

Electron-impact excitation and ionization cross sections for the Si, Cl, and Ar isonuclear sequences

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Electron-impact excitation and ionization cross sections are presented for all atomic ions in the Si, Cl, and Ar isonuclear sequences. These data contribute to the continuing effort to provide accurate collisional data for magnetic fusion and astrophysical modeling. For excitation processes, level-resolved cross section calculations are presented which were made using first-order many-body perturbation theory. For ionization processes, we present calculations made with the configuration-average approximation using a distorted-wave method. A selection of excitation and ionization cross sections are compared with experiment, where available. For ionization of Si^{2+} and Si^{3+} , we also compare with calculations made using time-dependent close-coupling theory, to assess the accuracy of the distorted-wave calculations. Our cross sections will be tabulated in several atomic collision databases for use in future kinetics modeling efforts.

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I. INTRODUCTION

The ongoing need for accurate atomic data for use in the astrophysical and magnetic fusion modeling communities is of continuing relevance as advances are made in the quality and quantity of observational data from recent x-ray satellites, and diagnostic measurements from fusion plasma devices. This need has motivated several groups to generate high-quality atomic collisional data for the systems of interest. For example, the Auburn group has used perturbative and nonperturbative approaches to compute excitation and ionization cross sections for all ion stages of Li [1] and Be [2], for which all data have been archived for use in plasma modeling. Recent comprehensive calculations have also been made for electron-impact ionization cross sections of all atomic ions of Kr [3], W [4], and of all ionization stages of Ar [5]. These systems are of much interest in fusion modeling and are expected to play a role in the upcoming ITER project. These calculations were made using a variety of distorted-wave techniques and were augmented by *R*-matrix with pseudostates calculations for neutral argon. Also, a recent effort has been initiated to calculate high-quality electron-impact excitation data for a wide range of ions of interest using the *R*-matrix approach [6]. This work builds on many previous efforts to compute excitation data using a variety of distorted-wave and *R*-matrix approaches (see Bhatia *et al.* for a review [7]), often motivated by the IRON project [8]. A comprehensive set of dielectronic recombination cross sections and rate coefficients for many isoelectronic sequences is also now available in the literature [9], and efforts continue to extend this work to more complicated (*M*-shell) ions.

In this paper, we contribute to these atomic data efforts by presenting excitation and ionization cross sections for all ions of Si, Cl, and Ar. Emission lines from Si ions are commonly seen in many observed astrophysical spectra, and all three ions are potential impurity candidates in proposed fusion devices. Furthermore, Ar is a candidate for the mitigation of tokamak disruptions [10]. Although some previous

calculations have been made on selected ions of these elements, we have calculated a consistent set of data for all ionization stages. This approach allows for the generation of a more consistent plasma kinetics model, which removes some potential ambiguities when computing plasma radiative properties.

In the following section we give a brief overview of the theoretical methods used in our calculations. We then present results for a selection of excitation and ionization cross sections, with most of the examples chosen from the Si isonuclear sequence, as it allows more comparison with available experimental data. For example, measurements are available for ionization of Si^{q+} , for $q=0-7$ [11–15]. Little, if any, data are available for the Cl isonuclear sequence, which has been rarely investigated by experiment due to its toxicity. Only one study of the elastic scattering cross sections of Cl [16] has been performed to the best of our knowledge. The recent work of Loch *et al.* [5] for ionization of Ar ions has given a comprehensive description of distorted-wave calculations and their comparison to available measurement. Our calculations of ionization cross sections are very similar to those of Loch *et al.* [5]. We end with a short conclusion.

II. THEORY

Our calculations of excitation and ionization cross sections for Si, Cl, and Ar ions were made using the Los Alamos suite of atomic collision codes. The first step was to run the semirelativistic structure code CATS [17], which is based on Cowan's codes [18]. All our calculations used the semirelativistic approximation in CATS, which includes the mass-velocity and Darwin terms in the Schrödinger equation. For fine-structure calculations, the spin-orbit interaction is also included when diagonalizing the appropriate Hamiltonian. For *M*-shell ions, configurations were included with all possible permutations of electrons within the $n=3$ manifold. One-electron promotions from all of these possible $n=3$ subshells into the $n=4$ and $n=5$ shells were added. For Na-like ions, one-electron promotions from the $n=2$ shell into the

$n=3$ shell were also included. For L -shell ions, configurations were included with all possible permutations of electrons within the $n=2$ manifold. One-electron promotions from all of these possible $n=2$ subshells into the $n=3$ and $n=4$ shells were also included. For Li-like ions, one-electron promotions from the $1s$ shell into the $n=2$ and $n=3$ shells were also included. For K -shell ions, all configurations were included containing one-electron promotions from $n=1$ into the $n=2, 3,$ and 4 shells. When constructing the Hamiltonian to obtain fine-structure levels, full configuration-interaction and spin-orbit coupling were included, using the default settings for scaling of spin-orbit and configuration-interaction parameters, as discussed in detail by Cowan [18]. These calculations resulted in quite accurate level energies for the majority of the ions considered here. For example, the level energies of the low-lying levels of Si^{2+} are within 3% of the experimental values. Excitation cross sections were computed using the ACE code [19], in which we used the first-order many-body perturbation theory option [20,21] to compute the excitation cross sections of interest. Our excitation data were tabulated as both cross sections (Q) and as collision strengths (Ω). The relation between these quantities for the transition from an initial level i to a final level k can be expressed as

$$Q_{ik}(\text{cm}^2) = \frac{\pi a_0^2}{g_i E(\text{Ry})} \Omega_{ik}, \quad (1)$$

where a_0 is the Bohr radius (in cm), g_i is the statistical weight of the initial level i , and E is the electron-impact energy. Excitation cross sections were computed in the fine-structure approximation. For M -shell ions, excitations from all $n=3$ levels to $n=3, 4,$ and 5 levels were computed, apart from the neutral Si, $\text{Cl}^{(0 \rightarrow 3)+}$, and $\text{Ar}^{(0 \rightarrow 4)+}$ ions, for which excitation cross sections from only levels within the ground configuration were computed. This restriction was made for these latter ions because of the extremely large run times required to compute excitation cross sections from all possible $n=3$ levels. For L -shell ions, excitations from all $n=2$ levels to $n=2, 3,$ and 4 levels were computed, and for K -shell ions, excitations from all $n=1$ levels to $n=2, 3,$ and 4 levels were computed.

Ionization cross sections were computed in the configuration-average approximation using distorted-wave theory via the multipurpose ionization code GIPPER [22] (for a description of the underlying theory, see Ref. [23]). Within the distorted-wave approximation, the incident electron is computed in a V^N potential (where N is the number of target electrons), whereas the scattered and ejected electrons are computed within a V^{N-1} potential [24]. Ionization cross sections between all possible configurations were included.

We also used the time-dependent close-coupling approach (TDCC) [25] to compute ionization cross sections from the ground and first excited configurations of Si^{2+} and Si^{3+} , as a check on the accuracy of our distorted-wave calculations. The TDCC calculations solve the coupled partial differential equations which result after expanding the two-electron wave function for the outgoing electrons and inserting this wave function into the time-dependent Schrödinger equation

[25]. We assume a frozen core of the remaining bound electrons, and used a pseudopotential to smoothly remove the inner nodes of the lowest angular momentum orbitals. This method is necessary to eliminate unphysical superelastic scattering [26], and has been used successfully to obtain configuration-average ionization cross sections from a number of heavier ions [25]. TDCC calculations were computed for all partial waves up to $L=9$, and “topped-up” with distorted-wave calculations for higher partial waves. A Fourier transform method [27] is used to extract ionization cross sections for multiple incident electron energies for only a single time propagation of the Schrödinger equation. A very similar previous TDCC calculation for ionization from the ground configuration of Si^{3+} , made for three selected energy points [26], is in very good agreement with our current calculations.

III. RESULTS AND DISCUSSION

In this section, we present a small sample of our calculations, which are compared to experiment or previous calculations where available. We draw most of our examples from the Si isonuclear sequence, due to the availability of experimental measurements for many of the Si ions, and also because of the lack of measurements available for Cl. Comparisons of Ar ionization cross sections with available experiment were recently published [5] and so we present just one example from this isonuclear sequence. The complete set of our excitation and ionization cross sections will be tabulated in the atomic databases operated by the International Atomic Energy Agency (IAEA) [28] and the Oak Ridge National Laboratory’s (ORNL) atomic data center [29] for convenient use by the plasma modeling community.

In Fig. 1 we present excitation collision strengths for the $2s^2 2p^2 \ ^2P_{1/2} - 2s 2p^2 \ ^2D_{3/2}$ transition in B-like Si, Cl, and Ar. Relativistic distorted-wave calculations have previously been made for many isoelectronic sequences by the Sampson group and here we have compared with the calculations of Ref. [30]. In general, good agreement is found between the two sets of calculations. We also performed a subsequent calculation that included mixing only between states that arise from the three $n=2$ configurations $2s^2 2p$, $2s 2p^2$, and $2p^3$, as was done in Ref. [30], to assess the accuracy of the present calculations. The closer agreement found between this test calculation and the calculations of Ref. [30] indicates that the differences between our current calculations and the calculations of Ref. [30] are due to configuration-interaction effects. Relativistic effects (beyond the semirelativistic terms included in the current calculations) appear to play a minor role for these mid- Z elements. We consider our current calculations to be more accurate than those of Ref. [30] since we have included more levels and correspondingly more detailed configuration interaction. We also emphasize at this point that these perturbative calculations for excitation do not include any resonances which may be commonly found in excitation cross sections [6]. Such resonance contributions can sometimes dominate the cross section, but an accurate treatment of such processes is only usually available with large-scale nonperturbative treatments, such as the

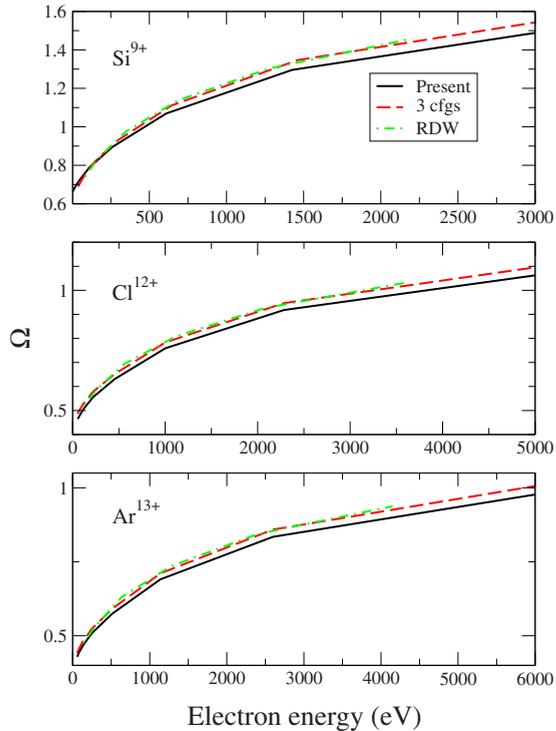


FIG. 1. (Color online) Collision strengths for the $2s^2 2p^2 P_{1/2} - 2s 2p^2 \ ^2D_{3/2}$ transition in three B-like ions: Si^{9+} , Cl^{12+} , and Ar^{13+} . We compare the present calculations with the results of Zhang and Sampson [30] and a test three-configuration calculation. See text for details.

R -matrix approach [6], which require significantly larger computational resources. However, the plasma kinetics modeling efforts at Los Alamos [31] typically include excitation cross sections between all possible levels, including doubly excited autoionizing levels. With this approach, the effect of resonances is automatically taken into account in the so-called isolated resonance approximation [18]. The use of R -matrix excitation data in this framework leads to a double counting of the resonance contribution. We therefore compute only nonresonant excitation cross sections to be consistent with the intended modeling application.

We now turn to a comparison of our ionization cross sections with results from other work. In Fig. 2 we present electron-impact ionization cross sections for neutral Si. We added the direct ionization contribution from the $3s$ and $3p$ subshells in order to compare with the measurements of Freund *et al.* [11] and binary-encounter-Bethe (BEB) calculations [32]. Our distorted-wave calculations are in good agreement with experiment in the threshold region, but overestimate the peak of the cross section by more than 50%. The BEB calculations are slightly lower than experiment, but only by around 10% or so. Another recent calculation [33] (not shown), made using a variant of the Born approximation to compute the ionization amplitude, was reported to be in reasonable agreement with the measurements of Freund *et al.* [11]. The overestimation by distorted-wave calculations of the ionization cross sections for neutral systems is not unexpected and has been observed for many other systems such as H [25] and He [34]. The overestimation arises from the

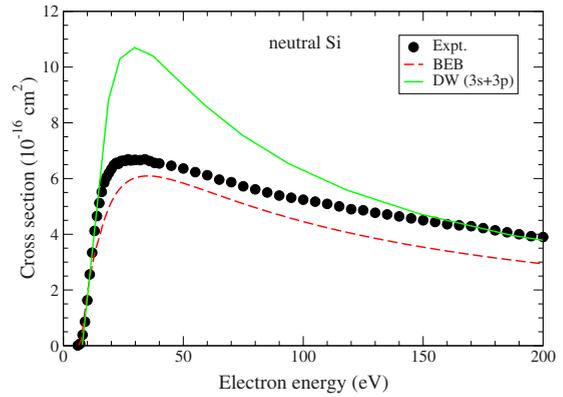


FIG. 2. (Color online) Electron-impact ionization cross sections for neutral Si. The partial cross sections from the $3s$ and $3p$ subshells of the ground $3s^2 3p^2$ configuration have been summed to compare with experiment. We compare our present distorted-wave calculations (DW) with the experimental measurements of Freund *et al.* [11] and binary-encounter-Bethe (BEB) calculations of Stone and Kim [32].

perturbative treatment of the electron-electron interaction between the outgoing electrons, which plays an important role in ionization from neutral systems.

In Fig. 3 we compare distorted-wave calculations of the ionization of Si^{2+} with experiment [12]. In the crossed beam experiment, the metastable ($3s 3p \ ^3P$) component of the Si^{2+} ion beam was unknown, and so we present calculations from both the ground $3s^2$ (upper part) and first excited $3s 3p$ (lower part) configurations of Si^{2+} , and compare both with the measurements of Ref. [12]. The distorted-wave calculations are in reasonable agreement with the measurements, and also in good agreement with previous distorted-wave calculations presented in Ref. [12]. However, it is difficult to draw a conclusion as to the accuracy of the distorted-wave calculations by comparison to experiment without knowing the metastable fraction of the ion beam. To assess the accuracy of the distorted-wave approach for this twice-ionized system, we also performed TDCC calculations from both the

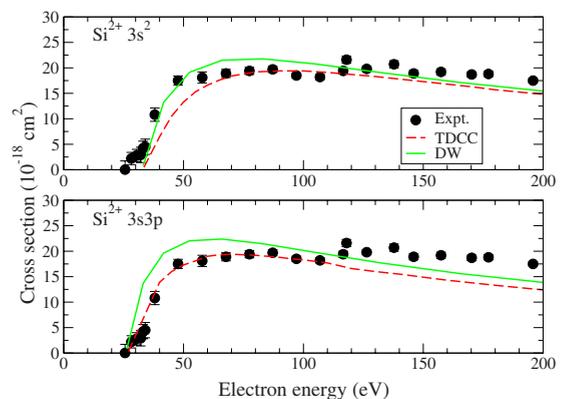


FIG. 3. (Color online) Electron-impact ionization cross sections for Si^{2+} from the ground $3s^2$ and excited $3s 3p$ configurations. In both cases, we compare our present distorted-wave calculations (DW) and time-dependent close-coupling (TDCC) calculations with the experimental measurements of Djurić *et al.* [12].

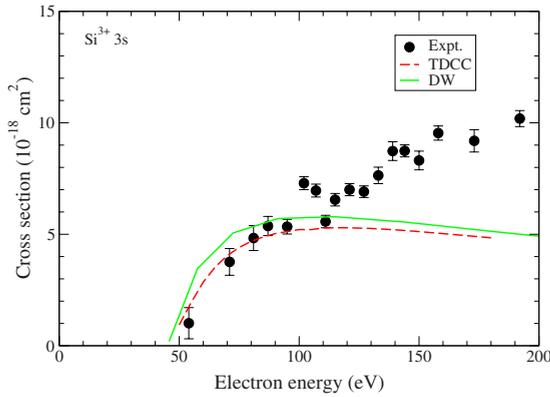


FIG. 4. (Color online) Electron-impact ionization cross sections for Si^{3+} from the ground $3s$ configuration. We compare our present distorted-wave calculations (DW) and time-dependent close-coupling (TDCC) calculations with the experimental measurements of Crandall *et al.* [13].

ground and first excited configurations, as previously described. The TDCC calculations are lower than the distorted-wave calculations by around 10–15 % near the peak of the cross section, and perhaps in better agreement with experiment over a broader range of energies. At higher electron energies, the distorted-wave calculations are in better agreement with the TDCC calculations from the ground configuration, but disagreement for the $3s3p$ data persists. The latter behavior can possibly be explained by previous work which demonstrated that distorted-wave approaches become less accurate for more highly excited systems [35].

At around 120 eV an increase in the experimental ionization cross section is observed, which arises from contributions from the two-step process of excitation autoionization (i.e., inner-shell excitation followed by autoionization). In this case the contributions are mainly from autoionization from the excited $2s^22p^33s^2nl$ configurations. Although it is possible to use distorted-wave methods to compute the excitation-autoionization contribution, we chose not to show it explicitly here, due to the issue of double counting mentioned previously. Since excitation to autoionizing states is considered explicitly in the isolated resonance approximation, the contribution of excitation autoionization to collisional ionization is included automatically. We also note that the threshold for direct ionization from the $2p$ subshell of Si^{2+} (not included in our calculations) is around 130 eV, and so may also contribute to the experimentally measured ionization cross section above this energy.

In Fig. 4 we show a comparison of our distorted-wave calculations of ionization of Si^{3+} with the experimental measurements of Ref. [13]. In this case the influence of metastable components in the ion beam was determined to be much less than in the Si^{2+} experiment. The agreement between the distorted-wave calculations and experiment is quite good. A further check on the accuracy of these calculations is also made by performing TDCC calculations from the ground configuration. The TDCC calculations are around 10% lower than the distorted-wave calculations, but both are within the error bars of experiment. The current TDCC calculations are in excellent agreement with previous TDCC

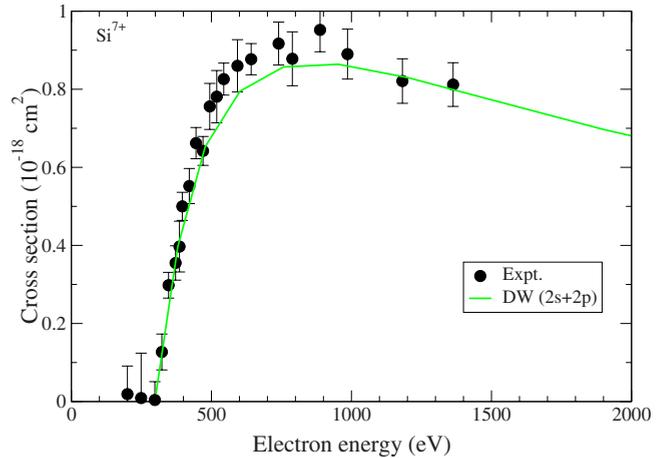


FIG. 5. (Color online) Electron-impact ionization cross sections for Si^{7+} . The partial cross sections from the $2s$ and $2p$ subshells of the ground $2s^22p^3$ configuration have been summed to compare with experiment. We compare our present distorted-wave calculations (DW) with the measurements of Zeijlmans van Emmichoven *et al.* [15].

calculations made for three low impact energies [26], which were shown to be in good agreement with convergent close-coupling and R -matrix pseudostate calculations. As in the previous case of Si^{2+} , a large excitation-autoionization contribution to the total ionization cross section is observed above 100 eV. Previous work has examined the excitation-autoionization contribution to this cross section using distorted-wave methods [36].

In Fig. 5 we present distorted-wave calculations of ionization cross sections for Si^{7+} , which are compared to the experimental measurements of Ref. [15]. We added the direct ionization contribution from the $2s$ and $2p$ subshells in order to compare with experiment. For this highly ionized case, the distorted-wave calculations are in very good agreement with experiment over the entire energy range. This behavior is consistent with previous findings that, in highly ionized systems where the nuclear Coulomb potential dominates over the electron-electron interaction, distorted-wave approaches are appropriate.

Finally, as an example of our ionization cross sections for Cl and Ar, we present in Fig. 6 ionization cross sections for Cl^{3+} and Ar^{4+} , which are isoelectronic with neutral Si. For Cl^{3+} there are no experimental measurements with which to compare, but for Ar^{4+} we can compare with the measurements of Müller *et al.* [37] and Zhang *et al.* [38]. The agreement of our calculations of the direct ionization cross sections (where we have summed the contributions of partial ionization from the $3s$ and $3p$ subshells) with experiment is good. It appears that, as expected, the distorted-wave approach is more accurate for these more ionized species than for the neutral Si atom, as shown in Fig. 2. Similar agreement between distorted-wave calculations and experiment was also demonstrated for Ar^{4+} by Loch *et al.* [5], where further comparisons of distorted-wave calculations with ionization measurements of other Ar ions were presented.

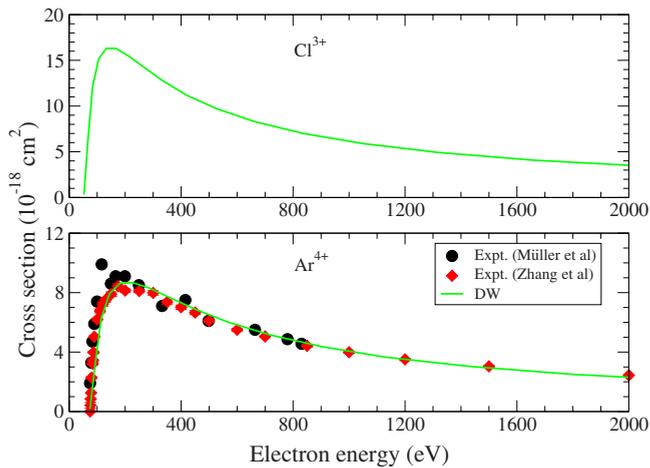


FIG. 6. (Color online) Electron-impact ionization cross sections for Cl^{3+} and Ar^{4+} . The partial cross sections from the $3s$ and $3p$ subshells of the ground $3s^2 3p^2$ configuration have been summed to compare with experiment. We compare our present distorted-wave calculations (DW) with the measurements of Müller *et al.* [37] and Zhang *et al.* [38].

IV. CONCLUSIONS

In this paper we have presented excitation and ionization cross sections calculated using first-order many-body perturbation and distorted-wave approaches for all ions in the Si, Cl, and Ar isonuclear sequences. We have made a comparison of a subset of our results with experiment and with previous calculations. The comparison of our distorted-wave calculations with experiment and other calculations allows an estimate of the accuracy of our calculations to be determined. For ionization of Si^{2+} and Si^{3+} , our distorted-wave calculations are within 20% of TDCC calculations. TDCC calculations for one or two electrons outside a closed shell have been previously found to be quite accurate in comparison with other nonperturbative calculations [25]. Good agreement between TDCC calculations and experiment has also been found for ionization of H [25] and He [34]. Based on these findings, and by considering the agreement shown in Figs. 3 and 4, we tentatively estimate that the distorted-

wave calculations for systems which are twice or more ionized are accurate to approximately 20%. We do caution though that this accuracy decreases as one considers ionization from excited configurations [35]. For neutral and once ionized systems, distorted-wave calculations appear to significantly overestimate the ionization cross sections, as demonstrated by comparison of our calculations for neutral Si with experiment and with BEB calculations. BEB calculations have previously been shown to be quite accurate for neutral systems, but have not been extended to treat ionization from ions. Therefore the distorted-wave ionization cross sections for neutral and near-neutral systems should only be regarded as accurate to approximately 50%. Although this level of agreement is far from ideal, very few accurate ionization cross sections for heavy neutral targets have been produced by nonperturbative calculations, for a wide range of impact energies. This issue is currently an outstanding problem in atomic collision physics and the focus of much effort [39].

It is more difficult to assess the accuracy of our excitation calculations, as there are few experiments against which comparisons can be made. We have demonstrated that our calculations are consistent with, and possibly more accurate than, previous relativistic-distorted-wave calculations for the highly ionized ions considered in the present work. For systems which are neutral or near-neutral, the accuracy of our approach is expected to decrease, due to the perturbative treatment of the electron-electron interaction.

Finally, we emphasize that our excitation and ionization calculations presented here form a complete data set of distorted-wave collisional data, and were made in a consistent manner with respect to the number of configurations included for each ion stage and the type of calculations performed. Thus, the resulting data, which will be archived in several international atomic data centers, should be quite suitable for use in kinetics modeling efforts.

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- [1] S. D. Loch, J. Colgan, M. C. Witthoef, M. S. Pindzola, C. P. Ballance, D. M. Mitnik, D. C. Griffin, M. G. O'Mullane, N. R. Badnell, and H. P. Summers, *At. Data Nucl. Data Tables* **92**, 813 (2006).
 - [2] S. D. Loch, M. S. Pindzola, C. P. Ballance, D. C. Griffin, J. Colgan, N. R. Badnell, M. G. O'Mullane, and H. P. Summers, *At. Data Nucl. Data Tables* **94**, 257 (2008).
 - [3] S. D. Loch, M. S. Pindzola, C. P. Ballance, D. C. Griffin, D. M. Mitnik, N. R. Badnell, M. G. O'Mullane, H. P. Summers, and A. D. Whiteford, *Phys. Rev. A* **66**, 052708 (2002).
 - [4] S. D. Loch, J. A. Ludlow, M. S. Pindzola, A. D. Whiteford, and D. C. Griffin, *Phys. Rev. A* **72**, 052716 (2005).
 - [5] S. D. Loch, Sh. A. Abdel-Naby, C. P. Ballance, and M. S. Pindzola, *Phys. Rev. A* **76**, 022706 (2007).
 - [6] M. C. Witthoef, A. D. Whiteford, and N. R. Badnell, *J. Phys. B* **40**, 2969 (2007).
 - [7] A. K. Bhatia, *At. Data Nucl. Data Tables* **57**, 253 (1994).
 - [8] D. G. Hummer, K. A. Berrington, W. Eissner, A. K. Pradhan, H. E. Saraph, and J. A. Tully, *Astron. Astrophys.* **279**, 298 (1993).
 - [9] N. R. Badnell, M. O'Mullane, H. P. Summers, Z. Altun, M. A. Bautista, J. Colgan, T. W. Gorczyca, D. M. Mitnik, M. S. Pindzola, and O. Zatsarinny, *Astron. Astrophys.* **406**, 1151 (2003).

- [10] D. G. Whyte, T. C. Jernigan, D. A. Humphreys, A. W. Hyatt, C. J. Lasnier, P. B. Parks, T. E. Evans, M. N. Rosenbluth, P. L. Taylor, A. G. Kellman, D. S. Gray, E. M. Hollmann, and S. K. Combs, *Phys. Rev. Lett.* **89**, 055001 (2002).
- [11] R. S. Freund, R. C. Wetzell, R. J. Shul, and T. R. Hayes, *Phys. Rev. A* **41**, 3575 (1990).
- [12] N. J. Djurić, E. W. Bell, X. Q. Guo, G. H. Dunn, R. A. Phaneuf, M. E. Bannister, M. S. Pindzola, and D. C. Griffin, *Phys. Rev. A* **47**, 4786 (1993).
- [13] D. H. Crandall, R. A. Phaneuf, R. A. Falk, D. S. Belić, and G. H. Dunn, *Phys. Rev. A* **25**, 143 (1982).
- [14] J. S. Thompson and D. C. Gregory, *Phys. Rev. A* **50**, 1377 (1994).
- [15] P. A. Zeijlmans van Emmichoven, M. E. Bannister, D. C. Gregory, C. C. Havener, R. A. Phaneuf, E. W. Bell, X. Q. Guo, J. S. Thompson, and M. Sataka, *Phys. Rev. A* **47**, 2888 (1993).
- [16] D. C. Griffin, M. S. Pindzola, T. W. Gorczyca, and N. R. Badnell, *Phys. Rev. A* **51**, 2265 (1995).
- [17] J. Abdallah, R. E. H. Clark, and R. D. Cowan, Los Alamos National Laboratory, Los Alamos Manual No. LA 11436-M-I, 1988 (unpublished), <http://aphysics2.lanl.gov/tempweb/>
- [18] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
- [19] R. E. H. Clark, J. Abdallah, Jr., G. Csanak, J. B. Mann, and R. D. Cowan, Los Alamos National Laboratory, Los Alamos Manual No. LA 11436-M-II 1988 (unpublished).
- [20] G. Csanak, H. S. Taylor, and R. Yaris, *Phys. Rev. A* **3**, 1322 (1971).
- [21] G. Csanak, H. S. Taylor, and R. Yaris, *Adv. At. Mol. Phys.* **7**, 287 (1971).
- [22] R. E. H. Clark, J. Abdallah, and J. B. Mann, *Astrophys. J.* **381**, 597 (1991); B. J. Archer, R. E. H. Clark, C. J. Fontes, and H. L. Zhang, Los Alamos Memorandum No. LA-UR-02-1526, 2002 (unpublished).
- [23] M. S. Pindzola, D. C. Griffin, and C. Bottcher, in *Atomic Processes in Electron-Ion and Ion-Ion Collisions*, Vol. 145 of NATO Advanced Studies Institute, Series B: Physics, edited by F. Brouillard (Plenum, New York, 1986), p. 75.
- [24] S. M. Younger, *Phys. Rev. A* **24**, 1278 (1981).
- [25] M. S. Pindzola, F. Robicheaux, S. D. Loch, J. C. Berengut, T. Topcu, J. Colgan, M. Foster, D. C. Griffin, C. P. Ballance, D. R. Schultz, T. Minami, N. R. Badnell, M. C. Witthoef, D. R. Plante, D. M. Mitnik, J. A. Ludlow, and U. Kleiman, *J. Phys. B* **40**, R39 (2007).
- [26] N. R. Badnell, M. S. Pindzola, I. Bray, and D. C. Griffin, *J. Phys. B* **31**, 911 (1998).
- [27] J. Colgan, M. S. Pindzola, and F. Robicheaux, *Phys. Rev. A* **66**, 012718 (2002).
- [28] <http://www-amdis.iaea.org/ALADDIN/>
- [29] <http://www-cfadc.phy.ornl.gov>
- [30] H. L. Zhang and D. H. Sampson, *At. Data Nucl. Data Tables* **56**, 41 (1994).
- [31] P. Hakel, M. E. Sherrill, S. Mazevet, J. Abdallah, Jr., J. Colgan, D. P. Kilcrease, N. H. Magee, C. J. Fontes, and H. L. Zhang, *J. Quant. Spectrosc. Radiat. Transf.* **99**, 265 (2006).
- [32] P. Stone and Y. K. Kim (private communication).
- [33] P. L. Bartlett and A. T. Stelbovics, *Phys. Rev. A* **66**, 012707 (2002).
- [34] M. S. Pindzola and F. J. Robicheaux, *Phys. Rev. A* **61**, 052707 (2000).
- [35] D. C. Griffin, C. P. Ballance, M. S. Pindzola, F. Robicheaux, S. D. Loch, J. A. Ludlow, M. C. Witthoef, J. Colgan, C. J. Fontes, and D. R. Schultz, *J. Phys. B* **38**, L199 (2005).
- [36] D. C. Griffin, C. Bottcher, and M. S. Pindzola, *Phys. Rev. A* **25**, 154 (1982).
- [37] A. Müller, E. Salzborn, R. Frodl, R. Becker, H. Klein, and H. Winter, *J. Phys. B* **13**, 1877 (1980).
- [38] H. Zhang, S. Cherkani-Hassani, C. Bélenger, M. Duponchelle, M. Khouilid, E. M. Oualim, and P. Defrance, *J. Phys. B* **35**, 3829 (2002).
- [39] C. P. Ballance, D. C. Griffin, M. S. Pindzola, and S. D. Loch, *J. Phys. B* **40**, F27 (2007).