

Criteria for Selection of Well-Validated Atomic Data

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There are a large number of papers, theoretical and experimental, published on different aspects of Atomic and Molecular Physics. These include the measurement and computation of oscillator strengths, radiative lifetimes, line shapes, line shifts, energy levels, ionization energies etc. for neutral and ionized atoms. Also, more than adequate data is available on electron and photon impact of molecules leading to many processes like excitation, dissociation, ionization and dissociative ionization, electron attachment, photo-ionization, photo-dissociation etc. All these data are needed to give a better understanding and insight regarding the different phenomena occurring at different sites and also help in putting forward better explanations and mechanisms.

But all these data need to be validated for accuracy in spite of the fact that the latest developments in science and technology are now capable of producing better results with higher resolution and sensitivity. However, all data still cannot be considered as the benchmark data which may be used further without ambiguity by different scientists in different fields.

It is the foremost duty of the scientific community to well-validate different atomic and molecular data. But unfortunately, it is not being done systematically as the criteria for rejection of data followed in the process have not been used in a consistent manner. That is why we have to ascertain and fix these criteria once for all.

Any data leading to relative measurements normalized using other standard data should not be considered for evaluation. Only absolute measurements should be included for validation. Measurements or computations which are obtained at a few electron or photon energies and not in the continuous range of energies should also be avoided even though new innovative approach may have been used to obtain the required data.

Measurement/computation of cross section if made by two different techniques can be used as a cross-check on one another and on theory.

Sometimes, only single set of data is available for a given parameter. Such data may only be considered if repeatability is ensured.

It is strongly believed that the experimental data should be preferred to one obtained by theoretical computation. This is mostly true for polyatomic molecules where target wave function cannot be represented unambiguously.

Cross checking experimental data could also be useful if carried out choosing some standard values provided by theory.

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In some experiments, accuracy is claimed to a large number of decimal places. It should be ascertained by checking different parameters used in the experimental system such as resolution of the projectile beam, the instrumental accuracy for measuring the number of atomic or molecular species involved in the collision etc. Otherwise, the claim for higher accuracy should not be entertained.

It should be made sure that the new technologies are used in the experiment to bring drastic improvement in the measurement of different atomic/molecular parameters. Where ever the atomic lines or molecular bands are observed as emission features due to projectile-target collisions, the absolute cross sections can be obtained only when the emission intensities are measured absolutely using standard radiometric techniques.

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