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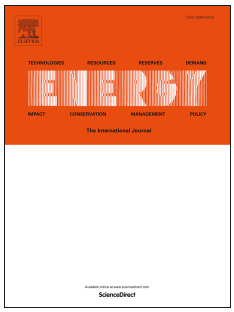

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Understanding the thermodynamic and kinetic performances of the substituted phosphorus ylides as a new class of compounds in carbon dioxide activation

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ABSTRACT

The investigation of thermodynamic and kinetic behavior of the carbon dioxide activation in the presence of the phosphorus ylides (P-ylides) is the main purpose of this study. Different substituents on the carbon atom of the P-ylides have different effects on the P-ylides performances in the carbon dioxide activation. The accessibility of the lone pair electrons on the carbon atom has a remarkable effect on the thermodynamic features of the reaction. A greater involvement of this carbon atom with the orbitals of the substituted groups decreases its reactivity in the CO_2 fixation and Gibbs energy increment. A similarity in the energy levels of the involved orbitals of the carbon dioxide and P-ylides is another factor that affects the thermodynamics of the reaction. The proximity of the energy levels corresponding to the lone pair electrons on the carbon atom of the P-ylides and π*C=O of the carbon dioxide has a good relationship with the ΔG values and progress of the reaction. However, the results of the activation strain model reveal that the activation energy of the reaction is influenced by the strain activation energy of CO_2 and a greater distortion from the equilibrium geometry of CO_2 increases the global energy barrier.

Keywords: Phosphorus ylides, Carbon dioxide, activation strain model, global electron density transfer, Molecular electrostatic potential