

## Synthesis and Properties of 2,6-Dinitro-3,7-dis(nitroimino)-2,4,6,8-tetraazabicyclo[3.3.0]octane

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**Abstract:** A novel high energetic density compound 2,6-dinitro-3,7-dis(nitroimino)-2,4,6,8-tetraazabicyclo[3.3.0]octane (TNGG) was synthesized using 3,7-bis(nitroimino)-2,4,6,8-tetraazabicyclo[3.3.0]octane as raw material and acetic anhydride as acylation reagent by acylation reaction and nitration reaction. Its structure was characterized. The factors affecting the yield of TNGG were investigated. Its thermal decomposition behavior was studied by thermogravimetric-differential scanning calorimetry (TG-DSC) analysis. Based on the density, the detonation performance of TNGG were obtained by isodesmic reaction and Kamlet-Jacobs formula. Results indicate that the yield of TNGG is up to 31.3% under the optimum synthetic conditions of reaction time 15 min, reaction temperature 25 °C and 98% fuming nitric acid/phosphorus pentoxide as nitrating system. The TG-DSC curves show that the thermal decomposition of the compound is completed within 700 °C, with the mass loss about 100%. The thermal decomposition peak temperature of TNGG is 182.6 °C, indicating that it has a good thermal stability. Theoretical calculations show that the hydrolysis stability of TNGG is better than that of tetranitroglycoluril (TNGU). The theoretical detonation velocity and detonation pressure of TNGG are 9.76 km · s<sup>-1</sup> and 44.0 GPa, respectively, better than those of HMX and RDX.

**Key words:** high energetic density compound; nitration reaction; 2,6-dinitro-3,7-dis(nitroimino)-2,4,6,8-tetraazabicyclo[3.3.0]octane (TNGG); thermal behavior; detonation performances

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