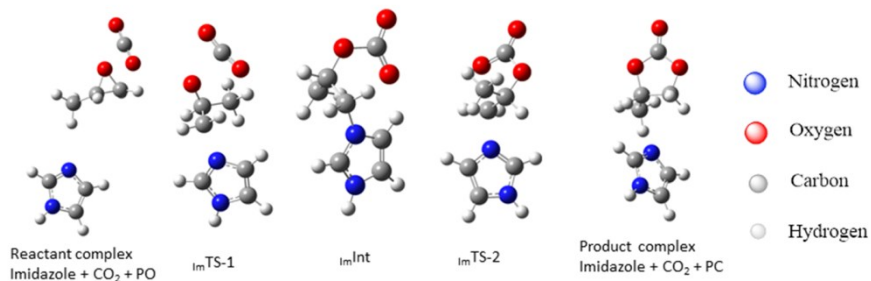


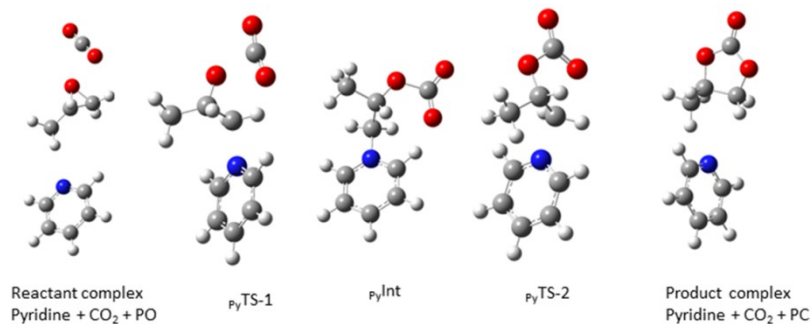
Supplementary information

A computational study into the mechanistic insights of base catalysed synthesis of cyclic carbonates from CO₂: Bicarbonate anion as active species

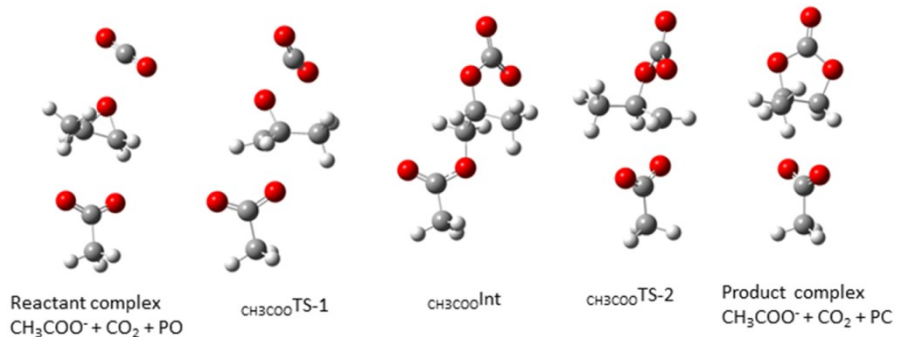
Kuruppathparambil Roshith Roshan, Revi Achuthan Plaissery, Amal Cherian Kathalikkattil,
Robin Babu, George Mathai, Hwa- Soo Lee, Dae-Won Park*



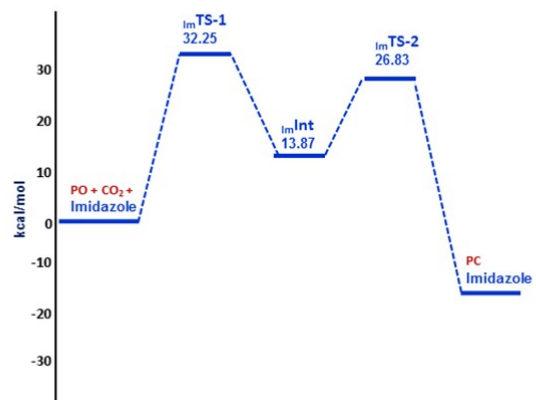
S1a. Optimized structural images of imidazole catalyzed PC synthesis from DFT simulations.



S1b. Optimized structural images of pyridine catalyzed PC synthesis from DFT simulations.



S1c. Optimized structural images of acetate ion catalyzed PC synthesis from DFT simulations.



S2. Relative energy profile from DFT for imidazole mediated PC synthesis