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Article

Upgrading of Biobased Glycerol to Glycerol Carbonate as a Tool to Reduce the CO_2 Emissions of the Biodiesel Fuel Life Cycle

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SUPPLEMENTARY

Products characterization.

After preliminary evaluation, Gly-urea mixtures were processed within the DoE domain, that is: reactor temperature from 175 to 195 °C, recirculation time from 90 to 210 min, urea:Gly MR from 1.2 to 1.8. After solvent extraction (EtOAc:Et_2O 4:1) and drying, a colorless oil was obtained. This raw material was directly analyzed with ^1H NMR spectroscopy and two main groups of signals were detected:

- a set of signals (Figure S1) was assigned to GC;

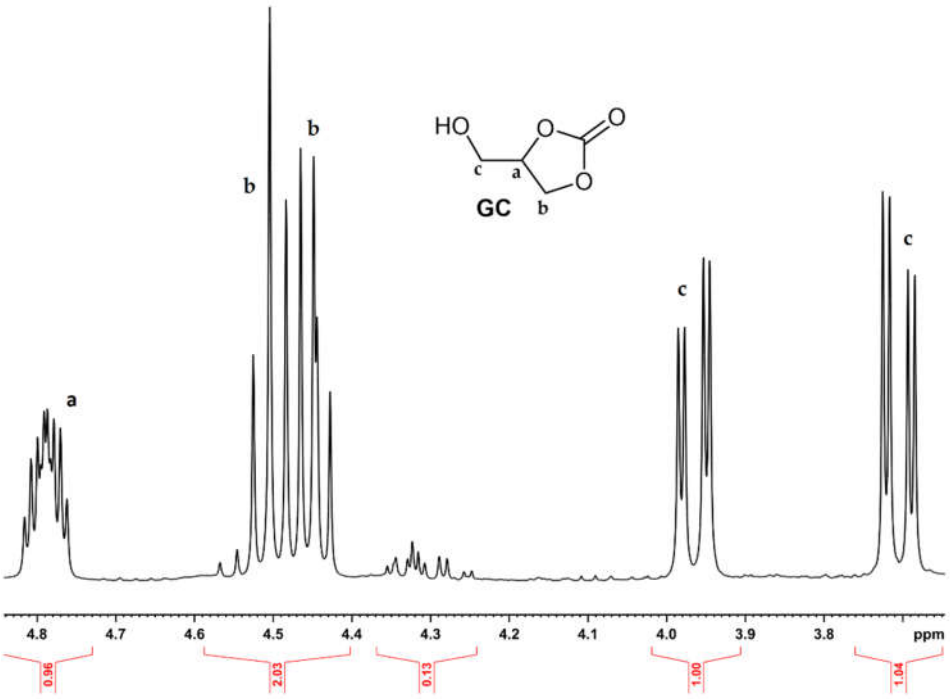

Figure S1. Typical ^{1}H-NMR spectra ($CDCl_3$, 400 MHz) of a GC-rich raw mixture.

- a second set of signals was assigned to DGTC. DGTC was always detected as contaminant of the main product (GC) and its identity was gathered from the literature [94-96]. In Figure S2 is shown a typical ^{1}H NMR spectra of a DGTC-rich raw mixture.

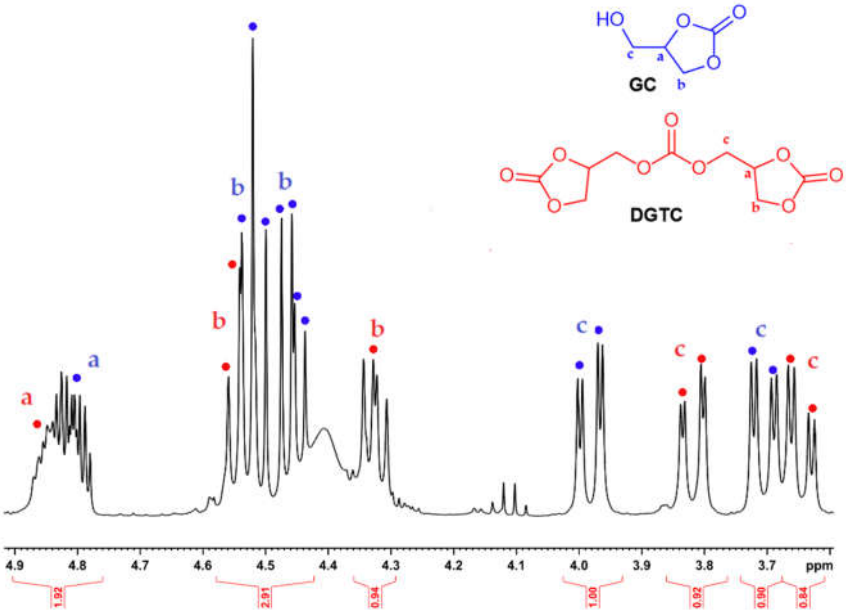

Figure S2. Typical ^{1}H NMR spectra ($CDCl_3$, 400 MHz) of a DGTC-rich raw mixture.

As DGTC was the only recurring and largely predominant detected side-product, we approximated the raw (extracted) reaction mixture as a binary mixture. Given that, GC molar selectivity was calculated from the integrated area of isolated -CH-C<u>H</u>$_2$-OH signals (**c** in Figg S1 and S2) of the desired product (GC, dd at δ 3.99 ppm, 1H) and the contaminant (DGTC, dd at δ 3.82 ppm, 2H), as follows:

$$\text{GC Sel \%} = \frac{100 \cdot \text{Area } (\delta\ 3.99\ \text{ppm})}{\text{Area } (\delta\ 3.99\ \text{ppm}) + (\text{Area } (\delta\ 3.82\ \text{ppm})\ /2)}$$

Figure S2 depicts the ^{1}H NMR spectra of the raw mixture obtained after solvent extraction from experiment n. 3 (Table 2). In this case, the calculated value for GC selectivity% equals to 68 (= 100·(1.00/1.00+(0.92/2))).