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Electronic Supplementary Information for the Manuscript:

DBU and TU Synergistically Induced Ring-Opening Polymerization of Phosphate Esters: A Mechanism Study

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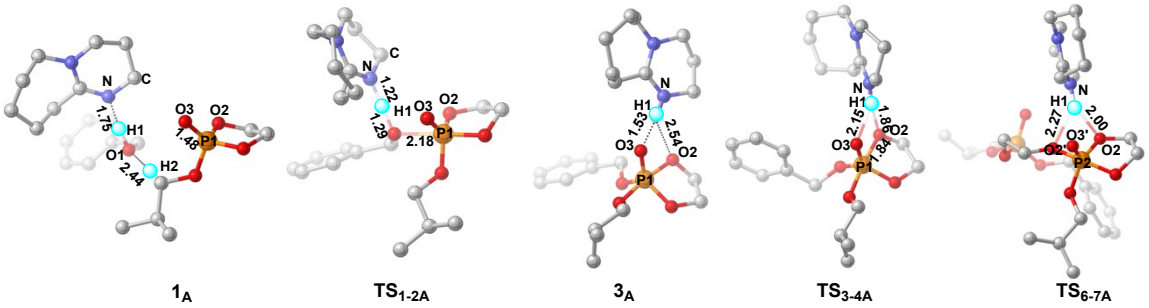

Fig. S1 Optimized structures (distances in Å) of key intermediates and transition states for ROP of *i*BP catalyzed by binary DBU/BnOH.

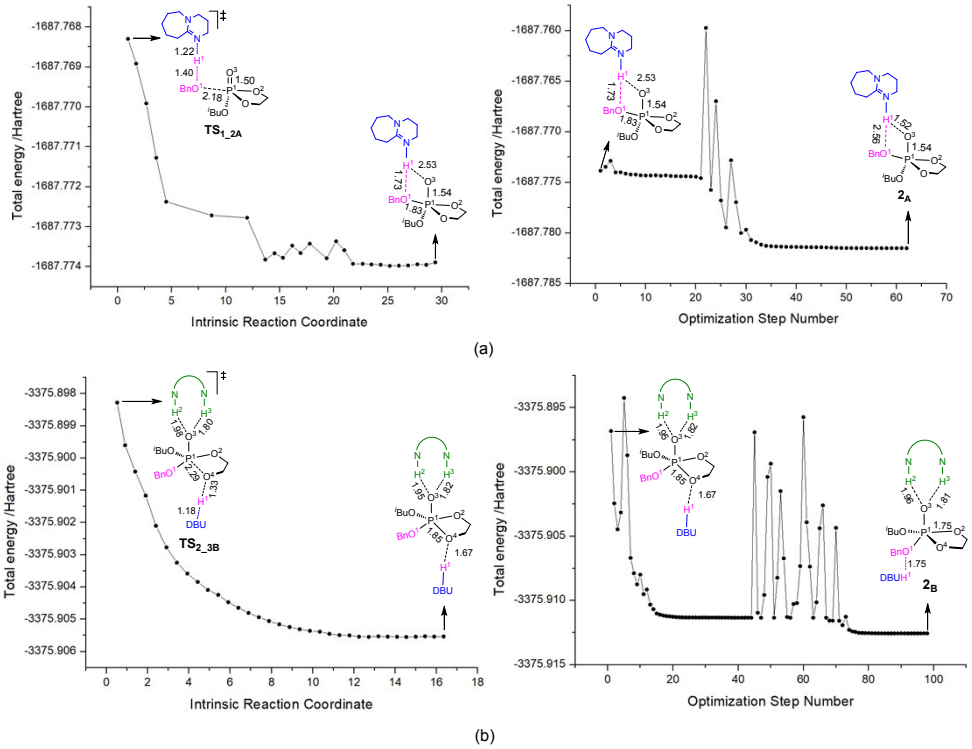

Fig. S2 (a) IRC following of $\mathbf{TS_{1\_2A}}$ and the optimization curve of $\mathbf{2_A}$. (b) IRC following of $\mathbf{TS_{2\_3B}}$ and the optimization curve of $\mathbf{2_B}$.

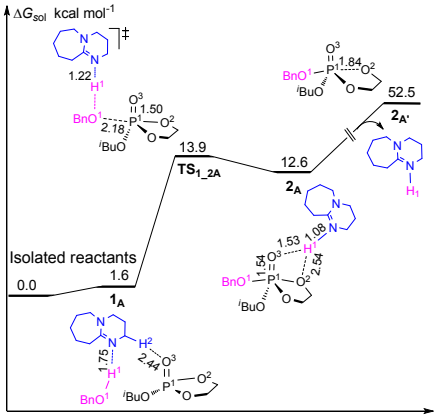

Fig. S3 The potential energy surface of $DBUH^+$ departure from $\mathbf{2_A}$.

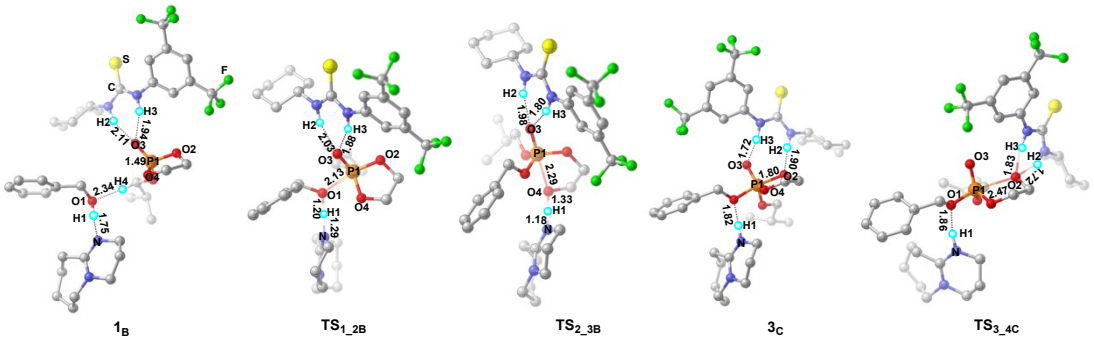

Fig. S4 Optimized structures (distances in Å) of key intermediates and transition states for ROP of *i*BP catalyzed by ternary DBU/TU/BnOH.

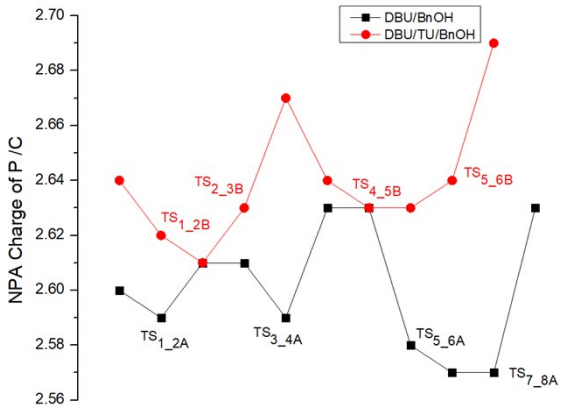

Fig. S5 NPA charge on P atom of *i*BP in binary DBU/BnOH (black curve) and ternary DBU/TU/BnOH (red curve) systems.

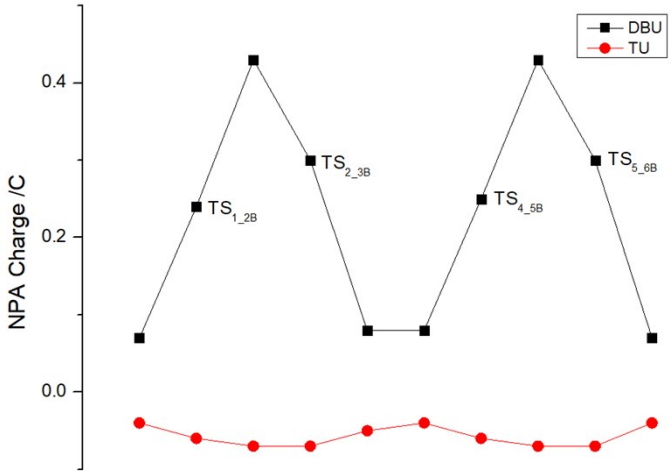

Fig. S6 Changes in NPA charge on DBU (black curve) and TU (red curve) in ternary DBU/TU/BnOH system.