# A Stepwise Procedure to Explore Uncertainty and Reliability in Theoretical Cross Section Data for Electron and Positron Scattering

**Bobby Antony***

*Indian Institute of Technology (ISM) Dhanbad, Jharkhand 826 004, India*

Many areas of science require accurate values of electron/positron induced scattering cross section data to probe various physio-chemical reactions occurring in those environments. For instance, electron collision data have applications in areas like modeling of electrical discharges, semiconductor processing, gas lasers, low and high-temperature laboratory plasmas, fluorescent lighting, the upper atmosphere, interstellar medium and quantitative mass spectrometry [1]. Similarly, interactions of positrons have potential technical applications in atomic physics, surface sciences, mass spectrometry, atmospheric modeling and medical imaging technique like positron emission tomography (PET) [2].

There is large amount of data set on electron scattering cross sections reported and compiled by various experimental and theoretical groups around the globe. However, we lack a mechanism to check the reliability of such data. Hence, it is critical to qualify and quantify legitimate data in the present scenario to benchmark the prevalent experimental and theoretical datasets. Experimentalists usually provide uncertainties to their measured data. However, theoretically it is quite demanding to envisage an effective methodology to estimate uncertainty for the calculated cross section data, but has been the urge of atomic and molecular physics community today. Hence, the present report is intended to address this issue and contribute a productive effort in this direction.

The first step in our approach is to benchmark the theoretical methodology employed against existing measurements/calculations. Next, a set of correlation relations are studied and verified for the calculated data to ensure consistency. This step is to make sure the reliability of the computed results. Then the variation in cross section due to a change in each input parameter used is quantified. This step is very crucial in speculating the sensitivity of cross sections for various input properties intrinsic to a target. Finally the spread in cross section due to various approximation methods used will be probed. It is to be noted that the aforementioned steps for uncertainty estimation are exclusive to the present method.

The atomic and molecular physics group at Indian Institute of Technology (ISM) Dhanbad, India has been in the forefront of calculating various cross section data for about a decade now. Electron and positron scattering cross sections are computed through SCOP formalism [3,4] (and R-matrix method) for a number of targets having applications in thrust areas of science. The cross section data includes electron induced DCS, total elastic, inelastic, ionization and momentum transfer cross sections [3] and positron impact cross sections like total, positronium formation and ionization (both direct and total) cross sections [4]. Employing above steps, we intend to provide recommended cross section dataset for many unknown targets to form a unified and complete database [5] with appropriate uncertainties.

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* bobby.iit.ism@gmail.com