

Opponent's Report on Maria Lugaro' DSc Thesis Submitted to the Hungarian Academy of Sciences

First of all, I have to apologize that my reviewing time was a bit longer than it should have been. Part of the reason is that although my research field is astrochemistry, and I know and teach the basics of the astrophysical formation of chemical elements, I am not an expert and I have never conducted a research project and have not even followed the most recent research papers on nucleosynthesis, which is the topic of the thesis. My research field start where this thesis is finished: how molecules can be formed from atoms in astrophysical objects. Why I have accepted the invitation to accept to review the DSc thesis of Maria Lugaro entitled „Origin of the chemical elements heavier than iron and of meteoritic stardust from asymptotic giant branch stars”? I had two main reasons. First, the thesis is backed by impressive publications in high-impact journals, predicting that the author is by far worthy of the MTA DSc title. The second reason is my own selfish interest in this topic, I wanted to learn and extend my knowledge in a field closely connected to my research interests.

The work is beautifully presented, the structure of the dissertation is logical and the text is easy to follow, – excluding some technical details – even for an outsider. The figures are also well-planned, and the captions are well worded. The dissertation contains almost no punctuation, I have noticed only a couple of them, but these are not worth mentioning one by one. In a very correct way, in the case of collaborations, the co-workers are named, and both in these cases, and in the case of working with students and postdocs, the contribution of the authors to publications is presented in detail.

In her research works, Maria Lugaro has very innovatively combined and partially developed computer codes for modelling the kinetics of nucleosynthesis with stellar evolution models. The models and the codes were applied to a variety of problems of astrophysics to better understand both the nucleosynthesis and stellar processes and the elemental and isotopic distributions of stellar atmospheres and interstellar/meteoritic dust particles.

I accept all the thesis points listed at the end of the dissertation. Instead of repeating all the thesis points, I would like to highlight only a few results that I found the most important or the most interesting.

One of the most important outcomes of the work of Maria Lugaro, is that she has shown that slow and rapid neutron capture processes themselves cannot explain the elemental distributions in the stellar environments of AGB stars, a third process, the intermediate neutron capture process should also be taken into account.

I found exciting the results on SiC grains. It was shown that the size of the grains is increasing with the metallicity of the parent star. From the distribution of Si in SiC grains, the age-metallicity of the AGB parent stars could be derived, which revealed that the stardust grains recovered from meteorites must have originated from AGB stars with a higher metallicity than that is observed in the solar neighborhood. The analysis of the silicate grains have shown the origin from AGB stars with an initial mass roughly above 4 solar mass. It is also an important value of these simulations that they have shown that the $^{17}\text{O}(p,\alpha)^{14}\text{N}$ reaction rate constants were inaccurate. This conclusion inspired new nuclear physics measurements that could provide more accurate rate constants for this important nuclear reaction.

The analysis of the formation and decay processes of radioactive isotopes, which are now extinct, but were present at the time when the Sun was formed, together with the analysis of the distribution of daughter species, it could be e.g. shown that the last r-process and s-process events that contributed to the Solar System matter occurred at different times, roughly 100 Myr and 30 Myr before the formation of the Sun, respectively.

If I could gently raise some mild criticism, I would mention that in some cases I had the impression that either the uncertainty in the input parameters, the uncertainties in the measured chemical or isotopic distribution, or the neglects in the physical models, or the limitations in the numerical computations (i.e., simulation time or resolution) could limit the accuracy of the results or could weaken the robustness of conclusions. Many times the main limitations are highlighted in the thesis. Nonetheless, it could have been interesting to see a rigorous sensitivity analysis of the parameters. I wonder if at least intuitively, the results and the conclusions could be located (visualized) in a coordinate system with coordinate axes of uncertain-robust input parameters or measured data used for comparison (i.e., nuclear physics rate constants and/or elemental or isotopic ratios) *vs* uncertain-robust modelling simulations. (Maybe these axes could be separated into more axes.) Either a mathematically rigorous sensitivity analysis or a semi-qualitative coordinate system representation could demonstrate how rigorous a conclusion is or what should be revised in the future to make the statement more rigorous.

Further questions and comments:

- It seems to me that $^{96}\text{Zr}(n,\gamma)^{97}\text{Zr}(\beta^-)^{96}\text{Mo}$ and $^{96}\text{Zr}(n,\gamma)^{96}\text{Mo}$ on p29 are wrong.
- Why Se, Rb, and Cd do not condense into dust (p38)? (Or did I misunderstand the sentence?)
- It is well-explained in the dissertation, that in the case of stellar spectra – due to limited spectral resolution – the abundances of different elements, while in the case of dust particles – due to possible chemical separations of different elements – the isotopic mixing ratios could be compared to the results of the simulations. As it is mentioned in the dissertation, at cooler spectral atmospheres the formation of molecular species can result in uncertainties in elemental ratios. In geochemistry and in planetary atmospheric chemistry there are well-known thermal and photochemical processes that cause isotopic fractionations. Similar processes could also occur on the surface of dust particles. Can X-processes considerably change the isotopic ratios on grain surfaces? Are there any attempts in the literature to consider and take into account these effects, and correct the elemental/isotopic ratios?

The DSc thesis, and the publications in highly reputed international journals that form the basis of the thesis, contain many interesting results important both for the astrophysics and the nuclear physics community. Both the quantity and quality of the new results amply satisfy the requirements for the title of Doctor of the Hungarian Academy of Sciences, so it is clear that I recommend both the setting of a public debate and the acceptance of the DSc thesis.

Budapest, 13 November, 2022

György Tarczay

Institute of Chemistry
ELTE Eötvös University, Budapest