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TOTAL CROSS SECTION MEASUREMENTS FOR ELECTRON SCATTERING ON METHYL FORMATE ($HCOOCH_3$) MOLECULE: METHYLATION EFFECT

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Abstract. We present the absolute total cross section (TCS) for electron scattering from the methyl formate ($HCOOCH_3$) molecule measured in the 10-300 eV energy range, with electrostatic electron spectrometer working in the linear transmission mode. Comparison of TCS for the $HCOOCH_3$ molecule with that measured earlier for the formic acid (HCOOH) compound manifests the methylation effect i.e. the response of the electron scattering dynamics on replacing of the hydrogen atom in the hydroxy group in HCOOH with the methyl group ($-CH_3$). It is also shown that the TCS for methyl formate can be estimated with simple additivity rule, using TCSs for the formic acid, ethane and hydrogen molecules. The energy dependence of determined this way TCS for $HCOOCH_3$ and the measured values are in very good agreement above 20 eV.

1. INTRODUCTION

Small organic molecules trapped in icy grains in the interstellar space, see e.g. Herbst and Dishoeck 2009, can interact with free electrons, coming from ionization events inside bulk or from other sources. Such interactions can significantly contribute to processes resulting in synthesis of complex organic molecules in space, see Boamah et al. 2013. Methyl formate ($HCOOCH_3$) has been detected towards many extraterrestrial sources, e.g. hot molecular cores, see e.g. Cazaux et al. 2003, or on Hale-Bopp comet, see Despois et al. 2005. Therefore, accurate and comprehensive electron scattering data for the methyl formate and its isomers, glycolaldehyde and acetic acid, as precursors to larger compounds are of great astrobiological importance. Interest in methylation increased when it has been recently revealed that DNA methylation plays an important role in the formation of many common human diseases, see in Jin and Liu 2018.

Total cross section (TCS) for electron scattering is the sum of the partial cross sections for all possible processes occurring during the electron-target molecule collisions. It can be measured in an absolute scale, yielding useful information over wide electron impact energy range, see e.g. Szmytkowski and Możejko 2020. However, not all compounds can be easily investigated experimentally, e.g. due to chemical instability, high toxicity or environmental risk. It is therefore desirable to employ theoretical and/or semiempirical methods for determining scattering cross sections. One of such methods is the additivity rule, see e.g. Domaracka et al. 2008, which allows to estimate cross section at the medium and high collisional energies by adding contributions from functional groups constituting the target molecule.

In this work we present preliminary results of experimentally obtained total cross sections for electron scattering on methyl formate ($HCOOCH_3$) in 10-300 eV energy range. Effects of the formic acid methylation is illustrated by the comparison of TCS data for HCOOH and $HCOOCH_3$ molecules.

2. EXPERIMENT

Presented experimental total cross section data have been obtained using electrostatic electron spectrometer working in the linear-transmission mode. The electron beam with given energy E, within the limits from 0.3 up to 300 eV and resolution of about 80 meV (FWHM), is directed into scattering chamber filled with studied molecules. Electrons leaving the collision volume by exit orifice, are energy discriminated by retarding-field analyzer and collected in Faraday cup. TCS, σ(E), at given energy E, is determined using the Bouguer-de Beer-Lambert attenuation formula, in which thermal transpiration effect was included:

$$\sigma(E) = \frac{k\sqrt{T_t T_m}}{pL} \ln \frac{I(E,0)}{I(E,t)}, \tag{1}$$

where $I(E,0)$ and $I(E,t)$ are transmitted electron currents taken in the absence and presence of target in the scattering chamber of the length L, p is the vapour pressure of studied target, T_t is the scattering cell temperature, T_m is the temperature of manometer head and k is the Boltzmann constant. Statistical uncertainties (about 1%) were estimated as standard deviation of the weighted mean of the results obtained in the successive measurement series. Potential systematic uncertainties are less than 10% at low collision energies and decrease to 5% at intermediate energies. For detailed description of the experimental equipment and measurement procedure see e.g. Szmytkowski and Możejko 2001.

3. RESULTS AND DISCUSSION

Figure 1 shows the TCS we recently measured for methyl formate in 10-300 eV energy range. Change in the TCS slope around 100 eV is most probably due to the maximum of ionization cross section, see e.g. Możejko 2007. For comparison, in Fig. 1, we also show experimental TCS for formic acid, see Możejko et al. 2017.

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With respect to the shape, both TCS curves are very similar. However, over whole presented energy range TCS values for the $HCOOCH_3$ are distinctly higher than those for the HCOOH. Larger TCS for $HCOOCH_3$ is mainly related to the increase in the geometrical size of the molecule due to presence of the methyl group.

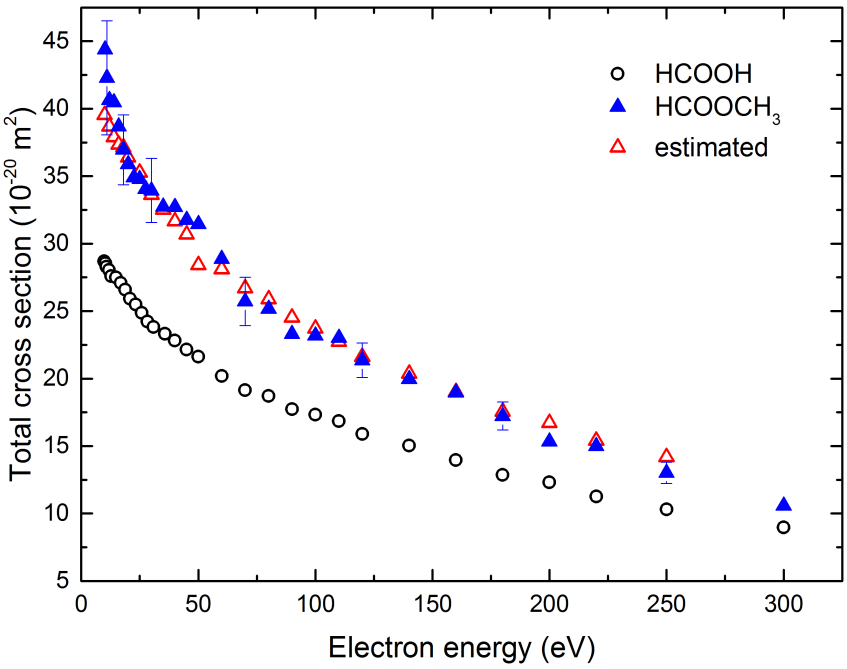

Figure 1: Comparison of preliminary TCS for electron scattering from methyl formate ($HCOOCH_3$), full blue triangles, with TCS for formic acid (HCOOH), Możejko et al. 2017, open circles. The error bars, at selected energies, correspond to overall estimated experimental uncertainties. The TCS for $HCOOCH_3$, estimated with additivity rule, is also shown, red open triangles.

Because above 20 eV no efficient resonant-like processes are expected, we can assume that beyond this energy scattering process can be approximately seen as independent electron scattering from each atom (or group of atoms), so the additivity rule can be applied, see Domaracka et al. 2008. That is why the cross section for $HCOOCH_3$ can be expressed with the formula:

$$\sigma_{HCOOCH_3} = \sigma_{HCOOH} - \sigma_H + \sigma_{CH_3}, \quad (2)$$

where σ_{HCOOH}, can be directly used as the TCS for the formic acid molecule, see Możejko et al. 2017, while σ_H and σ_{CH_3} can be estimated as one half of TCS for the

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hydrogen and ethane molecules, respectively. It is worth noting, that TCS values for H_2 and C_2H_6 come from measurements performed earlier with the same experimental system, see Szmytkowski et al. 1996 and Szmytkowski and Krzysztofowicz 1995. Above around 20 eV, TCS for methyl formate estimated according to the formula (2) is in excellent agreement with the experimental data, except for the small jump near 50 eV. Below 20 eV the curves diverge, as at low electron impact energies the geometry and structure of the target molecule grow in importance.

4. CONCLUSIONS

Total cross section for electron scattering on methyl formate is presented for the 10-300 eV energy range. The additivity rule was applied to estimate the TCS for this molecule based on TCSs for formic acid, molecular hydrogen and ethane. Above 20 eV, the estimated TCS values for $HCOOCH_3$ are in excellent agreement with the TCS obtained experimentally, showing that the reasonable accuracy can be obtained with the use of such simple approach.

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