Synthesis and Characterization of 3-Amino(nitro)-5-nitro- 1,2,4-triazole derivatives

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Abstract: Two new heat-resistant explosives of 1-picryl-3-amino-5-nitro-1,2,4-triazole(TNTA-TNB) and 4-picryl-3,5-dinitro-1,2,4-triazole(DNT-TNB) were synthesized via condensation of 3-amino-5-nitro-1,2,4-triazole(ANTA)(or ammonium 3,5-dinitro-1,2,4-triazole(ADNT)) with 2,4,6-trinitrochlorobenzene. The condensation mechanism was explored and discussed. The effects of some key reaction conditions, such as media, temperature, time and catalysts, on condensation were investigated. The explosive synthesis was carried out at 70 ℃, 8 h in DMF and NaF as catalyst. IR, NMR and elemental analysis confirmed the synthesized compound structures. In addition, we imroved the synthetic process of 2,4,6-tris(3-amino-5-nitro-1,2,4-triazole-1-yl)-1,3,5-triazine by means of direct reaction of ANTA with 2,4,6-trichloro-1,3,5-triazine omitting the preparation of ANTA-Na and without using phase transfer catalyst, lowering the production cost, simplifing the procedure, and improving the reaction safety.

Key words: organic chemistry; 3-amino-5-nitro-1,2,4-triazole(ANTA); 3,5-dinitro-1,2,4-triazole; synthesis; characterization
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