Theoretical study of alkaline acetylation of diphenylamine

Silvana Caglieri*, Héctor Macaño, Gustavo Servetti
CIQA-Centro de Investigación y Transferencia en Ingeniería Química Ambiental.
Universidad Tecnológica Nacional - Facultad Regional Córdoba. Córdoba, Argentina.
*scaglieri@quimica.frc.utn.edu.ar

Abstract:

The acetylation of amines is one of the most frequently used transformations in organic synthesis as it provides an efficient and inexpensive means for protecting amino groups in a multistep synthetic process and the amide bond is found to be present in a large number of pharmacologically active molecules.

Acetylation of amine is a nucleophilic substitution reaction. This reaction is carried out with acetic anhydride in the presence of amine bases such as tertiary amine and pyridine. Computational investigation[1] and an experimental work[2], agreed that this reaction takes place with the formation of a tetrahedral intermediate.

A theoretical study of alkaline acetylation of diphenylamine from the analysis of intermediate of the reaction was carried out. Geometries of all species involved in the acetylation were made and identified. Energies of all reagents and products and the energy of activation for the reaction were calculated using the method DFT - Density Functional Theory with B3LYP level of theory and was adopted the 6-31+G* basis set. Following the same procedure it was identified the geometric parameters and energy of intermediate. All the calculations were executed using Gaussian 09 software package. The calculations show 18.01 kcal/mol of activation energy.

References:

1. Tong, X.; Ren, Z.; Qü, X.; Yang, Q.; Zhang, W. *Research on Chemical Intermediates* **2012**, *38*, 1961-1968.
2. Yadav, V. K.; Babu, K.G.; Mittal, M. *Tetrahedron* **2001**, *57*, 7047-7051.