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## Synthesis and Properties of 3-Cyano-4-nitrofurazan

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**Abstract:** 3-Cyano-4-nitrofurazan was synthesized from dicyanopropane via diazotisation, addition, cyclization and oxidation reactions, and its structure was characterized by IR, <sup>13</sup>C NMR and <sup>15</sup>N NMR and elemental analysis. The yields of cyclization and oxidation reactions are 55.1% and 83.6%, respectively. In the <sup>13</sup>C NMR, the chemical shifts were assigned by comparing with 3-cyano-4-nitrofurazan, which further confirm the configuration of 3-cyano-4-nitrofurazan. The bond order, density, enthalpy of formation and detonation parameters of 3-cyano-4-nitrofurazan were calculated theoretically. Results show that the minimum bond order are N(1)—O(4) (0.84) and C(6)—N(9) (0.91), the density is up to 1.74 g · cm<sup>-3</sup>, the enthalpy of formation is 352.6 kJ · mol<sup>-1</sup>, and the detonation velocity and detonation pressure are 8352 m · s<sup>-1</sup> and 30.9 GPa, respectively.

**Key words:** 3-cyano-4-nitrofurazan; synthesis; quantum chemistry

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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研究工作介绍。

## 《含能材料》“损伤与点火”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材料学界的高度重视,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新性研究论文。来稿请注明“损伤与点火”专栏。

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