

## Measurements of electron cross sections of small molecules

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Low-energy electron interactions with molecules play an important role in many natural phenomena, laboratory and industrial applications which was shown by the increase of publications on the topic in last decades. The range of fields and topics where these processes need to be considered ranges from plasmas through focused electron beam-induced processing, radiation damage of DNA to atmospheric processes, astrophysics and astronomy. To understand the processes and to be able to utilize them it is necessary to characterize and evaluate them.

The internal energy of molecules is concealed within their degrees of motion, leading to quantized energy levels. For each type of motion, there exist corresponding energy levels: electronic state energy levels, vibrational energy levels, and rotational energy levels. The interaction of a molecule with another particle or an electromagnetic wave can induce a change in its motion, thereby altering the energetic level and the internal molecular energy. The probability of this change is known as the cross section, which is one of several parameters used to characterize the kinetics of the interaction process and depends on the collision energy [1]. Many environments in which electron-molecule interactions play a significant role are highly complex, with multiple concurrent processes influencing each other. Plasmas and atmospheres serve as excellent examples, where it is practically impossible to experimentally determine all parameters. This is where modelling comes into play, but even the simplest models require reliable input data that precisely characterize the processes. Probabilities of processes - cross sections, are crucial among these data. For models considering a wider range of interaction energies, cross sections must be defined for every energy value within the range. Currently, the lack of data is often a challenge, with cross sections either being unknown, or their values determined only for a few specific energies, necessitating estimation based on known processes for similar molecules or utilizing other forms of approximate data. Consequently, the reliability and precision of model results may be compromised. The cross section values for electron-molecule collisions span in a relatively large range of values. For example, according to Itikawa et al. [2] the values for low-energy electron impact on water reach the order of  $10^{-13}$  cm<sup>2</sup> for rotational transitions and less than  $10^{-18}$  cm<sup>2</sup> for some dissociative excitations.

The relatively wide range of expected values affects the possibilities of experimentally determining the cross sections. Nowadays, perhaps the most commonly used experimental setup is based on crossed beams of molecules and electrons, with some variations regarding the electron beam source and molecular source. The electron beam is typically generated by a relatively simple electron gun with a heated filament as a source of electrons. If a narrower distribution of kinetic energy of the electrons in the beam is desired, the gun can be accompanied by some kind of kinetic energy monochromator, such as a hemispherical or trochoidal type. The molecular source is often an effusive capillary, which creates the beam by restricting the motion of molecules in the direction perpendicular to the desired beam and allows for the thermal effusion of molecules into the reaction chamber. This setup enables conditions that ensure binary collisions, allowing the interactions to be studied almost one by one. The rest of the experimental setup is given by the kind of electron-molecule interaction that is supposed to be studied. For example, the detection method and detector will be determined by the products of the selected reaction. For ions it can be mass spectrometer, for photons spectrometer, for scattered electrons electron energy analyser, etc.

The results can vary from relative curves (Fig. 1.), which often depict the dependence of signal intensity corresponding to a specific product on the incident electron energy, to absolute cross section values for a range of conditions (Fig. 2.). The relative curves provide an overview of the relative process efficiency, and threshold value(s). Transitioning from relative to absolute results requires more sophisticated calibration methods. The simplest procedure assumes the availability of at least one cross

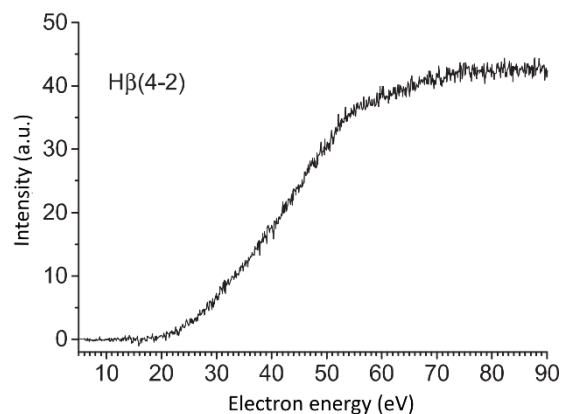


Fig. 1. Relative dependence of intensity for electron-impact induced production of excited hydrogen atom from the molecule of acetylene [3].

section value from the measured range. Then it is possible to bootstrap the data to this value and determine the cross sections for other processes. While the first procedure is based on data processing, the second method is experimental and requires the use of calibration compound. The cross section value of the calibration compound is known, and it is introduced into the experimental system at a known ratio with the studied compound. The third, most sophisticated method involves the experimental determination of all parameters for the direct calculation of the cross section (i.e., molecule and electron concentration in the beams, angles and efficiency of collection, etc.).

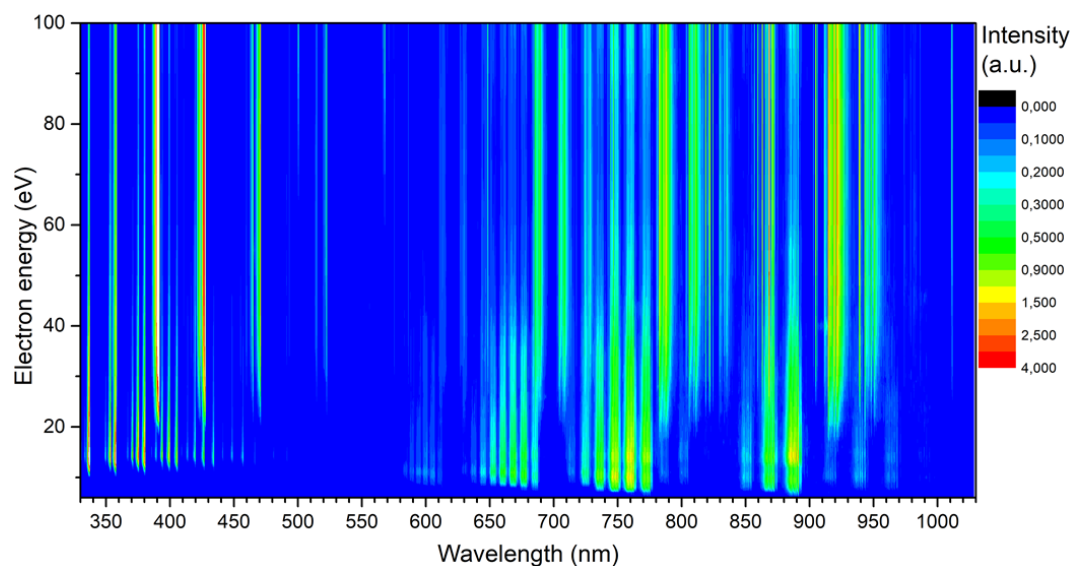


Fig. 2. Spectral electron energy map of electron impact induced emission of nitrogen from which the cross section for any detected process can be determined within the experimental energy and spectral limits [4].

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