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The Synthesis of 2, 6 diamino- 3, 5-dinitropyridine from Direct Nitration Reaction of 2, 6 diamino pyridine in Different Temperature Conditions by Density Functional Theory

Neda Hajizadeh*

Department of Chemistry, Yadegar-e-Imam Khomeini (RAH) Shahre-rey Branch, Islamic Azad University, Tehran, Iran

*Corresponding author Fax number: Tel.: +98 9358778448

*E-mail: nedahajizadeh83@gmail.com

ABSTRACT

In this article, synthesis of the explosive 2, 6 (diamino) 3, 5 dinitro pyridine (ANPY) of the direct nitration reaction of 2, 6 diamino pyridine in different conditions of temperature, with density functional theory method were studied. For this purpose, at first the material contained in the both sides of reaction were geometrically optimized, then the calculation of the thermodynamic parameters performed on all of them. The amount of ΔH , ΔS and ΔG of this reaction at different temperatures in form of sum of parameters discrepancy in the products than reactants is obtained and finally, the best temperature for the synthesis of explosive according to the obtained thermodynamic parameters were evaluated.

Keywords: Explosives, ANPY, synthesis, 2, 6 diamino 3, 5 – dinitro pyridine, nitration reaction