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[Lecture]

Experimental and theoretical investigation of electron interaction with molecules

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Abstract: In response to escalating concerns regarding the environmental implications of anesthetic compounds on both global warming and ozone layer degradation, a rigorous investigation combining theoretical and experimental methodologies was conducted to elucidate the elastic electron scattering dynamics of halothane, sevoflurane, and isoflurane. These anesthetic gases, which are predominantly excreted into the atmosphere without degradation post-use, contribute to increasing concentrations of halogenated compounds that possess both elevated Global Warming Potentials (GWP) and significant Ozone Depletion Potentials (ODP). Our experimental methodology involved measuring elastic differential cross sections (DCS) using a crossed-beam apparatus, relative-flow method, with argon as a standard, to calibrate the absolute scale of the cross sections. Theoretical analyses were further executed

through the Independent Atom Model coupled with the Screening Corrected Additivity Rule (IAM-SCAR+I), accounting for interference effects.

Introduction

Halogenated anaesthetics, including sevoflurane ($C_4H_3F_7O$) (Vukalović et al., 2022a), isoflurane ($C_3H_2ClF_5O$) (Vukalović et al., 2024) and halothane ($C_2HBrClF_3$) (Maljković et al., 2023), are widely used in clinical settings for inhalational anaesthesia due to their effective anaesthetic properties (Robinson and Toledo, 2012). These compounds, however, are released into the atmosphere largely unchanged (Shiraishi and Ikeda, 1990; Gadani and Vyas, 2011), raising environmental concerns due to their significant global warming potential (GWP) and varying impacts on ozone depletion [Brown et al., 1989; Langbein et al., 1999; Sulbaek et al., 2012; Ryan and Nielsen, 2010). The molecular structures and halogen content play crucial roles in determining their atmospheric behaviour and interaction with other chemical species. Sevoflurane (Vukalović et al., 2022a), characterized by a relatively high molar mass and a dipole moment of 2.33 D, is preferred for its rapid induction and recovery and lower environmental impact compared to other halogenated anaesthetics. Isoflurane (Vukalović et al., 2024), with a molar mass of 184.5 g/mol and dipole moment of 2.47 D, exhibits moderate onset and recovery times. Halothane (Maljković et al., 2023), synthesized in 1954, has the highest ozone depletion potential among these anaesthetics due to its bromine content and a substantial GWP. Research into the electron scattering behaviour of these molecules is crucial for understanding their atmospheric lifetimes and reactivity. Elastic electron scattering cross sections provide insights into the physical interactions and potential fragmentation processes. This study presents experimental and theoretical cross sections for elastic

electron scattering from these three anaesthetics at 100 eV, contributing to the broader understanding of their environmental effects.

Methods and data

To derive differential and integral elastic scattering cross sections for the anesthetic molecules under study, the IAM-SCAR+I method was employed. This sophisticated approach synthesizes the Independent Atom Model (IAM) with the Screening Corrected Additivity Rule (SCAR) and incorporates interference effects (I). Detailed descriptions of this methodology are available in previous literature (Blanco et al., 2010; Fuss et al., 2013; Blanco et al., 2016; Traore Dubuis et al., 2017; Lozano et al., 2018); thus, only a concise summary is presented herein. Each molecular target, including sevoflurane ($C_4H_3F_7O$), isoflurane ($C_3H_2ClF_5O$), and halothane ($C_2HBrClF_3$), is represented as an ensemble of constituent atoms (C, H, F, O, Cl, and Br). For each atomic unit, an "ab initio" optical potential was derived as $(r) = VR(r) + iVabs(r)$, where the imaginary component accounts for inelastic processes, while the real component describes elastic scattering events. Molecular scattering cross sections were calculated by summing individual atomic amplitudes with phase corrections applied through SCAR, accommodating interference effects. For molecules with substantial dipole moments, such as isoflurane (2.47 D), rotational excitation effects were incorporated using the first-Born approximation, under the assumption of rigid rotor behavior. Corrections for large-angle scattering, based on Dickinson's approach (for details see (Sanz et al., 2012)) were applied to ensure rigorous representation of the scattering dynamics. Considering the experiment, elastic electron scattering measurements were conducted using a high-precision spectrometer, composed of an electron gun, gas inlet, energy analyzer, and detector, enclosed within a chamber shielded by two concentric μ-metal layers to minimize external magnetic interference

(Vukalović et al., 2022b). The electron gun directed a beam into the interaction region at an energy of 100 eV, achieved through careful adjustment of the potential difference between the filament and a grounded electrode. Anaesthetic gases (isoflurane, sevoflurane, and halothane) were introduced into the chamber via a gas needle connected to a handling system, raising the chamber's base pressure from $6 \cdot 10^{-7}$ mbar by approximately one order of magnitude. After gas-molecule interaction, scattered electrons were channeled into a two-stage cylindrical energy analyzer, allowing passage of elastically scattered electrons based on precisely calibrated potential differences. These electrons were subsequently focused by a three-electrode lens into a channeltron detector to measure scattering intensity. Measurements were recorded across a 25°–125° angular range with an energy resolution exceeding ±2°. Relative DCSs were normalized via the relative flow method (Srivastava et al., 1975), using argon as the reference. Absolute DCS values were determined through comparative measurement of electron intensities and flow rates for both the target gas and argon (Williams and Willis, 1975; Ranković et al., 2018) adjusting the gas flow behind the needle to achieve equivalent mean free paths (Olander and Kruger, 1970). This measurement cycle was repeated to ensure data consistency, with uncertainty assessments accounting for statistical variance, apparatus stability, and reference cross-section accuracy. The primary source of uncertainty (~20%) was associated with argon reference cross sections, particularly at small angles, where uncertainties were compounded by adjustments to the interaction volume.

Results and discussion

Absolute differential cross sections (DCSs) for elastic electron scattering from the anesthetic molecules halothane, isoflurane, and sevoflurane were measured and presented Figure 1. as a function of scattering angle. These measurements were conducted at an incident electron energy of 100 eV over an angular range of 25° to 125°, with

5-degree increments, except for halothane, where the range was 20° to 110°. All three anesthetic molecules exhibit a similar angular trend in their DCSs. The values decrease from small angles to approximately 60°–90°, reach a minimum, and then show a increase towards higher angles (approaching 180°). This behavior, characterized by a pronounced forward peak and a broad dip, is typical of molecular targets, as noted in previous studies (Maljković et al., 2019; Vukalović et al., 2022c). It is important to note that our experimental setup did not differentiate between elastic scattering and rotational excitations, and thus, the experimental DCSs represent quasi-elastic cross sections. The experimental data were normalized using the relative flow method, with argon as the reference gas (Williams and Willis, 1975; Ranković et al., 2018). Two absolute DCS points (three for halothane) were obtained and used to normalize the relative differential cross sections. These normalized points align well with the experimental data demonstrating the reliability of our normalization procedure. In summary, the experimental and theoretical DCSs show strong agreement for all three anesthetic molecules, contributing valuable insights into their scattering behavior and atmospheric interactions. These results are crucial for understanding the broader implications of halogenated anesthetics in environmental and physical chemistry contexts.

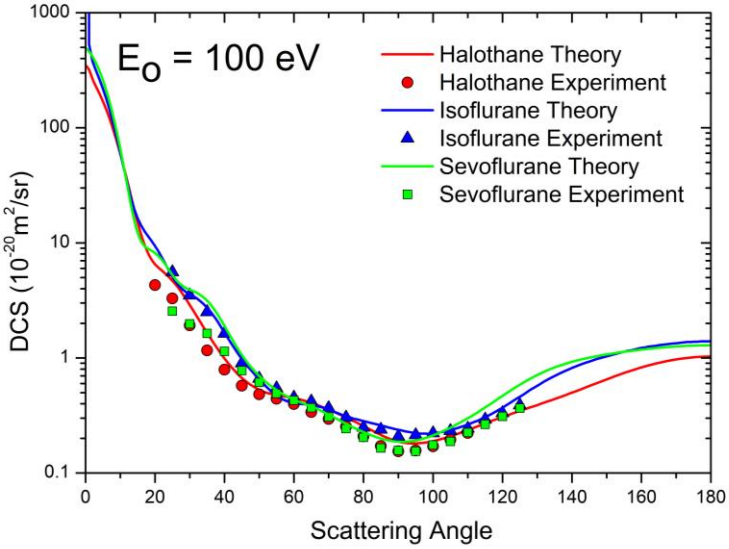

Figure 1. This graph presents the differential cross sections (DCS) for elastic electron scattering from halothane, isoflurane and sevoflurane at an incident electron energy of 100 eV, plotted together for a direct comparison.

Conclusion

This investigation provides a comprehensive analysis of elastic electron scattering from three halogenated anesthetic molecules: halothane, isoflurane, and sevoflurane at 100 eV. Differential cross sections (DCSs) were measured across an angular range of 25°–125°,for halothane, 20°–110°, using the relative flow method with argon as the reference gas to achieve absolute scaling. The resultant experimental data were normalized to absolute values, displaying strong alignment between normalized relative DCSs and absolute reference points, thus confirming the robustness of the experimental approach. Theoretical DCSs were computed using the IAM-SCAR+I method, which integrates the Independent Atom Model with the Screening Corrected Additivity Rule while incorporating interference

effects, yielding a high degree of congruence with experimental observations. These findings advance the understanding of the scattering dynamics of halogenated anesthetics, providing valuable insights into their atmospheric lifetimes and reactivity. By presenting novel DCS data alongside theoretical modeling, this work lays the groundwork for future investigations into the environmental impacts of anesthetic emissions, particularly regarding their contributions to global warming and ozone layer depletion.

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