

Supporting Information

Degradation of poly(ethylene terephthalate) catalyzed by nonmetallic dibasic ionic liquids under UV radiation

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Section A: Characterization of the [HDBU][Im]

FT-IR and ¹H NMR were used to determine the structure of [HDBU][Im]. FT-IR spectra of [HDBU][Im] is shown in Fig. S1.

The peak at 3106 cm⁻¹ is attributed to the stretching vibration of unsaturated C-H ^[1]. The peak at 2853 cm⁻¹ is attributed to the stretching vibration of saturated C-H ^[1]. The peak at 1643 cm⁻¹ is attributed to C=C stretching vibration of imidazole ring ^[2]. The peak at 1613 cm⁻¹ is attributed to C=N stretching vibration of imidazole ring and DBU ^[3]. The peaks at 1353 cm⁻¹ and 1368 cm⁻¹ are typical stretching vibration of C=N. These above FI-IR results demonstrated the successful synthesis of [HDBU][Im].

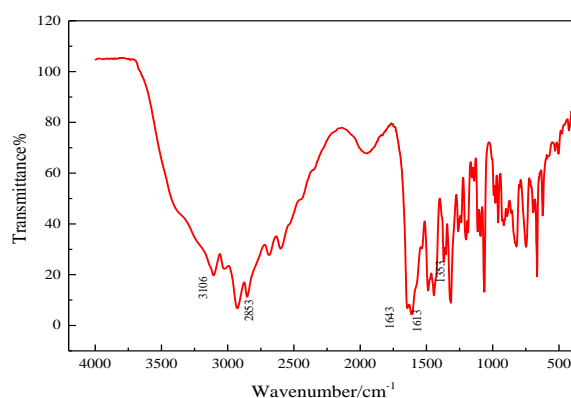


Figure S1 FT-IR spectrum of [HDBU][Im]

In the ¹H NMR spectrum (Fig.S2), the single peak at δ 7.63 ppm corresponds to the H-14 in imidazole ring. The single peak at δ 7.05 ppm represents H-12 and H-16. The triplet at δ 3.26 ppm indicates H-4. The multiple peaks from δ 3.18 ppm to δ 3.21 ppm represent H-6 and H-7, their chemical environment is similar, so their signals cannot be separated. The single peak at δ 2.38 ppm represents H-11. The multiple peaks at δ 1.79 ppm corresponds to H-5. The multiple peaks at δ 1.63 ppm corresponds to H-9 and H-10. The single peak at

$\delta 1.56$ ppm represents H-8. The NMR result is consistent with the data from literature, so [HDBU][Im] is successfully prepared^[4,5].

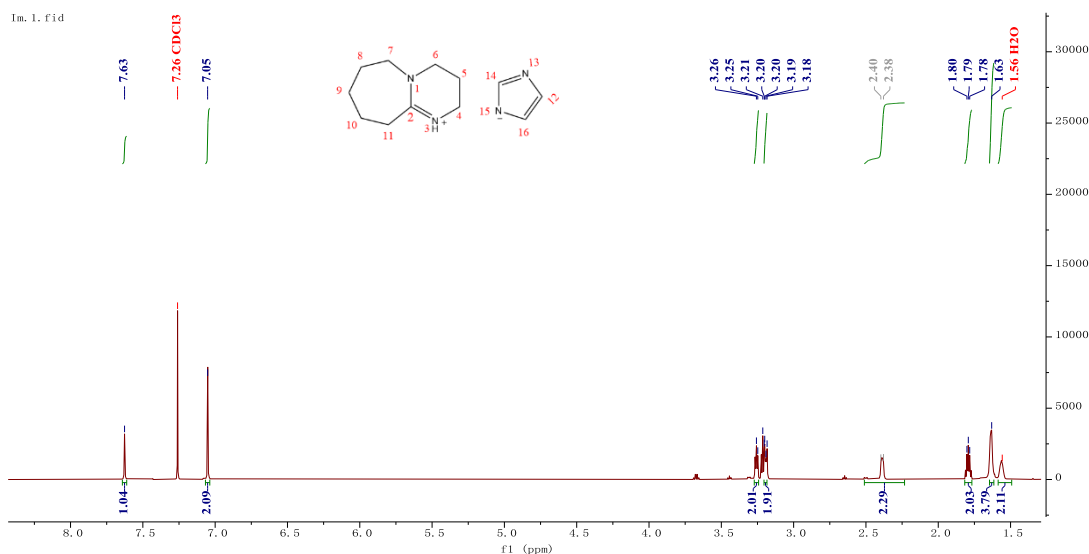


Figure S2 ^1H NMR spectrum of [HDBU][Im]

Section B: Characterization of the main product Thank you very much for your encouraging comments.

The structure of the main product obtained by glycolysis was determined by NMR, HPLC, TGA, DSC and FTIR. ^1H NMR spectrum was shown in Fig. S3. The signal at $\delta 8.13$ ppm indicates the presence of the four aromatic protons of the benzene ring (H-1). The signal at $\delta 4.32$ ppm $\delta 3.73$ ppm represents the methylene protons of COO-CH₂ (H-2) and CH₂-OH (H-3), respectively. The signal at $\delta 4.97$ ppm is the characteristic of the protons of the hydroxyl (H-4). It was demonstrated that the main product was BHET^[6].

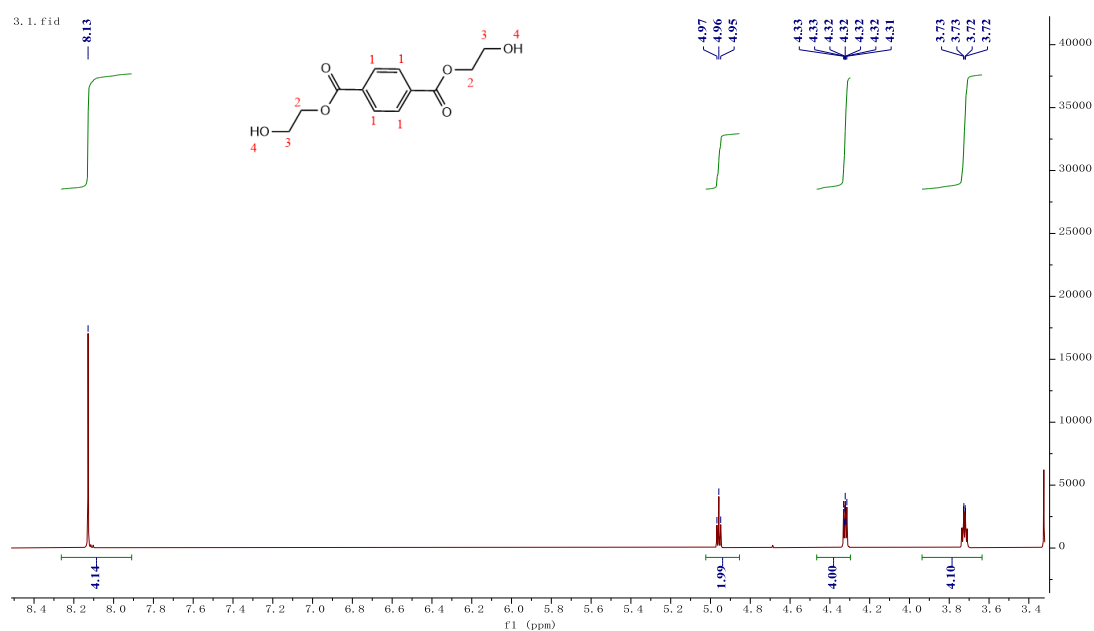


Figure S3 ^1H NMR spectrum of BHET

In the HPLC spectrum Fig. S4, only one peak appears other than solvent peak, which indicates that the purity of BHET is high.

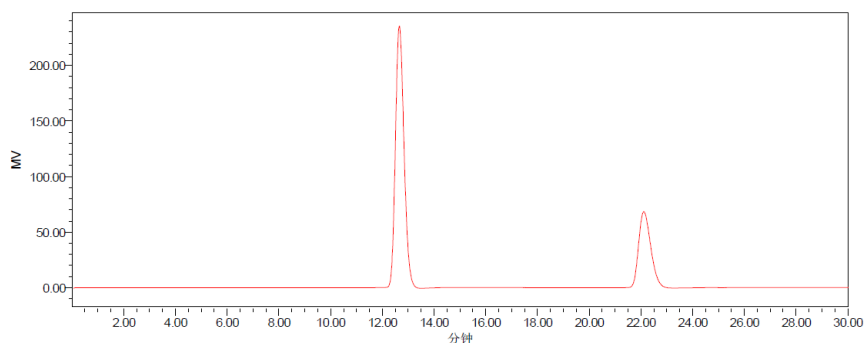


Figure S4 HPLC spectrum of BHET

Fig. S5 demonstrated the TGA curves of the BHET and PET raw material. The PET material experienced only one obvious weight loss process, while BHET experienced two weight loss processes. The TGA curve of PET showed an obvious weight loss at above 390 °C. The weight loss was more than 80% in the range from 390 °C to 461 °C, which was attributed to the thermal degradation of PET. For BHET, the thermal decomposition appeared in two different steps. The first weight loss at about 250 °C caused by thermal decomposition of BHET. In the second weight loss process, it was found that the weight loss temperature was around 390 °C, which is consistent with raw PET. It suggested that BHET may be polymerized into PET during the heating process, which is consistent with the literature reports and explains why the second weight loss process was similar to raw PET^[6].

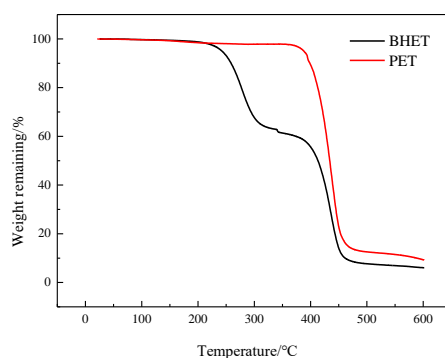


Figure S5 TGA curves of PET raw material and BHET

For BHET, a sharp endothermic peak appears at 110.09 °C (Fig. S6). The temperature of this peak is consistent with the melting point of the pure BHET (109.81 °C). The DSC analysis showed that the main product was BHET^[7].

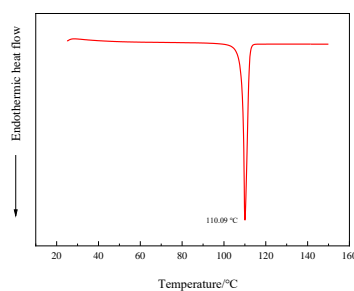


Figure S6 DSC curves of BHET

As shown in Fig. S7, BHET FT-IR spectrum demonstrated strong absorption peaks at 3299.19 cm^{-1} correspond to the characteristic stretching vibration of OH, peaks at 2955.45 and 2873.10 cm^{-1} appeared due to the stretching vibrations of aliphatic $-\text{CH}_2-$ group at different position; the strong absorption peaks at 1723.90 and 1271.98 cm^{-1} indicate the presence of ester functional groups, corresponding to the stretching vibrations of $\text{C}=\text{O}$ and $\text{C}-\text{O}$ respectively; peaks from 1407 to 1503 cm^{-1} indicate the presence of benzene rings corresponding to the stretching vibration and in-plane bending vibration of $\text{C}=\text{C}$ in the benzene ring. The transmission bands at 898.23 cm^{-1} and 727.20 cm^{-1} showed p-substitution on the benzene. These peaks are all consistent with reported BHET^[8–10].

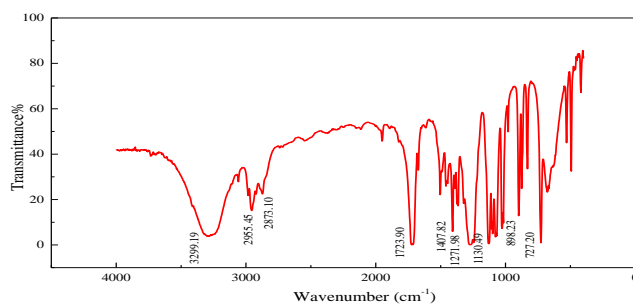


Figure S7 FTIR spectrum of BHET

Section C: Thermal stability analysis of [HDBU][Im]

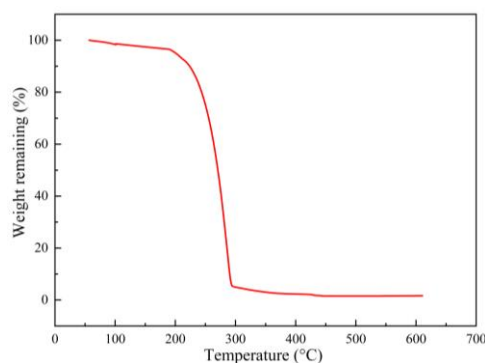


Figure S8 The TGA curve of [HDBU][Im]

Section D: The interaction between DBU and EG

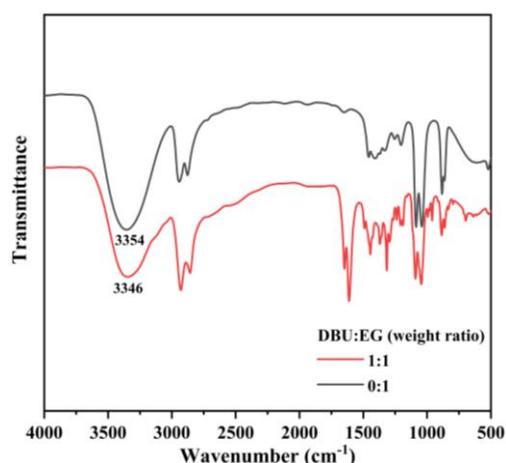


Figure S9 FT-IR spectra of DBU/EG mixtures.

Section E: The crystallinity of PET

FT-IR was used to measure the crystallinity of PET. The absorption peaks observed at 1370 and 1340 cm^{-1} were attributed to the gauche and trans conformations of CH_2 wagging in PET, respectively^[11]. In amorphous PET, PET mainly exhibits gauche conformation, while in crystalline PET, PET mainly exhibits trans conformation. It is a reliable quantitative method to assess the crystallinity of PET from gauche-to-trans conformation^[12,13]. Therefore, the crystallinity of PET could be calculated using the following equation^[14,15]:

$$\text{Trans content ratio} = A_{1340} / (A_{1340} + 6.6 A_{1370}) \quad (1)$$

where A_{1340} and A_{1370} are the areas of the absorption bands at 1340 and 1370 cm^{-1} , respectively.

Table S1 The changes in PET crystallinity during the degradation reaction¹

Reaction time (min)	The crystallinity of PET (%)
0	51.83
10	72.54
20	78.16
30	83.68

¹ Reaction conditions: 5.0 g PET, 5.0 wt% catalyst, 20.0 g EG, at 175°C under 10000 $\mu\text{W}\cdot\text{cm}^{-2}$

² UV radiation.

Reference

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