Single and Double Differential Cross Sections of PF3 Molecule

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Abstract : Partial and total (sum of partial cross sections) Single Differential Cross Sections (SDCS) as a function of fixed incident electron energy and Double Differential Cross Sections (DDCS) with their sums as a function of fixed incident electron energy and incident scattering angle have been evaluated through direct and dissociative ionization of PF_3. Here all calculations have been carried out by using modified Jain-Khare semi-empirical approach [1-5]. All these calculation were not available till now. So these results are predictive to the experimentalist for measurement.

Keywords : Cross Sections, Ionization Rate Coefficients, Jain-Khare Semi-Empirical Approach, Direct and Dissociative Ionization

INTRODUCTION:

Electron-molecule collision cross sections from very low energy up to threshold play a pivotal role in determining electron transport properties and electron energy distribution of a swarm of electrons drifting through various gases. Per-fluorinated compounds (PFC) are widely used in electrical industries, plasma-assisted fabrication of microcircuits, surface hardening, agriculture, and medicinal fields. PF_3 is also a potential reagent for the gasphase synthesis in microelectronic doping [1]. Theoretical works based on Binary Encounter Bethe (BEB) and Complex Potential Method (CPM) for total electron ionization cross sections of PF_3, both evaluated by M.Vinodkumar et al. [1] are available till now.

This letter reports the results of the single differential cross sections (SDCS) as a function of secondary electron energy and double differential cross sections (DDCS) as a function of secondary electron energy and incident angle of electron, by using modified Jain and Khare semi-empirical approach [2-8]. Modified Jain and Khare semi-empirical approach is the only formulation that evaluates the energy dependent partial cross sections for molecules in electron ionization. To the best of my knowledge, no other data (experimental and/or theoretical) of differential cross sections are available till now.

THEORETICAL:

Single differential cross sections (SDCS) formulism can be obtained by differentiation of (Equation (1)) w.r. to secondary electron energy i.e. [2-8]

$$\left(\left(\frac{1}{1+\frac{I_i}{E}}\right)\frac{R}{E}\frac{df}{dw}\,ln[\mathbf{1}+C_i(E-I_i)]@+\left(\frac{R(E-I_i)}{E}S_i\frac{1}{\varepsilon^3+\varepsilon_0^3}\left(\varepsilon-\frac{\varepsilon^2}{(E-\varepsilon)}+\frac{\varepsilon^3}{(E-\varepsilon)^2}\right)\right)\right| \quad \ldots(1)$$

Here all symbols have their usual meanings as defined in Refs [2-8].

For the evaluation of double differential cross sections (DDCS) we have used formula derived by Kumar et al. [7]

$$\left(\frac{8R^2Z^2}{W^2}\left(1-\frac{\varepsilon}{(E-\varepsilon)}\left(1-\frac{W}{E}\right)^{1/2}sin\theta\frac{df}{dW}\ln\left(1+C_i(E-I_i)\right)@+S_i\frac{\varepsilon^3}{\varepsilon^3+\varepsilon_0^3}\left(\frac{E-I_i}{E}\right)\left(\varepsilon-\frac{1}{(E-\varepsilon)}+\frac{1}{(E-\varepsilon)^2}\right)\frac{sin\theta}{2}\right)\right| \quad \ldots.(2)$$

and the total cross section is obtained by

$$Q_i^T(E,W,\theta)=\sum_i Q_i(E,W,\theta) \quad \ldots\ldots (3)$$

For PF_3 molecule the oscillator strengths and ionization potentials of various cations (PF_3^+, PF_2^+, PF^+, PF_3^{++}, PF_2^{++}, P^+, PF^{++}, F^+, and P^{++}) are taken from the experimental results of J. W. Au et al. [9]. Here, experimental partial oscillator strengths of PF_3^+, PF_2^+, PF^+, PF_3^{++}, PF_2^{++}, P^+, PF^{++}, F^+, and P^{++} are available up to 130 eV. For higher energies, the same data have been extrapolated by the Thomas–Reiche–Kuhn (TRK) sum rule, within 10% error bars [9]. The value of collisional parameter (C_i = 0.03789) and mixing parameters (ε_0 = 45eV) have been calculated as for other molecules [2–8].

RESULTS:

Partial and total single differential cross sections (SDCS) as a function of secondary electron energy produced in the ionization at fixed incident energies of 100 and 200eV are shown in Figure 1. Partial and total

double differential cross sections (DDCS) as a function of secondary electron energy and incident angle of electron at fixed incident electron energies of 100 and 200 eV, and fixed angles 30^0 and 60^0 are shown in Figure 2. 3D profile of DDCS as a function of secondary electron energy (in the range of 5 eV to $W_{max/2}$) and angle (10^0 to 180^0) are resented in Figure 3 at fixed incident electron energies 100 and 200 eV. To the best of my knowledge, no experimental and/or theoretical data is available for comparison to the present calculations for differential cross sections. However, the qualitative behavior of the cross sections are the same as for other molecules investigated [2–8]. The energy dependent cross sections are symmetric at $W_{max/2}$, where the energies of primary and the secondary electrons are almost equal, except some irregular behavior at lower energy side. The present calculations account the contribution of exchange effects and resonances through the second part of the formula (Eq. (1&2)). In the present formulation (Eq. (1&2)), the first part known as Born-Bethe cross section for slow secondary electron, corresponds to the growing contribution of the dipole-allowed interaction and resembles the photoionization cross-section and second part, the Mott cross section accounts for the electron exchange effect, is the non-dipole part which defines the knock-on collision. The figures clearly show the weight contribution of the molecular and atomic cations. The cross sections for molecular ions are much larger than the atomic ions.

CONCLUSION

The present calculation for energy dependent differential and integral ionization cross sections is an attempt towards the wider applicability of a modified Jain–Khare semi-empirical formalism. For the first time, we have evaluated the differential and partial ionization cross sections leading to the various cations in electron-PF_3 collision processes and the results are predictive to the experimentalist for measurement. These results are very much desirable in various phenomenons like etching, plasma simulation and modeling etc.

REFERENCES:

[1] M. Vinodkumar, C. Limbachiya, H. Desai and P. C. Vinodkumar, Electron-impact total cross sections for phosphorous triflouride, Physical Review A **89**, 2014, 062715.

[2] S.P.Khare, S.Prakash and W.J.Meath, Dissociative ionization of NH_3 and H_2O molecules by electron impact, Int. J. Mass Spectrom. Ion Procs., 88(2-3), 1989, 289.

[3] S. Pal, J. Kumar and T. D. Märk; J. Chem. Phys. **120**, 2004, 4658.

[4] Rajeev Kumar, Electron impact ionization cross sections of carbonyl sulfide, Int. J. Mass spectrom. **2011**, 303, 69.

[5] Rajeev Kumar and S. Pal, Electron ionization cross sections and rate coefficients for the N_2O molecule, Indian J. Phys. **2011**, 85(12), 1767.

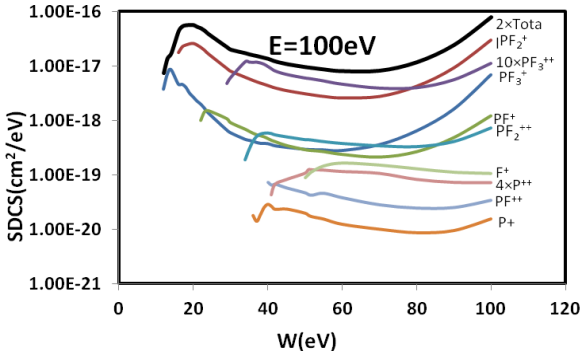
[6] R. Kumar and S. Pal, Evaluation of electron ionization cross sections of methyl halides, Rapid Commun. Mass Spectrom.Vol. **27**, 2013, 223

[7] Rajeev Kumar, Electron ionization cross sections for the PH_3 molecule, Chem. Phys. Letter, 604, 2014,108.

[8] S. Pal, R. Kumar and R. Singh, Electron impact ionization cross sections of the CO2 clusters, J. Electron Spect. and Related Phenomena xxx (2012) xxx– xxx

[9] J.W.Au, G. Cooper and C. E. Brion, Photoabsorption and photoionization of the valence and inner (P 2p, 2s) shells of PF_3: absolute oscillator strengths and dipole-induced breakdown pathways, Chem. Phys., **215**, 1997, 397.

Figure 1: Partial and total single differential cross sections (SDCS) of PF_3 at fixed impinging electron energies 100 and 200eV.



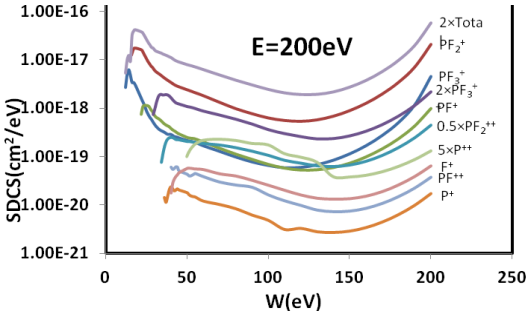


Figure 2: Partial and total double differential cross sections (DDCS) of PF_3 at fixed impinging electron energies of 100 and 200eVwith fixed incident angles 30^0 and 60^0.

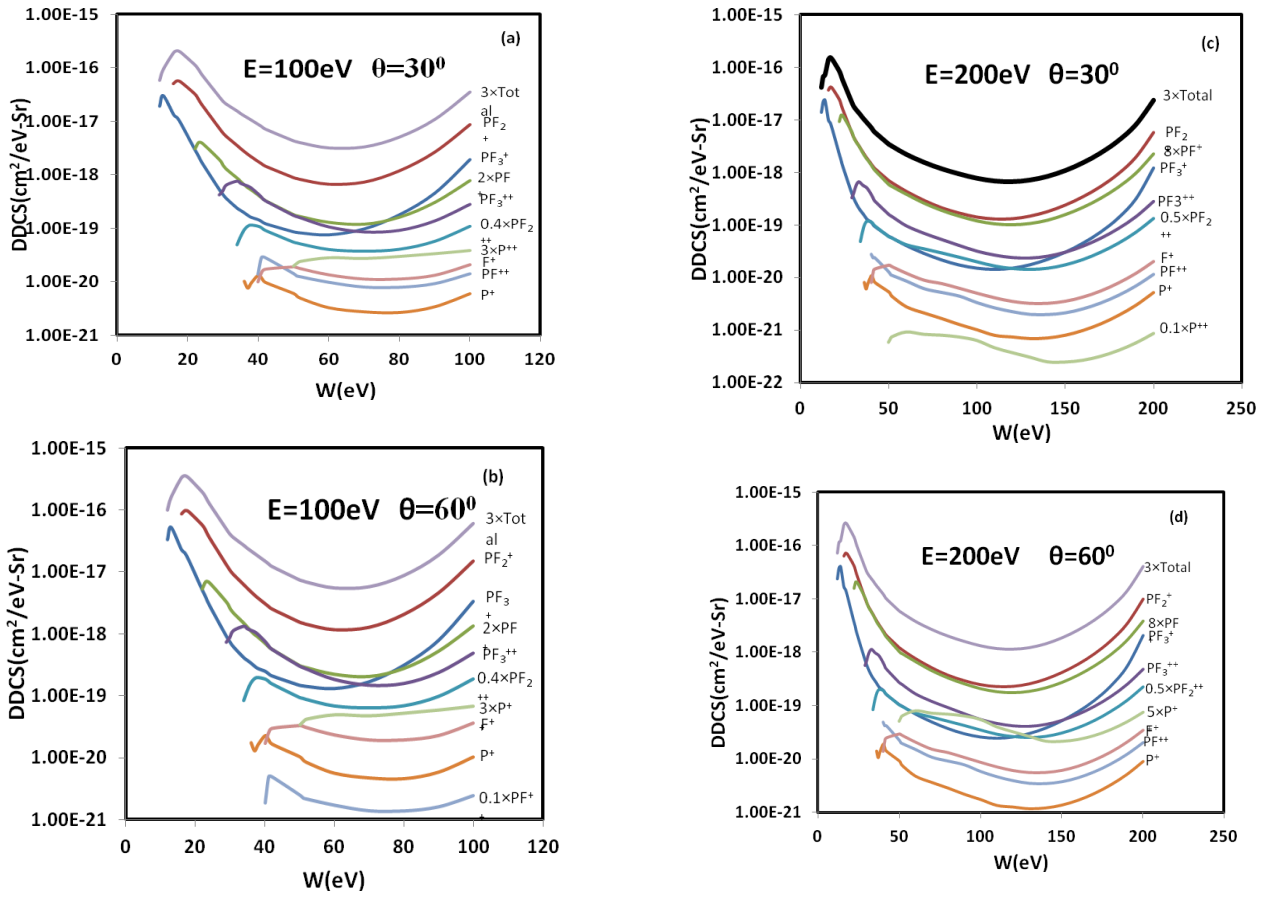
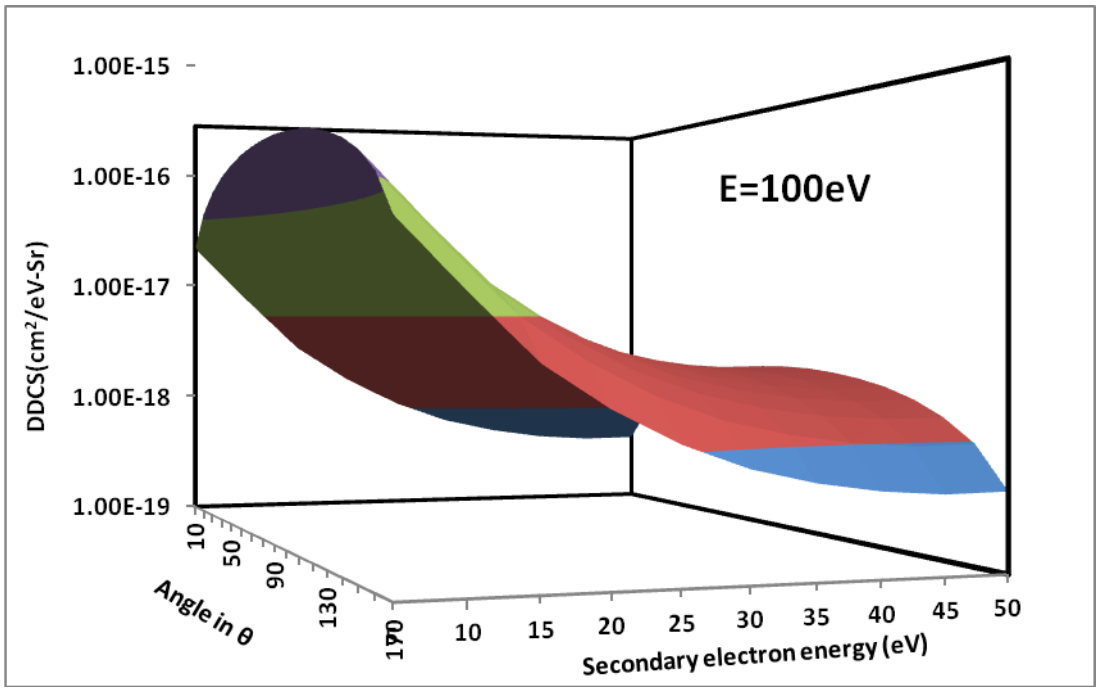
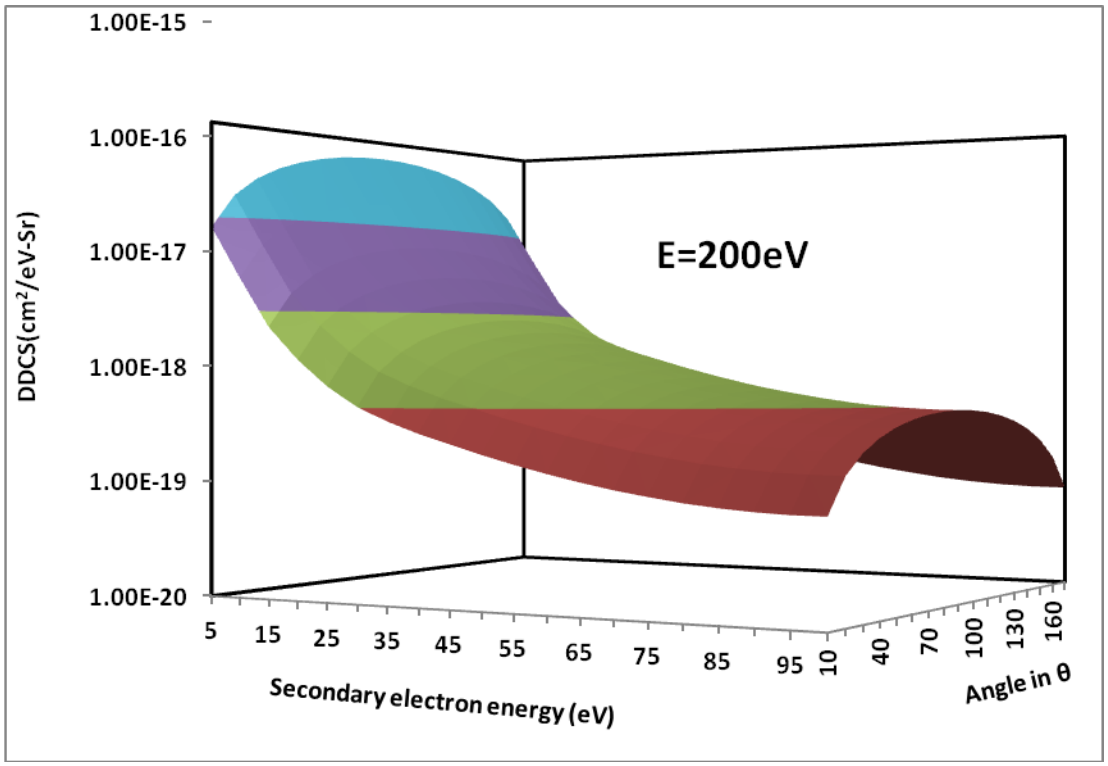


Figure 3: 3D profile of total double differential cross sections (DDCS) of PH_3 at fixed impinging electron energies of 100 and 200eV.




1.00E-15
1.00E-16
1.00E-17
1.00E-18
1.00E-19
1.00E-20
DDCS(cm²/eV-Sr)
E=200eV
5
15
25
35
45
55
65
75
85
95
10
40
70
100
130
160
Secondary electron energy (eV)
Angle in θ