

CHARACTERIZING SCATTERING IONIZATION PATHWAYS IN CHEMICAL MOLECULES THROUGH ELECTRON INTERACTION STUDIES

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Abstract

Using a new semiclassical method described in recent literature, this work explores the complex dynamics of scattering ionization routes in $\text{Ne}^(3P2,0)\text{-Ng}$ ($\text{Ng} = \text{Ar}, \text{Kr}, \text{Xe}$) systems. With the primary goal of clarifying the function of electron-molecule interactions, the study offers a thorough examination of experimental data, such as ionization cross sections and Penning ionization electron spectra (PIES), in order to identify underlying processes. Two basic microscopic reaction pathways are identified by the analysis: an indirect mechanism that is primarily controlled by noncovalent forces like dispersion and induction-polarization contributions at larger separations, and a direct mechanism that is driven by efficient charge transfer between reagents at short separation distances. The work provides insights into the development of reaction transition states by highlighting the crucial effects of collision energy, separation distance, and relative alignment of valence orbitals on reaction kinetics. Interestingly, ionization cross section energy dependency in Ne^* -molecule systems displays a variety of tendencies that are indicative of the distinct electronic structures of the molecules involved. Molecular characteristics, such as σ -holes and quadrupole moments, become important factors influencing the kinetics of interactions. With implications for atmospheric chemistry, materials science, and basic chemical kinetics, the discoveries advance our knowledge of chemical processes that are sparked by electron interactions. This work provides a framework for further investigation into scattering ionization routes and theoretical model improvement in the clarification of intricate chemical processes.*

Keywords: Scattering Ionization, Electron Interaction Studies, Chemical Molecules, Ionization Pathways, Semiclassical Treatment.

1. INTRODUCTION

Deciphering the underlying principles of ionization routes in chemical molecules is crucial to the advancement of several scientific areas as well as basic chemical processes. Important applications of ionization processes brought about by electron interactions may be found in atmospheric chemistry, materials science, and chemical kinetics. Electron interaction studies provide important insights into the molecular dynamics of chemical events by characterizing these scattering ionization routes.

Studies of electron interactions provide a potent way to look at the complex interactions that occur between electrons and molecules during collisions. These investigations combine experimental methods with theoretical models to provide contrasting views of the underlying chemistry and physics. With the use of complex experimental setups and cutting-edge theoretical models, scientists may investigate the dynamics of electron-molecule interactions with extreme resolution and accuracy.

Advances in semiclassical treatments in recent times have made it possible for scientists to study scattering ionization route dynamics in more detail. Through the use of advanced theoretical models and computer simulations, researchers can clarify the intricate mechanisms that underpin these phenomena. Branching ratios (BRs), total and partial ionization cross sections, and Penning ionization electron spectra (PIES) may all be thoroughly analyzed using this multidisciplinary method.

Because of their use in a variety of scientific situations, certain chemical systems, such $\text{Ne}^*(3\text{P}2,0)\text{-Ng}$ ($\text{Ng} = \text{Ar}, \text{Kr}, \text{Xe}$), are often the subject of research into scattering ionization routes. Researchers may learn essential things about electron-molecule interactions and how they play a part in starting chemical reactions by examining these systems. Furthermore, the examination of actual results serves as a foundation for creating theoretical frameworks that faithfully capture the phenomena that are seen.

Rationalizing experimental results and occurrences is a primary goal of characterization of scattering ionization routes. Scientists can clarify the variables affecting reaction kinetics, product distributions, and energy dependency by determining and examining the mechanisms driving ionization processes. This information is essential for expanding our understanding of chemical reactivity, creating effective analytical tools, and creating prediction models.

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February 2024

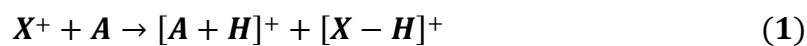
In this work, we use electron interaction studies to characterize scattering ionization processes in chemical compounds. We seek to shed light on the dynamics of electron-molecule interactions, clarify the fundamental principles guiding ionization processes, and advance our knowledge of molecular chemical reactions by applying a novel semiclassical treatment and examining experimental data. By using an interdisciplinary approach, we want to increase our understanding of basic chemical processes and how they affect other fields of science.

Scientific science research discoveries on atom and particle connections are straightforwardly utilized in the delicate ionization technique known as synthetic ionization(CI). Electron bombardment ionization (EI) was the first method of ionization. Dissecting the outcome created utilizing EI is trying because of its many pieces. CI began during the 1950s and has a great deal of commitment in scientific science, however it created generally couple of pieces.

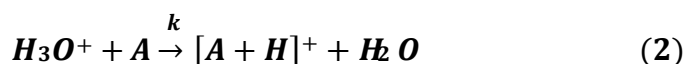
To make reagent particles in the CI cycle, electrons should initially attack the reagent gas. The reagent particles then ionize the example atoms by means of particle and sub-atomic response pathways. Throughout the entire existence of CI, the 1970s were viewed as a defining moment. Around that time, researchers sorted out some way to make CI capability in an air by fixing its imperfections in a vacuum. The variety of uses for corona discharge energy is substantially expanded by atmospheric chemical ionization, which does not need a vacuum environment. Currently, the mass spectrometry approach makes extensive use of CI.

2. THE PRINCIPLE OF CHEMICAL IONIZATION

The objective of CI is to ionize the analyte by responding the reagent particle X^+ with the analyte atom A:



The ionized response gas is the wellspring of X^+ in the process depicted previously. Smelling salts, water, isobutane, and methane are a couple of run of the mill reagent gases. You might get the equation's reaction time and rate consistent (k) by estimations or readings in the writing. For the situation where X^+ is a H_3O^+ reagent particle, equation (2) is:



Exploring Innovation Research Methodologies in a Variety of Multidisciplinary Fields and Their Prospective Future Impact

February 2024

A particle source creates reagent particles. Particle sources that are frequently utilized incorporate radiation sources, standard shine release power sources, and empty cathode release power sources. The two most incessant radiation sources are ^{210}Po and ^{241}Am . ^{210}Po and ^{241}Am delivery alpha particles, what start the ionization cycle. It might create reagent particles and electrons when it slams into the reagent gas because of its high energy. To make extra reagent particles and electronics, the delivered electrons might slam into the reagent gas in the event that their energy is sufficiently high. An empty cathode release powersource is in many cases used in the CI that involves H_3O^+ as a reagent particle and can create 99.5% of H_3O^+ .

2.1. Advantages and Disadvantages of CI

It is possible to determine the precise molecular weight of the analyte by simply resolving the CI spectrum. The analyte's molecules and ions make up the majority of the product produced by CI, which contains very few fragments. By choosing the right reagent ion, one may readily boost the selectivity of CI. For instance, only organic substances with a proton affinity larger than H_3O^+ would react with the reagent ion H_3O^+ . Furthermore, CI responds quickly (15 s) and with great sensitivity. However, mass spectrometry becomes challenging if the reactive ions are impure and many chemical ionization events happen simultaneously.

3. RESEARCH METHODOLOGY

We explored $\text{Ne}^*(3\text{P}_2,0)$ - Ng (Ng = Ar, Kr, Xe) frameworks utilizing a new semiclassical treatment that has been completely portrayed in late papers. The examination offered an inside steady legitimization of accessible exploratory outcomes, including Writing ionization electron spectra (PIES), aggregate and halfway ionization cross areas, and their stretching proportions (BRs). New understandings of the capability of revision and the rakish force coupling of valence electrons in chemical energy were gotten by the careful portrayal of the molecule ion response elements. These insights must be regarded as being of general importance for many other reactions. Specifically, the method's use indicates that:

- The optical potential model is described as a mix of a real and an imaginary portion. It was initially presented to explain the dynamics of nuclear processes and is also used to CHEMI. We have shown that, as they originate from the same interaction components, the two components—which regulate, respectively, the collision

Exploring Innovation Research Methodologies in a Variety of Multidisciplinary Fields and Their Prospective Future Impact

February 2024

dynamics and the "opacity" or likelihood of CHEMI—must be interdependent.

- Two competing microscopic response mechanisms are generated by the disparate balance of these components. Independently, they have been recognized as a backhanded system that starts from noncovalent powers, for example, scattering, enlistment polarization commitments, turn circle and outward Coriolis impacts, and an immediate instrument that is predominant at large separation distances of reagents driven by chemical powers. In particular, the immediate cycle is started by viable charge move (CT) impacts between reagents, which are improved by valence orbital cross-over. Ionization that likewise occurs because of a planned discharge retention of a "virtual" photon that is traded by reagents inside the feebly bound crash complex is made sense of by the roundabout interaction. Thusly, the roundabout system starts normal radiative (photograph)- ionization processes, while the immediate component coordinates the advancement of model rudimentary oxidation responses.
- The relative alignment of valence orbitals, separation distance R , and collision energy (E_{coll}) are crucial variables that impact the stability and structure of the adducts created when reagents collide, which in turn affects the reaction TS.
- Twelve reaction channels have been identified, each of which is impacted by a distinct relative role played by the two fundamental processes previously discussed. These channels are thought to represent certain transitions from a quantum state of reagents to that of products.

4. RESULTS AND DISCUSSION

4.1. General Trends

The notable examination of Beijerinck and partners demonstrates that the sub-atomic frameworks that produce CHEMI, which were all completely concentrated on tentatively in the gas stage under single crash conditions utilizing the sub-atomic shaft method, can be partitioned into two gatherings: those that show an unmistakable pattern toward a decline in cross segments and those that display an undeniable expansion in the all out ionization cross area as E_{coll} increments. An immediate and quantitative correlation of obtained discoveries is straightforward since the energy reliance of the complete ionization cross segment not entirely settled in that frame of mind in an inside predictable way for various frameworks utilizing Ne^+ . In Figure 1, a few prototype instances are provided.

Table 1: Collision Energy (meV)

	NH ₃	O ₂	Cl ₂	Co	N ₂	CH ₄	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆
10	70	40	70	12	5	12	25	25	15
100	50	45	28	15	10	16	15	15	20
1000	45	20	18	20	20	19	16	15	25

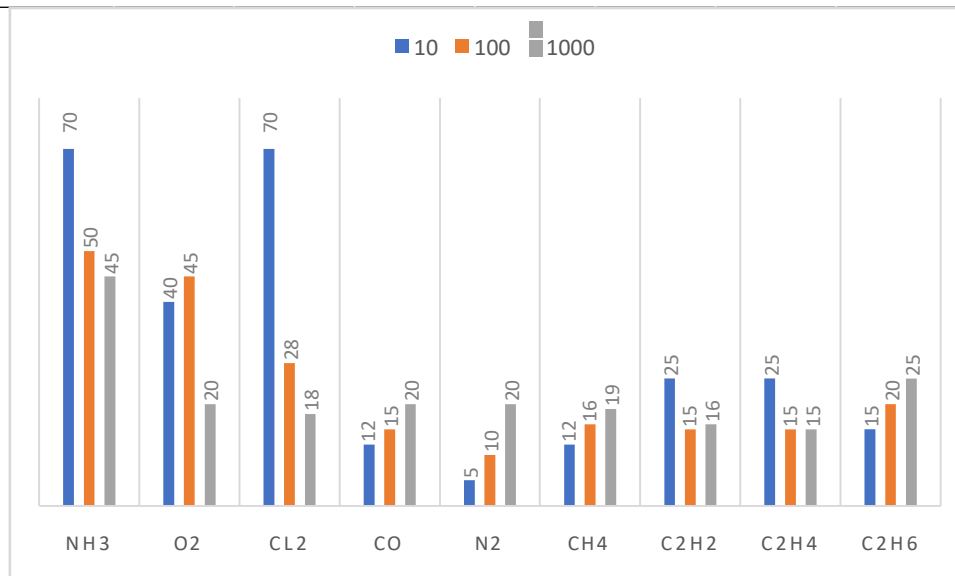


Figure 1: Collision Energy (meV)

Total ionization cross sections in relation to collision energy for some Ne*-molecule complexes. Third-degree polynomials of experimental data are interpolated by the curves in the following cases: (a) some inorganic compounds. (b) Saturated and unsaturated hydrocarbons in their most basic form.

The distinct behaviours shown by the different partners of the Ne* reagent is contingent upon their basic chemical and physical characteristics, as seen in Figure 2 for three instances of inorganic molecules. In the case of Ne*-Cl₂, when an effective ion pair is formed by harpooning, it is guessed that the limiting energy in the crash complex would ascend by something like two significant degrees contrasted with Ne*-N₂, leaning toward a nearer approach of reagents. By and by, here we likewise dissect exhaustively the Ne*-NH₃ framework, for which the intermolecular interaction is significantly anisotropic, shows a transitional strength between Ne*-Cl₂ and Ne*-N₂, and has been as of late detailed in logical structure, notwithstanding the exceptional properties of Ne*-Cl₂.

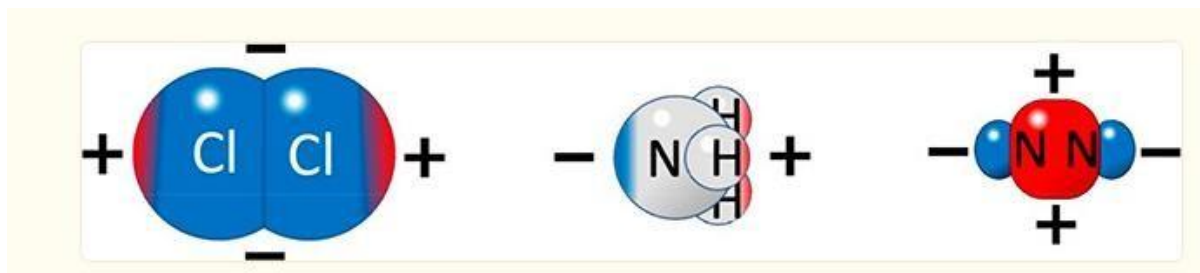


Figure 2: Fundamental features of Cl_2 , NH_3 , and N_2

Cl_2 , NH_3 , and N_2 molecules share basic characteristics related to varying electronic charge distribution along their molecular axis. There are two σ -holes in the chlorine molecule that are aligned with the bond axis. This explains why Cl_2 has a significant and positive quadrupole moment. There is a significant dipole moment in the ammonia molecule. The quadrupole moment of the nitrogen molecule is high and negative. The greater extent of the colour red roughly indicates an increase in positive charge density, whereas the colour blue similarly indicates an increase in negative charge density.

4.2. The $\text{Ne}^*\text{-Cl}_2$ Case

We first endeavor to defend the phenomenology noticed for the $\text{Ne}^*\text{-Cl}_2$ framework displayed in Figure 1a, fully intent on revealing insight into the basic job of the interaction parts that are supposed to specifically tweak the overall load of the two principal minuscule components demonstrated above as an element of impact energy. $\text{Ne}^*\text{-Cl}_2$ specifically is one of the frameworks showing the biggest cross-area esteem in the Ecoll warm reach. This way of behaving for the Cl_2 reagent should be connected with the electrical qualities of its design. Using the MRD-CI method, the interested reader may consult Peyer Imhoff and Buenker's probable bends for the ground and excited states of the chlorine atom, as well as its positive and negative particles. Specifically, this particle exhibits a σ -opening, a strong electron affinity (2.44 eV), and a large long-lasting electric quadrupole moment (+3.8 au). The positive electrostatic potential is restricted to the outer segments of the Cl bond.. A thorough examination of the σ -hole subject, using electron density plots of the ground electronic state of the Cl_2 molecule, is provided in ref (also refer to the references therein).

Even with lighter Ng atoms in their ground electronic state, the creation of the intermolecular halogen bond is in fact caused by these special properties of Cl_2 . As a result, the long-range intermolecular interaction field tends to polarize Ne^* 's "floppy" outer electronic cloud as it

approaches Cl_2 . The existence of the σ -hole in the collinear approach is what essentially initiates this electron transfer. The freshly formed Cl_2 -anion moves closer to its center along the interatomic $\text{Ne}\cdots\text{Cl}\cdots\text{Cl}$ division R, and the Coulomb attraction in the initial particle pair Ne^+-Cl_2 -suggests the capture of reagents, as seen schematically in Figure 3. Indeed, in Cl_2 -the extra electron in the external $3p_u^*$ antibonding orbital, which is part of the Cl bond's outer segment, entirely fills the σ -opening and significantly reduces the subatomic bond strength, rendering Cl_2 -an ecologically unsound animal group, particularly when exposed to Ne^+ .

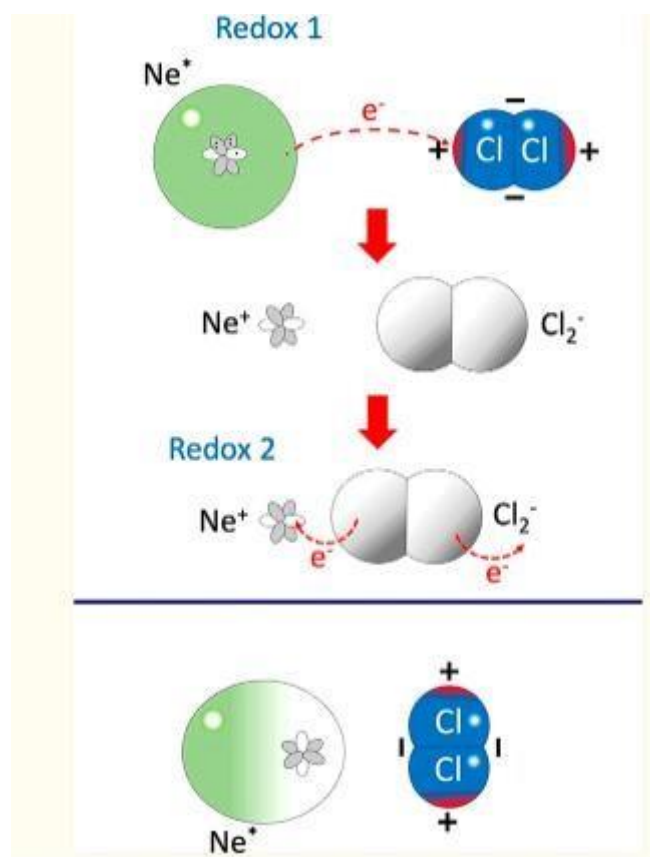


Figure 3: Microscopic Dynamics Schematic Diagram for the Ne^*-Cl_2 CHEMI Reaction

A schematic outline of the Ne^*-Cl_2 CHEMI response's minuscule elements. Redox 1 in the top board The Rydberg electron of Ne^* might fill the σ -opening of Cl_2 a good way off of around 6 \AA when collinear Cl_2 is available, prompting the making of Ne^+-Cl_2 -particle matches. The antibonding $3\sigma_u^*$ orbital contains the additional electron in Cl_2^- . Redox 2 on the centre panel Two electrons from the 3σ molecular orbitals may be involved in the ionization process at shorter distances. In this instance, the dissociative $\text{B}2\Sigma_g^+$ ion subsequently forms the Cl_2^+ ion. (bottom panel) The Ne^* atom is polarized in the event of a perpendicular approach, and the ionization may occur primarily at a short distance via an

Exploring Innovation Research Methodologies in a Variety of Multidisciplinary Fields and Their Prospective Future Impact February 2024

exchange (chemical-redox) process or at a wide distance via a radiative (physical photoionization) mechanism. The greater extent of the color red roughly represents the rise in positive charge density, whereas the color blue represents the equivalent shift in negative charge density.

Stronger attraction due to ion pair formation and Cl_2^- instability causes the highly excited NeCl^* adduct to form, which then autoionizes to produce $\text{Ne} + \text{Cl}^+ + e^-$ products. At a short R , the overlap between the populated 3σ molecular orbitals of Cl_2 and the half-filled orbital of Ne^+ initiates a further electronic rearrangement process, as seen in the center panel of Figure 3. In particular, this overlap generates enough energy to expel one of the two electrons that occupy the $3\sigma_g$ bonding molecular orbital of Cl_2 , together with a single electron transfer from the outer $3\sigma_u^*$ of Cl_2^- to the half-filled orbital of the Ne^+ core. Consequently, there is a tendency for the product Cl_2^+ to develop in the dissociative $\text{B}^2\Sigma_g^+$ state, where the bond order is 0.5. This unusual property of the chlorine molecule may be attributed to a chemical catalyst because electrons that populate both the $3\sigma_u^*$ and $3\sigma_g$ molecular orbitals are mostly contained in the σ hole region. On the other hand, a synchronization between the usual collision time and the amount of time needed by an interacting complex to produce an electronic rearrangement is necessary for the production of the fragment Cl^+ . As E_{coll} increases, this synchronization is both fully and partly loosened. Consequently, it is anticipated that Cl_2^+ production would rise with E_{coll} , which is in line with the experimental results obtained in our lab and by Kischlat and Morgner.

It is interesting to see that the chemical (direct) process predominates under these circumstances and that it follows these two fundamental steps: First, Cl_2 is reduced to Cl_2^- by CT, which results in a neon that acts as a reducing agent (Na, see Redox 1 in Figure 3). Besides, the Coulomb fascination supports the catching of the $\text{Ne}^+-\text{Cl}_2^-$ particle pair at nearer goes, where an organized CT including both inward $3\sigma_g$ and outside $3\sigma_u^*$ populated sub-atomic orbitals of Cl_2^- (where the external electron fills the p-orbital of the Ne and the other deepest electron is launched out) decides the oxidation to the last territory of Cl^+ . In the last option occasion, the Ne^+ oxidizes with similar qualities as a halogen ion (F).

The proficiency of this worldwide system, which is started by the Cl_2 with the sub-atomic pivot adjusted along R , does, be that as it may, decrease with expanding impact energy in light of the fact that the crash time abbreviates, the section through the going among

Exploring Innovation Research Methodologies in a Variety of Multidisciplinary Fields and Their Prospective Future Impact

February 2024

nonpartisan and ionic states assumes a less adiabatic personality, and arrangement impacts become more outlandish. In these conditions, the worldwide reactivity drops and impacts become genuinely doable for all overall directions of the two accomplices, including the Cl₂ particle's opposite way to deal with the Ne* molecule. Here, both backhanded (counting expected radiative impacts) and direct (chemical or trade) systems become cutthroat in the opposite arrangement of the shaped adduct, which is fairly shaky because of the absence of solid alluring parts. Most importantly, an electron expulsion from the external 3πu* atomic orbital becomes compelling, bringing about the single-step development of Cl₂⁺ in its ground electronic state, X²π_g. Comparable to Cl⁺, the creation probability of Cl₂⁺ is expanded by this clever channel.

Table 2: The Dependence of l_{\max} , Defining the Absolute Maximum of the Centrifugal Barrier, for the Two Selected Geometries for Each Collision Energy

$\theta = 90^\circ; \phi = 220^\circ$		$\theta = 15^\circ; \phi = 270^\circ$
$E_{\text{coll}} \text{ (meV)}$	l_{\max}	l_{\max}
0.1	10	10
0.3	15	15
1	23	23
3	34	34
10	52	37
30	78	44
100	114	55
300	140	110
1000	190	115

The acquired cross-segment values and their proportions show that just when E_{coll} is more noteworthy than the pivotal worth does the commitment from the most elevated b or values become recognizable. Subsequently, the outward hindrance's specific capability begins to decrease, and a particular scope of b or values empowers the response, making those values greater than b_{\max} or l_{\max} successful too since defining moments are distinguished at moderate and genuinely huge R .

5. CONCLUSION

Exploring Innovation Research Methodologies in a Variety of Multidisciplinary Fields and Their Prospective Future Impact

February 2024

The study on scattering ionization pathways in $\text{Ne}^*(3\text{P}_2,0)$ -Ng systems provide insights into chemical reactions initiated by electron-molecule interactions. The review uncovers the relationship of genuine and non-existent pieces of the optical likely model, which control crash elements and the likelihood of chemical ionization. Two cutthroat minute response instruments are recognized: an immediate system driven by compelling charge move and a roundabout component beginning from noncovalent powers. The reactivity of the frameworks relies upon impact energy, detachment distance, and valence orbital arrangement. Twelve response channels have been distinguished, each addressing explicit sections from the quantum condition of reagents to items. The findings have implications for atmospheric chemistry, materials science, and fundamental chemical kinetics.

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Exploring Innovation Research Methodologies in a Variety of
Multidisciplinary Fields and Their Prospective Future Impact
February 2024

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