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**Report on the doctoral dissertation of Ewa Erdmann**

The doctoral dissertation of Ewa Erdmann entitled "theoretical studies of fragmentation processes of neutral and ionized furan molecule" presents her work on theoretical molecular physics done under the co-supervision of Prof. J. Sienkiewicz and Dr. M. Łabuda. More precisely this work is within the field of the study of complex molecules and their stability after excitation and ionisation. She focused in this doctoral dissertation on the furan, a heterocyclic molecule. Due to the large number of degrees of freedom in such system, the decay can occur along numerous pathways in competition. Therefore, it is a very challenging task to look for a complete mapping of the decay channels. To this end, Ewa Erdmann has coupled three different theoretical approaches, namely molecular dynamics calculations, exploration of the potential energy surface, and a statistical method implemented in a new code named M3C (Microcanonical Metropolis Monte Carlo). Moreover, the studies cover three different charge states of the system over a wide energy range. Thus the present work represents a really impressive piece of work even more if one considers that Ewa Erdmann systematically compared her work with experimental results published or recently performed and motivated by her work. Therefore, Ewa Erdmann clearly showed that beside the excellent knowledge of the numerous theoretical studies she performed, she is also able to put in perspective her results with other works including experimental ones.

The dissertation is written in English and is really pleasant to read. Noteworthy, only few typing mistakes are present indicating a thorough proof reading before submission of the manuscript. It is subdivided in six chapters that I will detail below. Two appendices give further information on the inputs of the calculations with the M3C code. Particularly interesting is the first one which shows the extensive preparation necessary to perform these calculations even on a "small" complex system such as furan as one need to consider almost 500 fragments reflecting the different isomers and charge states possible. This again points out the difficulty to obtain a rather complete map of the dissociation channels and highlights the quality of the present work.

In the first and second chapter, Ewa Erdmann presents the context and the motivation of her work. The second chapter is specifically dedicated to the state-of-the-art on the study of furan dissociation. The complete bibliographic work done is well summarise and the striking results are extracted from the wealth of results. One can regret here the choice made by the author to focus on furan fragmentation. I suppose that a survey of the existing theoretical methods addressing molecular fragmentation may highlight the novelty of the present work. Considering the high quality of the bibliographic work done here, Ewa Erdmann may have written a very interesting section.

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The third chapter is dedicated to the theoretical methods. As an experimental physicist, this part of the dissertation may be looking boring but the present chapter is well written and easy to read. Again the important information are present.

Chapter four is the real beginning of Ewa's work. In this chapter she presents the computational details and she discusses the performances of the M3C code. This latter part is very interesting. The choice of the results shown is in my opinion excellent and their presentation is of very high quality. This part deeply helps to understand the M3C calculations. This also shows that Ewa Erdmann is among the very few (can be counted on the finger of one hands) able to manage calculations with M3C.

Chapter five is dedicated to the presentation of the results. Ewa Erdmann chooses to discuss the fragmentation of furan as a function of the charge state of the system. Again this choice seems pertinent as it is a really pleasant chapter to read particularly considering the amount of results shown due to the coupled approach proposed in the present work. The results obtained with the three different theoretical methods are discussed separately and in a coupled way. Moreover they are also compared with experimental results obtained after thermal decomposition, electron collisions, photoionisation, and ion collisions. All discussions are clear and very interesting. Again the graphical presentation of the wealth of results is of a very high standard. One small drawback in the present chapter is the fact that when comparing the theoretical results with experimental results is that there is no real discussion on the fact that in experiments, the target is usually electronically excited whereas all calculations are performed in the ground state and only consider vibrational excitation. This is particularly interesting when one considers the really good agreement between photoelectron-photoion coincidence (PEPICO) breakdown curves and the M3C ones. Nevertheless as stated before, the discussion of the present results and their comparison with existing ones and unpublished ones is of very high quality.

In the sixth chapter, the author concludes her dissertation and opens some perspectives.

In conclusion, the present dissertation by Ewa Erdmann is of very high grade. The text is very well written and pleasant to read. The amount of work done is impressive. Moreover the discussion of the results and their presentation show a lot of pedagogy. By this dissertation Ewa Erdmann clearly demonstrates that she possesses all the quality needed for a PhD. Thus I have no hesitations to recommend the defence of the thesis.

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