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Comparative study of elastic electron collisions on the isoelectronic SiN_2, SiCO, and CSiO radicals

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We report a theoretical study of elastic electron collisions on three isoelectronic free radicals, namely, SiNN, SiCO, and CSiO. More specifically, differential, integral, and momentum-transfer cross sections are calculated and reported in the (1–100) eV energy range. Calculations are performed at the static-exchange-polarization-absorption level of approximation. A combination of the iterative Schwinger variational method and the distorted-wave approximation is used to solve the scattering equations. Our study reveals that the calculated cross sections for the e^--SiNN and e^--SiCO collisions are very similar even at incident energies as low as 3 eV. Strong isomeric effects are also observed in the calculated cross sections for e^--CSiO and e^--SiCO collisions, particularly at incident energies below 20 eV. It is believed that the position of the silicon atom being at the center or extremity of the molecules may exert important influence on the calculated cross sections.

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I. INTRODUCTION

Silicon is one of the most abundant elements on Earth. Recently, there is an increasing interest in it and also in chemical compounds containing this element, due to their numerous applications in technology, for instance, in microelectronic and semiconductor industries. Particularly, silicon nitrides form one of the most important series of such compounds. Silicon nitrides, with a general formula Si_nN_m, play an important role in many fields of applications. For instance, SiN thin films are used as passivation layer to protect semiconductor devices [1,2] due to the important properties of this material, such as high dielectric constant, high breakdown voltage, low current leakage. Films of SiN are also used as insulate layers to fabricate metal-nitride-oxide-silicon devices [3,4] and as a gate dielectric layer in thin-film transistors [4,5]. In addition, Si_3N_4 and some silicon-nitride-oxide compounds have been suggested for interesting applications, such as ultra thin high dielectric materials which would possibly replace SiO_2 in field effect transistors reducing the gate lengths [6]. Moreover, Si_3N_4 is suggested to be used as a potential ultra hard material, due to its similarity to the hardest known material so far: C_3N_4 [7].

The thin films of silicon nitrides can be prepared by chemical vapor deposition (CVD), in particular, the plasma CVD is the mainly used [1,2,4,5,8]. This method has the advantage of lowering down the temperature of substrate to about 300 °C, much lower than that of the thermal CVD method (>600 °C). During the procedure of plasma CVD, the reactive environment is composed of many species such as electrons, molecules (in their ground and excited states), neutral radicals, ionic fragments, etc. The knowledge of cross sections for electron interaction with these constituents is important in determining the plasma properties and therefore is useful for plasma modeling. Nevertheless, experimental determination of cross sections for electron interaction with highly reactive species, such as radicals, is difficult. Therefore, theoretical calculations of various cross sections would contribute to fulfill this lacuna. In particular, the study of electron interaction with an isoelectronic series composed of diazasilene (SiNN), silaketenylidene (SiCO), and 2-sylaketenylidene (CSiO) would be very interesting. This series of molecules may be present in the environment of plasma CVD devices and so, such studies may contribute for the understanding of plasma media. Another important point is the fact that the possible presence of the SiNN radical in the interstellar medium [9].

The first experimental investigation on SiNN and SiCO was performed by Lembke *et al.* [10] in 1977. In their studies, infrared and electron-spin resonance (ESR) spectra for these radicals trapped in Ar, Ne, and N_2 matrices at 4 K were reported. Other experimental investigations for radicals containing Si include that of van Zee *et al.* [11]. In that work, ESR spectra for the $C_2{}^{17}O$, $SiC^{17}O$, and ${}^{29}Si_2O$ species were reported and the hyperfine splitting constant for the SiCO radical was also determined. Moreover, during the last two decades, there is a very intense activity of theoretical investigations on the SiNN, SiCO, and CSiO isoelectronic series. Quantum chemical calculations of several properties including molecular geometries, electronic distributions, dipole moments, harmonic vibrational frequencies, and associated infrared intensities, etc., for these radicals were carried out at various levels of approximations [12–22]. The SiNN is the

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most interesting of the three, because quantum chemical calculations suggested until recently that two distinct isomers, a tightly bound and a loosely bound structures, compete for the ground state. Nevertheless, to our knowledge, there has no study for electron interaction with these radicals ever been reported in the literature.

In this work, we present a theoretical investigation on elastic electron scattering by SiNN, CSiO, and SiCO radicals. More specifically, differential (DCS), integral (ICS), and momentum transfer (MTCS) cross sections for elastic electron collisions on these targets are calculated and reported in the (1–100) eV energy range. Besides these molecules being isoelectronic, SiCO and CSiO are also isomers. Recently, there have been an increasing interest on both theoretical and experimental studies of so-called isomeric effects in electron-molecule interactions [23–29]. Most of studies were performed on organic molecules, except that of Michelin *et al.* [29]. In the latter, electron scattering by the four isomeric CCNN, CNCN, NCCN, and CNNC inorganic molecules has revealed some interesting aspects. Strong isomeric effects are seen in both DCS and ICS in the low incident energy range. Thus the present study on the CSiO and SiCO isomers may contribute to understand the physical origins of the isomeric effects in small inorganic molecules. In this study, static-exchange-polarization-absorption (SEPA) potential is used to represent the electron-radical interaction, whereas the iterative Schwinger variational method (ISVM) is used to solve the Lippmann-Schwinger scattering equations [30,31].

The organization of the present article is as follows. In Sec. II, an outline of the theory used is presented, providing also some details of the calculations. In Sec. III we present our calculated data and a summary of conclusions.

II. THEORY AND CALCULATION

The details of the basic theory used in this work has already been presented elsewhere [30,31] and, therefore, they will only be briefly outlined.

The Schrödinger equation for the scattering electron, in atomic units, is given by

$$\left(\frac{1}{2}\nabla^2 + V_{\mathrm{opt}}(\vec{r}) - \frac{1}{2}k^2\right)\Psi(\vec{r},\vec{k}) = 0. \qquad (1)$$

Here, the dynamics of electron-molecule interaction is represented by a complex optical potential, given as

$$V_{\mathrm{opt}}(\vec{r}) = V_{\mathrm{SEP}}(\vec{r}) + iV_{ab}(\vec{r}), \qquad (2)$$

where V_{SEP} is the real part of the interaction potential composed of the static (V_{st}), the exchange (V_{ex}), and the correlation-polarization (V_{cp}) contributions, whereas V_{ab} is the absorption potential. In our calculation, V_{st} and V_{ex} are derived exactly from a restricted open shell Hartree-Fock self-consistent-field (ROHF-SCF) target wave function. A parameter-free model potential introduced by Padial and Norcross [32] is used to account for the correlation-polarization contributions. In this model, a short-range correlation potential between the scattering and target electrons is defined in an inner interaction region and a long-range polarization potential in an outer region. The first crossing of the correlation and polarization potential curves defines the inner and outer regions. The correlation potential is calculated by a free-electron-gas model derived using the target electronic density according to Eq. (9) of Padial and Norcross [32]. In addition, an asymptotic form of the polarization potential is used for the long-range electron-target interactions. The dipole polarizabilities (α_0 and α_2) are needed to generate the asymptotic form of V_{cp}. No cutoff or other adjusted parameters are needed in the calculation of V_{cp}.

Although the main features of the absorption effects are known, taking these effects into account in an *ab initio* treatment of electron-molecule scattering is very difficult. For instance, close-coupling calculations would require all discrete and continuum open channels to be included in the open-channel P space, which is computationally unfeasible. In view of these difficulties, the use of the model absorption potential seems to be presently the only practical manner to account for absorption effects in electron-molecule scattering calculations. In this work, a modified version of the quasifree scattering model version 3 of Staszewska *et al.* [33] is used to represent the absorption effects. The generation of such absorption potentials requires some molecular parameters as ionization potential (IP) and average excitation energy (Δ).

Since the SiN_2, SiCO, and CSiO are open-shell molecules with the ground-state configuration $X\,^3\Sigma^-$, the coupling between the incident and the target electrons leads to two spin-specific scattering channels, namely, the doublet ($S=1/2$) and quartet ($S=3/2$) couplings. The main difference between doublet and quartet scattering channels would reflect on the treatment of the electron-exchange terms in the potential operator. On the other hand, contributions such as V_{st}, V_{cp}, and V_{ab} are calculated in the present study using the target electronic density and some molecular properties such as ionization potential, dipole polarizability, etc. Thus, they are not explicitly dependent on the spin couplings.

In principle, the spin-specific scattering equations for elastic electron-molecule collisions should be solved with the full complex optical potential. Nevertheless, a tremendous computational effort would be required, particularly due to the large number of coupled equations involved, which makes such calculations practically prohibitive. On the other hand, our calculation has revealed that the magnitude of the imaginary part (absorption) of the optical potential is considerably smaller than its real counterpart. Therefore, it can be treated as a perturbation. In our work, the distorted-wave approximation (DWA) [34–36] is used to treat this interaction. Accordingly, the absorption part of T-matrix calculated via DWA is given as

$$T_{\mathrm{abs}} = i\langle \chi_f^- | V_{ab} | \chi_i^+ \rangle, \qquad (3)$$

where χ's represent the continuum wave functions which are the solutions of the Lippmann-Schwinger equation with the real part of the optical potential (V_{SEP}). In the ISVM calculations, the continuum wave functions are single-center expanded as

TABLE I. Calculated properties of SiNN, SiCO, and CSiO for the ground state configuration, $X\,^3\Sigma^-$. Except as noted, the energies, geometries, and dipole moments were calculated using the ROHF-SCF method, the dipole polarizabilities using the CISD method, and the IP using the CIS method.

	SiNN (tight)	SiNN (loose)	SiCO	CSiO
Energy (Hartree)	−397.8045	−397.8373	−401.6498	−401.5380
	−398.3158[a]	−397.8270[c]	−401.6401[c]	−401.5375[d]
	−398.2485[b]			
Internuclear distances (bohr)	$r_{\mathrm{SiN}}=\ldots$	$r_{\mathrm{SiN}}=6.404$	$r_{\mathrm{SiC}}=3.517$	$r_{\mathrm{CSi}}=3.454$
	2.238[a]	6.321[c]	3.530[c]	3.453[d]
	$r_{\mathrm{NN}}=\ldots$	$r_{\mathrm{NN}}=2.015$	$r_{\mathrm{CO}}=2.110$	$r_{\mathrm{SiO}}=2.789$
	2.145[a]	2.013[c]	2.107[c]	2.717[d]
Dipole moment (D)	0.715	0.286	0.058	0.653
	0.407[b]	0.310[c]	0.320[c]	0.613[d]
α_0 (a.u.)	59.024	50.520	53.262	41.062
α_2 (a.u.)	37.553	2.335	20.124	18.866
IP (eV)	7.86	7.793	8.27	10.48
			8.17[e]	

[a] Reference [17], at the CCSD(T) level.

[b] Our calculated results at the CISD level of approximation.

[c] Reference [12].

[d] Reference [21].

[e] Reference [22], at the CASSCF-MP2 level.

$$\chi^{\pm,S}_{\vec{k}}(\vec{r}) = (2/\pi)^{1/2}\sum_{lm}\frac{(i)^l}{k}\chi^{\pm,S}_{klm}(\vec{r})Y_{lm}(\hat{k}), \tag{4}$$

where the superscripts (−) and (+) denote the incoming- and outgoing-wave boundary conditions, respectively, and $Y_{lm}(\hat{k})$ are the usual spherical harmonics.

Moreover, the spin-specific, rotationally unresolved DCS for elastic e^--radical scattering are calculated via a summation of all rotationally resolved DCS

$$\left(\frac{d\sigma}{d\Omega}\right)^S = \sum_{j=0}\left(\frac{d\sigma}{d\Omega}\right)^S(j \leftarrow j_0), \tag{5}$$

where $(d\sigma/d\Omega)^S(j \leftarrow j_0)$ is the spin-specific DCS for the rotational excitation from an initial level j_0 to a final level j, calculated within the adiabatic-nuclei-rotation (ANR) framework.

Finally, the spin-averaged scattering DCS are given as

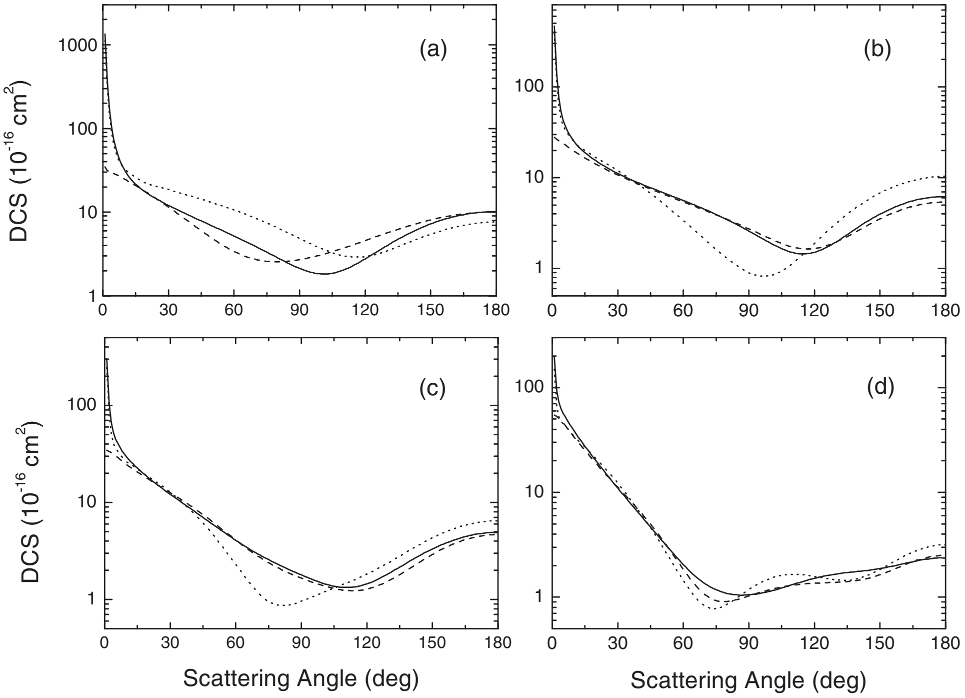

FIG. 1. Spin-averaged and rotationally summed DCS calculated for elastic electron collisions on radicals at (a) 1 eV, (b) 3 eV, (c) 5 eV, and (d) 10 eV. Solid line, results for e^--SiNN (tightly bound) interaction; dashed line, results for e^--SiCO interaction; and, short-dashed line, results for e^--CSiO interaction.

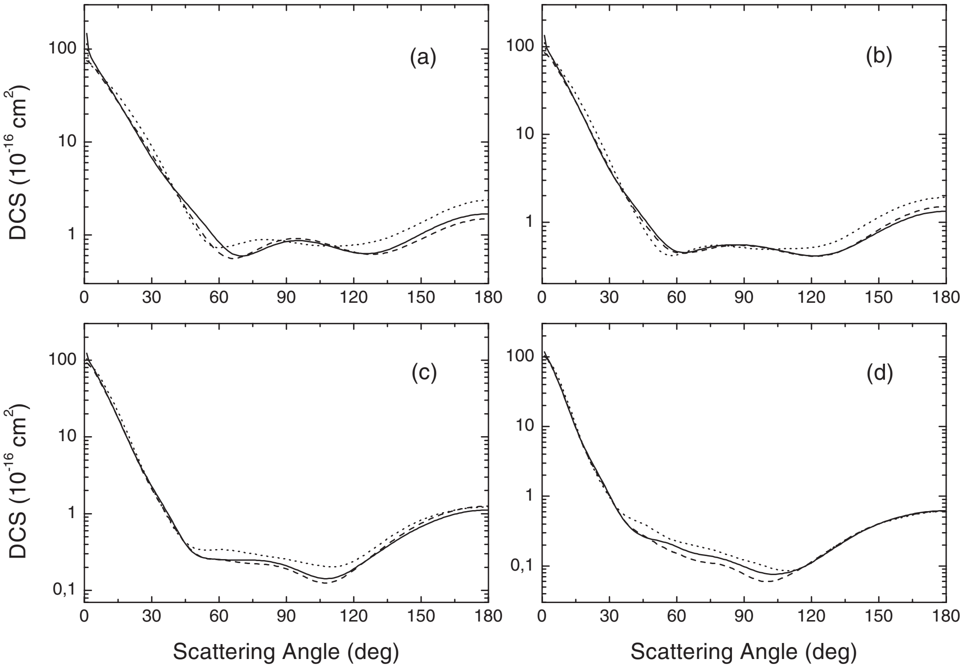

FIG. 2. Same as Fig. 1 except at (a) 20 eV, (b) 30 eV, (c) 50 eV, and (d) 100 eV.

$$\frac{d\sigma}{d\Omega}=\frac{1}{6}\left[2\left(\frac{d\sigma}{d\Omega}\right)^{1/2}+4\left(\frac{d\sigma}{d\Omega}\right)^{3/2}\right], \qquad (6)$$

where $(d\sigma/d\Omega)^{1/2}$ and $(d\sigma/d\Omega)^{3/2}$ are the spin-specific DCS for the total (e^{-}+target) spin $S=1/2$ (doublet) and $S=3/2$ (quartet) couplings, respectively. In Eq. (6), the numerical factors 2/6 and 4/6 are the corresponding statistical weights for the doublet and quartet couplings.

All matrix elements appearing in these calculations are computed using a single-center expansion technique with radial integral evaluated using a Simpson quadrature. The contributions from the direct and exchange parts of the interaction potential are truncated at $l=80$ and $l=50$, respectively. In the ISVM calculation, the partial-wave expansion of the scattering wave functions is limited to $l_{\max}=50$ and $m_{\max}=16$. A Born-closure procedure is used to account for the contribution of higher partial-wave dipole components to scattering amplitudes [31].

In the present study, standard triple-zeta-valence basis sets of Dunning [37], augmented by one s ($\alpha=0.0438$), one p ($\alpha=0.0438$), and three d ($\alpha=2.88,0.72,0.18$) uncontracted functions for carbon; one s and one p with the same exponent ($\alpha=0.0639$) and three d ($\alpha=3.92,0.98,0.245$) for nitrogen; one s ($\alpha=0.0845$), one p ($\alpha=0.0845$), and three d ($\alpha=5.12,1.28,0.32$) for oxygen; and one s ($\alpha=0.0331$), one p ($\alpha=0.0331$), and three d ($\alpha=1.552,0.388,0.097$) for silicon, are used for the calculation of the SCF wave function of the targets. All the radicals are linear on their ground-state configurations. The equilibrium geometries of SiCO and CSiO were optimized with ROHF-SCF calculations. For SiNN, the geometry optimization was also carried out at the ROHF level of approximation. Nevertheless, we found that the ROHF calculations were unable to provide tightly bound structure, but only the loosely bound structure, for this radical. Since it is expected that the tightly bound structure would be more stable than the loosely bound structure, and so, its interaction with electrons would be more interesting. Although the wave function of this radical at the tightly bound geometry can be obtained using more elaborated quantum chemistry methods such as CCSD, etc., the use of such complex target wave functions for electron-radical collisional investigation is, so far, computationally unfeasible in our group. In order to overcome the difficulties, we calculated the wave function of SiNN at the ROHF level using the tightly bound geometry optimized by Ornellas *et al.* [17] at the CCSD(T) level. In fact, it is quite often in theoretical studies of electron-molecule collisions, the use of experimental geometry to generate target wave functions. In the case of SiNN, the lack of experimental data made us to use the geometry optimized at the CCSD(T) level.

The electronic structures and the molecular properties were calculated using the GAMESS computational package [38]. The results of some calculated properties are summarized in Table I, where the results of deKock *et al.* [12], Petraco *et al.* [21], Ornellas *et al.* [17], and Bu and Han [22] are also shown for comparison. For SiNN in its tightly bound structure, a calculation at the CISD level of approximation using the geometry reported by Ornellas *et al.* [17] was also carried out. The calculated results are also shown in Table I. It is seen a significant difference between the calculated dipole moment for SiNN at the geometry given by Ornellas *et al.*, obtained by the ROHF (0.715 D) or by CISD (0.407 D). This discrepancy is somehow expected because the different levels of approximation were used in the calculations. However, it is quite surprising the discrepancy seen between our calculated dipole moment (0.058 D) and that of deKock *et al.* [12] (0.32 D) for SiCO, since both calculations were performed at the HF level of approximation. Therefore, this difference maybe caused by the different basis set used in the calculation. We noticed that the basis set used by deKock *et al.* has less polarization and diffuse functions than ours. In

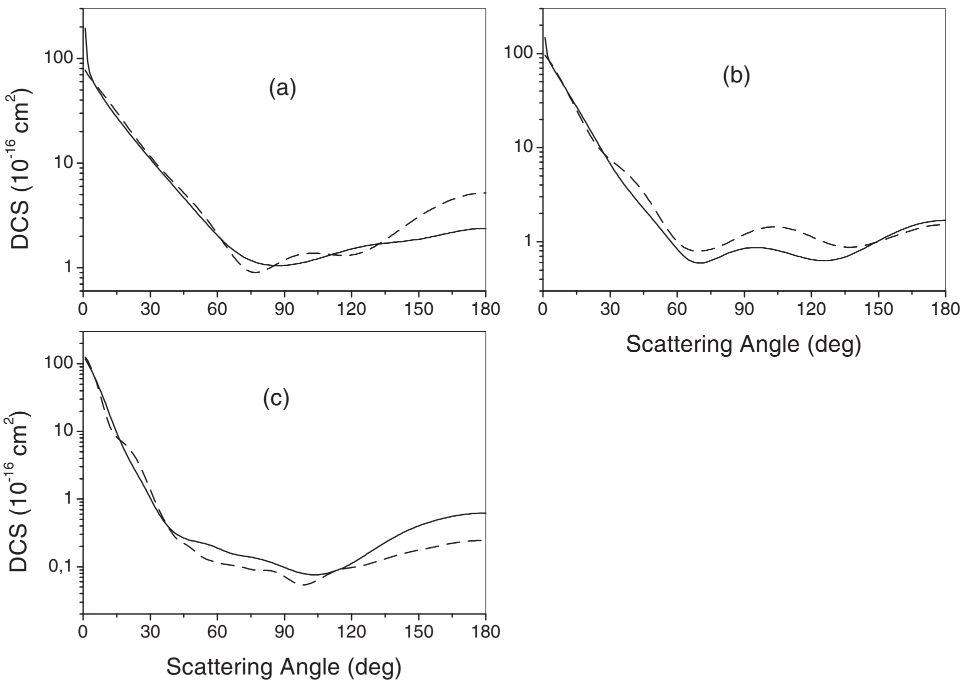

FIG. 3. Isomeric effects in the DCS calculated for elastic electron collision on SiNN radical at (a) 10 eV, (b) 20 eV, and (c) 100 eV. Solid line, results for the tightly bound isomer; dashed line, results for the loosely bound structure.

order to verify the physical origin of this discrepancy, some additional test runs were carried out. First, we repeated the calculation of deKock *et al.*, by using their basis functions and molecular geometry, we reproduced their reported dipole moment. Next, we added to their basis set, the same set of polarization and diffuse functions used in our calculation, and then the calculated dipole moment is 0.064 D, much closer to our calculated value. Since there are no experimental or theoretical values of ionization potentials and dipole polarizabilities for the SiNN, SiCO, and CSiO molecules reported in the literature, except the IP for the SiCO radical [22], they were calculated in this work. The dipole polarizabilities were calculated at the CISD level of approximation, whereas ionization potentials were calculated at the CIS level. The calculated results are also shown in Table I. Our calculated IP for the SiCO radical is 8.27 eV, in good agreement with the value of 8.17 eV predicted by Bu and Han [22] using the CASSCF-MP2 approach. On the other hand, although the dipole moments for SiNN, calculated at the ROHF level of approximation, differ significantly from those obtained at the CISD level, both at the geometry optimized by Ornellas *et al.* [17], we expect that this difference will not

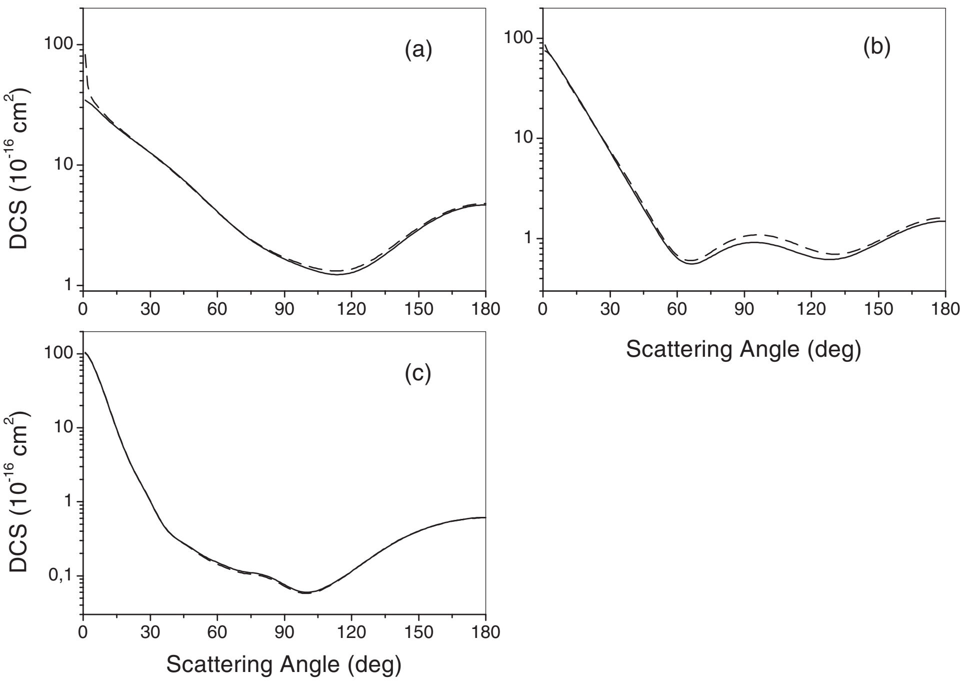

FIG. 4. Influence of the basis functions used in the calculated spin-averaged and rotationally summed DCS calculated for elastic electron collisions on SiCO radical at (a) 5 eV, (b) 20 eV, and (c) 100 eV. Solid line, calculated results using our basis functions; dashed line, results calculated using the basis set of deKock *et al.* [12].

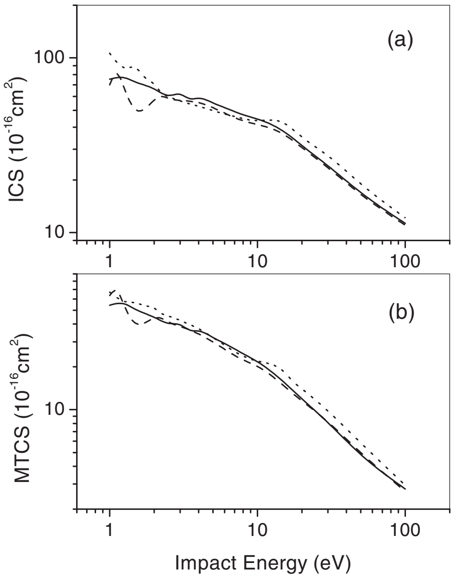

FIG. 5. (a) ICS and (b) MTCS for elastic electron collisions on radicals. The symbols used are the same as in Fig. 1.

affect significantly the calculated DCS, except at very small scattering angles.

III. RESULTS AND DISCUSSION

In Figs. 1 and 2 we present the spin-averaged and rotationally summed DCS calculated using the SEPA potential for elastic electron scattering by the isoelectronic targets SiNN (tightly bound), SiCO and CSiO in the (1–100) eV energy range. Qualitatively, it is seen that there is a strong enhancement in the calculated DCS for SiNN and CSiO near the forward direction in contrast to the DCS for SiCO. This enhancement is due to the larger dipole moments of SiNN (μ=0.715 D) and CSiO (μ=0.653 D) than that of SiCO (μ=0.058 D). Nevertheless, the influence of the dipole interaction becomes less important with increasing incident energies. As shown in Fig. 2, the DCS at small angles for the three targets are almost identical for energies equal to 20 eV or above. Another interesting aspect is the occurrence of strong isomeric effects between the calculated DCS of SiCO and CSiO, clearly seen in Figs. 1 and 2. These effects are more pronounced at low incident energies. But even at incident energies as high as 100 eV, differences in the DCS of the two isomers are apparent. Due to the dissimilar geometrical arrangement of their constituent atoms and therefore different electronic distribution of the outer valence orbitals, isomers may exhibit distinct permanent and/or induced dipole moments. Specifically for the two radicals studied herein, SiCO is very weakly polar whereas CSiO is moderately polar. Although such diversities can certainly contribute partially to the so-called isomeric effects at the small scattering angles, they cannot explain the differences shown at intermediate and large angles. It is known that at relatively low incident energies, the interaction between the incident electron and outer-valence-shell electrons of the target contributes significantly to the collisional dynamics. Since Si atom is much heavier than C and O, positioning the silicon atom at the center or at extremities of the molecule would affect substantially the distribution of the valence-orbital charge densities. Some valence orbitals of SiCO and CSiO are shown in Fig. 1 of Ref. [22]. From that figure, it is clearly shown that the electronic density distribution of the valence orbitals of SiCO, particularly that of the 3σ orbital, is significantly different from those of corresponding orbitals of CSiO. This fact may be the physical origin of the strong

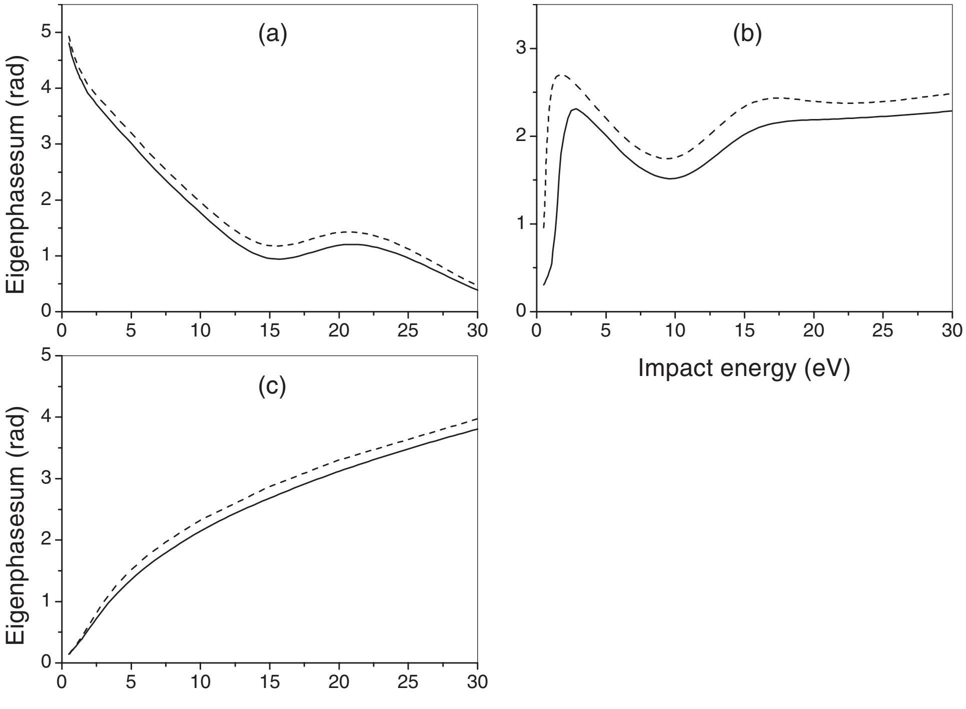

FIG. 6. Eigenphase sum analyses for the partial (a) $k\sigma$, (b) $k\pi$, and (c) $k\delta$ scattering channels for elastic electron collisions on CSiO. Solid line: Results obtained for the doublet spin coupling Dashed line: Results obtained for the quartet spin coupling.

isomeric effects exhibited in the DCS at intermediate and large angles. On the other hand, the calculated DCS for the isoelectronic molecules SiNN and SiCO are very similar even at energies as low as 3 eV, except at scattering angles near the forward direction. This fact may indicate the similarity of the charge distribution of the valence electrons of these targets, since the silicon atom is positioned at the extremity of both molecules. Moreover, the discrepancy seen in the DCS near the forward direction is due to the different dipolar nature of the targets.

At incident energies equal to or above 20 eV, shown in Figs. 2(a)–2(d), the DCS for elastic electron scattering by the three targets are remarkably similar with each other. It is probably due to the fact that electrons with increasing kinetic energies have more penetration power into the electronic clouds of the targets. Therefore, the interaction with inner-valence-shell electrons also becomes relevant. Consequently, the influence of the position of Si in the radicals becomes less important.

It would also be interesting to verify if the isomeric effects are demonstrated in the scattering cross sections for electron collisions with SiNN of different geometries. In Fig. 3, we compare the calculated DCS for the tightly bound and loosely bound structures of SiNN at incident energies of 10, 20, and 100 eV. It is seen that the magnitude of the DCS calculated from the two different geometries are rather similar. Nevertheless, the DCS obtained from the loosely bound structure present more oscillations, particularly at 100 eV, probably reflecting the large Si-N bond distance.

In Table I, it is verified that the dipole moment calculated for SiCO at the HF level of approximation is strongly influenced by the basis set used in the calculation, particularly, by the use of polarization and diffuse functions. Therefore, it would also to interesting to investigate the influence of the basis set on the calculated DCS. In Fig. 4, we compare the present DCS for electron scattering by SiCO with those calculated using the potential generated from the SCF wave functions obtained with the original basis set of deKock *et al.* [12] at 5, 20, and 100 eV incident energies. It is seen that in general there is a good agreement between the two set of DCS, particularly at 100 eV the difference between the calculated DCS is almost imperceptive. Nevertheless, the DCS obtained using their basis set is more forward peaked, reflecting the larger dipole moment of the target.

Figure 5 presents a comparison of the spin-averaged ICS and MTCS, calculated at the SEPA level of approximation for elastic electron scattering by the isoelectronic SiNN (tightly bound), SiCO, and CSiO targets in the (1–100) eV energy range. On qualitative aspects, one broad shoulder is seen at incident energy around 15 eV in the calculated ICS and MTCS for e^--CSiO collision, indicating a possible existence of a resonance. Besides, one additional resonance at about 1.6 eV in the ICS for e^--CSiO and two additional resonance features centered at about 1 and 2 eV, respectively, in the calculated cross sections for e^--SiCO collisions are seen. In order to clarify the physical origin of these resonancelike structures, in Figs. 6 and 7 we present eigenphase analyses for electron scattering by CSiO and SiCO, respectively. The three most important scattering channels, namely $k\sigma$, $k\pi$, and $k\delta$, are included in these analyses. It is verified that the resonance seen at about 1.6 eV in the ICS for e^--CSiO collisions is due to a combination of the contributions of both $k^2\Pi$ and $k^4\Pi$ scattering channels [see Fig. 6(b)]. Moreover, the shoulder shown at about 15 eV is also due to a combination of the occurrence of shape resonances at the $k\sigma$ (at around 17 eV) and $k\pi$ (at about 13 eV) channels for both the doublet and quartet couplings, as shown in Figs. 6(a) and 6(b). For e^--SiCO collisions, the feature at about 1 eV in the ICS and MTCS is identified as mainly due to the $k\pi$ channel at the quartet coupling, and that at about 2 eV is due to the $k\pi$

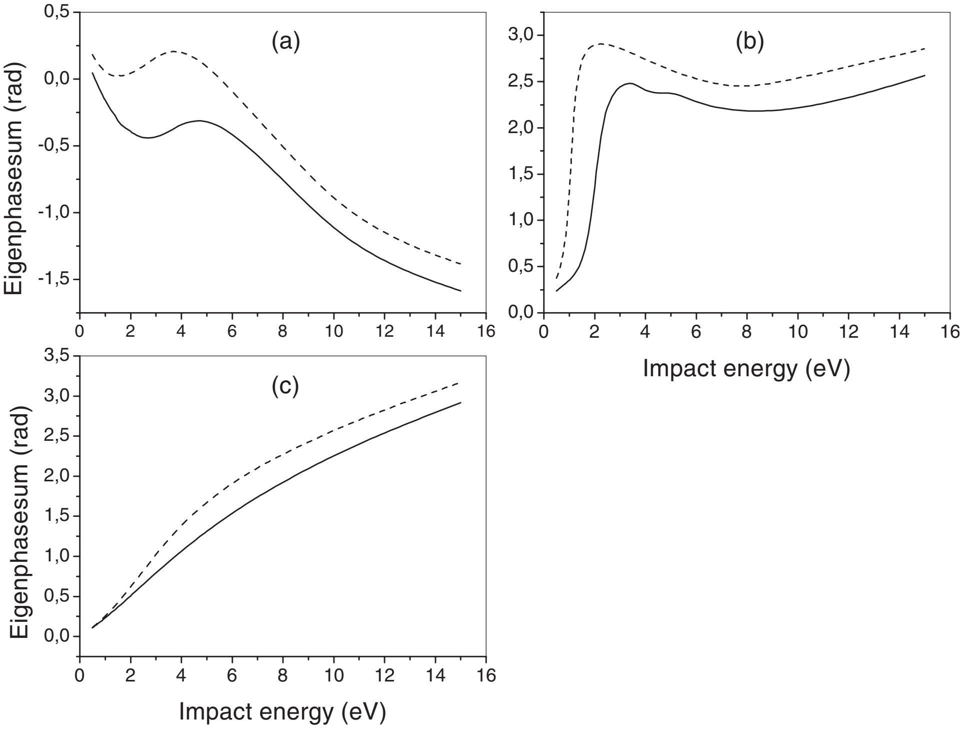

FIG. 7. Eigenphase sum analyses for the partial (a) $k\sigma$, (b) $k\pi$, and (c) $k\delta$ scattering channels for elastic electron collisions on SiCO. The symbols used are the same as in Fig. 6.

channel at the doublet coupling, shown in Fig. 7(b). On the other hand, although the eigenphase-sum analyses shown in Fig. 7(a) also indicate the occurrence of a weak shape resonance in the $k^2\Sigma$ (at about 3 eV) and $k^4\Sigma$ (at about 2 eV) scattering channels, their presence is not evident in the calculated cross sections.

Quantitatively, there is a good agreement between the calculated results for SiNN and SiCO for incident energies above 2 eV. It is interesting to note that the isomeric effect is again observed in the calculated ICS and MTCS for SiCO and CSiO. In general, the calculated cross sections for e^--CSiO collisions are larger than those for e^--SiCO interactions, except in a limited energy range between 2 to 10 eV.

In summary, the elastic electron scattering by isoelectronic SiNN, SiCO, and CSiO radicals has revealed some interesting aspects. Firstly, isomeric effects are clearly observed in both DCS and ICS for electron collisions on SiCO and CSiO radicals, particularly at the lower end of incident energies. The isomeric effects is also seen in the calculated DCS for electron collisions with tightly bound and loosely bound structures of SiN_2. Moreover, it seems that Si being the central or peripheric atom in the molecule has significant influence in the calculated cross sections. Moreover, the general good agreement between the calculated cross sections for e^--SiNN (tightly bound) and SiCO collisions seems to indicate the similarity of the charge distribution of the outer-valence orbitals of the two isoelectronic species. The discrepancies seen in the DCS near the forward direction at incident energies below 20 eV are due to the different dipole moments of the two targets.

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