ABSOLUTE DIFFERENTIAL CROSS SECTION FOR ELASTIC ELECTRON SCATTERING FROM HALOTHANE at 100eV

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Abstract. Absolute differential cross sections (DCSs) for elastic scattering of electrons from halothane (HC_2BrClF_3) are measured at incident electron energy of 100 eV. The measurements were performed using the relative flow technique for scattering angles 40º, 70º and 100º. The experimental results are compared with theoretical cross sections calculated by screen corrected additivity rule (SCAR) procedure.

1. INTRODUCTION

Fluorinated compounds are of particular interest due to their unusual physical and chemical properties and a wide range of applications from medicine to modern technology materials. Halofluorocarbons are being used as inhalation anesthetics and first of this type is 2-bromo-2-chloro-1,1,1-trifluoroetane (halothane). Halothane (HC_2BrClF_3), is a substituted ethane molecule, where one of carbon atoms is bonded to H, Cl, Br atoms, and of CF_3 group, having a chiral structure. It has a few undesired side-effects and particular advantages of high chemical stability, high vapor pressure and no flammability (Olejniczak et al. 2009). Souza et al. (2005) presented the valence excitation spectrum for the halothane molecule determined in the 5 to 50 eV energy range using high energy electron energy-loss spectroscopy. They also obtained the mass spectrum for this molecule, using a Helium lamp. Santos et al. (2005) have been studied a fragmentation of halothane using synchrotron radiation as ionizing agent. Czarnik-Matusewicz et al. (2006) have reported both experimental and theoretical study of vibrational spectra of ha-

lothane. Olejniczak et al. (2009) have been investigated intermolecular interactions for a halogenated –ethane anesthetic.

In the present contribution, experimental results on elastic electron scattering from halothane have been reported. The experimental absolute DCSs for 100eV incident electron energy at 40°, 70° and 100°, are shown and compared with theoretical calculations.

2. EXPERIMENTAL SET –UP

The absolute DCSs for elastic electron scattering from halothane were measured using a crossed electron-molecular beam setup which has been described in detail previously by Milosavljevic et al. (2006). Thus, we will only give a brief outline of the apparatus and measurement procedure. The relative flow method will be described in more detail.

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 20-500 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 angular range from about -40° to 110°. 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. The angular resolution is better than ±2°. Halothane was introduced into scattering region from a glass container via a gas line system, which was recently upgraded to allow relative flow measurements and more operative measurements of relative DCSs. The whole gas-handling system (sample container, pipes, needle) was heated to provide stable experimental conditions and to improve the signal. Temperature of the pipes, needle and container were kept at about 40°-50^oC.

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°, 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 (here Ar), with its known differential cross sections (Williams 1975), at a given incident electron energy (E_O) and a scattering angle (θ) under identical collision region geometry 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.

The absolute cross section is then obtained according to Nickel et al. (1989) as:

$$DCS_{Hal}(E,\theta) = DCS_{Ar}(E,\theta)\frac{N_{Hal}F_{Ar}}{N_{Ar}F_{Hal}}\sqrt{\frac{M_{Ar}}{M_{Hal}}} \tag{1}$$

Here, $DCS_{Hal}(E_0, \theta)$ and $DCS_{Ar}(E_0, \theta)$ represent absolute differential cross sections for elastic electron scattering from Halothane and referent gas, respectively; N_{Hal} and N_{Ar} measured signal intensities; F_{Hal} and F_{Ar} are measured mass flow rates and M_{Hal} and M_{Ar} are molecular weights. Since the flow rate condition depends on molecular diameters and masses, it is important to discuss the question of how errors in molecular properties affect the final cross section. If interaction volume, which is defined by electron and molecular beam intersection, is well within the viewcone of the detector and the electron beam flux is uniform, then Eq. (1) holds without any flow-rate condition. This means that although the shape of molecular beam may vary with flow rate, the total number of target particles in the scattering volume remains the same. If detector view-cone is smaller than the intersecting volume of two beams, the flow rate condition must be strictly used for Eq. (1) to be valid.

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 ($\pm15\%$) that absolute values of the cross sections do not depend significantly. We have taken the diameter for Halothane to be 5.6 Å (Lewis et al. 1997). Silva et al. (2008) have recently made a modification of relative flow method, which obviates a need to know the molecular diameters of the gases used.

In the present experiment, the mass flow rates of the gases (F_{Ar} and F_{Hal}) have been measured by closing the outlet to the gas chamber and recording the increase of the absolute pressure in the gas line behind the needle as a function of time (using an automated acquisition controlled by a PC LabView program). Flow rates have been obtained from experimental curves, which were fitted by a least squares method to a linear function.

3. PRELIMINARY RESULTS

The absolute DCSs for elastic scattering of electrons from halothane molecule have been experimentally obtained using relative flow technique. Absolute measurements were performed for 100eV incident electron energy at 40°, 70° and 100°. Experimental results are compared with theoretical curve (Fig. 1) based on a corrected form of the independent-atom method, known as the SCAR procedure and using an improved quasifree absoption model (Blanco and García 2003). The calculated DCSs using the SCAR procedure generally agree very well with experiment, regarding the shape and absolute values.
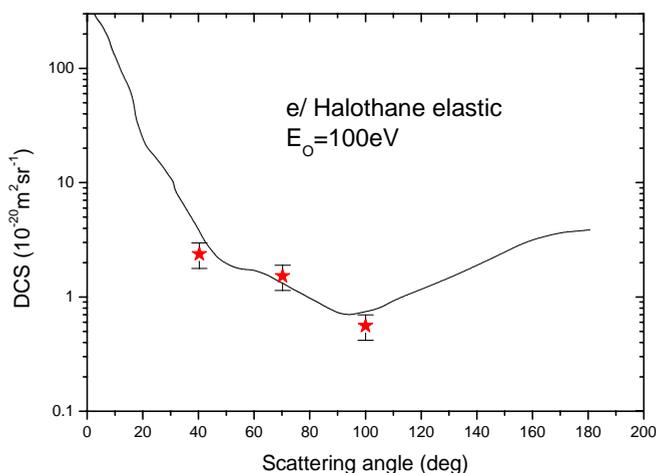
Figure 1: Angular dependence of absolute differential cross sections for elastic electron scattering from halothane at 100eV. Values obtained by relative flow method (full stars) are presented together with theoretical calculations SCAR (full line).Overall error is dominantly defined by the error of referent absolute DCSs for Ar (about 25%)

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