

# International Summit on Current Trends in Mass Spectrometry

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### Fully Relativistic Electron Impact Excitation Cross-sections and Plasma Modeling

**Rajesh Srivastava**

Indian Institute of Technology (I.I.T.) Roorkee, India

There is need to develop collisional radiative (CR) models for both inert gases and tungsten plasma. Addition of inert gases in trace amounts does not perturb the plasma and its non-invasive feature makes it attractive option for plasma diagnostics. Tungsten is planned to be used in the divertor region of International Thermonuclear Experiment Reactor (ITER) due to advantage of its lower erosion rate and longer life time. Optical emission spectroscopy coupled with a population kinetic model provides very effective route to plasma diagnostic. To extract basic plasma parameters viz. electron temperature, electron density and species populations an appropriate population kinetic model accounting the various population and depopulation mechanisms is needed. The accuracy of such approach highly depends upon the cross sections of various processes used in the model. We have developed CR models by incorporating our detailed fine structure excitation cross sections calculated by using fully relativistic distorted wave (RDW) theory for argon and krypton plasma. For tungsten ions, we have performed fully relativistic calculations to obtain the electron impact excitation cross-section for the transitions in Zr-like W34+ through Se-like W40+ ions in the light of wavelength measurements in the range 45-82Å carried out at electron beam ion trap at NIST. Different results along with the theoretical details will be presented.

[rajsrfph@iitr.ac.in](mailto:rajsrfph@iitr.ac.in)

### Demonstration of homotropic positive cooperativity in antibody-antigen binding reactions

**Robert Blake**

Xavier University of Louisiana, USA

We used macroion mobility spectrometry (macroIMS) to quantify the percentages of antibody complexes that contained 0, 1, and 2 protein antigens in different reaction mixtures of antibody and antigen. These measurements tested the following hypothesis: A bivalent antibody that exhibits positive cooperativity when it binds its protein antigen will have a higher ratio of doubly occupied to singly occupied antibody than that anticipated for an antibody that binds its protein antigens in separate and independent binding events. The binding of human peroxiredoxin 4 (PRDX4) to two different monoclonal antibodies was studied by kinetic exclusion assays on a KinExA flow fluorimeter. One antibody (PRDX4-1) exhibited positive cooperativity with a Hill coefficient of 1.6 when it bound PRDX4, while the other antibody (9D2) bound PRDX4 with no evidence of cooperativity whatsoever. MacroIMS measurements revealed that the ratios of Ab•Ag<sub>2</sub> to Ab•Ag<sub>1</sub> were 0.5 and 1.4 when half of the antigen binding sites on antibodies 9D2 and PRDX4-1, respectively, were filled with antigen. The lower value was precisely the ratio expected for the distribution of antibody complexes when each of the antigen binding sites behaved separately and independently. The higher ratio that was expected for the distribution of antibody complexes when binding of the second equivalent of antigen occurred with higher affinity than that of the first equivalent. These studies independently verified the existence of homotropic positive cooperativity in an antibody-antigen binding event. To our knowledge, no other laboratory has reported the occurrence of homotropic positive cooperativity in selected antibody-antigen binding reactions.

[rblake@xula.edu](mailto:rblake@xula.edu)

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