

Title: **Theoretical study of the relative stability of iminium ions**

Student: Alba Herrera Marcer

Date: June 2019

Supervisor/s: Dra. Anna Maria Costa Arnau
Department of Inorganic and Organic Chemistry
Dr. Jaume Vilarrasa Llorens
Department of Inorganic and Organic Chemistry

Nowadays, organocatalysis has become a very useful tool for the synthesis of chiral molecules. The catalyst in these processes is an organic molecule, very often an amine. Amines condense with aldehydes or ketones resulting in an equilibrium in which iminium ions are generated. Secondary amines have become the most used catalysts in organocatalysis.

The objective of this work is to quantify the ease with which different carbonyl compounds treated with pyrrolidine, a secondary amine, form their corresponding iminium ions. We have used the Gaussian 16 program to evaluate this tendency. This software has allowed us to identify the equilibrium geometry of each molecule and calculate its B3LYP, MP2 and M06-2X energies. Based on these energy values, a graph has been created in which different aldehydes and ketones are arranged according to their tendency to generate the iminium cation.