

**PRODUCTION OF A HIGHLY EFFICIENT METAL-FREE CATALYTIC SYSTEM
FROM MELAMINE BARBITURATE AND ITS PRECURSORS BY THERMAL
DECOMPOSITION**

Pyarnits D.Yu. (ITMO University), **Yurova V.Yu.** (ITMO University)
Scientific supervisor – Professor, PhD Smirnov E.A. (ITMO University)

Introduction. In the modern world, switching to more environmentally friendly ways of producing raw materials and generating energy is a growing tendency. Therefore, the development and synthesis of new unique catalysts is an important task. One of the promising materials for these purposes is the photocatalyst such as $g\text{-C}_3\text{N}_4$. This catalyst is environmentally friendly, has high selectivity, resistance to various aggressive environments, and most importantly, is inexpensive to produce. $g\text{-C}_3\text{N}_4$ is an effective photocatalyst along with metal oxides [1]. It can be synthesized by thermal condensation of nitrogen-rich precursors such as urea, thiourea, cyanamide, dicyandiamide, and melamine [2,3]. The structural unit of $g\text{-C}_3\text{N}_4$ is heptazine, which upon heating transforms into a highly ordered polymer structure of melon [4]. This catalyst has a smaller bandgap than titanium dioxide, 2.7 eV compared to 3.2 eV respectively, so $g\text{-C}_3\text{N}_4$ exhibits photocatalytic properties when exposed to visible light [5].

The main part. The synthesis of $g\text{-C}_3\text{N}_4$ was carried out by co-precipitation of melamine with barbituric acid followed by thermal condensation in a tubular muffle furnace in an Ar atmosphere at different temperatures ranging from 300 to 550 °C with a heating rate of 5-10 °C/min and a reaction time ranging from 1 hour to 8 hours [6]. Powder X-ray diffraction (PXRD) from melamine sample revealed two characteristic peaks at 13.5° and 27.5°. The weak peak at 13.5° (6.55 Å) is related to the arrangement of heptazine units in the plane. The strong peak at 27.5° (3.24 Å) is related to the characteristic reflection of the interlayer arrangement of conjugated aromatic systems. However, when synthesizing $g\text{-C}_3\text{N}_4$ from melamine barbiturate, we obtained a different structure, on which the peak at 13.5° is absent, so triazine structure was obtained instead of heptazine. To understand the phase transformation upon heating of melamine barbiturate, a thermal analysis was carried out using thermogravimetric (TG) and differential scanning calorimetric analysis (DSC). A temperature ranges from 30 °C to 700 °C was detected with a heating rate of 3 °C/min. During the analysis, an aluminum crucible with a lid was used to prevent sublimation of melamine barbiturate. From the DSC data, several phase transformations are observed in the system. The most pronounced endothermic peak appears in the temperature range of 300-380 °C, and the mass of the sample quickly decreases by 86%. This indicates that sublimation and thermal condensation of melamine barbiturate occurred simultaneously in this temperature range. Two weak endothermic peaks at 335 and 361 °C should be noted, which correspond to further deammoniation and decomposition of the material, respectively.

Conclusions. Based on the PXRD and TGA data obtained, we have demonstrated the synthesis of a new $g\text{-C}_3\text{N}_4$ -like structure from melamine and barbituric acid. In the future, we plan to develop a platform for logic device based on the photocatalytic material that will work with visible and ultraviolet radiation. For this, we will investigate the synthesis process, properties and applications of our material, as well the correlation between the chemical structure and photoelectronic properties of the material.

References:

1. Tahir N. et al. Metal oxide-based ternary nanocomposites for wastewater treatment //Aquananotechnology. – Elsevier, 2021. – C. 135-158.
2. Wang X. et al. A metal-free polymeric photocatalyst for hydrogen production from water under visible light //Nature materials. – 2009. – T. 8. – №. 1. – C. 76-80.
3. Li J. et al. A facile approach to synthesize novel oxygen-doped $g\text{-C}_3\text{N}_4$ with superior visible-light photoreactivity //Chemical communications. – 2012. – T. 48. – №. 98. – C. 12017-12019.

4. Darkwah W.K., Ao Y. Mini Review on the Structure and Properties (Photocatalysis), and Preparation Techniques of Graphitic Carbon Nitride Nano-Based Particle, and Its Applications // *Nanoscale Res. Lett.* 2018. Vol. 13, № 1. P. 388.
5. Mohini R., Lakshminarasimhan N. Coupled semiconductor nanocomposite g-C₃N₄/TiO₂ with enhanced visible light photocatalytic activity // *Materials Research Bulletin.* – 2016. – T. 76. – C. 370-375.
6. Vinu A. et al. Preparation and characterization of well-ordered hexagonal mesoporous carbon nitride // *Adv. Mater. Wiley Online Library*, 2005. Vol. 17, № 13. P. 1648–1652.