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22 September 2009

Report on the PhD thesis by Mgr. Michal Tarana entitled *Collisions of slow electrons with molecules*

The research presented in this PhD thesis focuses on the study of slow electron-molecule collisions, with particular emphasis on the description and understanding of resonant processes. Elastic scattering, electronic excitation, dissociative electron attachment and vibrational excitation have been studied for several test targets (F_2, Li_2 and CF_3Cl). The aim of the work, however, is not just to provide collisional data for these systems, but to analyse and develop computational approaches to their study.

Dissociative electron attachment leads to the production of negative ions and radicals and is thus, in many cases, and initiator of chemical reactions. For this reason, it is a process of great applied significance, of relevance in radiation damage phenomena, both biological and non-biological, plasma processing, etc.. In spite of its relevance, calculations for these processes are still not very accurate when the target is a polyatomic molecule. This is due to the computational demands that treating a problem with a large number of degrees of freedom (electronic and nuclear) entails. The work presented in this thesis makes an important contribution towards understanding and improving the theoretical description of this and other resonant processes.

The research presented can be divided into two parts. The first one deals with the electronic part of the problem (treating the collision within the fixed-nuclei approximation) and it involves a careful analysis of the effect of the quality of the polarisation and correlation description on cross sections and resonance characteristics. Very interestingly, two different computational implementations of the same technique (the R-matrix method) are used to study the short and long range polarization effect in collisions with Li_2. This allows for the comparison of the results obtained with both implementations, something not done before, in spite of the fact that these computer programmes have been available for more than fifteen years. The work also confirms the effectiveness of the molecular R-matrix with pseudostates method to provide a good description of the polarisability, even for this highly polarisable target.

The second part deals with the nuclear dynamics in the dissociative electron attachment and vibrational excitation processes, focusing on the application of a local complex potential approximation. This work is exciting because it takes into account two vibrational modes, whereas most of the previous work on these processes only took into account one. The resonant data required (that can be determined from fixed-nuclei calculations) has not been obtained from state-of-the art calculations. This somehow subtracts form the quality of the cross

sections obtained; it would certainly be interesting to see in the future how these results are affected by the use of more accurate data. Encouragingly, this work is already being planned.

To summarize, this thesis presents excellent research, at the forefront of current work on low energy electron-molecule collisions. Mgr. Tarana has sought the collaboration of highly regarded scientists in the field. This has allowed him to make use of methods and their implementations (computer programs) that are among the best available. In addition, it shows remarkable flexibility and ability to learn. The work is outstanding for its thoroughness and determination to analyse the different factors that affect the computational description of low energy electron collisions with molecules. It is of more than sufficient depth, quality an interest to justify the award of the PhD degree to Mgr. Tarana.

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