

3-硝基-1, 2, 4-三唑-5-酮二甲胺盐 (CH₃)₂NH²⁺+C₂N₄O₃H⁻的合成、晶体结构和量子化学研究

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摘要 利用3-硝基-1, 2, 4-三唑-5-酮(NTO)的乙醇溶液与二甲胺的水溶液合成了 NTO的二甲胺盐(CH₃)₂NH₂⁺+C₂N₄O₃H⁻, 在二甲基甲酰胺(DMF)和甲醇的混合溶剂(体积比为1:5)中培养出单晶。通过X射线单晶结构分析法测定分子结构和晶体结构, 晶体属单斜晶系, 空间群为P2(1)/c, 晶胞参数为: a=0.7116(1)nm, b=0.8735(2) nm, c=1.3160(3)nm, β=101.12(2)°, V=0.8026(3)nm³, D_c=1.450 g/cm⁻³, Z=4, F(000)=368。采取HF/6-31+G(d)和MP2/6-31+G(d)以及B3LYP/6-31+G(d)方法对标题化合物进行了几何全优化, 并对其成键情况、原子净电荷分布及化合物的稳定性进行了分析。

关键词 [三唑酮](#) [硝基化合物](#) [二甲胺](#) [二甲胺 P](#) [晶体结构](#) [X射线衍射分析](#) [稳定性](#)

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Preparation, Crystal Structure and Theoretical Calculation of (CH₃)₂NH₂⁺+C₂N₄O₃H⁻

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Abstract (CH₃)₂NH₂⁺+C₂N₄O₃H⁻ was prepared by mixing 3-nitro-1,2,4-triazol-5-one (NTO) ethanol solution and the dimethylamine aqueous solution. Single crystals suitable for X-ray measurement were obtained by recrystallization with the mixed solvent of dimethyl formamide and methanol (V:V = 1 : 5) at room temperature. The crystal is monoclinic, space group P2(1)/c with crystal parameters of a = 0.7116(1) nm, b = 0.8735(2) nm, c = 1.3160(3) nm, β = 101.12(2)°, V = 0.8026(3) nm³, D_c = 1.450 g/cm⁻³, Z = 4 and F(000) = 368. The theoretical investigation of the title compound as structure unit was carried out by HF/6-31 + G(d), MP2/6-31 + G(d) and B3LYP/6-31 + G(d) methods, and the atomic net charges and the population analysis have been discussed.

Key words [TRIADIMEFON](#) [NITRO COMPOUNDS](#) [DIMETHYLAMINE](#) [DIMETHYLAMINE P](#) [CRYSTAL STRUCTURE](#) [XRD](#) [STABILITY](#)

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