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COMPARATIVE STUDY OF THERMAL STABILITY AND COMBUSTION OF DINITROPYRAZOLE ISOMERS

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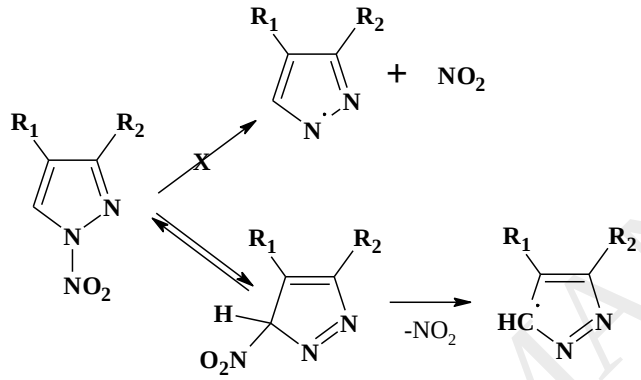
Graphical abstract



Highlights

- Decomposition of N-nitropyrazoles is controlled by reaction of isomerization.
- The following C-NO_2 bond rupture is not rate-limiting stage.
- Isomeric dinitropyrazoles have different thermal stability and volatility
- Despite different properties all dinitropyrazoles have close burning rates.
- Melt-castable isomeric dinitropyrazoles burn at the same rates as well-known HMX.

Abstract

A comparative study of the thermal stability and combustion peculiarities of three dinitropyrazole isomers was carried out. It has been found that the rate-limiting stage of the decomposition of 1,3-dinitropyrazole (1,3-DNP) and 1,4-dinitropyrazole (1,4-DNP) both having the N-bounded nitro group, is the N→C migration of the nitro group rather than its elimination, followed by secondary decomposition reactions of non-aromatic 3H-pyrazole. In the case of 3,4-dinitropyrazole (3,4-DNP) the rate-limiting stage is assumed to be the nitro group elimination. All the studied pyrazole isomers revealed close burning rate vs. pressure dependences despite significant differences in the thermal stability and volatility.

Key words: combustion, thermal decomposition, dinitropyrazoles, kinetics.