Contrib. Astron. Obs. Skalnaté Pleso **55/2**, 54 – 61, (2025)
https://doi.org/10.31577/caosp.2025.55.2.54

Electron energy loss spectra of magnesium in autoionization region

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Received: November 23, 2024; Accepted: December 12, 2024

Abstract. An experimental study of the autoionization spectra of magnesium by electron impact is given. Electron impact excitation of neutral magnesium atoms above the ionization limit leads to the states that auto-ionize. Energy loss spectra up to 12 eV are recorded at impact electron energies of 30 and 40 eV and scattering angles of 6 and 10 degrees. The two features at 10.09 and 10.46 eV we assigned to the 3s3d $^1D_2$ and 3s3d $^3D_{1,2,3}$ states.

Key words: Electronic spectroscopy – Autoionization – Electron impact excitation – Atomic data

1. Introduction

Magnesium is an element of significant astrophysical importance. Its significant abundance, combined with its array of spectral features across the UV, visual, and IR spectrum, means that it is observable in stars of all spectral types and even in the most metal-poor stars. The abundances of magnesium and other elements were reviewed by Suess & Urey (1956) who also gave the constraints based on different theories of the formation of the elements. The cosmic evolution of magnesium with its three stable isotopes (^{24}Mg, ^{25}Mg, ^{26}Mg) and their evolution after production in massive and intermediate-mass stars was followed by Vangioni & Olive (2019). Magnesium abundance measured in stars have, in recent years, served as a key tracer of Galactic chemical evolution (Fuhrmann (1998); Weinberg et al. (2019)), benefiting from data for hundreds of thousands of stars from the Apache Point Observatory Galactic Evolution Experiment (APOGEE - Abdurro'uf et al. (2022)) and Galactic Archelogy with Hermes (GALAH - Buder et al. (2021)) surveys.

For the particular study, spectral lines are selected based on the spectral type of the star. The optically thin Mg emission line at 880.7 nm from the transition 3s3p $^1P_1 \leftarrow$ 3s3d $^1D_2$ is utilized to track the level of chromospheric activity in active pre-main sequence stars Yamashita et al. (2024). Infrared Mg lines are used for precise observations of polarization in Solar emission Chang (1987). Esteva & Mehlman (1974) identified 24 resonances in neutral magnesium absorption spectra that belong to autoionization lines.

In the Laboratory for Atomic Collisions Processes at the Institute of Physics Belgrade there have been many studies of electron interactions with metal atom vapors Marinković et al. (2007) and in particular with Mg atom. Studies include elastic electron scattering Predojević et al. (2007), differential cross sections for excitations of the 3s3p $^1P_1$ Filipović et al. (2006), the 3s3p $^3P_1$ Predojević et al. (2011) and the 3s4s $^1S_0$, 3s3d $^1D_2$ and 3s4p $^1P_1$ Predojević et al. (2008) states. Autoionizing levels have been studied for Zn atom Predojević B. et al. (2004) and for Bi atom Marinković et al. (2008).

Most recently, the study of elastic electron scattering from magnesium atom below 1 keV impact energy have been done by Adibzadeh et al. (2024). They employed a semi-empirical approach in order to calculate elastic differential cross sections, integrated and momentum transfer cross sections. The comprehensive calculations of excitation cross sections of states below the first ionization limit have been performed by Gedeon et al. (1999). Calculations for the electron impact ionization of the Mg ground state leading to Mg^+(3s) and Mg^+(3p) were performed by Bartschat et al. (2007). Fung & Yih (2001) have measured the absolute photoabsorption cross sections in the wide spectral range that also covers the autoionizing series $3pns\ ^{1,3}P_1$ and $3pnd\ ^1P_1$.

Here we present autoionizing energy loss spectra of the magnesium atom at electron impact energies of $E_0 = 30$ and 40 eV and scattering angles of 6°and 10°. The first ionization limit of Mg is 7.646 eV with the ground cation state 3s $^2S_{1/2}$. The autoionizing spectra are presented from the ionization limit up to 12 eV energy loss.

2. Experimental method

For the experiments of electron collisions with metal atom vapors we have used a specially designed electron spectrometer that is presented elsewhere in greater detail Panajotović et al. (2004); Marinković et al. (2007), so here it will be just briefly presented. It consists of thoroughly covered units of the monochromator and analyzer based on hemispherical energy selectors. The source of electrons is a thoriated hairpin cathode that is brought to the potential of the desired electron impact energy with respect to the grounded vacuum chamber and the last exit electrode. All electrodes are made of oxygen-free high-conductivity gold-plated copper making three or four electrode electrostatic lenses. The hemispheres are made of molybdenum with the mean radius of 49.8 mm. A single channeltron is used as an electron detector. The angular range of the rotating analyzer is from $-30°$ to $+150°$.

An effusive beam of magnesium atom vapor is produced by non-magnetic stainless steel oven of Knudsen type. It ends with the cylindrical channel that has an aspect ratio of $\gamma = 0.075$. The oven is filled with 99.9% pure magnesium granules. The oven bottom temperature was about 780 K, while the exit nozzle was 50 K higher. This temperature is higher than that used for measurements of magnesium spectra below ionization limit due to requirements for high-intensity atomic beam. That results in the occurrence of the double scattering features in the spectra.

The energy resolution of the energy loss spectra was 65 meV. The energy scale is calibrated by the position of the most pronounced peak in the spectrum, i.e. the 3s3p$^1P_1$ state excitation at 4.346 eV.

3. Results and discussion

In Figure 1 we present the energy loss spectra of the neutral magnesium atom at the impact electron energy $E_0 = 30$ eV and the scattering angle 10°, and in Figure 2 at $E_0 = 40$ eV and 6°. This covers the region of autoionization states, from the ionization threshold up to 12 eV. The observerd autoionizing states are presented in Table 1 together with the energy level list from NIST database Kramida et al. (2024). All these autoionizing states come from the simultaneous excitation of two s electrons to the higher orbitals. The first observed state is assigned as $3p^2\ ^1S_0$ states, while the other states are of the $3pnl$ symmetry where l orbitals are s, p, d and n=3-7. The second ionization Mg$^+$ limit is doublet $3p$ $^2P_{1/2,3/2}$ at 12.069 and 12.080, respectively.

All autoionizing states that come from the excitation of the inner-shell orbital, $2p$, may be shown in the electron energy loss spectra above 54.8 eV. In the absorption spectrum, they have first been identified by Newsom (1971) and calculated by Mansfield & Connerade (1972). Kim & Tayal (2000) have calculated the photoionization cross sections and resonances of the ground state atomic magnesium to the Mg$^+$(3s) and Mg$^+$(4p) thresholds using the variational R-matrix method and the multichannel quantum defect theory. Their values for the Mg$^+$(3s) levels are also presented in Table 1.

Mg autoionizing levels and Auger transitions were measured by Pejčev et al. (1977) using ejected electron spectroscopy. They exploited electrons of incident energy from 62 to 400 eV and observed ejected electrons at 75°with respect to an incident electron beam. The autoionizing states of neutral magnesium were recorded in the energy range from 35 to 50 eV, while for the Mg cation the excited ion state energies were from 57 to 74 eV. Rassi et al. (1977) also measured with high resolution ejected electron spectra of magnesium autoionizing levels that come from the two-electron excitation assigned as $1s^2 2s^2 2p^6 3pnl$ by low-energy electron impact. They were able to identify eight levels assigned as $3pns\ ^1P$ n=4-11, two levels $3pnd\ ^1P$ n=3,4, five levels $3pns\ ^3P$ n=4-8, five levels $3pnd\ ^1F$ n=3-7, three levels $3pnd\ ^1D$ n=3-5, six levels $3pnp\ ^1S$ n=3-8, nine lev-

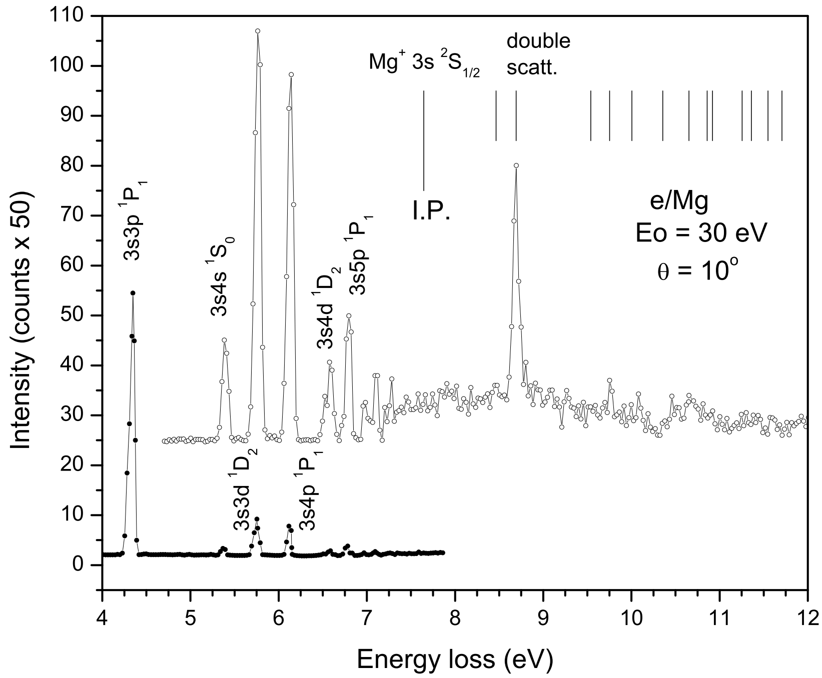

Figure 1. Energy loss at impact energy of $E_0 = 30$ eV and scattering angle of 10°. Vertical lines designate positions of autoionization energies according Kramida et al. (2024) and values are listed in Table 1.

els $3pnp\ ^1D$ n=4-12 and two levels $3pnp\ ^3P$ n=4,5. Tabulated energies of these series of autoionizing states from 8.45 eV to the ionizing limit $Mg^+\ 3p\ ^2P_{1/2}$ can be found in Rassi et al. (1977). The same group of authors has extended the measurements of autoionizing states up to the next ionization limit Mg^+(4s $^2S_{1/2}$) at 16.3 eV.

Trajmar & Williams (1976) provided a series of metal atom cross sections and also examined the autoionization region of the Mg atom. They made a comprehensive review of many atomic metals and gave trends in energy dependencies of cross sections. The energy range of the Mg energy loss spectrum is given from 5 to 19 eV, thus covering both regions, below and above the first ionization limit.

In the spectrum at $E_0 = 40$ eV and the scattering angle of 6°two features are distinctive and we attribute them as $^1D_2$ and $^3D_{1,2,3}$ states. The energies of these states are 10.09 and 10.46 eV, respectively, while the NIST data are 10.005 and 10.355 eV. The singlet-triplet splitting is in both cases the same, 350 meV. The assignment of the spectral features is obscured by the presence

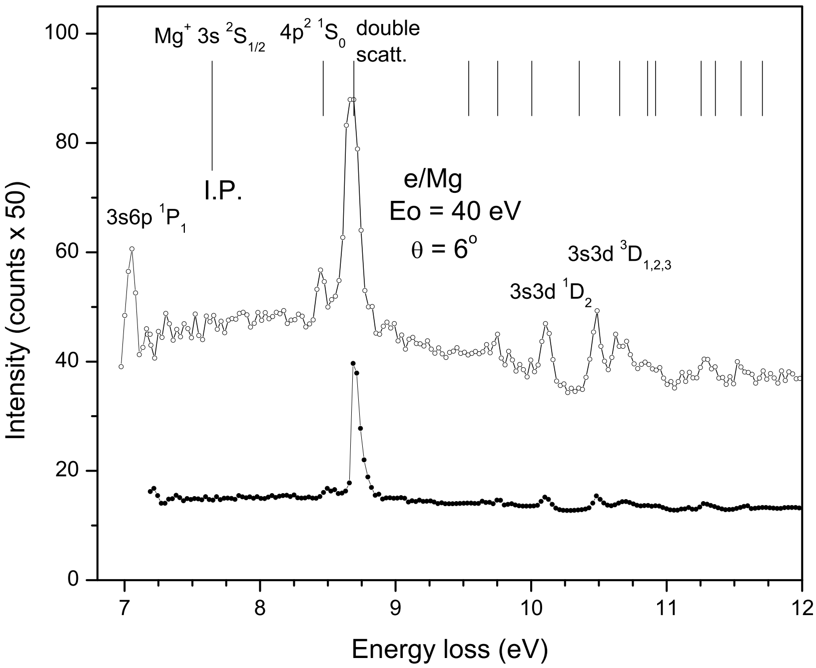

Figure 2. Energy loss at impact energy of $E_0 = 40$ eV and scattering angle of 6°.

of the 3p3d ^1F and 3p4d ^1F levels found by Rassi et al. (1977) at 10.03 and 10.44 eV, respectively. The levels of F symmetry have not been recorded in the NIST data tables. The sum of the ionization energy and the energy of ejected electrons found by Rassi et al. (1977) correspond to the observed energies of the autoionizing states in our energy loss spectra.

4. Conclusions

The Mg autoionizing states between two ionization limits, the $Mg^+(3s\ ^2S_{1/2})$ at 7.646 eV and $Mg^+(3p\ ^2P_{1/2})$ at 12.069 eV have been recorded by electron energy loss spectroscopy at $E_0 = 30$ eV and the scattering angle 10°, and $E_0 = 40$ eV and 6°. The autoionizing states are identified as two-electron excited states of the type $3pnl$. In all spectra the double scattering feature of the most intense peak in magnesium energy loss, 3s3p $^1P_1$, is recorded at 8.69 eV. The two features at 10.09 and 10.46 eV we assigned to the 3s3d $^1D_2$ and 3s3d $^3D_{1,2,3}$ states. This assignment needs further studies in order to resolve the contributions of the 3p3d ^1F and 3p4d ^1F levels observed previously by Rassi et al. (1977).

Table 1. Observed energies of autoionization states, their energies in NIST table Kramida et al. (2024), calculated resonances by Kim & Tayal (2000) and assignment.

energy present	energy NIST	energy Kim & Tayal (2000)	assignment
8.45 ± 0.03	8.465	-	3p^2 ^1S_o
8.79	-	-	double scattering
-	9.539	-	3p4s $^3P_1$
9.74 ± 0.03	9.753	9.706	3p4s $^1P_1$
10.09 ± 0.03	10.005	-	3p3d $^1D_2$
10.46 ± 0.03	10.354, 10.355, 10.357	-	3p3d $^3D_{1,2,3}$
10.65 ± 0.03	10.653	10.651	3p3d $^1P_1$
10.83 ± 0.03	10.859	-	3p5s $^3P_1$
10.91 ± 0.03	10.918	10.922	3p5s $^1P_1$
11.26 ± 0.03	11.255	11.247	3p4d $^1P_1$
11.36 ± 0.03	11.359, 11.387	-	3p4d $^{3,1}P_1$
11.57 ± 0.03	11.549	11.538	3p5d $^1P_1$
-	11.597, 11.615	11.610	3p7s $^{3,1}P_1$
11.70 ± 0.03	11.707	11.698	3p6d $^1P_1$

Presented data is of interest for astrophysical and plasma communities as well as for our fundamental knowledge of autoionization processes and atomic energy level structure.

Acknowledgements. The authors are extremely thankful to late Prof. Dr. Vladimir M. Pejčev for his contributions to experimental work and stimulating discussions on autoionization states and ejected electron spectra. This work has been supported by the Institute of Physics Belgrade through the grant from Ministry of Science, Technological Development and Innovation. B.P.M. acknowledges support of the Science Fund of the Republic of Serbia, Grant No. 6821, Atoms and (bio)molecules - dynamics and collisional processes on short time scale – ATMOLCOL.

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