[1]何飘,张建国,殷昕,等.5,8-二硝基四唑并三嗪的理论研究[J].火炸药学报,2015,38(3):27-31.[doi:DOI：10.14077/j.issn.1007-7812.2015.03.004]

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5,8-二硝基四唑并三嗪的理论研究

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Title:]Theoretical Study of 5,8-Dinitro-5,6,7,8-tetrahydrotetrazolo［1,5□b］［1,2,4］triazine (DNTzTr)

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Keywords: physical chemistry; density functional theory; DFT; polynitro substituted tetrazolotriazine; enthalpy of formation; detonation performance

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摘要: 运用量子化学方法研究了5,8-二硝基四唑并三嗪化合物的结构和性能。在B3LYP/6-311+G(2d)理论水平下，对其进行了几何优化及计算了电子密度、IR和NMR，以探究其电子结构性质和化学键本质，预估了密度、生成焓和爆炸性能等关键参数。结果表明，5,8-二硝基四唑并三嗪生成焓为497.64kJ/mol，密度为1.82g/cm3，其爆速和爆压分别为8.73km/s和33.97GPa，具有良好的爆炸性能，有望成为潜在的含能材料。

Abstract: The structure and properties of 5,8-Dinitro-5,6,7,8-tetrahydrotetrazolo［1,5□b］［1,2,4］triazine (DNTzTr) were investigated by using quantum chemistry methods.The optimized geometry and electronic density, IR and NMR spectrum data were calculated for inspecting the electronic structure properties and nature of chemical bonds at B3LYP/6-311+G(2d) level. The critical macroscopic properties such as density, enthalpy of formation and detonation performance have been also predicted. The results show that the enthalpy of formation and density of DNTzTr are 497.64kJ/mol and 1.82g/cm3,respectively. The detonation velocity and pressure are 8.73km/s and 33.97GPa, respectively.It possesses good detonation properties and can be the potential energetic materia.

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