Electron-impact single ionization of Si⁺

Valdas Jonauskas

Institute of Theoretical Physics and Astronomy, Vilnius University, Saulėtekio Av. 3, 10257 Vilnius, Lithuania
 e-mail: valdas.jonauskas@tfai.vu.lt

Received 25 April 2020 / Accepted 9 August 2020

ABSTRACT

Electron-impact single ionization is studied in the Si⁺ ion by considering transitions among energy levels. The study includes excitation-autoionization (EA) and collisional ionization processes. The excitations are investigated up to shells with the principal quantum numbers $n \leq 10$. It is shown that correlation effects included in the EA calculations play a crucial role in explaining measurements. The correlation effects diminish the EA cross sections by $\sim 30\%$ compared to single-configuration calculations. However, the collisional ionization is not significantly affected by an extension of the basis of interacting configurations. Good agreement between the presented level-to-level distorted wave data and experimental measurements is found for the single ionization of the Si⁺ ion.

Key words. atomic data – atomic processes

1. Introduction

Silicon is the seventh most abundant element in the Universe and the second most abundant element on Earth. Modeling of the silicon emission in astrophysical or laboratory plasmas requires reliable atomic data. The structure of the emission spectra is defined by a charge state distribution in the plasma. Electron-impact ionization along with the radiative and dielectronic recombination define the charge state distribution in the collisionally ionized plasma, such as those formed in the stellar coronae, supernova remnants, galaxies, and the intracluster medium of galaxy clusters. Multiple ionization is important for systems that are suddenly exposed to an abundance of energetic electrons (Müller 1986; Hahn & Savin 2015). On the other hand, the study of multiple ionization is quite complicated (Pindzola et al. 2007; Colgan & Pindzola 2012; Jonauskas et al. 2014; Liu et al. 2018) since it has to deal with the four-body Coulomb problem.

Electron-impact single-ionization cross sections for Si⁺ were measured and analyzed by Djurić et al. (1993). The semiempirical Lotz formula (Lotz 1968) was adopted to determine the fraction of metastable ions in the parent beam. Additional assessments were taken to eliminate contamination from the N₂⁺ and CO⁺ ions in experimental data since these ions have the same mass-to-charge ratio M/q as Si²⁺. Theoretical values were calculated using the configuration average distorted wave (CADW) method (Pindzola et al. 1983). A good agreement of the theoretical data with measurements was obtained (Djurić et al. 1993). The study included direct and indirect processes of electron-impact single ionization. Direct ionization (DI) was investigated for the 3s and 3p subshells. The excitations from the 2p and 3s subshells to shells with the principal quantum numbers $n = 4, 5$ were considered for the indirect process. However, the strong 3s → 3d excitations were missing from the CADW calculations (Djurić et al. 1993). Furthermore, the excitations to the higher shells ($n > 5$) were not investigated in that work (Djurić et al. 1993). On the other hand, it was demonstrated that the excitations to the high- n shells have

to be analyzed to determine the reliable cross sections for the excitation-autoionization (EA) process (Zhang & Kwon 2014; Jonauskas et al. 2015; Kynienė et al. 2015, 2016; Borovik et al. 2016; Jin et al. 2020). As such, a convergence of the cross sections has to be confirmed for the indirect process. The electron-impact single-ionization cross sections for the Si⁺ ion were later investigated by performing level-to-level distorted wave (LLDW) calculations (Dere 2007). It was noted that the LLDW values showed a fair reproduction of the Si⁺ cross sections; however, details of the calculations were not provided. It can be assumed that the same type of excitations that was presented in the CADW study (Djurić et al. 1993) were analyzed. The CADW study also omitted the influence of the radiative damping for the doubly excited states of the Si⁺ ion. The autoionization branching ratio was taken to be unity for all autoionizing configurations. The radiative damping diminishes the EA cross sections since the autoionizing states can also decay through the radiative transitions to the lower states of the Si⁺ ion.

Therefore, the aim of the current work is to study the electron-impact single-ionization process for the Si⁺ ion. Excitations to shells with $3 \leq n \leq 10$ for EA are investigated. Radiative damping is taken into account for all levels above the single-ionization threshold of the Si⁺ ion. Furthermore, an influence of the correlation effects for the direct and indirect processes of the electron-impact ionization is investigated.

The rest of the paper is organized as follows. Section 2 presents a brief outline of the theoretical approach. In addition, the main channels of the direct and indirect processes are defined. In Sect. 3, the obtained results are discussed. Finally, we end with the conclusions from the present investigation.

2. Theoretical approach

The cross section for the electron-impact single ionization from level i to level f includes direct and indirect processes:

$$\sigma_{if}(\varepsilon) = \sigma_{if}^{\text{DI}}(\varepsilon) + \sum_j \sigma_{ij}^{\text{CE}}(\varepsilon) B_{jf}^{\text{a}}, \quad (1)$$

where $\sigma_{if}^{\text{DI}}(\varepsilon)$ is the cross section of the direct single collisional ionization process and ε is an energy of the incident electron. The second term in Eq. (1) corresponds to the indirect process: electron-impact excitation with subsequent autoionization. Therefore, $\sigma_{ij}^{\text{CE}}(\varepsilon)$ is the electron-impact excitation cross section to the intermediate level j of the initial ion, and B_{jf}^a is a branching ratio for the autoionization process from level j to the final level, level f . The autoionization branching ratio diminishes cross sections of the EA process since the autoionizing levels can decay through radiative transitions to the energetically lower levels of the same ion. It defines a part of the population transferred from level j to level f by Auger transition and is expressed by the equation

$$B_{jf}^a = \frac{A_{jf}^a}{\sum_m A_{jm}^r + \sum_n A_{jn}^a}, \quad (2)$$

where A^r and A^a are the radiative and Auger transition probabilities, respectively. The summation in the denominator goes through all levels that can be reached by the radiative and Auger decays from level j .

The direct process studied for the Si^+ ion includes collisional ionization from the 3s and 3p subshells:

The collisional ionization from the 2p subshell produces ions above the double ionization threshold, and this mainly leads to states of the Si^{2+} ion. Therefore, the ionization from the 2p subshell was not included in the study of the single-ionization cross sections. The EA channels for the Si^+ ion were determined by excitations from the 2p and 3s subshells to autoionizing levels of the produced configurations:

where $4 \leq n \leq 10$, $l < n$, and $l \leq 5$. The $3s \rightarrow 3p$ excitation was not included in calculations since the $3s^1 3p^2$ configuration is below the single-ionization threshold. Furthermore, the excitations from the 3p subshell of the ground configuration do not contribute to the single ionization since all levels of the produced configurations are below the single-ionization threshold of the Si^+ ion. On the other hand, the valence shell excitations can be significant for cross sections close to the ionization threshold (Kwon & Savin 2012).

Energy levels, radiative and Auger transition probabilities, electron-impact excitation, and single-ionization cross sections were studied using Flexible Atomic Code (FAC) (Gu 2008), which implements the Dirac-Fock-Slater (DFS) approach. Continuum orbitals of the incident and scattered electrons were estimated in a potential of the ionizing ion since the obtained cross sections provide better agreement with experimental data (Djurić et al. 1993). The electron-impact excitation and ionization cross sections were investigated using the distorted wave (DW) approximation. Calculations of the single-ionization cross sections using the DW approximation usually provide a good agreement with the experimental data for highly ionized ions (Pindzola & Griffin 1997; Loch et al. 2005; Kwon & Savin 2012; Borovik et al. 2015; Jonauskas et al. 2019). It is well

Fig. 1. Energy levels of the ground configurations for the Si^+ , Si^{2+} , and Si^{3+} ions in addition to energy levels of the $3s^1 3p^1 3d^1$, $3s^1 3p^1 4s^1$, $3s^1 3p^1 4p^1$, $3s^1 3p^1 4d^1$, and $3s^1 3p^1 4f^1$ configurations. The first excited configuration of Si^{2+} is also presented. The red represents even configurations and the blue represents odd configurations.

known that the DW approximation often overestimates the single-ionization cross sections for neutral atoms and near neutral ions. Previously, the binary-encounter-dipole (BED) and binary-encounter-Bethe (BEB) models were developed for the direct process to deal with these ionization stages (Kim & Rudd 1994). These models, with the scaled plane-wave-Born cross sections, demonstrated a good agreement with experimental data (Kim 2001; Kim & Desclaux 2002; Kwon et al. 2005, 2006). It was suggested to use the scaled DW cross sections for the atoms and low-ionization ions (Jonauskas 2018; Kynienė et al. 2019a). However, previous DW calculations of the cross sections for the single ionization in Si^+ showed good agreement with the measurements (Djurić et al. 1993). Therefore, the same approximation was used in this study.

The Maxwellian rate coefficients were calculated using cross sections obtained for electron-impact direct and indirect ionization processes in the Si^+ ion. The rate coefficient $\alpha_{ij}(T_e)$ for the Maxwellian-Boltzmann electron energy distribution at electron temperature T_e was determined by the equation

$$\alpha_{ij}(T_e) = \left(\frac{1}{k_B T_e} \right)^{\frac{3}{2}} \left(\frac{8}{m_e \pi} \right)^{\frac{1}{2}} \int_0^\infty \varepsilon \sigma_{ij}(\varepsilon) \exp\left(-\frac{\varepsilon}{k_B T_e}\right) d\varepsilon. \quad (5)$$

Here, k_B is the Boltzmann constant and m_e is the electron mass.

3. Results

Energy levels of the ground configurations for the Si^+ , Si^{2+} , and Si^{3+} ions are presented in Fig. 1. In addition, configurations corresponding to the $3s \rightarrow 3d$, $3s \rightarrow 4l$ ($l = 0, \dots, 4$) excitations are shown. It can be seen that the energy levels of the $3s^1 3p^1 3d^1$, $3s^1 3p^1 4s^1$, and $3s^1 3p^1 4p^1$ configurations straddle the ionization threshold. The energy levels of the $3s^1 3p^2$ configuration are below the ionization threshold and, therefore, are not presented in Fig. 1. The theoretical single-ionization threshold for the ground $[\text{Ne}] 3s^2 3p^1$ configuration is 15.67 eV. This is slightly below the National Institute of Standards and Technology's (NIST) recommended value of 16.35 eV (Kramida et al. 2019). On the other hand, the same tendency for the FAC ionization thresholds compared to the NIST data were also determined for other ions (Jonauskas et al. 2015; Konevičiūtė et al. 2018; Jonauskas 2018; Kynienė et al. 2019b).

Fig. 2. Single-ionization cross sections for the ground level of the Si⁺ ion. The DI cross sections were obtained in the potential of the ionized ion. The solid (green) line represents the total LLDW cross sections, the dashed (green) line represents the LLDW DI cross sections, the dashed-dotted (blue) line represents the total CADW cross sections (Djurić et al. 1993), and the dotted (blue) line represents the DI CADW cross sections (Djurić et al. 1993). Experiment is shown by open circles with error bars (Djurić et al. 1993).

Single-ionization cross sections obtained in a potential of the ionized ion are compared to the CADW calculations and experimental measurements (Djurić et al. 1993) in Fig. 2. The LLDW values are higher than the measurements on the low-energy side. On the other hand, the theoretical cross sections are lower than the experimental ones from the peak to the higher energies of the incident electron. What is more, the DI cross sections obtained using the DFS approximation are lower by approximately a factor of two compared to the CADW values. This is the main reason why the total LLDW cross sections are lower than the CADW calculations at the higher energies.

Electron-impact single-ionization cross sections obtained in a potential of the ionizing ion are shown in Fig. 3. The CADW DI cross sections (Djurić et al. 1993) are slightly higher than the LLDW values at higher energies of the incident electron. However, the total LLDW cross sections are well above measurements at the peak values. It should be noted that a good agreement with the experimental values is obtained for the CADW calculations at the lower energies. However, these calculations omit the strong 3s → 3d excitations. The produced 3s³3p³3d¹ configuration has energy levels that straddle the single-ionization threshold (Fig. 1). This configuration may have had an average energy below the ionization threshold in the CADW calculations and, therefore, the excitations to this configuration were not investigated (Djurić et al. 1993). What is more, the excitations to the shells with $n > 5$ were not included in the previous calculations. Therefore, all omitted EA channels should lead to the much higher values of the total single-ionization cross sections obtained using the CADW approximation. The LLDW cross sections that include the EA channels corresponding to the excitations to the shells with $4 \leq n \leq 5$ are shown in Fig. 3. The CADW values are slightly above the presented LLDW cross sections starting from the peak. The difference can be explained by the higher CADW DI cross sections compared to the LLDW calculations. A similar situation for the CADW DI cross sections compared to the LLDW ones was previously determined (Zhang & Kwon 2014). Furthermore, the CADW method can provide different EA results for configurations with energy levels that straddle the single-ionization threshold.

Fig. 3. Single-ionization cross sections for the ground level of the Si⁺ ion. The DI cross sections were obtained in the potential of the ionizing ion. The solid (green) line represents the total LLDW cross sections, the dashed (green) line represents the LLDW DI cross sections, the dashed-dotted-dotted (red) line represents the total LLDW cross sections for excitations to $4 \leq n \leq 5$, the dashed-dotted (blue) line represents the total CADW cross sections (Djurić et al. 1993), and the dotted (blue) line represents the DI CADW cross sections (Djurić et al. 1993). Experiment is shown by open circles with error bars (Djurić et al. 1993).

Fig. 4. Accumulated cross sections of the EA channels contributing to the ionization of the ground level of Si⁺. The EA channels correspond to excitations to shells with a different principal quantum number.

Autoionization branching ratios studied for all EA channels lead to diminished cross sections for indirect process by ~5%. Therefore, radiative damping does not play a significant role when comparing the LLDW and CADW (Djurić et al. 1993) values.

The contribution of the EA channels corresponding to excitations to various shells is presented in Fig. 4. The excitation to the 3d subshell dominates compared to the other channels of indirect process. The excitations to the shells with $n > 5$ provide ~14% for the peak value of the EA process. All this shows that the previously omitted EA channels increase the EA cross sections by a factor of two. Therefore, if the total single-ionization CADW cross sections included the excitations to shells with $n = 3$ and $n > 5$, it would lead to strongly overestimated values compared to measurements (Djurić et al. 1993).

The EA channels corresponding to excitations to subshells with the orbital quantum number $l = 2$ dominate for indirect process (Fig. 5). These excitations amount to ~50% of the EA

Fig. 5. EA channels corresponding to excitations to various orbitals.

cross sections. As mentioned above, the main part is provided by the $3s \rightarrow 3d$ excitation (Fig. 4). The contribution of the excitations to the subshells with $l = 0$ or $l = 1$ is more than a factor of two lower compared to the $l = 2$ case. What is more, the excitations to the subshells with $l = 4$ give a negligible contribution to the EA cross sections. It should be noted that the excitations to the subshells with $l = 4$ are important for ions with the open $4f$ subshell in the ground configuration (Jonauskas et al. 2015; Kynienė et al. 2015, 2016).

Correlation effects play an important role in the study of energy levels, radiative transitions (Jonauskas et al. 2010), and Auger cascades (Jonauskas et al. 2008, 2011; Palaudoux et al. 2010). What is more, it was demonstrated that the correlation effects have to be included in the analysis of electron-impact ionization cross sections (Kynienė et al. 2019a; Jonauskas et al. 2019). The configuration interaction (CI) strength (Karazija 1996; Kučas et al. 1997; Karazija & Kučas 2013) was previously used to determine the bases of interacting configurations. In this work, the influence of the correlation effects for the direct and indirect ionization processes in the Si^+ ion were analyzed using the CI method. The admixed configurations with the largest weight in an expansion of the intermediate wavefunction were determined from the diagonalization of the Hamiltonian matrix. The initial CI bases that were used to determine the main admixed configurations were produced by making one electron excitation up to shells with $n = 9$ and two electron excitations up to shells with $n = 4$ from the $n = 3$ shell of the ground configuration of the Si^+ or Si^{2+} ions.

The $3s^2 3p^1$, $3p^3$, $3s^1 3p^1 3d^1$, $3s^2 4p^1$, and $3s^1 3p^1 4s^1$ configurations were used to build a basis of the interacting configurations in the study of the DI process for the Si^+ ion. Furthermore, the even parity CI basis consists of the $3s^2$, $3p^2$, $3s^1 3d^1$, $3s^1 4s^1$, $3d^2$, and $3p^1 4p^1$ configurations in Si^{2+} . The odd parity CI basis includes the $3s^1 3p^1$, $3p^1 3d^1$, and $4s^1 4p^1$ configurations. All this leads to a decrease in the cross sections of the direct process by $\sim 2\%$ for the peak values. Furthermore, since the theoretical single-ionization threshold is slightly below the NIST-recommended value, all energy levels of the Si^{2+} ion are increased by 0.78 eV for the direct processes in this work. As such, the DI cross sections were decreased by an additional $\sim 4\%$.

The basis of interacting configurations consists of the $3s^2 3p^1$, $3p^3$, $3s^1 3p^1 3d^1$, $3s^2 4p^1$, $3s^1 3p^1 ns$, $3s^1 3p^1 nd$, and $3p^1 n's^2$ ($n = 4, 5, 6$, $n' = 4, \dots, 9$) configurations for the EA channels corresponding to the $3s \rightarrow 3d$, $3s \rightarrow ns$, and $3s \rightarrow nd$ excitations. The inclusion of correlation effects diminishes the EA cross sections

Fig. 6. Single-ionization cross sections for the ground level of Si^+ . The solid (green) line represents the total CI LLDW cross sections, the dashed-dotted (magenta) line represents the single-configuration cross sections when DI values are obtained in the potential of the ionizing ion, the dashed-dotted-dotted (red) line represents single-configuration cross sections when DI values are obtained in the potential of the ionized ion, and the dotted (blue) line represents the total CADW cross sections (Djurić et al. 1993). Experiment is shown by open circles with error bars (Djurić et al. 1993).

by $\sim 5 \times 10^{-16} \text{ cm}^2$ ($\sim 36\%$). The correlation effects improve the agreement with measurements on the low-energy side and for peak values (Fig. 6). The CADW calculations that omit many EA channels are $\sim 6\%$ lower than the LLDW cross sections for the values at the peak of the cross sections. However, very good agreement is obtained between the LLDW and CADW values on the high-energy side. Single-configuration cross sections show large discrepancies from the measurements (Fig. 6).

The weight of the $3p^3$ configuration in expansion of the intermediate wavefunction for levels of the ground configuration amounts to $\sim 3\%$. This agrees with the NIST value (Kramida et al. 2019). Therefore, the EA channels corresponding to excitations from the $3p^3$ configuration were studied for the intermediate wavefunction of the ground configuration. The $3p \rightarrow nl$ ($n = 3, \dots, 10$, $l < n$, $l < 5$) excitations were investigated for the $3p^3$ configuration. The contribution to cross sections of the excitations from the $3p^3$ configuration in expansion of the intermediate wavefunction for the ground level is shown in Fig. 7. These cross sections appear from $\sim 24 \text{ eV}$. The total single-ionization cross sections are increased by $\sim 6\%$ and are slightly above the measurements for a peak value. The theoretical cross sections are in better agreement with the measurements compared to the CADW data from 70 eV to high energies of incident electrons.

The weight of the $3s^1 3p^1 3d^1$ configuration is $\sim 2\%$ in the expansion of the intermediate wavefunction of the ground configuration. However, the EA channels corresponding to excitations from the $3s$ and $3p$ subshells of this configuration contribute cross sections that are approximately two orders of magnitude lower than the total single-ionization cross sections. It should be noted that the excitations from the $3d$ subshell have already been included in calculations by considering the excitations from the $3s$ subshell of the $3s^2 3p^1$ configuration using the intermediate wavefunction.

The remaining discrepancies among the LLDW cross sections and measurements may be attributed to correlation effects that are missing in our study. A large basis of interacting configurations may help resolve this problem. Furthermore,

Fig. 7. Single-ionization cross sections for the ground level of Si⁺. The solid (black) line represents the total CI LLDW cross sections that include excitations from the 3p³ configuration in the intermediate wavefunction of the ground configuration (see text for explanation), the dashed (green) line represents cross sections without excitations from the 3p³ configuration, the dashed-dotted (magenta) line represents single-configuration cross sections when DI values are obtained in the potential of the ionizing ion, the dashed-dotted-dotted (red) line represents single-configuration cross sections when DI values are obtained in the potential of ionized ion, and the dotted (blue) line represents the total CADW cross sections (Djurić et al. 1993). Experiment is shown by open circles with error bars (Djurić et al. 1993).

Fig. 8. Comparison of the contribution from the DI and EA channels for the ground level of Si⁺. Experiment is shown by open circles with error bars (Djurić et al. 1993).

the electron-impact single-ionization cross sections would have to be diminished by the direct double ionization cross sections if it is assumed that the direct double ionization is formed by the sequential ionization. This effect for the single-ionization cross sections has to appear from the double ionization threshold (47.71 eV). It was previously demonstrated that the single-ionization calculations have to include the diminishing contribution from the direct double ionization to explain the measurements (Pakalka et al. 2018; Jonauskas 2019). What is more, additional measurements may be needed to determine the reason for the discrepancies between the theoretical and experimental data.

A comparison of the contribution from direct and indirect single-ionization processes is made in Fig. 8. The DI cross sections dominate in practically all energy ranges except the low-

energy side. The DI from the 3p subshell is ~10% stronger than the ionization from the 3s subshell for the peak values.

Finally, single-ionization cross sections for direct and indirect single-ionization processes are presented in Table A.1. The corresponding Maxwellian rate coefficients are shown in Table A.2.

4. Conclusions

Electron-impact single-ionization cross sections for the Si⁺ ion were studied using the DFS approximation. The direct and indirect ionization processes were investigated by considering transitions among energy levels. The contribution of the EA process to the total single-ionization cross sections is larger compared to the DI process obtained in the single-configuration approximation. The DI from the 2p subshell provides a slightly higher contribution than the DI from the 3s subshell. The strongest EA channel corresponds to the 3s → 3d excitation (~35%). The excitations to shells with $n > 5$ increases the EA cross sections by ~14%.

It is demonstrated that correlation effects play a crucial role in explaining measurements. The correlation effects decrease the total single-ionization cross sections by ~20% for the peak value. The influence of the correlation effects is less pronounced for the DI process. The DI cross sections are diminished by ~2% when the correlation effects are taken into account. Finally, the theoretical single-ionization cross sections are above the measurements by ~4% at the peak value and below the experimental values on the high-energy side. On the other hand, additional measurements may help resolve the disagreement between the theoretical and experimental cross sections.

Acknowledgements. Part of computations was performed on resources at the High Performance Computing Center “HPC Saulėtekis” in Vilnius University Faculty of Physics.

References

- Borovik, A., Jr., Gharaibeh, M. F., Schippers, S., & Müller, A. 2015, *J. Phys. B: At. Mol. Opt. Phys.*, **48**, 035203
- Borovik, A., Jr., Ebinger, B., Schury, D., Schippers, S., & Müller, A. 2016, *Phys. Rev. A*, **93**, 012708
- Colgan, J., & Pindzola, M. 2012, *Eur. Phys. J. D*, **66**, 284
- Dere, K. P. 2007, *A&A*, **466**, 771
- Djurić, N., Bell, E. W., Guo, X. Q., et al. 1993, *Phys. Rev. A*, **47**, 4786
- Gu, M. F. 2008, *Can. J. Phys.*, **86**, 675
- Hahn, M., & Savin, D. W. 2015, *ApJ*, **800**, 68
- Jin, F., Borovik, A., Jr., Ebinger, B., & Schippers, S. 2020, *J. Phys. B: At. Mol. Opt. Phys.*, **53**, 075201
- Jonauskas, V. 2018, *A&A*, **620**, A188
- Jonauskas, V. 2019, *J. Quant. Spectrosc. Radiat. Transf.*, **239**, 106659
- Jonauskas, V., Karazija, R., & Kučas, S. 2008, *J. Phys. B: At. Mol. Opt. Phys.*, **41**, 215005
- Jonauskas, V., Kisieliū, R., Kynienė, A., Kučas, S., & Norrington, P. H. 2010, *Phys. Rev. A*, **81**, 012506
- Jonauskas, V., Kučas, S., & Karazija, R. 2011, *Phys. Rev. A*, **84**, 053415
- Jonauskas, V., Pranciševičius, A., Masys, Š., & Kynienė, A. 2014, *Phys. Rev. A*, **89**, 052714
- Jonauskas, V., Kynienė, A., Merkelis, G., et al. 2015, *Phys. Rev. A*, **91**, 012715
- Jonauskas, V., Kynienė, A., Kučas, S., et al. 2019, *Phys. Rev. A*, **100**, 062701
- Karazija, R. 1996, *Introduction to the Theory of X-ray and Electronic Spectra of Free Atoms* (New York: Plenum Press)
- Karazija, R., & Kučas, S. 2013, *J. Quant. Spectrosc. Radiat. Transf.*, **129**, 131
- Kim, Y.-K. 2001, *Phys. Rev. A*, **64**, 032713
- Kim, Y.-K., & Desclaux, J.-P. 2002, *Phys. Rev. A*, **66**, 012708
- Kim, Y.-K., & Rudd, M. E. 1994, *Phys. Rev. A*, **50**, 3954
- Koncevičiūtė, J., Kučas, S., Masys, Š., Kynienė, A., & Jonauskas, V. 2018, *Phys. Rev. A*, **97**, 012705

Kramida, A., Ralchenko, Yu., Reader, J., & NIST ASD Team 2019, *NIST Atomic Spectra Database (ver. 5.7.1)*, [Online]. Available: <https://physics.nist.gov/asd> [2020, April 10]. National Institute of Standards and Technology, Gaithersburg, MD

Kučas, S., Jonauskas, V., & Karazija, R. 1997, *Phys. Scr.*, **55**, 667

Kwon, D.-H., & Savin, D. W. 2012, *Phys. Rev. A*, **86**, 022701

Kwon, D.-H., Rhee, Y.-J., & Kim, Y.-K. 2005, *Int. J. Mass Spectrom.*, **245**, 26

Kwon, D.-H., Rhee, Y.-J., & Kim, Y.-K. 2006, *Int. J. Mass Spectrom.*, **252**, 213

Kynienė, A., Masys, Š., & Jonauskas, V. 2015, *Phys. Rev. A*, **91**, 062707

Kynienė, A., Pakalka, S., Masys, Š., & Jonauskas, V. 2016, *J. Phys. B: At. Mol. Opt. Phys.*, **49**, 185001

Kynienė, A., Kučas, S., Pakalka, S., Masys, Š., & Jonauskas, V. 2019a, *Phys. Rev. A*, **100**, 052705

Kynienė, A., Kučas, S., Masys, Š., & Jonauskas, V. 2019b, *A&A*, **624**, A14

Liu, P., Zeng, J., & Yuan, J. 2018, *J. Phys. B: At. Mol. Opt. Phys.*, **51**, 075202

Loch, S., Ludlow, J., Pindzola, M., Whiteford, A., & Griffin, D. 2005, *Phys. Rev. A*, **72**, 052716

Lotz, W. 1968, *Z. Phys.*, **216**, 241

Müller, A. 1986, *Phys. Lett. A*, **113**, 415

Pakalka, S., Kučas, S., Masys, Š., et al. 2018, *Phys. Rev. A*, **97**, 012708

Palaudoux, J., Lablanquie, P., Andric, L., et al. 2010, *Phys. Rev. A*, **82**, 043419

Pindzola, M. S., & Griffin, D. C. 1997, *Phys. Rev. A*, **56**, 1654

Pindzola, M. S., Griffin, D. C., & Bottcher, C. 1983, *J. Phys. B: At. Mol. Opt. Phys.*, **16**, L355

Pindzola, M. S., Robicheaux, F., Loch, S. D., et al. 2007, *J. Phys. B: At. Mol. Opt. Phys.*, **40**, R39

Zhang, D.-H., & Kwon, D.-H. 2014, *J. Phys. B: At. Mol. Opt. Phys.*, **47**, 075202

Table A.1. continued.

Energy (eV)	DI:3s	DI:3p	EA	Total
62	3.701+3	4.767+3	5.816+3	1.457+4
65	3.659+3	4.664+3	5.589+3	1.420+4
68	3.612+3	4.561+3	5.379+3	1.384+4
70	3.579+3	4.493+3	5.263+3	1.363+4
72	3.548+3	4.426+3	5.175+3	1.345+4
75	3.495+3	4.329+3	5.050+3	1.317+4
80	3.407+3	4.173+3	4.856+3	1.274+4
100	3.060+3	3.631+3	4.223+3	1.121+4
200	1.942+3	2.166+3	2.793+3	7.117+3
300	1.423+3	1.551+3	2.024+3	5.162+3
500	9.294+2	9.902+2	1.426+3	3.456+3
1000	5.026+2	5.239+2	7.427+2	1.830+3
2000	3.326+2	3.455+2	4.224+2	1.140+3
3000	2.365+2	2.438+2	2.908+2	7.994+2

Notes. $a \pm b = a \times 10^{\pm b}$.

Table A.2. Maxwellian rate coefficients (in $10^{-10} \text{ cm}^3 \text{ s}^{-1}$) for the ground level.

Energy (eV)	DI:3s	DI:3p	EA	Total
1+4	2.452–10	6.989–7	1.668–6	2.982–6
2+4	1.686–4	1.180–2	2.406–2	3.835–2
4+4	1.637–1	1.662+0	3.460+0	5.370+0
6+4	1.720+0	8.887+0	1.793+1	2.877+1
8+4	5.681+0	2.072+1	4.007+1	6.688+1
1+5	1.172+1	3.452+1	6.406+1	1.109+2
2+5	5.051+1	9.534+1	1.526+2	3.012+2
4+5	1.028+2	1.525+2	2.151+2	4.777+2
6+5	1.269+2	1.723+2	2.321+2	5.416+2
8+5	1.385+2	1.793+2	2.367+2	5.665+2
1+6	1.442+2	1.810+2	2.368+2	5.750+2
2+6	1.470+2	1.718+2	2.225+2	5.528+2
4+6	1.362+2	1.517+2	1.944+2	4.860+2
6+6	1.247+2	1.363+2	1.750+2	4.403+2
8+6	1.156+2	1.248+2	1.603+2	4.062+2
1+7	1.084+2	1.162+2	1.479+2	3.771+2
2+7	8.566+1	9.007+1	1.022+2	2.648+2
4+7	5.900+1	6.122+1	5.615+1	1.469+2
6+7	4.289+1	4.429+1	3.606+1	9.458+1
8+7	3.269+1	3.367+1	2.553+1	6.705+1
1+8	2.589+1	2.662+1	1.926+1	5.062+1
2+8	1.134+1	1.163+1	7.590+0	1.997+1
4+8	4.492+0	4.597+0	2.837+0	7.470+0
6+8	2.541+0	2.600+0	1.573+0	4.144+0
8+8	1.683+0	1.722+0	1.031+0	2.717+0
1+9	1.219+0	1.246+0	7.422–1	1.955+0
2+9	4.412–1	4.511–1	2.654–1	6.993–1
4+9	1.579–1	1.614–1	9.436–2	2.486–1
6+9	8.627–2	8.819–2	5.146–2	1.356–1
8+9	5.615–2	5.739–2	3.346–2	8.816–2

Notes. $a \pm b = a \times 10^{\pm b}$.

Appendix A: Tables

Table A.1. Single-ionization cross sections (in 10^{-20} cm^2) for the ground level.

Energy (eV)	DI:3s	DI:3p	EA	Total
16	0.000+0	0.000+0	1.060+3	1.060+3
17	0.000+0	7.845+2	1.197+3	1.985+3
18	0.000+0	1.730+3	1.754+3	3.484+3
19	0.000+0	2.526+3	4.715+3	7.238+3
20	0.000+0	3.128+3	7.577+3	1.070+4
21	0.000+0	3.620+3	9.554+3	1.317+4
22	0.000+0	3.959+3	9.985+3	1.393+4
23	1.411+2	4.215+3	9.735+3	1.408+4
24	5.713+2	4.460+3	1.004+4	1.507+4
25	9.263+2	4.694+3	1.013+4	1.575+4
26	1.244+3	4.920+3	1.001+4	1.617+4
27	1.493+3	5.055+3	9.657+3	1.621+4
28	1.826+3	5.142+3	9.567+3	1.653+4
29	2.079+3	5.226+3	9.491+3	1.680+4
30	2.322+3	5.307+3	9.306+3	1.693+4
35	3.139+3	5.480+3	8.596+3	1.726+4
38	3.432+3	5.483+3	8.182+3	1.719+4
40	3.538+3	5.460+3	7.929+3	1.706+4
42	3.639+3	5.427+3	7.692+3	1.691+4
45	3.717+3	5.349+3	7.359+3	1.661+4
48	3.770+3	5.254+3	7.049+3	1.629+4
50	3.778+3	5.183+3	6.852+3	1.604+4
52	3.786+3	5.115+3	6.663+3	1.581+4
55	3.768+3	5.018+3	6.393+3	1.544+4
58	3.742+3	4.912+3	6.137+3	1.506+4
60	3.721+3	4.839+3	5.974+3	1.481+4