Habilitation Thesis Report

"ASTROPHYSICALLY RELEVANT REACTIONS OF IONS WITH MOLECULAR AND ATOMIC HYDROGEN"

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1 THE CANDIDATE

I have followed the work of Dr. Roučka for last 10 years due to my own interest in gas phase ion chemistry. Thus, I am familiar with his publications in this area and can thus state that Dr. Roučka is now an internationally known researcher in the specific area of reactions of ion-molecule interactions relevant to hydrogen in interstellar medium. Also, it is interesting to note that his most cited article relates to symbolic computing in Python. Unfortunately, am not that familiar with his lecturing or teaching. Nevertheless, his publication record and this submitted habilitation thesis demonstrate his potential to push forward frontiers of challenging research subjects and to inspire new generation of students.

2 REVIEW OF THE PRESENTED WORK

2.1 SCIENTIFIC LEVEL

The habilitation theses summarizes the post-doctoral work of Dr. Roučka that has been largely already published in leading physics and chemistry journals. In three of the included articles he is the first author and in six of them he is a corresponding author. This demonstrates the high level of scientific rigor and citations of his work (the paper on "Formation of H_2O^+ and H_3O^+ Cations in Reactions of OH^+ and H_2O^+ with H_2" received 18 citations) indicate that it is well received by the scientific community. The habilitation thesis brings the individual studies together and shows their mutual relation.

The Introduction covers the background of the ionic processes in the interstellar medium and discusses the current state of the art of various experimental techniques used for the author's original research. Also clearly outlined are the author's contributions to specific technical developments including the above-mentioned symbolic computing in Python. Subsequent chapters outline the motivation and the rationale for the candidate's work in a clear and logical fashion from studies of anions in interstellar medium, via studies of H_3O^- reaction complex to a range of studies related to formation of interstellar hydrides. Finally, an outlook is presented for future work, which is perhaps too brief, but clearly covers the future plans for absolute measurements of rate coefficients of $H_2 + H_3^+$ rotational state-changing collisions and for construction of a new source of vibrationally excited H_2.

2.2 RELEVANCE

The presented work is highly relevant to widening the understanding of ionic processes in the interstellar medium, especially concerning the hydrogen reactions. The importance of the results is

fundamentally in providing reliable new experimental data on rate coefficients of the species essential for the formation of molecules in the interstellar medium. Perhaps a weakness that can be seen in this thesis is that whilst the importance of providing the rate coefficients for modelling is mentioned (especially in the included articles), their actual use in this area is not retrospectively reviewed (e.g. who and why was citing the article Tran et al. 2018).

2.3 ORIGINALITY

The chosen area of interstellar medium ion interaction research as a whole represents one of the frontiers of experimental ion chemistry; as such, the work is highly original due to the methodology alone. In addition to that, the studies of individual reaction systems are highly original, each in its own right. It may be said that the field of research chosen by the candidate is perhaps too original, in a sense that nobody else is doing similar work in Czechia and very few researchers in the world pursue active experimental research on low-temperature reactions of small ions with hydrogen molecules in defined internal states.

The automated originality report Turnitin highlights mostly the references and commonly used phrases, it certainly does not indicade any plagiarism whatsoever.

3 OUTSTANDING QUESTIONS

When studying the candidate's work, some questions arise to which it would be eminently interesting to hear the candidate's reaction:

1) Concerning the first paragraph of the Introduction: Would it be possible to use the latest advanced ab-initio methods to calculate reaction energetics and spectral lines with better accuracy than what was possible ten or twenty years ago?
2) Regarding the relating enthalpy difference to the ground state energy difference (e.g. equation 27): does this involve some assumptions about the very low temperature, so no rotational and vibrational levels are populated? (This reviewer does not have immediate access to Light et al. 1969). Why is equation (5) in the publication "I" written with ΔE instead of ΔH_0 as in equation 27?

4 CONCLUSION

The presented work, together with the cited previous work of the candidate, demonstrates that his research outputs are of a high-quality scientific level, directly relevant to the current interest in astrochemistry, and very original. Thus, I recommend that it is accepted as a Habilitation Thesis for and fully support his habilitation as a "Docent".

[redacted]

Prof. Dr. Patrik Španěl, Dr. Rer. Nat.

In Prague 3. June 2022

RNDr. Patrik Španěl

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