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## Thermal Decomposition of Nitropyrazoles

A. Bragin<sup>a\*</sup>, Alla Pivkina<sup>a, b</sup>, N. Muravyev<sup>a</sup>, K. Monogarov<sup>a</sup>, Olga Gryzlova<sup>a</sup>, Tatyana Shkineva<sup>c</sup>, I. Dalinger<sup>c</sup>

<sup>a</sup> *Semenov Institute of Chemical Physics, RAS, Kosygin str. 4, Moscow 119991 Russia,*

<sup>b</sup> *National Research Nuclear University MEPhI, Kashirskoye shosse 31, Moscow 115409, Russia*

<sup>c</sup> *Zelinsky Institute of Organic Chemistry, Moscow 119991, Russia*

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### Abstract

Fully nitrated five-membered heterocycles (pyrazoles), polynitropyrazoles in particular, have been actively studied as promising high-energy materials. Polynitropyrazoles have high density and high enthalpy of formation combined with reduced sensitivity to external stimuli. We have studied non-equilibrium processes of thermal decomposition of the first members of high-energy polynitropyrazoles row, i.e., 3,4-dinitropyrazole, 3,5-dinitropyrazole, and 3,4,5-trinitropyrazole, under atmospheric and increased pressures. The use of increased pressure allowed to reduce the influence of evaporation process of 3,5-dinitropyrazole and to determine the temperature and heat effect of its decomposition, which was found to exceed this value for HMX. For the first time evolved gas products were identified for each stage of decomposition. As a result the probable thermal decomposition pathway for the investigated materials was suggested.

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*Keywords:* nitropyrazole; thermal analysis; high-pressure calorimetry; FTIR spectrometry; evolved gases analysis

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\* Corresponding author. *E-mail address:* [aabragin@gmail.com](mailto:aabragin@gmail.com)

**Nomenclature**

|       |                                    |
|-------|------------------------------------|
| $T_m$ | melting temperature                |
| $Q_m$ | heat of fusion                     |
| $T_o$ | onset temperature for heat release |
| $Q_d$ | heat release at decomposition      |

**1. Introduction**

Among new high-energy materials with higher performance and/or lower sensitivity fully nitrated five-membered heterocycles (pyrazoles) have high enthalpy of formation and high density. Recently synthesized 3,4,5-trinitropyrazole (TNP) has impact sensitivity value close to TNT, and detonation velocity close to ones of RDX and HMX [1-2]. 3,4-dinitropyrazole (DNP-1) could be used as a melt cast matrix, alternatively to TNT [4]. The aim of the present study is to investigate thermal stability both in atmospheric and high pressures for three polynitropyrazoles: 3,4-dinitropyrazole, 3,5-dinitropyrazole, and 3,4,5-trinitropyrazole (Fig. 1).

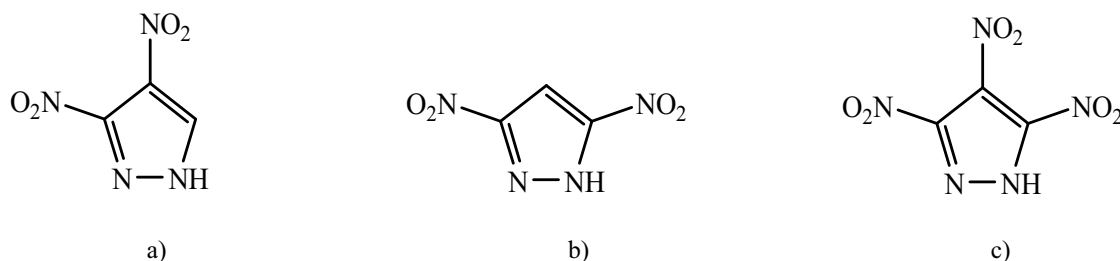


Fig. 1 Synthesized monocyclic polynitropyrazoles: a) - DNP-1 (3,4-dinitropyrazole), b) - DNP-2 (3,5-dinitropyrazole), c) - TNP (3,4,5-trinitropyrazole).

**2. Experimental study and results***2.1. Physical measurements*

The samples of the synthesized compounds were investigated by simultaneous thermal analysis DSC/TG at a scanning rate of 10 K/min using STA 449 F3 (Netzsch) apparatus. Samples of mass about 2 mg were placed into closed alumina pans with pierced lids and then heated in dynamic argon atmosphere 70 ml/min. In order to estimate the thermal stability under elevated pressure DSC 204 HP (Netzsch) was used. The scanning rate and the sample mass were the same. Samples were placed into the aluminum crucibles, covered with a pierced lids, sealed, and heated in dynamic nitrogen atmosphere (flow rate 100 ml/min) under 50 bar pressure. The temperature range for both DSC/TG and DSC HP was from 30 to 600°C.

Simultaneously with DSC/TG analysis, FTIR-spectroscopy via coupling Bruker ALPHA FTIR device was used to study the gas phase products. As a result a full set of FTIR spectra for the whole range of time (temperature) was obtained. The most intense peaks were selected, analyzed, and identified. Some of the peaks, however, were impossible to identify using NIST database. In order to identify these spectra and, probably, to attribute them to the vapors of investigated materials, IR spectra of initial compounds in chloroform solution were obtained. The matching of these peaks allowed indicating the evaporation of the initial materials. Concentration curves for the main gas products were calculated in relation to CO<sub>2</sub> [5]. For main products the relative concentration was plotted in the same scale, unlike the curves of the evaporated initial materials. message, with clear lines of thought and validation of the techniques described.

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