Published in "Journal of Physics B 39: L139-L144 , 2006"
which should be cited to refer to this work.

Absolute angle-differential cross sections for electron-impact excitation of neon atoms from threshold to 19.5 eV

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Abstract

Absolute angle-differential cross sections for electron-impact excitation of neon atoms to the four levels with the ($2p^5 3s$) configuration have been determined both experimentally and theoretically for incident energies from threshold up to 19.5 eV at scattering angles of 135° and 180°. Excellent agreement between the experimental data and theoretical predictions, obtained by a Breit–Pauli *B*-spline *R*-matrix method with non-orthogonal orbitals, has been found in terms of both absolute values and the energies and widths of the numerous resonant features.

Absolute cross sections for inelastic electron scattering from rare-gas atoms are of great importance for gaseous discharge physics [1], but—except for helium—the theoretical description of these processes has remained a substantial challenge. Recently, however, significant progress has been made by means of a *B*-spline *R*-matrix method [2–4]. The key feature of this method is the possibility to use *non-orthogonal* sets of term-dependent one-electron orbitals. This allows for an accurate target description with relatively small configuration expansions. Excellent agreement was observed, for instance, between the calculated energy-dependent cross sections for the production of metastable Ne [2] and Ar [3] atoms with those measured in high-resolution experiments [5–7]. For Ne, a very sharp resonance (energy 18.527 meV, width 0.8 meV) was theoretically predicted [2] and subsequently confirmed experimentally [7].

For thorough tests of theoretical approaches, it is highly desirable to compare the computed results with detailed experimental information, such as angle-differential excitation cross sections, obtained in *absolute units* at energies *near threshold,* where the excitation process is dominated by prominent resonance structure [5]. A particular point of interest is the coupling of the various anion resonances to specific final states. Apart from numerous work on He (see, e.g., [5, 8, 9]) and some results for Ar [5, 6] and Kr [5, 10], such data are currently missing in the literature.

Here, we report on the first absolute angle-differential cross sections for excitation of neon atoms to the four levels of the Ne ($2p^53s$) configuration in the near-threshold energy range up to 19.5 eV incident energy. Most of the prominent anion resonances in this range [2, 5–7] have been resolved. Previous angle-differential work on Ne ($2p^53s$) excitation was carried out at a few discrete impact energies $\geqslant$20 eV. The two studies, which include measurements at 20 eV and therefore come close to the present energy range, are that of Register *et al* [11] and the more recent work by Khakoo *et al* [12].

The experimental results were obtained with a high-resolution electron scattering apparatus [9] involving two-stage hemispherical analysers. The incident beam possesses an energy width (FWHM) of 9 meV. The energy loss peaks have a width of 14 meV, thus permitting the resolution of all four Ne ($2p^53s$) levels. The present letter reports cross sections recorded as a function of electron energy at the scattering angles of 135° and 180°. The angle of 180° was reached with a magnetic angle changer [13] of special design [14]. The raw signal was corrected for the variations of the instrumental response with energy and scattering angle, as described in detail recently [15].

The absolute values for the inelastic cross sections at discrete energies were obtained in two steps. First, the values of the absolute elastic cross sections of neon were determined at 18 eV and 20 eV by normalizing to helium results [16] using the relative flow method [17]. They are reliable within about ±15%. Electron energy-loss spectra including both the elastic and the inelastic peaks were then recorded at constant incident energies of 18 eV and 20 eV and corrected for the analyser response function. Absolute inelastic values were determined from the elastic and inelastic signal intensities in the energy-loss spectra by normalizing to the absolute elastic values determined in the first step. The energy-loss spectra span a large range of scattered electron energies, and hence an accurate knowledge of the response function over this energy range is critical for an accurate determination of the values of the inelastic cross sections. The uncertainty of the response function makes the errors of the absolute inelastic cross sections larger than those of the elastic cross section; they become about ±20% for energies more than 0.3 eV above each threshold. At lower energies, the response function becomes more difficult to determine and the error bars increase gradually, reaching ±50% very close to threshold.

Finally, excitation functions for the four ($2p^53s$) levels were recorded, corrected for the instrumental response function, and normalized to the absolute values at 18 eV, where no sharp resonant features occur. The absolute values obtained at 20 eV and 135° can be compared with the results of Register *et al* [11], who show graphically (in their figure 6) the cross sections measured at 20 eV as a function of scattering angle up to 140°. Interpolation of their data between 130° and 140° reveals satisfactory agreement for the $^3P_2$ and $^3P_0$ states. The present value is about 25% lower, which is still within the combined error limits, for the $^1P_1$ state. The difference is more substantial for the $^3P_1$ state, however, where the present value is about two times larger. A detailed comparison of the present absolute values with the results of the extensive study by Khakoo *et al* [12] is not possible at the present stage, because their measurements only extend to $\theta = 120°$, with an extrapolation to 130°. A visual extrapolation of their data to 135° reveals overall agreement, although the present cross sections are generally somewhat lower, in some cases by up to 30%.

The numerical calculations performed for the present work are based upon the semi-relativistic B-spline R-matrix approach described in [2, 3]. Details of this particular method and references to earlier work can be found in these papers. As mentioned above, the key feature of this approach is to significantly improve the target description by using compact configuration-interaction expansions involving non-orthogonal sets of term-dependent one-electron orbitals. We used the program `MJK` of Grum-Grzhimailo [18] to calculate the differential cross sections

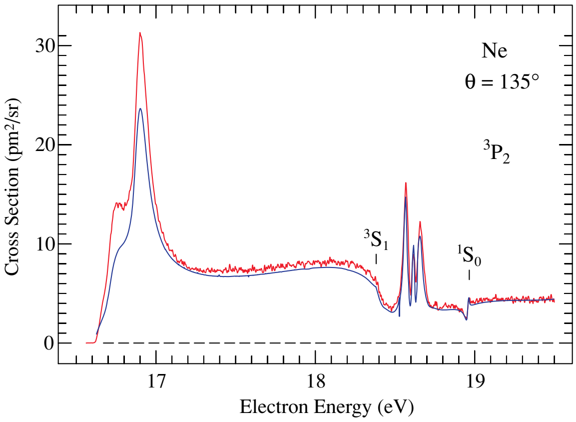

Figure 1. Absolute experimental and calculated (smooth line) cross section for excitation of the Ne $(2p^53s)\ ^3P_2$ level at $\theta = 135°$.

from the $\boldsymbol{T}$-matrix elements produced by the asymptotic program `FARM` [19]. Contributions up to a total electronic angular momentum $J = 11$ of the projectile–target collision system were sufficient to converge the partial-wave expansion for all transitions and energies of interest.

In figure 1, we compare the measured and the calculated cross section for the excitation of the $(2p^53s)\ ^3P_2$ lowest excited level, at the scattering angle of 135°. Theory and experiment agree within about 8% at energies more than 0.3 eV above threshold, well within the experimental error limit. The difference increases closer to threshold, where the theoretical values are below experiment by 25% at 16.9 eV and by 40% at 16.7 eV. Note that these differences are still within the error limits stated above. They may be due to the difficulty of determining the response function for an inelastic process on the elastic scattering in helium [15]. No contradiction between theory and experiment is thus found over the entire energy range.

Figure 1 exhibits two prominent and relatively broad bands around 16.7 eV and 16.9 eV in the energy dependence of the cross section. These can be assigned as core-excited shape resonances with the dominant configuration $(2p^53s3p)$ [7]. As shown in table II of the latter paper, there are actually six partially overlapping resonances in this energy regime. Starting with 'feature A', the lowest $J = 5/2^e$ resonance manifests itself in the shoulder just above threshold, followed by $J = 1/2^e$ and $J = 3/2^e$ resonances that fit well with the peak seen experimentally between 16.75 eV and 16.80 eV. Furthermore, 'feature B', made up by another triplet of $J = 1/2^e$, $J = 5/2^e$ and $J = 3/2^e$ resonances, is seen in the peak at 16.90 eV.

These two resonant features are followed by a nearly constant cross section up to about 18.3 eV. A prominent downward Wigner cusp is found at the threshold for excitation of the lowest $(2p^53p)$ level with $^3S_1$ symmetry, followed by a group of narrow resonances associated with higher lying $(2p^53p)$ levels, namely the triplet of peaks located (with an experimental uncertainty of 3 meV) at 18.573 eV, 18.615 eV and 18.662 eV [7], respectively, and the sharp Feshbach resonance located at 18.957 eV, which is attached to the highest $(2p^53p)$ level with $^1S_0$ symmetry [7]. Figure 2 shows that the former three resonances cause strong peaks in the cross sections for the three ^3P levels and window-type features in the excitation function for the ^1P level, in contrast to the latter resonance. These resonances are also prominent in the previous measurements of the total yield for production of metastable Ne $(2p^53s)\ ^3P_{2,0}$ atoms [5–7]. Theory and experiment agree remarkably well on the shapes, widths and energies of these narrow resonant features, as illustrated in figures 1 and 2. Note that neither the absolute

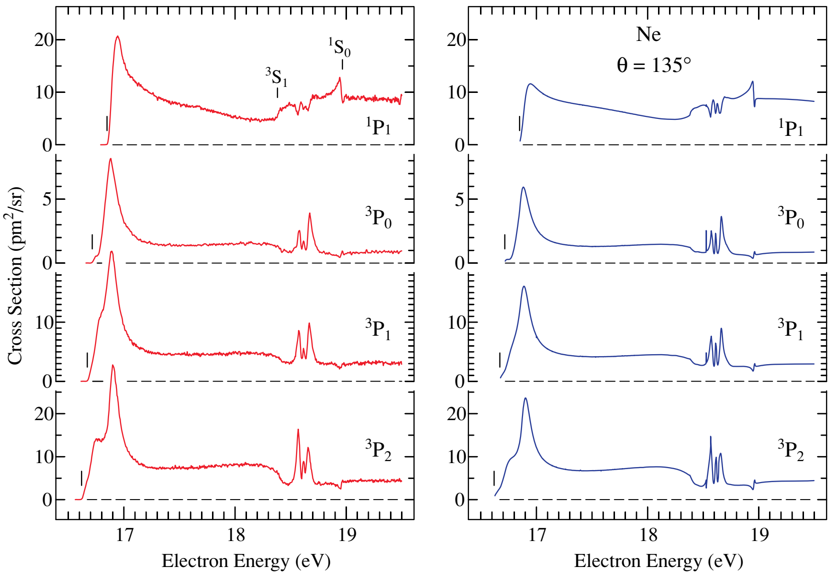

Figure 2. Absolute cross sections (experiment in the left panels, theory in the right panels) for excitation of the Ne ($2p^53s$) levels at $\theta = 135°$. The vertical bars indicate the excitation thresholds, including those of the $^3S_1$ and $^1S_0$ levels.

magnitudes nor the energy scale have been adjusted for the comparison. The resonance calculated at 18.527 eV [7] is too narrow to be observed in the present experiment.

We note that the general features in the energy dependence of the cross section for the lowest excited state of neon in figure 1 resemble qualitatively those of the lowest excited state in helium [8, 9]. In both cases, the cross section is dominated by two relatively broad core-excited shape resonances in the first few tenths of an eV above threshold, followed by a region where the energy dependence is smooth and then a range in which the cross section is dominated by a series of sharp Feshbach resonances associated with higher lying excited states.

The conclusions for the higher levels shown in figure 2 are the same as for the $^3P_2$ state: theory and experiment agree remarkably well on both the absolute values and the details of the sharp resonant structures at energies more than about 0.3 eV above threshold. Within the first 0.3 eV, experiment and theory agree on the overall shapes, but the experimental values are consistently higher by about the same factor for all four states. As already mentioned for the $^3P_2$ state above, this difference may be due to the experimental difficulty of determining the analyser response function at low energies.

The 16.90 eV core-excited shape resonance dominates the threshold region of the $^3P_1$ and $^3P_0$ cross sections. The lower lying 16.76 eV shape resonance is clearly seen in the $^3P_2$ cross section and can be discerned as a shoulder just above threshold in the $^3P_1$ cross section. The threshold peak in the $^1P_1$ cross section is due to the 16.90 eV shape resonance. It is noteworthy that experiment and theory agree that there is no threshold peak in the $^3P_0$ excitation—the cross section is small within 100 meV above threshold. The downward step at the threshold for excitation of the $^3S_1$ level is also observed in the $^3P_1$ and $^3P_0$ cross sections; an upward step is observed at this energy in the $^1P_1$ cross section. The group of resonances in the 18.3–19 eV range strongly affects the cross sections for the excitation of all four ($2p^53s$) states.

Figure 3 compares the experimental and calculated cross sections at $\theta = 180°$. Excellent agreement is also found at this scattering angle at energies higher than about 0.3 eV above

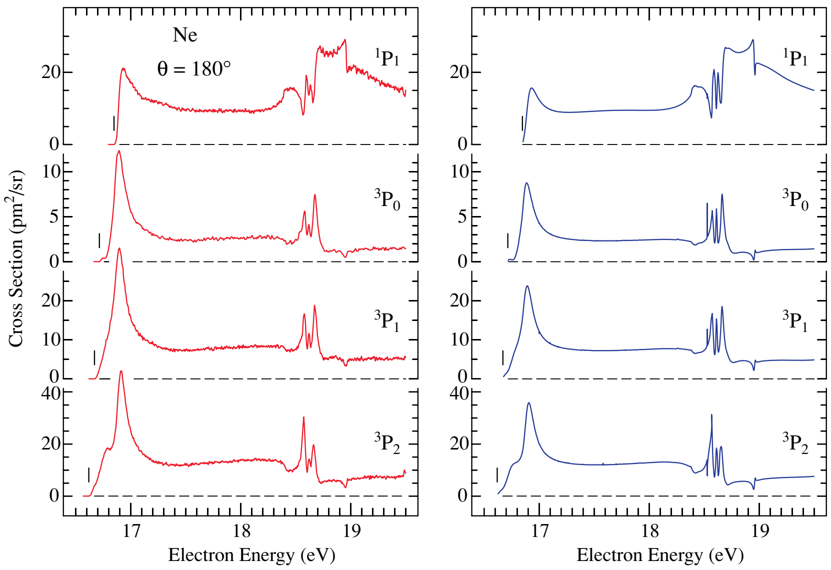

Figure 3. Absolute cross sections (experiment in the left panels, theory in the right panels) for excitation of the Ne (2p^{5}3s) levels at $\theta = 180°$.

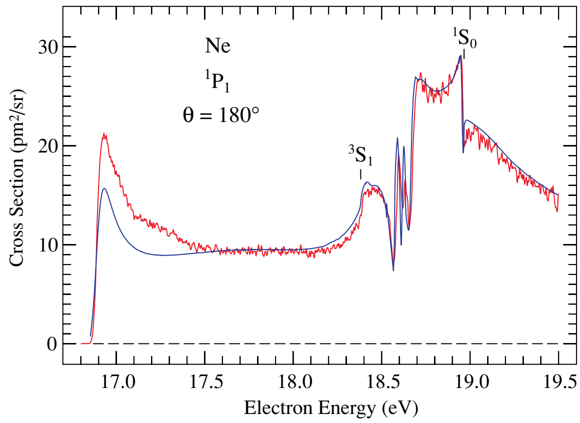

Figure 4. Absolute experimental and calculated (smooth line) cross section for excitation of the Ne (2p^{5}3s) $^1P_1$ level at $\theta = 180°$.

threshold. The experimental cross sections are higher than calculated within the first 0.3 eV above threshold, possibly for the same reason as the cross sections recorded at $\theta = 135°$, namely the difficulty of determining the response function in the experiment. Experiment and theory agree that the cross sections for the triplet levels have similar shapes at 135° and 180°, whereas the energy dependence of the $^1P_1$ cross section dramatically depends on the scattering angle in this angular range, particularly between 18.3 and 19 eV. The peculiar shape of the cross section in this energy range and at 180° is excellently reproduced by theory, as shown in detail in figure 4.

We conclude that substantial progress has been made both by theory and experiment in the ability to accurately determine the cross sections for excitation of neon in the near-threshold regime, even at the extreme scattering angle of 180°. The near-threshold energy range is particularly interesting for many applications. The *B*-spline *R*-matrix method with non-orthogonal orbitals has proven to be a powerful tool, which is apparently capable of predicting all details of the angle-differential electron-impact excitation cross sections for the first four excited levels of neon from threshold to 19.5 eV: the absolute magnitude, the overall energy dependence of the cross sections, and the energies and widths of resonances. At energies higher than about 0.3 eV above threshold, the agreement of the calculated and the measured values is within 10% for all levels and angles studied in the present work. The measured cross sections are systematically larger than the theoretical values within the first 0.3 eV above threshold, but this may well be due to the difficulty of determining the instrumental response function for very slow electrons.

Further experiments and calculations are currently in progress to follow the cross sections for excitation of the ($2p^5 3s$) levels toward higher incident energies and to also determine, at several angles, the cross sections for excitation of selected levels of the ($2p^5 3p$) configuration. Since the present theoretical model does not treat the $n = 4$ levels as physical, the basis set used in this work is probably not sufficient for a detailed description of the cross section at these higher energies. This suspicion has indeed already been confirmed by preliminary results. We therefore plan to include more physical states in the calculation and also to include coupling to the ionization continuum, which is known to become increasingly important with increasing energies, especially for optically forbidden transitions [20].

Acknowledgments

This work has been supported by the European Science Foundation (EIPAM Network), by the Swiss National Science Foundation (MA), by the Deutsche Forschungsgemeinschaft (KF and HH) and by the United States National Science Foundation (OZ and KB). KF and HH thank T H Hoffmann for helpful cooperation.

References

[1] Christophorou L G and Olthoff J K 2001 *Adv. At. Mol. Opt. Phys.* **44** 59
[2] Zatsarinny O and Bartschat K 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 2173
[3] Zatsarinny O and Bartschat K 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 4693
[4] Zatsarinny O and Bartschat K 2005 *Phys. Rev.* A **71** 022716
[5] Buckman S J and Clark C W 1994 *Rev. Mod. Phys.* **66** 539
[6] Buckman S J, Hammond P, King G C and Read F H 1983 *J. Phys. B: At. Mol. Phys.* **16** 4219
[7] Bömmels J, Franz K, Hoffmann T H, Gopalan A, Zatsarinny O, Bartschat K, Ruf M-W and Hotop H 2005 *Phys. Rev.* A **71** 012704
[8] Phillips J M and Wong S F 1981 *Phys. Rev.* A **23** 3324
[9] Allan M 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 1559
[10] Phillips J M 1982 *J. Phys. B: At. Mol. Phys.* **15** 4259
[11] Register D F, Trajmar S, Steffensen G and Cartwright D C 1984 *Phys. Rev.* A **29** 1793
[12] Khakoo M A *et al* 2004 *Phys. Rev.* A **65** 062711
[13] Read F H and Channing J M 1996 *Rev. Sci. Instrum.* **67** 2372
[14] Allan M 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** L215
[15] Allan M 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** 3655
[16] Nesbet R K 1979 *Phys. Rev.* A **20** 58
[17] Nickel J C, Mott C, Kanik I and McCollum D C 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 1867
[18] Grum-Grzhimailo A N 2003 *Comput. Phys. Commun.* **152** 101
[19] Burke V M and Noble C J 1995 *Comput. Phys. Commun.* **85** 471
[20] Ballance C P and Griffin D C 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 2943