RESONANCE EXCITATION CROSS SECTION OF Al-LIKE P^{2+} AND S^{3+} AT LOW ENERGIES

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الخلاصـــة :

عُـيِّـنـتْ المقاطع المستعرضة للإثارة الرنـيـنـيَّـة لأيوني الفوسفور والكبريت ذات تركيب إلكتروني شبيهة بالألونيوم عند الطاقات المنخفضة . وقد تم حساب احتمالات كلٍّ من الانبعاث الإشعاعي وإنبعاث أوجيه للإليكترونات باستخدام حساب الإقتران الزاوي المغزلي مع استخدام دوال هارتري - فوك غير النسبية . وتمت الحسابات لثمانية أنماط مختلفة للإثارة من حالة الخمود الإبتدائية . وقد وجُـد أنَّ المساحات المستعرضة للإثارة الرنـيـنـيَّـة أكبر بكثير من المساحات المستعرضة لإعادة الربط الثنائي الإليكتروني ، وهذا ناتج عن صغر الإنتاج البريقي لمستويات الرنين . ووجُـد أيضاً أن معدلات التشتت الرنيني المرن هى السائدة ، وأنَّ قيم المساحات المستعرضة للإثارة الرنينية تقل مع زيادة العدد الذري وعكس ذلك مع إعادة الربط الثنائي الإليكتروني .

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ABSTRACT

Resonance excitation (RE) cross sections of the ground state $(3s^2\ 3p)^2$P configuration of Al-like P^{2+} and S^{3+} ions are calculated at low energies. Contributions from the multiplets of the first excited state $3s^2\ 3p$ are also included. The Auger and radiative transition probabilities were calculated using single configuration non-relativistic Hartree–Fock wavefunctions in LS coupling. There are eight different modes of excitation for the initial ground state configuration. The resonance excitation cross sections, for both ions, were found to be large, as much as a factor of 10^3 larger than that of dielectronic recombination (DR), mainly because of the smallness of the fluorescence yield of the resonance levels. It was also found that the resonance elastic scattering is dominant, and that the RE cross section decreases with increasing atomic number and *vice versa* for the DR process.

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1. INTRODUCTION

Resonant excitation (RE) which combines both resonant elastic and inelastic scattering is the complementary process to dielectronic recombination (DR). The probabilities of these processes are related by $P_{DR} + P_{RE} = 1$ [1]. It has been shown that electron-ion collision processes are often dominated by their resonant mode [2, 3]. In a recent paper we calculated the cross sections and rate coefficients for the DR process by the Al-like P^{2+} and S^{3+} ions at low energies [4]. We propose to extend the previous work by calculating the cross sections and rate coefficients for the RE process associated with the $3s \rightarrow 3p$ excitation mode for the same ions. To simplify the calculations, we limited the energy range to below the threshold of the first excited state $(3s3p^2)^1P$. This correspond to the incident kinetic energy e_c of 0.99 Ry and 1.21 Ry as measured from the ground state for P^{2+} and S^{3+} respectively. Moreover, it was found that this excitation mode was dominant over other excitation modes such as $3s^23p \rightarrow 3s^23d$, $3s^23p \rightarrow 3s^24s$, and so forth [5]. The calculations are done for eight different modes of excitation with 30 possible final states for each ion. The results have been tabulated to facilitate direct comparison with the previous calculation of the DR process.

The work reported here is a continuation of the comprehensive study of the resonant process involving ions of interest for pollution control and the "Greenhouse Effect". There are many substances that contribute to air pollution. The sulfur ions treated here exist in different substances, such as sulfur oxides. The primary source of these oxides are sulfur-bearing fuels used for heat and power, both industrially and domestically. Chemical and metallurgical plants of various kinds also emit SO_x as the results of processing activities, such as the manufacture of sulfuric acid. The phosphorus ion exists in organic phosphates. It contributes to pollution notably from crop dusting and spraying (pesticide control). Other substances are phosphoric acid, phosphorus-containing fertilizers, and detergents.

For that matter the two ions P^{III} and S^{IV}, present in our atmosphere, presumably play a crucial role in changing the composition of the ionosphere and depleting the ozone layer. Because of the complexity of the calculations involved in this type of work, only a limited number of ions has been treated so far [6–8], and much more additional effort is being made to obtain a more complete set of data for modeling the atmosphere.

In Section 2 we will give a brief description of the theoretical procedure adopted in the evaluation of RE cross sections which is closely related to that of DR. The results and discussion of the calculations will be presented in Section 3, followed by a conclusion in Section 4.

2. RESONANT EXCITATION THEORY

The basic formulation of the theory for RE in the isolated resonance approximation is identical to that for the DR and we simply refer to references [2] and [3] for details.

The RE process of interest here involves an initial excitation capture in going from the ground state $i = 3s^23p$ to an intermediate state d

$$(3s^23p)\,(i) + e \rightarrow (3s3p^2)\,nl(d) \qquad (1)$$

followed by an emission of an Auger electron

$$(3s3p^2)\,nl(d) \rightarrow (3s3p^2)\,(f) + e' \qquad (2)$$

while in the DR process the initial process, Equation (1), is followed by a radiative decay of the intermediate state d

$$(3s3p^2)\,nl(d) \rightarrow (3s3p^2)\,n'l'(f) + \gamma(nl \rightarrow n'l') \qquad (3)$$

(explicit reference to the core electrons and the multiplet states of the Al-like ions are omitted for simplicity).

The DR averaged cross sections are defined as follow

$$\bar{\sigma}^{DR} = \frac{1}{\Delta e_c} \int_{e_c - \frac{\Delta e_c}{2}}^{e_c + \frac{\Delta e_c}{2}} \sigma^{DR}(e_c')\, de_c', \qquad (4)$$

where the DR cross section σ^{DR} is given by

$$\sigma^{DR}(i, l_c \rightarrow d) = \frac{4\pi}{(k_c a_o)^2} V_a(i, l_c \rightarrow d)\tau_o \omega(d)\, \tilde{\delta}(\pi a_o^2), \qquad (5)$$

similarly, we define an energy-averaged cross section for the RE process as follow

$$\bar{\sigma}^{RE} = \frac{1}{\Delta e_c} \int_{e_c - \frac{\Delta e_c}{2}}^{e_c + \frac{\Delta e_c}{2}} \sigma^{RE}(e_c')\, de_c' , \qquad (6)$$

where the RE cross section σ^{RE} is given by:

$$\sigma^{RE}(i, l_c \rightarrow d) = \frac{4\pi}{(k_c a_o)^2} V_a(i, l_c \rightarrow d) \tau_o z(d)\, \tilde{\delta}(\pi a_o^2), \qquad (7)$$

where the Lorentzian factor $\tilde{\delta}$ provides the resonance profile in the isolated resonance approximation

$$\tilde{\delta} = \frac{\Gamma(d)}{2\pi\left[(e_i - e_d)^2 + \frac{\Gamma(d)^2}{4}\right]} \qquad (8)$$

and imposes energy conservation $e_i = e_d$ when $\Gamma(d) \ll 1$, in which case $\int \tilde{\delta}\, de_c = 1$.

V_a is the radiationless excitation capture probability which is related, by detailed balance, to the Auger emission probability $A_a(i \rightarrow d)$ by $V_a = (g_d/2g_i)\, A_a(i \rightarrow d)$, where g_d and g_i are the statistical weights of the intermediate and the initial states respectively; a_o and τ_o are the Bohr radius and the atomic unit of time respectively. Δe_c is a small energy bin which is chosen arbitrarily but with the requirement that it is small compared with the actual experiment continuum electron beam width. $z(d) = A_a(i \rightarrow d)/\Gamma(d)$ and $\omega(d \rightarrow f) = A_r(d \rightarrow f)/\Gamma(d)$ are the partial Auger and fluorescent yields of the state d, respectively. A_r is the radiative transition probability. $\Gamma(d) = \Sigma_f A_a(d \rightarrow i) + \Sigma_f A_r(d \rightarrow f)$ is the total width of the intermediate state.

We can clearly see that z and ω are closely related by:

$$\Sigma_f z(d \rightarrow f) + \Sigma_{f'} \omega(d \rightarrow f') = 1. \qquad (9)$$

Therefore, the theories for DR and RE are essentially the same, as they are constructed in terms of A_a and A_r.

The calculations presented here were carried out in the single configuration, non-relativistic Hartree–Fock approximation, isolated resonance approximation, and in LS coupling. The Cowan RCN/RC Code [9] was extensively used in the calculation of the transition energies as well as the relevant A_a and A_r needed in the evaluation of the DR and the RE cross sections. Some of the energies of the levels involved were adjusted in terms of better experimental and theoretical values [10], since the cross sections are very sensitive to the resonance energies.

For convenience, we define the various channels needed in our work as:

$$i_1 = (3s^2 3p)^2P,$$
$$i_2 = (3s3p^2)^4P, \qquad d_1 = (i_2)\, nl,$$
$$i_3 = (3s3p^2)^2D, \qquad d_2 = (i_3)\, nl,$$
$$i_4 = (3s3p^2)^2S, \qquad d_3 = (i_4)\, nl,$$
$$i_5 = (3s3p^2)^2P, \qquad d_4 = (i_5)\, nl.$$

3. RESULTS AND DISCUSSION

We will consider here the contribution to RE from the states which lie below threshold energy level $(3s3p^2)^2P$ only, which correspond to $e_c < 1.0$ Ry for P^{2+}, and $e_c < 1.21$ Ry for S^{3+}. This upper limit in energy is imposed to limit the extend of the calculations. Thus, the following excitation modes for the intrashell transitions contribute to the RE:

$e_c + i_1 \rightarrow d_{1,2,3,4} \rightarrow i_1 + e'$	purely resonant elastic scattering
$\rightarrow d_{1,2,3} + e'$	resonant inelastic scattering
$e_c + d_1 \rightarrow d_{2,3,4} \rightarrow d_1 + e'$	purely resonant elastic scattering
$\rightarrow (i_1, d_{2,3}) + e'$	resonant inelastic scattering
$e_c + d_2 \rightarrow d_{3,4} \rightarrow d_2 + e'$	purely resonant elastic scattering
$\rightarrow (i_1, d_{1,3}) + e'$	resonant inelastic scattering
$e_c + d_3 \rightarrow d_4 \rightarrow d_3 + e'$	purely resonant elastic scattering
$\rightarrow (i_1, d_{1,2}) + e'$	resonant inelastic scattering

Tables 1 and 2 from reference 4 have been added here for completeness. As seen from the above excitation modes, there are 30 different final states for each ion. Ten of them contribute to RE as purely elastic resonant scattering. The rest of the contribution to RE comes from resonant inelastic scattering. The RE cross sections for P^{2+} are tabulated in Tables 1–10 as functions of e_c (Ryd) and for S^{3+} in Tables 11–20. The DR cross sections have been added for comparison purposes. It can be seen that the cross sections due to resonant elastic scattering are dominant for the two ions with peaks at $2.48\times10^{-13}\,cm^2$ for P^{2+} and $4.81\times10^{-14}\,cm^2$ for S^{3+} for transition $i_1\rightarrow d_2\rightarrow i_1$ (see Tables 2 and 12). The DR cross sections, on the other hand, are the least dominant with highest values of $6.21\times10^{-17}\,cm^2$ for P^{2+} and $1.03\times10^{-16}\,cm^2$ for S^{3+} for the transition $i_1\rightarrow d_4$ (see Tables 7 and 11), and lowest values of $6.22\times10^{-20}\,cm^2$ for P^{2+} for the transition $i_1\rightarrow d_1$ (see Table 1) and $6.03\times10^{-19}\,cm^2$ for S^{3+} for the transition $d_1\rightarrow d_3$ (see Table 15).

Configuration interaction (CI) was not included in the present calculation even though the transitions studied here were very close to threshold, in which case the CI effects could be very strong. Therefore, its inclusion may refine our calculations, but it needs further careful study.

4. CONCLUSION

We have calculated the DR and the RE cross sections for the multiplet of the first excited state $(3s3p^2)^2P$ of the Al-like P^{2+} and S^{3+} ions. Explicit cross sections are listed in Tables 1–20 as a function of e_c (Ryd). We observe that the resonant elastic scattering cross sections are dominant over the RE and that they are larger than the DR by as much as 10^3, mainly because of the fluorescent yield of the resonance levels. The RE cross section decreases with increasing atomic number in a given isoelectronic sequence. The DR, on the other hand, increases with increasing atomic number in a given isoelectronic sequence.

Due to the unitary nature of the mixing matrix, the total cross sections are generally much less sensitive to the mixing (on the order of $\pm10\%$ change), although the individual states are sometimes very much affected by it. The dependence of our results on the coupling scheme used is also very weak in so far as the total is concerned. That is why we neglected these and other possible complications in the present calculations.

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Table 1. Values of $\bar{\sigma}^{DR}(cm^2)$ and $\bar{\sigma}^{RE}(cm^2)$ *vs.* e_c(Ry) for P^{2+} for the Transitions $i_1 \rightarrow d_1$, and $i_1 \rightarrow d_1 \rightarrow i_1$. $\Delta e_c = 0.01$ Ry. Powers of 10 are shown in Parenthesis.

	$i_1 \rightarrow d_1$	
e_c	DR	i_1
0.01	3.20(−20)	5.98(−14)
0.19	3.45(−21)	1.44(−15)
0.21	1.36(−20)	1.51(−15)
0.24	1.13(−20)	1.25(−15)
0.26	1.82(−28)	1.86(−17)
0.32	1.02(−21)	3.58(−16)
0.33	3.05(−21)	5.08(−16)
0.34	4.55(−22)	4.05(−16)
0.35	4.87(−29)	1.13(−17)
0.38	1.57(−22)	1.54(−16)
0.39	1.49(−21)	2.40(−16)
0.40	2.49(−22)	1.97(−16)
0.42	1.19(−21)	2.17(−16)
0.43	1.55(−22)	1.11(−16)
0.44	9.24(−22)	1.69(−16)
0.45	4.36(−22)	2.00(−16)
0.46	8.81(−22)	1.84(−16)
0.47	6.09(−22)	1.45(−16)
0.48	5.50(−22)	1.36(−16)
0.49	3.62(−22)	6.58(−17)
0.50	1.05(−22)	1.67(−17)
Total	6.22(−20)	6.71(−14)

Table 2. As Table 1 but for $i_1 \rightarrow d_2$, and $i_1 \rightarrow d_2 \rightarrow i_1, d_1$.

	$i_1 \rightarrow d_2$		
e_c	DR	i_1	d_1
0.02	4.78(−19)	6.63(−14)	
0.07	5.08(−19)	1.55(−13)	
0.17	7.73(−20)	6.22(−15)	
0.35	1.99(−20)	1.24(−15)	
0.37	9.66(−20)	5.86(−15)	
0.41	3.31(−20)	1.31(−15)	
0.42	1.26(−19)	2.27(−15)	
0.48	1.27(−20)	4.11(−16)	
0.49	7.33(−20)	1.76(−15)	
0.51	1.28(−19)	1.54(−15)	
0.52	1.25(−19)	1.39(−16)	1.73(−19)
0.55	5.29(−20)	8.48(−16)	1.53(−16)
0.56	2.12(−19)	9.44(−16)	3.34(−17)
0.57	1.33(−19)	7.99(−18)	1.41(−21)
0.58	8.88(−21)	1.07(−16)	4.13(−18)
0.59	3.71(−19)	1.03(−15)	1.03(−16)
0.61	4.04(−19)	8.89(−16)	6.88(−17)
0.62	1.44(−19)	4.14(−16)	5.48(−17)
0.63	1.00(−18)	8.13(−16)	4.37(−17)
0.64	1.99(−18)	4.39(−16)	3.02(−17)
0.65	4.33(−18)	4.08(−16)	3.01(−17)
0.66	1.14(−17)	2.77(−16)	2.24(−17)
0.67	8.22(−18)	1.35(−17)	3.00(−19)
Total	2.99(−17)	2.48(−13)	5.44(−16)

Table 3. As Table 1 but for $d_1 \rightarrow d_2$, and $d_1 \rightarrow d_2 \rightarrow i_1, d_1$.

	$d_1 \rightarrow d_2$		
e_c	DR	i_1	d_1
0.03	1.71(−19)	1.19(−15)	6.47(−15)
0.04	1.16(−19)	1.98(−16)	2.40(−15)
0.05	2.25(−20)	8.05(−19)	1.17(−19)
0.06	1.09(−21)	1.76(−17)	6.84(−19)
0.07	1.22(−19)	4.15(−16)	1.97(−14)
0.08	1.91(−20)	3.97(−19)	8.06(−20)
0.09	9.48(−20)	2.21(−16)	8.08(−16)
0.10	1.11(−19)	1.51(−16)	5.74(−16)
0.11	1.45(−19)	8.28(−17)	1.74(−16)
0.12	1.98(−19)	8.83(−17)	2.88(−16)
0.13	4.69(−19)	7.28(−17)	2.47(−16)
0.14	6.83(−18)	5.81(−17)	1.89(−16)
0.15	8.55(−19)	2.04(−18)	4.88(−19)
Total	9.16(−18)	2.49(−15)	1.31(−14)

Table 4. As Table 1 but for $i_1 \rightarrow d_3$, and $i_1 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$i_1 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.25	1.33(−20)	1.16(−15)		
0.30	4.55(−20)	5.54(−15)		
0.40	1.90(−20)	1.42(−15)		
0.58	4.47(−21)	1.51(−16)		
0.60	1.36(−20)	3.62(−16)	3.53(−16)	
0.64	9.82(−21)	2.54(−16)	7.25(−17)	
0.65	2.90(−20)	3.02(−16)	6.25(−18)	
0.71	3.62(−21)	5.57(−17)		
0.72	8.74(−20)	1.17(−16)	1.01(−16)	2.39(−17)
0.74	2.05(−20)	1.77(−16)	2.42(−17)	1.04(−16)
0.75	1.02(−20)	6.02(−18)	2.57(−21)	1.34(−17)
0.78	1.19(−20)	8.92(−17)	4.52(−17)	1.38(−17)
0.79	3.25(−20)	1.15(−16)	1.26(−17)	6.65(−17)
0.80	1.01(−20)	3.11(−19)		8.42(−19)
0.81	1.54(−21)	7.13(−19)		1.01(−18)
0.82	4.69(−20)	1.02(−16)	3.09(−17)	5.11(−17)
0.84	5.87(−20)	7.48(−17)	2.11(−17)	4.33(−17)
0.85	2.78(−20)	3.76(−17)	1.93(−17)	1.42(−17)
0.86	1.45(−19)	7.95(−17)	1.31(−17)	4.42(−17)
0.87	2.16(−19)	4.20(−17)	1.12(−17)	2.16(−17)
0.88	9.32(−19)	4.02(−17)	9.97(−18)	2.04(−17)
0.89	2.05(−18)	2.94(−17)	5.94(−18)	1.51(−17)
0.90	1.72(−18)	1.71(−18)	4.99(−20)	9.75(−19)
Total	5.43(−18)	1.02(−14)	7.26(−16)	4.34(−16)

Table 5. As Table 1 but for $d_1 \rightarrow d_3$, and $d_1 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$d_1 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.08	3.20(−20)	1.23(−15)	1.43(−15)	
0.12	5.61(−21)	1.88(−16)	5.43(−17)	
0.13	1.41(−21)	1.51(−17)	4.09(−19)	
0.20	1.11(−20)	1.77(−16)	1.59(−16)	2.45(−17)
0.22	2.85(−21)	4.01(−17)	1.07(−17)	2.16(−17)
0.23	7.03(−24)	4.15(−21)	2.28(−24)	8.85(−21)
0.26	7.56(−21)	6.65(−17)	4.98(−17)	1.12(−17)
0.27	2.23(−21)	1.80(−17)	3.83(−18)	8.45(−18)
0.28	7.84(−24)	4.30(−21)	2.54(−24)	6.44(−21)
0.30	7.61(−21)	4.03(−17)	2.66(−17)	1.09(−17)
0.31	5.33(−22)	1.49(−18)	5.23(−20)	7.99(−19)
0.32	9.08(−21)	2.73(−17)	1.46(−17)	9.00(−18)
0.33	1.34(−20)	2.42(−17)	1.45(−17)	6.69(−18)
0.34	1.07(−20)	1.16(−17)	5.13(−18)	4.18(−18)
0.35	2.51(−20)	1.50(−17)	8.34(−18)	4.54(−18)
0.36	2.52(−19)	1.34(−17)	7.45(−18)	4.03(−18)
0.37	7.15(−19)	8.28(−18)	5.16(−18)	1.95(−18)
0.38	4.95(−20)	1.55(−19)	5.92(−21)	7.37(−20)
Total	1.15(−18)	1.87(−15)	1.79(−15)	1.08(−16)

Table 6. As Table 1 but for $d_2 \rightarrow d_3$, and $d_2 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$d_2 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.04	3.69(−20)	2.21(−16)	1.29(−16)	1.56(−16)
0.06	9.27(−20)	6.90(−16)	8.89(−17)	5.57(−16)
0.07	1.41(−19)	8.26(−17)	3.38(−20)	1.85(−16)
0.10	1.69(−20)	6.04(−17)	3.32(−17)	2.70(−17)
0.11	1.56(−20)	8.52(−17)	1.99(−17)	8.16(−17)
0.12	2.93(−20)	1.80(−16)	3.93(−18)	1.43(−16)
0.14	1.75(−19)	7.22(−17)	2.75(−17)	5.94(−17)
0.15	5.21(−20)	1.01(−16)	1.97(−18)	8.47(−17)
0.16	1.78(−19)	6.04(−17)	1.94(−17)	5.82(−17)
0.17	3.37(−19)	8.89(−17)	8.55(−18)	7.82(−17)
0.18	5.48(−19)	1.09(−16)	1.54(−17)	8.97(−17)
0.19	2.28(−18)	7.87(−16)	1.09(−17)	6.62(−17)
0.20	2.48(−18)	5.09(−17)	8.40(−18)	4.23(−17)
0.21	2.48(−18)	3.58(−17)	4.31(−18)	2.62(−17)
0.22	4.80(−18)	8.61(−18)	1.94(−19)	6.17(−18)
Total	1.14(−17)	1.93(−15)	3.71(−16)	1.66(−15)

Table 7. As Table 1 but for $i_1 \rightarrow d_4$, and $i_1 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$i_1 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.33	1.01(−19)	2.33(−14)			
0.38	3.71(−19)	5.63(−14)			
0.48	1.53(−19)	8.38(−15)			
0.66	4.15(−20)	7.40(−16)	3.41(−17)		
0.68	1.41(−19)	4.04(−15)	2.13(−16)	9.54(−16)	
0.72	9.03(−21)	1.79(−15)	1.46(−17)	3.14(−16)	
0.73	3.46(−19)	2.33(−15)	8.09(−18)	1.43(−17)	
0.79	3.15(−20)	2.75(−16)	1.22(−17)	1.80(−17)	
0.80	1.24(−19)	1.38(−15)	4.51(−17)	3.00(−16)	
0.82	3.13(−19)	2.15(−15)	1.06(−17)	1.32(−16)	
0.83	3.88(−19)	1.57(−16)	4.33(−21)	3.66(−20)	
0.86	1.45(−19)	7.95(−16)	2.33(−17)	1.55(−16)	
0.87	2.93(−19)	1.24(−15)	5.81(−18)	7.10(−17)	
0.88	6.09(−19)	1.42(−16)	4.28(−21)	3.52(−20)	
0.89	2.75(−20)	8.14(−17)	3.29(−18)	6.78(−18)	
0.90	1.19(−19)	6.26(−16)	1.02(−17)	1.18(−16)	
0.91	8.60(−19)	6.19(−16)	2.15(−18)	4.46(−18)	
0.92	4.67(−19)	9.21(−16)	1.24(−17)	9.69(−17)	5.26(−17)
0.93	8.09(−19)	4.54(−16)	7.13(−18)	6.84(−17)	2.53(−17)
0.94	1.79(−18)	7.74(−16)	6.29(−18)	4.41(−17)	2.82(−17)
0.95	3.05(−18)	6.93(−16)	6.85(−18)	5.56(−17)	2.93(−17)
0.96	7.41(−18)	4.67(−16)	4.29(−18)	4.37(−17)	2.40(−17)
0.97	1.95(−17)	3.15(−16)	3.17(−18)	2.69(−17)	5.87(−18)
0.98	2.50(−17)	5.98(−17)	2.33(−19)	4.65(−19)	7.04(−20)
Total	6.21(−17)	1.08(−13)	4.23(−16)	2.42(−15)	1.65(−16)

Table 8. As Table 1 but for $d_1 \rightarrow d_4$, and $d_1 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_1 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.15	6.52(−21)	7.58(−17)	7.35(−18)		
0.16	8.68(−20)	4.33(−16)	5.79(−16)	2.33(−17)	
0.21	2.46(−20)	3.90(−17)	1.28(−16)	2.42(−18)	
0.27	2.99(−21)	1.74(−17)	1.60(−18)	1.71(−18)	
0.28	4.80(−20)	6.30(−17)	1.24(−16)	2.68(−18)	
0.30	1.18(−20)	6.67(−18)	3.96(−17)	9.39(−19)	
0.31	7.40(−21)	7.49(−18)	9.34(−20)	4.66(−20)	
0.34	4.11(−20)	2.90(−17)	5.04(−17)	1.64(−18)	
0.35	1.01(−20)	2.85(−18)	1.84(−17)	2.23(−19)	
0.36	6.37(−21)	4.24(−18)	5.27(−20)	2.75(−20)	
0.38	3.67(−20)	1.43(−17)	2.62(−17)	9.35(−19)	
0.39	1.56(−20)	4.08(−18)	1.05(−17)	1.39(−19)	
0.40	4.29(−20)	1.00(−17)	1.85(−17)	7.05(−19)	1.04(−18)
0.41	2.52(−20)	5.50(−18)	8.22(−18)	3.54(−19)	2.12(−18)
0.42	1.32(−19)	1.31(−17)	2.64(−17)	5.97(−19)	1.40(−18)
0.43	1.33(−19)	6.12(−18)	1.10(−17)	3.34(−19)	1.12(−18)
0.44	8.90(−19)	5.70(−18)	1.27(−17)	2.32(−19)	1.00(−18)
0.45	1.06(−18)	3.54(−18)	6.65(−18)	9.16(−20)	2.52(−20)
0.46	7.70(−19)	4.96(−19)	1.44(−19)	5.34(−21)	1.28(−21)
Total	3.35(−18)	7.42(−16)	1.07(−15)	3.60(−17)	6.71(−18)

Table 9. As Table 1 but for $d_2 \rightarrow d_4$, and $d_2 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_2 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.05	1.07(−19)	2.80(−15)	1.19(−17)	7.83(−16)	
0.12	7.90(−20)	1.20(−15)	1.20(−17)	6.89(−16)	
0.14	3.45(−21)	4.09(−16)	1.35(−18)	1.06(−16)	
0.15	4.44(−20)	3.49(−17)	1.15(−19)	2.97(−18)	
0.18	5.47(−20)	4.26(−16)	3.64(−18)	2.41(−16)	
0.20	3.81(−20)	1.87(−16)	5.40(−19)	4.36(−16)	
0.22	4.69(−20)	2.09(−16)	1.92(−18)	1.13(−16)	
0.23	3.29(−20)	1.00(−16)	2.81(−19)	2.28(−17)	
0.24	4.91(−20)	1.28(−16)	1.29(−18)	6.44(−17)	1.23(−18)
0.25	4.43(−20)	1.13(−16)	7.81(−19)	2.30(−17)	2.21(−17)
0.26	1.66(−19)	1.98(−16)	1.04(−18)	9.31(−17)	8.62(−18)
0.27	1.72(−19)	9.88(−17)	6.79(−19)	3.64(−17)	9.71(−18)
0.28	7.20(−19)	9.66(−17)	4.42(−19)	3.97(−17)	8.25(−18)
0.29	1.36(−18)	5.92(−17)	1.82(−19)	3.05(−17)	1.06(−18)
0.30	3.50(−18)	8.62(−18)	2.24(−20)	4.12(−18)	7.66(−20)
Total	6.41(−18)	6.06(−15)	3.62(−17)	2.29(−15)	5.11(−17)

Table 10. As Table 1 but for $d_3 \rightarrow d_4$, and $d_3 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_3 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.01	2.32(−18)	8.16(−15)	3.04(−16)	1.20(−15)	4.16(−15)
0.02	1.51(−18)	2.94(−15)	9.76(−17)	3.99(−16)	1.45(−15)
0.03	1.49(−18)	1.68(−15)	6.30(−17)	2.47(−16)	8.30(−16)
0.04	2.91(−18)	1.41(−15)	5.74(−17)	2.23(−16)	7.27(−16)
0.05	3.16(−17)	9.09(−16)	2.95(−17)	1.32(−16)	4.43(−16)
0.06	1.89(−17)	1.79(−16)	6.69(−19)	8.51(−18)	6.82(−17)
0.07	6.59(−19)	8.25(−19)	2.15(−21)	5.93(−23)	6.75(−21)
Total	5.94(−17)	1.53(−14)	5.53(−16)	2.21(−15)	7.68(−15)

Table 11. Values of $\bar{\sigma}^{DR}(cm^2)$ and $\bar{\sigma}^{RE}(cm^2)$ *vs.* e_c(Ry) for S^{3+} for the Transitions $i_1 \rightarrow d_1$, and $i_1 \rightarrow d_1 \rightarrow i_1$. $\Delta e_c = 0.01$ Ry. Powers of 10 are shown in Parenthesis.

	$i_1 \rightarrow d_1$	
e_c	DR	i_1
0.06	1.96(−19)	1.95(−16)
0.10	1.73(−20)	2.43(−15)
0.23	2.96(−21)	7.86(−16)
0.25	4.71(−21)	5.05(−16)
0.28	2.87(−20)	3.86(−17)
0.30	3.33(−21)	3.76(−16)
0.37	5.28(−22)	2.58(−16)
0.38	1.87(−21)	1.75(−16)
0.39	1.23(−20)	1.97(−17)
0.40	1.51(−21)	1.49(−16)
0.44		1.24(−16)
0.45	1.05(−21)	8.61(−17)
0.46	6.72(−21)	1.18(−17)
0.47	8.72(−22)	7.82(−17)
0.49		7.08(−17)
0.50	4.77(−21)	5.89(−17)
0.51	1.03(−21)	8.21(−17)
0.52	3.94(−22)	3.28(−17)
0.53	3.07(−21)	7.58(−17)
0.54	5.45(−22)	7.47(−17)
0.55	2.49(−21)	7.16(−17)
0.56	1.93(−21)	4.51(−17)
0.57	1.38(−21)	4.47(−17)
0.58	1.24(−21)	5.88(−17)
0.59	1.07(−21)	5.03(−17)
0.60	1.60(−21)	4.18(−17)
0.61	8.67(−22)	2.56(−17)
0.62	9.70(−22)	1.71(−17)
0.63	9.54(−22)	7.53(−18)
0.64	6.49(−23)	1.27(−19)
Total	3.01(−19)	5.99(−15)

Table 12. As Table 11 but for $i_1 \rightarrow d_2$, and $i_1 \rightarrow d_2 \rightarrow i_1, d_1$.

		$i_1 \rightarrow d_2$	
e_c	Γ	i_1	d_1
0.17	2.91(−19)	8.86(−15)	
0.21	7.21(−20)	2.69(−15)	
0.27	4.18(−19)	1.21(−14)	
0.30	8.56(−20)	4.93(−15)	
0.44	8.62(−20)	1.36(−15)	
0.46	2.40(−20)	5.86(−16)	
0.48	1.75(−19)	3.72(−15)	
0.49	1.08(−19)	8.10(−16)	
0.50	4.88(−20)	1.45(−15)	
0.57	6.64(−20)	5.15(−16)	
0.58	1.61(−20)	2.51(−16)	
0.60	3.22(−19)	2.36(−15)	
0.61	3.91(−20)	6.77(−16)	
0.65	3.83(−20)	2.15(−16)	5.42(−17)
0.66	8.95(−21)	1.24(−16)	1.20(−17)
0.67	4.05(−19)	1.72(−15)	9.41(−17)
0.70	3.72(−20)	2.02(−16)	3.87(−17)
0.71	4.44(−19)	9.13(−16)	2.76(−17)
0.72	2.00(−20)	2.14(−16)	3.23(−17)
0.73	3.56(−20)	1.35(−16)	2.52(−17)
0.74	5.58(−19)	8.26(−16)	4.57(−17)
0.75	6.06(−20)	2.22(−16)	3.61(−17)
0.76	5.50(−19)	6.18(−16)	3.79(−17)
0.77	5.83(−20)	1.21(−16)	2.09(−17)
0.78	5.96(−19)	4.96(−16)	3.86(−17)
0.79	1.07(−18)	5.84(−16)	3.45(−17)
0.80	1.36(−18)	4.18(−16)	3.17(−17)
0.81	2.43(−18)	3.34(−16)	2.60(−17)
0.82	4.47(−18)	2.52(−16)	1.45(−17)
0.83	5.15(−18)	2.49(−16)	1.37(−17)
0.84	2.07(−17)	1.48(−16)	4.63(−18)
Total	3.97(−17)	4.81(−14)	5.88(−16)

Table 13. As Table 11 but for $d_1 \rightarrow d_2$, and $d_1 \rightarrow d_2 \rightarrow i_1, d_1$.

	$d_1 \rightarrow d_2$		
e_c	DR	i_1	d_1
0.01	1.60(−19)	7.44(−16)	2.52(−16)
0.02	1.41(−19)	6.79(−16)	1.14(−15)
0.05	8.57(−20)	2.58(−16)	6.27(−16)
0.06	9.25(−20)	3.27(−16)	3.32(−16)
0.07	2.68(−21)	2.43(−17)	2.32(−18)
0.08	7.56(−20)	1.81(−16)	4.00(−16)
0.09	4.20(−20)	9.12(−17)	2.81(−17)
0.10	6.57(−20)	1.29(−16)	2.44(−16)
0.11	7.38(−20)	1.28(−16)	1.35(−16)
0.12	7.21(−20)	8.03(−17)	1.61(−16)
0.13	1.25(−19)	1.03(−16)	1.68(−16)
0.14	1.92(−19)	1.09(−16)	1.32(−16)
0.15	5.07(−19)	6.98(−17)	1.09(−16)
0.16	2.97(−18)	5.45(−17)	8.70(−17)
0.17	3.45(−19)	2.98(−17)	5.17(−17)
0.18	3.66(−18)	2.55(−17)	3.58(−17)
0.19	1.27(−18)	5.78(−18)	1.96(−18)
Total	9.87(−18)	3.04(−15)	3.91(−15)

Table 14. As Table 11 but for $i_1 \rightarrow d_3$, and $i_1 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$i_1 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.44	3.47(−20)	7.17(−16)		
0.48	9.54(−21)	2.38(−16)		
0.54	5.70(−20)	1.07(−15)		
0.58	4.89(−21)	5.32(−16)		
0.71	1.40(−20)	1.03(−16)	6.34(−17)	
0.73	4.84(−21)	7.36(−17)		
0.76	6.48(−20)	5.88(−16)	1.86(−17)	
0.77	9.72(−21)	1.60(−16)	3.07(−17)	
0.84	1.23(−20)	4.82(−17)	2.29(−17)	
0.85	2.00(−21)	2.41(−17)		1.02(−17)
0.87	3.12(−20)	1.90(−16)	6.74(−18)	1.27(−16)
0.88	1.58(−20)	5.60(−17)	1.01(−17)	3.73(−17)
0.92	3.96(−21)	1.35(−17)	6.29(−18)	1.88(−17)
0.93	1.55(−21)	1.35(−17)		5.80(−18)
0.94	5.68(−20)	1.17(−16)	4.04(−18)	8.41(−17)
0.95	4.38(−21)	3.20(−17)	5.80(−18)	1.81(−17)
0.97	3.67(−21)	7.81(−18)	3.59(−18)	1.14(−17)
0.98	7.79(−20)	8.90(−17)	2.75(−18)	5.82(−17)
0.99	4.24(−21)	2.06(−17)	3.66(−18)	1.15(−17)
1.00	1.45(−21)	6.10(−18)		2.60(−18)
1.01	2.04(−20)	6.16(−17)	6.73(−18)	4.08(−17)
1.02	8.79(−20)	1.89(−17)	1.39(−20)	1.49(−17)
1.03	2.28(−20)	4.94(−17)	4.87(−18)	3.15(−17)
1.04	1.03(−19)	3.92(−17)	4.72(−18)	2.70(−17)
1.05	1.09(−19)	4.18(−17)	3.05(−18)	2.80(−17)
1.06	2.09(−19)	5.72(−17)	4.09(−18)	4.00(−17)
1.07	1.59(−19)	3.44(−17)	2.85(−18)	2.28(−17)
1.08	4.88(−19)	3.31(−17)	2.76(−18)	2.30(−17)
1.09	9.77(−18)	2.63(−17)	2.13(−18)	1.92(−17)
1.10	6.61(−19)	2.45(−17)	1.50(−18)	1.82(−17)
1.11	3.91(−18)	2.00(−17)	7.79(−19)	1.39(−17)
1.12	9.74(−19)	1.46(−19)	6.02(−23)	1.18(−19)
Total	8.14(−18)	4.50(−15)	2.12(−16)	6.64(−16)

Table 15. As Table 11 but for $d_1 \rightarrow d_3$, and $d_1 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$d_1 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.06	3.34(−20)	3.76(−16)	2.34(−16)	
0.10	4.35(−21)	6.54(−17)	3.27(−18)	
0.11	4.67(−23)	1.56(−19)	9.09(−23)	
0.12	4.29(−21)	9.49(−17)	1.93(−17)	
0.19	8.60(−21)	4.96(−17)	2.38(−17)	
0.22	1.37(−21)	1.33(−17)	7.46(−19)	7.87(−18)
0.23	1.52(−21)	1.92(−17)	3.75(−18)	1.02(−17)
0.27	3.08(−21)	1.06(−17)	4.94(−18)	1.46(−17)
0.29	2.14(−21)	1.58(−17)	2.10(−18)	8.88(−18)
0.32	2.52(−21)	5.41(−18)	2.49(−18)	7.84(−18)
0.33	8.20(−22)	4.05(−18)	2.46(−19)	2.37(−18)
0.34	9.85(−22)	5.34(−18)	9.69(−19)	2.66(−18)
0.35	2.19(−21)	3.14(−18)	1.40(−18)	4.69(−18)
0.36	1.70(−21)	6.32(−18)	8.30(−19)	3.38(−18)
0.37	2.96(−21)	4.80(−18)	1.45(−18)	4.55(−18)
0.38	2.43(−21)	5.32(−18)	7.46(−19)	2.81(−18)
0.39	2.81(−21)	2.75(−18)	9.12(−19)	2.92(−18)
0.40	6.12(−21)	5.11(−18)	1.31(−18)	4.72(−18)
0.41	8.17(−21)	5.03(−18)	1.04(−18)	3.93(−18)
0.42	1.03(−20)	3.52(−18)	7.33(−19)	2.69(−18)
0.43	3.84(−20)	3.62(−18)	8.07(−19)	2.90(−18)
0.44	1.31(−19)	2.08(−18)	5.32(−19)	2.08(−18)
0.45	2.44(−19)	1.63(−18)	4.32(−19)	1.74(−18)
0.46	9.03(−20)	5.34(−19)	3.31(−20)	3.13(−19)
Total	6.03(−19)	7.04(−16)	3.05(−16)	9.11(−17)

Table 16. As Table 11 but for $d_2 \rightarrow d_3$, and $d_2 \rightarrow d_3 \rightarrow i_1, d_1, d_2$.

	$d_2 \rightarrow d_3$			
e_c	DR	i_1	d_1	d_2
0.01	3.24(−19)	3.04(−15)	1.30(−16)	1.92(−15)
0.02	9.72(−19)	1.63(−15)	1.03(−16)	1.54(−15)
0.06	7.32(−20)	1.51(−16)	6.98(−17)	3.81(−15)
0.07	1.03(−20)	4.28(−17)		3.85(−17)
0.08	4.00(−19)	5.56(−16)	1.72(−17)	4.20(−16)
0.09	2.24(−20)	1.12(−16)	1.83(−17)	9.28(−17)
0.11	4.35(−20)	5.66(−17)	2.58(−17)	1.35(−16)
0.12	4.00(−20)	1.75(−16)	7.33(−18)	1.15(−16)
0.13	3.25(−19)	1.42(−16)	8.16(−18)	1.19(−16)
0.14	5.44(−21)	1.09(−17)		9.78(−18)
0.15	7.47(−20)	1.51(−16)	2.26(−17)	1.56(−16)
0.16	3.30(−19)	6.39(−17)	3.73(−20)	5.24(−17)
0.17	5.50(−20)	5.33(−17)	1.20(−17)	7.57(−17)
0.18	3.78(−19)	1.48(−16)	1.44(−17)	1.32(−16)
0.19	3.06(−19)	7.59(−17)	3.05(−18)	5.48(−17)
0.20	4.24(−19)	1.25(−16)	1.46(−17)	1.27(−16)
0.21	6.13(−19)	5.97(−17)	6.28(−18)	5.98(−17)
0.22	1.13(−18)	7.28(−17)	6.79(−18)	6.49(−17)
0.23	2.07(−18)	5.22(−17)	5.11(−18)	5.04(−17)
0.24	1.76(−18)	4.74(−17)	4.29(−18)	4.58(−17)
0.25	6.68(−18)	3.96(−17)	2.00(−18)	3.11(−17)
0.26	4.74(−18)	2.18(−18)	3.40(−20)	1.60(−18)
Total	2.08(−17)	6.81(−15)	4.71(−16)	5.59(−15)

Table 17. As Table 11 but for $i_1 \rightarrow d_4$, and $i_1 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$i_1 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.53	3.40(−19)	4.31(−15)			
0.57	7.82(−20)	1.28(−15)			
0.63	5.12(−19)	9.51(−15)			
0.67	1.55(−19)	3.66(−15)	2.61(−17)		
0.80	1.96(−19)	1.06(−15)	2.82(−17)		
0.82	4.71(−20)	4.17(−16)	1.63(−17)		
0.85	6.53(−19)	4.69(−15)	1.94(−17)	1.34(−19)	
0.86	1.10(−19)	1.27(−15)	7.20(−18)	1.08(−16)	
0.93	1.83(−19)	3.80(−16)	1.07(−17)	7.60(−17)	
0.94	3.86(−20)	1.94(−16)	7.34(−18)	7.67(−18)	
0.96	5.53(−19)	2.53(−15)	1.07(−17)	3.33(−17)	
0.97	4.00(−19)	7.00(−16)	3.23(−18)	6.32(−17)	
1.01	8.59(−20)	1.55(−16)	3.22(−18)	3.84(−17)	
1.02	2.92(−20)	1.12(−16)	4.05(−18)	4.31(−18)	
1.03	1.22(−18)	1.64(−15)	6.53(−18)	1.73(−17)	
1.04	7.60(−20)	3.85(−16)	1.77(−18)	3.60(−17)	
1.06	1.15(−19)	1.27(−16)	3.41(−18)	2.33(−17)	
1.07	2.21(−19)	8.07(−16)	6.73(−18)	1.47(−17)	
1.08	1.28(−18)	6.18(−16)	1.15(−18)	2.27(−17)	9.47(−21)
1.09	2.74(−20)	5.14(−17)	1.79(−18)	1.92(−18)	
1.10	3.99(−19)	7.99(−16)	7.27(−18)	3.95(−17)	6.79(−21)
1.11	1.50(−18)	2.77(−16)	4.62(−20)	5.42(−20)	
1.12	4.45(−19)	6.20(−16)	6.70(−18)	3.03(−17)	5.03(−21)
1.13	1.79(−18)	5.04(−16)	3.16(−18)	3.04(−17)	5.13(−18)
1.14	1.87(−18)	5.52(−16)	3.54(−18)	1.75(−17)	2.79(−18)
1.15	3.51(−18)	7.12(−16)	4.95(−18)	2.35(−17)	3.91(−18)
1.16	2.71(−18)	4.24(−16)	3.46(−18)	1.68(−17)	2.56(−18)
1.17	6.92(−18)	4.04(−16)	2.35(−18)	1.60(−17)	2.43(−18)
1.18	1.33(−17)	3.37(−16)	2.15(−18)	1.18(−17)	2.13(−18)
1.19	1.04(−17)	3.02(−16)	1.81(−18)	7.70(−18)	1.62(−18)
1.20	4.54(−17)	2.43(−16)	9.77(−19)	2.92(−18)	6.06(−19)
1.21	8.53(−18)	1.31(−18)	1.82(−22)	1.90(−22)	1.44(−23)
Total	1.03(−16)	3.91(−14)	1.94(−16)	6.43(−16)	2.12(−17)

Table 18. As Table 11 but for $d_1 \rightarrow d_4$, and $d_1 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_1 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.01	2.94(−19)	4.86(−16)	1.55(−15)		
0.15	8.51(−20)	7.54(−17)	1.06(−16)		
0.17	6.14(−21)	3.94(−17)	2.91(−18)		
0.19	1.33(−20)	4.15(−17)	9.89(−19)		
0.20	1.95(−23)	6.84(−20)	4.06(−24)	3.65(−24)	
0.21	2.39(−20)	1.45(−17)	5.77(−17)	7.25(−19)	
0.28	3.82(−20)	1.75(−17)	2.01(−17)	4.68(−18)	
0.29	3.15(−21)	1.17(−17)	8.06(−19)	2.06(−19)	
0.31	9.59(−21)	1.65(−17)	4.47(−19)	2.28(−19)	
0.32	1.58(−20)	4.86(−18)	2.08(−17)	2.27(−19)	
0.36	6.75(−20)	4.49(−18)	1.06(−17)	2.95(−18)	
0.37	1.95(−21)	5.57(−18)	3.62(−19)	9.47(−20)	
0.38	2.01(−20)	1.12(−17)	1.07(−17)	2.25(−19)	
0.41	2.00(−20)	7.59(−18)	4.63(−18)	1.06(−18)	
0.42	6.47(−21)	5.41(−18)	1.68(−19)	7.65(−20)	
0.43	9.87(−21)	1.37(−18)	6.19(−18)	5.84(−20)	
0.44	1.79(−20)	4.98(−18)	2.76(−18)	6.35(−19)	
0.45	1.62(−20)	6.17(−18)	4.51(−18)	1.12(−19)	
0.46	2.76(−20)	4.75(−18)	5.08(−18)	4.81(−19)	
0.47	2.39(−20)	4.16(−18)	4.28(−18)	8.25(−20)	9.24(−21)
0.48	2.77(−20)	3.14(−18)	2.83(−18)	3.39(−19)	3.84(−20)
0.49	5.46(−20)	4.95(−18)	3.94(−18)	4.57(−19)	3.60(−20)
0.50	6.84(−20)	4.78(−18)	3.19(−18)	2.15(−19)	1.84(−20)
0.51	1.80(−19)	4.22(−18)	3.23(−18)	3.31(−19)	2.56(−20)
0.52	3.91(−19)	2.78(−18)	2.67(−18)	2.35(−19)	2.00(−20)
0.53	4.19(−19)	1.91(−18)	9.30(−19)	1.89(−19)	1.43(−20)
0.54	6.84(−19)	1.93(−18)	6.40(−19)	1.53(−19)	1.26(−20)
0.55	2.33(−19)	6.75(−19)	2.04(−20)	6.42(−21)	9.88(−22)
Total	2.76(−18)	7.88(−16)	1.83(−15)	1.38(−17)	1.75(−19)

Table 19. As Table 11 but for $d_2 \rightarrow d_4$, and $d_2 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_2 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.08	2.17(−19)	5.35(−16)	2.01(−17)	2.91(−16)	
0.09	7.24(−21)	4.80(−17)	8.06(−19)	2.61(−18)	
0.10	6.66(−20)	1.81(−16)	8.04(−19)	1.53(−17)	
0.11	4.99(−20)	3.15(−16)	7.50(−19)	5.71(−17)	
0.15	1.46(−19)	1.47(−16)	8.13(−18)	7.64(−17)	
0.16	3.16(−21)	1.60(−17)	2.55(−19)	8.57(−19)	
0.17	5.60(−20)	6.12(−17)	3.17(−19)	6.22(−18)	
0.18	2.08(−20)	1.23(−16)	2.66(−19)	2.13(−17)	
0.20	6.71(−20)	7.18(−17)	2.41(−18)	3.44(−17)	
0.21	3.71(−20)	4.36(−17)	3.02(−19)	1.01(−17)	
0.22	4.30(−20)	6.59(−17)	1.35(−19)	1.10(−17)	7.22(−21)
0.23	2.19(−21)	5.38(−18)	8.23(−20)	2.82(−19)	
0.24	1.01(−19)	1.03(−16)	1.52(−18)	3.27(−17)	4.83(−21)
0.25	1.14(−20)	3.92(−18)	5.78(−20)	2.00(−19)	
0.26	7.22(−20)	6.51(−17)	1.06(−18)	1.84(−17)	3.40(−21)
0.27	1.26(−19)	8.63(−17)	8.41(−19)	2.21(−17)	1.60(−18)
0.28	4.93(−20)	2.15(−17)	1.03(−19)	4.74(−18)	2.26(−19)
0.29	2.38(−19)	6.83(−17)	1.24(−18)	2.33(−17)	9.63(−19)
0.30	2.03(−19)	3.69(−17)	4.94(−19)	1.03(−17)	5.79(−19)
0.31	5.60(−19)	3.87(−17)	4.68(−19)	1.11(−17)	5.74(−19)
0.32	1.80(−18)	2.47(−17)	4.11(−19)	8.37(−18)	3.62(−19)
0.33	1.00(−18)	1.65(−17)	3.60(−19)	7.01(−18)	1.69(−19)
0.34	3.18(−18)	7.65(−18)	7.94(−20)	2.73(−18)	4.49(−20)
0.35	3.96(−19)	1.49(−19)	1.61(−22)	1.99(−20)	3.03(−23)
Total	8.45(−18)	2.09(−15)	4.09(−17)	6.68(−16)	4.54(−18)

Table 20. As Table 11 but for $d_3 \rightarrow d_4$, and $d_3 \rightarrow d_4 \rightarrow i_1, d_1, d_2, d_3$.

	$d_3 \rightarrow d_4$				
e_c	DR	i_1	d_1	d_2	d_3
0.01	1.46(−18)	1.08(−15)	6.78(−18)	1.24(−16)	8.51(−17)
0.02	5.46(−19)	2.80(−16)	1.57(−18)	2.26(−17)	1.88(−17)
0.03	7.06(−19)	2.08(−16)	1.45(−18)	1.96(−17)	1.85(−17)
0.04	1.07(−18)	1.74(−16)	1.30(−18)	1.76(−17)	1.70(−17)
0.05	2.09(−18)	1.44(−16)	9.73(−19)	1.42(−17)	1.25(−17)
0.06	9.49(−18)	8.91(−17)	6.70(−19)	6.38(−18)	9.14(−18)
0.07	8.35(−18)	1.96(−17)	7.42(−20)	2.74(−19)	8.54(−19)
Total	2.37(−17)	1.99(−15)	1.28(−17)	2.05(−16)	1.62(−16)