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International (Photo)-Ionization Cross-section Database

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Molecular Beam mass spectrometry has developed into a staple technique for the investigation of gas phase reactive systems including for instance kinetics (Sandia: Kinetics Machine, Univ. Colorado: Reactor, Argonne: Shock tubes), Flow and jet stirred reactors (Princeton, Bielefeld University, NSRL, DLR, Sandia, LBL) and flames (Université catholique de Louvain, Bielefeld University, Princeton, Sandia, University of Duisburg-Essen, Siberian Branch of the Russian Academy of Sciences). The quantitative and even qualitative results of all these experiments and many more rely heavily on the knowledge of ionizations properties of the investigated molecules (Thresholds, cross-sections, electronic structure of the ground and ion states, maybe even interaction between different components). The NIST Chemistry Webbook (http://webbook.nist.gov/chemistry/) only lists ionization thresholds and fragment appearance energies stating all the measurements known to them and sometimes an evaluated value. Even this database is maintained only in long cycles and does not keep pace with the measurements and needs of this Community or other communities which also rely on such data and measure them as byproducts of their work. Most recently Fei Qi et al at NSRL gathered all the published cross-sections in a database which was made available online. (http://flame.nsrl.ustc.edu.cn/database/) This list is likely not comprehensive as new cross-sections are generated frequently and are inefficiently stored in closed loops that could be easily accessible to all researchers. Furthermore an evaluation of the cross-sections in respect to their accuracy would be most useful. Accurate and reliable data is scarcely available in the literature. E.g. a given photoionization efficiency curve measured on different machines at the same beamline has led to different results. Obtaining cross-sections by computational methods is a route employed recently. The calculations can yield cross-sections with reasonable trustworthiness. The usual problem is that this work either needs some serious time commitment by the experimentalists who need the cross-section, or relies on computational chemists/physicists who usually does not have funding on which this type of work can be performed on. The Physikalisch Technische Bundesanstalt PTB as the German Metrology institute has the scope of improving the accuracy and precision of measurements. Therefore we would like to outline a concept to establish a network of institutions to coordinate the individual efforts and to acquire funding from the metrology community to establish, maintain and expand this crucial reference database.

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