Evaluation of elastic cross sections for electron scattering from PH_3 molecules

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Abstract

A parameter-free spherical optical potential (SOP) model is used to calculate the total cross sections for the elastic scattering of electrons from phosphine molecules at incident energies up to 30 eV. The optical potential is constructed from a near-Hartree-Fock one-center expansion of a phosphine (PH_3) wave function. This potential is then treated in a partial-wave analysis to extract total scattering cross sections using spherical approach. The qualitative feature of the scattering parameters (such as a Ramsauer-Townsend (RT) minimum around 1 eV) observed in recent experiments, is very well reproduced in the present model calculation.

1. Introduction

In matter, energy deposition is due to the interaction of radiation with atoms and molecules. So investigation of electron scattering cross section is an interesting area of radiation physics. The total cross sections for electron/positron collisions with a large number of atoms and polyatomic molecules have been measured from low (~ 1 eV) to keV energy region [1, 2]. These cross sections have important applications in space, plasma, laser, biomedical science and the environment. Many approaches ranging from as simple as independent atom models (IAM) [3] to *ab initio* methods [4] have been proposed. But in case of polyatomic molecules, *ab initio* calculations are quite difficult to perform. Therefore, our goal here is to apply a simple SOP model approach for calculating the total cross sections for PH_3 molecule. In the present paper, phosphine has been chosen because it is a major component in the fabrication of materials for micro- and opto- electronics.

2. Theoretical Methodology

In the present SOP model, the complicated interaction between the electron molecule system is approximated by an optical potential composed of three local and real terms, namely the static (V_{st}), exchange (V_{ex}) and polarization (V_p) potential without involving any adjustable parameter. The PH_3 molecule belongs to the C_{3v} symmetry and has an electronic $^1A_1$ ground state with the configuration $1a^2_1\ 1e^4\ 2a^2_1\ 3a^2_1\ 4a^2_1\ 2e^4\ 5a^2_1$. The central quantity in the calculations of the optical potential is the charge density $\rho(\boldsymbol{r})$. The quantity $\rho(\boldsymbol{r})$ is expanded in terms of symmetry-adapted functions belonging to the totally symmetric $^1A_1$ irreducible representation of the molecular point group

$$\rho(\vec{r}) = \sum_{L,H} \bar{\rho}_{LH}(r)\ \chi^{A_1}_{LH}(r) \qquad (1)$$

In the spherical approximation, we need only the first term (L = 0, H = 1) of the expansion of equation (1) in order to evaluate all the three potentials. Explicit expression for $V_{st}(\boldsymbol{r})$ is given in the literature [5]. We have used modified semi classical exchange (MSCE) form of $V_{ex}(\boldsymbol{r})$ [6]. Finally, the correlation polarization potential (COP) is calculated from the expression given by Padial and Norcross [7] and Gianturco *et a1* [8].

At larger distances the COP $V_p(\boldsymbol{r})$ is replaced by the correct asymptotic form $-\alpha_0/2r^4$ (α_0 is the dipole polarisability of PH_3; we employ the experimental value of 32.67 au for α_0). It is now a standard procedure to compute the l^{th} partial-wave phase shift from the solutions of following 2nd order differential equation:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - V_{opt.}(r)\right] f_l(kr) = 0 \qquad (2)$$

where k^2 is the electronic energy. Variable-phase approach (VPA) [9] was employed to find the solutions of equation (2). The total cross sections (σ_t) are then easily obtained from the S matrix at each energy. All our cross sections are converged with respect to number of partial waves up to a value of 0.000 01 rad.

3. Results and Discussion

We have calculated σt cross sections for the e - PH3 system in the energy range of 0.1 – 30 eV. Calculations have been performed in several combinations of different potentials but in this paper we present results in only SEP model (i.e. static plus MSCE plus correlation polarization potential). In figure 1, σt cross sections are presented in the energy range 0.1 – 10 eV and compared with the experimental measurements of Szmytkowski et al [10] along with theoretical calculations of Munjal and Baluja [11] as well as Bettega and Lima [12]. It is indeed remarkable that our SEP calculation is able to reproduce the R-T minimum at around 1 eV. Figure 2 presents σt cross sections at energies between 10 - 30 eV. It is clear from the figures that the present results are

in good agreement with experimental measurements in the entire energy region. Further it has been noticed that above 3 eV, our results are in better agreement with measurements.

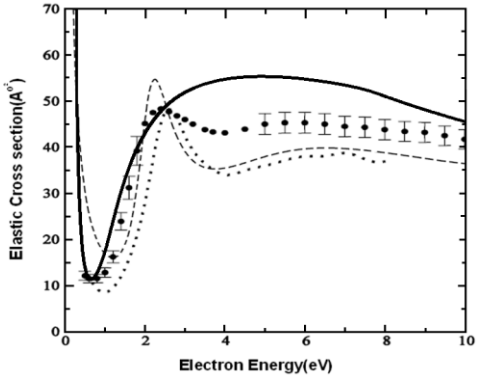

Fig 1: σ_t for *e* - PH_3 system in the energy range 0.1 - 10 eV. Calculations: ——— , Present results in SEP model; - - -, Munjal and Baluja [11]; …, Bettega and Lima [12]; Experiment: ⊥, Szmytkowski *et al* [10].

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4. Conclusion

We reported low-energy e - PH_3 total cross sections by using a parameter-free correlation polarization potential along with exact static and approximate exchange model interactions. The R-T minimum position reproduced here is in agreement with measurements and other calculations.

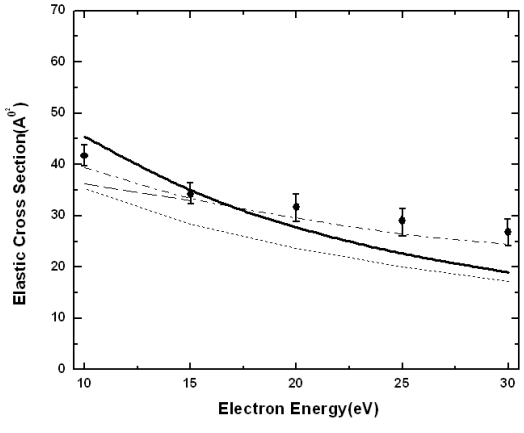

Fig 2: σ_t for e - PH_3 system in the energy range 10 - 30 eV. Calculations: ——— , Present results in SEP model; - - -, Munjal and Baluja [11]; …, Bettega and Lima [12]; ——·——·——, Limbachiya *et al* [13]. Experiment: ⊥ , Szmytkowski et al [10].

Acknowledgement

We gratefully acknowledge the financial support for this research work from Department of Science and Technology (DST), New Delhi, India under the Project No. SR/S2/LOP-0015/2010(G).

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