

Theoretical Study of Acid Acetylation of Ethylamine

S.C.Caglieri¹

scaglieri@quimica.frc.utn.edu.ar

¹CIQA-Centro de Investigación y Transferencia en Ingeniería Química Ambiental. Universidad Tecnológica Nacional - Facultad Regional Córdoba. Avenida Cruz Roja Argentina esquina Maestro López. X5016ZAA. Córdoba, Argentina.

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. Acetylation of amine is a nucleophilic substitution reaction. This reaction can be catalyzed by Brønsted acid. In the mechanism, the acetic anhydride first accepts a proton at the carbonyl oxygen and this change enhances the positive charge on the carbonyl carbon. This protonation facilitates the successive addition of amine at the position to form a tetrahedral intermediate, determining step of the rate of the reaction. Computational method to study the reaction using acid catalysis [1] and an experimental work [2], agreed that this reaction takes place with the formation of a tetrahedral intermediate. A theoretical study of acid acetylation of ethylamine from the analysis of intermediate of the reaction was carried out. Geometries of all species involved in the acetylation were made and identified. All of the geometry optimizations were performed by the method at the DFT - Density Functional Theory [3] with B3LYP level of theory and was adopted the 3-21+G* basis set. Energies of all reagents and products and the energy of activation for the reaction were calculated using the AM1- Austin Model 1 method. 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 33.89 kcal/mol of energy for the tetrahedral intermediate and the activation energy was 9.07 kcal/mol. It was observed a marked consistency between the theoretical results and bibliographic data, which validates the use of theoretical methods DFT and AM1 as tools for kinetic studying the reaction of acetylation of ethylamine.

Keywords. Acetylation, Ethylamine, AM1, DFT

Acknowledgements. This work was supported by UTN. We thank UTN 1403

References.

- [1] Kruger H.G., *Journal Molecular Structure (Theochem)*. **2002**. 577. 281- 285.
- [2] Prasad H.S., Srinivasa G.R., Channe Gowda D., *Synthetic Communications*. **2005**. 35. 1189- 1195.
- [3] Lee C., Yang W., Parr R.G., *Physical Review B*. **1988**. 37. 785-789.