Absolute differential cross section for elastic electron scattering from halothane molecule at 150eV

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Abstract

Motivated by its undeniable influence on global warming and ozone destruction, we present joint theoretical and experimental absolute differential cross section for elastic electron scattering from halothane molecule, for incident electron energy of 150 eV.

Introduction

2-bromo-2-chloro-1,1,1-trifluoroethane, commonly known halothane as (CF₃CHBrCl), is a multihalogenated derivate of ethane. It is mainly used as an inhalation aneaesthetic. Mostly because of its clinical usage, halothane 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). Halothane is known to have a high global warming potential (GWP) (Ishizawa et al. 2011). Its tropospheric lifetime is calculated to be 7 years (Langbein et al. 1999), long enough to reach the stratosphere in considerable quantities. There, halothane can damage the ozone layer, since its ozone depletion potential (ODP), relative to Freon-11, is 1,56 (Langbein et al. 1999), highest among all aneaesthetics. All the above-mentioned give enough motive for research of electron interaction with this molecule.

In this paper, experimental and theoretical results for elastic electron scattering from halothane molecule, for incident electron energy 150 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 halothane.

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 uA 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 u-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 126° . The base pressure of about $4x10^{-7}$ mbar was obtained by a turbo-molecular pump. The working pressure was usually less than 5×10^{-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. Halothane 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°-50°C. Absolute values for differential cross sections (DCSs) were obtained for 150eV incident electron energy, using relative flow technique (Nickel et al. 1989), at several scattering angles (40° , 70° and 100°). 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 (Williams 1975), at a given incident electron energy (E_0) 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.

We have taken the gas kinetic diameter for halothane to be 5.6 Å (Lewis et al. 1997). For the present experiment, the ratio of driving pressures (according to their gas-kinetic diameters) is p_{Hal} : $p_{Ar}=2.45$:1. During the measurement it has been proved by varying the ratio of the halothane and Ar pressures (±15%) that absolute values of the cross sections do not depend significantly.

Analysis and results

Experimentally measured (red 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 Williams and Willis.



Fig. 2. Angulary dependent differential cross section for elastic electron scattering from halothane molecule, for incident electron energy 150 eV.

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