

## CROSS SECTIONS CALCULATIONS FOR ELECTRON SCATTERING FROM RHODANINE AND CYANOACETIC ACID

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**Abstract.** Cross sections for electron-impact ionization and for elastic electron scattering for rhodanine ( $C_3H_3NOS_2$ ) and cyanoacetic acid ( $C_3H_3NO_2$ ) have been calculated in wide impinging electron energy range.

### 1. INTRODUCTION

New accurate experimental data on electron interactions with matter, including collisional cross sections are still crucial and desired for understanding a wide variety of natural and technological processes occurring and carried on in complex environments (see e.g. Szmytkowski and Możejko 2020). Recent interest in electron interaction with rhodanine ( $C_3H_3NOS_2$ ), its derivatives and cyanoacetic acid ( $C_3H_3NO_2$ ) is connected with their potential use in solar cells. Especially, the process of electron attachment to dye-sensitized solar cell components have been studied by Modelli *et al.* 2010 and Modelli and Burrow 2011.

In this contribution we report cross sections calculations for two different collisional processes i.e. elastic electron scattering (ECS) and electron-impact ionization (ICS). These cross sections have been computed for rhodanine ( $C_3H_3NOS_2$ ) and cyanoacetic acid ( $C_3H_3NO_2$ ) in a wide collisional energy range spanned between the ionization threshold and 4 keV. The geometrical structure of the studied molecules is shown in figure 1. Rhodanine is a 5-membered

heterocyclic organic compound possessing a thiazolidine core while cyanoacetic acid contains two functional groups, a nitrile NC and a carboxylic acid.

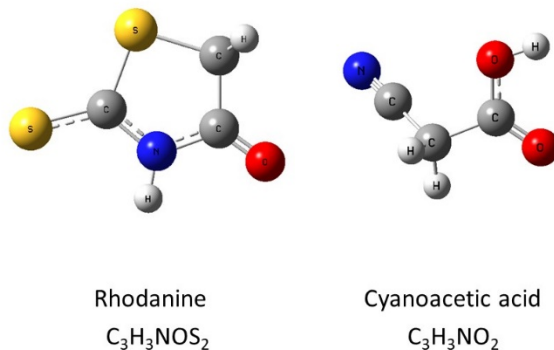


Figure 1: Geometrical structure of the studied molecules.

## 2. THEORETICAL METHODS

The electron-impact ionization cross section of a given molecular orbital can be calculated using the binary-encounter-Bethe method (BEB) see e.g. Kim and Rudd 1994 and Hwang *et al.* 1996:

$$\sigma^{BEB} = \frac{S}{t+u+1} \left[ \frac{\ln t}{2} \left( 1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1} \right], \quad (1)$$

where  $u=U/B$ ,  $t=T/B$ ,  $S=4\pi a_0^2 NR^2/B^2$ ,  $a_0=0.5292 \text{ \AA}$ ,  $R=13.61 \text{ eV}$ , and  $T$  is the energy of the impinging electron. The total cross section for electron-impact ionization can be obtained as a sum of ionization cross sections calculated for all molecular orbitals:

$$\sigma^{ION} = \sum_i^{n_{MO}} \sigma_i^{BEB}, \quad (2)$$

where  $n_{MO}$  is the number of the given molecular orbital. It is extremely important that in the BEB method there is no free parameter. All quantities have well defined physical meaning and can be quite precisely evaluated. The electron binding energy,  $B$ , kinetic energy of the given orbital,  $U$ , and orbital occupation number,  $N$ , have been calculated for the ground state of the geometrically optimized molecules with the Hartree-Fock method using quantum chemistry computer code GAUSSIAN (Frisch *et al.* 2003) and 6-31G+d Gaussian basis set. Obtained that way, ionization energies are not precise enough and are usually higher, even more than 1 eV, from experimental ones. For this reason, to include into account the

effect of electron correlations within molecule, we have performed also outer valence Green function (OVGF) calculations of ionization potentials using the GAUSSIAN code see e.g. Zakrzewski and Niessen 1994. It is worth to notice that the BEB method usually provides ionization cross sections which are in quite good agreement (within  $\pm 15\%$ ) with experimental data see e.g. Karwasz *et al.* 2014.

Elastic electron scattering from the studied molecules has been investigated on the static plus polarization level with well known, additivity rule (Raj 1991), in which the total elastic cross section can be calculated from cross sections for elastic electron scattering from constituent atoms of the target molecule.

### 3. RESULTS AND DISCUSSION

Figure 2 shows electron-impact ionization cross section for rhodanine molecule calculated for energies ranging from the ionization threshold at 8.59 eV up to 4 keV. The cross section maximum of  $12.98 \times 10^{-20} \text{ m}^2$  is located at 85 eV.

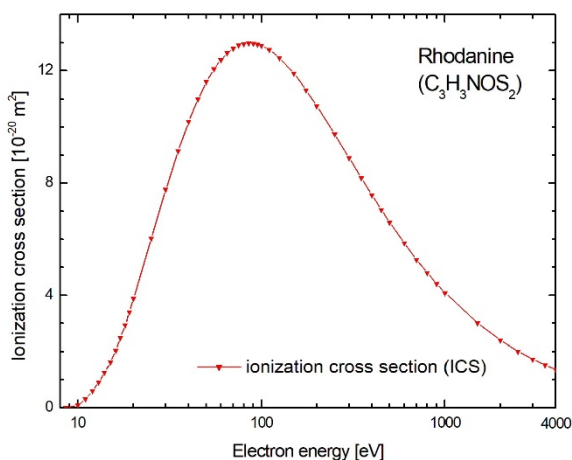


Figure 2: Electron-impact ionization cross section (ICS) calculated for rhodanine.

Figure 3 shows comparison of ICS and ECS cross sections calculated for cyanoacetic acid. The calculated ionization threshold for cyanoacetic acid is 11.464 eV. ICS maximum for this target reaches maximum of  $10.57 \times 10^{-20} \text{ m}^2$  at 90 eV. It can be easily seen that in the case of cyanoacetic acid contribution of elastic collisions and electron-impact ionization into overall electron scattering efficiency is almost equal for collisional energies higher than 1 keV.

The sum of the computed ECS and ICS can be used as approximation of total electron scattering cross section (TCS) for cyanoacetic acid. Basing on our



previous works the agreement between evaluated in such way TCS and measured one is quite satisfactory (see e.g. Szmytkowski et al. 2005, Szmytkowski et al. 2007, Szmytkowski et al. 2018).

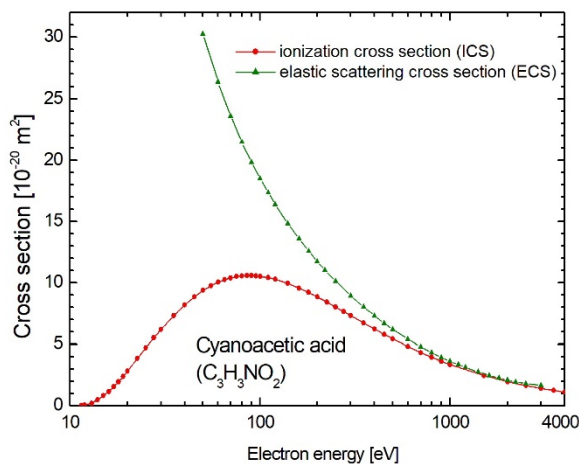


Figure 3: Cross section for elastic electron scattering (ECS) and electron-impact ionization cross section (ICS) calculated for cyanoacetic acid.

Numerical calculations have been performed at the Academic Computer Center (TASK) in Gdańsk.

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