Supplementary information

g-C_3N_4 and Tetrabutylammonium bromide catalyzed efficient conversion of Epoxide to Cyclic Carbonate under ambient condition

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Experimental Section:

Materials.

Melamine was purchased from LOBA Chemicals. tetrabutylammonium bromide (TBAB) was purchased from SRL. All epoxides used here were purchased from sigma aldrich. Chloroform-d was purchased from sigma and chloroform was used as internal standard. All chemicals were used as received.

Experimental Procedure.

Prepared g-C_3N_4 was characterized by PXRD, FTIR, solid state ^{13}C NMR (CP MAS) and, TGA analysis. Cyclic carbonates produced by the reaction of epoxide and CO_2 was characterized by solution state ^{1}H and ^{13}C NMR spectroscopy.

General Procedure: 13.7 mmol epoxides, g-C_3N_4 and TBAB were taken in 50 ml Schlenck round bottom flak with a small magnetic stirrer. One blank glass tube was kept as condenser above the round bottom flask. On the top of the glass tube, the balloon attached with the glass stopcock was fitted. All glass joints were sealed with both grease and teflon tape in order to minimize the gas lick-age. Subsequently, the set up was vacuumed and backfill with 99.995% CO_2 gas thrice to remove any dissolved air from the setup and heating was started. Subsequently, the reaction mixture was heated for 20 hours in the CO_2 environment. After the completion of the reaction, a small amount of the reaction mixture was taken in $CDCl_3$ and immediately precipitate of g-C_3N_4 appeared. Precipitates were separated by centrifugation and the solution was utilized for NMR measurement.

Recyclability Test:

Recyclability was checked using epichlorohydrin as substrate. For every cycle 13.7 mmol epoxides was added to the reaction mixture and using the CO_2 balloon reaction was started. In order to check the conversion small amount of aliquot was taken for ^{1}H NMR analysis. The results showed complete conversion.

Fig. S1: Experimental setup for g-C_3N_4 & TBAB catalyzed epoxide to cyclic carbonate conversion.

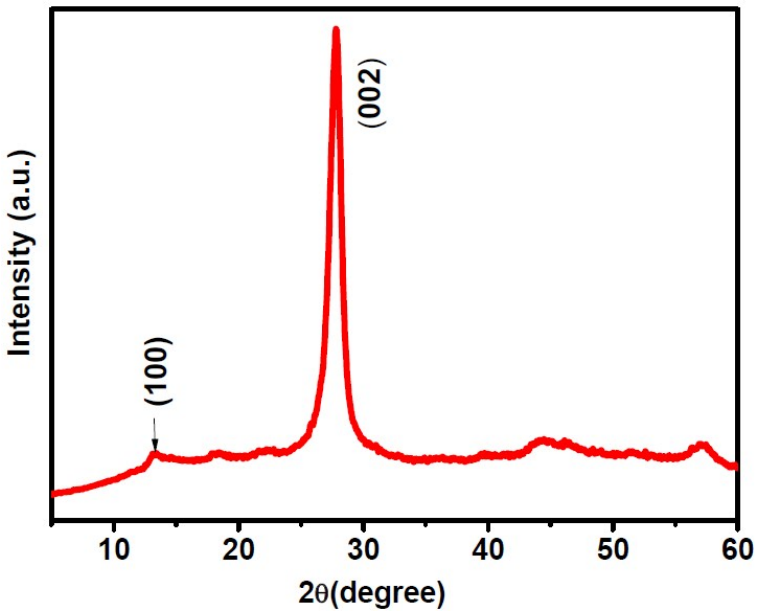

Fig. S2: PXRD spectrum of g-C_3N_4.

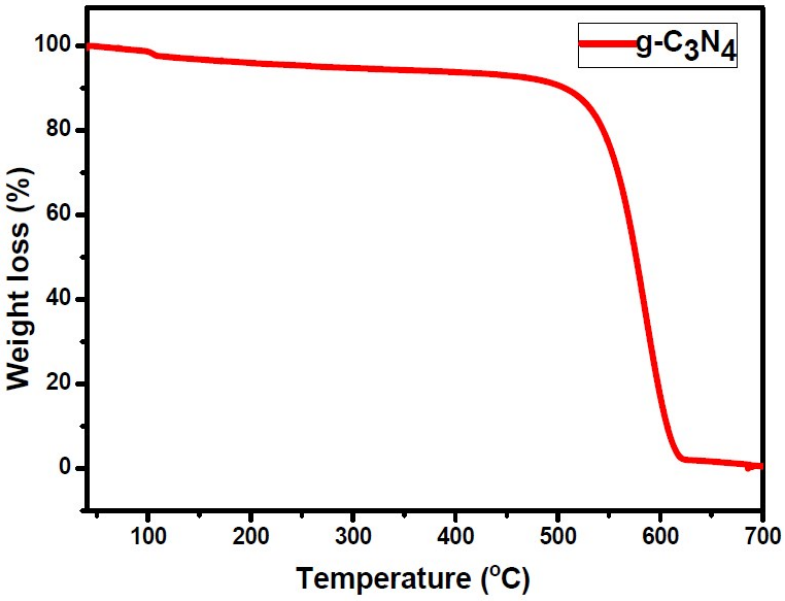

Fig.S3. Thermogravimetric analysis curves of g-C3N4.

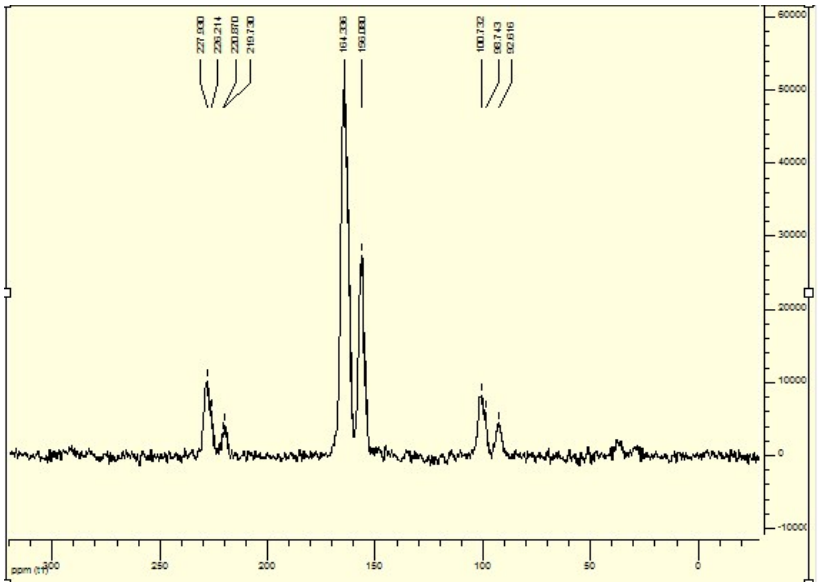

Fig. S4: ^{13}C (CP MAS) NMR of g-C_3N_4 (500 MHz).

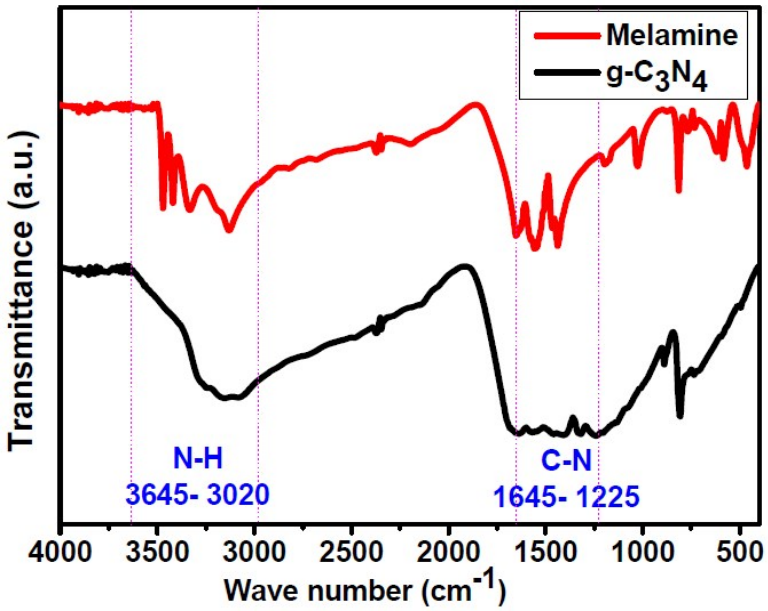

Fig. S5: IR Spectra of melamine and g-C_3N_4.

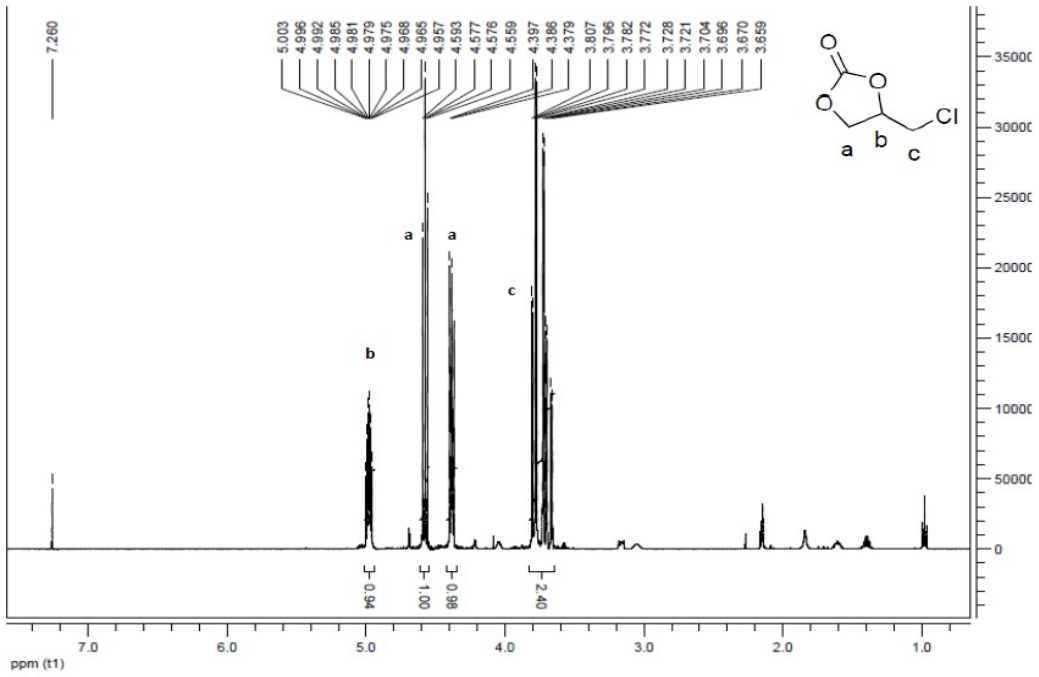

Fig. S6: 4-(chloromethyl)-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 500 MHz).

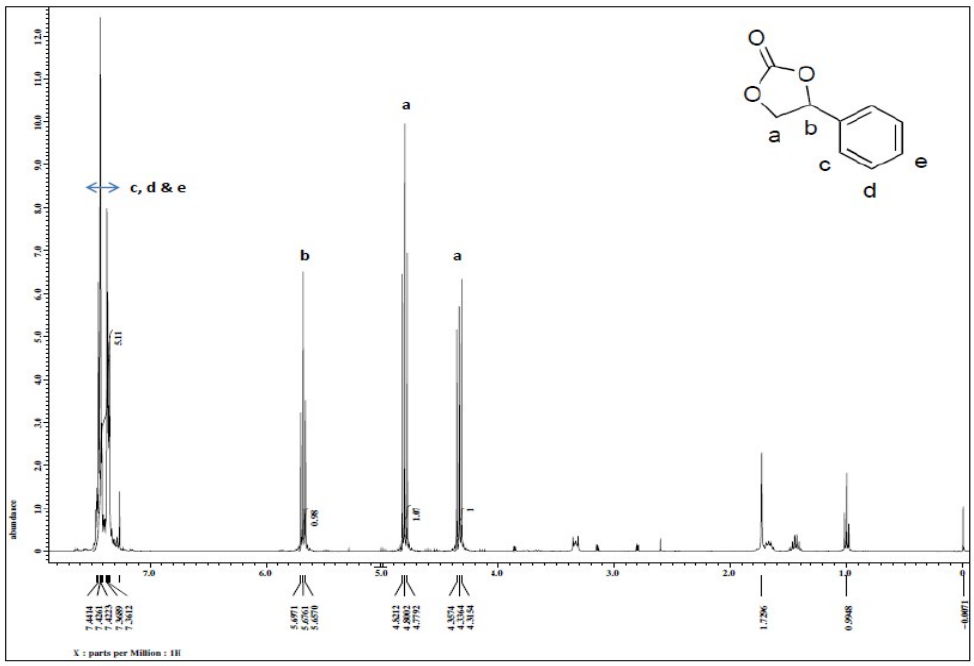

Fig. S7: 4-phenyl-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 400 MHz).

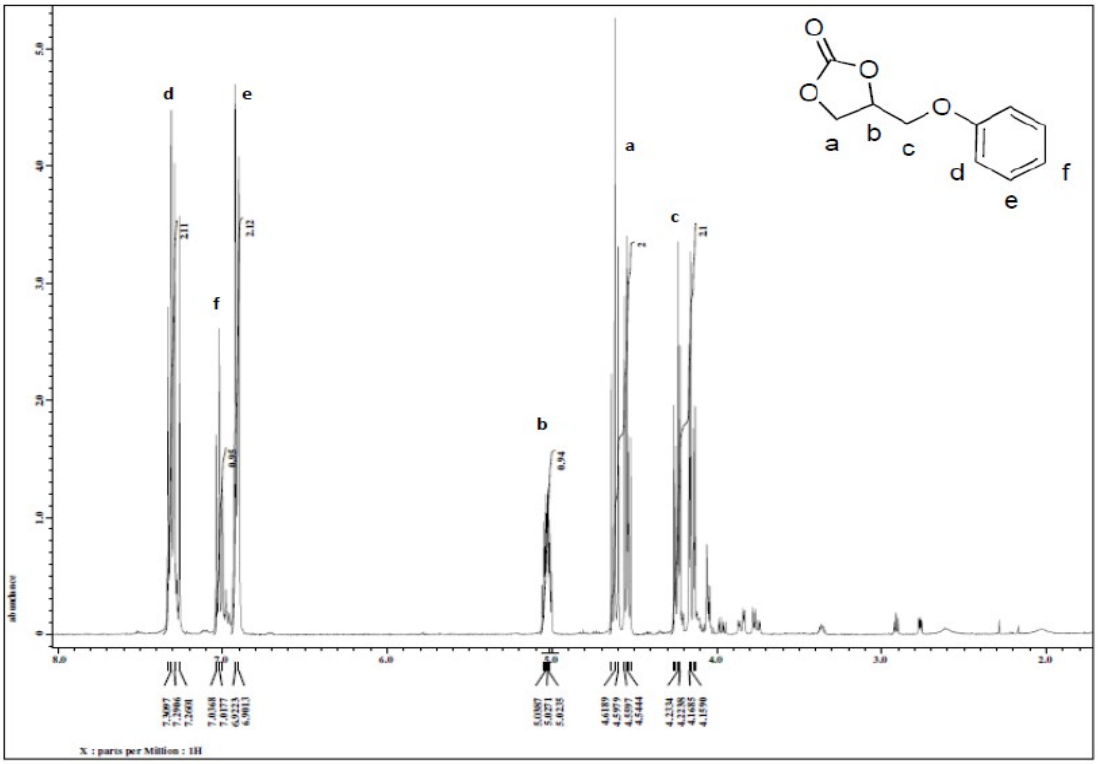

Fig. S8: 4-(phenoxymethyl)-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 400 MHz).

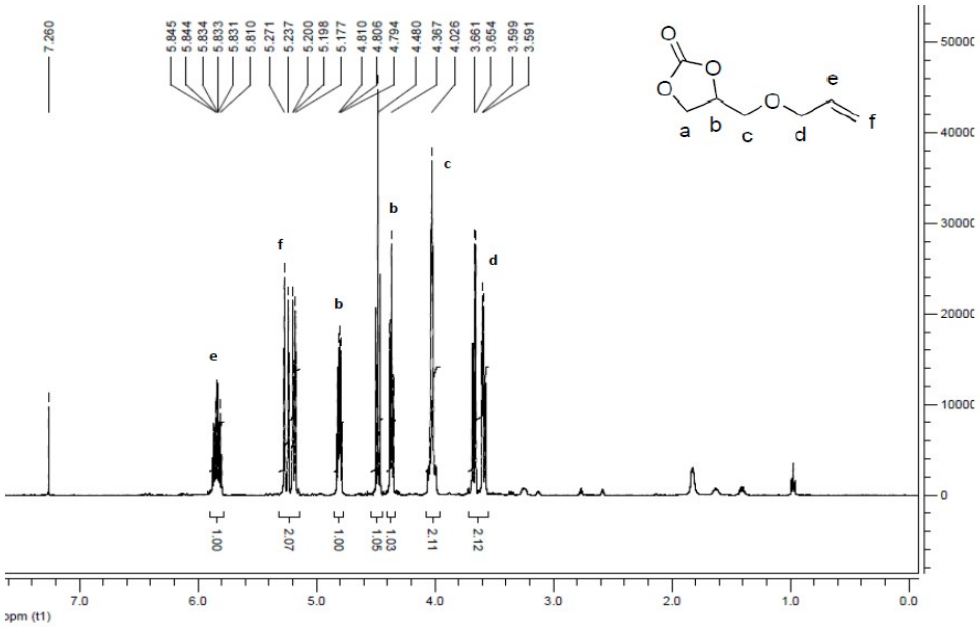

Fig. S9: 4-(allyloxymethyl)-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 500 MHz).

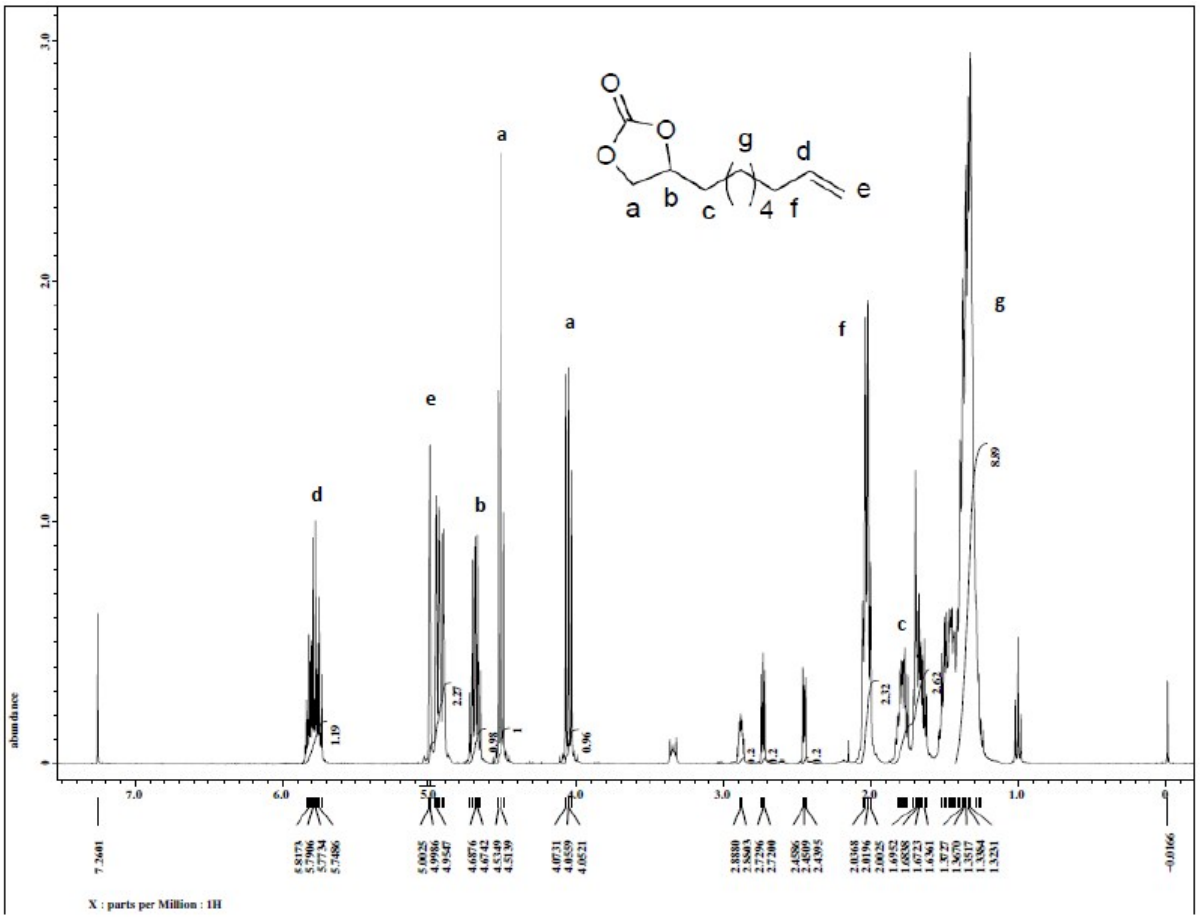

Fig. S10: 4-(oct-7-enyl)-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 400 MHz).

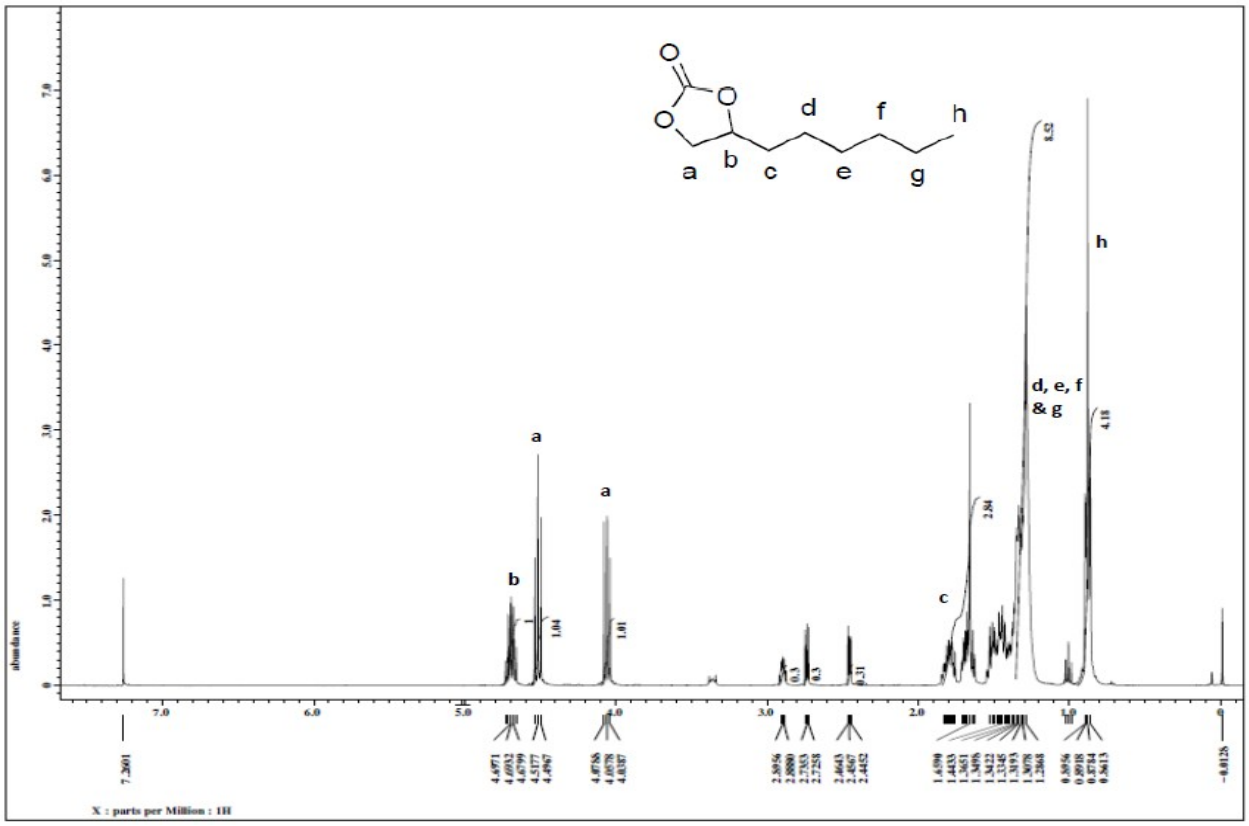

Fig. S11: hexyl-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 400 MHz).

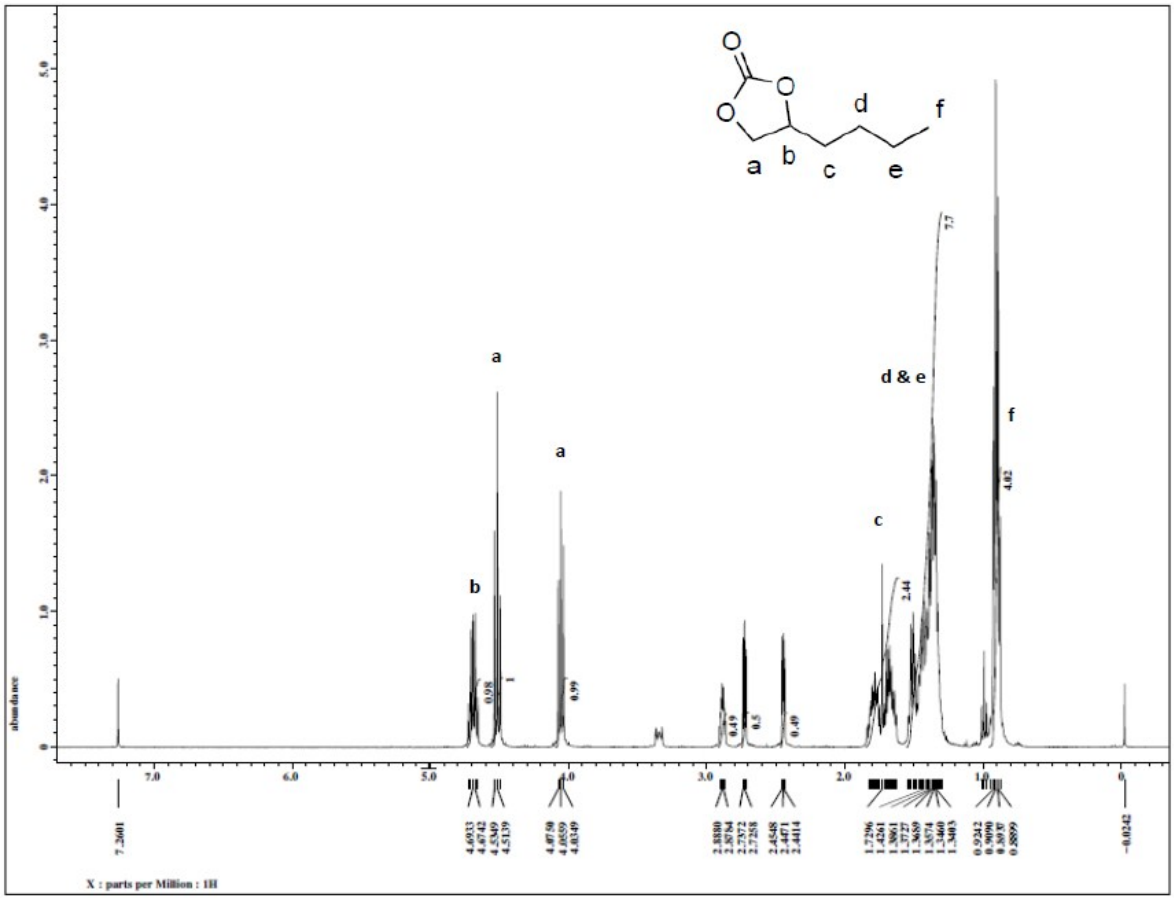

Fig. S12: 4-butyl-1,3-dioxolan-2-one: ^{1}H NMR ($CDCl_3$, 400 MHz).

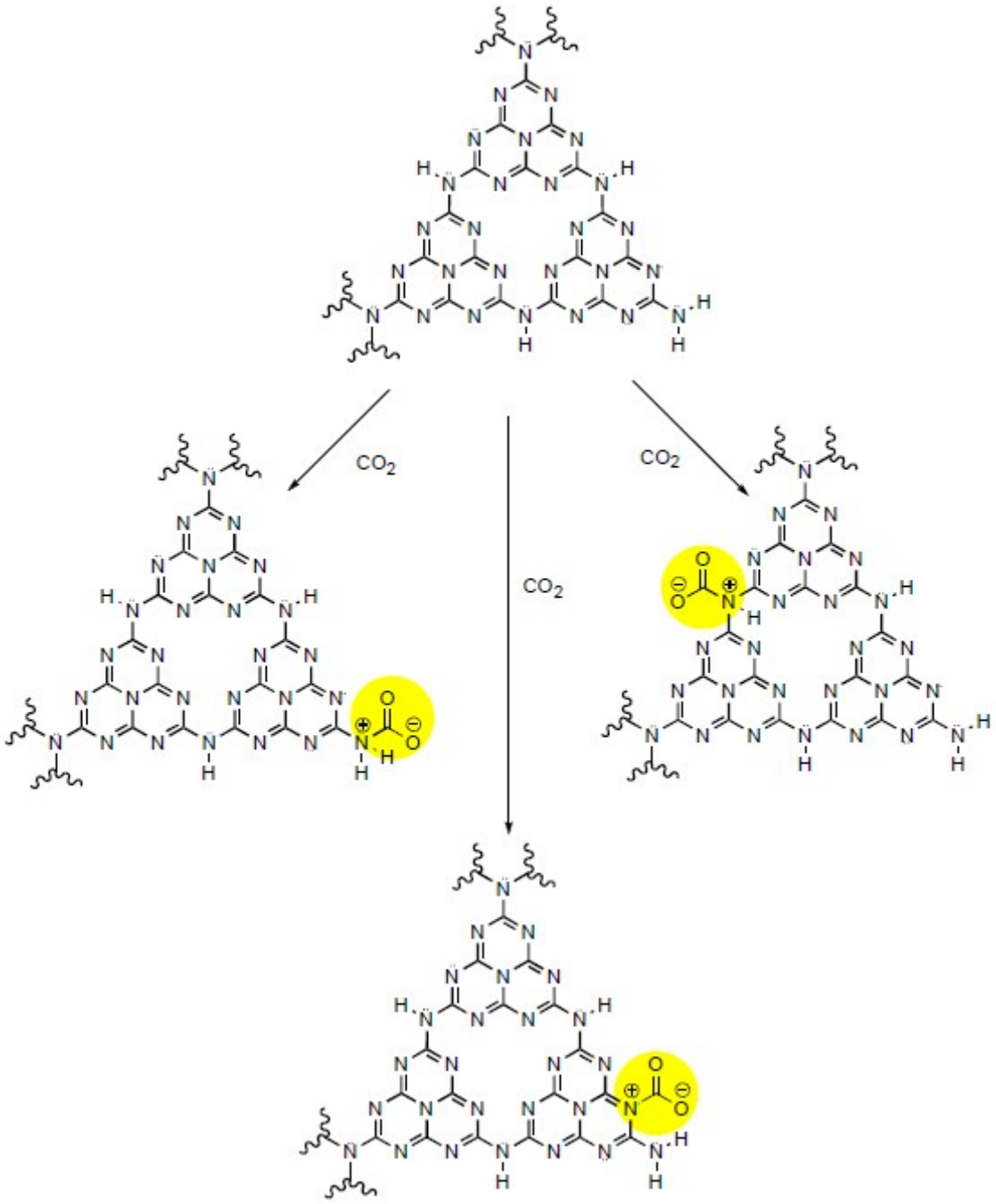

Fig. S13: Schematic illustration of the different pathways for CO_2 absorption by g-C_3N_4