.1016/j.radphyschem.2016.09.028
Received 8 March 2016; Received in revised form 19 September 2016; Accepted 24 September 2016
Available online 26 September 2016
0969-806X/

Table 1
The cross section of the 3s3p $^3P^o$ of Mg near the threshold.

σ (Mb)	Method	Reference
19.9	quantum defect method and hydrogenic approximations	Travis and Matsushima, 1968
16.2	close-coupling approximation	Butler et al., 1993
16.49/14.74 (LG/VG)	L^2 CI calculation	Moccia and Spizzo, 1988
<15	B-spline-based configuration interaction (BSCI) approach	Fang and Chang, 2000
16	enhanced non-iterative variational R-matrix approach	Kim, 2001
<14.5	the method of complex basis functions	Rescigno, 1985
<15	close-coupling approximation	Mendoza and Zeippen, 1987
20.2	through a quantum defect extrapolation of their oscillator strengths	Ueda et al., 1982
45	emission measurement, normalised assuming transition f=0.0185 for the 3s3p $^3P^o \rightarrow$ 3s5s $^3S^e$	Bötticher, 1958
38	normalised assuming f=0.0157 for the 3s3p $^3P^o \rightarrow$ 3s5s $^3S^e$ transition	Moccia and Spizzo, 1988
35 ± (9 ~ 18)	normalised assuming f=0.0144 for the 3s3p $^3P^o \rightarrow$ 3s5s $^3S^e$ transition	Lombardi et al., 1981
41	normalised assuming f=0.017 for the 3s3p $^3P^o \rightarrow$ 3s5s $^3S^e$ transition	Ueda et al., 1982
46 ± 12	absorption measurement	Lombardi et al., 1981
14.95/15.06 (LG/VG)	present nonrelativistic R-matrix calculation	
14.92/14.85 (LG/VG)	present relativistic R-matrix calculation	

method below.

In the R-matrix calculation, the wavefunction of the $N+1$ electron system is given by

$$\Psi_k(X_1, \ldots, X_{N+1}) = \widehat{A} \sum_{ij} c_{ijk}\Phi_i(X_1, \ldots, X_N, \hat{\mathbf{r}}_{N+1}\sigma_{N+1})u_{ij}(r) + \sum_j d_{jk}\phi_j(X_1, \ldots, X_{N+1}) \quad (1)$$

where $\widehat{A}$ is the antisymmetrization operator to take the exchange effects between the target electrons and the continuum electron into account. X_i stands for the spatial ($\mathbf{r}_i$) and spin (σ_i) coordinates of the ith electron. The functions $u_{ij}(r)$ in the first sum construct the basis set for the wave functions of the continuum electron, and Φ_i is the coupling wavefunctions between the target states and the angular and spin parts of the continuum electron. The correlation functions ϕ_j in the second sum are constructed by the square integrable orbitals to account for the correlation effects, which is not adequately considered because of the cutoff in the first sum.

In nonrelativistic calculations, the square integrable orbitals are expressed by a sum of Slater-type orbitals

$$P_{nl}(r) = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r) \quad (2)$$

The parameters ξ_{jnl} and coefficients C_{jnl} are determined by a variational optimization on the energy of a particular state, whilst the powers I_{jnl} remain fixed. In present nonrelativistic calculation, we included eleven real and three pseudo-orbitals (1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5s, $\overline{5p}$, $\overline{5d}$ and $\overline{5f}$). The 1s, 2s, 2p and 3s orbitals are taken from those of the Hartree-Fock orbitals given by Clementi and Roetti (1974) for the Mg^+ ground state $2p^6 3s\ ^2S$, while the other orbitals are obtained by optimizing on the energy of given states using the CIV3 code of Hibbert (1975) . We included eight LS target states of Mg^+ which are listed in Table 2, in which we have also given the comparison between the present calculated and experimental energies of these states relative to the ground state of Mg^+. Our results are uniformly lower than those of NIST. The differences result from the number of the configurations included in the calculation. The R-matrix boundary was chosen to be 41.8 au and the continuum orbitals are expressed as a linear combination of 60 numerical basis functions for each angular momentum and we employed a very fine energy mesh of 10^{-6} Ry. The present calculated ionization potential (IP) is 0.363 Ry, in good agreement with the experimental value 0.3625 Ry (Ralchenko et al., 2008).

In relativistic R-matrix calculations, on the other hand, the orbitals are obtained from multiconfiguration Dirac-Fock (MCDF) code GRASP92 (Parpia et al., 1996) by using an extended optimized level (EOL) scheme for the concerned energy levels of the ion Mg^+ in order to perform the close-coupling expansion. The relativistic electron wavefunctions have the form

$$\varphi(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} P_{n\kappa}(r)\chi_\kappa^m(\theta, \phi) \\ iQ_{n\kappa}(r)\chi_{-\kappa}^m(\theta, \phi) \end{pmatrix} \quad (3)$$

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are respectively the large and small component radial wavefunctions, and the functions $\chi_{\pm\kappa}^m(\theta, \phi)$ are two-component spinors made up of spherical harmonics and Clebsch-Gordan coefficients. The radial parts of the bound orbitals (i.e., $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$) are input into the fully relativistic R-matrix code in the form of numerical values on a suitable mesh of points.

In the present calculations, the Mg^+ target wavefunctions are described by a closed core $1s^2 2s^2 2p^6$ and twelve one-electron orbitals: $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, $3d_{5/2}$, $4s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$ and $4f_{7/2}$. In performing the relativistic R-matrix calculation, 10 lowest levels of Mg^+ are included in the expansion of wavefunctions and the theoretical energy levels are shown in Table 2 along with the experimental values (Ralchenko et al., 2008) . It can be seen that the calculated energy levels agree well with the experiment. The differences between them are less than 0.02 Ry similarly in nonrelativistic calculations. The R-

Table 2
Calculated nonrelativistic, relativistic and experimental energy levels from NIST (Ralchenko et al., 2008) (in Ry) for the target Mg^+ ion relative to its ground state $2p^6 3s$.

Configuration	Term/J	Level	
		Present	NIST
$2p^6 3s$	^2S	0.0000	0.0000
	$^2S_{1/2}$	0.0000	0.0000
$2p^6 3p$	$^2P^o$	0.3149	0.3256
	$^2P^o_{1/2}$	0.3185	0.3250
	$^2P^o_{3/2}$	0.3194	0.3259
$2p^6 4s$	^2S	0.6188	0.6361
	$^2S_{1/2}$	0.6225	0.6361
$2p^6 3d$	^2D	0.6332	0.6515
	$^2D_{5/2}$	0.6364	0.6515
	$^2D_{3/2}$	0.6364	0.6515
$2p^6 4p$	$^2P^o$	0.7216	0.7348
	$^2P^o_{1/2}$	0.7200	0.7347
	$^2P^o_{3/2}$	0.7203	0.7349
$2p^6 5s$	^2S	0.8273	0.8456
$2p^6 4d$	^2D	0.8299	0.8503
	$^2D_{5/2}$	0.8331	0.8503
	$^2D_{3/2}$	0.8331	0.8503
$2p^6 4f$	$^2F^o$	0.8329	0.8548