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Sustainable Synthesis of Zwitterionic Bases for CO_2 Capture

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ABSTRACT

Carbon dioxide (CO_2) capture is essential for reducing emissions and mitigating climate change effects. Developing new materials for CO_2 capture is crucial for enhancing efficiency and reducing energy costs. Zwitterionic bases are promising due to their high water solubility, thermal stability, recyclability, and low absorption enthalpy. This study explored an alternative synthesis route for zwitterionic bases using dimethyl carbonate (DMC) as a green alkylating agent. Various reaction conditions were tested. Extended reaction times (>4 hours) predominantly yielded fully alkylated products with high purity (93% ^{1}H NMR), whereas shorter times (30 minutes) resulted in mixed products, highlighting the need for optimized reaction conditions. Density functional theory (DFT) calculations elucidated the reaction mechanisms, revealing insights into transition states and energy profiles. These findings supported experimental results and deepened the understanding of the processes. This work demonstrates DMC's potential as a sustainable alkylating agent, advancing green chemistry and sustainable practices in environmental remediation.

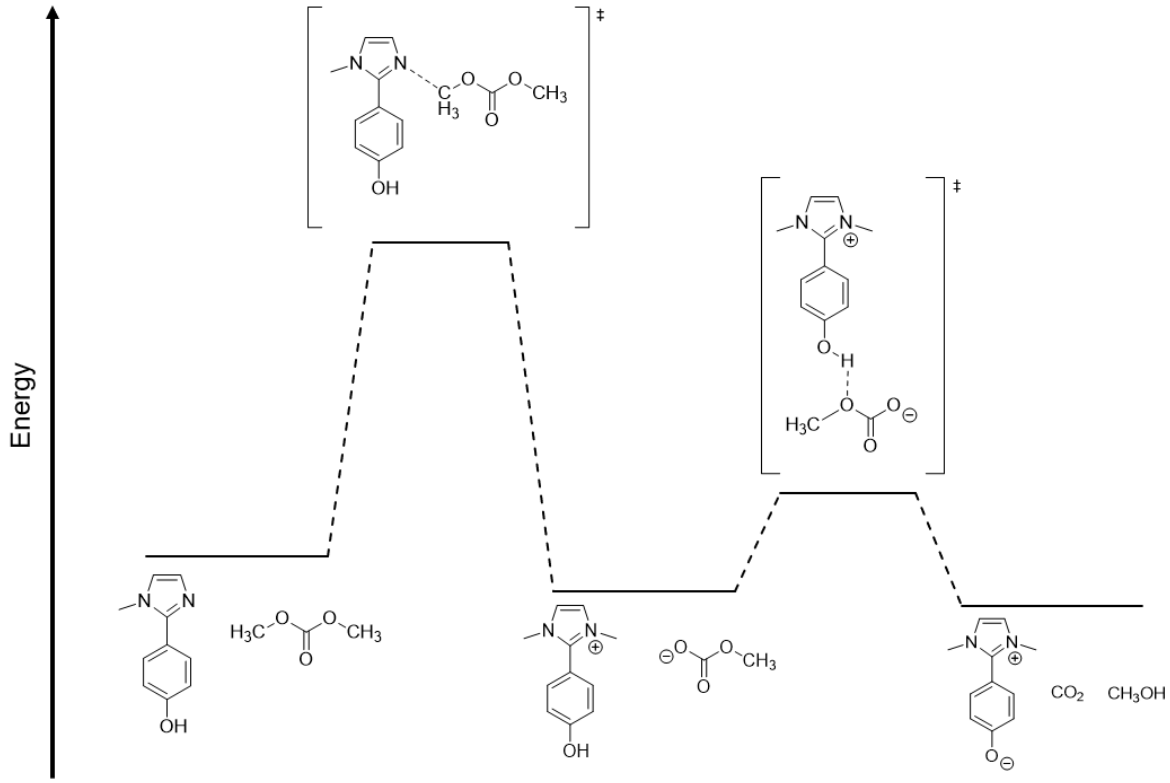

Figure 1 – Calculated energy profile for the reaction between DMC and 1-methyl-2-(4-hidroxiphenyl)-imidazole.

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