Supporting Information

PET recycling under mild conditions via substituent-modulated intramolecular hydrolysis

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1. Preparation of binuclear complexes

General synthetic procedure for 2-hydroxy-5-R-isophthalaldehyde (R_1 = OCH_3, R_2 = OH, R_3 = CH_3, R_4 = H, R_5 = F, R_6 = Cl, R_7 = Br, R_8 = NO_2, R_9 = ethyl, R_{10} = tert-butyl, R_{11} = n-pentyl, R_{12} = cyclohexyl, and R_{13} = adamantly)

2-hydroxy-5-R_1-isophthalaldehyde. The synthesis was conducted following the procedure detailed previously.[1] In brief, hexamethylenetetramine (11.2 g, 80 mol) was mixed with trifluoroacetic acid (TFA) (15 mL) and the mixture was heated up to 105 °C. When hexamethylenetetramine was dissolved, 4-methoxyphenol (2.5 g, 20 mmol) was added and the solution was stirred at 105 °C for 12 h. After that, 10 mL of water was poured into the reaction vessel and the reaction solution was refluxed for another 10 min. To quench the reaction, the reaction solution was slowly added into ice water (400 mL). Yellow solid was obtained by filtration and vacuum drying.

2,5-dihydroxy-isophthalaldehyde. The compound was synthesized via demethylation of 2-hydroxy-5-R_1-isophthalaldehyde according to procedures reported previously.[2] In a typical synthesis, 2-hydroxy-5-R_1-isophthalaldehyde (0.356 g, 2 mmol) was suspended in 26 mL of dry dichloromethane and the mixture was cooled to -70 ^oC in N_2 atmosphere. Then, tribromoborane solution (8.7 mL, 8.7 mmol) was added in dropwise. The resultant mixture was warmed up to 0 °C over 24 h. Once upon the temperature reached 0 ^oC, water (10 mL) was slowly added into the reaction. The product was extracted with ethyl acetate, washed by saturated solution of sodium thiosulfate and brine, and dried over Na_2SO_4. After filtration, the solvent was removed using a rotary-evaporator to yield orange-yellow solid.

2-hydroxy-5-R_3-isophthalaldehyde. The synthesis was the same as that of 2-hydroxy-5-R_1-isophthalaldehyde, except that 4-methoxyphenol (2.5 g, 20 mmol) was replaced by 4-methylphenol (2.16 g, 20 mmol). Yellow solid was obtained by recrystallization from methanol-water solution.

2-hydroxy-5-R_4-isophthalaldehyde. The synthesis was the same as that of 2-hydroxy-5-R_1-isophthalaldehyde, except that 4-methoxyphenol (2.5 g, 20 mmol) was replaced by phenol (1.9 g, 20 mmol). Yellow product was obtained by filtration and vacuum drying.

2-hydroxy-5-R_5-isophthalaldehyde. The synthesis was conducted according to previously reported procedures with minor modification.[3] Briefly, 4-fluorothiophenol (1.12 g, 10 mmol) was added into a TFA solution of hexamethylenetetramine (5.6 g, 40 mmol, 15 mL). The reaction was heated at 120 °C for 24 h. After cooling to room temperature, the reaction flask was charged with 60 mL of HCl (3 M).

The reaction mixture was heated up to 80 ℃ again and maintained at this temperature for another 5 h. After cooling to room temperature, the reaction solution was poured into 300 mL of ice water. Yellow precipitation was obtained by filtration and the solid was dried under vacuum.

2-hydroxy-5-R_6-isophthalaldehyde. The synthesis was similar to that of 2-hydroxy-5-R_5-isophthalaldehyde. In a typical synthesis, p-chlorophenol (1.86 g, 14.5 mmol) was added into a TFA solution of hexamethylenetetramine (8.3 g, 58 mmol, 25 mL). The reaction was left at 120 ℃ for 24 h. Then, 60 mL of HCl (3 M) was poured into the reaction after it was cooled down to room temperature. The reaction was heated up to 80 ℃ and kept at this temperature for another 5 h. After that, the reaction was left at room temperature for 24 h without stirring. Yellow crystals were obtained by filtration.

2-hydroxy-5-R_7-isophthalaldehyde. The synthetic method was the same as that of 2-hydroxy-5-R_6-isophthalaldehyde above, except that p-chlorophenol (1.86 g, 14.5 mmol) was replaced by *p*-bromophenol (2.51 g, 14.5 mmol). Yellow crystals were collected following the same post-treatment as 2-hydroxy-5-R_6-isophthalaldehyde.

2-hydroxy-5-R_8-isophthalaldehyde. The synthesis was conducted according to previously reported procedures with minor modification.[4] In brief, p-nitrophenol (1 g, 7.2 mmol) and hexamethylenetetramine (3 g, 21.4 mmol) in TFA (15 mL) was mixed and stirred at 120 °C for 6 d. Then, 30 mL of HCl (1 M) was added into the reaction at 50 °C. The reaction was stirred at this temperature for 10 min before cooling to room temperature. The reaction solution was extracted with CH_2Cl_2, washed with brine and water successively, and dried over Na_2SO_4. Orange solid was obtained after rotary-evaporation and vacuum-drying.

In the case of **R_9 -R_{13}**, the synthesis was similar to that of 2-hydroxy-5-R_1-isophthalaldehyde as detailed above, except that 4-methoxyphenol was replaced by equivalent amount of 4-R-phenol. Crude yellow solids were obtained by filtration and dried under vacuum.

General synthetic procedures for complexes 1–13. Binuclear complexes were prepared according to a modified procedure reported previously[5]. Typically, a methanol solution of 1,3-diamino propane (1 mmol, 84 μL) was added dropwise into a methanol solution of $Zn(NO_3)_2$ $6H_2O$ (0.3 g, 1 mmol, 5 mL) under stirring, followed by the addition of a methanol solution of 2-hydroxy-5-R-isophthalaldehyde (1 mmol, 5 mL). For complexes with R_2, R_4 and R_6–R_{13}, the resulting solutions were refluxed for 1 h under stirring. After standing for a while, products were collected by filtration and washed with methanol and

diethyl ether. For complexes with R_1 and R_3, the resulted mixtures were stirred for 10 minutes at room temperature. Yellow crystals precipitated after standing for several hours and were collected by filtration. For $Zn_2L–R_5(NO_3)_2$, the complex was prepared according to a modified procedure reported previously [6]. To a acetonitrile-methanol solution (v/v 1:1, 20 mL) of $Zn(NO_3)_2$ $6H_2O$ (1 mmol) and 5-fluoro-2-hydroxyisophthalaldehyde (1 mmol) was added dropwise a acetonitrile-methanol solution(1:1, 2 mL) contained 1,3-diamino propane (84 μL, 1 mmol) in the presence of 10 molar equivalents of triethylamine. White precipitate was filtered after refluxing for 1 h and standing at room temperature.

$Zn_2L–OH(NO_3)_2$. After standing for 3 days at room temperature, dark red rod-shaped crystals were collected and characterized without further purification. ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 9.28 (s, 2H, Ar-OH), 8.43 (s, 4H, N=CH), 7.10 (s, 4H, Ar), 3.94 (s, 8H, N–CH_2), 2.05 (s, 4H, CH_2). Anal. Calcd for $C_{22}H_{22}N_6O_{10}Zn_2$: C, 41.12; H, 3.42; N, 13.08. Found: C, 37.51; H, 3.32; N, 11.91.

$Zn_2L–OCH_3(NO_3)_2$. Yellow crystals were obtained after standing for several hours. ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.55 (s, 4H, N=CH), 7.41 (s, 4H, Ar), 3.98 (s, 8H, N-CH_2), 2.05 (s, 4H, CH_2). Anal. Calcd for $C_{24}H_{26}N_6O_{10}Zn_2$: C, 41.74; H, 3.91; N, 12.17. Found: C, 42.20; H, 4.06; N, 11.90.

$Zn_2L–CH_3(NO_3)_2$. Yellow tabular crystals were obtained after standing overnight and characterized without further purification. ^{1}H NMR (400 MHz, D_2O): δ 8.26 (s, 4H, N=CH), 7.34 (s, 4H, Ar), 3.92 (s, 8H, N–CH_2), 2.20 (s, 6H, Ar–CH_3), 2.04 (s, 4H, CH_2). Anal. Calcd (%) for $C_{25}H_{28}N_6O_9Zn_2$: C, 43.69; H, 4.11; N, 12.23. Found: C, 43.42; H, 4.21; N, 12.31.

$Zn_2L–H(NO_3)_2$. The precipitated product obtained after standing overnight was filtered out and yellow crystals were obtained by evaporating the solvent. ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.56 (s, 4H, N=CH), 7.72 (d, 4H, Ar), 7.03 (t, 2H, Ar), 3.99 (s, 8H, N–CH_2), 2.05 (s, 4H, CH_2). Anal. Calcd (%) for $C_{22}H_{22}N_6O_8Zn_2$: C, 42.22; H, 3.60; N, 13.63. Found: C, 42.04; H, 3.50; N, 13.37.

$Zn_2L–F(NO_3)_2$. White precipitate was dried and recrystallized in methanol-water to obtain pale yellow crystals. ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.52 (s, 4H, N=CH), 7.68 (d, 4H, Ar), 3.99 (s, 8H, N–CH_2), 2.06 (s, 4H, CH_2).

$Zn_2L–Cl(NO_3)_2$. Yellow crystals were obtained by recrystallization in methanol-water. ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.54 (s, 4H, N=CH), 7.85 (s, 4H, Ar), 3.99 (s, 8H, N–CH_2), 2.07 (s, 4H, CH_2). Anal. Calcd (%) for $C_{22}H_{24}Cl_2N_6O_{10}Zn_2$: C, 36.92; H, 3.36; N, 11.76. Found: C, 36.49; H, 3.10; N, 11.35.

$Zn_2L–Br(NO_3)_2$. Crystals were obtained by recrystallization similar to that of Zn_2L-$F(NO_3)_2$. ^{1}H NMR

(400 MHz, $(CD_3)_2SO$): δ 8.53 (s, 4H, N=CH), 7.94 (s, 4H, Ar), 3.96 (s, 8H, N–CH_2), 2.06 (s, 4H, CH_2). Anal. Calcd (%) for $C_{22}H_{24}Br_2N_6O_{10}Zn_2$: C, 32.88; H, 2.74; N, 10.46. Found: C, 32.24; H, 3.02; N, 10.14.

Zn_2L–$NO_2(NO_3)_2$. Yellow precipitate was filtered off after standing for 7 days and the crude product was crystallized by slow addition of diethyl ether to a DMF solution. Then, orange rod-like crystals were used for characterization. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.75 (s, 4H, N=CH), 8.70 (s, 4H, Ar), 4.03 (s, 8H, N–CH_2), 2.10 (s, 4H, CH_2). Anal. Calcd (%) for $C_{24}H_{28}N_8O_4Zn_2$: C, 36.80; H, 3.57; N, 14.31. Found: C, 37.12; H, 3.61; N, 14.74.

Zn_2L–ethyl$(NO_3)_2$. Yellow crystals were collected after slow evaporation at room temperature. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.54 (s, 4H, N=CH), 7.59 (s, 4H, Ar), 3.98 (s, 8H, N–CH_2), 2.59 (q, 4H, Ph-CH_2), 2.04 (s, 4H, CH_2), 1.20(t, 6H, CH_2-CH_3). Anal. Calcd (%) for $C_{26}H_{32}N_6O_8Zn_2$: C, 45.52; H, 4.38; N, 12.26. Found: C, 45.98; H, 4.47; N, 12.00.

Zn_2L–tert-butyl$(NO_3)_2$. Yellow precipitate was filtered off after standing overnight. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.60 (s, 4H, N=CH), 7.76 (s, 4H, Ar), 3.98 (s, 8H, N–CH_2), 2.04 (s, 4H, CH_2), 1.30 (s, 18H, C–$(CH_3)_3$). Anal. Calcd (%) for $C_{30}H_{40}N_6O_8Zn_2$: C, 48.42; H, 5.38; N, 11.29. Found: C, 48.41; H, 5.24; N, 11.30.

Zn_2L–n-pentyl$(NO_3)_2$. Yellow precipitate was filtered off after standing overnight. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.51 (s, 4H, N=CH), 7.54 (s, 4H, Ar), 3.97 (s, 8H, N–CH_2), 2.10 (s, 4H, CH_2), 1.81(m, 4H, Ar-CH_2), 1.58(m, 4H, CH_2-CH_2), 1.28(m, 8H, CH_2-CH_2), 0.86(t, 6H, CH_3). Anal. Calcd (%) for $C_{32}H_{44}N_6O_8Zn_2$: C, 49.77; H, 5.70; N, 10.89. Found: C, 39.30; H, 5.78; N, 13.06.

Zn_2L–cyclohexyl$(NO_3)_2$. Yellow precipitate was filtered off after standing overnight. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.55 (s, 4H, N=CH), 7.61 (s, 4H, Ar), 3.97 (s, 8H, N–CH_2), 2.05 (s, 4H, CH_2), 1.99 (m, 2H, Ph-CH), 1.81-1.24 (m, 20H). Anal. Calcd (%) for $C_{34}H_{44}N_6O_8Zn_2$: C,52.50; H, 5.59; N, 10.22. Found: C, 50.87; H, 5.41; N, 10.15.

Zn_2L–adamantyl$(NO_3)_2$. Yellow precipitate was filtered off after standing for several hours. ^1H NMR (400 MHz, $(CD_3)_2SO$): δ 8.59 (s, 4H, N=CH), 7.71 (s, 4H, Ar), 7.72 (s, 4H, Ar)3.97 (s, 8H, N–CH_2), 2.09 (s, 4H, CH_2), 2.03(m, 6H, C-CH_2-CH), 1.87(s, 12H, C-CH_2), 1.77(d, 12H, CH-CH_2). Anal. Calcd (%) for $C_{42}H_{52}N_6O_8Zn_2$: C,52.50; H, 5.86; N, 9.12. Found: C, 50.87; H, 5.92; N, 8.77.

2. PET hydrolysis.

Depolymerization of PET granules. PET hydrolysis was performed in a 20 mL vial placed in an aluminum heating block on a stirring hotplate. The vial was charged with a magnetic stirring bar, 10 mg of crystalline PET granule (crystallinity of 38%, Macklin, P875573, 80 mesh), and zinc-containing catalysts (0.12 mg or 0.4 mg in terms of zinc). 10 mL of NaOH aqueous solution (0.1 M) or a mixed solution of NaOH aqueous solution (0.1 M) and methanol (v/v = 4:1) was then added into the mixture under stirring at 400 rpm. The reaction solution was heated to designed temperatures to initiate the hydrolysis, and aliquots were taken and analyzed by ^{1}H NMR.

Depolymerization of daily-use PET products. Post-consumer PET beverage bottles (Danone, France; Coca-Cola, USA, crystallinity of 25%) was micronized into powders with diameters of 200 to 800 μm. Cloth fibers (shirt, labelled as 100% PET, crystallinity of 36%) and towel (labelled as 100% PET, crystallinity of 31%) were purchased online and were cut into 5 × 5 mm^2 pieces. The crystallinities of the PET were determined by differential scanning calorimetry (Figure S14). Then, PET hydrolysis was performed in a 60 mL vial placed in an aluminum heating block on a stirring hotplate.

The vial was charged with a magnetic stirring bar, 1.0 g of post-consumer PET products, and n-pentyl-substituted binuclear catalyst (2 mg in terms of zinc). 40 mL of NaOH aqueous solution (0.1 M) and 10 mL of methanol was added into the mixture under stirring at 400 rpm. The reaction mixture was heated up to 60 °C while periodically adding sodium hydroxide to maintain the pH at ca. 13. After the reaction, unreacted PET residual was removed by vacuum filtration using a Buchner funnel. Then n-pentyl-substituted binuclear catalyst in the filtrate was adsorbed by activated carbon and removed by vacuum filtration. Thereafter, acidification process was performed by adding sulfuric acid to convert soluble disodium terephthalate into terephthalic acid precipitation. After being washed with deionized water twice and dried in oven overnight, terephthalic acid (TPA) was gained.

PET hydrolysis under industrially relevant condition. PET hydrolysis was optimized at pH 13 and 90 °C in a 250 mL three-necked flask. The flask was charged with a mechanical stirrer, 50 g of PET (solids content of 100% w/v), and 5–50 mg complex supported on carbon. NaOH aqueous solution (40 mL, pH 13) and methanol (10 mL) was added into the mixture under stirring at 400 rpm. The reaction solution was heated to 90 °C. The kinetics of the PET depolymerization was determined by using base consumption (Figure S11). The pH value was maintained constant at 13 during the reaction by adding

NaOH aq. (10 M).

Recycling experiment. The 250 mL three-necked flask was charged with a mechanical stirrer, 50 g of PET, and 50 mg n-pentyl-substituted binuclear complex supported on carbon (Zn_2L complex/C), NaOH aqueous solution (40 mL, pH 13) and methanol (10 mL) under stirring at 400 rpm and 90 ^oC. After the reaction is complete and cooled to room temperature, the mixture is pumped to the primary filter to recycle the catalysts for the next reaction. In addition, Zn_2L complex/C is also redispersed into a hot solution, and the complex on the activated carbon can be maximally redissolved in the hot solvent depending on the difference in solubility at different temperatures. Finally, the activated carbon and the complex can be separated by hot filtration.

3. Characterizations.

Single-crystal X-ray diffraction (SCXRD) data were collected at 173 or 273 K on a SuperNova charge-coupled device (CCD) X-ray diffractometer, with Cu-Kα radiation (λ = 1.54184 Å). The structures were solved by directed methods with *SHELXS*. The final crystal structures were refined with the *SHELXL-2018* software package and *OLEX2 program*.[7,8] All non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least-squares fitting on F^2. The positions of hydrogen atoms were generated by calculated ideal geometries. Powder X-ray diffraction (XRD) patterns were recorded on a Rigaku D/MAX-2500 diffractometer using a filtered Cu-Kα radiation source (λ = 1.54056 Å). Elemental analyses (C, H, N) were carried out on a vario EL III analyzer. The change in particle size during the reaction was detected by a laser particle size analyzer (Nastersizer2000). XPS measurements were carried out on a Omicron XPS System using Al Kα X-rays as the excitation source at a voltage of 15 kV and a power of 300 W. All binding energies were referenced to the C1s peak (284.7 eV).

X-ray adsorption spectroscopy. The XAFS spectra at Zn K-edge were acquired at the BL14W1 station in Shanghai Synchrotron Radiation Facility (SSRF) and the 4B9A station in Beijing Synchrotron Radiation Facility (BSRF), operated at 2.5 GeV with a maximum current of 250 mA. The data for Zn_2L–$R(NO_3)_2$ were recorded in transmission mode using an ionization chamber. Zn foil, and ZnO were used as reference materials and measured in transmission mode using an ionization chamber. The acquired EXAFS data were processed according to the standard procedures using the ATHENA program integrated within the IFEFFIT (1.2.12) software packages.[9] The k^3-weighted EXAFS spectra χ(k) were

Fourier-transformed in a k-range of 3.0–12.5 $Å^{-1}$ for the Zn K-edge with a Kaiser-Bessel window function.

Diffuse reflection infrared Fourier transform spectroscopy (DRIFTS). DRIFTS experiments were performed via a Fourier transform infrared spectrometer (Thermo Nicolet iS50) equipped with a diffuse reflection accessory (Harrick Inc.). For the adsorption-desorption experiment, the catalyst was first mixed with the ethyl benzoate (EB) at room temperature. The catalyst was then heated to 100 ºC to remove the free EB. After that, the catalyst was packed in the cell and the spectra were collected.

^{1}H nuclear magnetic resonance (NMR). ^{1}H NMR was acquired on AVANCE III (Bruker). The ^{1}H NMR samples were prepared according to the following procedure: 0.1 mL of the reaction solution and 0.5 mL of D_2O with 1 mg mL^{-1} maleic acid (MA) as the internal standard were added into NMR tube and completely mixed. The peak positions of disodium terephthalate (Na_2-TP), ethylene glycol (EG), and MA are at around 7.80, 3.60, and 5.94 ppm, respectively. The molar quantity of analyte (nanalyte) in the reaction solution was calculated via the equation below:[10,11]

$$n_{analyte} = \frac{S_{analyte}}{S_{standard}} \times \frac{2}{4} \times \frac{m_{standard}}{M_{standard}} \times \frac{10}{0.1}$$

The conversion of PET was calculated by the equation below:

$$Conversion = \frac{n_{analyte}}{m_{PET}} \times M_{unit} \times 100\%$$

The S_{standard} and S_{analyte} represent the peak areas of MA and analyte (disodium terephthalate or EG), respectively. The m_{standard} and M_{standard} represent the mass and mole weight of MA, respectively. The m_{PET} represents the initial mass of PET. The M_{unit} represents the molecular weight of ethylene terephthalate ($C_{10}H_8O_4$), the repeating unit of PET.

Differential scanning calorimetry (DSC). DSC measurements were performed by Q200 of TA Inst. The temperature range was from 25 °C to 300 °C and the heating rate was 10 °C min^{-1}. The degree of PET crystallinity (XC) was calculated by the following equation: [12,13]

$$X_C = \frac{\Delta H_f - \Delta H_C}{\Delta H_f^0} \times 100\%$$

ΔH_f: the enthalpy of melting

ΔH_C: the enthalpy of cold crystallization

ΔH_f^0: the standard enthalpy of melting for a 100% crystalline PET

ΔH_f and ΔH_C could be calculated by integrating the endothermic melting peak and exothermic cold crystallization peak of DSC, and ΔH_f^0 was taken from literature as 140 J/g.[12,13]

4. DFT calculations

Density functional theory (DFT) calculations were performed in the Gaussian 09, Revision D. 01[14]. The structures of the involved complexes were optimized using the DFT/M06-L exchange-correlation functional[15] in combination with the 6-31G(d)[16] basis set for C, H, N, O, Cl, F, Br atoms, and the LANL2DZ basis set[17] for Zn atoms. The associated ECPs[18] for Zn atom were obtained from the EMSL basis set exchange site (https://www.basissetexchange.org/)[19]. The single point energy was further refined at the M06-L/def2-TZVP level[20] with zero-point-energy correction. The DFT calculations were converged with the tight convergence criteria (opt = tight) and an ultrafine grid (int = ultrafine). In the structural optimization process, the Generalized Direct Inversion in the Iterative Subspace (GEDIIS) method[21] was applied, and the frequencies were obtained with rigid rotor harmonic vibration approximation. The convergence criteria for geometry optimization were set as follows: the maximum force is less than 0.00045 au, the root-meansquare (RMS) force is less than 0.0003 au, maximum displacement is less than 0.0018 au, the root-meansquare (RMS) Displacement is less than 0.0012 au. All the stationary structures were confirmed to have no imaginary frequencies. The charge Model 5 (CM5) charge[22] value of Zn atom was obtained at M06-L/6-31G(d)+LANL2DZ level with Multiwfn[23]. The cation $[Zn_2L(OH)]^+$ was taken as the reactant based on the experimental observations, the structure of which is depicted in Figure S7. The abbreviations used are listed in Table S7. Considering that the electronic structure differences is the main factor of Hammett plot, we here choose the electronic energy changes to explain to differences causing by the different substituents, which have been reported in relevant literature[24–26]. The geometries and Cartesian coordinates of the species are depicted in Appendix.

5. Shrinking core model

The depolymerization of PET is a heterogeneous liquid–solid reaction and reaction proceeds at the liquid–solid interface. Considering that PET is nonporous material and virtually insoluble in the solution, so the reaction takes place at the surface of the PET particle. The depolymerized products

TPA-Na_2 and EG are readily soluble in NaOH solution, so TPA-Na_2 and EG is not deposited on the surface of PET particles. Therefore, the kinetics of depolymerization of PET can be described by shrinking core model. To describe the kinetics of the hydrolysis process of PET, the following assumptions and simplifications are used: (a) The PET particle of 80 mesh is so small that can be regarded as spheres during the hydrolysis process; (b) The influence of external diffusion resistance is negligible because of strong stirring, and the concentration of NaOH and catalyst on the main body of solution and particle surface is the same, and the hydrolysis process is controlled by the chemical reaction; (c) Reversible reaction of PET decomposition could be ignored due to the depolymerized products TPA-Na_2 and EG are readily soluble in NaOH solution. Since the rate is proportional to the available surface of unreacted core, the kinetic model can be represented as the following equation[27]:

$$-r_P = -\frac{1}{4\pi R_c^2}\frac{dN_p}{dt} = bC_{NaOH}(k_{No-Cat} + k_{Cat}C_{Cat}) = bk_{APP}C_{NaOH} \quad (1)$$

The decrease in radius of unreacted core accompanying the disappearance of dN_p moles of solid reactant is then given by

$$-dN_p = -\rho_p dV = -\rho_p d(\frac{4}{3}\pi R_c^3) = -\rho_p 4\pi R_c^2 dR_c \quad (2)$$

Based on equations (1) and (2), we can obtain

$$-\frac{1}{4\pi R_c^2}\rho_p 4\pi R_c^2\frac{dR_c}{dt} = -\rho_p\frac{dR_c}{dt} = bk_{APP}C_{NaOH} \quad (3)$$

which on integration becomes

$$-\rho_p\int_{R_0}^{R_c} dR_c = k_{APP}C_{NaOH}\int_0^t dt \quad (4)$$

or

$$t = \frac{\rho_p}{bk_{APP}C_{NaOH}}(R_0 - R_c) \quad (5)$$

The time required τ for complete conversion of a PET particle is given when $R_c = 0$, we can obtain

$$\tau = \frac{\rho_p}{bk_{APP}C_{NaOH}}R_0 \quad (6)$$

The conversion percentage of PET particle can also be represented as the following equation:

$$X_p = 1 - \left(\frac{\frac{4}{3}\pi R_c^3}{\frac{4}{3}\pi R_0^3}\right) = 1 - (\frac{R_c}{R_0})^3 \quad (7)$$

The decrease in radius or increase in fractional conversion of the particle in terms of τ is obtained by

dividing equation (5) by equation (6).

$$\frac{t}{\tau} = 1 - \frac{R_c}{R_0} = 1 - (1 - X_p)^{1/3} \quad (8)$$

or

$$Kt = 1 - (1 - X_p)^{1/3} \quad (9)$$

where $-r_p$ is overall reaction rate; N_p is moles of PET; $k_{NO\text{-}Cat}$ is the intrinsic non-catalytic depolymerisation rate constant; k_{Cat} is the intrinsic catalysed depolymerisation rate constant; k_{APP} is the apparent rate constant; b is stoichiometric coefficient; V is volume of PET; X_p is conversion percentage of PET; ρ_p is the molar density of PET; R_0 is initial radius of PET particle; R_c is radius of PET particle in the reaction; C_{NaOH} is the concentration of NaOH. Applying equation (9), the plots of $\{1–(1–X_p)^{1/3}\}$ *vs*. times for PET hydrolysis reaction over $Zn_2L–CH_3(NO_3)_2$ at 60 ºC is shown in Figure 2a. The results show that the kinetic model provides a good linear relationship ($r^2 > 0.99$). Apart from this, all other binuclear zinc complexes exhibit similar linear dependence at 40–80 ºC are shown in Figure S4. $K=1/\tau = bk_{APP}C_{NaOH}/\rho_p R_0$ can be determined from the slope of lines.

6. Techno-economic analysis

Economic calculation: The cost includes capital cost, maintenance cost, labor cost, chemical input, and utility cost. And the sales of TPA and ethylene glycol (EG) are the earnings in the process. The net profit (NP) is as the equation below:

$$NP = \sum Sales - \sum Costs$$

Capital cost: Capital cost is the cost to build a factory from scratch. To simplify the process, our calculation of capital cost included the cost of facilities and installation. The major facilities include serval batch reactors, filters, an adsorption tower, and a distillation tower. The capital cost wasn't calculated directly in the NP calculation but was reflected as depreciation.

Depreciation: Depreciation is related to capital cost. It's a variable to describe capital cost with its service life. In this process, we used the straight-line depreciation method, as described by the following equation:

$$D = (V - V_s)/n$$

where D means depreciation (USD/year), V means original value, V_s means salvage value, and n means service year. Here we assumed the salvage value would be zero when its service life reached ten years.

Maintenance cost: Maintenance cost is the cost of maintaining facilities, usually considered to be 10 %

of capital cost.

Labor cost: Labor cost is related to the cost of hiring workers. The estimation of labor cost was 10% of capital cost.

Chemical input & sales: Chemicals input and sales are the most influential factors in the simulation. It decides whether this simulation or this process can make positive NP. The chemical prices are shown in Table S4−6. All the data was acquired from a chemical trading platform called SunSirs (http://www.sunsirs.com/) and confirmed in another platform called made-in-china (https://www.made-in-china.com/) in 2021.

Utility cost: Utility cost refers to the cost of power, steam, compressed air, etc. In the whole process, separating steps, including evaporation, crystallization, and distillation, were the costliest steps. Therefore, our calculation of the utility cost mainly depended on salt crystallizer and distillation tower. The annual PET treatment capacity is set as 150 thousand tons, so the water annually recycled would be 150 thousand tons, which means recycled water and EG would evaporate twice during evaporation and distillation steps. Roughly, the rest of the utility cost would be estimated as equal to evaporation and distillation. And the evaporation cost was calculated as the price of the same amount of steam, where the price of steam was given by DOE benchmark.

Catalyst cost: In our experiments, the catalyst is recycled, and the loss of catalyst is around 1% per reaction. The cost of catalyst for processing 150 thousand tons of PET is calculated to be 0.18 million USD, which can be negligible compared to the others.

7. Figures S1-14

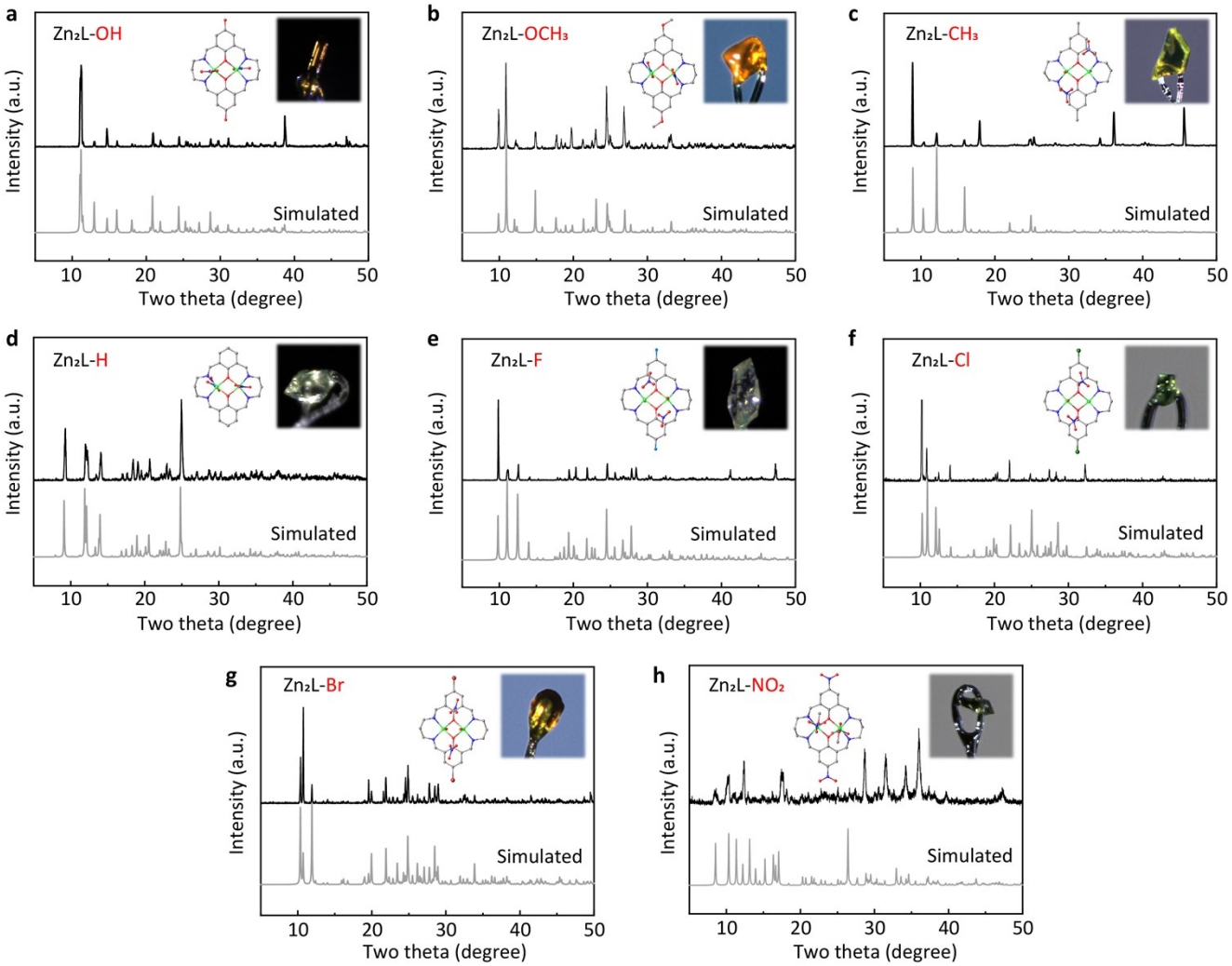

Figure S1. PXRD of binuclear zinc complexes. Experimental (gray) and simulated (light gray) PXRD patterns of $Zn_2L–OH(NO_3)_2$ (a), $Zn_2L–OCH_3(NO_3)_2$ (b), $Zn_2L–CH_3(NO_3)_2$ (c), $Zn_2L–H(NO_3)_2$ (d), $Zn_2L–F(NO_3)_2$ (e), $Zn_2L–Cl(NO_3)_2$ (f), $Zn_2L–Br(NO_3)_2$ (g), and $Zn_2L–NO_2(NO_3)_2$ (h). The insets show the optical images of the single crystals and the corresponding simplified crystal structures (green: Zn; blue: N; red: O; gray: C; sky blue: F; dark green: Cl; dark red: Br).

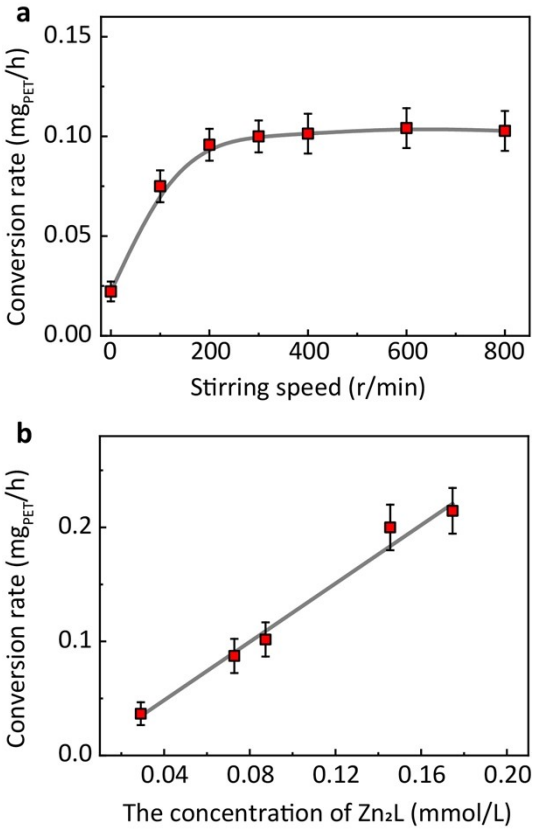

Figure S2. Mass transfer test. Effect of stirring speed (a) and catalyst mass (b) on the reaction rate of PET hydrolysis using the $–CH_3$ substituted catalyst $Zn_2L–CH_3(NO_3)_2$. Reaction temperature 60 ºC, 10 mL of 0.1 M NaOH, PET (80 mesh).

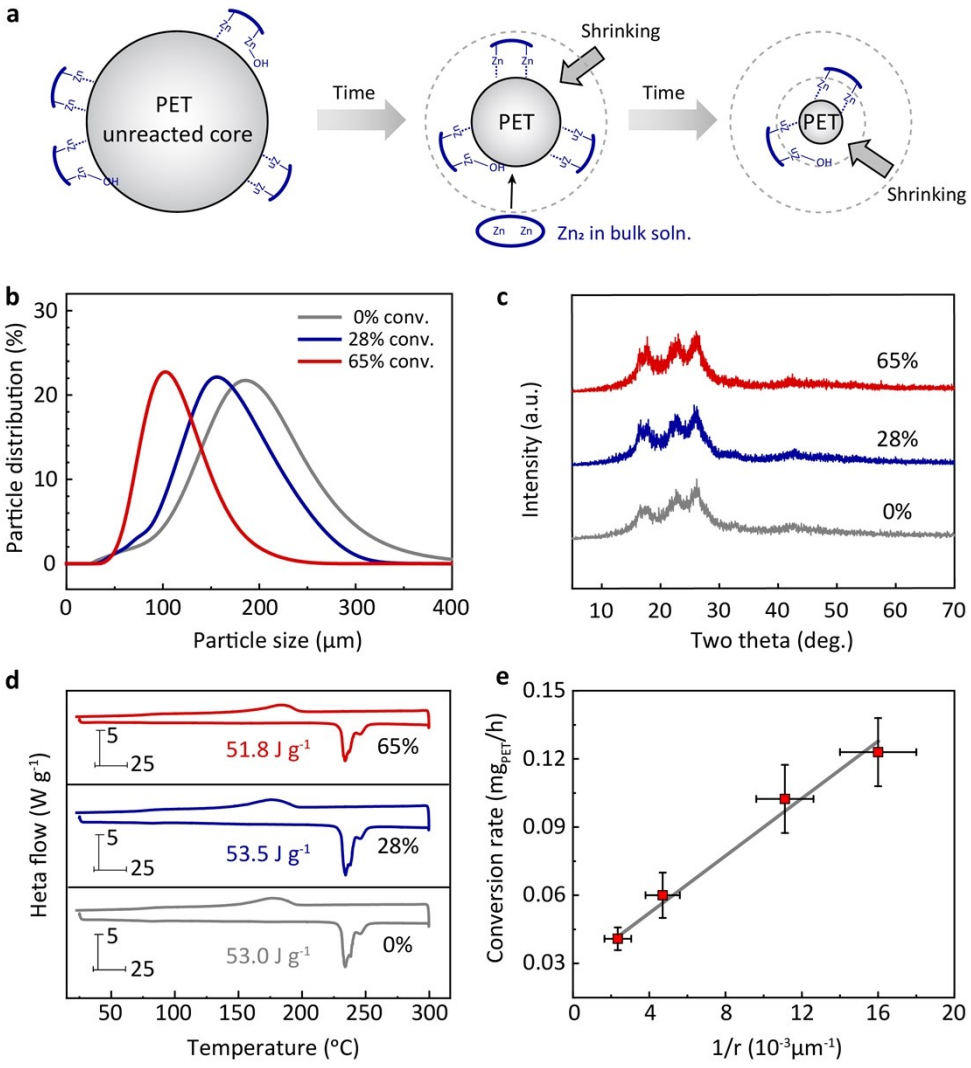

Figure S3. Kinetic modeling of PET hydrolysis over $Zn_2L–CH_3(NO_3)_2$. (a) Schematic illustration of a shrinking core model for PET hydrolysis. The size distribution profiles (b), PXRD patterns (c) and DSC (d) of the PET particles during hydrolysis at conversions of 0%, 28%, and 65%, respectively. (e) Effect of PET particle size on PET hydrolysis rate.

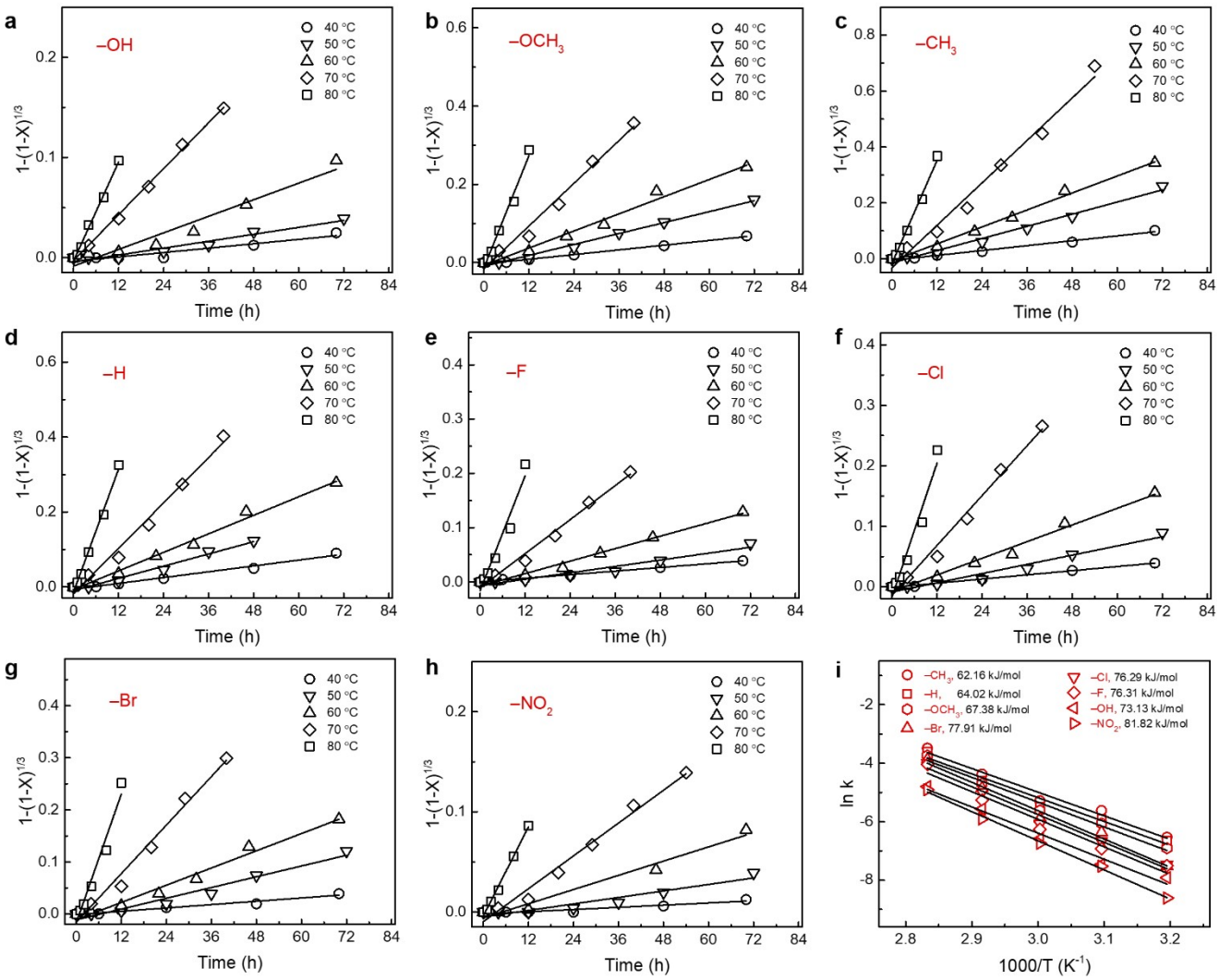

Figure S4. Reaction kinetics based on the shrinking core model. (a–h) Hydrolysis kinetics of PET over binuclear catalysts with different substituents at 40–80 °C. (i) The corresponding Arrhenius plots, showing the apparent activation energies are in the range of 62–82 kJ/mol.

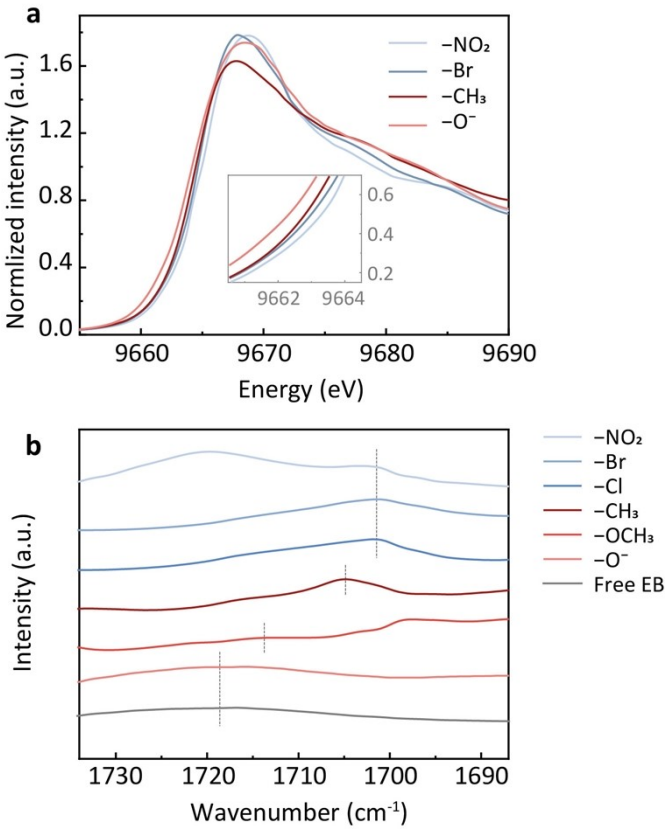

Figure S5. (a) Normalized XANES spectra of binuclear zinc catalysts with different substituents (R = $-O^-$, $-CH_3$, −Br and $-NO_2$). (b) DRIFTS spectra of ethyl benzoate in the presence of binuclear zinc catalysts with different substituents (R = $-O^-$, $-OCH_3$, $-CH_3$, −Cl, −Br and $-NO_2$).

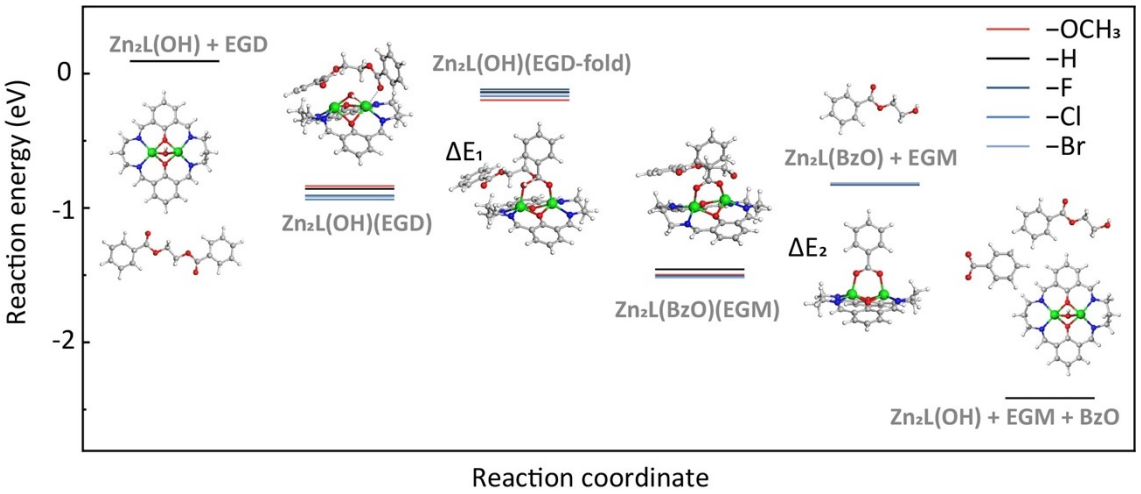

Figure S6. Potential energy profiles of ethylene glycol dibenzoate (EGD) decomposition on $Zn_2L{-}R(NO_3)_2$ (R= $-OCH_3$, −H, −F, −Cl, and −Br), which were computed at the M06L/def2-TZVP//M06L/6-31G(d)+LANL2DZ level.

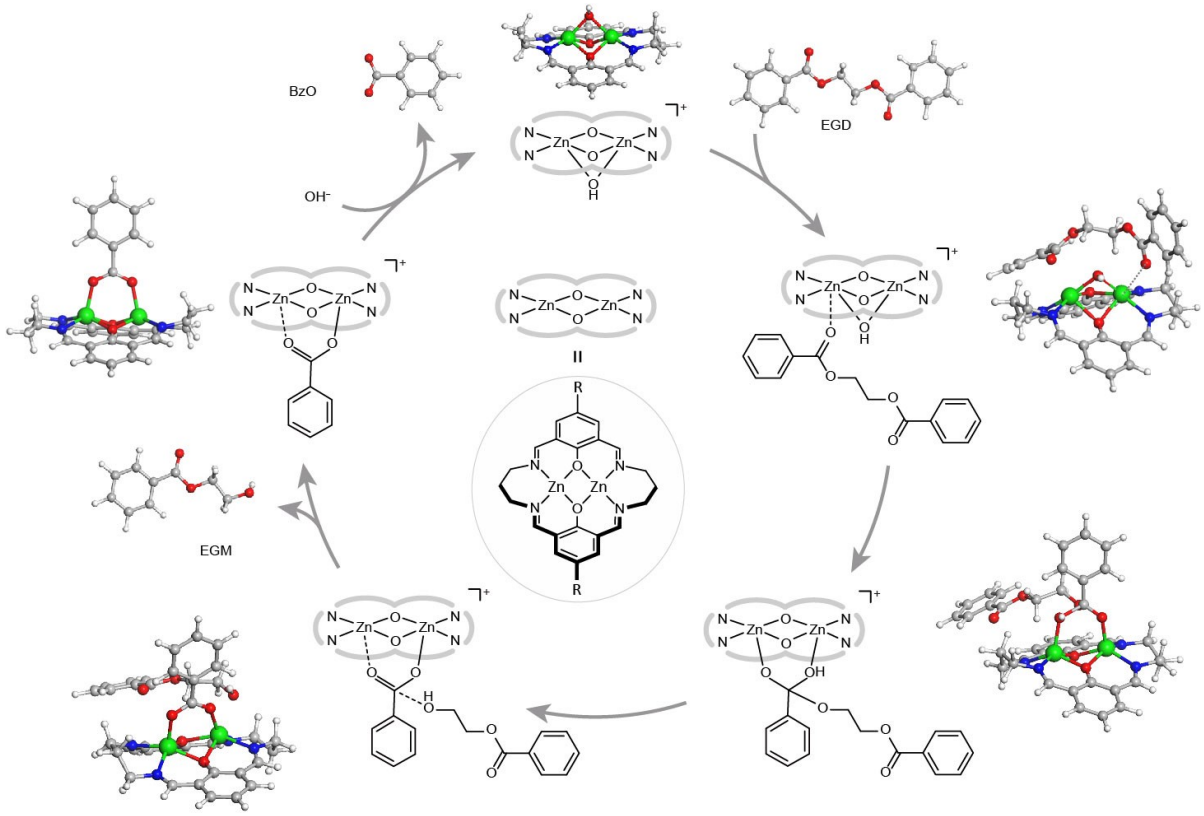

Figure S7. The PET hydrolysis mechanism proposed based on experimental and DFT results. Ball-and-stick models are given near the corresponding skeleton formulas. Ethylene glycol dibenzoate (EGD) is employed as the ester substrate for simplicity.

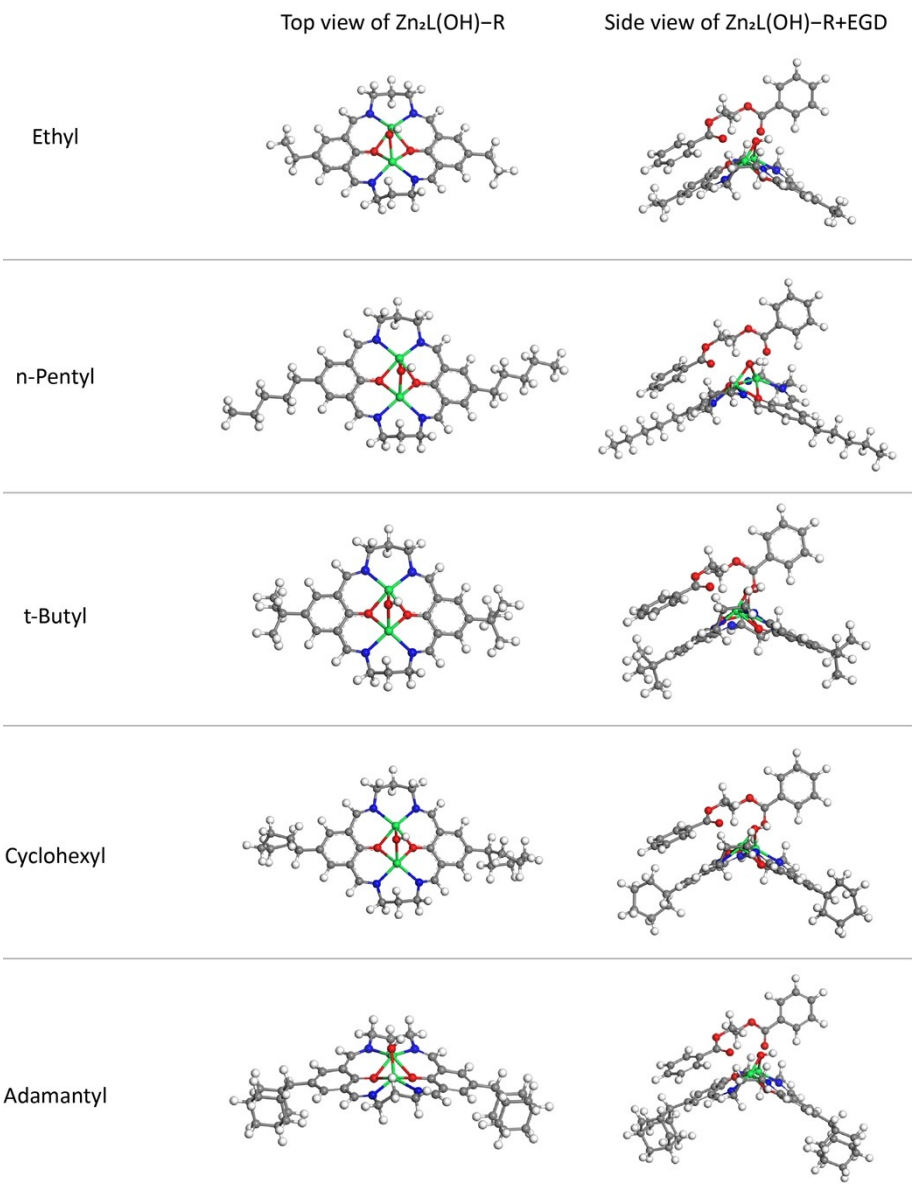

Figure S8. The geometry of $Zn_2L(OH)-R_2$ compound (R= −ethyl, −tert-butyl, −n-pentyl, −cyclohexyl, and −adamantyl) and $Zn_2L(OH)-R_2$ compound with EGD adsorbed on. The adsorption site Zn atoms connected with OH is slightly raised in $Zn_2L(OH)-R_2$ compound, which is beneficial for the adsorption of EGD. From the geometries with adsorbed EGD, the adsorbed EGD and the substituents almost have no overlap in space and have a certain distance, which indicates that the steric effect of these alkyl-substituents can be almost ignored, and this is also consistent with their similar adsorption energies (-0.96 eV) between EGD and $Zn_2L(OH)-R_2$ compounds, and similar CM5 charge of Zn (0.748).

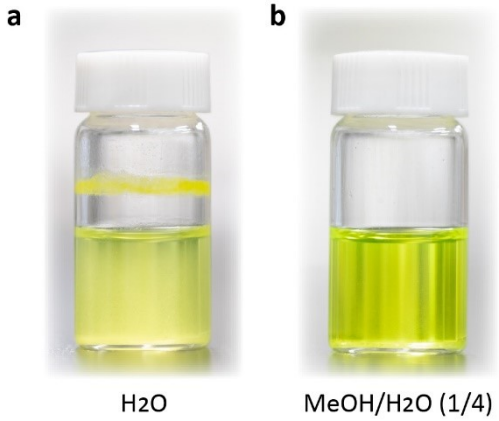

Figure S9. Photographs of n-pentyl-substituted binuclear catalyst (0.4 mg in terms of zinc) dissolved in 10 mL of NaOH aqueous solution (0.1 M) or in 10 mL of a mixed solution of NaOH aqueous solution (0.1 M) and methanol (v/v = 4:1) at 60 ºC.

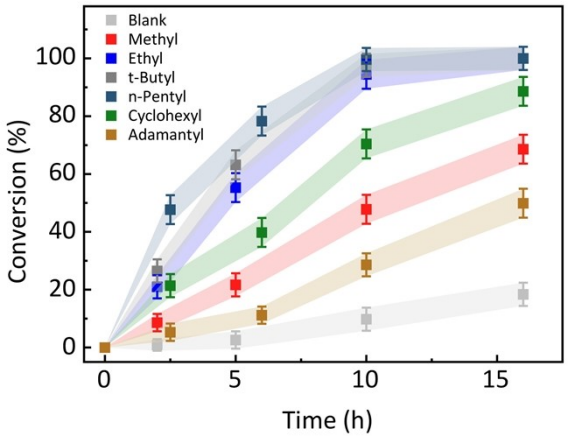

Figure S10. The hydrolysis kinetics of crystalline PET granules (38%) over binuclear zinc catalysts with different alkyl substituents. Reaction condition: 10 mL of a mixed solution of NaOH aqueous solution (0.1 M) and methanol (v/v = 4:1), 10 mg of PET, binuclear catalysts (0.4 mg in terms of zinc), 60 ºC.

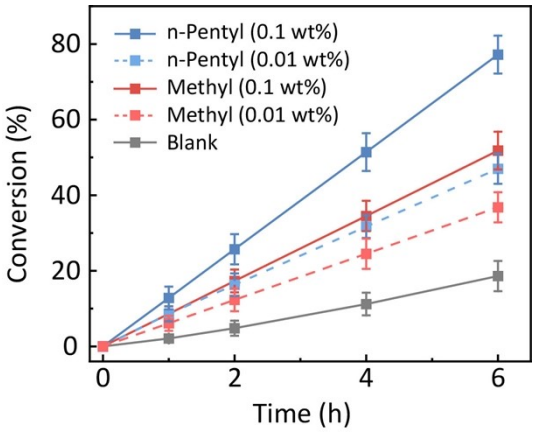

Figure S11. The hydrolysis kinetics of crystalline PET granules (38%) over Zn_2L–n-pentyl$(NO_3)_2$, Zn_2L–$CH_3(NO_3)_2$, and blank control at pH 13 and 90 °C. Reaction conditions: 50 mL of a mixed solution of NaOH aqueous solution (pH 13) and methanol (v/v = 4:1) containing 50 g of crystalline PET (38%) and 5 mg (0.1 wt%) or 50 mg (0.01 wt%) of the complex supported on carbon. All the error bars represent the standard deviations for three measurements.

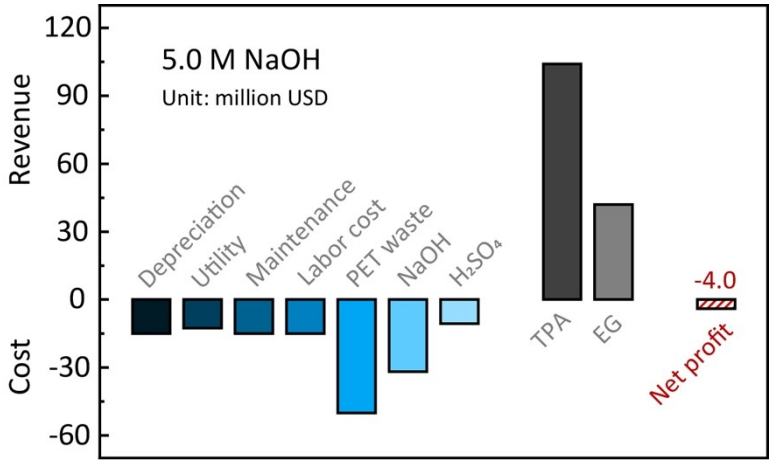

Figure S12. Techno-economic analysis based on a capability of 150 thousand tons of PET waste per year for alkaline hydrolysis conducted in 5.0 M NaOH.

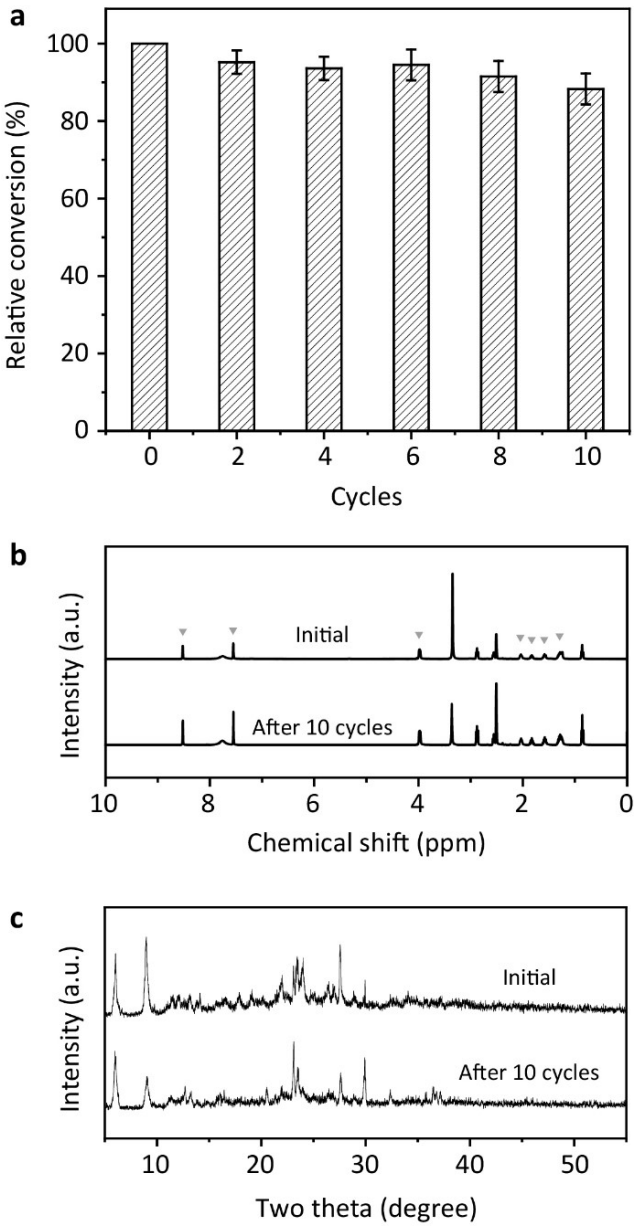

Figure S13. (a) Relative catalytic activity of the supported n-pentyl-substituted binuclear catalyst through recycling. The ^{1}H NMR (b) and XRD patterns (c) of the supported n-pentyl-substituted binuclear catalyst before and after recycling.

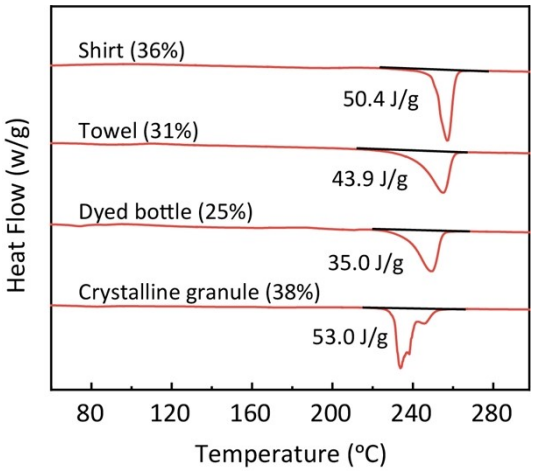

Figure S14. The differential scanning calorimetry (DSC) analysis of crystalline granule (Macklin,P875573), dyed water bottle (Coca-cola, USA), towel and shirt (online purchase).

8. Tables S1-8

Table S1. Comparison of the space-time yield and the specific activity of different catalysts for PET hydrolysis.

Catalysts	pH	C_{NaOH} (M)	T (^oC)	Space-time yield ($g_{TPA}\ L^{-1}h^{-1}$)	Reaction rate ($M_{TPA}\ h^{-1}$)	[a]Specific activity ($g_{PET}\ h^{-1}g_{cat}^{-1}$)	References
$ZnCl_2$	7.0	10^{-7}	180	7.0	0.04	0.0036	28
H^+@ZSM-5-25	7.0	10^{-7}	230	16.7	0.10	3.0	29
-	7.0	10^{-7}	230	19.2	0.11	-	30
$[(CH_3)_3N(C_{16}H_{33})]_3[PW_{12}O_{40}]$	7.0	10^{-7}	160	26.8	0.16	3.3	31
-	14.0	1.0	125	36.7	0.22	-	32
EtOH:H_2O/NaOH	14.1	1.1	80	49.4	0.29	-	33
TOMAB	14.1	1.1	95	1.49	0.009	10.6	34
CTAB	14.1	1.1	110	1.73	0.01	0.4	35
TBAI	14.4	3.0	90	51.3	0.3	33.3	36
-	14.4	3.0	110	30.8	0.18	-	37
-	14.4	3.0	120	0.68	0.004	-	38
-	14.6	4.0	150	5.7	0.03	-	39
-	14.6	4.4	180	3.3	0.02	-	40
-	14.7	5.0	120	4.2	0.025	-	38
Zn_2L–$CH_3(NO_3)_2$	13.0	0.1	60	7.6 ± 1	0.04	43.7 ± 3 ($0.2mg_{Cat}$/mL)	This work
Zn_2L–$CH_3(NO_3)_2$	13.0	0.1	60	11.0 ± 2	0.07	15.9 ± 2 ($0.8mg_{Cat}$/mL)	This work
Zn_2L–$CH_3(NO_3)_2$/C	13.0	0.1	90	50 ± 3	0.3	577 ± 35 ($0.1mg_{Cat}$/mL)	41
Zn_2L–$CH_3(NO_3)_2$/C	13.0	0.1	90	70 ± 4	0.42	79 ± 5 ($1.0mg_{Cat}$/mL)	41
Zn_2L–n-pentyl$(NO_3)_2$/C	13.0	0.1	90	67 ± 3	0.40	778 ± 40 ($0.1mg_{Cat}$/mL)	This work
Zn_2L–n-pentyl$(NO_3)_2$/C	13.0	0.1	90	111 ± 5	0.67	129 ± 5 ($1.0mg_{Cat}$/mL)	This work

[a]Blank correction is not included because the blank data is not available in most literatures

Table S2. Crystal data and structure refinements for $Zn_2L\text{-}R(NO_3)_2$.

Compound Name	$Zn_2L\text{-}OH(NO_3)_2$	$Zn_2L\text{-}OCH_3(NO_3)_2$	$Zn_2L\text{-}CH_3(NO_3)_2$	$Zn_2L\text{-}H(NO_3)_2$
CCDC number	2205612	2082453	2082457	2205615
Empirical formula	$C_{22}H_{22}N_6O_{10}Zn_2$	$C_{24}H_{26}N_6O_{10}Zn_2$	$C_{25}H_{28}N_6O_9Zn_2$	$C_{22}H_{22}N_6O_8Zn_2$
Formula weight/g mol^{-1}	661.19	689.25	687.27	629.19
Temperature/K	273	173.00(10)	173.00(10)	300.51(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P2_1/n$
a/Å	8.39710(10)	7.9192(3)	19.9701(3)	9.00730(5)
b/Å	15.80160(10)	9.0455(3)	17.0535(3)	13.58036(7)
c/Å	10.07390(10)	17.8728(6)	8.0230(2)	19.66015(10)
α/°	90	90	90	90
β/°	112.8580(10)	92.107(3)	97.808(2)	99.5336(5)
γ/°	90	90	90	90
Volume/Å^3	1231.71(2)	1279.42(7)	2706.98(9)	2371.66(2)
Z	2	2	4	4
ρ_{calc}g/cm^3	1.783	1.789	1.686	1.762
μ/mm^{-1}	3.028	2.944	2.751	3.043
F(000)	672	704	1408	1280
Reflections collected	8384	5973	17712	20522
Independent reflections	2037	2600	4551	4036
Goodness-of-fit on F^2	1.054	1.065	1.041	1.047
Final $R_1{}^a$ indexes [$I \geq 2\sigma(I)$]	0.0233	0.0310	0.0436	0.0261
Final $wR_2{}^b$ indexes [$I \geq 2\sigma(I)$]	0.0633	0.0830	0.1180	0.0714
Largest diff. peak/hole/e Å^{-3}	0.26/-0.24	0.44/-0.35	0.92/–0.58	0.47/-0.27

Compound Name	**Zn_2L-$F(NO_3)_2$**	**Zn_2L-$Cl(NO_3)_2$**	**Zn_2L-$Br(NO_3)_2$**	**Zn_2L-$NO_2(NO_3)_2$**
CCDC number	2205624	2205619	2205618	2205623
Empirical formula	$C_{22}H_{24}F_2N_6O_{10}Zn_2$	$C_{22}H_{24}Cl_2N_6O_{10}Zn_2$	$C_{22}H_{24}Br_2N_6O_{10}Zn_2$	$C_{24}H_{28}N_8O_{14}Zn_2$
Formula weight/g mol^{-1}	701.21	734.11	818.87	783.28
Temperature/K	272.1(8)	172.99(10)	271.26(13)	173.00(10)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	P-1
a/Å	8.14410(10)	8.37106(7)	8.50810(10)	7.97610(10)
b/Å	17.9862(2)	17.24574(11)	17.08160(10)	8.79990(10)
c/Å	9.44930(10)	9.47691(8)	9.70880(10)	10.5943(2)
α/°	90	90	90	98.6050(10)
β/°	109.2110(10)	105.3664(8)	104.2460(10)	97.1330(10)
γ/°	90	90	90	98.8420(10)
Volume/$Å^3$	1307.07(3)	1319.226(18)	1367.61(2)	718.204(18)
Z	2	2	2	1
ρ_{calc}g/cm^3	1.782	1.848	1.989	1.811
μ/mm^{-1}	3.006	4.72	6.155	2.84
F(000)	712	744	812	400
Reflections collected	8116	17264	10694	8217
Independent reflections	2092	2299	2372	2365
Goodness-of-fit on F^2	1.085	1.058	1.08	1.055
Final $R_1{}^a$ indexes [$I \geq 2\sigma(I)$]	0.0302	0.0222	0.0289	0.0218
Final $wR_2{}^b$ indexes [$I \geq 2\sigma(I)$]	0.0725	0.0546	0.0795	0.0547
Largest diff. peak /hole / e $Å^{-3}$	0.36/-0.24	0.33/-0.28	0.49/-0.61	0.35/-0.35

Table S3. Charge accumulation during step 2 and step 4 based on the DFT calculations.

Catalysts	Step 2		Step 4	
	CM5 charge at $Zn_2L(OH)(EGD)$	CM5 charge at $Zn_2L(OH)(EGD\text{-}fold)$	CM5 charge at $Zn_2L(BzO)(EGM)$	CM5 charge at $Zn_2L(BzO)$
$Zn_2L\text{-}OH(NO_3)_2$	-	-	0.0063	0
$Zn_2L\text{-}OCH_3(NO_3)_2$	-	-	0.1046	0
$Zn_2L\text{-}CH_3(NO_3)_2$	0.7558	1.1882	-	-
$Zn_2L\text{-}H(NO_3)_2$	0.7511	1.1948	-	-
$Zn_2L\text{-}F(NO_3)_2$	0.7461	1.1879	-	-
$Zn_2L\text{-}Cl(NO_3)_2$	0.7439	1.1876	-	-
$Zn_2L\text{-}Br(NO_3)_2$	0.7461	1.1887	-	-
$Zn_2L\text{-}NO_2(NO_3)_2$	0.7175	1.1612	-	-

Table S4. Simplified techno-economic analysis based on a capability of 150 thousand tons of PET waste per year for alkaline hydrolysis in 0.1 M NaOH catalysed by Zn_2L–n-pentyl$(NO_3)_2$.

Items			**Total price (million USD)**
Depreciation			-5.0
Utility cost			-4.2
Maintenance cost			-5.0
Labor cost			-5.0
Chemicals	Weight per ton_{PET} (ton)	Unit price (USD ton^{-1})	
Waste PET	1.000	333.9	-50.1
Sodium hydroxide (NaOH)	0.416	340.0	-21.2
Sulfuric acid (H_2SO_4)	0.510	92.7	-7.1
Terephthalic acid (TPA)	0.864	803.7	104.1
Ethylene glycol (EG)	0.323	865.5	42.0
Net profit			**48.5**

Table S5. Simplified techno-economic analysis based on a capability of 150 thousand tons of PET waste per year for alkaline hydrolysis in 1.0 M NaOH.

Items			**Total price (million USD)**
Depreciation			-15.0
Utility cost			-12.6
Maintenance cost			-15.0
Labor cost			-15.0
Chemicals	Weight per ton_{PET} (ton)	Unit price (USD ton^{-1})	
Waste PET	1.000	333.9	-50.1
Sodium hydroxide (NaOH)	0.456	340.0	-23.3
Sulfuric acid (H_2SO_4)	0.560	92.7	-7.8
Terephthalic acid (TPA)	0.864	803.7	104.1
Ethylene glycol (EG)	0.323	865.5	42
Net profit			**7.3**

Table S6. Simplified techno-economic analysis based on a capability of 150 thousand tons of PET waste per year for alkaline hydrolysis in 5.0 M NaOH.

Items			**Total price (million USD)**
Depreciation			-15.0
Utility cost			-12.6
Maintenance cost			-15.0
Labor cost			-15.0
Chemicals	Weight per ton_{PET} (ton)	Unit price (USD ton^{-1})	
Waste PET	1.000	333.9	-50.1
Sodium hydroxide (NaOH)	0.624	340.0	-31.8
Sulfuric acid (H_2SO_4)	0.765	92.7	-10.6
Terephthalic acid (TPA)	0.864	803.7	104.1
Ethylene glycol (EG)	0.323	865.5	42
Net profit			**- 4.0**

Table S7. Abbreviations used in DFT calculation.

Abbreviations	Synonyms	Formulas
PET	Polyester terephthalate	-
EGD	Ethylene glycol dibenzoate	$C_{16}H_{14}O_4$
EGM	Ethylene glycol monobenzoate	$C_9H_{10}O_3$
BzO	Benzoate	$[C_7H_5O_2]^-$

Table S8. Comparison of the methyl- and n-pentyl-substituted binuclear catalysts for PET hydrolysis.

	Conditions	Zn_2L-$CH_3(NO_3)_2$	Zn_2L-n-pentyl$(NO_3)_2$
Zn loss (wt%)	at 90 °C and pH 13	4.6	0.5
Specific activity (g_{PET} $h^{-1}g_{cat}^{-1}$)	at 60 °C and pH 13	0.23	0.90
	at 90 °C and pH 13	577	778
Space-time yield (g_{TPA} $L^{-1}h^{-1}$)	at 90 °C and pH 13	50	67
Net profit (million USD)	at 90 °C and pH 13	30.8	48.5

Notes: The advantages of the n-pentyl-substituted catalyst compared with the methyl-substituted catalyst include: (1) 4-fold enhancement in activity at 60 °C and pH 13; (2) 57% increase in profit under industrially relevant conditions (90 °C and pH 13); (3) easier catalyst recovery as shown by much less Zn loss during reuse; (4) more compatible with hydrophobic polyesters to form biodegradable blend.

9. References

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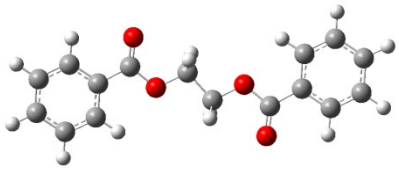
10. Appendix

The geometries and Cartesian coordinates of the species. Note that the values in the first line of Cartesian coordinate part present the charge and spin multiplicity, respectively. 1) EGD, EGM and $C_6H_5COO^-$, 2) R=O^-, 3) R=OCH_3, 4) R=CH_3, 5) R=H, 6) R=Br, 7) R=Cl, 8) R=F, 9) R=NO_2

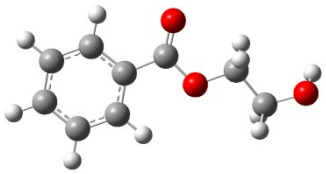
1) EGD, EGM and $C_6H_5COO^-$

EGD :

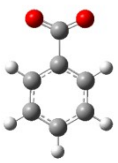


0 1			
C	-5.56354800	-1.64394400	-0.20500200
C	-4.28778500	-1.09937000	-0.11793900
C	-4.12726200	0.28419600	0.01479900
C	-5.25312100	1.11290500	0.06260100
C	-6.52609800	0.56450500	-0.02379500
C	-6.68230700	-0.81430000	-0.15929300
H	-5.68674200	-2.72012700	-0.30981900
H	-3.41084900	-1.74008600	-0.15284400
H	-5.10241300	2.18545000	0.16496500
H	-7.40012700	1.21182200	0.01169200
H	-7.68016500	-1.24401900	-0.23007600
C	-2.79687300	0.92493100	0.09558200
O	-2.60348300	2.11946600	0.19871400
O	-1.78956400	0.01799200	0.03416300
C	-0.47709900	0.58303500	0.07819400
H	-0.32168000	1.23102000	-0.79314000
H	-0.36723600	1.20562700	0.97359800
C	0.47710400	-0.58310600	0.07835700
H	0.36718400	-1.20550700	0.97389500
H	0.32175000	-1.23130500	-0.79282800
O	1.78955700	-0.01805000	0.03426900
C	2.79690700	-0.92496700	0.09568000
O	2.60355700	-2.11950400	0.19883700
C	4.12726400	-0.28419200	0.01484100
C	4.28774100	1.09938800	-0.11781100
C	5.25314500	-1.11288000	0.06250000
C	5.56348700	1.64399300	-0.20491900
H	3.41078600	1.74008200	-0.15261700
C	6.52610500	-0.56444900	-0.02395200
H	5.10246800	-2.18543600	0.16479000

EGM:



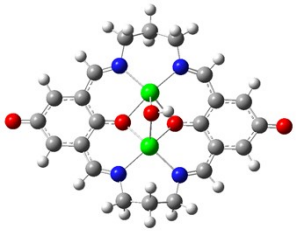
0 1			
O	4.76694600	-0.45546700	0.01593100
C	3.41518300	-0.85351100	-0.03118700
H	3.17557300	-1.42927200	-0.94151500
H	3.26463800	-1.52503500	0.82105700
C	2.49029800	0.33929100	0.07915400
H	2.66477100	0.89461700	1.00888400
H	2.63072700	1.04599300	-0.75054300
O	1.14766500	-0.15901100	0.05425300
C	0.18838800	0.79739000	0.02285100
O	0.43917500	1.98606600	0.00798300
C	-1.17453400	0.22175100	0.00699300
C	-1.41048100	-1.15738400	0.02134700
C	-2.25409600	1.11048100	-0.02307700
C	-2.71461400	-1.63776000	0.00507200
H	-0.56736600	-1.84317200	0.04538600
C	-3.55534100	0.62658100	-0.03884900
H	-2.04461500	2.17797400	-0.03306600
C	-3.78700800	-0.74825900	-0.02500800
H	-2.89673900	-2.71084800	0.01617800
H	-4.39348600	1.32054000	-0.06148500
H	-4.80749700	-1.12774100	-0.03735800
H	4.95692300	0.03275900	-0.79665700

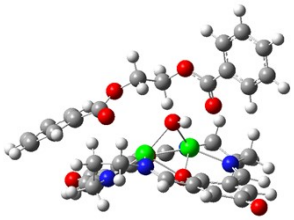


$C_6H_5COO^-$:

	-1 1			
	C	1.82659700	-1.20488900	-0.00022600
	C	0.43387600	-1.19901000	0.00024000
	C	-0.28353700	-0.00000600	0.00030200
	C	0.43386400	1.19901200	0.00054500
	C	1.82657600	1.20490400	0.00017000
	C	2.53080300	0.00000900	-0.00038600
	H	2.37346900	-2.15104000	-0.00047800
	H	-0.15251200	-2.11823600	0.00031600
	H	-0.15257900	2.11820800	0.00072300
	H	2.37345600	2.15105100	-0.00000900
	H	3.62251300	0.00003000	-0.00062400
	C	-1.82811900	-0.00000400	-0.00013200
	O	-2.35656300	1.13916100	-0.00056800
	O	-2.35652500	-1.13917500	0.00019300

2) R=O$^-$





-1 1				-1 1				
C	2.78449400	-2.49024300	-0.23958700	C	1.58509200	3.85626000	-0.65055300
C	2.61980000	0.00668500	-0.43472700	C	2.32785700	2.11421100	1.02174300
C	-3.39265700	-1.20423300	-0.39393100	C	-3.26817600	0.68755800	1.19734500
C	2.77244400	2.49435600	-0.13357900	C	3.48806700	0.33304900	2.36597200
C	-2.77498900	2.49529200	-0.11148800	C	-1.33881900	-2.29894900	2.40427700
C	4.79075300	-1.17046600	-0.50446900	C	3.74925800	4.03772200	0.39428800
C	-5.59764000	0.02523700	-0.60522000	C	-4.87047800	-0.92225600	2.30038600
C	4.78108100	1.20059400	-0.47817000	C	4.65191100	2.37692800	1.82797800
C	1.28228200	4.19152600	0.49590200	C	3.02037400	-1.90451200	2.89836500
C	-3.38082400	1.22455800	-0.35045800	C	-2.41512300	-1.43151900	2.02869100
C	0.00268000	4.71543900	-0.14216100	C	1.88486000	-2.58461900	3.65281700
C	5.59195900	0.01882200	-0.60220800	C	4.87704500	3.64652100	1.19409300
C	-1.27802000	4.19309500	0.49468600	C	0.79356300	-3.19153700	2.77524900
C	-4.78678200	1.20591900	-0.47058100	C	-3.70894800	-1.74783900	2.48976800
C	-0.00602200	-4.52976200	0.92017000	C	-1.72879300	3.82349200	-2.07977400
C	3.37345000	1.22192400	-0.37858900	C	3.46269600	1.62456500	1.75012000
C	-4.79997200	-1.16618400	-0.50088600	C	-4.53013400	0.34595900	1.71310000
C	3.38156200	-1.20608800	-0.41785800	C	2.53831600	3.32242900	0.27533900
C	-2.79468300	-2.48901300	-0.22493900	C	-3.15668700	1.96258200	0.54695800
C	-2.63253900	0.00746600	-0.38859100	C	-2.18418400	-0.23615500	1.28601400
C	-1.28128100	-4.23660800	0.14390100	C	-2.31333200	3.79224600	-0.66716700
C	1.27634900	-4.23624800	0.15643300	C	-0.23184300	4.11344700	-2.11769100
H	5.31128200	2.15577500	-0.43219000	H	5.48485400	1.96040700	2.40128000
H	3.48412600	3.33750600	-0.18870800	H	4.39933300	0.14241300	2.96199600
H	5.32726400	-2.12299600	-0.48474900	H	3.85643000	4.95938900	-0.18444900
H	3.50980500	-3.32251800	-0.28147500	H	1.84763900	4.86540600	-1.01635700
H	-3.52073000	-3.32074000	-0.26238100	H	-4.08897300	2.55713300	0.57239700
H	-5.33822300	-2.11790400	-0.49572900	H	-5.34172900	1.07064300	1.60489100
H	-5.31573700	2.16224700	-0.43604300	H	-3.84814900	-2.68516700	3.03568200
H	-3.48634900	3.33908100	-0.15847200	H	-1.65742400	-3.15721800	3.02523800
H	-2.13734300	-4.73854600	0.62647100	H	-3.38395800	4.06378800	-0.68257900
H	2.12921500	-4.73261500	0.65063000	H	0.14657600	3.90963000	-3.13287700

H	1.19983500	4.31904600	1.59034400
H	-1.19775300	4.32194400	1.58914500
H	-2.13457800	4.81112000	0.17399000
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H	1.19367800	-4.69302200	-0.84569100
H	2.14028300	4.80860100	0.17712900
H	-0.00627200	-5.59532000	1.18771600
H	-0.01202500	-3.97257000	1.87035300
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N	-1.54826300	-2.80983300	0.00762600
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Zn	-0.00194000	1.36032700	0.42108400
Zn	-0.00685600	-1.41107700	0.31431300
O	0.00253800	-0.08060500	1.88988500
H	0.82420700	-0.10148200	2.39811400
O	-6.84597800	0.03556600	-0.75158900
O	6.84216000	0.02728900	-0.73089200

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H	1.27093200	-3.77965100	1.97555500
H	0.18661300	-3.89051400	3.37879900
H	-1.80295200	4.54333100	-0.04150500
H	-0.05358800	5.18683800	-1.92787400
H	3.86874200	-1.73241500	3.58409900
H	-2.24002800	4.58806400	-2.68081300
H	-1.94030900	2.85559300	-2.55601100
H	2.32617200	-3.39923900	4.24581800
H	1.43496800	-1.88050800	4.36703500
N	-2.13652100	2.47952400	-0.06616200
N	-0.06185200	-2.18758000	2.16563100
N	2.63916000	-0.65226300	2.26426200
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O	-1.02889300	-0.01752100	0.71592400
O	1.16513100	1.52299000	1.08984800
Zn	0.94394100	-0.63270000	0.99558600
Zn	-0.29146900	1.46770700	-0.49010500
O	0.95595100	-0.10011500	-1.04673500
C	-6.14882500	-1.32188400	-0.67938000
C	-4.81848300	-1.47531000	-1.05254700
C	-4.12933500	-0.41531200	-1.65722900
C	-4.79608900	0.79363800	-1.89594100
C	-6.12893000	0.93553100	-1.53891900
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H	-6.65231300	-2.11520600	-0.13324000
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H	-4.24408600	1.61313400	-2.35445300
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O	1.10091700	-3.06758300	-1.94688200
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C	3.57974600	-3.14474100	-3.15693900
C	4.49239100	-2.08953800	-1.17642300
C	4.82029000	-3.04531400	-3.77403300
H	2.73442900	-3.58735200	-3.67811500
C	5.72468700	-1.97473500	-1.80529100
H	4.33848800	-1.71076100	-0.16725900
C	5.89263300	-2.45821900	-3.10248200
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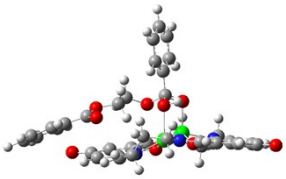

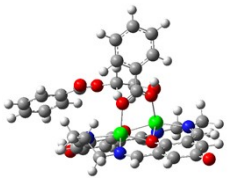

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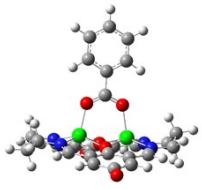

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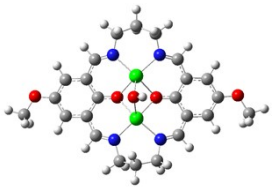

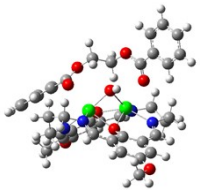

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C	-3.33804400	1.27292700	-0.36433900	C	-2.28627900	-0.95677200	2.29933700
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H	-2.02863000	-4.76809300	0.27961500	H	-3.39386900	3.52419300	-1.87853700
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N	1.53892800	2.86266300	0.29805400	N	2.62577600	-0.17779200	2.23425000
N	1.58970000	-2.73135400	0.36150800	N	0.48419000	2.80775000	-2.02508300
O	-1.28809600	0.07204600	-0.34333200	O	-1.05024600	-0.15672300	0.44660700

O	1.30669400	0.06012500	-0.26248700
Zn	-0.02782000	1.45638100	0.61407300
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C	-7.48318700	-1.05417000	-1.07405000
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H	7.48141900	-1.55554600	-0.23567700
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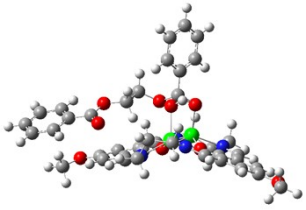

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C	-5.89925400	-1.37357800	-0.70995400
C	-4.58505000	-1.69753400	-1.02423100
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C	-4.42448900	0.30464800	-2.37651400
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H	-7.51521700	0.02279000	-1.00096700
C	-2.41817300	-1.11599200	-2.15757000
O	-1.64170400	-0.27098500	-2.59781000
O	-2.07853500	-2.38913500	-1.91699500
C	-0.72868100	-2.78759500	-2.21356500
H	-0.78836700	-3.52501900	-3.02083300
H	-0.13707000	-1.92108500	-2.51482500
C	-0.13682400	-3.38364100	-0.95710300
H	-0.17593800	-2.66400900	-0.13359700
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C	2.21970900	-3.23470100	-0.55113900
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C	4.66750500	-2.97123300	-0.50266200
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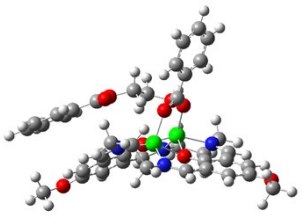

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C	4.53463200	1.13484300	-1.79215600	C	3.60359800	2.46432800	0.97267400
C	-0.74468200	2.28959100	-2.67929000	C	-1.71060200	3.06609600	1.16628300
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	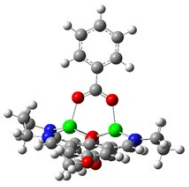						
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C	0.51439900	-4.79044100	0.82526800
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C	0.78806400	-5.91364600	-1.71147700
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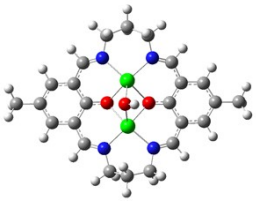

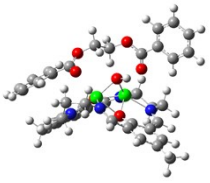

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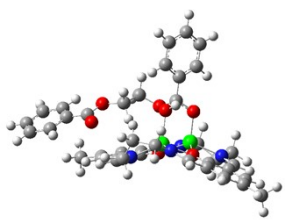

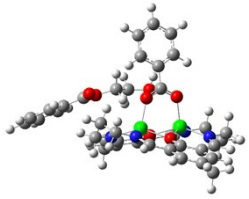

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C	0.20140200	-1.47734200	4.16964700	H	1.77152500	-0.47885500	0.85512500
C	-1.26086800	-3.23050300	3.39817700	C	2.41975900	-2.53068900	0.74756000
C	0.24048800	-2.06552900	5.43110700	H	2.63052000	-2.59183600	-0.32735100
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H	-1.77829400	-4.73310900	4.84532800	C	0.70636500	-0.52651800	4.16308100
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	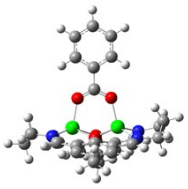						
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C	-4.80187000	-0.11407500	-1.70878900				
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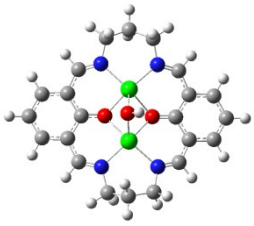

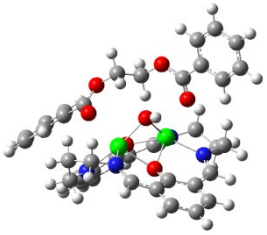

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C	-2.87008800	2.38881300	-0.17544900	C	-0.48758900	-1.71001200	3.10521600
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C	-5.40545100	-0.24462400	-0.84140800	C	-4.12629500	-1.00535100	3.36481900
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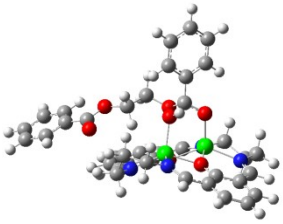

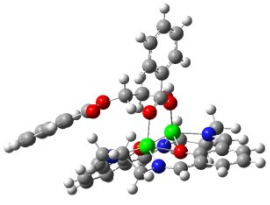

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O	3.80945300	1.50966500	1.15242600	O	-2.57372700	-1.60982800	0.99695000
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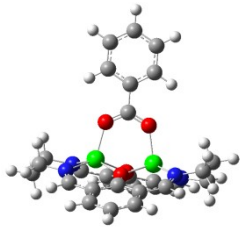

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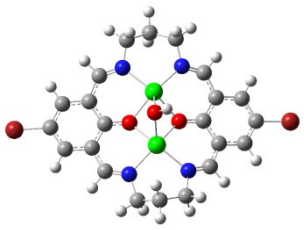
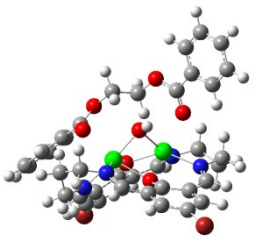
6) Br





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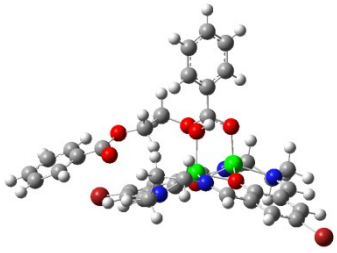				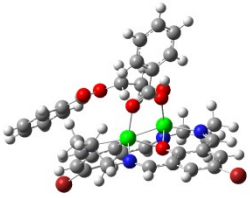
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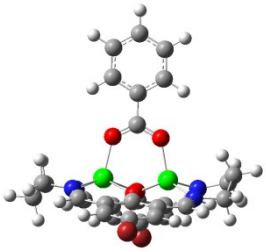

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H	3.18258000	-0.99597900	-3.49629600
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H	1.88371200	-0.01804000	-4.91685900
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H	0.33454400	4.16731700	2.58419400
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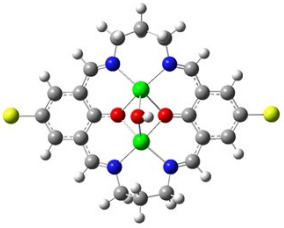

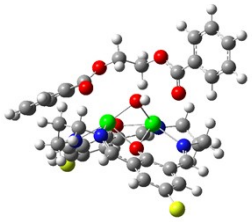

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C	4.69604700	1.22971500	-0.63151500	C	3.95807500	3.27340800	1.56383100
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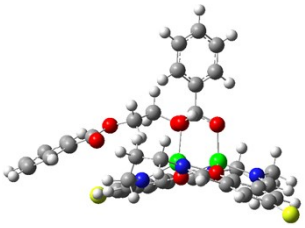

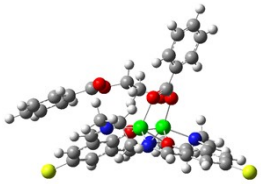

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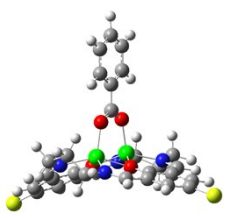

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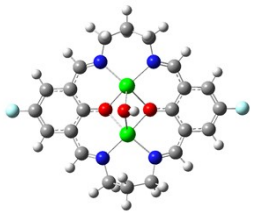

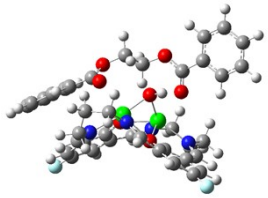

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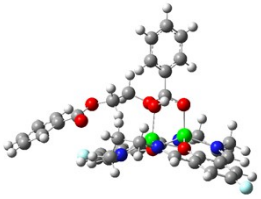

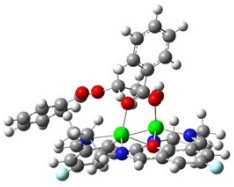

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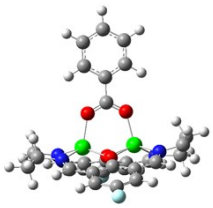

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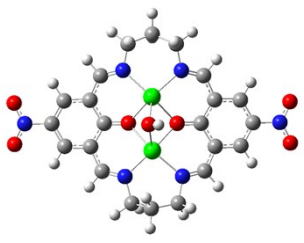	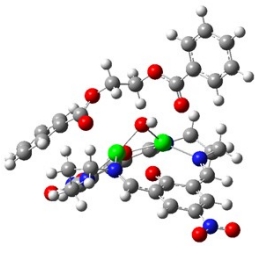

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	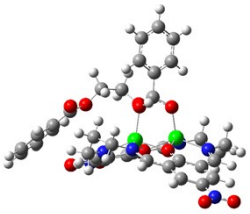				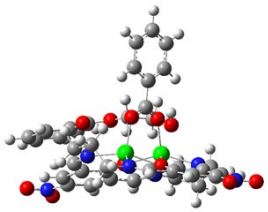		
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C	-5.62216900	-1.01810800	-0.26137500	H	-7.94281200	2.45160300	0.57665200
C	-4.92679900	-1.90662700	0.56867100	H	-5.54436600	2.36293500	1.21123800
C	-5.18336800	-3.28158400	0.48137400	H	-5.52807200	-1.88566900	0.58450200
C	-6.10172700	-3.76402200	-0.44228700	H	-7.93527600	-1.80197700	-0.06118600
C	-6.77960200	-2.87548000	-1.27717200	H	-9.13407000	0.37240200	-0.06316800
H	-7.07936100	-0.81124000	-1.82800100	C	-3.95696900	0.12362100	1.24414800
H	-5.43559900	0.05101100	-0.18324400	O	-3.28901400	-0.89092800	1.15635500
H	-4.65852100	-3.95159300	1.16035400	O	-3.41303200	1.31709400	1.61460600
H	-6.29842500	-4.83192600	-0.50718900	C	-2.00565100	1.27267200	1.83852400
H	-7.50131600	-3.25205800	-1.99911700	H	-1.78242100	0.66602400	2.72687800
C	-3.90840100	-1.46111100	1.54355000	H	-1.51692400	0.77622900	0.98932500
O	-3.34394300	-2.20063000	2.33048000	C	-1.52658900	2.70444300	1.96121100
O	-3.64778900	-0.13696000	1.44657500	H	-2.03833700	3.31851300	1.21174200
C	-2.77763600	0.40168200	2.46021000	H	-1.75413500	3.13141900	2.94670300

H	-3.38257300	0.57075300	3.36042200	O	-0.12897700	2.81807100	1.68742500
H	-2.00757000	-0.33624000	2.70334300	C	1.22107000	-0.63390100	2.22959100
C	-2.18136600	1.69822100	1.95622300	O	1.06913500	0.53513500	1.74072300
H	-2.84044300	2.13222400	1.19567500	C	1.29819000	-0.77139900	3.70421300
H	-2.10120100	2.41731200	2.77995500	C	1.37880800	-2.04560200	4.27862700
O	-0.91531100	1.56545600	1.30794300	C	1.27990800	0.35401600	4.53691800
C	0.25946600	1.42822000	2.08918200	C	1.43626500	-2.19002200	5.65881200
O	1.30280600	1.85744100	1.45042000	H	1.39155100	-2.91403000	3.62513000
C	0.15474900	1.92443100	3.51631900	C	1.34088900	0.20983000	5.91692400
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C	-0.44262500	1.69186000	5.85073300	H	1.49647000	-3.18306000	6.09871500
H	-0.64818900	0.12363100	4.39330700	H	1.33208500	1.08942100	6.55683400
C	0.44312400	3.78092900	5.04230700	H	1.46372800	-1.17704400	7.56055900
H	0.95034000	3.83260800	2.94409500	H	0.34360000	2.21501700	2.29540100
C	-0.05321600	3.00682000	6.08912900	N	7.79702500	0.55246000	-1.45042600
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H	0.75452000	4.80768200	5.22361000	O	8.42876900	-0.47769700	-1.67298500
H	-0.13237200	3.42690800	7.08956000	N	-5.62760500	-0.68270200	-2.63429000
O	0.33860000	-0.17301000	2.18809500	O	-6.09057200	-1.81875100	-2.71798800
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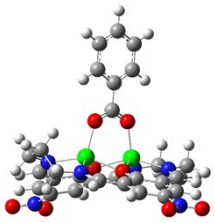

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C	0.91780700	-0.04090900	-4.34134800
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H	3.10157000	0.94913400	-3.62853200
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C	0.85535200	-6.28292300	-0.06862700
H	0.62454800	-4.54782500	-1.33191300
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H	0.77147400	-6.23761800	3.33251400
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O	6.86085600	2.70359200	-1.69688900
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