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# A comparative study of elastic scattering of low-energy electrons by boron, aluminum and gallium trihalides

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In this paper we present integral, differential and momentum transfer cross sections for elastic scattering of low-energy electrons by some metal-halogen molecular compounds, namely,  $\text{BF}_3$ ,  $\text{BCl}_3$ ,  $\text{BBr}_3$ ,  $\text{BI}_3$ ,  $\text{AlF}_3$ ,  $\text{AlCl}_3$ ,  $\text{AlBr}_3$ ,  $\text{AlI}_3$ ,  $\text{GaF}_3$ ,  $\text{GaCl}_3$ ,  $\text{GaBr}_3$ , and  $\text{GaI}_3$ . The pseudopotential based calculations were carried out with the Schwinger multichannel method at the static-exchange level of approximation. It is the purpose of this work to make a comparative study of the scattering processes involving aluminum and gallium trihalides with previous results for the boron ones [M. H. F. Bettega, *Phys. Rev. A* **61**, 042703 (2000)]. We find through direct comparison of the elastic cross sections that, at low energies, the scattering processes are mainly dominated by the halogen atoms. © 2003 American Institute of Physics. [DOI: 10.1063/1.1523902]

## I. INTRODUCTION

Electron–molecule collision cross sections have been increasingly important for modeling and controlling discharge environments in low-temperature plasma reactors. The driving mechanism in these plasmas is closely related to general electron–molecule scattering phenomena that occur in the precursor gases during the discharges. Indeed, the active fragments (ions, radicals and atoms) generated when electrons hit the molecular systems are responsible for several chemical reactions, like etching, coating, polymerization and nitriding, leading to surface and materials treatment or modification. Processes of this kind, especially those involving metallic species, are of great interest in semiconductor manufacturing.<sup>1–6</sup> Despite this fact, the data basis concerning electron–molecule collision cross sections (elastic, inelastic, ionization, etc.) are still very scarce. The situation, at least from the theoretical point of view, could be understood since all-electron calculations for scattering cross sections of large molecules demand substantial computer power and quickly reach limitation of memory and/or processing time. Therefore, it remains necessary to make use of some alternative methodologies which allow us to perform calculations for molecules composed by one or more heavy atoms.

In this paper we report elastic integral, momentum transfer, differential and partial wave contribution cross sections for scattering of electrons by  $\text{XY}_3$  molecules ( $X = \text{B, Al, and Ga}$ ;  $Y = \text{F, Cl, Br, and I}$ ) for energies from 5 up to 40 eV. To calculate the cross sections we used the Schwinger multichannel method<sup>7–9</sup> with pseudopotentials (SMCPP).<sup>10</sup> The idea behind this procedure is that the nuclei and the core electrons of each atom in the molecule are replaced by an effective potential, the pseudopotential (PP), and only the

valence electrons are actually taken into account in the calculations. This simplification has an enormous impact in studies of low-energy electron scattering by heavy molecules. Since polyatomic systems having the same number of valence electrons can, in principle, be studied with the same amount of computational effort, we are able to obtain cross sections for entire families of molecules formed by atoms of the same column in the periodic table.

The target molecules investigated in the present work are planar, belong to the  $D_{3h}$  symmetry group, and have the same number of valence electrons. In this way, it is possible to make use of the pseudopotential advantages to perform a comparative study of low-energy electron scattering by boron, aluminum and gallium trihalides. We also show, for completeness, previous results for the  $\text{BCl}_3$ ,  $\text{BBr}_3$ , and  $\text{BI}_3$  molecules.<sup>11</sup> Some of these molecules, like  $\text{AlCl}_3$ ,  $\text{AlBr}_3$ ,  $\text{GaF}_3$ , and  $\text{GaCl}_3$ , have interesting applications for modeling of industrial plasmas,<sup>12–18</sup> widely used in processes of etching and chemical vapor deposition. It has been pointed out that boron-halogen compounds play an important role as reaction precursors in discharge environments.<sup>19–22</sup> The present study is motivated by the increasing interest in plasma applications of the boron trihalides and also to extend previous studies to include aluminum and gallium halogen compounds.

The paper is outlined as follows: In Sec. II we briefly describe the theoretical formulation of SMCPP method. Section III contains details of calculation and discussion for our integral, momentum transfer, differential and partial wave contribution cross section results. Conclusions are finally presented in Sec. IV.

## II. METHOD

The Schwinger multichannel method (SMC) and its implementation with pseudopotentials (SMCPP) have been

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discussed in other papers<sup>7-10</sup> and here we will give only a brief description of the main features concerning the present work.

The SMC is an *ab initio* method that is obtained as a multichannel extension of the Schwinger variational principle (SVP). Since the SVP is a variational method for the scattering amplitude, the total scattering wave function can be expanded in a trial basis set

$$|\Psi_{\vec{k}}^{(\pm)}\rangle = \sum_m a_m^{(\pm)}(\vec{k}) |\chi_m\rangle. \quad (1)$$

The variational determination of the coefficients  $a_m^{(\pm)}(\vec{k})$  allows us to write

$$[f_{\vec{k}_f, \vec{k}_i}^-] = -\frac{1}{2\pi} \sum_{m,n} \langle S_{\vec{k}_i}^- | V | \chi_m \rangle (d^{-1})_{mn} \langle \chi_n | V | S_{\vec{k}_f}^- \rangle, \quad (2)$$

which is the expression for the scattering amplitude in the body frame, where we have

$$d_{mn} = \langle \chi_m | A^{(+)} | \chi_n \rangle \quad (3)$$

and

$$A^{(+)} = \frac{1}{2}(PV + VP) - VG_p^{(+)}V + \frac{1}{N+1} \left[ \hat{H} - \frac{N+1}{2}(\hat{H}P + P\hat{H}) \right]. \quad (4)$$

In these equations  $|S_{\vec{k}_i}^- \rangle$  is the product of a target state and a plane wave with momentum  $\vec{k}_{i(f)}$ , and is an eigenstate of the unperturbed Hamiltonian  $H_0$ ;  $V$  is the interaction potential between the incident electron and the target;  $|\chi_m\rangle$  is a  $(N+1)$ -electron Slater determinant used in the expansion of the trial scattering wave function;  $\hat{H} = E - H$  is the total energy of the collision minus the full Hamiltonian of the system, with  $H = H_0 + V$ ;  $P$  is a projector operator onto the open-channel (energetically accessible) space defined by target eigenfunctions  $|\Phi_l\rangle$

$$P = \sum_{l \in \text{open}} |\Phi_l\rangle \langle \Phi_l|, \quad (5)$$

and  $G_p^{(+)}$  is the free particle Green's function projected in the  $P$ -space.

This method allows us to deal with the following aspects of the electron-impact collision process: Elastic scattering with and without inclusion of polarization effects on the target, multichannel electronic excitations and multichannel coupling with polarization effects (accounting for competition between open and closed channels). In this work we are dealing with elastic scattering at the static-exchange approximation and, to this level of calculation, the  $P$  operator is composed only by the ground state of the target  $|\Phi_0\rangle$

$$P = |\Phi_0\rangle \langle \Phi_0|, \quad (6)$$

and the configuration space is composed by combinations of Slater determinants  $|\chi_m\rangle$  of the type

$$|\chi_m\rangle = \{ \mathcal{A} |\Phi_0\rangle |\phi_m\rangle \}, \quad (7)$$

where  $|\phi_m\rangle$  is a one-particle function represented by one molecular orbital and  $\mathcal{A}$  is the antisymmetrization operator. In our calculations we use the virtual molecular orbitals to represent the functions  $|\phi_m\rangle$ .

The final expression for scattering amplitude presented in Eq. (2) contains matrix elements of the Hamiltonian operator  $H$  of the system. Despite this, the scattering wave function does not need to satisfy any specific boundary condition, which is included in the Green's function. Besides, it always appears multiplied by the interaction potential  $V$ , and therefore, must be well described only in the region where  $V$  is appreciable. This property allows an expansion of the wave function in terms of  $L^2$  functions (in the present implementation Cartesian Gaussian functions, which are especially designed for integration with multicenter reference systems). In this way, the matrix elements that appear in the final expression of the scattering amplitude can be computed analytically, except those involving the Green's function. The  $\langle \chi_m | VG_p^{(+)} V | \chi_n \rangle$  (VGV) terms, being evaluated by numerical quadrature,<sup>23</sup> represent the most expensive step in the SMC method. The construction of the VGV term requires the evaluation of a very large number of the primitive two-electron integrals of the form

$$\langle \alpha \beta | V | \gamma \vec{k} \rangle = \int \int d\vec{r}_1 d\vec{r}_2 \alpha(\vec{r}_1) \beta(\vec{r}_1) \times \frac{1}{r_{12}} \gamma(\vec{r}_2) e^{i\vec{k} \cdot \vec{r}_2}, \quad (8)$$

which must be calculated for all possible combinations of Cartesian Gaussian functions  $\alpha$ ,  $\beta$ , and  $\gamma$ , and for a wide range of  $\vec{k}$  in both magnitude and direction.

In a way to overcome this troublesome task we introduced pseudopotentials in the formulation giving rise to the Schwinger multichannel method with pseudopotentials (SMCPP).<sup>10</sup> In our applications of the SMCPP method, we have been using the norm-conserving pseudopotentials of Bachelet, Hamann, and Schlüter (BHS).<sup>24</sup> By construction, these PP include core-core and core-valence correlation and also incorporate relativistic effects, which are important to give an accurate description of heavier atoms.

In the PP approach, the two-electron integrals, Eq. (8), are calculated only for valence electrons. Integrals involving core electrons are, in this case, replaced by one-electron integrals of the type

$$\langle \alpha | V^{\text{PP}} | \vec{k} \rangle = \int d\vec{r} \alpha(\vec{r}) V^{\text{PP}} e^{i\vec{k} \cdot \vec{r}}. \quad (9)$$

The BHS pseudopotentials are represented by the following expression:

$$\hat{V}^{\text{PP}}(r) = \hat{V}_{\text{core}}(r) + \hat{V}_{\text{ion}}(r), \quad (10)$$

which is given as a sum of two terms, a Coulombic potential contribution:

$$\hat{V}_{\text{core}}(r) = -\frac{Z_v}{r} \left[ \sum_{i=1}^2 c_i^{\text{core}} \text{erf}[(\alpha_i^{\text{core}})^{1/2} r] \right], \quad (11)$$

and an  $l$ -dependent short range term

TABLE I. Experimental bond length ( $\text{\AA}$ ) for  $\text{XY}_3$  molecules.

$\text{BF}_3$	1.313	$\text{AlF}_3$	1.630	$\text{GaF}_3$	1.880
$\text{BCl}_3$	1.742	$\text{AlCl}_3$	2.068	$\text{GaCl}_3$	2.108
$\text{BBr}_3$	1.893	$\text{AlBr}_3$	2.210	$\text{GaBr}_3$	2.243
$\text{BI}_3$	2.118	$\text{AlI}_3$	2.439	$\text{GaI}_3$	2.458

$$\hat{V}_{\text{ion}}(r) = \sum_{n=0}^1 \sum_{j=1}^3 \sum_{l=0}^2 A_{njl} r^{2n} e^{-\alpha_j r^2} \sum_{m=-l}^{+l} |lm\rangle \langle lm|, \quad (12)$$

where  $Z_v$  is the atomic valence charge. The coefficients  $c_i^{\text{core}}$ ,  $A_{njl}$  and decay constants  $\alpha_i^{\text{core}}$  and  $\alpha_{jl}$  are tabulated in the BHS article, Ref. 24.

The cross sections for electron scattering by molecules with different atoms but same number of valence electrons can then be calculated with almost the same amount of computational effort. Here we are dealing with three types of central atoms (B, Al, and Ga) and four types of peripheral atoms (F, Cl, Br, and I). Thus, for the present application, the computational saving behind the use of pseudopotentials is substantial, considering that the total number of electrons of the studied molecules goes from 32 to 190 while all the molecules have only 24 valence electrons.

### III. RESULTS

We have performed a comparative study for the electron-impact scattering by boron, aluminum and gallium trihalides. Cross sections for these processes were initially obtained in the static-exchange (SE) approximation. Since we are not including the relaxation effects of the target, the results are presented only for energies above 5 eV, where we could expect reasonable results of the SE approach. For energies lower than this value it remains necessary to perform a more elaborated calculation including polarization effects.

In order to compute the target wave function  $|\Phi_0\rangle$  and to describe the scattering orbitals  $|\phi_m\rangle$  for each molecular system, we have used the Cartesian Gaussian basis sets presented in Ref. 25. The basis sets were generated by a variational method<sup>26</sup> and specifically designed for pseudopotential based calculations. The 3s combinations of the d-type Cartesian Gaussian functions, namely  $[(x^2 + y^2 + z^2)\exp(-\alpha r^2)]$ , are not included in the calculations in order to avoid linear dependency in the basis set. The calculations were carried out at the experimental equilibrium geometries for the ground state of neutral molecules, as shown in Table I.

#### A. Integral cross sections

In Fig. 1 we show a comparison of the elastic integral cross sections for the boron, aluminum and gallium trihalides for energies from 5 eV up to 40 eV. Initially, we observe that integral cross sections (ICS) of metal-trifluorines are always smaller than the other metal-trihalides ICS. Comparing the results for molecules with the same central atom, as for example  $\text{AlY}_3$  ( $\text{Y}=\text{Cl}, \text{Br}, \text{I}$ ), we notice that in the energy range between 5 and about 20 eV, the magnitude of the ICS are ordered as follows:  $\sigma_{\text{AlCl}_3} < \sigma_{\text{AlBr}_3} < \sigma_{\text{AlI}_3}$ . Above 20 eV there is a crossing among the curves and the ICS for  $\text{AlCl}_3$

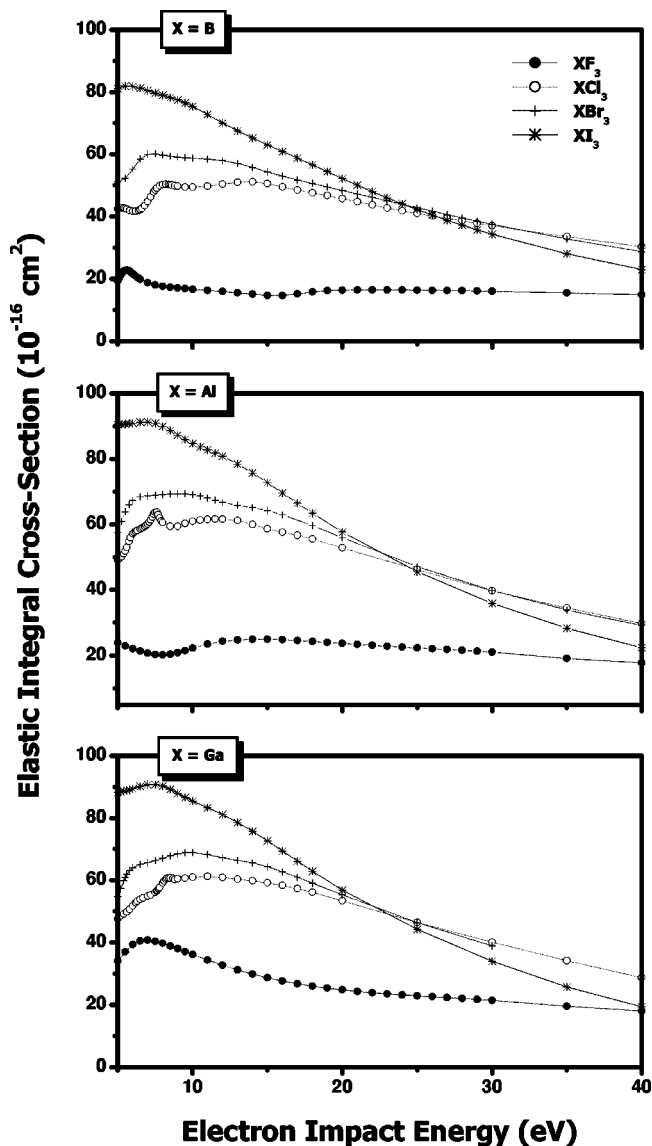


FIG. 1. Elastic integral cross section for  $e^- - \text{XY}_3$  ( $\text{X}=\text{B}, \text{Al},$  and  $\text{Ga}; \text{Y}=\text{F}, \text{Cl}, \text{Br},$  and  $\text{I}$ ) scattering. Study of the influence of the peripheral atoms.

and  $\text{AlBr}_3$  become very similar to each other and both greater in magnitude than the  $\text{AlI}_3$  one. The same pattern is observed for  $\text{BY}_3$  and  $\text{GaY}_3$  ( $\text{Y}=\text{Cl}, \text{Br}, \text{I}$ ) families of molecules. In the  $\text{BCl}_3$ ,  $\text{AlCl}_3$ , and  $\text{GaCl}_3$  integral cross sections we notice the presence of structures at around 8.0 eV, which may represent shape resonances.

In Fig. 2 we observe the influence of the central atom on the ICS as a function of the impact energy. The four plots show that distinct central atoms produce small differences in the cross sections, except for  $\text{BY}_3$  ( $\text{Y}=\text{F}, \text{Cl}, \text{Br}, \text{I}$ ). The ICS for  $\text{AlY}_3$  and  $\text{GaY}_3$  ( $\text{Y}=\text{Cl}, \text{Br}, \text{I}$ ) molecules are actually very similar in shape and present a broad structure around 10 eV. For the trifluorines we have the following behavior in the ICS:  $\text{BF}_3$  shows a very sharp maximum around 5 eV,  $\text{AlF}_3$  presents a pronounced minimum at  $\sim 8$  eV and finally, for the  $\text{GaF}_3$  molecule we observe a broad structure at 7.5 eV. It becomes clear, from these elastic ICS results, that heavier

peripheral atoms, namely Cl, Br, and I, provide larger cross sections than F.

## B. Momentum transfer cross sections

Momentum transfer cross sections (MTCS) for electron-impact scattering are used to model electron diffusion in a low-temperature plasma reactor.<sup>27,28</sup> In fact, the Boltzmann equations required in the determination of electron transport properties have been solved using the MTCS to describe the momentum loss rates for elastic collisions. MTCS can be calculated by theoretical methods or indirectly deduced from measured elastic differential cross sections (DCS), and are given by

$$\sigma_{\text{MTCS}} = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta (1 - \cos\theta) \frac{d\sigma(\theta, \varphi)}{d\Omega}. \quad (13)$$

From the above expression we see that the most significant contribution to the MTCS comes from the higher scattering angles, since its integrand is weighted by the  $(1 - \cos\theta)$  term.

We have calculated the momentum transfer cross sections for  $XY_3$  molecules ( $X = \text{B, Al, and Ga}$ ;  $Y = \text{F, Cl, Br, and I}$ ). Although not shown here (see Ref. 25), the same behavior described previously for the ICS curves could be seen in the MTCS plot. Once again we have found that the compounds containing fluorine atoms have smaller MTCS when compared to the molecules composed by the other halogen atoms. The low energy MTCS region is rich in structures, with the chlorine compounds ( $\text{BCl}_3$ ,  $\text{AlCl}_3$ , and  $\text{GaCl}_3$ ) showing the most remarkable data.

## C. Differential cross sections

We have carried out a large set of calculations for comparison of elastic differential cross sections of boron, aluminum and gallium trihalides. In Figs. 3–6 we study the influence of central atoms (which is also directly related to the molecular size) in the differential cross sections at 5, 7.5, 10, 15, 20, 25, 30, and 40 eV. The plots show that distinct central atoms produce very similar differential cross sections, except for  $\text{XF}_3$  ( $X = \text{B, Al, Ga}$ ) molecules at low energies. In fact, in Fig. 3 we observe that the DCS for these three molecules are actually dissimilar, the results for  $\text{GaF}_3$  being greater in magnitude, especially at the forward region. At these same energies the  $\text{BF}_3$  molecule, which is the lighter system, presents a distinguished behavior in its DCS curves. These results pointed out that the possible effects produced with the use of different central atoms are shielded by the heavier outer atoms Cl, Br, and I. This also clearly denotes the importance of these halogen atoms in the scattering processes.

Although not shown here, we have also compared the differential cross section (DCS) for trihalides with same central atoms. We have learned that the DCS for the  $\text{BCl}_3$ ,  $\text{BBr}_3$ , and  $\text{BI}_3$ , previously discussed in other papers<sup>11,29,30</sup> are in general bigger than those obtained for boron trifluorine. For the whole family, we can notice that as the scattering energy raises, the presence of oscillations also increases

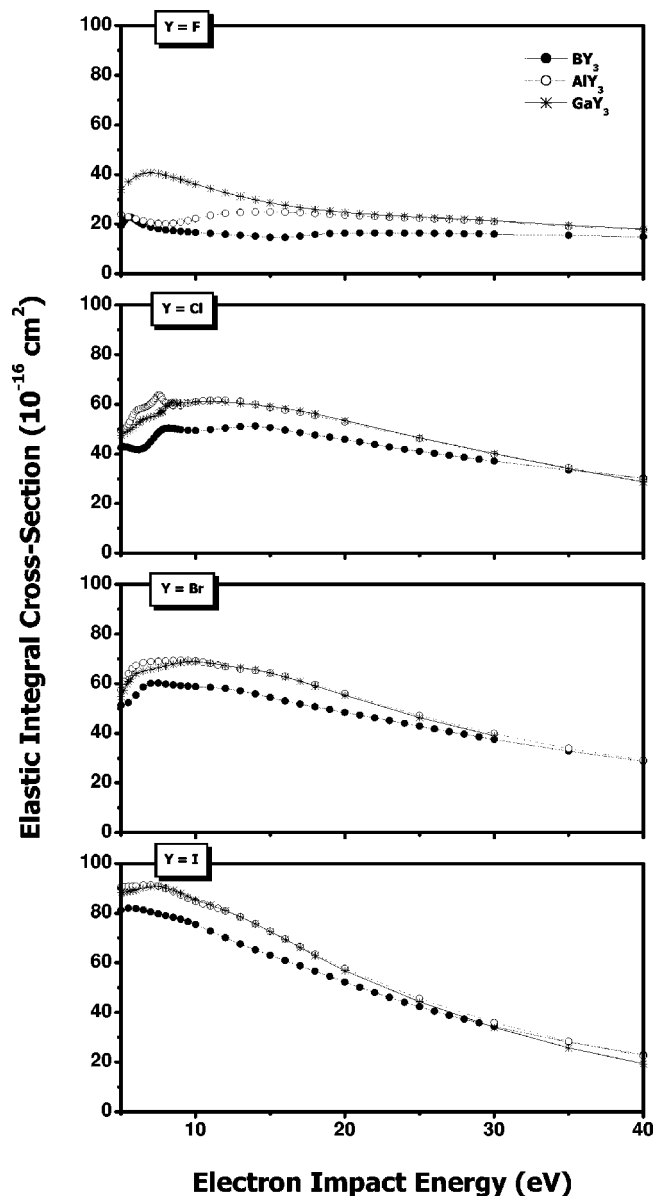


FIG. 2. Elastic integral cross section for  $e^- - \text{XY}_3$  ( $X = \text{B, Al, and Ga}$ ;  $Y = \text{F, Cl, Br, and I}$ ) scattering. Study of the influence of the central atom.

and for lower energies, from 5 to 15 eV, the DCS curves become more forward peaked.<sup>25</sup> This pattern indicates that there is a strong mixing between components of angular momentum.

For the heavier systems, we have compared our DCS for  $\text{AlY}_3$  and  $\text{GaY}_3$  ( $Y = \text{F, Cl, Br, and I}$ ) and have found that the peripheral atoms, Cl, Br, and I, have greater influence on the DCS than F atoms and, in general, they present small differences among themselves. At low energies the most significant discrepancies are basically located at the forward direction. In particular, we have observed that the  $\text{XI}_3$  ( $X = \text{Al and Ga}$ ) differential cross sections at 5 and 7.5 eV present a distinct behavior, being greater in magnitude in all angular range if compared with the corresponding trichlorides and tribromides. At higher energies, beyond 15 eV, this tendency undergoes an inversion and the ordering of the DCS curves is changed. However, we have found that even at these higher

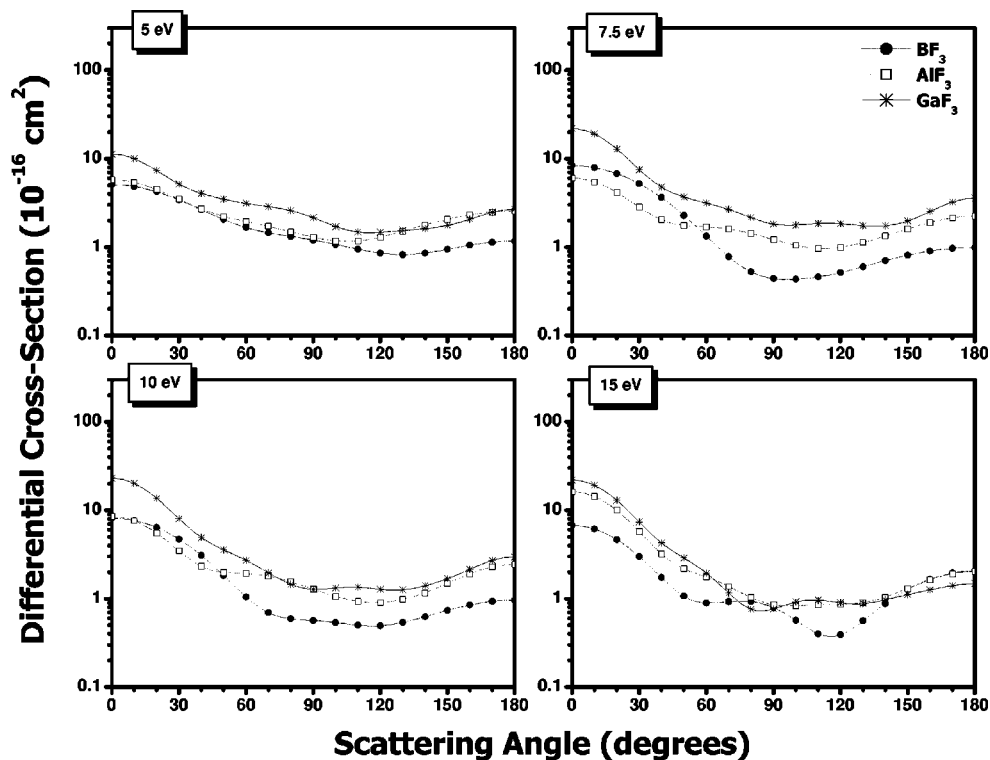


FIG. 3. Elastic differential cross section for  $e^-$ - $\text{XF}_3$  ( $X=\text{B}$ ,  $\text{Al}$ , and  $\text{Ga}$ ) scattering at 5, 7.5, 10, and 15 eV. Study of the influence of the central atom.

energies, trifluorine compounds present features which evidently distinguish its DCS curves from those belonging to the other aluminum and gallium halogen molecules. Furthermore, the same oscillation pattern that arises from augment-

ing the impact energy, observed for the  $\text{BY}_3$  compounds, is seen for the  $\text{AlY}_3$  and  $\text{GaY}_3$  ( $Y=\text{F}$ ,  $\text{Cl}$ ,  $\text{Br}$ , and  $\text{I}$ ) sets of molecules. Additional figures illustrating the above comments can be found in Ref. 25.

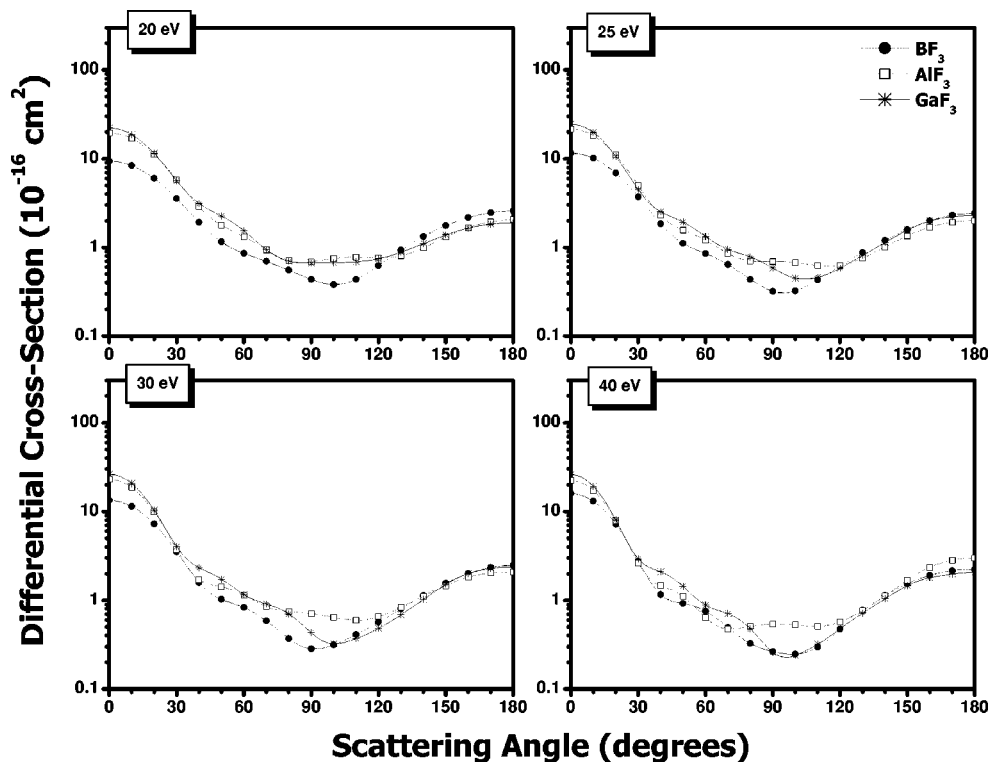


FIG. 4. Elastic differential cross section for  $e^-$ - $\text{XF}_3$  ( $X=\text{B}$ ,  $\text{Al}$ , and  $\text{Ga}$ ) scattering at 20, 25, 30, and 40 eV. Study of the influence of the central atom.

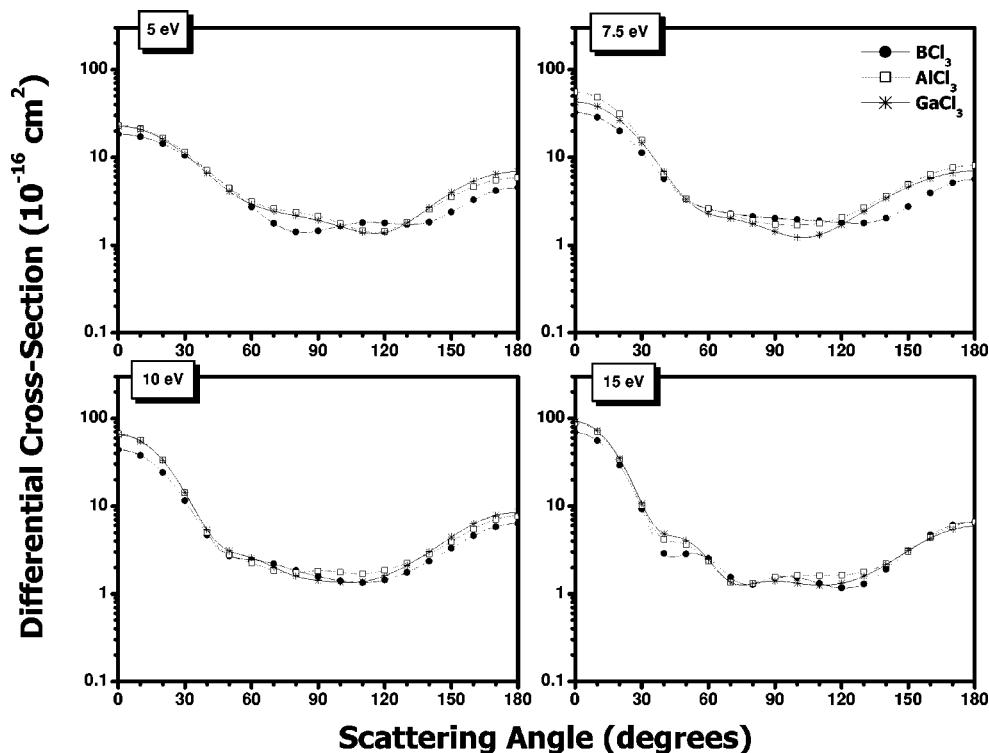


FIG. 5. Elastic differential cross section for  $e^-$ - $XCl_3$  ( $X=B$ , Al, and Ga) scattering at 5, 7.5, 10, and 15 eV. Study of the influence of the central atom.

#### D. Partial wave coupling and halogenation effects

We know from the general theory of potential scattering<sup>31</sup> that the scattering amplitude can be written in terms of Legendre polynomials and, due to this fact, the

presence of oscillations in the differential cross sections (DCS) can be related to polynomials of high degree.

Looking at the above DCS plots we notice that the oscillation pattern is directly related to the size of the periph-

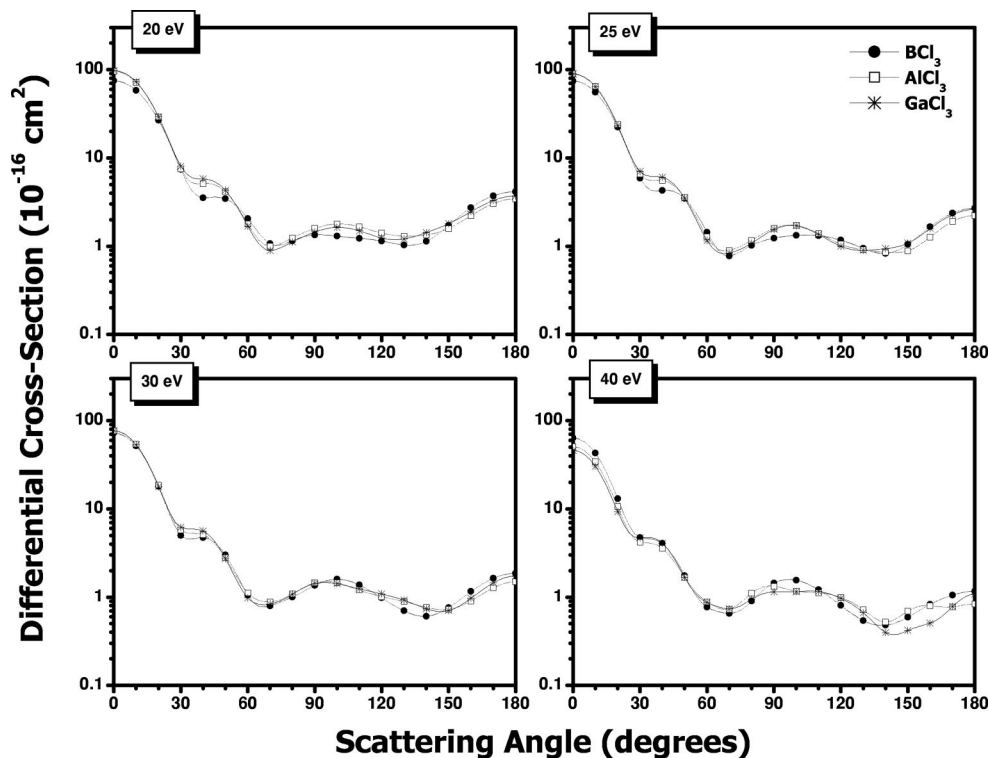


FIG. 6. Elastic differential cross section for  $e^-$ - $XCl_3$  ( $X=B$ , Al, and Ga) scattering at 20, 25, 30, and 40 eV. Study of the influence of the central atom.

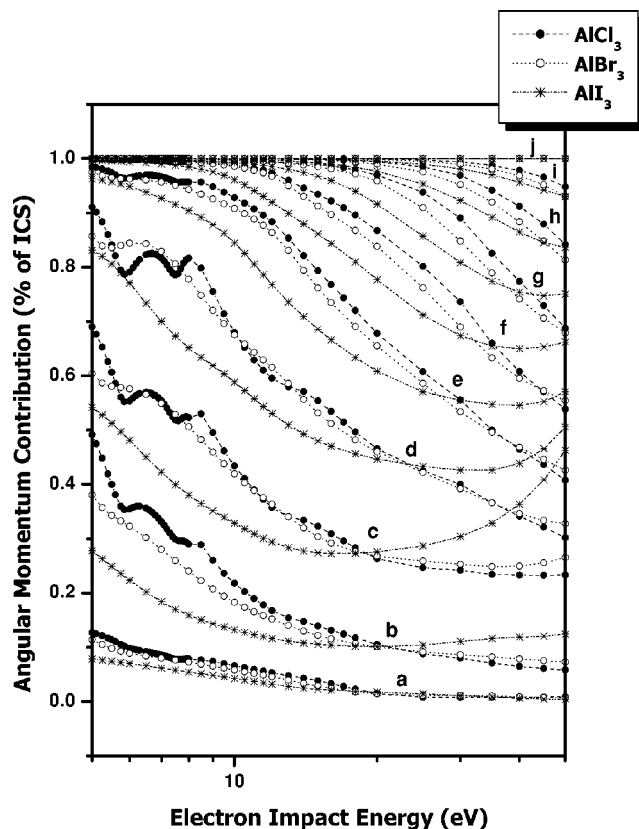


FIG. 7. Partial wave cross sections as a fraction of elastic integral cross section for  $e^-$ - $\text{AlY}_3$  [ $Y=\text{Cl}$  (full circle),  $\text{Br}$  (open circle), and  $\text{I}$  (star)] scattering from 5 to 40 eV. Study of the influence of the peripheral atom. Index a:  $L = 0$ , b:  $L = 0 + 1$ , c:  $L = 0 + 1 + 2$ , d:  $L = 0 + 1 + 2 + 3$ , e:  $L = 0 + 1 + 2 + 3 + 4$ , f:  $L = 0 + 1 + 2 + 3 + 4 + 5$ , g:  $L = 0 + 1 + 2 + 3 + 4 + 5 + 6$  and h:  $L = 0 + 1 + 2 + 3 + 4 + 5 + 6 + 7$ , i:  $L = 0 + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8$ , j:  $L = 0 + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9$ .

eral atoms in the molecule. Motivated by these results we have performed a study on partial wave contribution to the behavior of the aluminum trihalides cross sections.

The partial wave cross sections (PWCS) used in this analysis are obtained for collision processes of incoming electrons in a plane wave to outgoing electrons in a sum of partial waves ( $l'$ ,  $m'_l$ ) averaged in all molecular orientations. In order to analyze the angular momentum contribution to the calculated cross sections, we have defined the following fraction:

$$f^{(l)} = \frac{\sum_{l'=0}^l \sum_{m=-l'}^{l'} \int d\vec{k}_i |f^{LAB}(\vec{k}_i, l' m')|^2}{\sum_{l'=0}^9 \sum_{m=-l'}^{l'} \int d\vec{k}_i |f^{LAB}(\vec{k}_i, l' m')|^2}. \quad (14)$$

The denominator in these expression is calculated up to  $l'=9$  and it is converged in better than 5%, even for the higher energies and heavier molecules.

In Fig. 7 we show the partial wave contribution  $f^{(l)}$  for the cross sections of the aluminum trihalides at energies from 5 to 40 eV. At first we observe that at energies below 20 eV, aluminum triiodide presents higher partial wave coupling

than aluminum tribromide and this one, higher coupling than aluminum trichloride. That is, the highest partial wave with significant contribution increases with the size of the peripheral atom in the molecule. It is also known that low-angle scattering is highly influenced by high partial waves, which may cause the DCS magnitude to increase at this angular region as the peripheral atom in the molecule changes from Cl to I. This behavior is most prominent at energies of 5, 7.5, and 10 eV. Besides, another interesting characteristic is that the partial wave  $l=1$  seems to provide important contribution in the description of the resonance observed in the  $\text{AlCl}_3$  integral cross section.

For energies ranging 20–25 eV we notice that occurs a change in the ordering of the PWCS curves. That is, the hierarchy established by the size of the peripheral atom in the molecule it is no longer supported at high energies. The results also pointed that the contribution of partial waves with large angular momentum are not negligible, which indicates that in this energy range the convergence is not completely attained.

To get a better understanding of the interesting features discussed above, we have calculated the partial wave cross sections for each aluminum trihalide molecule separately (see Ref. 25). The low energy region for the  $\text{AlCl}_3$  molecule presents a large number of maxima and minima structures, indicating a high interference pattern. However the overall effect is apparently smoothed out as we sum all the angular momentum components together. At high energies, ranging from 20 to 40 eV, we have observed a meaningful contribution of the partial wave with angular momentum  $l=2$  to the PWCS behavior of the  $\text{AlI}_3$  molecule.

The results presented in this section show that, at the low energy range, the oscillatory pattern observed in the DCS is related to the electron scattering from heavier peripheral atoms (from Cl to I), which favors the coupling of high partial waves. That is, this type of undulation in the differential cross sections is a signature of the so called *halogenation effect* (confirming the previous halogenation and fluorination effects, respectively, observed by Natalense *et al.*<sup>32</sup> and Tanaka *et al.*<sup>33</sup>).

#### IV. CONCLUSIONS

In summary, we have presented the results of elastic calculations on electron- $\text{XY}_3$  scattering, where  $X=\text{B, Al, Ga}$ ;  $Y=\text{F, Cl, Br, I}$ . To our knowledge, this is the first calculation of elastic cross sections for all molecules belonging to aluminum and gallium trihalide families. From our preliminary results we may conclude that, in the low energy range (below 20 eV), the elastic scattering is mostly dominated by the halogen atoms, except for molecules containing fluorine. In other words, it was found that heavier peripheral atoms play a significant role as scattering centers. At higher energies these halogenation effects could not be identified.

The partial wave cross section results reinforce the features mentioned above and clearly display that the importance of the high angular momentum contribution increases with the raising in the size of the outer atom in the molecule.

In order to investigate the resonances which appears in the  $\text{XCl}_3$  ( $X=\text{B, Al, and Ga}$ ) integral cross sections, it re-



mains necessary to perform calculations including polarization effects (due to energetically closed channels). This is the next step towards a deeper comprehension on collisional processes involving the metal-trihalide molecules investigated in the present study.

Unfortunately, even more detailed comparisons could not be made since there are no available elastic cross sections in the literature. Nevertheless, we hope that our results serve as a base reference and motivation for future studies on electron-XY<sub>3</sub> scattering.

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