Supporting Information

Niobate Salts of Organic Base Catalyzed Chemical Fixation of Carbon Dioxide with Epoxides to Form Cyclic Carbonates

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Catalyst characterization

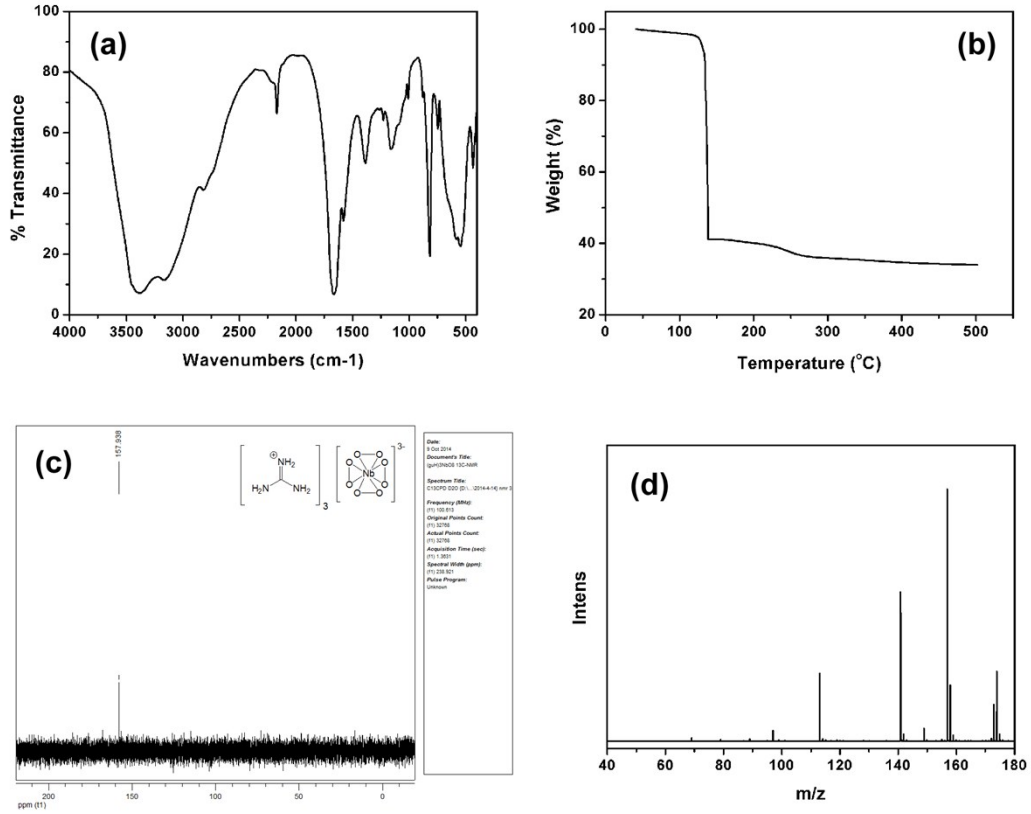

Figure S1. Characterization of $(guH)_3NbO_8$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{13}C NMR spectrum; (d) mass spectrum.

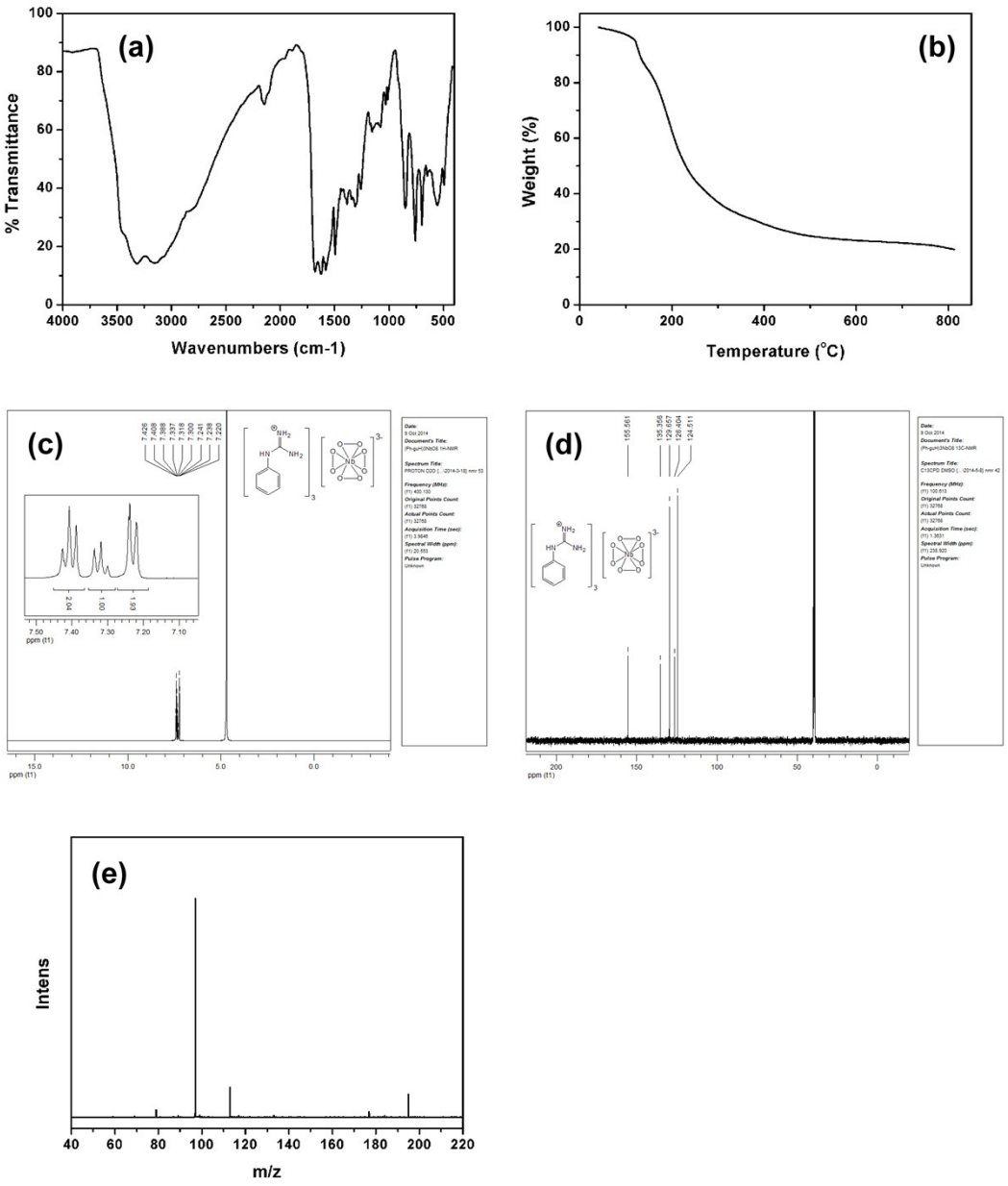

Figure S2. Characterization of $(Ph\text{-}guH)_3NbO_8$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{1}H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

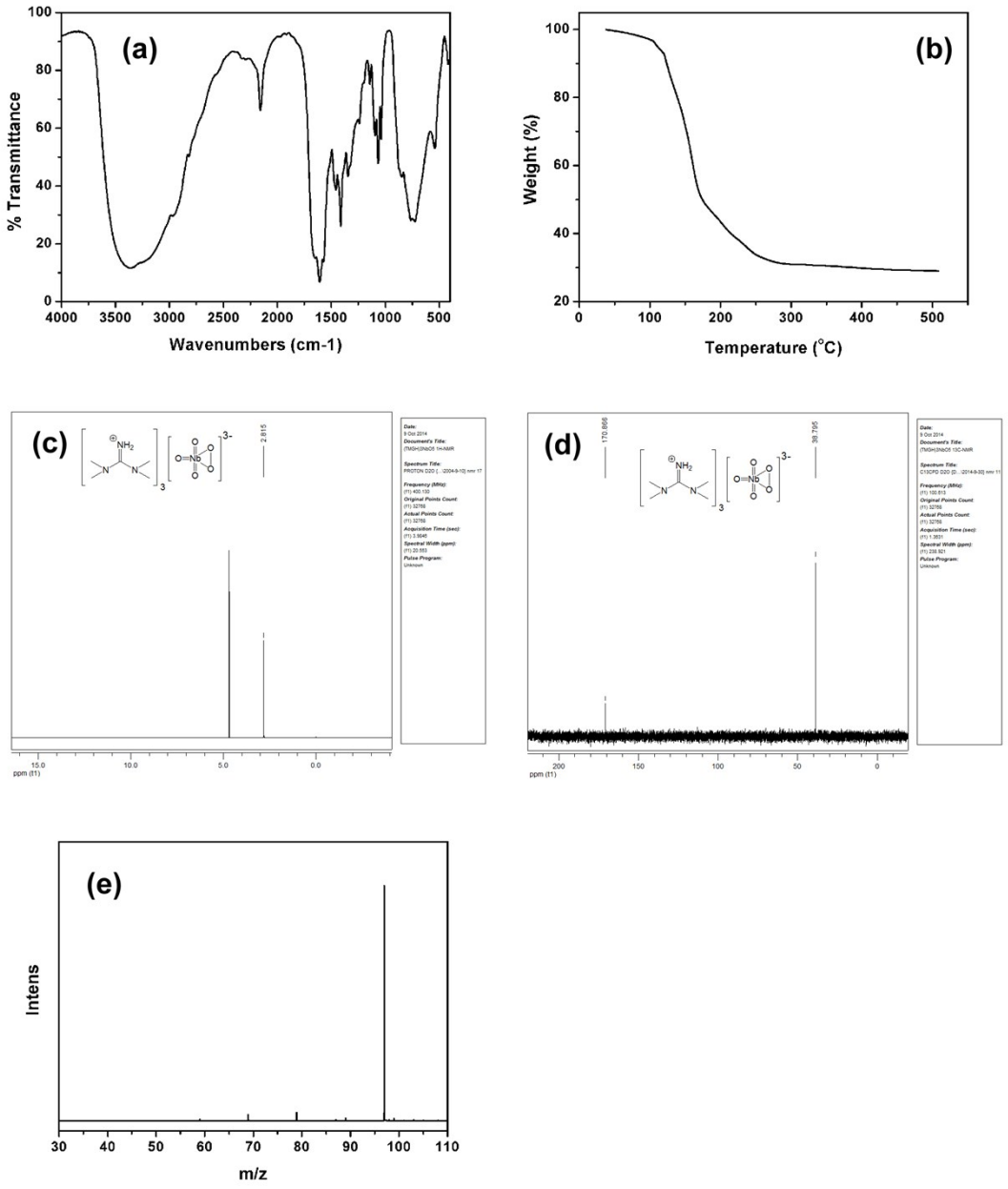

Figure S3. Characterization of $(TMGH)_3NbO_5$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{1}H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

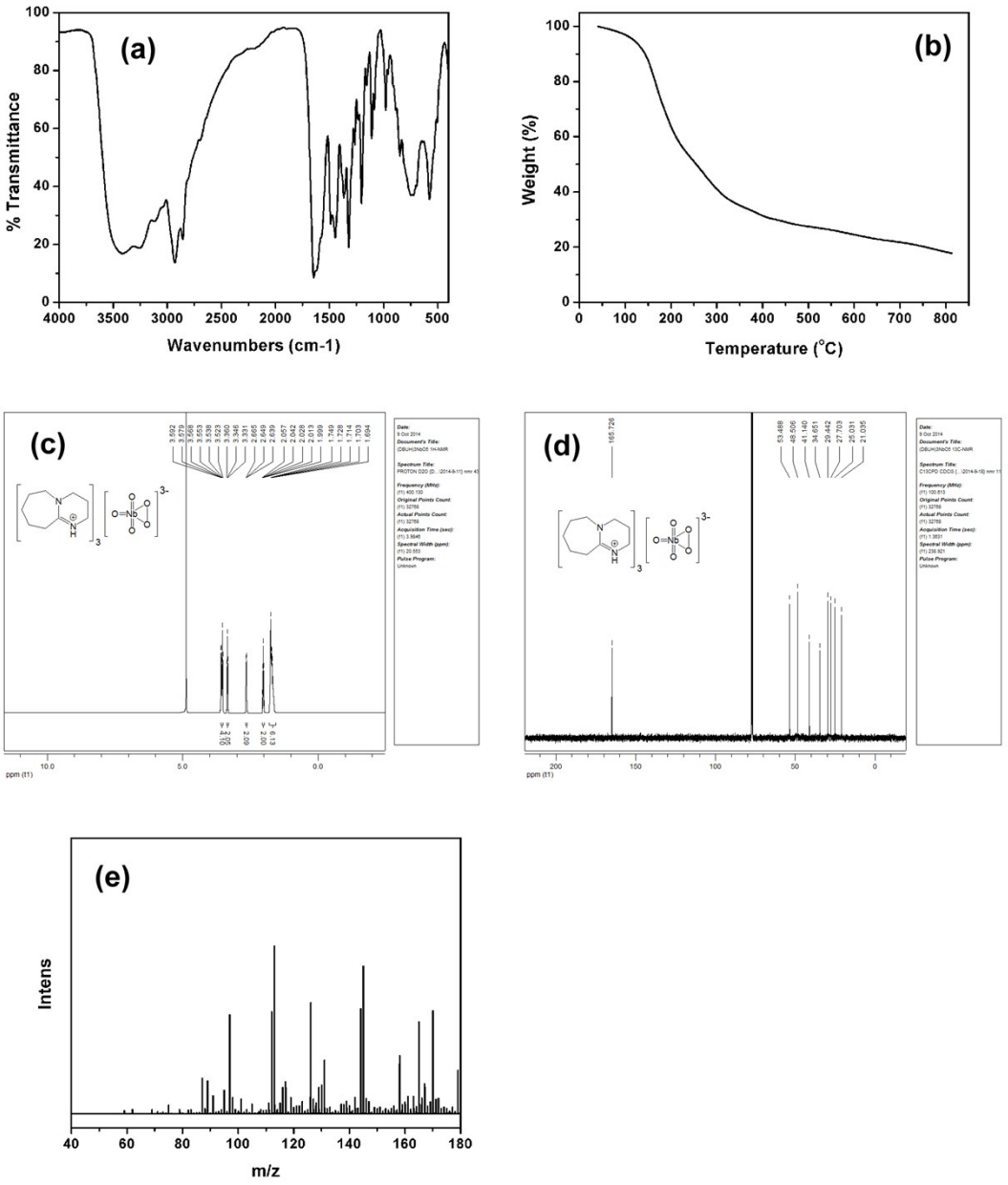

Figure S4. Characterization of $(DBUH)_3NbO_5$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^1H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

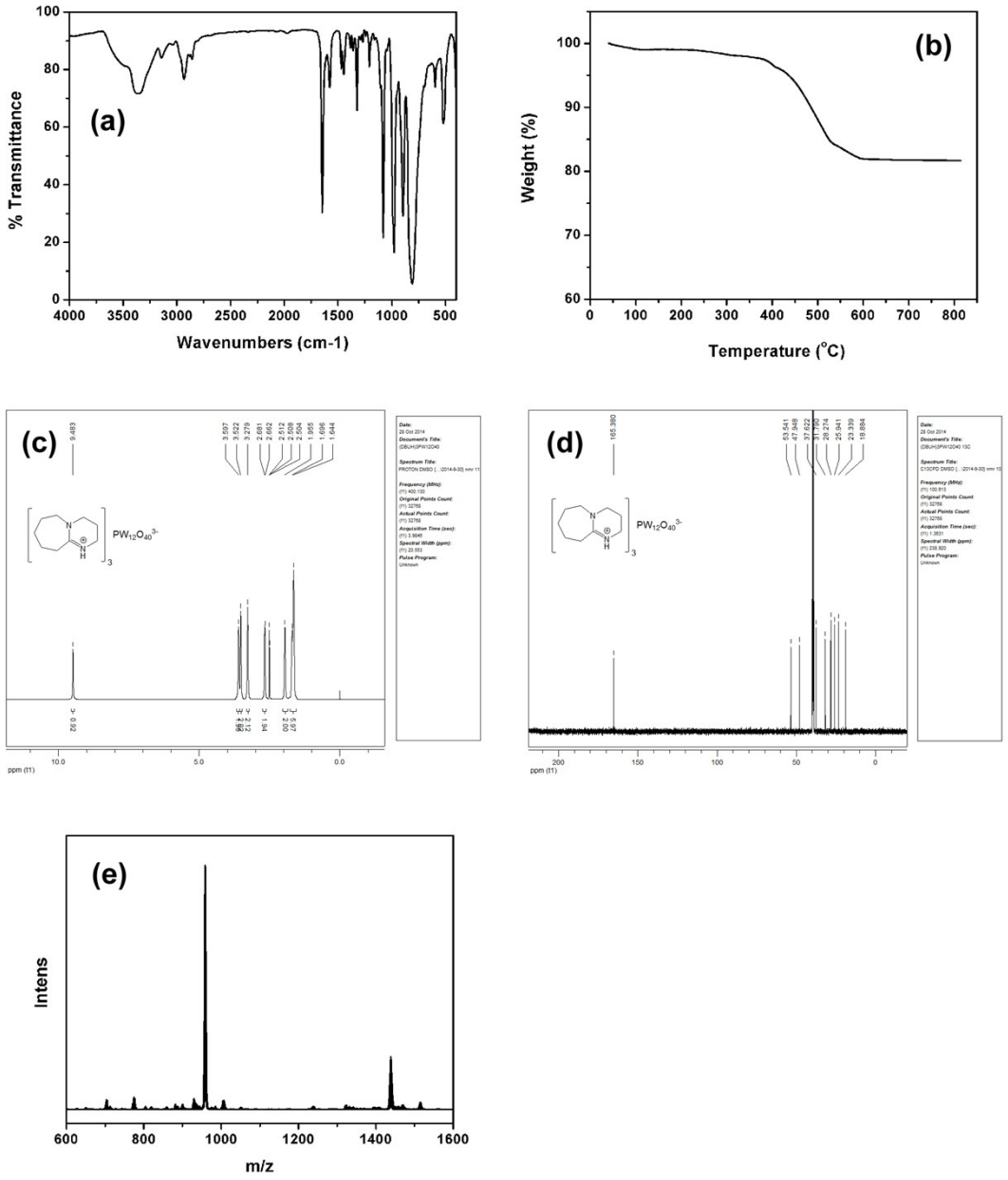

Figure S5. Characterization of $(DBUH)_3PW_{12}O_{40}$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{1}H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

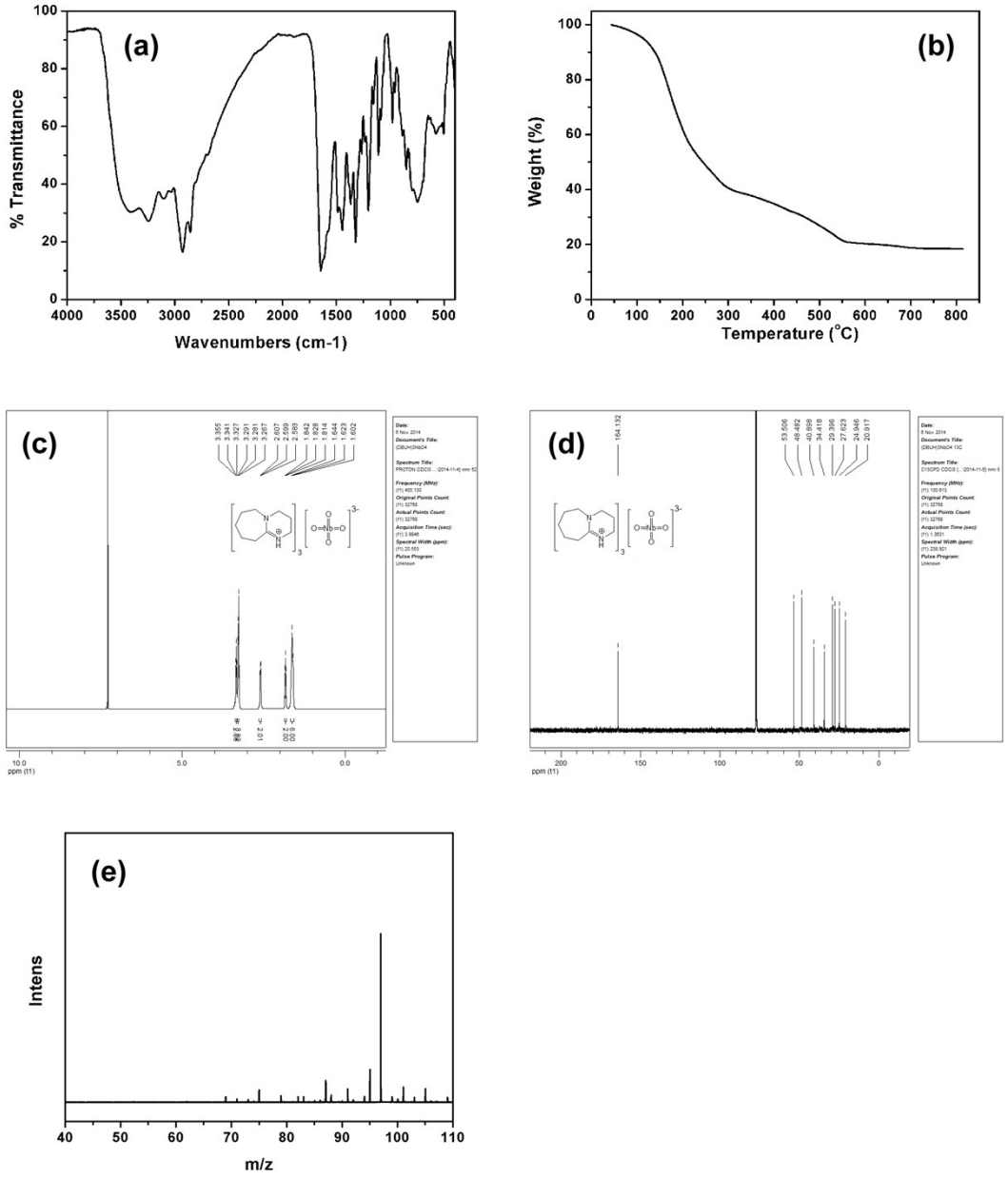

Figure S6. Characterization of $(DBUH)_3NbO_4$: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{1}H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

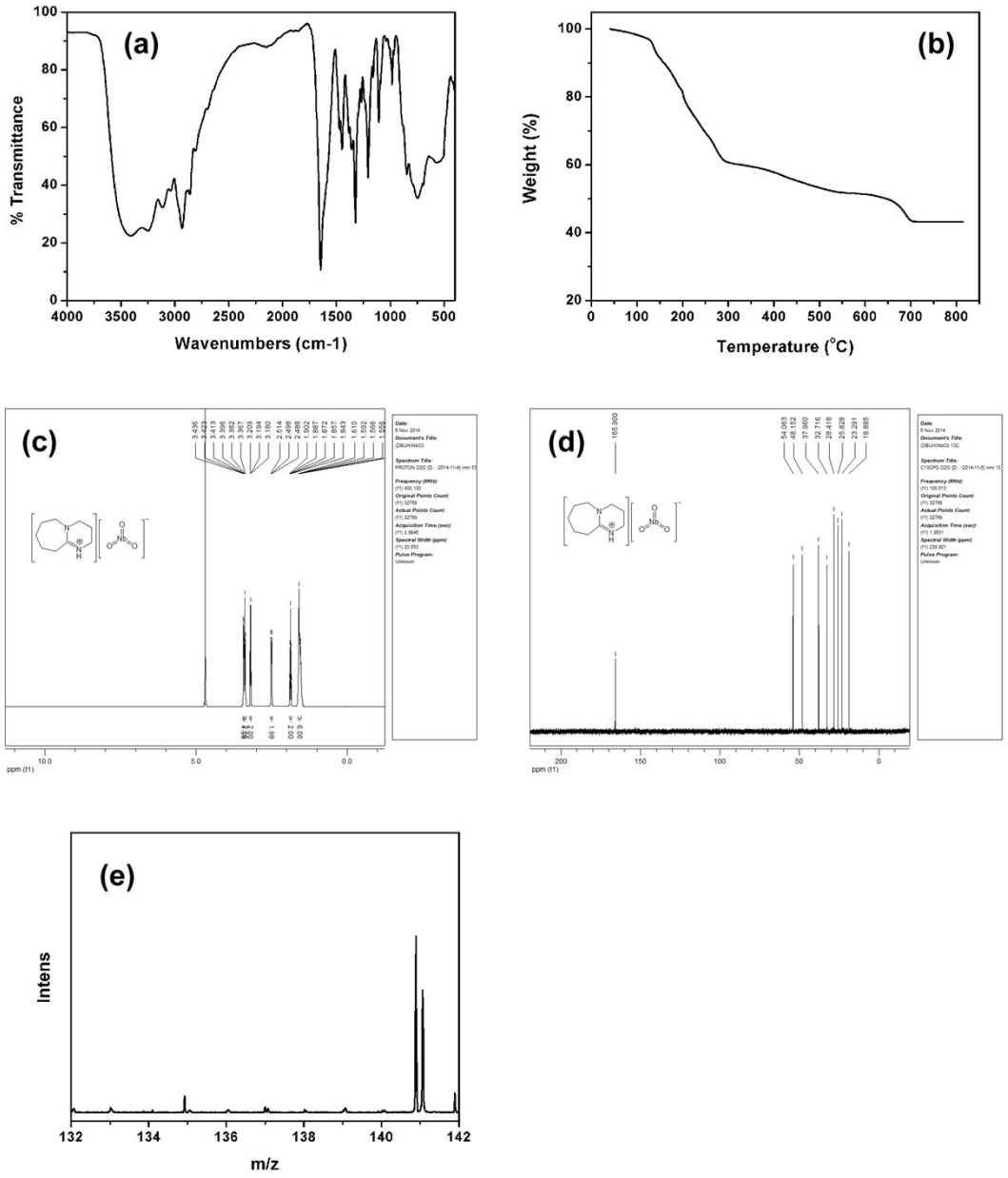

Figure S7. Characterization of (DBUH)NbO_3: (a) FT-IR spectrum; (b) TGA pattern; (c) ^{1}H NMR spectrum; (d) ^{13}C NMR spectrum; (e) mass spectrum.

Reaction kinetics of propylene carbonate synthesis

The procedure for investigating the kinetic parameters for the cycloaddition of carbon dioxide to propylene oxide (PO) was adapted from the literature.[27] PO (0.7 ml, 10 mmol), $(DBUH)_3NbO_5$ (0.204 g, 0.3 mol) were loaded into an autoclave. Carbon dioxide was introduced to the reaction and kept at 3.0 MPa bar by CO_2 pump (DB-80, made by Beijing Satellite Manufacturing Factory). The reaction mixture was stirred vigorously using a magnetic stirrer and heated to the desired temperature (110-140^oC). The reaction was monitored every 1 hour using gas chromatography. The rate constant was determined from the experimental data assuming pseudo-first order reaction kinetics and the activation energy for the process was determined using the Arrhenius equation based on the calculated rate constants at different temperatures.

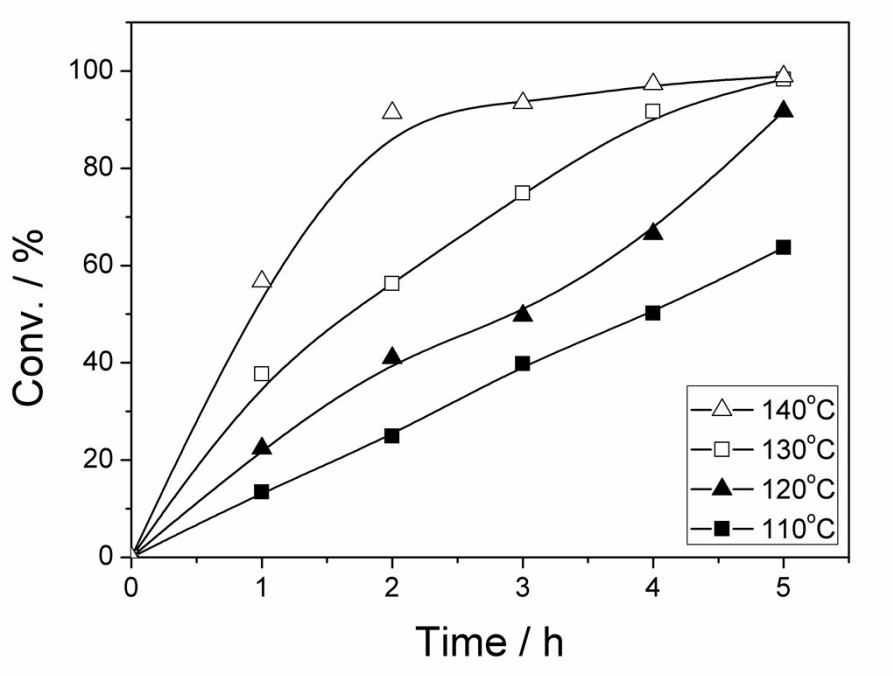

Figure S8. Conversion/time profiles of cycloaddition reactions catalyzed by $(DBUH)_3NbO_5$ at different temperatures. Reaction conditions: PO 0.7 ml (10 mmol), $(DBUH)_3NbO_5$ 0.3 mmol, 3 MPa.

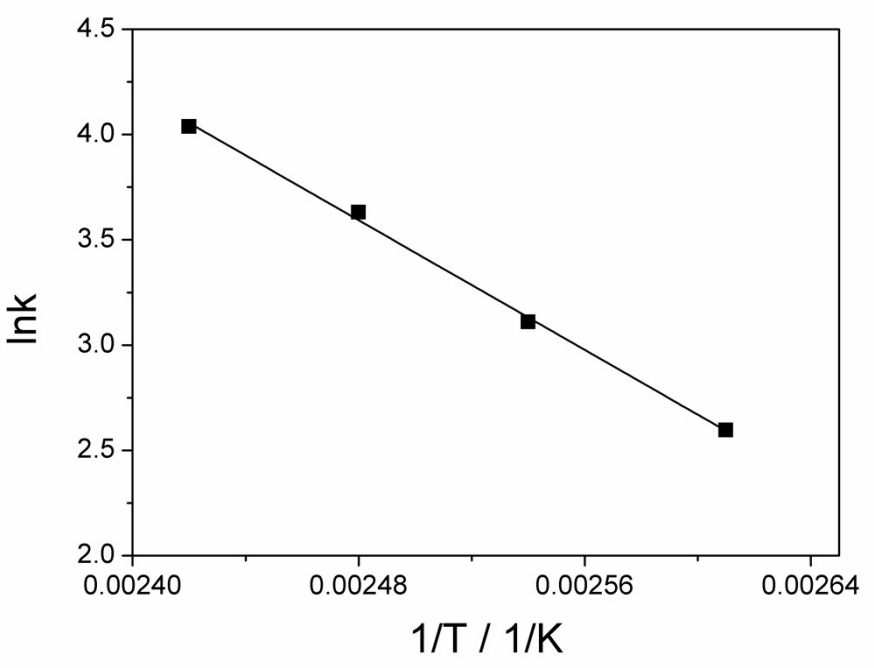

Figure S9. Arrhenius plots for the cycloaddition reaction of PO and carbon dioxide. The observed rate constants (k) were calculated with the initial rates by Figure S8 at different temperatures.

The TGA curves of the catalyst

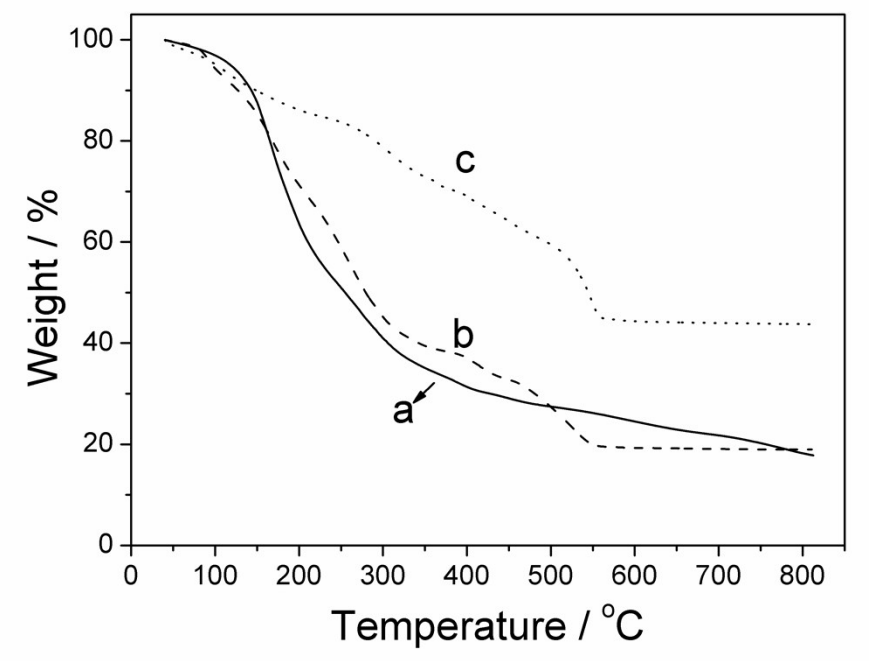

Figure S10. The TGA pattern of (a) fresh catalyst: $(DBUH)_3NbO_5$; (b) the catalyst after the first run; (c) the catalyst after the eighth run.

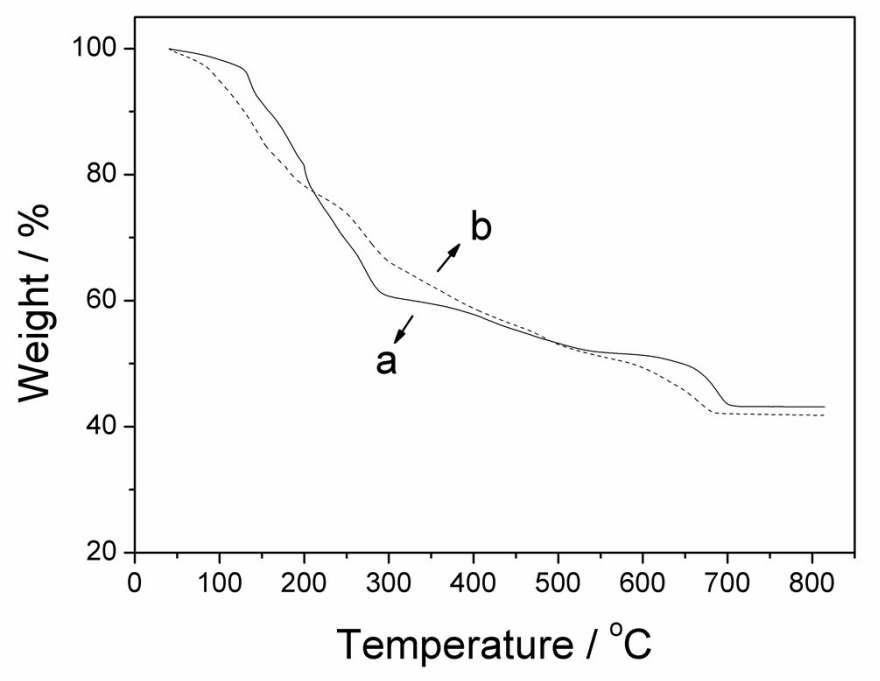

Figure S11. The TGA pattern of (a) fresh catalyst: (DBUH)NbO_3; (b) the catalyst after the sixth run.

Spectroscopic data for the isolated products

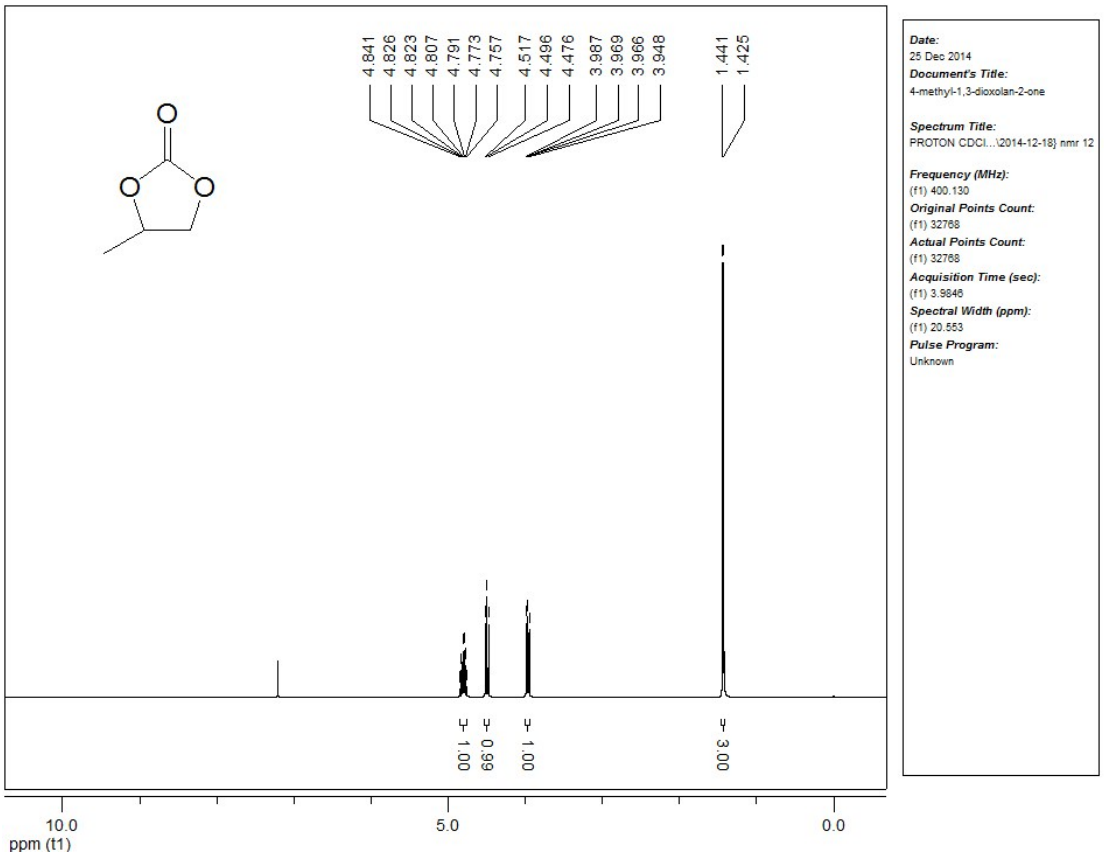

Figure S12. ^{1}H NMR spectrum of 4-methyl-1, 3-dioxolan-2-one.

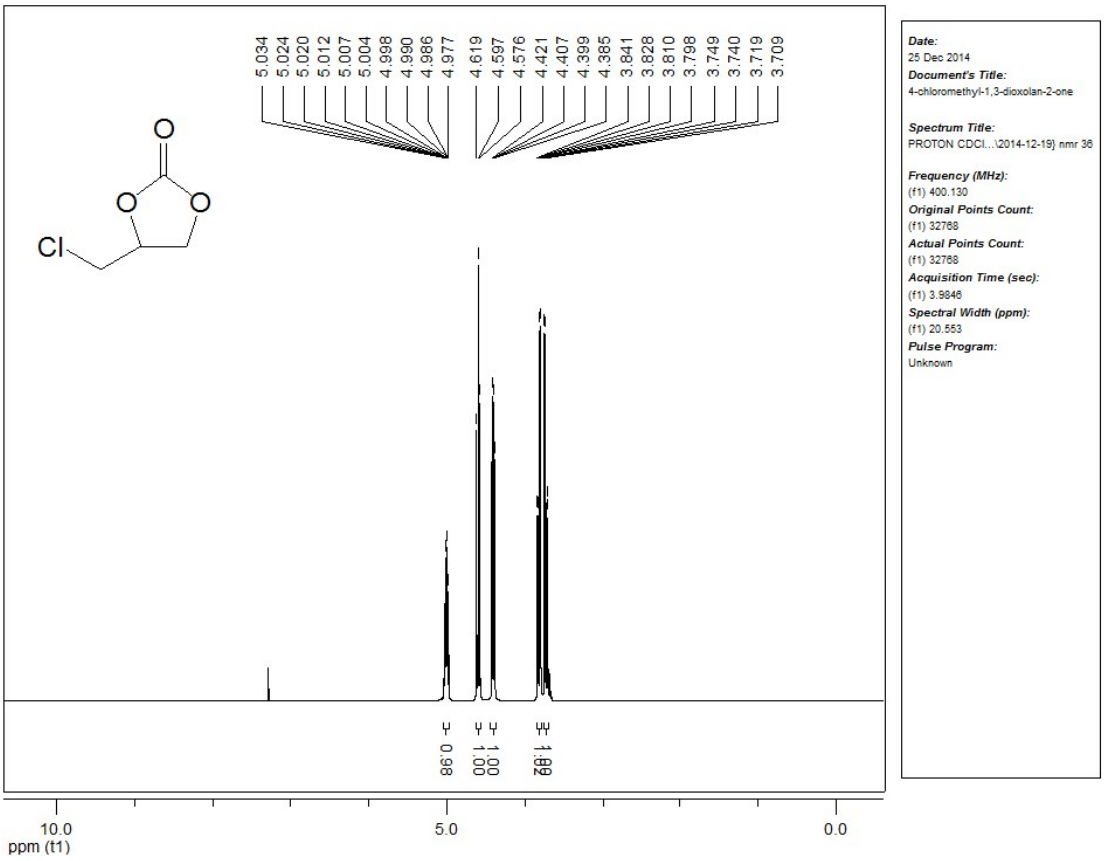

Figure S13. ^{1}H NMR spectrum of 4-chloromethyl-1, 3-dioxolan-2-one.

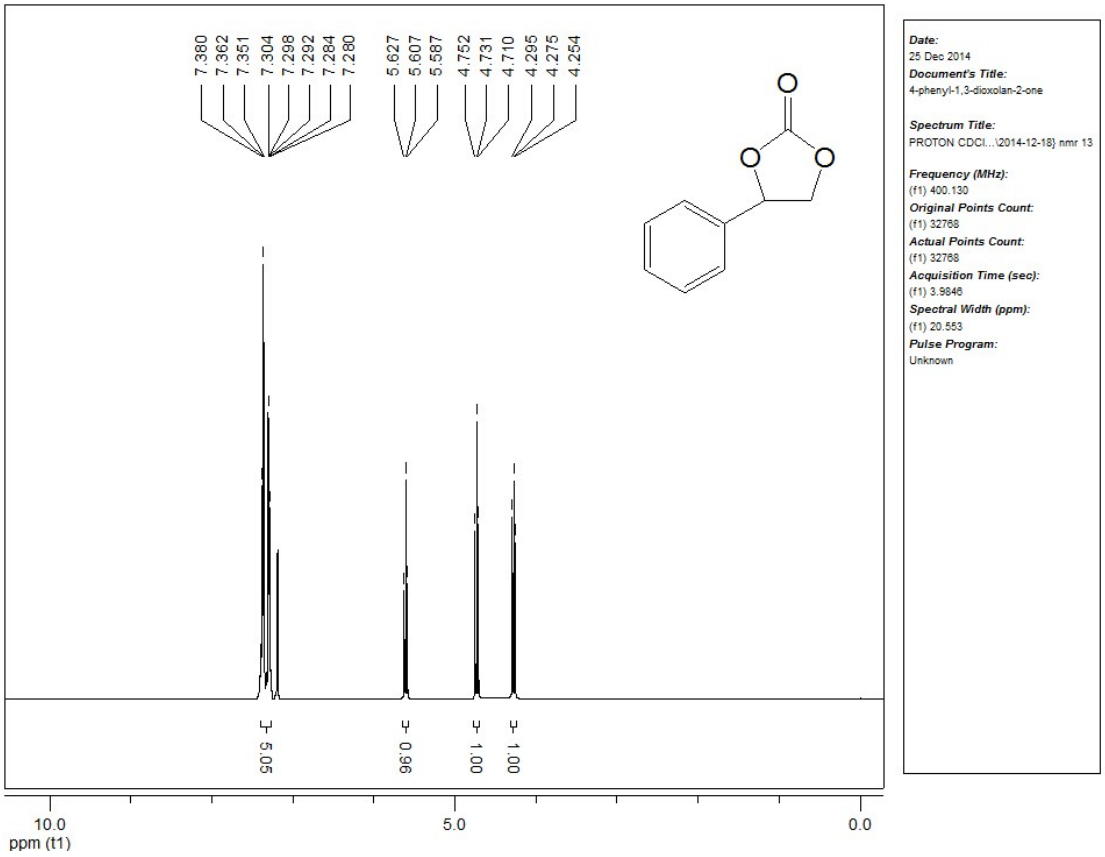

Figure S14. ^{1}H NMR spectrum of 4-phenyl-1, 3-dioxolan-2-one.

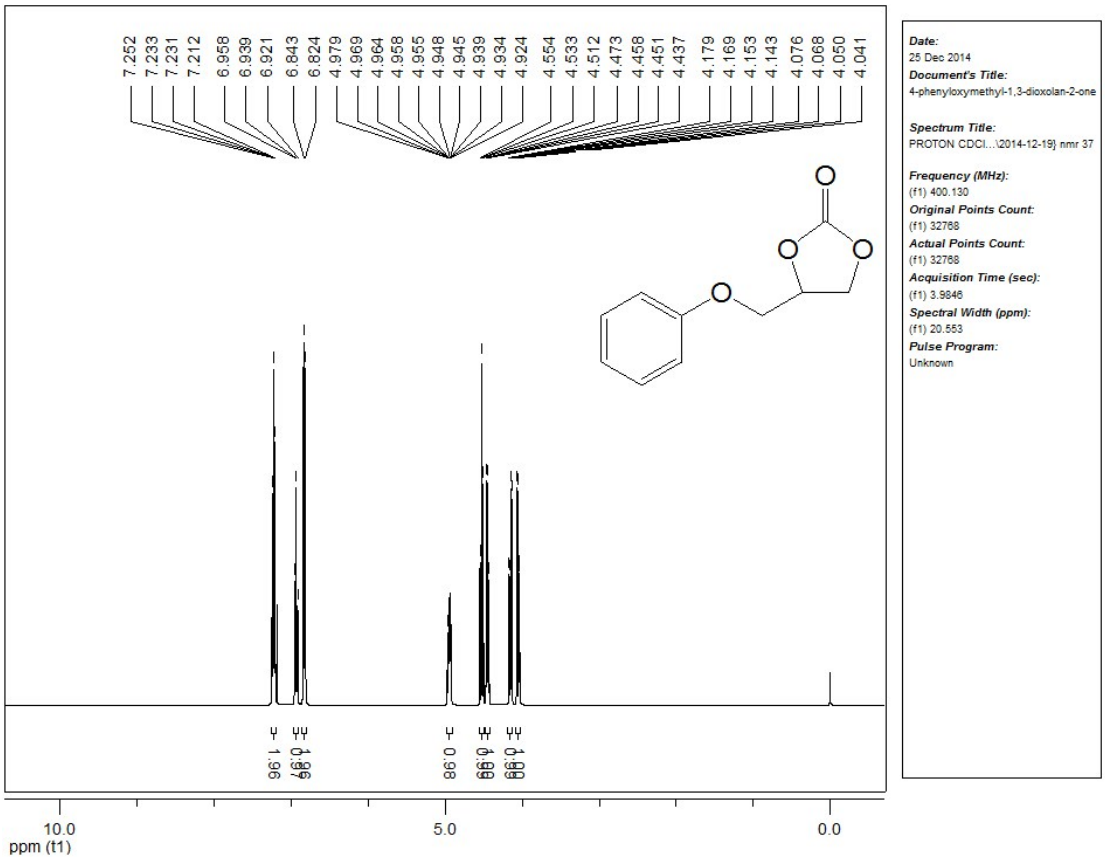

Figure S15. ^{1}H NMR spectrum of 4-phenyloxymethyl-1, 3-dioxolan-2-one.

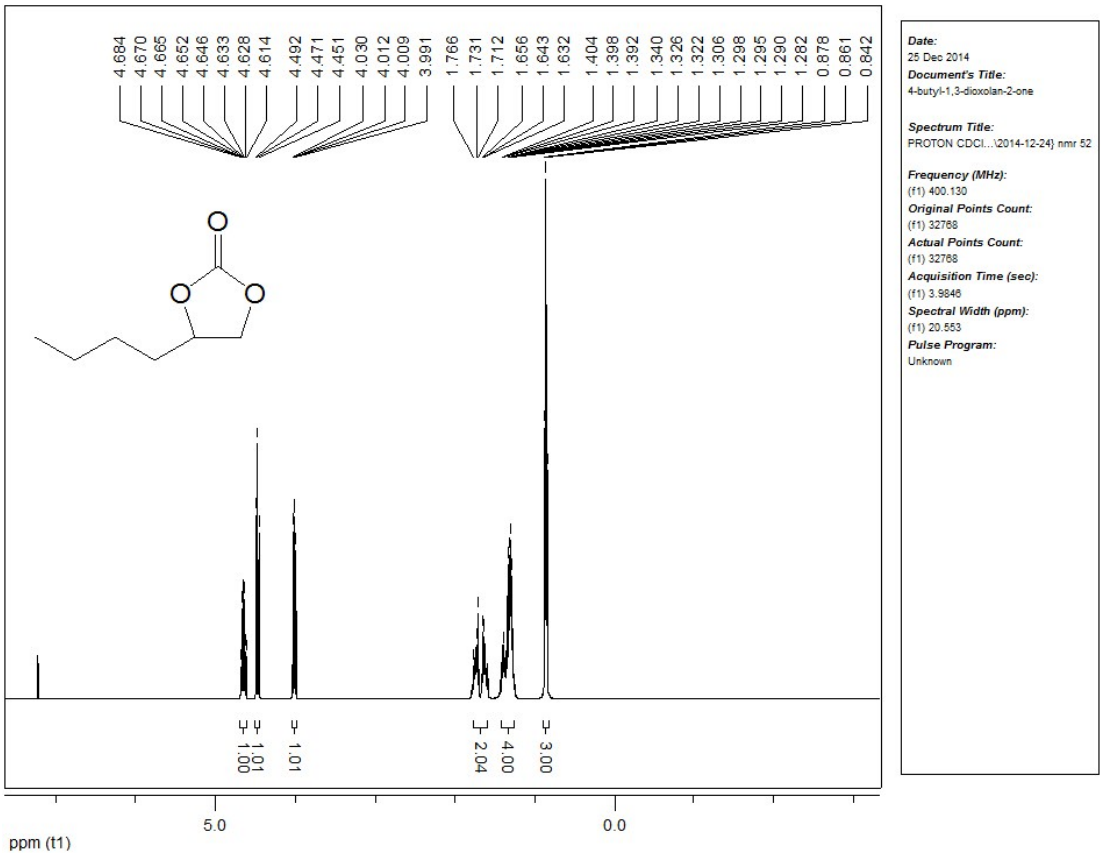

Figure S16. ^{1}H NMR spectrum of 4-butyl-1, 3-dioxolan-2-one.

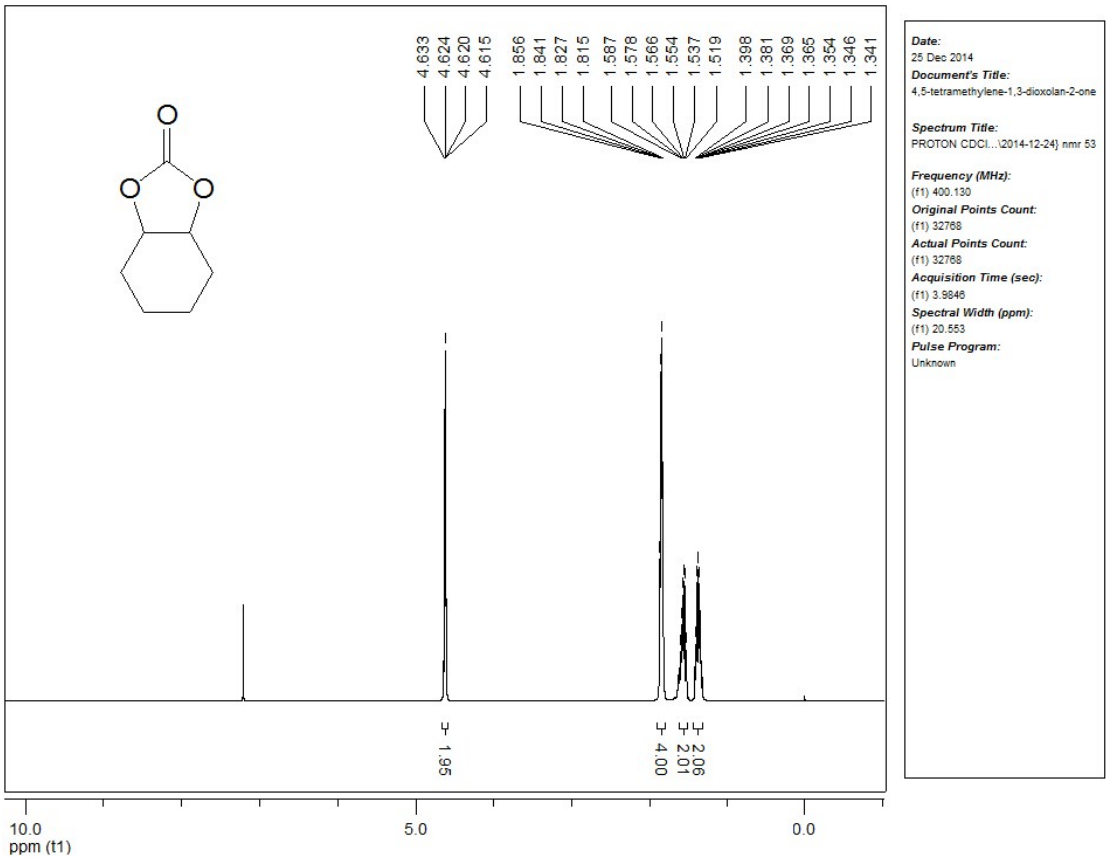

Figure S17. ^{1}H NMR spectrum of 4, 5-tetramethylene-1, 3-dioxolan-2-one.