## Supporting information

# Mechanistic Insights into the Ring-Opening Polymerization of Cyclic Esters Catalyzed by Phosphonium Carboxybetaines and Catalyst Design

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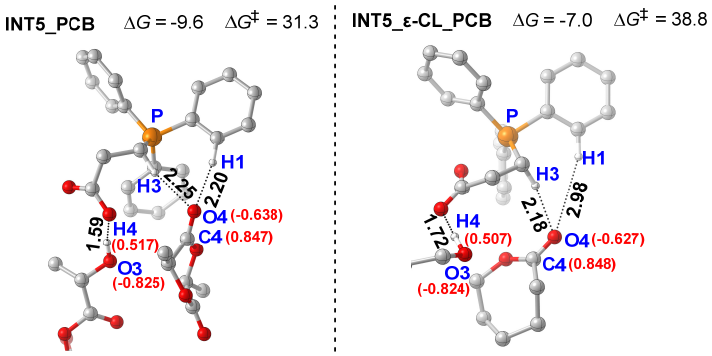



**Figure S1**. The optimized geometrics of the **INT5** for the ROP of *L*-LA and *ε*-CL catalyzed by PCB (the NBO charge is shown in red font, energy is in kcal/mol, "‡" represents energy barrier).

**Table S1.** Energies (kcal/mol) of intermediates and transition states in the gas phase.

| Structures | $\Delta G_{gas}$ |
|---|---|
| TS1 | 12.5 |
| INT2 | 12.6 |
| TS3 | 11.2 |
| INT6 | 10.7 |