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Synthesis and Property Prediction of 1,1-Bis(picrylamino)-2,2-dinitroethylene

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Abstract: 1,1-Bis(picrylamino)-2,2-dinitroethylene (TFT) was synthesized using 2,4,6-trinitrochlorobenzene and 1,1-diamino-2,2-dinitroethylene (FOX-7) as raw materials and KF and imidazole as catalysts by condensation with the yield of 71.3% and melting point of 225-226 ℃. Its structure was identified by IR, NMR and MS. Its thermal stability was analyzed by DSC and the decomposition temperature was 331.3 °C, which indicating that its thermal stability was better than that of FOX-7. The theoretical density of TFT after optimizing predicted by Monte-Carlo method is 1.85 g · cm⁻³. The heat of detonation, detonation velocity and detonation pressure predicted by Kamlet-Jacobs formula are 1751.26 J \cdot g⁻¹, 8.83 km \cdot s⁻¹ and 36.25 GPa, respectively. Impact sensitivity (H_{50}) is 156 cm. All the results show that TFT is more insensitive and has higher detonation pressure than FOX-7.

Key words: 1,1-bis(picrylamino)-2,2-dinitroethylene(TFT); synthesis; detonation performance; thermal performances

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《含能材料》"观点"征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了"观点"栏目。"观点" 栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要 erials.or 研究工作介绍。

《含能材料》损伤与点火专栏征稿

含能材料的损伤特征与点火过程有密切的联系,炸药、推进剂的内部损伤及其对力学特性、安全特性和点火行为的影 响规律受到了含能林料学界的高度重视,为推动这一重要研究方向的学术交流,本刊特设立"损伤与点火"专栏。专栏主要 征集炸药、推进剂等含能材料的损伤观测与多尺度表征技术、含损伤的本构方程、准静态与动态损伤演化规律、损伤与破坏 的宏(细)观模式、损伤对起爆、爆炸、爆轰成长以及非冲击起爆行为的影响等方向的原创性研究论文。来稿请注明"损伤与

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