THEORETICAL STUDY OF ACETYLATION OF ETHYLAMINE CATALYZED BY Co^{2+} IONS

S.C.Caglieri, G.I.Servetti, *Universidad Tecnológica Naciona, Facultad Córdoba, Argentina*
scaglieri@quimica.frc.utn.edu.ar

Theoretical study of acetylation of ethylamine catalyzed by Co^{2+} ions from the analysis of intermediate of the reaction was carried out. The study of acetylation of amines is of great interest by the utility of its products of reaction and 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 Lewis acid[1], metallic ion. In reaction mechanism, the metallic ion formed a complex with the oxygen of the acetic anhydride carbonyl, facilitating the polarization of the same and the successive addition of amine at the position to form a tetrahedral intermediate, determining step of the rate of the reaction. Experimental work[2] agreed that this reaction takes place with the formation of a tetrahedral intermediate. In the present theoretical work were investigated the structure and energy of the tetrahedral intermediate of the reaction catalyzed by Co^{2+} ions. 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/B3LYP level of theory and the method MP2. Were adopted the 6-31+G* basis sets. Energies were calculated using DFT, MP2 and the Mechanics-UFF method. Following the same procedure it was identified the geometric parameters and energy of reaction intermediate. The reaction and the compounds studied are shown in Figure 1.

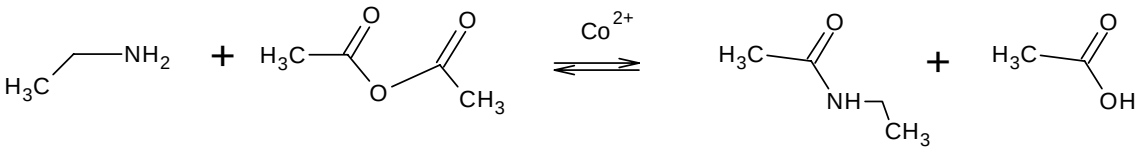

Fig.1. General Scheme of Acetylation of Ethylamine

The Mechanics-UFF method reported lower energy values for the studied chemical system. The calculations show 63.12 kcal/mol of energy for the tetrahedral intermediate and the energy of activation for the reaction was 14.85 kcal/mol. It was observed a marked consistency between the theoretical results and bibliographic data.

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1. K. Jeyakumar, D.K.Chand, Journal of Molecular Catalysis A: Chemical, 255, 275 (2006)
2. S. Farhadi, S. Panahandehjoo, Applied Catalysis A: General, 382, 293 (2010)