



Original Article.

Determination of Amino-1,2,3,4-tetrazole (PAT) from the reaction of Article 5 - Amino-1,2,3,4-tetrazole with Chloride Pyr-Chloride

Neda Hajizadeh* and Azade Saadat

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 research, the synthesis of Article 5 -Pacrylamino-1,2,3,4-tetrazole (PAT) from the reaction of the 5-amino-1,2,3,4-tetrazole with chloride picral in various temperature conditions was studied by the method of density functional theory it placed. For this purpose, the materials were first geometric optimization reaction sides, then the thermodynamic parameters were calculated for all of them. Then the values of H, ΔG , $\Delta S\Delta$ of this reaction are obtained at different temperatures as the sum of these parameters in the products to the raw materials. Finally, the best temperature for the synthesis of explosives was evaluated according to the thermodynamic parameters

Keywords: 5 - Amino-1,2,3,4-tetrazole (PAT), Synthesis, 5-Amino-1,2,3,4-tetrazole, Chloride Pyridine.
