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Thermal decomposition peculiarities and combustion behavior of nitropyrazoles

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Abstract

Physico-chemical characterization of high energetic nitropyrazoles has been conducted, including studies on the thermal decomposition under non-isothermal and isothermal conditions, burning behavior, and flame structure. The thermal stability of dinitropyrazoles, such as 3,4-dinitro-1*H*-pyrazole (3,4-DNP), N-(3,5-dinitro-1*H*-pyrazol-4-yl)-[1,2,4]triazolo[4,3-*b*][1,2,4,5]tetrazin-6-amine (ADNPTrTz), and 3,3',4,4'-tetranitro-1,1'*H*-bipyrazole-5,5' (TNBP) in the liquid phase lies between stability of nitramines RDX and HMX. The decomposition of dinitropyrazole moiety in 3,4-DNP and TNBP starts from a nitro group loss. If the nitropyrazole molecule contains the amino group, the thermal decomposition may begin with NO₂ group isomerization followed by decomposition of either the pyrazole ring or formed furazan cycle. The pyrazole moiety is resistant to oxidation by NO₂, leading to low heat effect at the initial decomposition stages and bringing about difficulties in determining real kinetics from DCS experiments. The activation energy of decomposition of 4-amino-3,5-dinitro-1*H*-pyrazole (ADNP) appeared to be rather low (108.8 kJ/mol) that might be indicative of possible hazard in handling this compound, even though its decomposition temperature is high enough. Combustion studies have shown that the burning rate of the nitropyrazoles depends on the surface temperature as well as on the condensed-phase heat release rate which, in turn, is subject to the decomposition kinetics. Thermocouple-aided measurements have revealed the surface temperatures of 3,4-DNP and ADNP both to be high enough and close to that of RDX. A shortage of heat to warm up the compound to the surface temperature is supposed to be a reason for (a) the observed combustion instability of ADNP and ADNPTrTz at low pressures, (b) occurrence of high pressure limit of 3,4-DNP combustion, and (c) inability of TNBP to burn at pressures up to 20 MPa.

Introduction

Nitro derivatives based on mono, two or more bonded nitrogen heterocyclic rings have recently been studied extensively for their wide applications in the materials science [1-4]. Nitropyrazole unit has become a quite popular building block and has been shown to be very successful in producing thermally stable and relatively insensitive to friction and impact energetic materials [5-9]. Progress in the synthesis and chemistry of nitropyrazoles has been the subject of several reviews [10,11].

As the thermal and combustion behaviors determine a number of the desirable

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