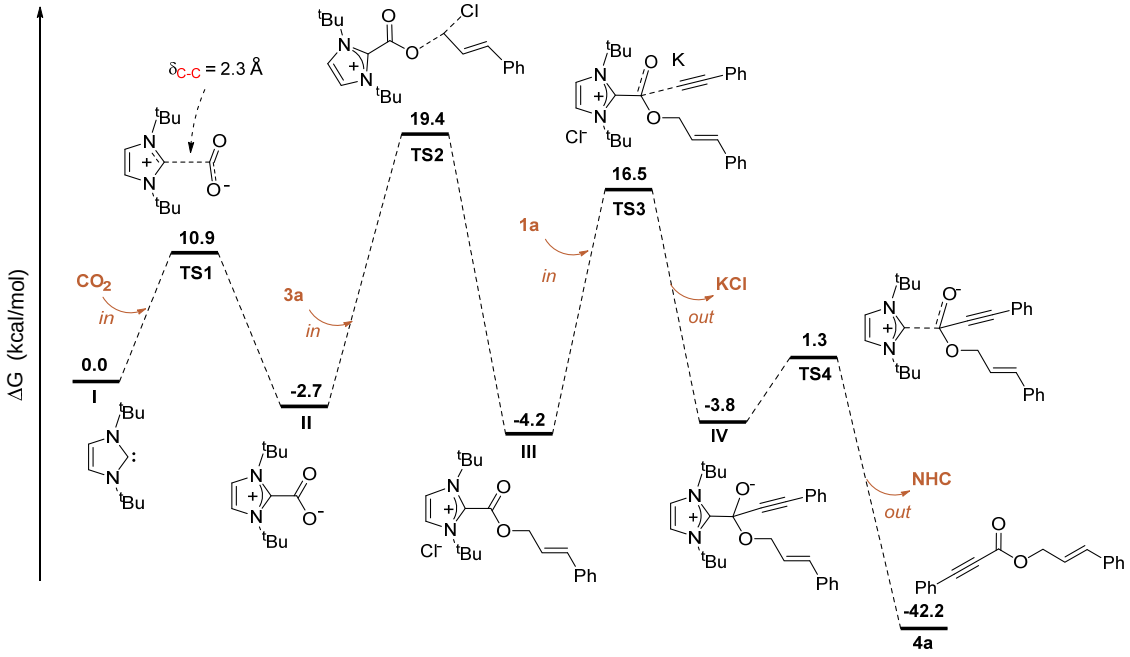
UNPRECEDENTED MULTICOMPONENT ORGANOCATALYTIC SYNTHESIS OF PROPARGYLIC ESTERS VIA CO_2 ACTIVATION

Martin Pauze[a], Argyro T. Papastavrou[b], Enrique Gómez-Bengoa[a], Georgios C. Vougioukalakis[b]

[a] Department of Organic Chemistry I, Faculty of Chemistry, University of the Basque Country UPV-EHU, 20018 Donostia-San Sebastian, Spain
[b] Laboratory of Organic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Athens GR-15771, Greece

Valorisation of CO_2 is, in the actual society, a real challenge and any new method is valuable. We report a new method for the synthesis of propargylic ether. This three components method uses CO_2, organochlorides and terminal alkynes. The catalyst, 1,3-Di-tert-butyl-1H-imidazol-3-ium chloride, is widely-available, stable, and usage friendly N-heterocyclic carbene (NHC). The method allows using a wide range of organochloride and terminal alkynes, containing electron-withdrawing or electron-donating substituents, from low to good yields. Mechanism has been investigated by DFT calculations. Starting by the condensation of the NHC and the CO_2 followed by the addition of the organochloride to finish with the attack of the alkyne. More investigation has been done by calculation for explaining the non-reactivity of certain substrates.



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