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**POTENTIAL ELECTRON SCATTERING
 BY P₂ AND P₃ PHOSPHORUS MOLECULES**

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Potential electron scattering by P₂ and P₃ phosphorus molecules at scattering energies of 0.5–30 eV has been studied theoretically for the first time. The research is carried out in the framework of the independent-atom model and using a real parameter-free relativistic optical potential for the electron interaction with atoms in the molecule. For the consistent description of the electron scattering by the atoms in the molecule, the potential parameters and the atomic characteristics are calculated in the local approximation of the stationary and time-dependent variants of the density functional theory. The comparison of the angular behavior of the differential cross-sections and the energy dependences of the integral ones in the cases of electron scattering by phosphorus molecules and phosphorus atoms testifies to their similarity.

Keywords: independent-atom model, optical potential, scattering amplitude, partial phase shift, differential and total cross-sections, optical theorem.

1. Introduction

A theoretical consideration of the potential electron scattering by a molecule, when it is regarded as a multiatomic system, is much more difficult than the description of this process in the case of atom. However, the former is extremely important from the fundamental (research of the electron interaction with targets characterized by various shapes and complicated structures) and applied (physics and chemistry of gases, surface science, solid state physics, and plasma physics) aspects. A very important task consists in finding the accuracy of theoretical approximations that are used in researches and for the description of the scattering by molecular systems at low, medium, and high collision energies. In the absence of experimental data for scattering parameters, the results of calculations carried out in various approximations should be compared with various theoretical data.

A description of this kind is performed, first of all, using rather a simple Independent-Atom Model (IAM) [1–4]. In the framework of this model, the amplitude of electron scattering by a molecule is reduced to a sum of scattering amplitudes for atoms. In works [5, 6], the IAM was improved by introducing a correction to the interatomic screening (the Screening Correction Additivity Rule, IAM-SCAR). The corresponding correction for total cross-sections was developed in work [5], and, for differential ones, in work [6]. In this work, we also use the IAM [7–9] together with the optical potential (OP) method [10], which is based on the approach of works [11, 12], with regard for the interaction between an electron and the atoms in a molecule.

In more complicated approaches, the methods of electron gas theory are used to find the potentials of the electron interaction with a target molecule. The application of the electron density of a target molecule for this purpose was proposed and applied for the first time to the electron scattering by

atoms and molecules in works [11, 12]. In particular, in work [12], the non-spherical character of the correlation-polarization potential for the electron interaction with the molecule was taken into account in the form of the two-term series expansion of the potential in Legendre polynomials. At large distances from the target, those terms, with the corresponding polarizabilities, represent the spherical and non-spherical potentials. In the cited work, one can find references to the standard methods used for molecular parameter calculations.

Basing on this approach, the methods of spherical [13, 14] and single-center [15] molecular interaction potentials were developed. For instance, in works [13, 14], the total wave function of a molecule and the corresponding electron density were determined in the framework of the Hartree–Fock method. At the same time, in work [15], the description used molecular parameters that were found by applying a much more complicated procedure, namely, a symmetry-adapted, single-center expansion of the total multi-center wave function of electrons in a target molecule.

A detailed research of the scattering characteristics for electrons, positrons, and photons was also carried out in the framework of the R -matrix method, which is the most advanced today [16]. In the cases of electron scattering by an N -electron molecule at small distances from the target in the internal region, the wave function of the $(N+1)$ -electron complex for the given configuration of interatomic distances is determined, by using the methods of coupled molecular states, with regard for the exchange and correlation interactions. In particular, the Gaussian- or Slater-type orbitals are used as basis functions. Those orbitals are centered at the nuclei; then they are combined with continuous basis functions.

A single work, where the scattering $e + P_2$ was studied theoretically, is [17]. The cited authors applied the Schwinger multichannel method with pseudopotentials for the calculation of the cross-sections of elastic electron scattering by X_2 and XH_3 molecules ($X = N, P, As,$ and Sb) at collision energies of 10, 15, 20, 25, and 30 eV in the static-exchange approximation. In this approximation, the electron interacts with the whole molecule, similarly to the methods used in works [12–15], but owing to the static and exchange potentials only. The introduction of a pseudopotential allows one to change a real potential arising due to the combined action of the nucleus and the

core electrons in every atom of the molecule. The authors of work [17] used many-particle methods, e.g., the Hartree–Fock method, for valence electrons. This approach is described in more details in the short review [18] (see also references therein). Below, we compare our results obtained for the $e + P_2$ scattering with the data of work [17].

2. Theoretical Method

2.1. Scattering parameters

For studying the behavior of elastic differential cross-sections (DCSs) and integral – elastic, momentum-transfer, and viscosity – ones for the potential scattering of electron by molecules in the IAM framework [1–4], we applied the OP method [7–9] (see also work [10]). In the IAM, when an electron is scattered by an N -atomic molecule, the following scattering amplitudes are used [19, 20]:

$$\begin{aligned} F(\theta, E) &= \sum_{m=1}^N f_m(\theta, E) \exp(i\mathbf{s}\mathbf{r}_m), \\ G(\theta, E) &= \sum_{m=1}^N g_m(\theta, E) \exp(i\mathbf{s}\mathbf{r}_m). \end{aligned} \quad (1)$$

Here, $\mathbf{s} = \mathbf{k}_i - \mathbf{k}_f = k(\mathbf{n}_i - \mathbf{n}_f)$ is the vector of transferred momentum; \mathbf{k}_i and \mathbf{k}_f are the initial and final, respectively, momenta of the incident electron; \mathbf{r}_m is the radius vector of the nucleus of the m -th atom in the molecule (reckoned from molecule's center of mass); θ the scattering angle; E the energy of an incident electron, $E = k^2/2$; and f_m and g_m are the direct and spin-flip, respectively, amplitudes of electron scattering by the m -th atom in the molecule. The factors $\exp(i\mathbf{k}\mathbf{n}_i \cdot \mathbf{r}_m)$ in the amplitudes $F(\theta, E)$ and $G(\theta, E)$ (see Eqs. (1)) involve the wave phase shifts, which are associated with a shift of the reference mark with respect to the position \mathbf{r}_m for the m -th scattering center [1].

The differential cross-section of the elastic electron scattering by an N -atomic molecule in the IAM framework with the use of the averaging over the rotational and vibrational molecular degrees of freedom is given by the expression [1, 2, 19, 20]

$$\frac{d\sigma_{\text{el}}^{\text{IAM}}}{d\Omega} = \langle |F|^2 + |G|^2 \rangle, \quad (2)$$

where the atomic units $\hbar = e = m_e = 1$ are used. In terms of atomic amplitudes of DCS, Eq. (2) looks like

$$\frac{d\sigma_{\text{el}}^{\text{IAM}}}{d\Omega} = \sum_{m=1}^N \sum_{n=1}^N [f_m(\theta, k) f_n^*(\theta, k) + g_m(\theta, k) g_n^*(\theta, k)] \exp(-\ell_{mn}^2 s^2 / 2) \frac{\sin(sr_{nm})}{sr_{nm}}. \quad (3)$$

The differential cross-section (3) can be written differently in the form of two terms: (i) the sums of DCSs for the scattering by each atom; this is the direct term

$$\sum_{m=1}^N d\sigma_{\text{el},m}/d\Omega = d\sigma_{\text{el}}^{\text{Ad}}/d\Omega$$

(according to the sum rule, the ‘‘additivity rule’’ (Ad) approximation); and (ii) the interference (or indirect) term

$$\frac{d\sigma_{\text{el}}^{\text{IAM}}}{d\Omega} = \frac{d\sigma_{\text{el}}^{\text{Ad}}}{d\Omega} + \frac{d\sigma_{\text{el}}^{\text{Int}}}{d\Omega}, \quad (4)$$

where

$$\frac{d\sigma_{\text{el}}^{\text{Int}}}{d\Omega} = \sum_{m,n \neq m}^N [f_m(\theta, k) f_n^*(\theta, k) + g_m(\theta, k) g_n^*(\theta, k)] \exp(-\ell_{mn}^2 s^2 / 2) \frac{\sin(sr_{nm})}{sr_{nm}}. \quad (5)$$

In expressions (3) and (5), ℓ_{mn} and r_{nm} are the amplitude of vibration and the distance, respectively, between the n -th and m -th atoms in the molecule, and the function $s(\theta, k) = 2k \sin(\theta/2)$.

To describe the important effects of spin polarization at the electron scattering by molecules, the spin polarization parameters $S(\theta, E)$, $T(\theta, E)$, and $U(\theta, E)$ are used, which are related to the scattering amplitudes $F(\theta, E)$ and $G(\theta, E)$ (see works [21, 22]). For instance, the Sherman function $S(\theta, E)$, which describes the electron polarization at the scattering of a non-polarized electron beam owing to the spin-orbit interaction, has a standard form [21, 22] that takes the above-indicated averaging into account [19]:

$$S(\theta, E) = i \frac{\langle FG^* - F^*G \rangle}{\langle |F|^2 + |G|^2 \rangle} = i \left(\sum_m [f_m g_m^* - f_m^* g_m] + \sum_{m,n \neq m} [f_m g_n^* - f_n^* g_m] \right) \times$$

$$\times e^{-\ell_{mn}^2 s^2 / 2} \frac{\sin(sr_{nm})}{sr_{nm}} \Big) / (d\sigma_{\text{el}}^{\text{IAM}}/d\Omega). \quad (6)$$

The energy and angular dependences of the DCS and the spin polarization parameters are very sensitive to the quality of every approximation used for the description of the potential electron scattering by molecules.

For the electron scattering by homonuclear molecules – in our case, these are two- and three-atomic ones – the differential scattering cross-sections (3) and (4) in the IAM framework have much simpler forms (see also work [20]):

$$\frac{d\sigma_{\text{el}}^{\text{IAM}}}{d\Omega} = 2 \frac{d\sigma_{\text{el},A}}{d\Omega} \left[1 + \exp(-\ell_{12}^2 s^2 / 2) \frac{\sin(sr_{12})}{sr_{12}} \right], \quad (7)$$

$$\frac{d\sigma_{\text{el}}^{\text{IAM}}}{d\Omega} = 3 \frac{d\sigma_{\text{el},A}}{d\Omega} \left[1 + \frac{2}{3} \left(\exp(-\ell_{12}^2 s^2 / 2) \times \frac{\sin(sr_{12})}{sr_{12}} + \exp(-\ell_{13}^2 s^2 / 2) \frac{\sin(sr_{13})}{sr_{13}} + \exp(-\ell_{23}^2 s^2 / 2) \frac{\sin(sr_{23})}{sr_{23}} \right) \right]. \quad (8)$$

Here, $d\sigma_{\text{el},A}/d\Omega$ is the DCS of the scattering by one of the atoms in the molecule. One can see that the behavior and the features of the DCS $d\sigma_{\text{el}}^{\text{IAM}}/d\Omega$ for the electron scattering by such molecule in the IAM framework are mainly governed by the angular and energy dependences of the DCS $d\sigma_{\text{el},A}/d\Omega$ – as well as by all their features, i.e. minima and maxima – for the electron scattering by a separate atom in the molecule.

In the indicated IAM and Ad approximations, the integral cross-sections of elastic scattering are coupled with each other. They can be calculated by directly integrating the DCS over the scattering angles. In particular, for the DCS $d\sigma_{\text{el}}^{\text{IAM}}/d\Omega$, we obtain

$$\sigma_{\text{el}}^{\text{IAM}}(E) = 2\pi \int_0^\pi d\theta \sin \theta \frac{d\sigma_{\text{el}}^{\text{IAM}}(E, \theta)}{d\theta} = \sigma_{\text{el}}^{\text{Ad}} + \sigma_{\text{el}}^{\text{Int}}, \quad (9)$$

where

$$\sigma_{\text{el}}^{\text{Ad}}(E) = 2\pi \int_0^\pi d\theta \sin \theta \frac{d\sigma_{\text{el}}^{\text{Ad}}(E, \theta)}{d\theta}, \quad (10)$$

and the interference term equals

$$\sigma_{\text{el}}^{\text{Int}}(E) = 2\pi \int_0^\pi d\theta \sin\theta \frac{d\sigma_{\text{el}}^{\text{Int}}(E, \theta)}{d\theta}. \quad (11)$$

It is worth to note that the integral cross-section of elastic scattering $\sigma_{\text{el}}^{\text{Ad}}(E)$ can also be determined from the optical theorem [1–3, 23]. For the IAM, this theorem coincides with the “additivity rule” of the Ad approximation [2–6]. Therefore, on the basis of expressions (3)–(5) for the DCS and with the use of the relations

$$\begin{aligned} \sin(sr_{nm})/sr_{nm} |_{\theta \rightarrow 0} &\rightarrow 1, \\ \sin(sr_{nm})/sr_{nm} |_{r_{nm} \rightarrow 0} &\rightarrow 1, \end{aligned}$$

we obtain

$$\sigma_{\text{el}}^{\text{Ad}}(E) = \frac{4\pi}{k} \sum_{n=1}^N \text{Im}[f_n(\theta = 0, k)] = \sum_{n=1}^N \sigma_{\text{el},n}(E) \quad (12)$$

for this cross-section.

In the case of forward scattering, the “spin-flip” amplitude (see below) gives no contribution, because of the properties of associated Legendre functions of the first kind $P_\ell^1(\cos\theta)$; i.e. $g_n(\theta = 0, k) = 0$. From expressions (7) and (8) for the DCS, we see that the optical theorem (12) results in the following expressions for the integral cross-sections: $\sigma_{\text{el}}^{\text{Ad}}(E) = 2\sigma_{\text{el},A}(E)$ and $\sigma_{\text{el}}^{\text{Ad}}(E) = 3\sigma_{\text{el},A}(E)$, respectively. Similarly, expressions (9) and (10) in the IAM or Ad approximation can be used to determine the integral cross-section of momentum transfer, $\sigma_{\text{mom}}^{\text{IAM}}(E)$ or $\sigma_{\text{mom}}^{\text{Ad}}(E)$, with the weight function $(1 - \cos\theta)$, and the integral cross-section of viscosity, $\sigma_{\text{vis}}^{\text{IAM}}(E)$ or $\sigma_{\text{vis}}^{\text{Ad}}(E)$, with the weight function $\sin^2\theta$. Note that the integral cross-sections for the $e+P$ scattering, which were calculated by us by integrating DCS (9) over the angles and using the optical theorem, coincide, which testifies to the correctness of those calculations.

The IAM approach is valid under the conditions that the electron is fast enough: $k(r_{nm})_{\text{min}} \gg 1$, and the scattering by atoms occurs only once: $(r_{nm})_{\text{min}} \gg (a)_{\text{max}}$ [1]. Here, $(r_{nm})_{\text{min}}$ is the minimum distance between the atoms, and $(a)_{\text{max}}$ the maximum radius of the particle interaction with each atom. For instance, if $(r_{nm})_{\text{min}} = 4a_0$, which corresponds the an interatomic distance of about 2.1 Å, and $k = 1$ a.u., which corresponds to an incident electron energy of about 14 eV, the simple inequality $k(r_{nm})_{\text{min}} > 1$ is

obeyed. Here, $a_0 = 5.2918 \times 10^{-11}$ m is the Bohr radius, the atomic length unit. Note that $k(r_{nm})_{\text{min}} \sim 1$ at an electron energy of 1 eV.

We consider that the application of a rather good consistent quantum-mechanical description of the electron scattering in the potential field of molecular atoms will also allow us to describe well the electron scattering by the whole molecule in the IAM framework. In our opinion, this description of the scattering by the molecule will be valid even in the case where the simple inequality $k(r_{nm})_{\text{min}} > 1$ is satisfied. Note also that, e.g., the IAM-SCAR approximation [5, 6] was proposed just in order to use the IAM at medium and even low, lower than 10 eV, collision energies.

The amplitudes of electron scattering by the atom can be found from the real partial phase shifts $\delta_\ell^\pm(E) = \varepsilon_\ell^\pm(E)$ in the case of real OP of interaction [10] or the complex ones $\delta_\ell^\pm(E) = \varepsilon_\ell^\pm(E) + i\xi_\ell^\pm(E)$ in the case of complex OP, which makes allowance for absorption effects [22]. In particular, the formulas for the scattering amplitudes in terms of the real partial phase shifts $\delta_\ell^\pm(E) = \varepsilon_\ell^\pm(E)$ look like

$$\begin{aligned} f_m(\theta, k) = \frac{1}{2ik} \sum_{\ell=1}^{\infty} \{(\ell+1) [\exp(2i\varepsilon_\ell^+) - 1] + \\ + \ell [\exp(2i\varepsilon_\ell^-) - 1]\} P_\ell(\cos\theta), \end{aligned} \quad (13)$$

$$\begin{aligned} g_m(\theta, k) = \frac{1}{2ik} \sum_{\ell=1}^{\infty} [\exp(2i\varepsilon_\ell^-) - \exp(2i\varepsilon_\ell^+)] \times \\ \times P_\ell^1(\cos\theta), \end{aligned} \quad (14)$$

where $P_\ell(\cos\theta)$ are Legendre polynomials.

The partial phase shifts for the initial values of orbital momentum of the incident electron, $\ell < \ell_{\text{min}}$, are obtained by solving the real or complex phase equations (see works [10], [22], and references therein) with the OP $V_{\text{opt}}^\pm(r, E) = V^\pm(r, E)$ or $V_{\text{opt}}^\pm(r, E) = V^\pm(r, E) + iV_A^\pm(r, E)$, respectively. Here, V_A is the absorption potential. The asymptotic (at $\ell_{\text{max}} > \ell > \ell_{\text{min}}$) values of phase shifts are calculated, by using the expression [23]

$$\tan \delta_\ell^{\text{as}} = \pi\alpha_d(0)k^2 / [(2\ell+3)(2\ell+1)(2\ell-1)]. \quad (15)$$

Here $\alpha_d(0)$ is the static dipole polarizability of the corresponding atom of the molecule.

It is worth to note that the availability of data in the scientific literature concerning the calculated

partial phase shifts of particle scattering by various atoms allows them to be widely applied to the calculation of the parameters of scattering by various multiatomic molecules, by using the IAM.

2.2. Optical potential

We use the real part of OP, which is independent of the fitting (arbitrary) or empirical parameters (the RSEP LA approximation) [10] (see also work [9]):

$$V^\pm(r, E) = V_S(r) + V_e(r, E) + V_P(r) + V_R(r, E) + V_{so}^\pm(r, E). \quad (16)$$

Here, the signs “ \pm ” in the potential of spin-orbit interaction correspond to the total angular momenta of the incident electron, $j = \ell \pm 1/2$. The potential components of the OP are the static V_S , exchange V_e , polarization V_P , scalar-relativistic V_R , and spin-orbit interaction V_{so}^\pm , potentials. These components are determined, in general, by the total and spin electron densities of atoms in the molecule. The electron density can be calculated in the approximations presented by various theories, such as the Thomas–Fermi theory, the Hartree–Fock one, and the density functional theory (DFT). Analytical expressions with parameters can also be used for those quantities, which is very convenient in calculations (see, e.g., work [24]). The values of electron density parameters calculated for atoms from hydrogen to krypton ($Z = 1\div 36$) in the Hartree–Fock approximation are quoted in work [24]. The corresponding parameters calculated for the phosphorus atom in the local spin density approximation of the DFT and for the mercury atom calculated in the local density approximation are given, respectively, in works [10] and [25]. Note that, in the approaches of works [11–15], the potential components of the OP are determined by the electron density of a molecule.

The exchange and polarization potentials are used in the local spin-non-polarized (or local) or spin-polarized (or local-spin) [7, 26] approximations for the (free) inhomogeneous electron gas. In the former approximation, the exchange potential $V_e(r, E)$ can be either non-relativistic, $V_e(r, E) = V_e^N(r, E)$ [10] or, for heavy atoms, include relativistic corrections, $V_e(r, E) = V_e^R(r, E)$. For the polarization potential V_P^{SR} at short distances from the molecule’s atom, a parameter-free expression for the potential of the correlation-polarization interaction between electrons

is used (see works [9, 10]). At large (asymptotic) distances, the polarization potential looks like $V_P^{\text{LR}}(r) = -\alpha_d(0)/2r^4$. The dependences $V_P^{\text{SR}}(r)$ and $V_P^{\text{LR}}(r)$ intersect at a definite point r_c . For the calculation of the atomic polarizability $\alpha_d(0)$, the local approximation of the time-dependent density functional theory is applied.

Absorption effects influence the scattering parameters at collision energies $E > \Delta$, where Δ is the first inelastic threshold energy for the n -th atom. In the case of phosphorus atom, they have to be taken into account starting from the energy $\Delta = 6.9667$ eV [27]; this is the average energy of the term 4P of the configuration $3p^24s$, which is dipole-excited from the ground state $3p^3\ ^4S$ of a phosphorus atom (the ionization energy of the phosphorus atom amounts to 10.4868 eV [27]). In the OP method, those effects are taken into consideration with the help of the non-empirical, $V_A(r, E) = V_{\text{af}}(r, E)$ (of the Staszewska-type [28]), or empirical, $V_A(r, E) = V_{\text{aMc}}(r, E)$ (of the McCarthy-type [29]), absorption potentials (see also work [26]). Generally speaking, we may assert that making allowance for absorption will result in a certain reduction of the elastic differential cross-section and, as a consequence, a reduction of the integrated elastic scattering, momentum-transfer, and viscosity cross-sections.

Note that the approaches, in which spherical [13, 14] and single-center [15] potentials are used, take absorption effects into consideration more consistently, as the absorption performed by the whole molecule, which is determined by the excitation of its spectra: electronic, vibrational, and rotational ones.

Hence, the scattering parameters for the description of the electron interaction with an atom in the molecule can be calculated in various approximations, taking and not taking absorption effects into account; for example, in the spin-non-polarized [25], spin-polarized [26], and completely relativistic approaches, using the $V_e^R(r, E)$, $V_R(r, E)$, and $V_{so}^\pm(r, E)$ potentials; and in the semirelativistic, or partially relativistic, approach using only $V_R(r, E)$ or $V_{so}^\pm(r, E)$.

2.3. Structural calculations for P₂, P₃, and P₄ molecules

The structural characteristics of the P₂, P₃, and P₄ molecules were calculated using the theoretical methods of the computer software program GAMESS [30]. In all cases, the initial matrix of electron den-

sity was self-consistently and iteratively calculated in the framework of the unrestricted Hartree–Fock method. In order to take the correlation interactions of electrons into account, the further calculations were carried out within the coupled cluster method with single and double excitations and with the triple correction (CCSD(T)). In so doing, we used an expanded Gaussian basis set “triple- ζ ” with additional functions for taking the polarization and correlation interactions into account.

The equilibrium structures of the P_2 and P_3 molecules were obtained as a result of the geometrical optimization following the quadratic approximation algorithm. The equilibrium distances between the atoms obtained in CCSD(T) calculations are as follows (in a_0 units): for the P_2 molecule, $r_{12} = 3.610$ (cf. $r_{12} = 3.579$ [27] and $r_{12} = 3.578$ (for the $^{31}P_2$ isotope) [31]); for the P_3 molecule, $r_{12} = 3.7403$, $r_{13} = 3.7148$, and $r_{23} = 7.4552$. Note that work [17] contains no data on the calculated interatomic distance in the P_2 molecule.

In addition, let us indicate here that the geometrical structure of a P_4 molecule is not planar. It is characterized by the following interatomic distances (in a_0 units): $r_{12} = 4.1094$, $r_{13} = 4.1094$, $r_{14} = 4.5494$, $r_{23} = 6.4074$, $r_{24} = 4.1094$, and $r_{34} = 4.1094$.

3. Discussion of Results

The real OP (16), which was found in the local spin-density approximation of the DFT, was applied in work [10] to describe the potential scattering of an electron by a P atom. The amplitudes of the $e + P$ scattering determined in work [10] in the local density approximation of the DFT (the RSEP LA approximation) were used in this work to calculate the electron scattering by P_n molecules ($n = 2, 3$) (see also our previous publications [7–9]). In our calculations, we neglected the amplitudes of vibrations ℓ_{mn} between the n -th and m -th atoms in the molecule; i.e. we considered them to equal zero.

3.1. Differential scattering cross-sections

Figure 1 demonstrates the angular dependences of the DCS for the elastic electron scattering by a phosphorus atom [10] and the DCSs $d\sigma_{el}^{IAM}/d\Omega$ and $d\sigma_{el}^{Ad}/d\Omega$ for the electron scattering by the indicated phosphorus molecules calculated in the RSEP LA approximation for eight values of collision energy: 0.5, 1, 5, 10,

15, 20, 25, and 30 eV (see also work [8]). The obtained cross-sections are compared with the corresponding results of calculations carried out in work [17]. One can see that the DCSs of electron scattering by the phosphorus molecules obtained according to expressions (7) and (8) are expectedly very similar by their structure to the cross-sections of scattering by a phosphorus atom, being larger than the latter by a factor that corresponds to the number of phosphorus atoms in the molecule.

At low collision energies of 0.5 and 1 eV, the DCS $d\sigma_{el}^{Ad}/d\Omega$ lies between the atomic DCS and the DCS $d\sigma_{el}^{IAM}/d\Omega$ (for $e + P_2$) within the whole interval of angles. As the collision energy grows, even at 5 eV, the DCSs $d\sigma_{el}^{Ad}/d\Omega$ for the scattering by P_2 and P_3 atoms grow from large angles to medium and small ones and approach $d\sigma_{el}^{IAM}/d\Omega$. However, even at 30 eV, the DCS $d\sigma_{el}^{IAM}/d\Omega$ remains larger than $d\sigma_{el}^{Ad}/d\Omega$ within the angular interval of $0 \div 30^\circ$. This fact means that the interference terms (the sum in Eq. (4)) dominate at the scattering at small angles. From Fig. 1, d , one can see that, at an energy of 10 eV, the DCS from work [17] remains almost invariant and equal to approximately 1.4×10^{-20} m²/sr within the angular interval from 60° to 140° . Our results for the DCS at those angles have a smooth minimum of 0.42×10^{-20} m²/sr at 112° . At small ($< 60^\circ$) and large ($> 150^\circ$) angles, the DCS data from work [17] are close to our results obtained for the electron scattering by a P atom at all collision energies.

For higher electron energies, the angular behavior of DCS from work [17] becomes more structured: it contains two smooth minima and one maximum. At the minima, the DCSs from work [17] considerably exceed our values. Those features become the most pronounced at 30 eV, when, at medium angles ($75^\circ < \theta < 130^\circ$) and in the interval around the maximum, the data of work [17] are between our DCSs for the scattering by a P atom and a P_2 molecule. In our opinion, the understated values of theoretical DCSs in work [17], which were obtained in the static-exchange approximation, are a consequence of neglecting the polarization interaction between the electron and the P_2 molecule at calculations. This fact may explain why the lowest analyzed collision energy in work [17] was rather high (10 eV). On the other hand, maybe, it is the application of the molecular electron density in work [17] that is responsible for a little reduced, by magnitude, interaction between the incident electron

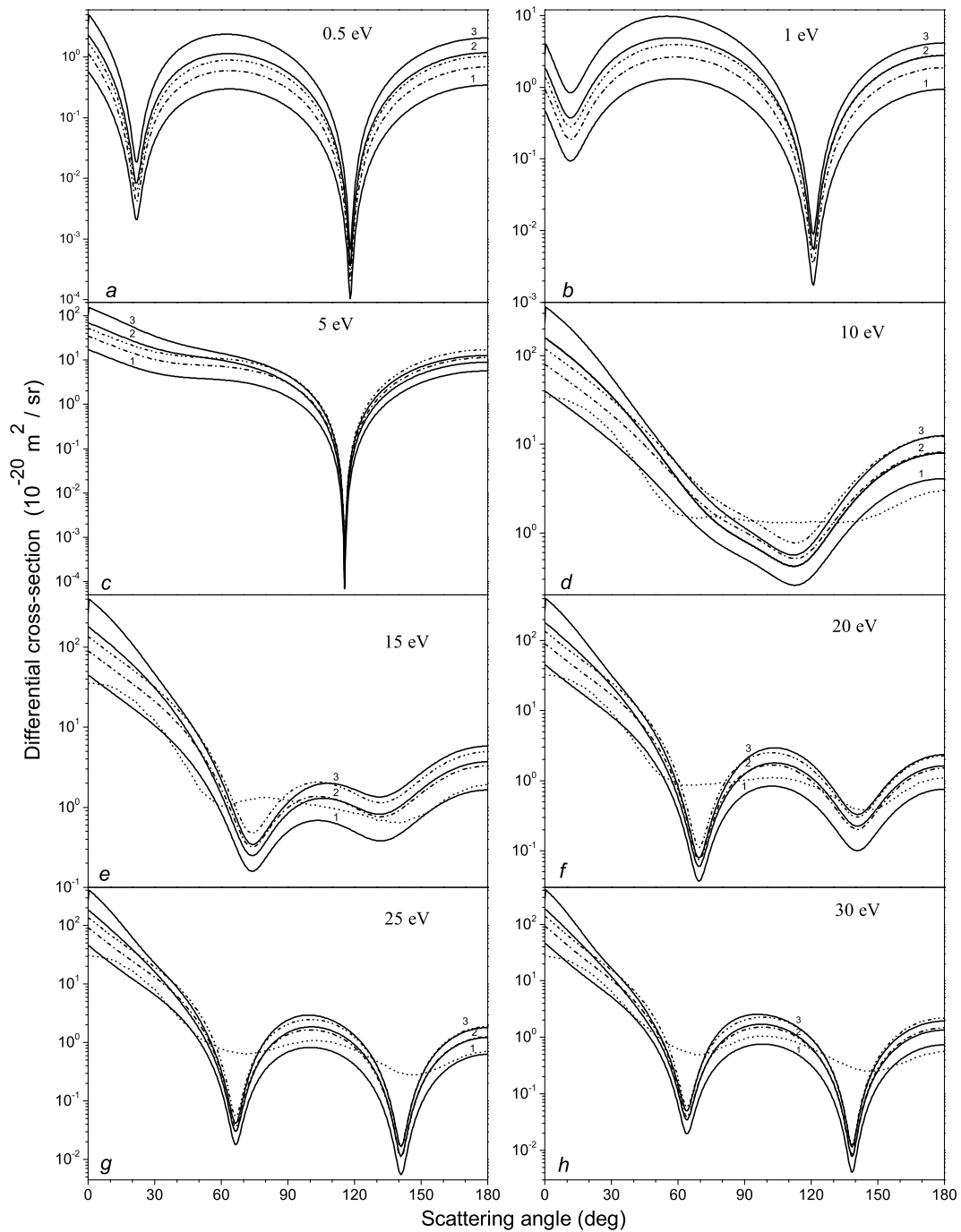


Fig. 1. Angular dependence of the differential cross-sections for the elastic electron scattering by a phosphorus atom and molecules at collision energies of 0.5 (a), 1 (b), 5 (c), 10 (d), 15 (e), 20 (f), 25 (g), and 30 eV (h). RSEP-LA theory: $d\sigma_{el}/d\Omega$ for $e + P$ scattering (solid curves 1) [10], $d\sigma_{el}^{IAM}/d\Omega$ for $e + P_2$ scattering (solid curves 2), $d\sigma_{el}^{IAM}/d\Omega$ for $e + P_3$ scattering (solid curves 3), $d\sigma_{el}^{Ad}/d\Omega$ for $e + P_2$ scattering (dash-dotted curves), $d\sigma_{el}^{Ad}/d\Omega$ for $e + P_3$ scattering (dash-dot-dotted curves). The Schwinger multichannel method in the static-exchange approximation [17]: $d\sigma_{el}/d\Omega$ for $e + P_2$ scattering (short-dashed curves)

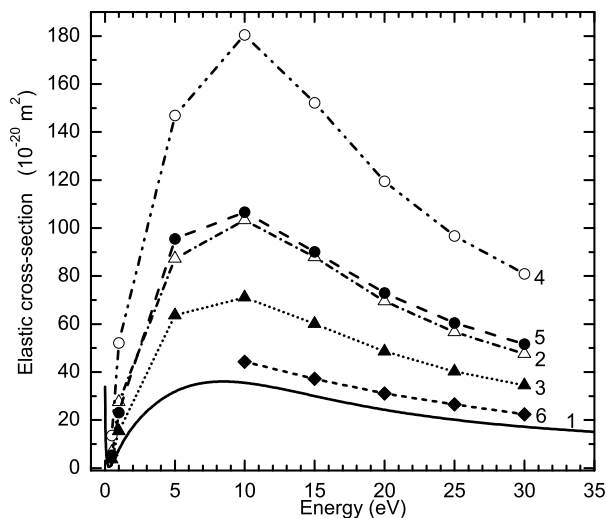


Fig. 2. Energy dependence of the integral elastic cross-sections $\sigma_{el}^{IAM}(E)$ and $\sigma_{el}^{Ad}(E)$ for the electron scattering by a phosphorus atom and molecules. RSEP-LA theory: (1) $e + P$ scattering [10], (2) IAM-approach, (3) Ad-approach, $e + P_2$ scattering, (4) IAM-approach, (5) Ad-approach, $e + P_3$ scattering. The Schwinger multichannel method in the static-exchange approximation [17]: (6) $e + P_2$ scattering

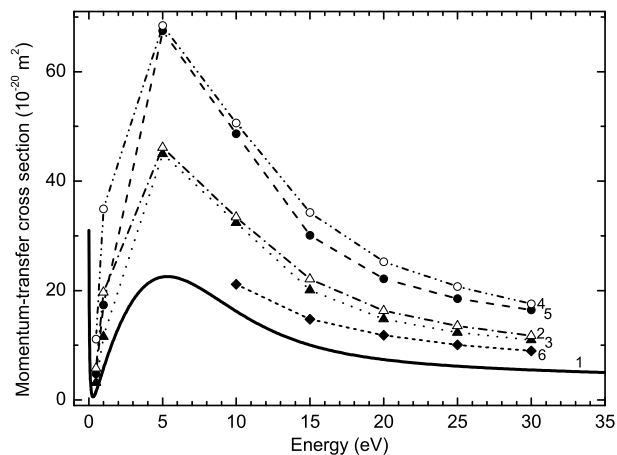


Fig. 3. The same as in Fig. 2, but for the integral momentum-transfer cross-sections $\sigma_{mom}^{IAM}(E)$ and $\sigma_{mom}^{Ad}(E)$

and the molecule, which results in the presented angular behavior of their DCS.

3.2. Integrated scattering cross-sections

In Figs. 2–4, the energy dependences of various integral cross-sections calculated for the elastic electron scattering by a P atom [10] and by the indicated

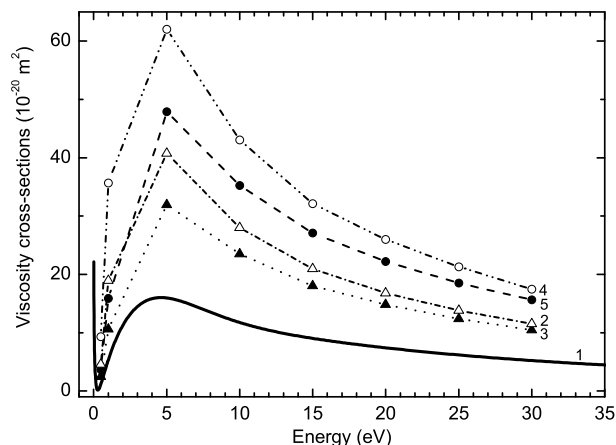


Fig. 4. The same as in Fig. 2, but for the integral viscosity cross-sections $\sigma_{vis}^{IAM}(E)$ and $\sigma_{vis}^{Ad}(E)$

phosphorus molecules are shown: elastic, $\sigma_{el}^{IAM}(E)$ and $\sigma_{el}^{Ad}(E)$ (see also work [8]), momentum-transfer, $\sigma_{mom}^{IAM}(E)$ and $\sigma_{mom}^{Ad}(E)$, and viscosity, $\sigma_{vis}^{IAM}(E)$ and $\sigma_{vis}^{Ad}(E)$, ones. One can see that the qualitative behaviors of all indicated cross-sections are similar. The behaviors of cross-sections for the scattering by molecules – the presence of the minimum and the maximum, and the dependence on the energy – are also structurally similar in all approximations. As the collision energy increases, the cross-sections come closer to one another and approach the cross-section of the $e + P$ scattering from above.

Figures 2 and 3 testify that the magnitudes of integral elastic and momentum-transfer cross-sections of the $e + P_2$ scattering from work [17] slightly exceed the corresponding cross-sections of the $e + P$ scattering [10]. This is a result of the understated DCS values in work [17]: by an order of magnitude at small angles and by several times at large ones. That is why the integral cross-sections from work [17] turned out rather small. From Fig. 2, one can also see that the cross-section $\sigma_{el}^{IAM}(E)$ exceeds $\sigma_{el}^{Ad}(E)$ rather strongly at the maximum located at 10 eV: by a factor of about 1.4 for the $e + P_2$ scattering and by a factor of about 1.8 for the $e + P$ one. In other words, the role of the interference (indirect) term $\sigma_{el}^{Int}(E)$ (see Eq. (11)) in Eq. (9) (see also Eqs. (4) and (5)) is rather important.

Figure 3 demonstrates that, at every collision energy, the cross-sections $\sigma_{mom}^{IAM}(E)$ and $\sigma_{mom}^{Ad}(E)$ calculated for the scattering by either of the examined

phosphorus molecules are close to each other. This fact means that the contribution made by the sum

$$\sum_{m,n \neq m}^N [f_m(\theta, k)f_n^*(\theta, k) + g_m(\theta, k)g_n^*(\theta, k)] \times \exp(-\ell_{mn}^2 s^2/2) \frac{\sin(sr_{nm})}{sr_{nm}}$$

of the products of the amplitudes of scattering by different atoms (or, in the case of identical atoms, by the terms containing the multipliers $\sin(sr_{nm})/sr_{nm}$ in expressions (7) and (8)) to the DCS in expression (5) is small and decreases, as the energy grows. Note that the integrand in Eq. (11) used for the calculation of this cross-section contains the function

$$(1 - \cos \theta)/s(\theta, k) = \sin(\theta/2)/k,$$

which gives a substantial contribution only at the medium and large scattering angles. We would like to emphasize that, as was numerically shown in work [2], for the growing collision energy (for the energies above 100 eV), the equality $\sigma_{\text{mom}}^{\text{IAM}}(E) \approx \sigma_{\text{mom}}^{\text{Ad}}(E)$ for the momentum-transfer cross-sections becomes valid. The approach of cross-sections $\sigma_{\text{mom}}^{\text{IAM}}(E)$ and $\sigma_{\text{mom}}^{\text{Ad}}(E)$ at higher energies can also be seen from Fig. 3.

From Fig. 4, one can see that, as the collision energy grows, the cross-sections $\sigma_{\text{vis}}^{\text{IAM}}(E)$ and $\sigma_{\text{vis}}^{\text{Ad}}(E)$ calculated for the scattering by both phosphorus molecules also become close enough. The integrand in Eq. (11) used for the calculation of this cross-section contains the function

$$\sin^2 \theta/s(\theta, k) = 2 \sin(\theta/2) \cos^2(\theta/2)/k,$$

which gives a substantial contribution only at the medium scattering angles.

4. Conclusions

To summarize, we may assume that the applied description of the potential electron scattering by a molecule in the framework of the independent-atom model and making use of the method of parameter-free real optical potential for the electron interaction with atoms in a molecule is quite satisfactory and can be fruitful. A further account of the absorption by atoms has to affect, to a larger extent, the magnitude and, to a less extent, the angular and energy

dependences of molecular scattering parameters. The account of well-known corrections to the interatomic screening at the scattering, IAM-SCAR, can also be essential. From this point of view, the issue concerning the correspondence of scattering parameters calculated in the examined approximations at low and medium collision energies to available experimental data remains urgently important. The further development of the potential scattering description in the direction, where the application of structural characteristics of molecular targets is required, seems to be the most important.

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1. N.F. Mott and H.S.W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, Oxford, 1965).
2. D. Raj, Phys. Lett. A **160**, 571 (1991).
3. P. Mozejko, B. Zywicka-Mozejko, and Cz. Szmytkowski, Nucl. Instrum. Methods B **196**, 245 (2002).
4. P. Mozejko, B. Zywicka-Mozejko, and Cz. Szmytkowski, Nauk. Visn. Uzhgorod. Nat. Univ. Ser. Fiz. **8**, 108 (2000).
5. F. Blanco and G. Garcia, Phys. Lett. A **317**, 458 (2003).
6. F. Blanco and G. Garcia, Phys. Lett. A **330**, 230 (2004).
7. Sh. Demesh, E. Remeta, and V. Kelemen, in *Contributed Papers of the 6th Conference on Elementary Processes in Atomic Systems (CEPAS)*, edited by Š. Matejíček, P. Papp, and O. Bogár (Bratislava, 2014), p. 65.
8. Sh.Sh. Demesh, V.I. Kelemen, and E.Yu. Remeta, J. Phys. Conf. Ser. **635**, 072020 (2015).
9. Sh.Sh. Demesh, Nauk. Visn. Uzhgorod. Nat. Univ. Ser. Fiz. **38**, 149 (2015).
10. V.I. Kelemen, M.M. Dovahnych, and E.Yu. Remeta, Ukr. J. Phys. **59**, 569 (2014).
11. J.K. O'Connell and N.F. Lane, Phys. Rev. A **27**, 1893 (1983).
12. N.T. Padiál and D.W. Norcross, Phys. Rev. A **29**, 1742 (1984).
13. A. Jain and K.L. Baluja, Phys. Rev. A **45**, 202 (1992).
14. G. Kaur, A.K. Jain, H. Mohan, P.S. Singh, S. Sharma, and A.N. Tripathi, Phys. Rev. A **91**, 022702 (2015).
15. F.A. Gianturco, J.A. Rodriguez-Ruiz, and N. Sanna, Phys. Rev. A **52**, 1257 (1995).
16. P.G. Burke, *R-Matrix Theory of Atomic Collisions* (Springer, Berlin, 2011).
17. M.H.F. Bettega, M.A.P. Lima, and L.G. Ferreira, J. Phys. B. **31**, 2091 (1998).
18. R.F. da Costa, M.T. do N. Varella, M.H.F. Bettega, and M.A.P. Lima, Eur. Phys. J. D **69**, 159 (2015).
19. A.C. Yates, Phys. Rev. **176**, 173 (1968).

20. J. Kessler, H. Lorenz, H. Rempp, and W. Buring, *Z. Phys.* **246**, 348 (1971).
21. E.Yu. Remeta and V.I. Kelemen, *Dopov. Nat. Akad. Nauk Ukr.* **11**, 84 (2011).
22. V.I. Kelemen and E.Yu. Remeta, *Dopov. Nat. Akad. Nauk Ukr.* **1**, 65 (2013).
23. P.G. Burke, *Potential Scattering in Atomic Physics* (Plenum Press, New York, 1977).
24. T.G. Strand and R.A. Bonham, *J. Chem. Phys.* **40**, 1686 (1964).
25. V.I. Kelemen and E.Yu. Remeta, *J. Phys. B* **45**, 185202 (2012).
26. E.Yu. Remeta and V.I. Kelemen, *J. Phys. B* **43**, 045202 (2010).
27. A.A. Radtsig and B.M. Smirnov, *Reference Data on Atoms, Molecules, and Ions* (Springer, Berlin, 1986).
28. G. Staszewska, D.W. Schwenke, and D.G. Truhlar, *Phys. Rev. A* **29**, 3078 (1984).
29. I. McCarthy, C. Noble, B. Phillips, and A. Turnbull, *Phys. Rev. A* **15**, 2173 (1977).
30. M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.J. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, and J.A. Montgomery, *J. Comput. Chem.* **14**, 1347 (1993).
31. K.P. Huber and G. Herzberg, *Constants of Diatomic Molecules. NIST Chemistry WebBook, NIST Standard Reference Database Number 69* (NIST, Gaithersburg, MD, 2015).

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ПОТЕНЦІАЛЬНЕ РОЗСИЮВАННЯ ЕЛЕКТРОНА МОЛЕКУЛАМИ ФОСФОРУ P₂ ТА P₃

Резюме

Теоретично вперше розглянуто потенціальне розсіювання електрона молекулами фосфору P₂ та P₃ в області енергій зіткнень 0,5–30 еВ. Дослідження проведено у рамках моделі незалежних атомів з використанням дійсного безпараметричного релятивістського оптичного потенціалу взаємодії електрона з атомами молекули. Для узгодженого опису розсіювання електрона на атомах молекул потенціали взаємодії та атомні характеристики визначено у локальному наближенні стаціонарної та нестаціонарної теорії функціонала густини. Проведене порівняння кутової поведінки диференціальних та енергетичної поведінки інтегральних перерізів розсіювання електрона на молекулах та на атомі фосфору показує їх подібність.