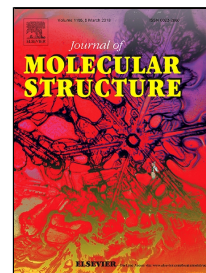


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# Effects of hydrogen bond on the melting point of azole explosives

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## Abstract

Melting point is an important index to determine whether an explosive can be a melt cast carrier. In this study, the relationship among the molecular structure, crystal structure, and melting point of explosives was investigated by using nitroazole compounds. Hydrogen bonds influence crystal packing modes in chemically understandable ways. Hydrogen bonds also affect the changes in entropy and enthalpy in balancing melting process. Hence, different types of hydrogen bonds in explosive crystal structures were compared when the relationship between the molecular structure and the melting point of nitroazole explosives were analyzed. The effects of methyl and amino groups on intermolecular hydrogen bonds were also compared. Results revealed that the methyl and amino groups connected on the N(1) of the heterocyclic compound can reduce the melting point of azole explosive. This finding is possible because methyl and amino groups destroy the intermolecular hydrogen bond of the heterocyclic compound.

## Keywords

hydrogen bond, melting point, carriers for melt-cast explosives, methyl, amino

## 1. Introduction

Melt cast explosive is a loading technique widely used in local and foreign armaments. It is a molding method that melts and mixes 2,4,6-trinitrotoluene or other explosives through calefaction at 90 °C and then injects the mold or cartridge to cool, solidify, and form various shapes and dimensions.<sup>1,2</sup> In accordance with the casting and forming requirements of explosives, the melting point of carriers for melt cast explosives are usually not higher than 120 °C to accommodate steam melting explosives.<sup>3</sup> The development of new carriers for melt cast explosives mainly focuses on molecular design and performance prediction.<sup>4</sup> Compared with the features of other explosives, the major characteristics of carriers for melt cast explosives are low melting point and narrow melting

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