



## CLAFOO-XIV

**14<sup>a</sup> Conferencia Latinoamericana de Físico-Química Orgánica**  
**14<sup>th</sup> Latin American Conference on Physical Organic Chemistry**

**7<sup>th</sup> – 11<sup>th</sup> of May 2017, Concón, Chile**

---

Presenter's Name: Caglieri SilvanaClaudia

Mailing Address: Avenida Cruz Roja Argentina esquina Maestro López. X5016ZAA, Ciudad Universitaria, Córdoba, República Argentina.

Telephone: +54-9-351-4684317

E-mail: [scaglieri@quimica.frc.utn.edu.ar](mailto:scaglieri@quimica.frc.utn.edu.ar)

Title of the contribution: Theoretical Study of Acetylation of p-methylaniline catalyzed by Ni<sup>2+</sup> ions

Authors' names: Caglieri Silvana C., Macaño Héctor R. and Servetti Gustavo I.

Preferred mode of presentation is (check one)

Oral Presentation

Poster

Date:

Files should be named by presenter's last name followed by the first letters of name (i.e BrownJG.doc) and save as Word document.

Send this filled document to: [clafqo14@gmail.com](mailto:clafqo14@gmail.com)

DEADLINE FOR SUBMISSION OF ABSTRACTS: March 3<sup>rd</sup>, 2017

## Theoretical Study of Acetylation of p-methylaniline catalyzed by Ni<sup>2+</sup> ions

S. C. Caglieri<sup>a,\*</sup>; H.R. Macaño<sup>a</sup> and G.I. Servetti<sup>a</sup>

<sup>a</sup>CIQA- Centro de Investigación y Transferencia en Ingeniería Química Ambiental,  
Facultad Regional Córdoba - Universidad Tecnológica Nacional, Córdoba, República Argentina

\* scaglieri@quimica.frc.utn.edu.ar

A theoretical study of acetylation of p-methylaniline catalyzed by Ni<sup>2+</sup> 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<sup>1</sup>, metallic ion. The reaction and the compounds studied are shown in Figure 1.

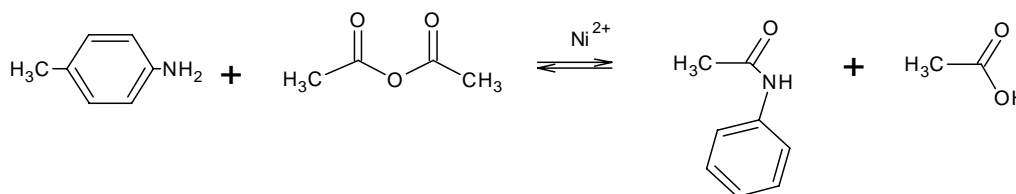


Fig. 1: General Scheme of Acetylation

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<sup>2</sup> 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 Ni<sup>2+</sup> 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 was adopted the 6-31+G\* basis set. Energies were calculated using the Mechanics-UFF method. Following the same procedure it was identified the geometric parameters and energy of reaction intermediate.

The calculations show 61.89 kcal/mol of energy for the tetrahedral intermediate and the energy of activation for the reaction was 16.05 kcal/mol.

### References

1. Aerry, S., Kumar, A., Saxena, A., De, A. and Mozumdar, S., "Chemoselective acetylation of amines and thiols using monodispersed Ni-nanoparticles", *Green Chem. Lett. Rev.*, Vol. 6, No. 2, 2013, pp.183-188, <http://dx.doi.org/10.1080/17518253.2012.737029>
2. Farhadi S. and Panahandehjoo, S., "Spinel-Type Zinc Aluminate (ZnAl<sub>2</sub>O<sub>4</sub>) Nanoparticles Prepared by the Co-Precipitation Method: A Novel, Green and Recyclable Heterogeneous Catalyst for the Acetylation of Amines, Alcohols and Phenols under Solvent-Free Conditions", *Appl. Catal., A.*, Vol. 382, 2010, pp. 293-302.