Experimental and theoretical differential cross sections for elastic electron scattering from isoflurane molecule at 100eV

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Abstract

We present joint theoretical and experimental absolute differential cross section for elastic electron scattering from isoflurane molecule, for incident electron energy of 100 eV. Motivation for this research has been found in influence on global warming and ozone destruction.

Introduction

Isoflurane(2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane,CF_3CHCl-O-CHF_2) It is a non-flammable halogenated ether, with a molecular weight of 184.49 g/mol, a boiling point of 48.5°C, a vapor pressure of 330 mmHg (Pub Chem), and an estimated dipole moment of 2.47D (Atomistic Models of General Anesthetics for Use in in Silico Biological Studies). Mostly because of its clinical usage, isoflurane is widely investigated, but lately, its impact on the environment has motivated further research. Namely, it is known that most of the inhaled aneaesthetics are eliminated from the patient's body without being metabolized, so they are released into the lower atmosphere (Shiraishi et al. 1990). Atmospheric lifetime of isofurane is calculated to be between 2 and 5.9 years (Langbein et al. 1999), long enough to reach the stratosphere in considerable quantities. Isoflurane is known to have a high global warming potential (GWP) and it is calculated to be 545 according to (Langbein et al. 1999) and there, isoflurane can damage the ozone layer. All the above-mentioned give enough motive for research of electron interaction with this molecule.

Absolute differential cross sections of elastic electron scattering from isoflurane molecule, for incident electron energy 100 eV are reported. The experiment is performed in crossed beam setting. Relative differential cross section (DCS) is normalized on the absolute scale using the relative flow method, with Ar as a reference gas. The theory is obtained with IAM+SCAR method (Independent Atom Model + Screening Corrected Additivity Rule). A schematic drawing of halothane is shown in Fig. 1.

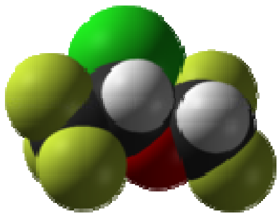

Fig. 1. Schematic drawing of isoflurane.

Experimental set up

Crossed electron-molecular beam apparatus UGRA which has been described in detail previously by Milosavljevic et al. (2006), was used for measuring absolute differential cross sections for elastic electron scattering on a halothane. The experimental set-up consists of an electron gun (hairpin electron source, up to about 1 μA incident beam current in the energy range from 40-300 eV, a double cylindrical mirror energy analyzer (DCMA) and a channel electron multiplier as a detector. All of these components are enclosed in a double μ–metal shielded vacuum chamber. The incident electron beam is crossed perpendicularly by a molecular beam produced by stainless still needle. The electron gun can be rotated around the needle in the in a limited angular range, from -40° to 125°.The base pressure of about $4x10^{-7}$ mbar was obtained by a turbo-molecular pump. The working pressure was usually less than $5x10^{-6}$ mbar and was checked for each experimental point. The energy resolution is limited by a thermal spread of primary electrons to about 0.5 eV. Isoflurane was introduced into scattering region from a glass container via a gas line system which was heated (sample container, pipes, needle) to provide stable experimental conditions and to improve the signal. Temperature of the pipes, needle and container were kept at about 40^{o}-50^{o}C. Absolute values for differential cross sections (DCSs) were obtained for 100eV incident electron energy, using relative flow technique (Nickel et al. 1989), at several scattering angles (40 and 70, 80 or 90 degrees.). In the relative flow method, the DCS for scattering of the unknown gas is determined by comparing scattering signals from a standard target (Ar), with its known differential cross sections (Ranković et al 2018), at a given incident electron energy (E_O) and a scattering angle (θ) under identical experimental conditions. To obtain the same profiles for both gas beams, the gases must be operated at pressures behind the needle so that their mean-free paths are the same.

Gas kinetic diameter for argon (D_{ref}=D_{Ar}) is known to be 3.58 Å and the estimated value for isoflurane (D_x=D_{IF}) is 5.57 Å. For the present experiment, the ratio of driving pressures (according to their gas-kinetic diameters) is p_{Hal}: p_{Ar}=2.4:1. During the measurement it has been proved by varying the ratio of the halothane and Ar pressures (±20%) that absolute values of the cross sections do not depend significantly.

Analysis and results

Experimentally measured (green circles, for scattering angles from 20° to 110°) and theoretically calculated (black full line, 0°-180°) DCSs, for incident electron energy 150 eV, are shown graphically in Fig. 2. DCS has characteristic behavior for molecular targets, as noticed before (Vukalović et al. 2021). It exhibits a wide minimum at about 90°. Experiment and theory are, in general, in very good agreement, considering absolute scale and shape. Concerning the normalization procedure, described in detail elsewhere (Vukalović et al. 2021), relative flow measurements are shown in Fig. 2. as yellow stars. The reference gas used was Ar, and its absolute DCS values were taken from a paper by Ranković et al.

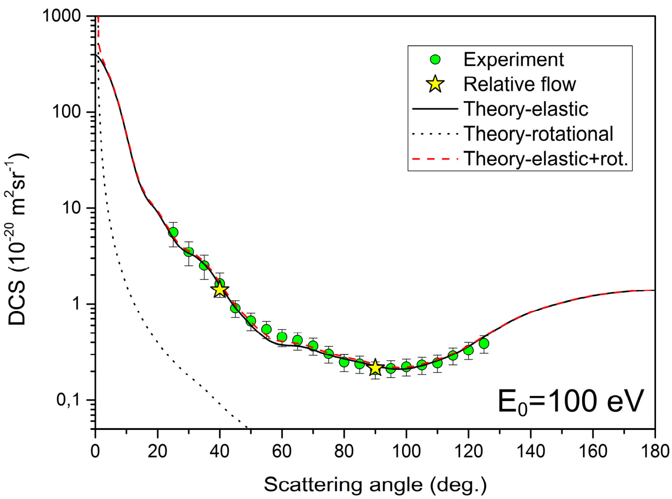

Fig. 2. Angulary dependent differential cross section for elastic electron scattering from isoflurane molecule, for incident electron energy 100 eV.

Acknowledgments

We acknowledge the financial support of MESTD supplied via Institute of Physics Belgrade. This collaborative work has been undertaken under COST Actions: CA18212 MD-GAS and CA 20129 MultIChem.

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