

REPORT

by **Prof. Dr. Eng. Petar Todorov Todorov**

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Member of the Academic Jury set to render a decision

on a procedure for the acquisition of Academic Degree “Doctor of Philosophy” (PhD) in the Professional Field 4.2. Chemical Sciences according to the Classifier of the Areas of Higher Education and the Professional Fields (Scientific Specialty “Polymers and Polymer Materials”) Doctoral thesis with title "Preparation of phosphor-containing products with added value based on recycled PET"

prepared by **Eng. Simona Miroslavova Zahova**

This Report is prepared in response to Order № ПД-09-178 of 19.12.2024 issued by the Director of the Institute of Polymers, Bulgarian Academy of Sciences, following the decision made by the Academic Jury that was held on 17.12.2024. The Report is in compliance with Development of Academic Staff in the Republic of Bulgaria Act (DASRB), the Rules for the Application of the Development of Academic Staff in the Republic of Bulgaria Act, the Rules of BAS and with the Rules set at the Institute of Polymers, Bulgarian Academy of Sciences, for applying the Act aforementioned.

1. Assessment of the scientific and research accomplishments of the candidate

1.1. Assessment to meet the minimal criteria in accordance with Specific the Rules for Granting Academic Degrees set at the Institute of Polymers, Bulgarian Academy of Sciences, Application 1.

According to the requirements of the Law on the Acquisition of Scientific Degrees and the Regulations for Acquiring Scientific Degrees and Occupying Academic Positions of the Bulgarian Academy of Sciences, the minimum total number of points from the indicators in groups A to E is 80 points. Simona Zahova participated with 116 points, which significantly exceeds the required points. Under indicator A, which brings 50 points, she has fulfilled the requirement and has submitted a dissertation. Its results are formed in 2 scientific publications in journals that are indexed and referenced in the world databases SCOPUS/Web of Science. Both publications have quartile Q1. According to these publications, the points under indicator D are 50 points, with a minimum of 30 points required. The relevance and significance of the obtained and published scientific results is evidenced by the fact that they have already been cited 8 times by foreign authors in journals referenced in SCOPUS/Web of Science and the respective points are 16 points.

1.2. Assessment of the scientific accomplishments of the doctoral thesis, as well as to the relevance of the topic

For the first time, a degraded product has been obtained that is used directly, without the need for its additional purification or processing, for the synthesis of new phosphorus-containing products via reaction of polycondensation with phenylphosphonic acid dichloride

or transesterification with trimethyl phosphate. Products of the interaction between a degraded product and phenylphosphonic acid dichloride have been obtained. It was found that the resulting oligomeric product has increased resistance to combustion. Thermogravimetric analysis of this product has shown an amount of charred residue of ~ 17%, which suggests the possibility of its application as a flame-retardant additive of polymers (polyurethanes, polyethylene terephthalate). The interaction between the degradation product of polyethylene terephthalate and trimethyl phosphate has resulted in the production of phosphoric acid triesters, which, in addition to being thermal stabilizers of polymeric materials or lithium-ion cells, can be part of the composition of additives that slow down the combustion of polymers. This is confirmed by the amount of carbon residue obtained after thermogravimetric analysis (~ 13 %).

In her dissertation, Eng. Simona Zahova has used a wide range of modern research methods and techniques, which prove the scientific results achieved. When characterizing the newly synthesized compounds, the appropriate methods such as: NMR spectroscopy, FT-IR spectroscopy, UV-Vis spectroscopy, thermogravimetric analysis, differential scanning calorimetry, X-ray diffraction analysis and other analyzes have been used.

The scientific achievements in the dissertation are presented through three conclusions and contributions:

➤ For the first time, titanium(IV) phosphate was used as a catalyst for the degradation of polyethylene terephthalate, through the process of glycolysis in MW heating.

➤ For the first time, value added products have been obtained by using directly the degraded product of polyethylene terephthalate glycolysis without the need for its additional processing, isolation or purification.

➤ For the first time, a method has been described to increase the value of products obtained from the glycolysis of waste polyethylene terephthalate by phosphorylating with phenylphosphonic acid dichloride and trimethyl phosphate to obtain new materials that have the potential to be used as additives that retard the combustion of polymers.

The contributions of the research arm of a scientifically applied nature and reflect the results presented.

In summarizing what has been said so far, it can be concluded that the PhD student has successfully coped with the tasks. Within the framework of the dissertation, sufficient quantity and quality of experimental work has been carried out, which reveals a huge potential for the future development of this extremely interesting and modern topic, both in the direction of fundamental research and in the direction of their practical application.

1.3. Assessments of the scientific production of the candidate and his contribution, as well as the reflection of the results in the works of other authors.

The results of the dissertation have been published in 2 prestigious international journals. One has been published in the journal *Polymer Degradation and Stability* (publisher: ELSEVIER) with quartile Q1, and the other in the journal *Molecules* (publisher: MDPI) with quartile Q1. In both publications, Eng. Zahova is the first author, and in one of them she is also a corresponding author. 8 citations of one of the publications have already been noticed, which is proof of the relevance of the research carried out and the interest in them in the scientific community.

During the development of his dissertation, Eng. Zahova has participated as a co-author with 4 oral and 3 poster papers presented at national scientific conferences. Part of the results of the dissertation are included in the development of the topic "Glycolysis of PET waste under conventional and microwave heating", selected as the most significant scientific and applied achievement of IP-BAS for 2023.

2. Notes and recommendations

I have no critical remarks on the merits. The dissertation is written clearly and accurately at a high scientific level. All documents are submitted as required. The PhD student has successfully passed the necessary exams. The abstract reflects correctly and accurately the results of the dissertation.

3. Conclusion

The presented dissertation is completely dissertable, with an original contribution to science in an interesting and promising field for application, such as polymer chemistry. The results obtained are up-to-date and have a scientifically applied nature. The conclusions made are supported by a sufficient volume of experimental results. During the development of the dissertation, Eng. Simona Zahova has mastered and upgraded various methods and techniques for synthesis and characterization of phosphorus-containing materials, which are described and interpreted very well with understanding and in good scientific language. The results are presented in 2 scientific publications with a high IF /quartile Q1/ and 7 reports at scientific forums. The presented materials and results fully comply with the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria and the Regulations for Acquiring Scientific Degrees and Occupying Academic Positions of the Bulgarian Academy of Sciences.

Based on the above, I confidently give a positive assessment of the dissertation of Eng. Simona Miroslavova Zahova and recommend to the esteemed members of the scientific jury to support her awarding the educational and scientific degree "Doctor" in the scientific specialty *4.2. Chemical Sciences, scientific specialty: Polymers and Polymeric Materials*.

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Sofia

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