

April 02, 2020, Prague

Referee report for evaluation of doctoral thesis:

Mgr. Thuy Dung Tran: “Water formation in reactions of anions and/or cations with molecular hydrogen at low temperature”

The doctoral thesis of Mgr. Thuy Dung Tran concerns several experiments related to ion-molecule reactions leading to both formation and destruction of water at astrochemical relevant temperatures. The experimental work was carried out under the supervision of doc. Radek Plašil in the laboratory of prof. Juraj Glosík, where experiments using 22-pole ion trap apparatus have a long tradition. The high scientific standard of the group itself guarantees quality of the presented work. The thesis of Thuy Dung Tran brings the work of the group further and can be divided into two main topics:

1. Reactions with negative ions: $OD^- + p-H_2$; $O^- + H_2$, $O^- + D_2$; $O^- + HD$
2. Reactions with positive ions: $OH^+ + H_2$; $H_2O^+ + H_2$; $D_2O^+ + H_2$; $D_2O^+ + D_2$

The work itself is divided into 4 chapters followed by a brief summary. In Introduction, all the necessary information is brought together – chemistry of negative ions in interstellar space, their role in atmosphere of planets, H_2O origin and detection in interstellar space and also general introduction to reaction rate coefficient theory of ion-molecule reactions. Then, various experimental techniques for the study of ion-molecule reactions are introduced and a separate chapter is dedicated for description of the 22-pole ion trap apparatus, which was used for all the experiments. Para-enriched H_2 generator and data analysis procedure are also explained. All the experimental results for the aforementioned reactions are given in the fourth chapter.

The thesis is written in a relatively good English, however, there are frequent mistakes and typos throughout the text. The results are well documented in figures. The literature survey used in the work is very well documented with plenty of references, including also the work

of the group. The formal standard of the thesis is good. The author also includes her own contribution both in the introduction and in the conclusion and often refers to the other work published by the former and present members of the group.

Both chapters describing experimental techniques contain enough information about various approaches to measuring reaction rate coefficients of ion-molecule reactions and about the 22-pole ion trap apparatus used for the presented experiments, respectively. However, neither of the two chapters contains schematic drawings of the apparatus or any of its parts. This is a significant drawback of the work. It would greatly beneficial to include such figures instead of references to other works.

Another drawback of the thesis is the overwhelming and thus confusing amount of reactions and their coefficients included in the results section. The thesis would be better understandable if it included more tables and reaction schematics throughout the text, so any readers could navigate more easily.

The thesis is accompanied by five papers published in well established and impacted journals: 2 × Astronomy & Astrophysics; 2 × The Astrophysical Journal (including one letter to the editor; Physical Review A. Thuy Dung Tran is the main author of “Formation of H₂O⁺ and H₃O⁺ Cations in Reactions of OH⁺ and H₂O⁺ with H₂: Experimental Studies of the Reaction Rate Coefficients from T=15 to 300 K, The Astrophysical Journal, 854:25, 2018”. This paper already has four citations according to Web of Science what proves the high level of the publication. Scientific quality of the five papers has been verified in a peer review process, so I do not add any comments on them.

Major comments and/or questions:

1. I missed a sketch or drawing of the experimental apparatus and its parts. There is no such schematics in whole work, nor in the attached publications. Any reader of the thesis would certainly appreciate if it was included.
2. The importance of the work for astrochemistry is stressed out in the introductory part of the thesis. Therefore, I would like to see more comprehensive comment from the author about the influence of the measured reaction rate coefficients on astrochemical models, not just a short statement in the last two paragraphs of the work.
3. On p. 50, there is a factor ξ describing ratio of the detection efficiencies of OD⁻ to OH⁻

introduced. Since it is naturally close to 1, how does it affect behaviour of the equations 4.21 and 4.22 and which specific value was used for the solving?

In summary, the thesis demonstrates the author's ability to perform independent and creative scientific work. Despite the abovementioned comments, I fully recommend the presented thesis for the defence, and the author to be awarded the Ph.D. title after a successful defence.

RNDr. Peter Rubovič, Ph.D.