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研究论文

含能材料的密度、爆速、爆压和静电感度的理论研究

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摘要 用密度泛函理论(DFT) B3LYP方法, 在6-31G*基组水平下, 全优化计算了系列硝胺类和硝基芳烃类爆炸物的几何构型, 用Monte-Carlo方法和自编程序, 基于0.001 e•bohr^{-3}等电子密度面所包围的体积空间求得分子平均摩尔体积(V)和理论密度(ρ). 用Kamlet-Jacobs方程基于理论密度(ρ)和PM3计算生成焓(ΔH_f)估算标题物的爆速(D)和爆压(p), 发现多环硝胺类化合物的爆轰性能优于芳烃硝基类化合物, 故此, 在寻求高能量密度材料(HEDM)时, 我们应特别关注多环硝胺化合物. 与ρ和D文献值比较, 表明本理论计算方法和结果是适用可靠的. 将爆速(D)和爆压(p)计算值与静电感度实验值(E_{ES})进行比较和关联, 发现: 若对化合物进行细致分类讨论, 则它们之间存在较好的线性关系. 据此建议, 在含能材料分子设计中, 可通过理论计算爆轰性质(D或p)去预估难以定量求得或尚未合成的含能材料的静电火花感度值(E_{ES}). 此外, 我们还讨论了取代基对ρ, D和p的影响, 也有助于分子设计.

关键词 硝胺和硝基芳烃类化合物 密度泛函理论 密度 爆速 爆压 静电感度

分类号

Theoretical Studies on Densities, Detonation Velocities and Pres-sures and Electric Spark Sensitivities of Energetic Materials

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Abstract The DFT-B3LYP method, with basis set 6-31G*, is employed to optimize molecular geometries and electronic structures of a series of nitramines and nitro arenes. The averaged molar volume (V) and theoretical density (ρ) are estimated using the Monte-Carlo method based on 0.001 e•bohr^{-3} density space. Subsequently, on the basis of the theoretical density and en-thalpy of formation (ΔH_f) which is calculated by using the PM3 method, the detonation velocity (D) and pressure (p) of the explosives are estimated by using the Kamlet-Jacbos equation, and we found that the detonation characteristics of the multicyclic nitramines is superior to nitro arenes. Consequently, we ought to pay more attention to the multicyclic nitramines in seeking high energy density materials (HEDM). The reliability of this theoretical method and results are tested by comparing the theoretical values of ρ and D with the experimental or referenced values. The theoretical val-ues of D and p are compared with the experimental values of electric spark sensitivity (E_{ES}). It is found that, there are quantitative relationships between the experimental E_{ES} values and the theoretical values of D and p if the titled com-pounds are particularly classified. In addition, we have discussed that the substituting groups have effects on density, detonation velocity and pressure, and the result suggests that such a theoretical approach can be used to predict their E_{ES} values which are difficult to predict quantitatively or to synthesize. In addition, we discussed the effects of substituting groups on density, detonation velocity and detonation pressure, and the obtained result is advantageous to design the molecules.

Key words a series of nitramines and nitro arenas density functional theory density detonation velocity detonation pressure electric spark sensitivity

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