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Empirical Calculation of the Explosion Parameters of Nitrodiazole Explosives

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Abstract: New polynitroimidazole explosive molecules were designed using 2, 4, 5-trinitroimidazole as "matrix" structural unit. The explosion parameters of designed explosives were calculated by Brinkley-Wilson(B-W) rule for predicting explosion decomposition products, Rothsteine′s method for estimating detonation velocity and Kamlet method for estimating C-J pressure. And the calculated detonation parameters were compared with those of RDX and HMX explosives. Results show that the designed explosives are a new class of high energy density material compounds with high density, detonation velocity and detonation pressure approaching to that of RDX even HMX. As imidazole ring in the molecules, having aromacity, the stability of these explosives molecules designed is favorable for potential application.

Key words: organic chemistry; high energy density material compound; polynitroimidazole; explosion parameters; empirical calculation

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《含能材料》创刊 20 周年纪念活动——专刊征稿

2013 年,《含能材料》迎来创刊 20 周年。过去的 20 年,是我国含能材料科学技术事业大发展的 20 年,也是《含能材料》稳步发展、茁壮成长的 20 年。作为以董海山院士为代表的我国火炸药科技事业的开拓者们创建的专业学术期刊,《含能材料》见证了我国火炸药、推进剂等领域 20 年来的光辉发展历程。20 年来,《含能材料》凝炼出"传承火药文明,创新能源材料"的办刊理念。

重温过去,展望未来,为纪念《含能材料》创刊 20 周年,《含能材料》将于 2013 年 4 月(第 2 期)出版"《含能材料》创刊 20 周年纪念专刊",并特设新能源材料专栏,报道聚变能源材料、储氢材料、金属氢等新能源材料的研究成果。

为此,特向国内外广大专家征集研究快报、研究论文和综述,以期集中反映我国近年来在含能材料、新概念含能材料及其相关领域取得的重要学术成果。

稿件类型:(1) 简要报道新概念含能材料最新研究成果的研究快报(英文),以基金项目为主;(2) 具有较高创新性的原创研究论文;(3) 具有较高水平的综述文章。

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