Supporting Information

The Al(III)-Based Polydentate chelate Complex Catalyzed Cycloaddition of Carbon Dioxide and Epoxides: Synthetic Optimization and Mechanistic Study

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Experiment

The detail procedure for Figure 4

The topical procedure for Figure 4 as following: Propylene oxide (1.4 mL, 20 mmol), catalyst (0.0938 g, 0.2mmol) and 10 mL (DMF) were added to a 50mL stainless steel autoclave which equipped with a mechanical stirrer. The reactor was kept connected to a CO_2 tank to keep the 2 MPa CO_2 pressure. The reaction mixture was heated to 120 ℃ and kept stirring for 8 hours. After the reaction, the reactor was cooled in an ice water for 30 minutes and then slowly release excess CO_2. (A) To investigate the influence of CO_2 pressure, the pressure of CO_2 was adjusted to 0.1 MPa(balloon), 0.5 MPa, 1.0 MPa, 1.5 MPa, 2.0 MPa and 2.5 MPa respectively under the other conditions unchanged. (B) Under the topical condition, the product was detected after stirring for 2 h, 4 h, 6 h, 8 h, 10 h, and 12 h respectively to investigate the product generation with the reaction time extending. (C) The reaction was processed at 80 ^{o}C, 100 ^{o}C, 120 ^{o}C and 140 ^{o}C respectively to test the influence of temperature for the cyclic addition reaction. (D) The PO/catalyst ratio (200:1, 100:1, 50:1, 25:1 and 10:1) was involving to investigate the influence of catalyst amounts.

Supporting Figures

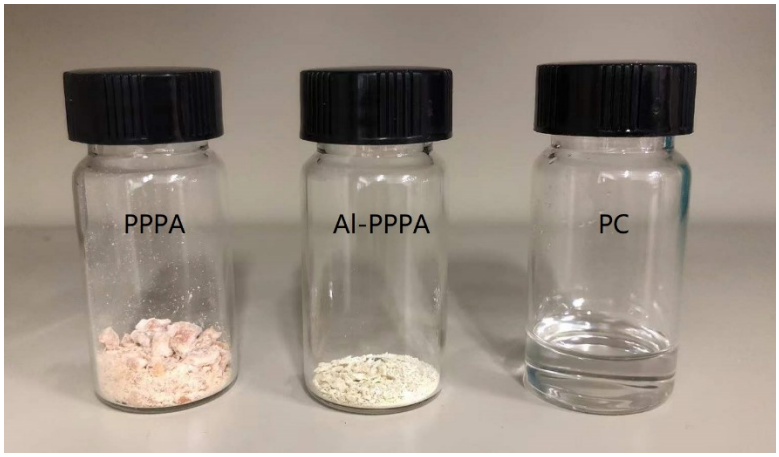

Figure S1. Physical state of ligand PPPA, catalyst Al-PPPA and product PC

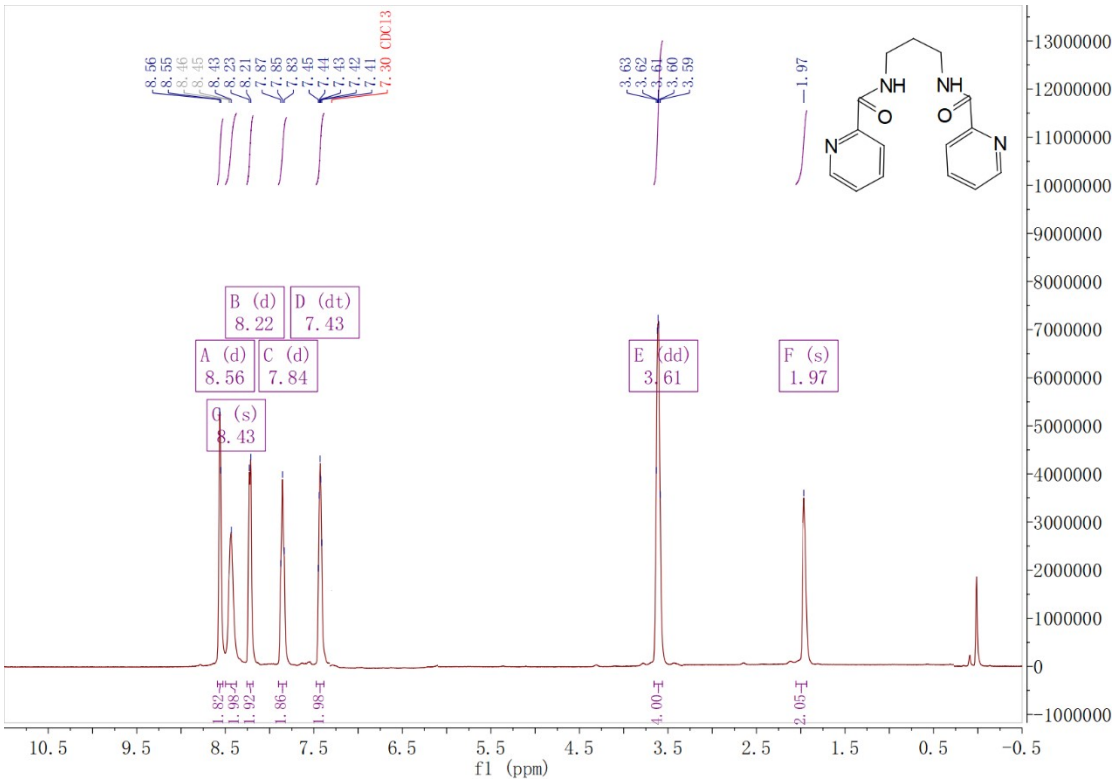

Figure S2. ^{1}H NMR spectrum of ligand PPPA

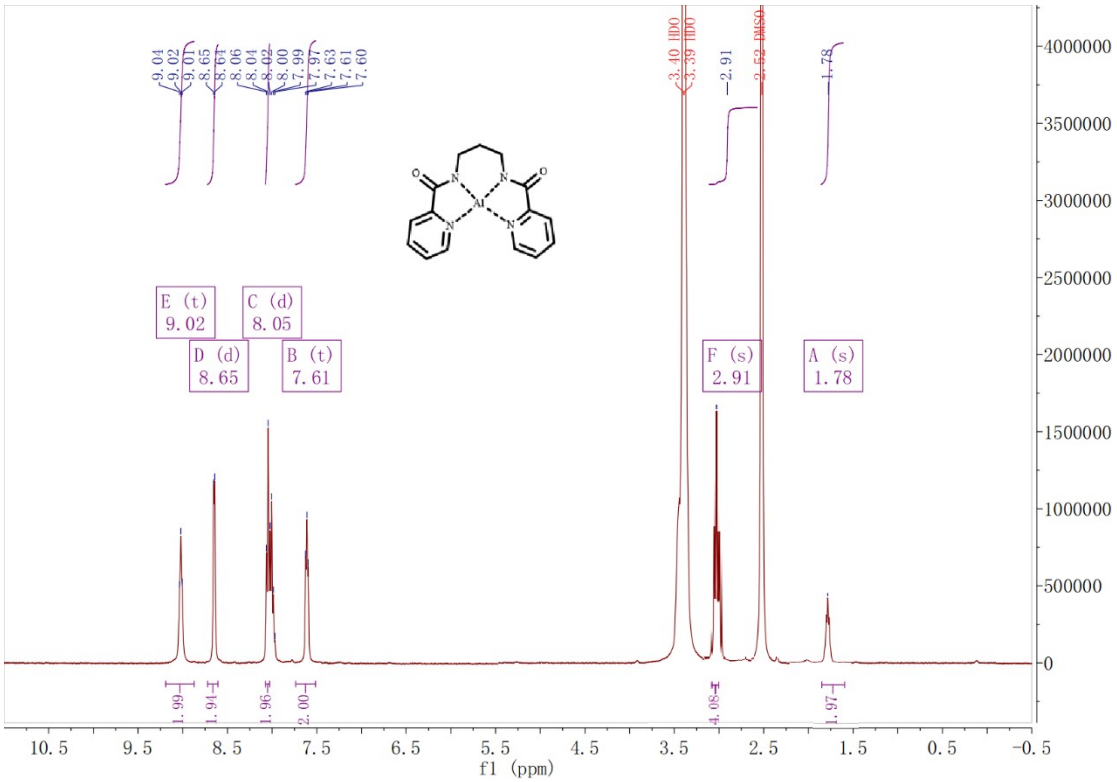

Figure S3. ^{1}H NMR spectrum of catalyst Al-PPPA

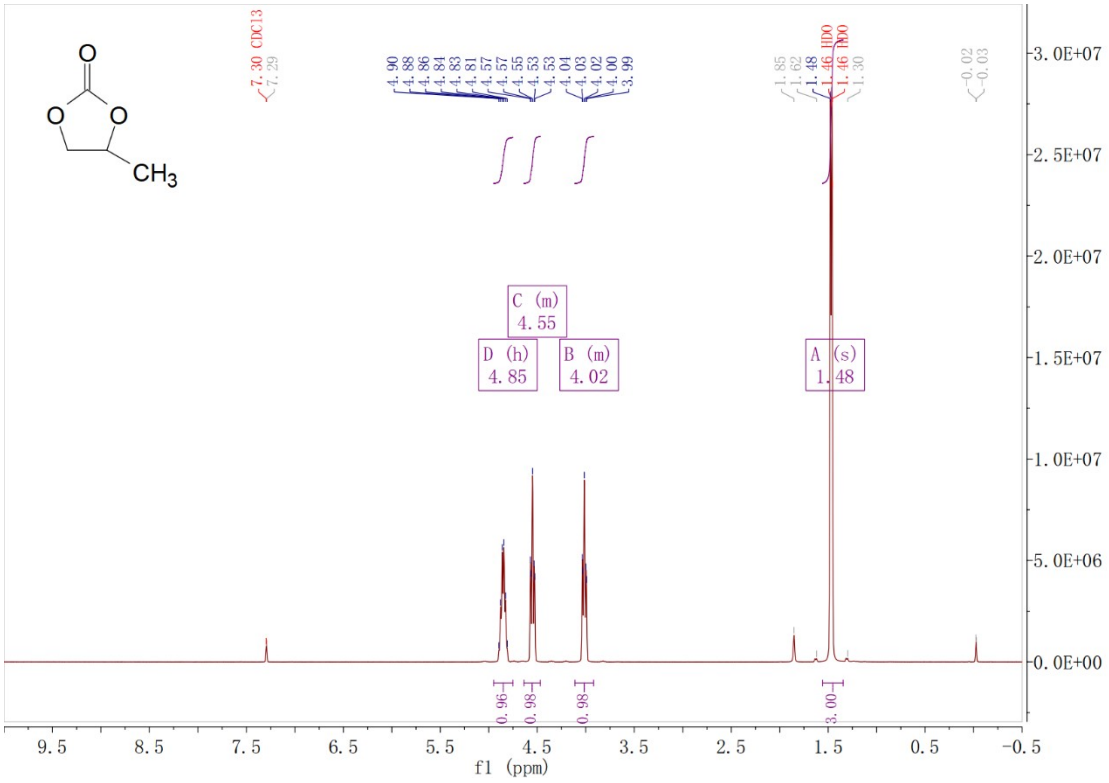

Figure S4. ^{1}H NMR spectrum of product PC

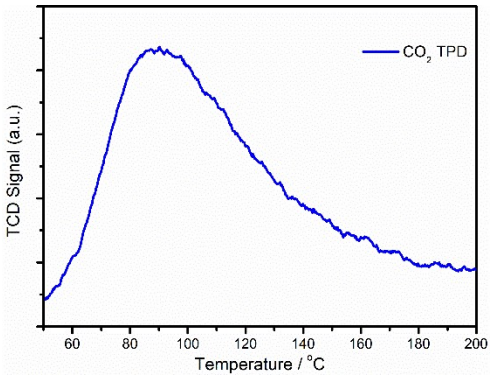

Fig.S5 CO_2-TPD of representative polymer catalysts.

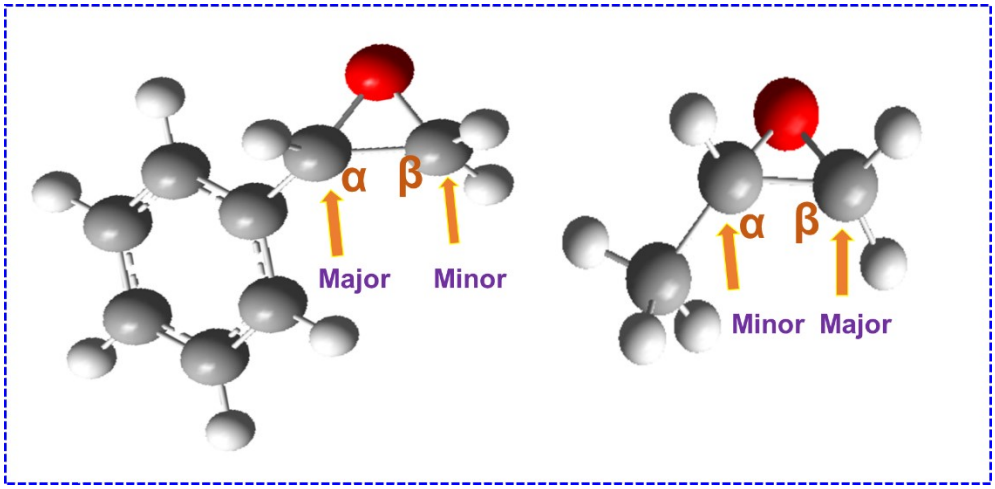

Fig. S6 Difference in Nucleophilic Ring-Opening between Styrene Oxide and Propylene Oxide

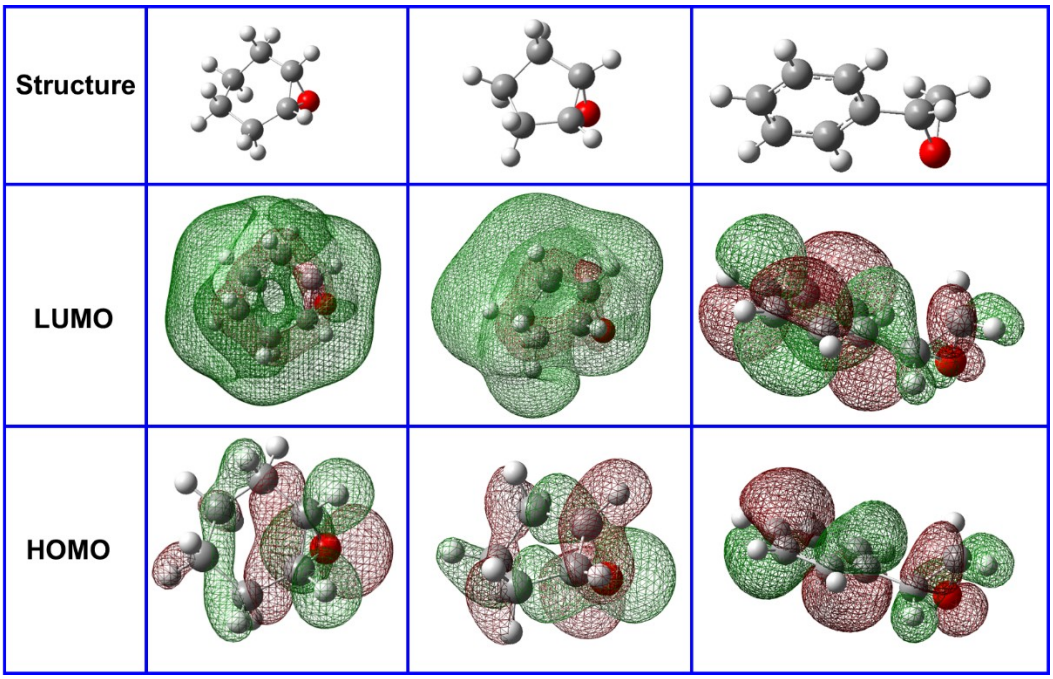

Fig. S7 The calculated the electron cloud density of styrene oxide, cyclopentane oxide and cyclohexene oxide.

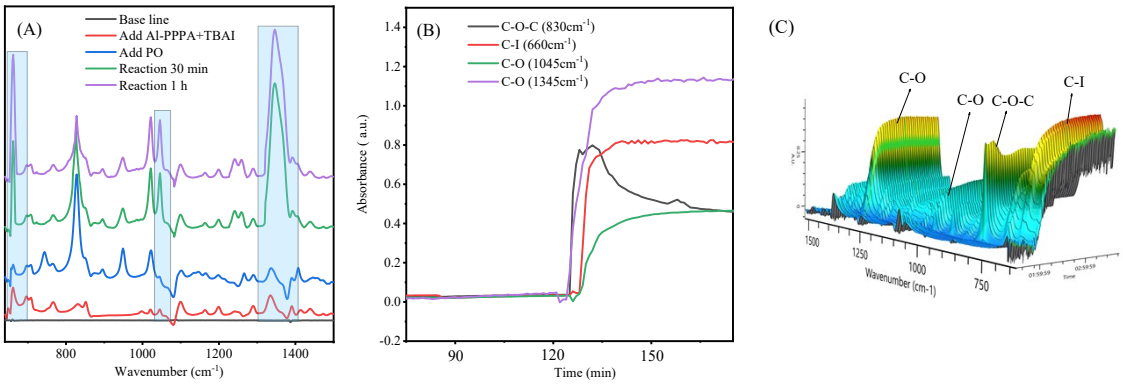

Fig.S8 *In-situ* ATR-IR monitoring of ring opening process of PO: (a) overall spectra during ring opening process; (b) IR profile of PO (black) and ring open intermediate (red, green, purple); (c) 3D ATR-IR variation diagram during PO ring opening.

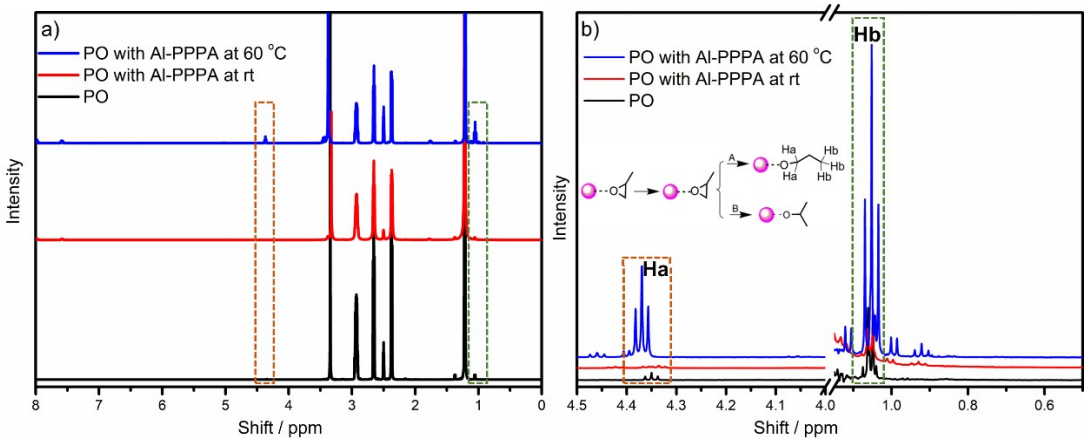

Fig.S9 The ^{1}H NMR spectra of PO, PO with Al-PPPA at room temperature and PO with Al-PPPA at 60 °C.