Title: **Organocatalysis. DFT Calculations on the Relative Tendency of Carbonyl Compounds to Afford Chiral Iminium Ions.**

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Organocatalysis is defined as the synthetic process where an organic molecule is used to catalyse reactions. Nowadays, secondary amines are the most commonly used catalysts in organocatalysis, due to their capacity to condense with aldehydes and ketones and generate, in equilibrium, iminium ions, which in many cases may give rise to the corresponding enamines. The reactions of iminium ions and enamines arising from chiral secondary amines, with nucleophiles and with electrophiles respectively, afford chiral products that can be useful as fragments or chiroblocks for the total synthesis of bioactive natural products and enantiopure drugs.

The main goal of this work is to calculate the relative tendency of 24 different carbonyl compounds to afford (chiral) iminium ions by means of the Gaussian 16 package. Optimizations of the equilibrium geometries at B3LYP, M06-2X and ω-B97X-D levels and calculations of the total energies with the MP2/6-31G(d) and M06-2X/6-311+G(d,p) methods from these geometries allowed us to compare the performance of the different methods. In accordance with these energy values we have been able to sort the different aldehydes and ketones regarding the stability of their iminium ions, from pyrrolidine, 2-*tert*-butylpyrrolidine and 2-triphenylmethylpyrroline.