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Electron and Positron Impact Ionization Cross Sections of O and Hg Atoms

Research Article

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Abstract. Total ionization crosssections for O and Hg atoms have been calculated for electron and *positron impact scattering*. A quantum mechanical formulation originating from complex atomic spherical potential is adapted in the scattering calculations on two targets. Then we obtain *total ionization cross sections* and cumulative total excitation cross sections by applying *variant CSP-ic method*. Our calculated results are presented for impact energy starting from the first threshold of ionization and going up to about 2000 electron volts (eV). For positron-atom scattering, our total inelastic cross sections include positronium formation together with ionization and excitation channels. Because of Ps formation channel it is difficult to separate our ionization cross sections from the total inelastic cross sections. An approximate method has been applied in this regard. Electron impact studies on Hg atom are scarce in literature. Similarly positron impact ionization in relation to electronic ionization discussed presently has not been highlighted much.

Keywords. Spherical complex potential; Total inelastic and total ionization cross sections; Positron impact scattering; Variant CSP-*ic* method

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1. Introduction

In terms of relative abundance in the universe, oxygen is one of the elements next to H and He. Interactions of oxygen atoms with electrons/positrons play an important role in atmospheric and planetary science. Being heavy atom, mercury is a very attractive target for the study of relativistic effects in electron scattering processes. Interest arises from the use of mercury in important technological processes. Knowledge of electron impact mercury cross sections is particularly important for modeling fluorescent and high energy discharge lamp and in modeling low-temperature plasmas containing Hg. It has been shown in recent literature [1, 3] that methodology based on complex atomic spherical potential can be employed to deduce the relative contribution of ionization in the cumulative inelastic scattering. This line of argument is followed presently to examine electron or positron impact oxygen atoms as well as mercury atoms. In this paper, we abbreviate the method of Complex Scattering Potential – ionization contribution by 'CSP-ic', and select the well-known O atom along with a lesser known target Hg to highlight our results.

2. Theory

In our previous papers [1, 3], we have successfully calculated ionization and total cross sections of several atomic as well as molecular targets using the CSP-ic formalism for electron and positron impact. We have employed this to calculate total (complete) cross sections Q_T, as sum of total elastic cross sections Q_{el} and total inelastic cross sections Q_{inel}.

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i). \tag{2.1}$$

Further,

$$Q_{inel}(E_i) = \Sigma Q_{ion}(E_i) + \Sigma Q_{exc}(E_i), \tag{2.2}$$

where E_i is the incident electron/positron energy. In equation (2.2) the first term represents the summation over the total cross sections of all allowed, namely single doubleand higherionizations in the target atoms. For simplicity we denote this term by Q_{ion}, and second term stands for the summation over all accessible discrete transitions in the atom by the impacting projectile. Also theoretical efforts have been directed towards extracting the ionization cross sections Q_{ion} from the total inelastic cross section Q_{inel} derived from a complex scattering potential formalism.

The e^-/e^+-target system is represented by complex spherical potential

$$V(r, E_i) = V_R(r, E_i) + iV_I(r, E_i), \tag{2.3}$$

where r is the radial distance from the target (atom). In equation (2.3) the real part V_R of the complex potential includes the static potential, the exchange potential [5] and the polarization potential. The potential terms are constructed from the electronic charge density, of the target and this is generated from the atomic wave functions given by [6].

The polarization potential used here is of the form given by Zhang *et al*. [7]. The total complex potential comprises of an imaginary part V_I, vide equation (2.3). The imaginary potential term

referred to as the absorption potential and denoted by V_{abs} was given by Staszewska *et al*. [8]. Modification in the original V_{abs} is discussed in [9–11]. The Schrödinger equation with the modified V_{abs} is solved by the variable phase approach [12], in order to determine Q_{el}, Q_{inel} and Q_T [13]. We denote by E_p the incident energy corresponding to the peak position of Q_{inel}.

For positron scattering, the total inelastic contribution must include positronium formation apart from electronic excitation and ionization of the target atom. Therefore, equation (2.2) for positron scattering can be expressed as

$$Q_{inel}(E_i) = Q_{Ps}(E_i) + \Sigma E_{ion}(E_i) + \Sigma Q_{exc}(E_i)\,. \tag{2.4}$$

Equation (2.4) is an expression of cumulative total inelastic cross section Q_{inel} which consists of the total cross section for the formation of positronium Ps represented by the first term (Q_{Ps}).

Apart from this the inelastic flux must contain the outgoing positrons corresponding to ionizations and electronic excitations. Accordingly, the second term of equation (2.4) i.e. ΣQ_{ion} stands for total (admissible) ionization cross sections and total cumulative excitation cross sections $\Sigma Q_{exc}$for the transitions that are accessible at the given energy.

The basic static potential along with polarization interaction is included in the real part i.e. the first term of the equation (2.3). The atomic target offers a repulsive static potential to the incident positrons, while polarization potential $V_{pol}(r)$ is attractive and dynamic, i.e. energy dependent. Thus at low-to-intermediate energies the static potential and the polarization potential tend to cancel each other and at high energies only the static potential dominates. The total positron complex potential consists of three potentials as shown below:

$$V(r,E_i) = V_{st}(r) + V_{pol}(r) + iV_I(r,E_i)\,. \tag{2.5}$$

The polarization potential for positron scattering is defined below as per the detailed expression given Ref [14]:

$$V_{pol}(r) = \begin{cases} V_{corr}(r), & r \le r_c\,, \\ -\frac{\alpha_d}{2r^4}, & r \le r_c\,, \end{cases} \tag{2.6}$$

where r_c is the radial distance of the first crossing of the correlation term $V_{corr}(r)$ and the asymptotic form $-\alpha_d/2r^4$. We have adopted absorption model from Reid and Wadehra [15].

The absorption probability per unit time is given by $\overline{\sigma}_b v$, where the symbol v denotes the (local) speed of the incident positron in the target region. The symbol $\overline{\sigma}_b$ shows the average positron-electron binary collision cross section. Thus

$$V_{abs} = -\frac{1}{2}\rho\overleftarrow{\sigma}_b v\,. \tag{2.7}$$

Then the absorption potential is given by,

$$\overline{\sigma_b} = \frac{\pi}{(\varepsilon E_F)^2} \times \begin{cases} f(0), & \varepsilon^2 - \delta \le 0 \\ f(\sqrt{(\varepsilon^2 - \delta)}, & 0 < \varepsilon^2 - \delta \le 1 \\ f(1), & 1 < \varepsilon^2 - \delta \end{cases} \tag{2.8}$$

$$\delta = \frac{\omega}{2E_F}, \quad \varepsilon = \sqrt{\frac{E}{E_F}}, \quad \text{and} \quad f(x) = \frac{2}{\delta}x^3 + 6x + 3\varepsilon \ln\left(\frac{\varepsilon - x}{\varepsilon + x}\right). \tag{2.9}$$

As far as the role of energy parameter Δ in V_{abs} is concerned, there is a difference between positron and electron scattering, and it arises due to the positronium formation observed with positrons [16]. With the full complex potential inserted into the Schroedinger equation, we treat it exactly in partial wave analysis by solving the corresponding first order differential equations for the real (δ_R) and the imaginary (δ_I) parts of the complex phase shift function, in order to determine Q_{el}, Q_{inel}, and Q_T [17].

Now, transitions to continuum leading to ion formation become dominant as incident energy increases. Hence ionization contribution in Q_{inel} increases with E_i exceeding 'I', so that the cross section Q_{ion} turns out to be the main contribution to Q_{inel}. Therefore, we conclude in general as follows:

$$Q_{inel}(E_i) \geq Q_{ion}(E_i) \tag{2.10}$$

Although the ionization cross section is contained in the inelastic cross section, there seems to be no rigorous treatment to project out Q_{ion} from Q_{inel}. However, a meaningful theoretical procedure has been in vogue in literature of the last two decades [1–4, 9–11]. The theoretical method CSP-ic starts with the following function of incident energy E_i.

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}, \quad 0 \leq R \leq 1 \tag{2.11}$$

In the next step in this theoretical procedure the ratio R is made target sensitive by expressing it as a function of a dimensionless variable $U = E_i/I$, as

$$R(E_i) = 1 - C_1 \left[\frac{C_2}{U+a} + \frac{\ln(U)}{U} \right]. \tag{2.12}$$

The above expression defines three parameters a, C_1 and C_2, and for their evaluation we employ three conditions exhibiting the general behaviour of the ration function R, as stated hereunder.

$$R(E_i) = \begin{cases} 0, & \text{at } E_i = I \\ R_p, & \text{at } E_i = E_p \\ R', & \text{for } E_i \gg E_p \end{cases} \tag{2.13}$$

where the symbol E_p stands for the impact energy at which our cross section Q_{inel} reaches the peak. The ratio value 'R_p' is chosen to be 0.7, which though approximate, turns out to be a meaningful input. This particular choice has been discussed in literature [9–11]. The peak position E_p of the cross section Q_{inel} occurs at incident energy where the discrete-excitation sum is decreasing while Q_{ion} is rising fast, suggesting the R_p value to lie between 0.5 and 1. We follow the general trends observed in a large number of atoms and molecules [9–11] that at energies of the peak of Q_{inel} the Q_{ion} is about 70-80% of the total inelastic cross section Q_{inel} and the ionization contribution increases with energy. Admittedly, the approximate input R_p results into theoretical uncertainty in the calculated cross sections.

In the variant of the usual CSP-ic method, we start by taking $a = 0$ in (2.12) and determine initial R' of equation (2.13). The alternative calculation provides $R_p \approx 0.69$, which we employ to calculate the parameters a, C_1 and C_2, hence to obtain Q_{ion} from Q_{inel} using the equation (2.11). In Table 1 various properties of the targets are given.

Table 1. Various properties of the present targets

Target	First Ionization Energy I (eV)	Polarizability α_0 (Å^3)
O	13.618	0.802
Hg	10.437	5.02

3. Results and Discussion

The theoretical approach CSP-*ic*together with the variant CSP-*ic*aims to calculate all the total cross sections defined in the above outline of the theory. This work covers all the major TCSs of electron impact on the present atomic targets;we have exhibited all cross sections for heavy atomic target Hg which is a lesser known target.

Atomic Oxygen (electron and positron impact)

Figure 1 exhibits various total cross sections of electron impact on atomic O, while Figure 2 corresponds to positron scattering with this atom.

In Figure 1, the upper most two solid curves show present total cross section Q_T and total elastic cross section Q_{el} for which no other comparisons are available. The lower curve for total ionization cross section (Q_{ion}) values determined in variant CSP-*ic* approach for atomic Oxygen are in good accord with the experimental data of Oxygen atom, as measured by Thompson *et al*. [18] and also with experimental data by Brook *et al*. [19], measured using crossed beam. Our results shows good agreement with other theoretical data by Bartlett *et al*. [20] and also with Kim and Desclaux [21]. The lower most solid line shows summed total excitation cross section (ΣQ_{exc}) present.There is a good agreement of the present Q_{ion} with the compared data.

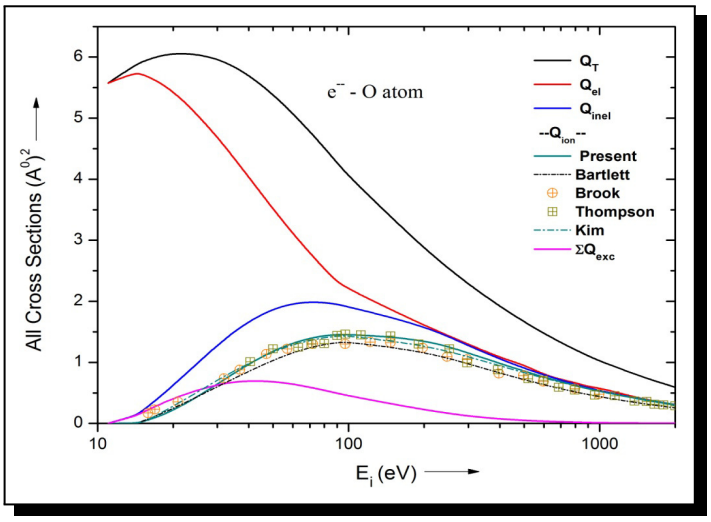

Figure 1. All cross sections for atomic Oxygen by electron impact (Black solid line-present Q_T; Red solid line – present Q_{el}; Blue solid line – present Q_{inel}; Dark cyan solid line – present Q_{ion}; Circle + center – E Brook [19] Q_{ion}; Square + circle – Thompson [18] Q_{ion}; Black short Dash – Bartlett [20] Q_{ion}; Dark cyan Dash Dot – Kim [21] Q_{ion}; Solid Magenta – present ΣQ_{exc})

In Figure 2 for positrons on O, the upper most two solid curves show present total cross section Q_T and total elastic cross section Q_{el} are compared with calculated data of Reid and Wadehra [15]. We are not aware of any experimental measurements for positron impact scattering cross sections from this atomic target. Considering the present calculations from Figure 2, we observe that results of Reid and Wadehra [15] for Q_T is slightly higher than our present results. Our total elastic cross section show good agreement with results of Reid and Wadehra [15]. We have employed the variant CSP-*ic* approximation as in [3]. As Q_{Ps} (positronium formation cross section) results are not available for atomic Oxygen, we take $R_p = 0.8$, considering that our Q_{ion} cross sections results must include Q_{Ps} cross sections.

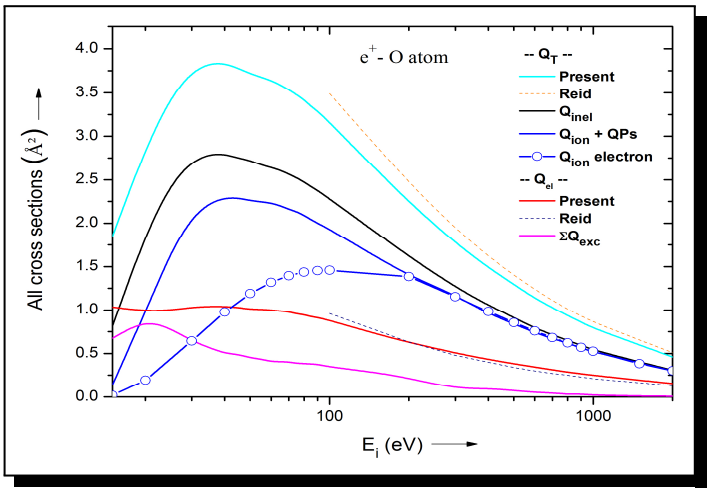

Figure 2. All the present cross sections for atomic Oxygen by positron impact (Cyan solid line-present Q_T; Orange Dash – Reid [15] Q_T; Black solid line – present Q_{inel}; Blue solid line – present $Q_{ion} + Q_{Ps}(e^+)$; Blue circle + solid line – $Q_{ion}(e^-)$; Red Solid line – present Q_{el}; Navy Dash – Reid [15] Q_{el}; Solid Magenta – present ΣQ_{ex})

Atomic Mercury (electron and positron impact)

The calculated cross sections for electron/positron scattering with atomic Mercury are shown in Figure 3 and Figure 4.

First of all, since Hg is a heavy atom with 80 electrons, the electron charge-density is calculated in the relativistic DHFS approach of [22]. The electronic charge density is given by [22];

$$\rho(r) = \frac{Z}{4\pi r}\left[A_1\alpha_1^2\exp(-\alpha_1 r) + A_2\alpha_2^2\exp(-\alpha_2 r) + A_3\alpha_3^2\exp(-\alpha_3 r)\right], \tag{3.1}$$

where A_i and α_i are the parameters of the expression in [22].

$$A_1 = 0.2098,\ A_2 = 0.6004,\ A_3 = 0.1898,\ \alpha_1 = 24.408,\ \alpha_2 = 3.9643 \text{ and } \alpha_3 = 1.5343.$$

In Figure 3, we have shown total inelastic cross sections (Q_{inel}), total ionization cross sections Q_{ion} and the excitation sum ΣQ_{exc} along with comparison data for electron impact on atomic mercury in Figure 3. Our ionization cross section (Q_{ion}) for Model-2 (Δ variable with 6.8 eV to I) are shows agreement with the experimental data for total ionization cross sections (SICS+DICS) measured by Almedia [23]. Our results also show agreement with other theoretical data by

Gryzinski and Zecca [24, 25]. Our results are higher than DM formalism [26].

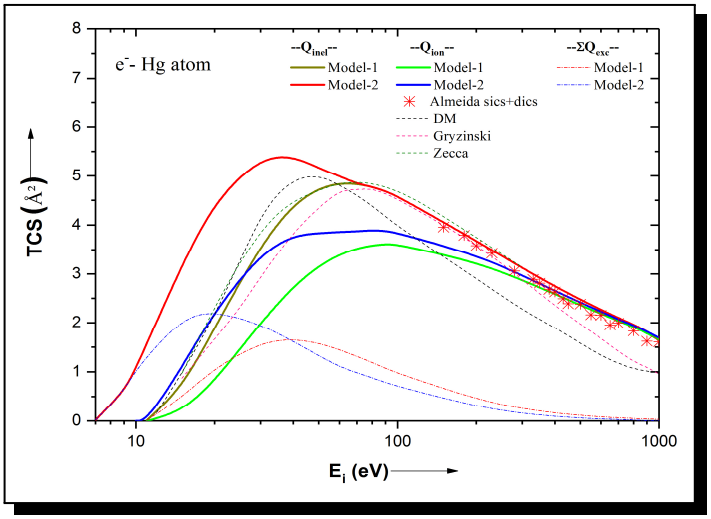

Figure 3. Ionization and total excitation cross sections for Mercury atoms by electron impact (Red solid line – present Q_{inel} (Model-2); Blue solid line – present Q_{ion} (Model-2); Red star – Q_{ion} SICS+DICS Almedia [23]; Black dash line – Q_{ion} DM [26]; Red active dash Q_{ion} Gryzinski [24]; Olive dash line – Q_{ion} Zeccai [25]; Dark yellow solid line – present Q_{inel} (Model-1); Green line – present Q_{ion} (Model-1); Red dash dot line – present ΣQ_{exc} (Model-2); Blue dash dot line – present ΣQ_{exc} (Model-1))

In Figure 4, we have shown total inelastic cross sections (Q_{inel}), total ionization cross sections Q_{ion} and the excitation sum ΣQ_{exc} for positron impact on atomic Mercury. We are not aware of any theoretical data or experimental measurement results for positron impact scattering cross sections.

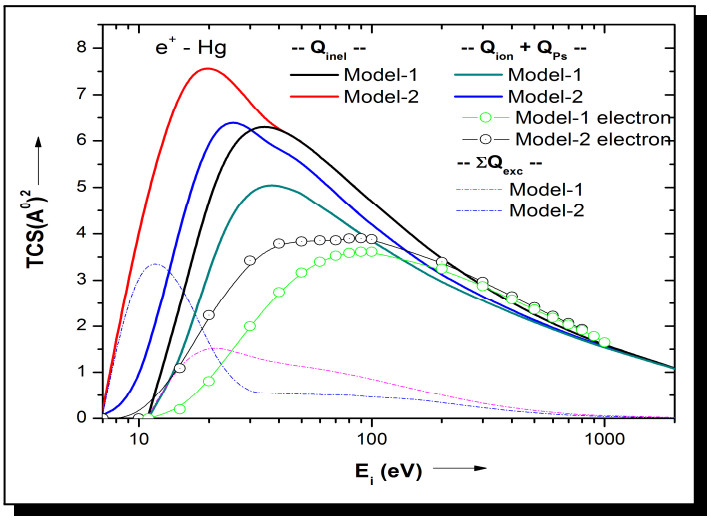

Figure 4. Ionization and total excitation cross sections for Mercury atoms by positron impact (Red solid line – present Q_{inel} (Model-2); Blue solid line – present Q_{ion} (Model-2); Black solid line + circle present Q_{ion} (E^--Model-2); Green solid line + circle Q_{ion} (e^--Model-1); Black solid line – present Q_{inel} (Model-1); Dark cyan solid line – present Q_{ion} (Model-1); Blue dash dot line – present ΣQ_{exc} (Model-2); Magenta dash dot line – present ΣQ_{exc} (Model-1))

4. Conclusions

In conclusion, in this paper we have considered O atom which is extensively studied, and the Hg atom which is less studied. The methodology of SCOP and CSP-*ic* and variant CSP-*ic* formalism are used by several authors to derive the total ionization cross section and has given reasonably good agreement for many atoms and molecules in the past studies. Presently in case of atomic Oxygen our results for electron impact, our calculated ionization cross sections find a good accord with the literature data, this fact confirms the validity of our theoretical method. The importance of the present study is that Hg atom has not been investigated much. Our results on Hg with assumption (Model-2) show good agreement with other results.

In the case of positron impact, the employed theory works well; Q_{ion} of electron and positron are quit close for fast collisions, while it differs at low and intermediate energies. Our conclusion is that in positron scattering with atomic target, the formation of Ps is important up to 200 eV. From variant *CSP-ic* method we can calculate Q_{ion} successfully with an important by-product as ΣQ_{exc}. It is also found that in case of O-atom positrons are more ionizing projectiles than electron at low energies.

Finally for a less studied atomic target like Hg, the positron impact results would be of interest to stimulate further investigations.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

References

[1] M. J. Pindariya, A. Chaudhari, F. M. Joshi, K. N. Joshipura and H. N. Kothari, Comparative study of electron and positron scattering with N atom and N_2 molecule, in *National Conference on Improve Conceptual Learning in Physics*, M.N. Science College, Patan, India (2018), ISBN 978-1-387-61856-9.

[2] K. N. Joshipura and N. J. Mason, *Atomic?molecular Ionization by Electron Scattering, Theory and Applications*, Cambridge University Press (2019), ISBN 9781108551489, DOI: 10.1017/9781108551489.

[3] F. M. Joshi, K. N. Joshipura, A. S. Chaudhari, H. S. Modi, M. J. Pindariya, *Digital identifier*, arXiv:1602.01928[physics.atom-ph], (submitted on 5 February 2016), 7 pages.

[4] K. N. Joshipura, S. S. Gangopadhyay, H. N.. Kothari and F. A. Shelat, *Phys. Lett. A* **373**(32), 2876 – 2881 (2009), DOI: 10.1016/j.physleta.2009.05.075.

[5] S. Hara, *J. Phys. Soc. Jpn*. **22**(3), 710 – 718 (1967), DOI: 10.1143/JPSJ.22.710.

[6] B. C. F. and J. A. Barrientos, *At. Data Nucl. Data Tables* **53**(1), 113 – 162 (1993), DOI: 10.1006/adnd.1993.1003.

[7] X. Z. Zhang, J. F. Sun and Y. F. Liu, *J. Phys. B: At. Mol. Opt. Phys*. **25**, 1893 (1992), DOI: 10.1088/0953-4075/25/8/021.

[8] G. Staszewska, D. M. Schwenke and D. G. Truhlar, *J. Chem. Phys*. **81**, 3078 (1984).

[9] K. N. Joshipura, S. Gangopadhyay and G. Vaishnav Bhushit, *J. Phys. B: At. Mol. Opt. Phys.* **40**, 199 (2007); see also K. N. Joshipura, M. Vinodkumar, C.G. Limbachiya and B.K. Antony, *Phys. Rev. A* **69**, 022705 (2004), DOI: 10.1103/PhysRevA.69.022705.

[10] K. N. Joshipura, B. G. Vaishnav and S. Gangopadhyay, *Int. J. Mass Spectrum* **261**(2-3), 146 – 151 (2007), DOI: 10.1016/j.ijms.2006.08.014.

[11] K. N. Joshipura, S. Gangopadhyay, C. G. Limbachiya and M. Vinodkumar, *J. Phys. Conf. Series* **80**, 012008 (2007), DOI: 10.1088/1742-6596/80/1/012008.

[12] F. Calogero, *Variable Phase Approach to Potential Scattering*, *American Journal of Physics* **36**, 566 (1968), DOI: 10.1119/1.1975005.

[13] C. J. Joachain, *Quantum Collision Theory*, Amsterdam North-Holland, (1984).

[14] K. L. Baluja and A. Jain, *Phys. Rev. A* **46**, 1279 (1992), DOI: 10.1103/PhysRevA.46.1279.

[15] D. D. Reid and J. M. Wadehra, *J. Phys. B* **29**, l127 (1996), DOI: 10.1088/0953-4075/29/4/002.

[16] H. N. Kothari and K. H. Joshipura, *Prajñā – J. Pure and Appl. Sci.* **17**, 185.

[17] H. N. Kothari and K. H. Joshipura, *Chin. Phys. B* **10**, 103402 (2010), DOI: 10.1088/1674-1056/19/10/103402.

[18] W. R. Thompson, M. B. Shah and H. B. Gilbody, *J. Phys. At. Mol. Opt. Phys. B* **28**, 1321 (1995), DOI: 10.1088/0953-4075/29/13/018.

[19] E. Brook, M. F. Harrison and A. C. H. Smith, *J. Phys. B* **11**, 3115 (1978), DOI: 10.1088/0022-3700/11/17/021.

[20] P. L. Bartlett and A. T. Stelbovics, *Phys. Rev. A* **66**, 012707 (2002), DOI: 10.1103/PhysRevA.66.012707.

[21] Y. K. Kim and P. M, Stone, *Phys. Rev. A* **64**, 052707 (2001), DOI: 10.1103/PhysRevA.64.052707.

[22] F. Salvat, J. M. Martmez, R. Mayol and J. Parellada, *Phys. Rev. A* **36**, 467 (1987), DOI: 10.1103/PhysRevA.36.467.

[23] D. P. Almeida, M. A. Scopel, R. R. Silva and A. C. Fonts, *Chem. Phys. Lett.* **341**, 490 (2001), DOI: 10.1016/S0009-2614(01)00520-6.

[24] M. Gryzinski and J. A. Kunc, *J. Phys. B. At. Mol. Opt. Phys*. **32**, 5789 – 5804 (1999), DOI: 10.1088/0953-4075/32/24/314.

[25] A. Zecca, G. P. Karwasz and R. S. Brusa, *Rivista Del Nuovo Cimento* **19**, 1 (1996), DOI: 10.1088/0953-4075/32/24/314.

[26] H. Deutsch, P. Scheier, S. Matt-Leubner, K. Becker and T. D. Mark, *Int. J. Mass. Spec.* **243**, 215 – 221 (2005), DOI: 10.1016/j.ijms.2005.03.003.