

Electron-Impact Ionization of the Rn Atom

M. S. PINDZOLA¹, S. D. LOCH² AND J. P. COLGAN³

^{1,2}*Department of Physics, Auburn University, Auburn, AL*

³*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM*

ABSTRACT: Electron-impact ionization cross sections for the ground configuration of the Rn atom are calculated using a combination of non-perturbative close-coupling and perturbative distorted-wave methods. Direct ionization of the 6p and 6s subshells leading to single ionization are presented.

1. INTRODUCTION

Radon is the leading environmental cause of cancer. The development of means to reduce radon levels in homes and workplaces is an ongoing business concern. Knowledge of the ionization cross sections for neutral Rn allow for an approximate estimation of the likelihood of Rn redepositing, however there is a current lack of accurate ionization cross section data for Rn.

A combination of the classical binary encounter approximation and Sommerfeld's quantization of electronic atomic orbits was used to calculate electron ionization cross sections for the heavy rare gas atoms including the outer subshell of the Rn atom[1]. In this paper we carry out non-perturbative close-coupling and perturbative distorted-wave calculations for the direct ionization of the 6p⁶ and 6s² subshells for Rn. For direct ionization of the 6p⁶ subshell we examine the effects of adding a polarization potential. We note that the inclusion of a polarization potential in the non-perturbative close-coupling method was shown to be important for complex atomic systems such as W[2] and Pb[3]. We also carry out perturbative distorted-wave calculations for the excitation of the 6s² subshell for Rn to investigate the possibility of excitation-autoionization contributions.

The rest of this paper is organized as follows. In Section 2 we give a brief review of the non-perturbative close-coupling and the perturbative distorted-wave methods used to calculate electron-impact ionization cross sections. In Section 3 we present our cross section results for the electron-impact ionization of the Rn atom. We conclude with a brief summary and future plans in Section 4. Unless otherwise stated, we will use atomic units.

2. THEORY

The non-perturbative close-coupling ionization cross section is given by[4]:

$$\sigma_{ion}(n_0l_0) = \frac{\pi w_0}{8(2l_0 + 1)E} \times \sum_{LS} (2L + 1)(2S + 1)P(n_0l_0LS) , \quad (1)$$

where $P(n_0l_0LS)$ is the non-perturbative theory partial ionization probability.

The perturbative distorted-wave ionization cross section is given by[5]:

$$\sigma_{ion}(n_0l_0) = \frac{32w_0}{k_i^3} \int_0^{E/2} \frac{d(k_e^2/2)}{k_e k_f} \times \sum_{l_i l_e l_f} (2l_i + 1)(2l_e + 1)(2l_f + 1) S(n_0l_0k_i l_i \rightarrow k_e l_e k_f l_f), \quad (2)$$

where $S(n_0l_0k_i l_i \rightarrow k_e l_e k_f l_f)$ is the first order perturbation theory partial scattering probability. The bound and continuum orbitals are calculated in the Hartree-Fock Relativistic (HFR) approximation[6].

For both the non-perturbative close-coupling and the perturbative distorted-wave ionization calculations we use a polarization potential given by:

$$V_{pol}(r) = - \frac{\alpha r^2}{2(r^2 + r_c^2)}, \quad (2)$$

where $\alpha = 35.0$ and $r_c = 2.54338$ for Rn [7]. The polarization potential corresponds to the incoming electron polarizing the electron charge cloud.

3. RESULTS

3.1. Direct Ionization of the 6p subshell with no polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 6p subshell of Rn using Eq.(1) with no polarization potential were made on a 480×480 point lattice with a mesh spacing of $\delta r = 0.20$ ranging from $r = 0.0$ to $r = 96.00$ for both sets of points. The non-perturbative close-coupling cross sections for direct ionization of the 6p subshell with no polarization potential are presented in Table 1. Perturbative distorted-wave calculations were used to topup the non-perturbative close-coupling calculations for $l = 9 - 50$. We note that the previous classical binary encounter approximation and Sommerfeld's quantization of electronic atomic orbits calculations[1] at an incident energy around 25 eV range from 800 Mb to 1000 Mb, substantially above the cross sections found in Table 1.

Both the non-perturbative close-coupling and the perturbative distorted-wave ionization cross sections for the 6p subshell of Rn are presented in Figure 1. The configuration-average ionization potential for the 6p subshell is 11.40 eV. We use simple analytical formulae to smoothly join the the 5 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[8].

3.2. Direct Ionization of the 6p subshell with polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 6p subshell of Rn using Eq.(1) with the polarization potential of Eq.(3) were made on a 480×480 point lattice with a mesh spacing of $\delta r = 0.20$ ranging from $r = 0.0$ to $r = 96.0$ for both sets of points. The non-perturbative close-coupling cross sections for direct ionization of the 6p subshell with a polarization potential are presented in Table 2. Perturbative distorted-wave calculations with a polarization potential were used to topup the non-perturbative close-coupling calculations for $l = 9 - 50$.

Both the non-perturbative close-coupling and the perturbative distorted-wave ionization cross sections for the 6p subshell of Rn with the polarization potential are presented in Figure 2. We use simple analytical formulae to smoothly join the 5 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[8].

3.3. Direct Ionization of the 6s subshell with no polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 6s subshell of Rn using Eq.(1) with no polarization potential were made on a 480×480 point lattice with the same mesh as used before for the 6p subshell.

The non-perturbative close-coupling cross sections for direct ionization of the 6s subshell with no polarization potential are presented in Table 3. Perturbative distorted-wave calculations were used to topup the non-perturbative close-coupling calculations for $l = 8 - 50$.

Both the non-perturbative close-coupling and the perturbative distorted-wave cross sections for the 6s subshell of Rn are presented in Figure 3. The configuration-average ionization potential for the 6s subshell is 29.33 eV. We use simple analytical formulae to smoothly join the 3 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[8].

Non-perturbative close-coupling and perturbative distorted-wave cross sections for the 6s subshell of Rn with the polarization potential of Eq.(3) were not made since previous calculations[2] for the 5d subshell of W yielded only small changes in the cross sections.

3.4. Excitation of the 6s subshell

Perturbative distorted-wave excitation cross sections are calculated for the 6s subshell of Rn. Excitation cross sections for the $6s \rightarrow 6d$, $6s \rightarrow 7l$, and $6s \rightarrow 8l$ transitions are presented in Table 4. The excitation energies are all above the configuration-average ionization energy of the 6p subshell. In the configuration-average approximation the 6s subshell excitations contribute to the ionization of the Rn atom through excitation-autoionization.

4. SUMMARY

Electron-impact ionization cross sections for the single ionization of the neutral Rn atom have been presented. The overall perturbative distorted-wave and non-perturbative close-coupling calculations for the 6p subshell with and without a polarization potential were presented for energies ranging from threshold to 150 eV. The overall perturbative distorted-wave and non-perturbative close-coupling calculations for the 6s subshell without a polarization potential were presented for energies ranging from threshold to 200 eV. In the future we plan to carry out perturbative distorted-wave and non-perturbative close-coupling calculations for the outer subshells of other heavy atoms.

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References

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Table 1. Non-perturbative close-coupling calculations for the ionization of the $6p$ subshell of Rn

Initial Channel	L Values	Coupled Channels	20 eV	30 eV	40 eV	50 eV	60 eV
$6pks$	1	16	3.77 Mb	3.75 Mb	3.04 Mb	2.42 Mb	2.03 Mb
$6pkp$	0	9	2.15 Mb	2.56 Mb	2.35 Mb	1.87 Mb	1.46 Mb
$6pkp$	1	8	5.55 Mb	5.22 Mb	4.12 Mb	3.21 Mb	2.53 Mb
$6pkp$	2	22	7.29 Mb	7.65 Mb	6.45 Mb	5.38 Mb	4.56 Mb
$6pkd$	1	16	12.21 Mb	11.12 Mb	7.88 Mb	5.67 Mb	4.49 Mb
$6pkd$	2	14	9.74 Mb	8.85 Mb	6.90 Mb	5.44 Mb	4.47 Mb
$6pkd$	3	26	20.38 Mb	18.19 Mb	13.49 Mb	10.45 Mb	8.58 Mb
$6pkf$	2	22	15.08 Mb	18.59 Mb	16.88 Mb	14.19 Mb	11.66 Mb
$6pkf$	3	19	17.30 Mb	17.26 Mb	13.82 Mb	10.82 Mb	8.66 Mb
$6pkf$	4	29	27.53 Mb	38.80 Mb	35.72 Mb	29.65 Mb	24.07 Mb
$6pkg$	3	26	7.16 Mb	11.22 Mb	12.81 Mb	13.10 Mb	12.68 Mb
$6pkg$	4	22	5.75 Mb	9.24 Mb	8.90 Mb	8.09 Mb	7.47 Mb
$6pkg$	5	30	16.82 Mb	30.19 Mb	32.78 Mb	30.31 Mb	26.63 Mb
$6pkh$	4	29	6.47 Mb	11.37 Mb	11.87 Mb	11.81 Mb	11.34 Mb
$6pkh$	5	24	4.12 Mb	8.27 Mb	8.09 Mb	7.33 Mb	6.45 Mb
$6pkh$	6	30	15.12 Mb	34.01 Mb	36.01 Mb	34.23 Mb	30.64 Mb
$6pki$	5	30	5.47 Mb	11.34 Mb	12.88 Mb	12.57 Mb	11.75 Mb
$6pki$	6	24	1.79 Mb	5.32 Mb	6.82 Mb	6.82 Mb	6.22 Mb
$6pki$	7	28	9.10 Mb	27.28 Mb	35.88 Mb	36.16 Mb	32.74 Mb
$6pkj$	6	28	3.01 Mb	8.32 Mb	10.67 Mb	11.25 Mb	10.99 Mb
$6pkj$	7	23	0.83 Mb	3.37 Mb	5.12 Mb	5.72 Mb	5.66 Mb
$6pkj$	8	25	4.93 Mb	21.03 Mb	32.76 Mb	36.72 Mb	35.82 Mb
$6pkk$	7	24	1.76 Mb	6.60 Mb	9.95 Mb	11.42 Mb	11.76 Mb
$6pkk$	8	20	0.43 Mb	2.36 Mb	4.18 Mb	5.14 Mb	5.42 Mb
$6pkk$	9	20	2.54 Mb	15.32 Mb	28.46 Mb	35.58 Mb	37.46 Mb
		partial total	206.33 Mb	337.21 Mb	367.81 Mb	355.34 Mb	325.52 Mb
		topup	1.65 Mb	26.38 Mb	86.53 Mb	158.35 Mb	224.86 Mb
		final total	207.98 Mb	360.59 Mb	454.34 Mb	513.69 Mb	550.38 Mb

Table 2. Non-perturbative close-coupling calculations with a polarization potential for the ionization of the $6p$ subshell of Rn

Initial Channel	L Values	Coupled Channels	20 eV	30 eV	40 eV	50 eV	60 eV
$6pks$	1	16	3.30 Mb	3.47 Mb	2.85 Mb	2.32 Mb	2.00 Mb
$6pkp$	0	9	1.86 Mb	2.33 Mb	2.15 Mb	1.74 Mb	1.35 Mb
$6pkp$	1	8	4.73 Mb	4.83 Mb	3.89 Mb	3.09 Mb	2.47 Mb
$6pkp$	2	22	6.39 Mb	7.14 Mb	6.06 Mb	5.11 Mb	4.37 Mb
$6pkd$	1	16	10.16 Mb	10.16 Mb	7.32 Mb	5.37 Mb	4.34 Mb
$6pkd$	2	14	8.08 Mb	8.11 Mb	6.47 Mb	5.24 Mb	4.38 Mb
$6pkd$	3	26	17.51 Mb	16.56 Mb	12.48 Mb	9.88 Mb	8.25 Mb
$6pkf$	2	22	11.90 Mb	17.17 Mb	16.00 Mb	13.64 Mb	11.28 Mb
$6pkf$	3	19	13.41 Mb	15.93 Mb	13.16 Mb	10.51 Mb	8.49 Mb
$6pkf$	4	29	21.86 Mb	36.04 Mb	33.62 Mb	28.19 Mb	23.00 Mb
$6pkg$	3	26	6.31 Mb	10.13 Mb	12.00 Mb	12.64 Mb	12.38 Mb
$6pkg$	4	22	5.56 Mb	8.35 Mb	8.17 Mb	7.76 Mb	7.31 Mb
$6pkg$	5	30	15.94 Mb	28.37 Mb	31.18 Mb	29.09 Mb	25.65 Mb
$6pkh$	4	29	6.47 Mb	10.86 Mb	11.19 Mb	11.23 Mb	10.91 Mb
$6pkh$	5	24	4.82 Mb	8.46 Mb	7.95 Mb	7.15 Mb	6.33 Mb
$6pkh$	6	30	15.50 Mb	40.87 Mb	35.94 Mb	33.73 Mb	29.93 Mb
$6pki$	5	30	5.01 Mb	10.99 Mb	12.54 Mb	12.27 Mb	11.46 Mb
$6pki$	6	24	2.33 Mb	5.74 Mb	6.98 Mb	6.94 Mb	6.32 Mb
$6pki$	7	28	8.96 Mb	27.63 Mb	36.39 Mb	36.47 Mb	32.64 Mb
$6pkj$	6	28	3.46 Mb	8.49 Mb	10.63 Mb	11.21 Mb	11.00 Mb
$6pkj$	7	23	1.63 Mb	3.86 Mb	5.32 Mb	5.95 Mb	5.92 Mb
$6pkj$	8	25	5.24 Mb	20.87 Mb	32.80 Mb	37.11 Mb	36.27 Mb
$6pkk$	7	24	2.55 Mb	7.01 Mb	10.03 Mb	11.48 Mb	11.92 Mb
$6pkk$	8	20	1.48 Mb	2.99 Mb	4.43 Mb	5.40 Mb	5.76 Mb
$6pkk$	9	20	3.48 Mb	14.92 Mb	27.69 Mb	35.31 Mb	37.75 Mb
		partial total	187.94 Mb	324.53 Mb	357.24 Mb	348.82 Mb	321.48 Mb
		topup	5.03 Mb	44.64 Mb	105.59 Mb	162.22 Mb	206.61 Mb
		final total	192.97 Mb	369.17 Mb	462.83 Mb	511.04 Mb	528.09 Mb

Table 3. Non-perturbative close-coupling calculations for the ionization of the 6s subshell of Rn

Initial Channel	L Values	Coupled Channels	40 eV	50 eV	60 eV
<i>6sks</i>	0	9	0.09 Mb	0.11 Mb	0.13 Mb
<i>6skp</i>	1	16	0.60 Mb	0.78 Mb	0.76 Mb
<i>6skd</i>	2	22	1.24 Mb	1.72 Mb	1.79 Mb
<i>6skf</i>	3	26	1.97 Mb	2.61 Mb	2.78 Mb
<i>6skg</i>	4	29	1.22 Mb	2.46 Mb	2.91 Mb
<i>6skh</i>	5	30	0.52 Mb	1.65 Mb	2.67 Mb
<i>6ski</i>	6	30	0.43 Mb	1.40 Mb	2.31 Mb
<i>6skj</i>	7	28	0.19 Mb	0.96 Mb	2.02 Mb
		partial total	6.26 Mb	11.69 Mb	15.36 Mb
		topup	0.04 Mb	0.68 Mb	2.49 Mb
		final total	6.29 Mb	12.37 Mb	17.84 Mb

Table 4. Perturbative distorted-wave calculations for the excitation of the 6s subshell of Ta

Transition	Excitation Energy	Incident Energy	Cross Section
<i>6s</i> → <i>6d</i>	26.85 eV	27.79 eV	3.61 Mb
		28.74 eV	5.74 Mb
		29.70 eV	6.63 Mb
<i>6s</i> → <i>7s</i>	25.02 eV	25.89 eV	2.06 Mb
		26.79 eV	2.78 Mb
		27.70 eV	3.62 Mb
<i>6s</i> → <i>7p</i>	26.53 eV	27.46 eV	1.53 Mb
		28.41 eV	1.76 Mb
		29.35 eV	1.73 Mb
<i>6s</i> → <i>7d</i>	27.85 eV	28.82 eV	2.88 Mb
		29.82 eV	2.84 Mb
		30.81 eV	2.74 Mb
<i>6s</i> → <i>8s</i>	27.34 eV	28.30 eV	0.92 Mb
		29.27 eV	0.93 Mb
		30.25 eV	0.93 Mb
<i>6s</i> → <i>8p</i>	27.76 eV	28.73 eV	0.62 Mb
		29.73 eV	0.59 Mb
		30.72 eV	0.57 Mb
<i>6s</i> → <i>8d</i>	28.26 eV	29.25 eV	1.48 Mb
		30.25 eV	1.42 Mb
		31.26 eV	1.36 Mb

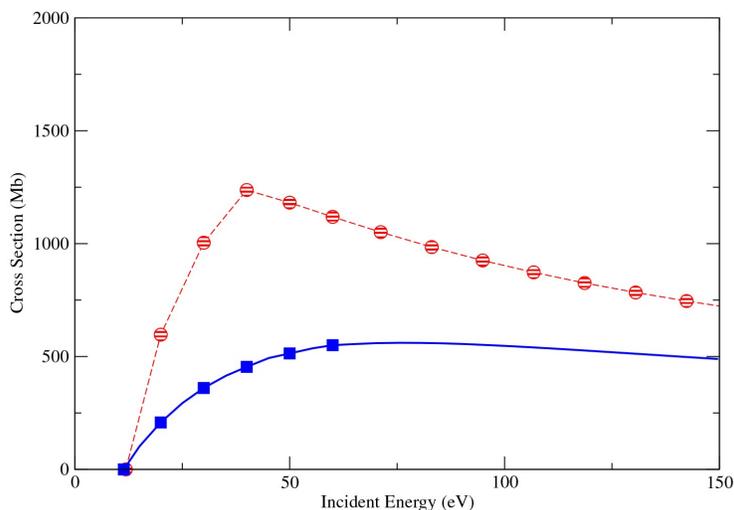


Figure 1. Electron-impact direct ionization of the 6p subshell of Rn. Dashed line (red): distorted-wave method, Solid squares (blue): non-perturbative close-coupling method ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).

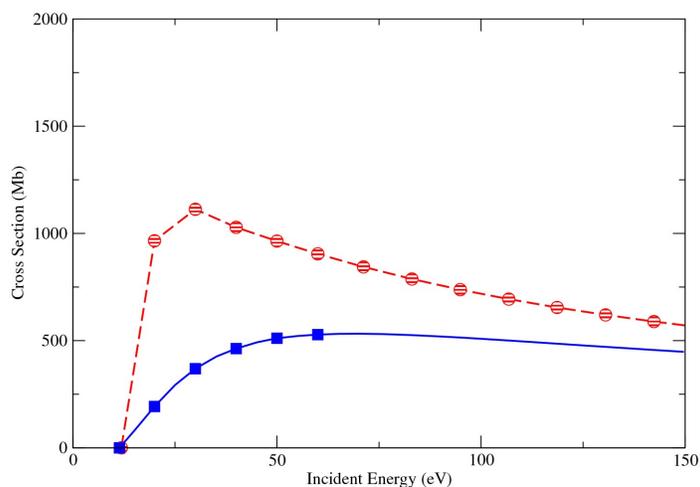


Figure 2. Electron-impact direct ionization of the 6p subshell of Rn. Dashed line (red): distorted-wave method with a polarization potential, Solid squares (blue): non-perturbative close-coupling method with a polarization potential ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).

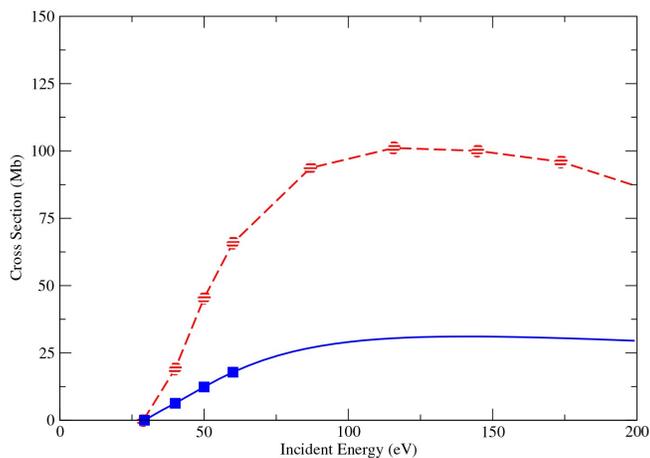


Figure 3. Electron-impact direct ionization of the 6s subshell of Rn. Dashed line (red): distorted-wave method, Solid squares (blue): non-perturbative close-coupling method ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).



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