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**ЭКСПЕРТНОЕ ЗАКЛЮЧЕНИЕ О ВОЗМОЖНОСТИ ОПУБЛИКОВАНИЯ**

Руководитель-эксперт Федерального государственного бюджетного учреждения науки Института элементоорганических соединений им. А.Н.Несмеянова Российской академии наук, рассмотрев статью Sinditskii V.P., Burzhava A.V., Usuntsinova A.V., Egorshv V.Yu, Palysaeva N.V., Saponitsky K.Yu, Ananiev I.V., Sheremetev A.B. «Increasing the burning rate through energetic compound tuning: Hybrids of the furazan and [1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine ring systems», направляемую в журнал *Combustion and Flame*, подтверждает, что в материале не содержатся сведения, предусмотренные Постановлением Правительства РФ №1233 от 30.11.1994г. и на публикацию материала не следует получать разрешение Минобрнауки России и/или Президиума РАН

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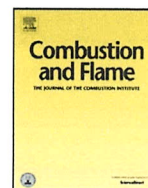
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# Increasing the burning rate through energetic compound tuning: Hybrids of the furazan and [1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine ring systems

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## ABSTRACT

Combustion behavior, flame structure, and thermal decomposition of hybrid compounds based on tetrazine, triazole and furazan rings have been described. It has been found that the introduction of [1,2,4]triazolo[4,3-b][1,2,4,5] tetrazine core into the molecules of energetic materials allows obtaining energetic hybrid compounds with combustion rates greater than those of common explosive HMX and RDX. These hybrids have good thermal stability, which depends on the substituent at the furazan ring, and not on the triazolotetrazine core. Combustion with thermocouple-aided studies has shown that all triazolotetrazine hybrids are nonvolatile and have high burning surface temperatures which cause their condensed-phase combustion mechanism. Based on the condensed-phase combustion model, the constants of the leading combustion reactions were determined. It turned out that the burning rates of nitrogen-rich compounds of this study are controlled by the decomposition kinetics at surface temperature. It is shown that the two-stage decomposition of substances leads to the appearance of two regions in the burning rate-pressure dependences that related to each other by the instability region. The incorporation of the triazolotetrazine moiety into an energetic compound is a promising way to design new propellant components with high burning rates and attractive performance.

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## 1. Introduction

Currently, hybrid compounds based on endothermic heterocycles such as furazan, tetrazole and triazole are of wide interest and importance due to their utilization in synthetic chemistry and as key backbone of energetic materials [1–7]. As a potential alternative to conventional explosives or components of rocket propellants, nitrogen-rich compounds form a promising class of energetic materials whose energy is derived, to a large degree, from their very high enthalpy of formation. The disadvantage of mononuclear furazan derivatives that prevent their practical use is high volatility. At the same time, 1,2,4,5-tetrazines and, especially, their fused derivatives are characterized by very high melting and boiling points and low volatility [8,9]. It can be assumed that the

synthesis of hybrids combining tetrazine and furazan rings can eliminate the above furazan's disadvantages and will allow obtaining new compounds with a novel set of properties.

Approaches to the production of hybrid compounds whose cores are a combination of the (un)fused tetrazine ring systems with various azoles have been described previously [1,5,10–12]. However, the properties of these hybrids have not been studied in sufficient detail. First of all, the burning rate is of interest, since nitrogen-rich compounds may be used as components that lower the flame temperature of the powders, as well as combustion modifiers of the powders and solid rocket propellants [13,14].

Recently [15], it was found that the binding of the triazolotetrazine backbone with 3,5-dinitro-1H-pyrazole unit through the NH-bridge leads to an increase in the burning rate and a decrease in the pressure index of burning law, that is very important for the components of gunpowder and solid rocket propellants. In this regard, the purpose of this work is to study the effect of the triazolotetrazine moiety on the combustion

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decomposition of substances leads to the appearance of two regions in the burning-rate dependences that related to each other by the transition or instability region.

The introduction of a triazolotetrazine moiety into a molecule of energetic compounds could open a new way to advanced propellant components with high burning rates and good practical properties as thermal stability and sensitivity.

### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.combustflame.2019.12.006.

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