Electronic Supplementary Information

Deep Eutectic Solvents as highly active catalysts for the fast and mild glycolysis of poly(ethylene terephthalate)(PET)

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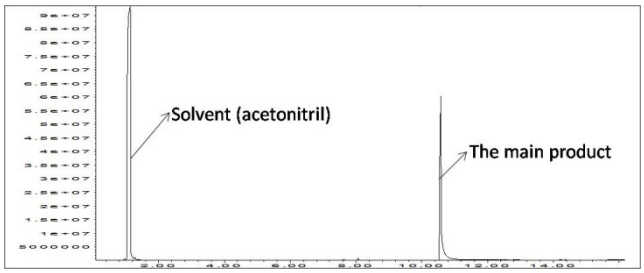
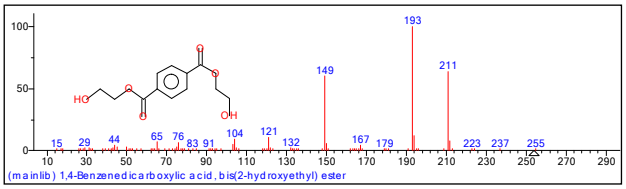
Qualitative analysis of the main degradation product:



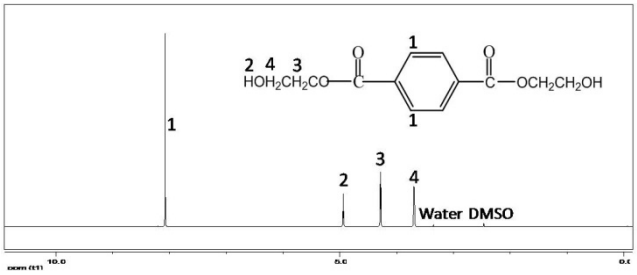
(a) GC spectrum of the main product



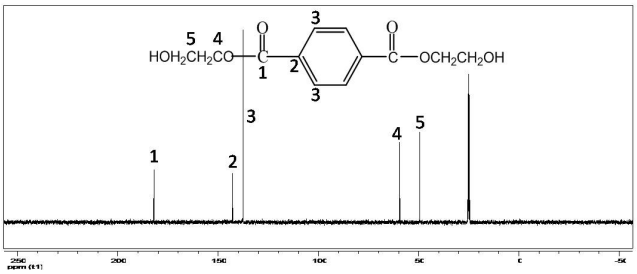
(b) MS spectrum of the main product

Fig. S1 GC-MS spectra of the main product

GC-MS spectra in Fig. S1 show that the main product is BHET at 10.577 min and the product is pure because there is no extra peak except the solvent peak at1.133 min (acetonitrile).



(a) ^{1}H NMR patterns of the main product

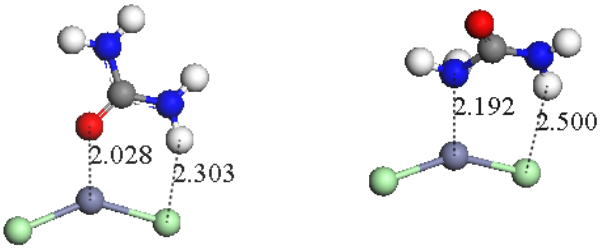


(b) ^{13}C NMR patterns of the main product

Fig. S2 NMR patterns of the main product

Structure optimizations of the urea/$ZnCl_2$: It was found that there are different energy minimum structures for the coordination $ZnCl_2$ and urea by calculations while the coordination numbers are 1, 2, 3, 4. The structures with 5, 6 coordination numbers couldn't be found.

The interaction of $ZnCl_2$ with one urea will lead to the formation of two kinds of structure A and B. The coordination position will be N atom or O atom of urea, and the structure with O-coordination position is with the energy advantage as shown in **Fig. S3**. The hydrogen atom of urea will also interact with Cl of $ZnCl_2$ while the coordination formed between Zn and O/N.

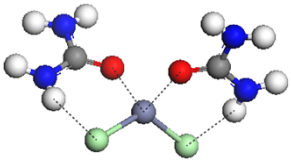


0.0 kcal/mol 9.1 kcal/mol

A B

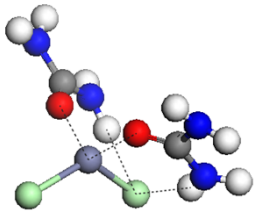
Fig. S3 Optimized structures of coordinated structure $ZnCl_2$ with one urea with relative energies, the structure B is with higher energy than A by 9.1 kcal/mol. Red: O; green: Cl; blue: N; white: H; dark grey: C; light gray: Zn.

There are four kinds of possible coordination structure $ZnCl_2$ with two urea 2A, 2B, 2C and 2D. Two structures are with O-coordination between $ZnCl_2$ and urea, and other two are with N-coordination position.



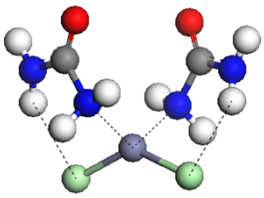
0.0 kcal/mol

2A



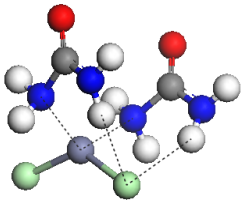
1.6 kcal/mol

2B



13.4 kcal/mol

2C

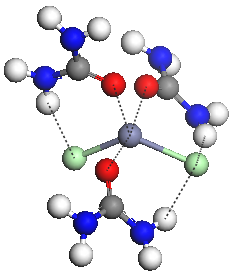


14.5 kcal/mol

2D

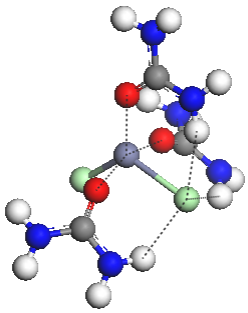
Fig. S4 Optimized structures of coordinated structure $ZnCl_2$ with two urea. The structure B is with lower energy than A by 2.7 kcal/mol, and the structure C is with lower energy than D by 4.4 kcal/mol. Red: O; green: Cl; blue: N; white: H; dark grey: C; light gray: Zn.

The interaction of $ZnCl_2$ with three urea will lead to the formation of two kinds of structure 3A and 3B with O-coordination interaction, and stable N-coordination structures couldn't be found. The structures 3A is with two urea on the one side of $ZnCl_2$, and one urea on another side (H of the two urea molecules interact with Cl-1 of $ZnCl_2$, and H of the one urea interacts with Cl-2 of $ZnCl_2$). The structure 3B is with three urea on the one side of $ZnCl_2$ (H of three urea molecules interact with Cl-1 of $ZnCl_2$).



0.0 kcal/mol

3A

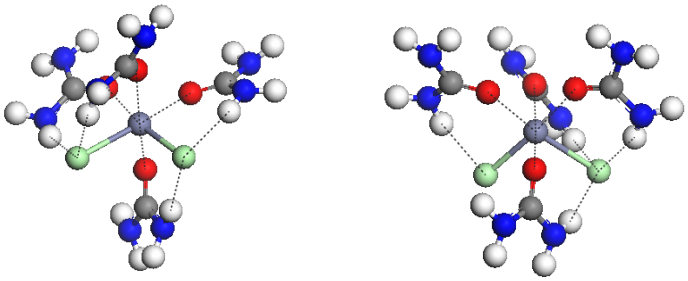


0.7 kcal/mol

3B

Fig. S5 Optimized structures of coordinated structure $ZnCl_2$ with three urea. The structure B is with lower energy than A by 2.7 kcal/mol. Red: O; green: Cl; blue: N; white: H; dark grey: C; light gray: Zn.

The interaction of $ZnCl_2$ with four urea will lead to the formation of two kinds of structure 4A and 4B, and both of them are O-coordination structures. The structures 4A is with two urea on the one side of $ZnCl_2$ (H of the two urea molecules are interact with Cl-1 of $ZnCl_2$), and other two urea on another side (H of the two urea molecules are interact with Cl-2 of $ZnCl_2$). The structures 4B is with three urea on the one side of $ZnCl_2$ (H of the three urea molecules interact with Cl-1 of $ZnCl_2$), and the last one on another side (H of the one urea interacts with Cl-2 of $ZnCl_2$).



0.0 kcal/mol　　0.4 kcal/mol

4A　　4B

Fig. S6 Optimized structures of coordinated structure $ZnCl_2$ with four urea. The two structures almost are not with any energy difference. Red: O; green: Cl; blue: N; white: H; dark grey: C; light gray: Zn.