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Report on the habilitation thesis of Dr. Lucie Augustovičová *QUANTUM DYNAMICS OF SMALL MOLECULAR SYSTEMS FROM DIATOMICS TO POLYATOMICS* submitted to Charles University Prague.

This habilitation thesis provides an excellent introduction to, and overview of the research carried out by Dr. Augustovičová over the last ten years. Dr. Augustovičová has undertaken a programme of original research that straddles the fields of Theoretical Chemistry and Molecular Physics, but with a clear aim to generate results that can inform other areas of scientific endeavour, for example Astronomy. Her most significant contributions are presented in the thesis and include the study of the following:

- Radiative processes of astrochemical relevance. This research aims to provide information that sheds light on molecule formation and the growth of molecular complexity in the early Universe. The study of radiative association also enables the investigation of the depopulation of metastable levels of helium through radiative collisions in astrophysical environments.
- Rotational and vibrational radiative transitions that could be used to determine the variability of some fundamental constants with time and space, specifically the proton to electron mass ratio. In particular, transitions in diatomic hydrides amenable to astronomical detection are identified: strong magnetic fields (like those present in many stars) lead to significant enhancement of the spectral sensitivity to the mass ratio in these transition making them particularly suitable for the quantification of the mass ratio. Similarly, the study of hyperfine structure of the rotation-inversion lines of ammonia also provides data to probe (and constrain) this ratio.
- Utracold molecular collisions in the presence of electromagnetic fields in order to provide guidance for the improvement of molecular cooling techniques. The investigation of some polar diatomic and triatomic molecules shows how, for the latter, evaporative cooling can be enhanced by the application of 'experimentally reasonable' electric fields and thus potentially lead, for example, to the experimental realization of molecular Bose-Einstein Condensates.
- The emergence of quantum chaos in cold atom collisions. Semi-analytic results show that for diatomic molecules where chaos is shown, both theoretically and experimentally, to manifest in the below-dissociation energy spectrum, chaotic behaviour is also exhibited by the Feshbach-Fano resonance spectrum.

The coherent theme that links this research is the detailed study of the physics of small molecular systems, employing a number of theoretical and computational techniques. There is, however, a clear and sustained effort to link to experimentation: some of the

research provides accurate data where laboratory investigations are difficult, if not simply unfeasible at the moment, whereas other work puts forward suggestions for measurements and new experiments.

The thesis shows both the breadth of Dr. Augustovičová's interests and the depth with which she has applied her knowledge and expertise to scientific problems of contemporary relevance. This is demonstrated by the fact that her work has led to a number of publications in high quality journals, both in the areas of Molecular Physics and Quantum Chemistry (*Phys. Rev.* A, *J. Chem Phys.*, etc.) and those where the outputs of Dr. Augustovičová's research can be used to shed light on more complex phenomena both of applied and fundamental interest (e.g. MNRAS).

The thesis is clear, well structured and well written. Dr. Augustovičová has conveyed, in each of the sections, the research questions addressed, how this has been done and what the challenges and limitations of the research are. She has also chosen, from amongst the work she has carried out, the most appropriate examples to illustrate the different strands of her research so far. I have found the concise and clear way in which she has explained the motivation for each of these strands particularly appealing: it demonstrates a capacity to communicate scientific ideas with both clarity and precision.

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In summary, this habilitation thesis presents a significant, high-quality body of research that explores and exploits the ability of theoretical chemistry and molecular physics methods to provide answers to scientific questions, both fundamental and of applied relevance. I believe it also shows the potential of Dr. Augustovičová to make further significant contributions to her area of expertise in the future.

Dr. Jimena D. Gorfinkiel
Head of Physics Research Discipline
School of Physical Sciences
The Open University
United Kingdom