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ACCEPTED MANUSCRIPT

Thermal behaviour and safety of 1,3,7,9-tetranitrodibenzo-1,3a,4,6a-tetraazapentalen (z-TACOT)

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Highlights

- z-TACOT is a highly thermostable explosive
- Kinetic parameters were determined for initial stage of z-TACOT decomposition
- Calculated maximum safe temperature for processing z-TACOT is 263 °C

Abstract: 1,3,7,9-tetranitrodibenzo-1,3a,4,6a-tetraazapentalen (z-TACOT) is a thermostable compound which exhibits low-sensitivity to external stimuli. At elevated temperature it undergoes thermal decomposition. Thermal properties and safety of z-TACOT use in terms of the heat-explosion hazard were examined. The obtained kinetic parameters of the decomposition reaction and thermal capacity of z-TACOT were used to determine the maximum safe temperature of technological processes which involve z-TACOT. The temperature is 266 °C. Based on the attained safety parameters z-TACOT can be classified as a non-reactive, stable compound which does not exhibit dangerous behaviour in the Koenen test.

Keywords: thermal decomposition, kinetic parameters, ADT24, explosives, thermal explosion

1 Introduction

1,3,7,9-tetranitrodibenzo-1,3a,4,6a-tetraazapentalen (z-TACOT) is an explosive known since 1959 [1,2]. This compound is known under another name: TACOT [3]. At first, due to high production costs, this compound was not considered for prospective use. The growing requirements regarding the thermostability of explosives in special applications, such as the mining, cosmic and defense industries, make z-TACOT applicable in such areas [4,5]. z-TACOT is extremely thermostable, withstands heating for 10 h at 315° C without noticeable signs of decomposition [6]. z-TACOT belongs to the group of C-nitro explosive compounds. Its structure is shown in Fig. 1.

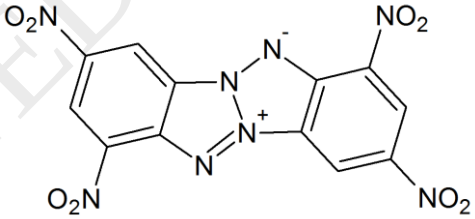

Fig. 1. Structure of z-TACOT.

Despite the fact that z-TACOT has been known for decades, there are no detailed studies of its thermal properties, and the available numbers exhibit significant discrepancies (activation energy 292 kJ · mol^{-1} [7], 234.3 kJ · mol^{-1} [8]). In the literature there is no information available about changes in kinetic parameters of the z-TACOT decomposition reaction as a function of the conversion. The kinetic parameters of the decomposition reactions determined by the Kissinger method which can be found in the literature do not allow the assessment of the safety of application of z-TACOT [7,9]. In the Kissinger method, kinetic parameters are determined based on the minimum of the decomposition peak, which are determined for a high degree of conversion. During the decomposition high energy material, many simultaneous and subsequent reactions take place. Analysis of the sample's properties with a high degree of conversion refers to a mixture of the starting compound and its degradation products (for a one-step reaction) or a mixture containing only traces of the starting compound (for multi-stage reactions, e.g. TNT decomposition, 94% of the substance reacts until 64% of the heat has been produced [10]). Kinetic parameters are the resultant of all of the processes occurring during sample decomposition and can undergo substantial changes as the conversion rate changes [11,12].

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