Supplementary Information

Co-upcycling of mixed polypropylene and polyester

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Method

Materials

Polypropylene pellets (PP-T30S, Mw=4.20×10^5 g/mol, PDI 3.52) were purchased from China National Petroleum Corporation. PET powders (Mw=4.59×10^5 g/mol, PDI 1.7) were purchased from Sigma-Aldrich. $FeSO_4\cdot7H_2O$ were purchased from Jinshan Chemical Test. Sodium dodecyl sulfate (SDS, $\geq$99.0%) were purchased from adamas-beta. 36% HCl and 30% H_2O_2 were purchased from Chron Chemicals. Potassium hydroxide (AR), xylene (AR) and tetrahydrofuran (AR) were purchased from Tianjin Zhiyuan Reagent Co. Ltd..

Characterization

Fourier-Transform Infrared Spectroscopy (FT-IR). FT-IR spectroscopy was performed on a Nicolet 6700 FT-IR System. Infrared testing was performed using potassium bromide compressions with a wave number range of 4000-400 cm^{-1}.

Nuclear Magnetic Resonance (NMR). The degradation products were analyzed by a Bruker Avance 400 nuclear magnetic resonance spectrometer operating at 400 MHz.

Gel permeation chromatography (GPC). Molecular weight distributions of PET and HPET were analyzed on an Agilent PL-GPC 220 gel permeation chromatograph, equipped with a PL-Gel Mixed B guard column, three PL-Gel Mixed B columns, and a refractive index (RI) detector. HFIP was used as a mobile phase. Molecular weight was determined from a calibration curve obtained using polystyrene standards.

Liquid-mass spectrometry (LC-MS). 10 mg of the sample was dissolved in 5 ml of THF, and then filtered through the organic phase filter head. The sample solution was analyzed on Thermo TSQ Fortis plus, equipped with a C18 column and an ESI-MS detector. The mobile

phase of column A was 1 wt% formic acid aqueous solution and the mobile phase of column B was methanol solution. The experiment took a gradient elution with a total flow rate of 0.2 mL/min.

High Performance Liquid Chromatography (HPLC). PP/PBS degradation solution was diluted with deionized water and analyzed on a Shimadzu HPLC system equipped with a UV-VIS detector and a refractive index detector. The liquid products were separated in an Aminex Column, using 5 mM H_2SO_4 as the mobile phase (0.6 mL/min of flow rate) with a column temperature of 50 ^oC.

Degradation of PET in the ITGH system

0.4 g PP and 0.4 g PET powders were added to 50 mL of PTFE liner, 5.6 mL of 30% H_2O_2, 0.18 g of SDS and 7 mg of $FeSO_4 \cdot 7H_2O$ were added sequentially. The liner was sealed in a hydrothermal reactor. The hydrothermal synthesis kettle was heated in an 80 ^oC oil bath for 5 min, and removed from the oil bath. The reaction was continued at room temperature for 25 min. At the end of the reaction, the kettle was snap-cooled with cold water. The solid and liquid products were obtained by filtration, and the solid products were separated by dissolution with THF. The part dissolved in THF was DPP/PET-solTHF, and the insoluble part was DPP/PET-insolTHF. DPP/PET-insolTHF was added to xylene and dissolved at 100 ^oC for 30 min. The solution was filtered while hot. The filtrate residue was PET **residual**. Ethanol was added to the filtrate to precipitate a solid, which was filtered and dried to obtain **DPP-1**.

DPP/PET-solTHF contain PET degradation products **TPAs** and PP degradation products **DPP-2**. In order to calculate the yield of TPAs, DPP/PET-solTHF was hydrolyzed to convert

TPAs into TPA. At the end of the reaction, the pH of the reaction solution was adjusted to 1 with 1 M HCl. At this time, a large number of solids were precipitated. DPP-2 has a density less than 1 and floated on the surface of the water, while TPA has a density greater than 1 and settled to the bottom of the container. **DPP-2** and **TPA** were separated by different densities.

The yield of TPAs form PET degradation (Y_{TPAs}) were calculated according to Eq.1. M_{TPA} and M_{PET} are molar masses, which are 166 g/mol and 192 g/mol, respectively.

$$Y_{TPAs}(wt\%) = \frac{W_{TPA}}{W_{PET} \times {}^{M_{TPA}}/_{M_{PET}}} \times 100\% \quad (1)$$

The selectivity of TPAs from PET degradation (S_{TPAs}) was calculated according to Eq. 2 and 3. C_{PET} is the conversion rate of PET in PP/PET mixed degradation.

$$C_{PET}(\%) = \frac{W_{PET} - W_{residual}}{W_{PET}} \times 100\% \quad (2)$$

$$S_{TPAs}(\%) = \frac{Y_{TPA}}{C_{PET}} \times 100\% \quad (3)$$

The yield of terminal functionalized PP oligomers from PP degradation (Y_{TFDPP}) was calculated according to Eq. 4, where W_{DPP-1}, W_{DPP-2} and W_{PP} are the mass of DPP-1, DPP-2 and PP, respectively.

$$Y_{TFDPP}(wt\%) = \frac{W_{DPP-1} + W_{DPP-2}}{W_{PP}} \times 100\% \quad (4)$$

The selectivity of terminal functionalized PP oligomers from PP degradation (S_{TFDPP}) was calculated according to Eq. 5, where C_{DPP-1}, C_{DPP-2} and C_{PP} are the carbon contents of DPP-1, DPP-2 and PP, respectively.

$$S_{TFDPP}(\%) = \frac{C_{DPP-1} + C_{DPP-2}}{C_{PP}} \times 100\% \quad (5)$$

Content of methyl ketone and isopropenyl groups. ^{1}H NMR was performed on a mixture of TFDPP and 2.0 μL DCE in $CDCl_3$. The contents of methyl ketone and isopropenyl groups are calculated using eq. 6-8.

$$mol\ of\ isopropenyl\ (mmol) = \frac{integration\ of\ isopropenyl}{integration\ of\ DCE} \times mol\ of\ DCE \times \frac{4}{2} \quad 6$$

$$mol\ of\ methyl\ ketone\ (mmol) = \frac{integration\ of\ Methy\ ketone}{integration\ of\ DCE} \times mol\ of\ DCE \times \frac{4}{3} \quad 7$$

$$Content\ of\ functional\ group\ (mmol/g) = \frac{mol\ of\ function\ group}{mass\ of\ TFDPP} \quad 8$$

Monitoring of reaction internal temperature

The degradation reactions were carried out in a reactor with the temperature sleeve. The internal temperature of the reaction was tested three times in parallel and the sensor sensitivity of the measured temperature was at ± 0.5 ^{o}C. In order to prevent the metal sleeve from affecting the degradation reaction, the temperature measuring point was designed above the reaction liquid level. The temperature of the gas in the reactor was measured, and the test temperature would be lower than the actual reaction temperature. The internal temperature of the reaction PP degradation and PP/PET mixed degradation was recorded, and the curve of the internal temperature with time was plotted.

Simulation of relay degradation

The PET powder was added to a crucible with a lid and heated in a muffle furnace at 600 ^{o}C for 45 s. The crucible was immediately removed and cooled at room temperature to obtain HPET.

HPET or PET powder was added to an aqueous solution of pH=1 (conditioned by H_2SO_4) and heated in a hydrothermal synthesizer at 180 ^{o}C for different time. After the reaction was finished, the solid product was collected by filtration. The solid product was dissolved with 1 M KOH and the filtrate and residue were obtained by filtration. The filtrate was adjusted to pH 1 with 1 M HCl to precipitate solid product, which was analyzed by LC-MS. The degradation rate (*D%*) was calculated according to Eq. 9.

$$D\% = \frac{W_{HPET} - W_{residue}}{W_{HPET}} \times 100\% \quad (9)$$

Expanded application of the ITGH system

The mixed degradation of PP/PBT, PP/PBAT and PP/PBS were conducted according to the procedure for PP/PET. Differently, in the case of PP/PBS, the solid and liquid products were obtained by filtration, and the obtained solid product was **DPP** and the liquid product was analyzed by HPLC for quantification of **SA**.

Y_{TFDPP} and S_{TFDPP} were calculated according to Eq. 10 and Eq. 11, respectively.

$$Y_{TFDPP}(wt\%) = \frac{W_{DPP}}{W_{PP}} \times 100\% \quad (10)$$

$$S_{TFDPP}(\%) = \frac{C_{DPP}}{C_{PP}} \times 100\% \quad (11)$$

Y_{SA} and S_{SA} were calculated according to Eq. 12 and Eq. 13, respectively.

$$Y_{SA}(mol\%) = \frac{W_{SA}/M_{SA}}{W_{PBS}/M_{PBS}} \times 100\% \quad (12)$$

$$S_{SA}(\%) = \frac{Y_{SA}}{C_{PBS}} \times 100\% \quad (13)$$

Three domestic wastes, PP/PET beverage bottle, PP/PET composite film, or PP/PET carpet, was added in HFIP to dissolve the PET component therein. The PP fraction was obtained by filtration and the PET fraction was precipitated by adding methanol to the filtrate. The mass ratio of PP and PET in the actual sample was calculated.

The mixed degradation of three domestic wastes was conducted according to the procedure for PP/PET.

Figure S1. Hydrothermal reactor with temperature sensor.

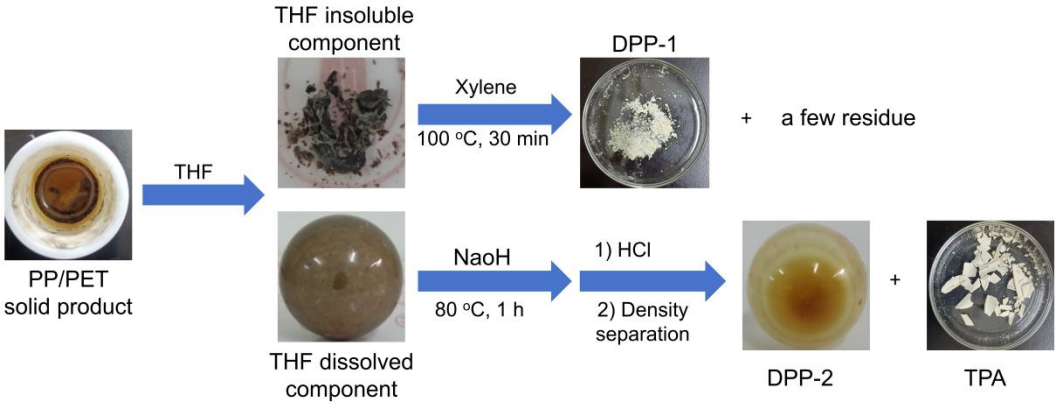


Figure S2. Separation process of solid degradation product.

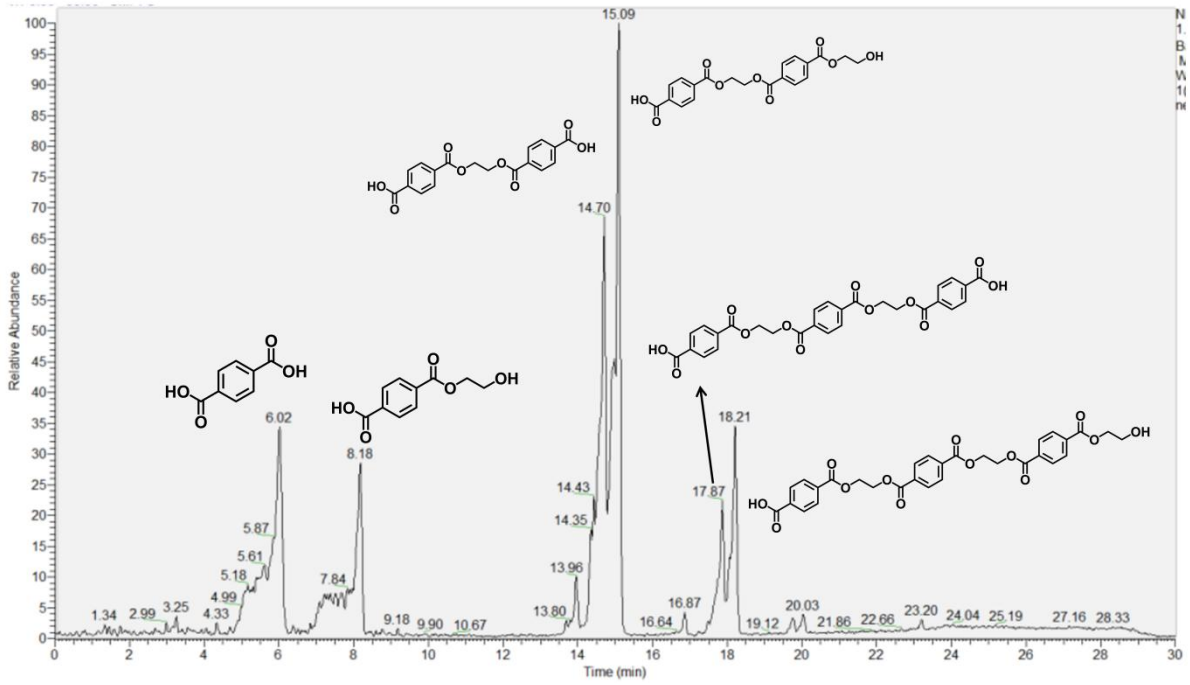


Figure S3. LC-MS analysis of the products dissolved in THF from PP/PET mixed degradation.

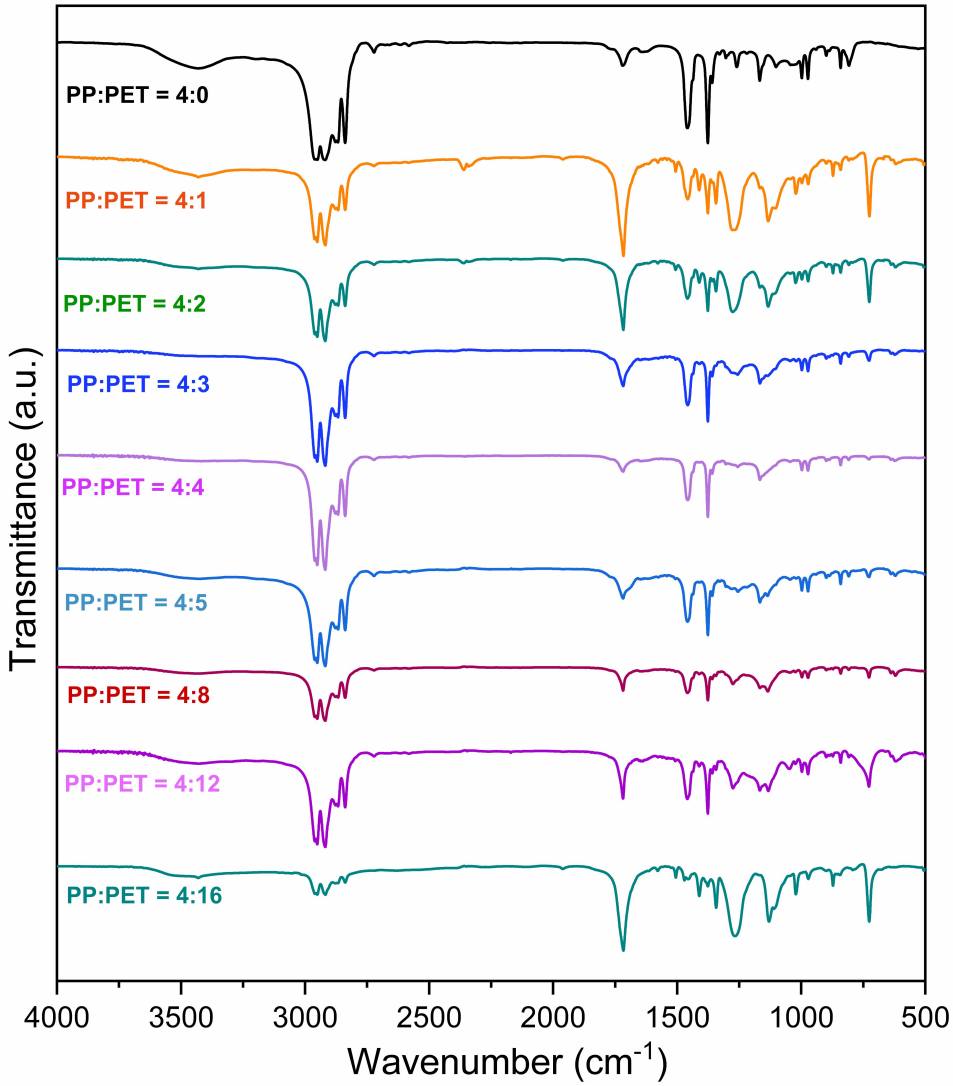


Figure S4. Comparative infrared spectra of PP degradation product DPP-1 under different PP/PET.

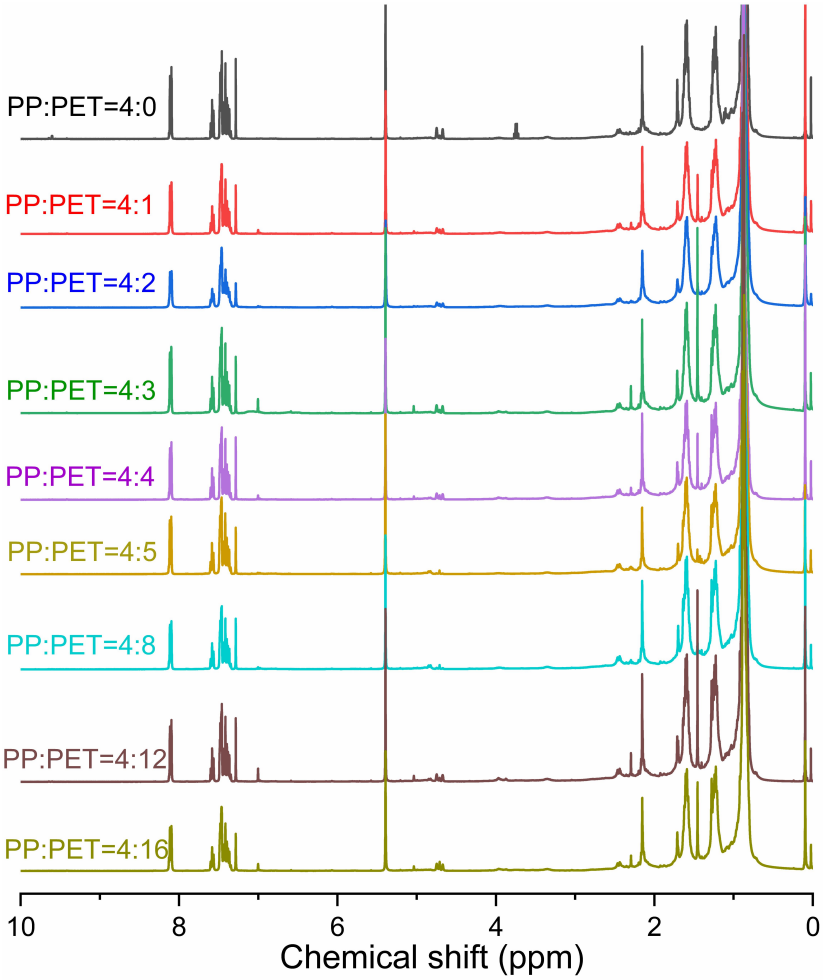


Figure S5. Comparative ^{1}H NMR spectra of PP degradation product DPP-2 under different PP/PET.

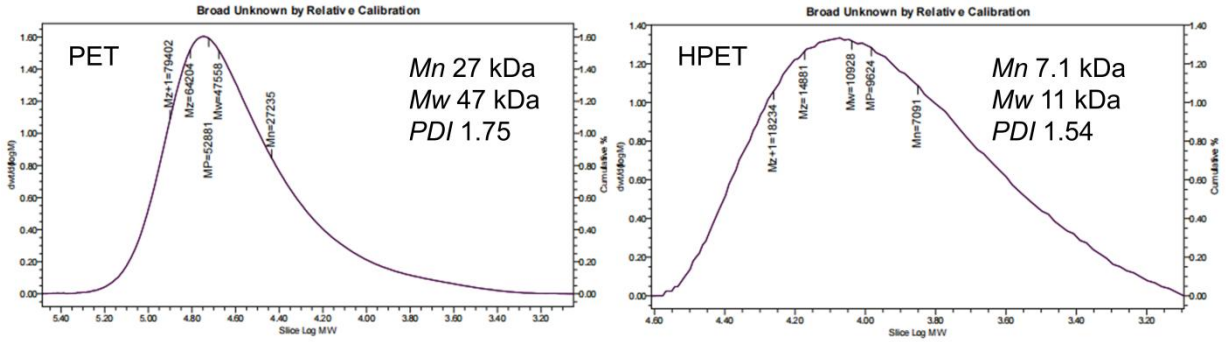


Figure S6. GPC chromatograms of PET and HPET performed in HFIP.

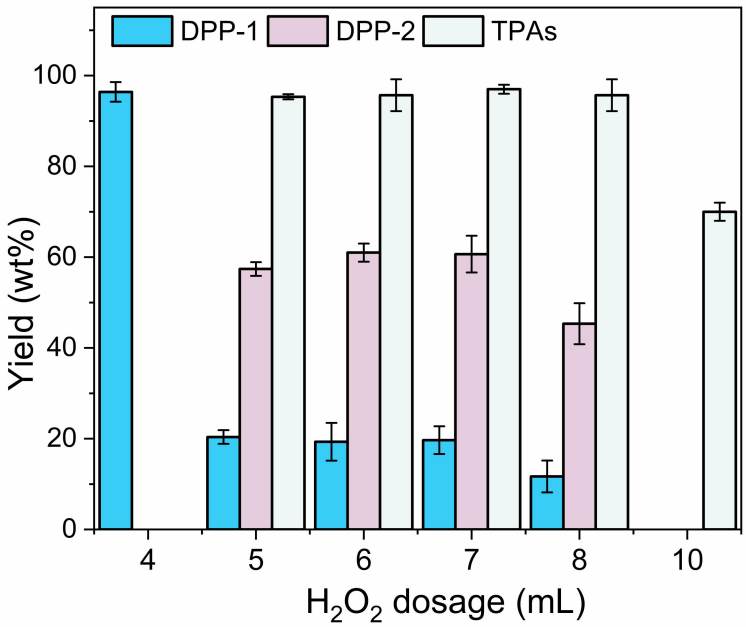


Figure S7. Variation of the yields of mixed PP/PET degradation products with the amount of H_2O_2.

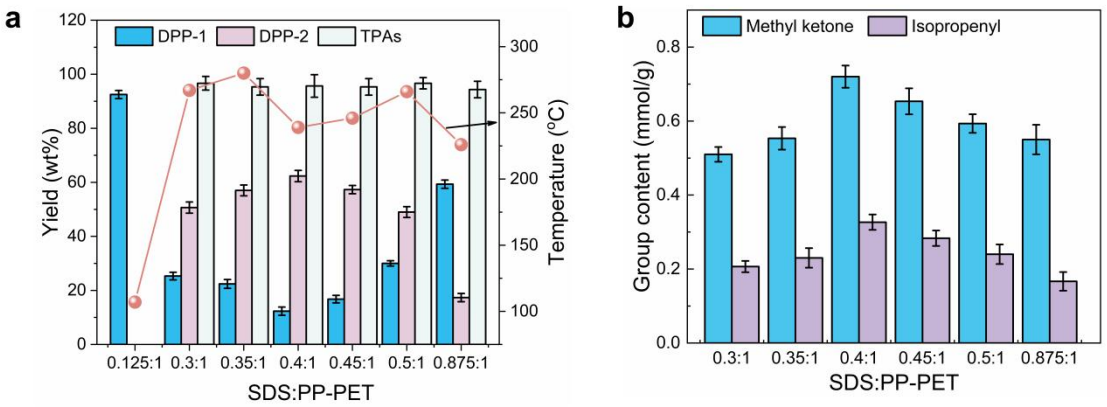


Figure S8. The effect of SDS dosage on the mixed PP/PET degradation. a) Variation of internal peak temperature and degradation product yields with SDS dosage. b) Variation of functional group contents in DPP-2 with SDS dosage.

Table S1. Functional group contents of PP degradation products under different PP/PET ratios.

Entry	PP:PET	DPP-2	
		Methylketone* (mmol/g)	Isopropenyl * (mmol/g)
1	4:0†	0.57	0.35
2	4:1	0.68	0.21
3	4:2	0.77	0.19
4	4:3	0.65	0.25
5	4:4	0.65	0.23
6	4:5	0.65	0.22
7	4:8	0.64	0.26
8	4:12	0.68	0.23
9	4:16	0.67	0.24

*Calculated from ^{1}H NMR, using an internal standard. † The degradation products of PP without PET .

Computational details

All calculations were performed using Gaussian 09 program package[1], employing the B3LYP density functional[2] with the 6-31G* basis set[3-4]. Geometries were optimized in water and characterized by frequency analysis at 528 K. The self-consistent reaction field (SCRF) method based on the universal solvation model SMD[5] was adopted to evaluate the effect of solvent. The intrinsic reaction coordinate (IRC) path[6] was traced to check the energy profiles connecting each transition state to two associated minima of the proposed mechanism. All single-point energies were computed by using B3LYP density functional with the 6-311G** basis set[7-8]. Homolytic bond dissociation enthalpies (BDEs) were calculated by the enthalpy change for the reaction at 528 K:

$$A\text{-}B \rightarrow A\bullet + B\bullet$$

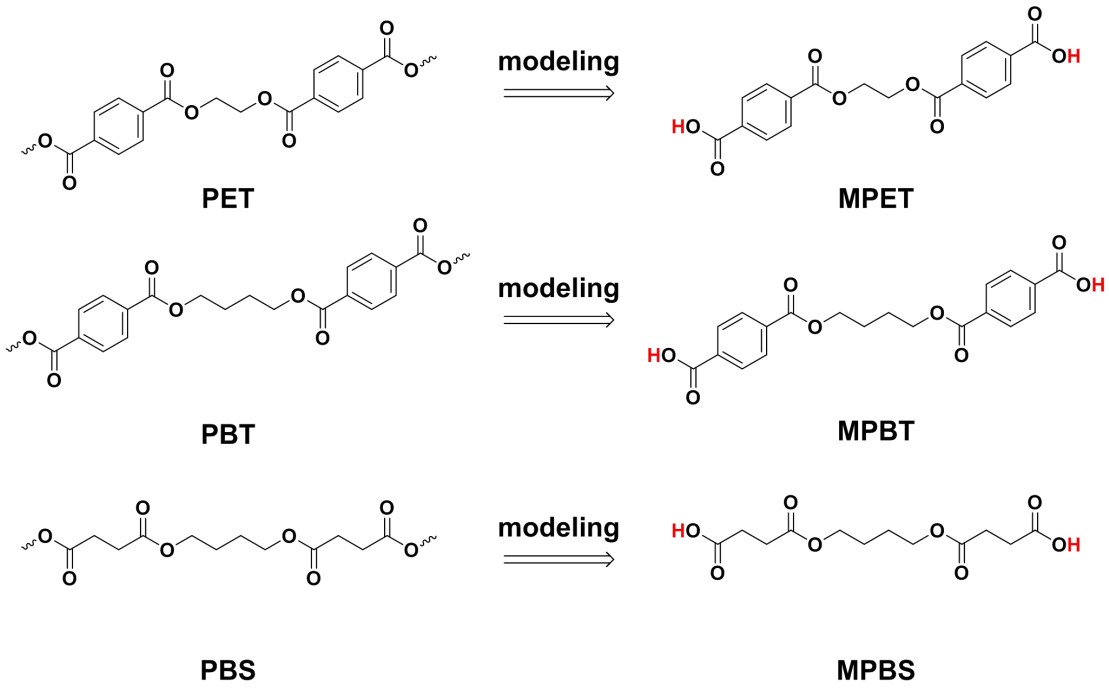


Figure S9. Model compound MPET, MPBT, MPBS used in the present work.

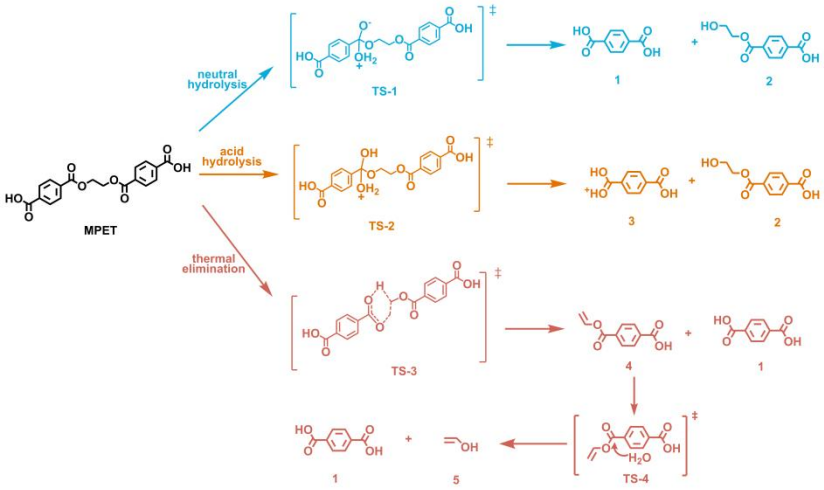


Figure S10. Possible reaction paths in the depolymerization of MPET.

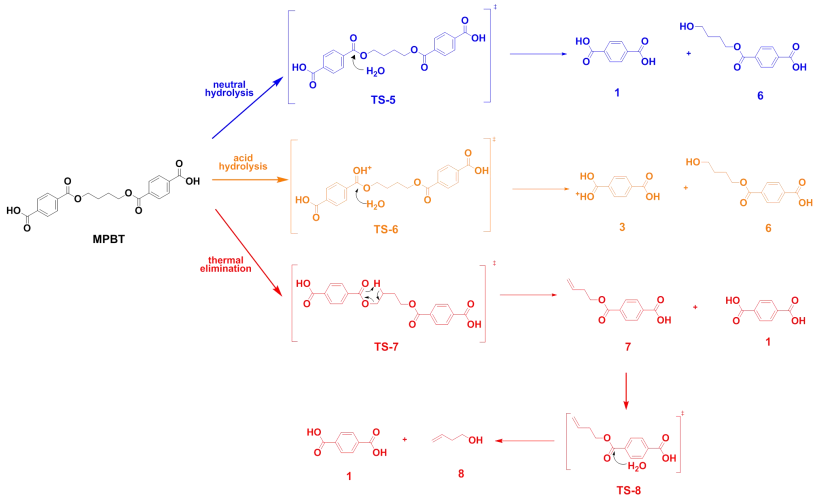


Figure S11. Possible reaction paths in the depolymerization of MPBT.

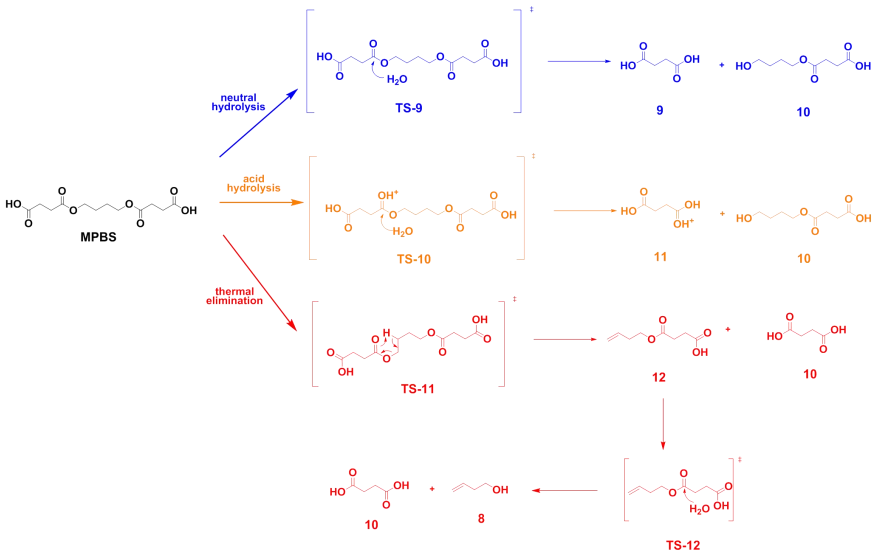


Figure S12. Possible reaction paths in the depolymerization of MPBS.

Table S2. Bond dissociation enthalpies (BDEs, kcal mol^{-1}) of MPET, obtained at B3LYP/6-311G**(SMD,H_2O)//B3LYP/6-31G*(SMD,H_2O) theoretical level.

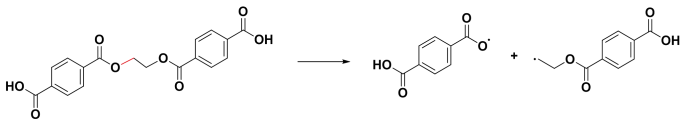
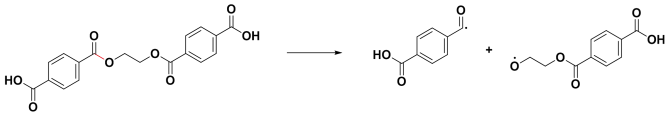
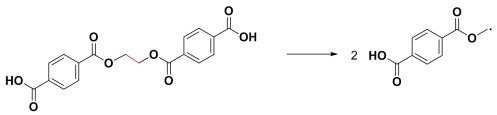
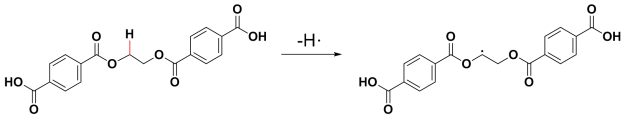
Reaction	BDEs
	83.3
	93.2
	86.2
	97.6

Table S3. Possible reactions of 1,4-dicarboxybenzene (TPA). Bond dissociation enthalpies (BDEs) and activation barrier are in kcal mol^{-1}.

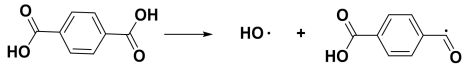
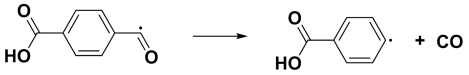
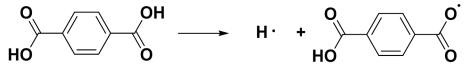
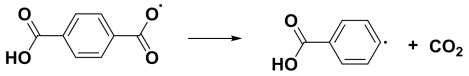
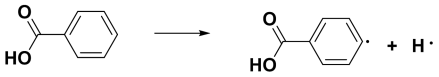
		Reaction	BDE	$\Delta^{\neq}G$
Path 1	Step 1		107.3	-
	Step 2		31.5	-
Path 2	Step 1		109.7	-
	Step 2		-	8.5
Path 3	Step 1		-	61.7
	Step 2		114.0	-

Table S4. Electronic energies (E_e), enthalpies (H) and Gibbs free energies (G) for all stationary points (in Hartree), obtained at the B3LYP/6-311G**(SMD,H_2O)//B3LYP/6-31G*(SMD,H_2O) theoretical level at 528 K.

Structures	[a]*ZPE*	E_e	[b]H_{corr}	*H*	[c]G_{corr}	*G*
MPET	0.29827	-1296.32134	0.36344	-1296.25616	0.16595	-1296.45366
TS-3	0.29032	-1296.26339	0.35516	-1296.19854	0.16773	-1296.38598
TS-4	0.18446	-763.12454	0.22536	-763.08364	0.09111	-763.21789
TS-1	0.31849	-1372.51225	0.38864	-1372.44210	0.18050	-1372.65023
TS-2	0.33314	-1372.91509	0.40309	-1372.84513	0.19698	-1373.05125
MPET-C-O-frag1-a	0.17161	-687.39266	0.20938	-687.35489	0.08008	-687.48419
MPET-C-O-frag2-a	0.11653	-608.79750	0.14542	-608.76861	0.03700	-608.87703
MPET-C-O-frag1-b	0.17708	-762.62763	0.21645	-762.58826	0.08130	-762.72341
MPET-C-O-frag2-b	0.11198	-533.54635	0.13900	-533.51932	0.03480	-533.62352
MPET-C-C-frag	0.14303	-648.09342	0.17707	-648.05937	0.05722	-648.17923
MPET-C-H-frag	0.28331	-1295.67026	0.34879	-1295.60478	0.14831	-1295.80526
H·	0.00000	-0.49999	0.00418	-0.49581	-0.02126	-0.52125
TPA/1	0.13003	-609.46887	0.15960	-609.43931	0.05151	-609.54740
OH·	0.00832	-75.75491	0.01417	-75.74906	-0.02503	-75.78826
TPA-IM1-a	0.11211	-533.54623	0.13903	-533.51931	0.03546	-533.62289
CO	0.00500	-113.33215	0.01088	-113.32627	-0.03224	-113.36939
TPA-IM2	0.10236	-420.16473	0.12429	-420.14280	0.03429	-420.23280
TPA-IM1-b	0.11653	-608.79750	0.14542	-608.76861	0.03700	-608.87703
TPA-TS-b	0.11395	-608.78220	0.14314	-608.75302	0.03264	-608.86352
TPA-TS-c	0.12291	-609.36886	0.15242	-609.33935	0.04277	-609.44900
TPA-IM1-c	0.11557	-420.84266	0.13787	-420.82036	0.04850	-420.90973
MPBT	0.35563	-1374.92318	0.42832	-1374.85048	0.21389	-1375.06492
MPBT-TS-7	0.34852	-1374.86942	0.42078	-1374.79717	0.21542	-1375.00252
MPBT-TS-8	0.24077	-841.80493	0.28899	-841.75671	0.13658	-841.90912
MPBT-TS-5	0.37636	-1451.29265	0.45377	-1451.21524	0.23134	-1451.43767
MPBT-TS-6	0.39014	-1451.71526	0.46779	-1451.63761	0.24319	-1451.86222
MPBS	0.30825	-1070.03647	0.36737	-1069.97735	0.17988	-1070.16484
MPBS-TS-11	0.30020	-1069.98637	0.35932	-1069.92724	0.18001	-1070.10655
MPBS-TS-12	0.21702	-689.36767	0.25848	-689.32620	0.12019	-689.46449
MPBS-TS--9	0.32922	-1146.42170	0.39233	-1146.35859	0.20416	-1146.54676
MPBS-TS-10	0.34478	-1146.84407	0.40731	-1146.78154	0.22375	-1146.96510

2	0.192198	-763.28856	0.23195	-763.24881	0.09813	-763.38263
3	0.144419	-609.86785	0.17415	-609.83812	0.066544	-609.94573
5	0.056457	-153.81075	0.06722	-153.79999	0.007823	-153.85938
6	0.249518	-841.88823	0.29683	-841.84091	0.144695	-841.99305
8	0.114144	-232.40049	0.13219	-232.38244	0.053688	-232.46095
9	0.105989	-457.02603	0.129	-457.00301	0.033685	-457.09833
10	0.225062	-689.44612	0.26576	-689.40542	0.128569	-689.54261
11	0.11958	-457.43581	0.14243	-457.41296	0.051011	-457.50438

[a] Zero-point correction energy;

[b] Thermal correction to enthalpy obtained at the B3LYP/6-31G*(SMD, H_2O) level of theory;

[c] Thermal correction to Gibbs free energy obtained at the B3LYP/6-31G*(SMD, H_2O) level of theory.

Table S5. Electronic energies (E_e), enthalpies (H) and Gibbs free energies (G) for all stationary points (in Hartree), obtained at the B3LYP/6-311G**(SMD,H_2O)//B3LYP/6-31G*(SMD,H_2O) theoretical level at 298 K.

Structures	[a]*ZPE*	E_e	[b]H_{corr}	*H*	[c]G_{corr}	*G*
MPET	0.29826	-1296.32134	0.32217	-1296.29743	0.24064	-1296.37896
TS-3	0.29032	-1296.26339	0.31353	-1296.24017	0.23797	-1296.31574
TS-1	0.31848	-1372.69276	0.34415	-1372.66709	0.25897	-1372.75227
TS-2	0.333136	-1373.11206	0.35837	-1373.08683	0.274498	-1373.17070
1	0.130034	-609.46887	0.14094	-609.45796	0.093487	-609.50542
4	0.162775	-686.83579	0.17611	-686.82245	0.122449	-686.87611
2	0.192199	-763.28856	0.20698	-763.27378	0.149582	-763.33118
3	0.144419	-609.86785	0.15516	-609.85712	0.108208	-609.90406

[a] Zero-point correction energy;

[b] Thermal correction to enthalpy obtained at the B3LYP/6-31G*(SMD, H_2O) level of theory;

[c] Thermal correction to Gibbs free energy obtained at the B3LYP/6-31G*(SMD, H_2O) level of theory.

Cartesian coordinates of all structures

4

C	4.84779000	0.68489300	-1.73096200
C	4.13782700	1.33682300	-0.81856000
O	2.74702400	1.25098800	-0.85376700
C	2.02264700	1.88035000	0.11082900
O	2.52580600	2.51129900	1.02512200
C	0.56009300	1.70459100	-0.08583900
C	-0.30097100	2.29053500	0.85353600
C	0.03165000	0.98359900	-1.16757000
C	-1.67805000	2.15966900	0.71674800
C	-2.20633200	1.43964000	-0.36494100
C	-1.34537700	0.85383200	-1.30356700
C	-3.67268700	1.27047000	-0.55878400
O	-4.17383600	0.64759800	-1.48400300
O	-4.41184200	1.87649200	0.39322000
H	5.93001700	0.75148200	-1.71294000
H	4.37721500	0.08102800	-2.50110800
H	4.54170400	1.95249700	-0.02403700
H	0.11600200	2.84557200	1.68653700
H	0.69213100	0.52932100	-1.89631600
H	-2.33872800	2.61406700	1.44569300
H	-1.76283700	0.29940800	-2.13674400
H	-5.35378600	1.71386800	0.18715500

2

O	-1.58777500	1.12868000	-0.65239500
C	-0.26061300	0.75141700	-0.28977700
H	0.26016100	1.55992000	0.23907900
H	-0.34581600	-0.10260700	0.38842800
H	-1.52480700	1.97178200	-1.13237300
C	0.53116400	0.34776500	-1.53150600
H	0.06926400	-0.50864700	-2.02471600
H	0.60611300	1.18112100	-2.23539100
O	1.85850700	-0.10134100	-1.16064600
C	2.79491900	0.84473100	-0.95839400
O	2.58982000	2.04163800	-1.10459400
C	4.10718300	0.27432900	-0.54113300
C	5.17084400	1.16234400	-0.32403100
C	4.29594200	-1.10280900	-0.35531200
C	6.40997700	0.67891300	0.07544100
H	5.01666800	2.22582200	-0.46959300
C	5.53734700	-1.58706000	0.04537500
H	3.47596300	-1.79156300	-0.52007500
C	6.59978800	-0.69777000	0.26335300
H	7.23707700	1.35921400	0.24583700
H	5.67808900	-2.65185600	0.18961600
C	7.94399300	-1.16674400	0.69775000
O	8.89237600	-0.42543000	0.91326900
O	8.02482200	-2.50659500	0.83457800
H	8.93406100	-2.72196500	1.12255000

3

O	-2.42567300	2.00909500	1.84756400
C	-3.00860100	1.79781200	0.71364800
H	-2.72978000	1.41284700	2.56293300
O	-2.49328400	2.51141200	-0.23253600
H	-2.97809700	2.44700400	-1.08149800
C	-4.11623000	0.86552300	0.52539200
C	-4.33740900	0.28998500	-0.73939600
C	-4.95511700	0.54699500	1.61014200
C	-5.38662300	-0.60262000	-0.91380200
H	-3.67685100	0.50439500	-1.57324300
C	-6.00806500	-0.33597300	1.42263700
H	-4.81236200	1.00974300	2.58112300
H	-5.54926900	-1.05554400	-1.88398300
H	-6.66894600	-0.57948300	2.24623600
C	-6.22525200	-0.91474600	0.16517000
C	-7.37046900	-1.86533900	0.02222400
O	-8.12691100	-2.15522500	0.93510100
O	-7.48212100	-2.37136000	-1.21836700
H	-8.25022700	-2.97676000	-1.23129000

5

O	2.89320000	1.61356500	-0.99597100
H	2.95460500	1.39867900	-0.04794300
C	3.83997800	0.88495100	-1.67644000
H	3.79313700	1.10472400	-2.74006100
C	4.71091300	0.02159700	-1.15001900
H	4.74339000	-0.18619300	-0.08268200
H	5.41309800	-0.49591200	-1.79486700

6

O	2.78550400	-0.98210100	-0.52356800
C	1.43977200	-0.82889800	-0.05413600
H	1.06068800	-1.77936200	0.35180600
H	1.49236000	-0.11461000	0.77502400

H	2.76108800	-1.64730900	-1.23161800
O	-3.18739600	0.64007600	-1.21080500
C	-4.01336300	-0.41543500	-1.12937900
O	-3.70868000	-1.54640000	-1.48565500
C	-5.34650200	-0.06052600	-0.56171900
C	-6.30058500	-1.08013700	-0.43358300
C	-5.66080200	1.24584000	-0.16020800
C	-7.55601200	-0.79723500	0.08907400
H	-6.04949200	-2.08816500	-0.74475800
C	-6.91879100	1.52972000	0.36248900
H	-4.92589300	2.03626900	-0.25566900
C	-7.87224200	0.50918100	0.48889800
H	-8.29866500	-1.58091100	0.19051100
H	-7.15764800	2.54099200	0.67036500
C	-9.23026000	0.76389600	1.04164300
O	-10.08298900	-0.10000300	1.19067900
O	-9.44130900	2.05584800	1.36928100
H	-10.35081900	2.12943200	1.72069200
C	0.50199900	-0.31143300	-1.14178800
H	0.89355100	0.64122000	-1.52159900
H	0.50959900	-1.02102000	-1.98136000
C	-0.93044300	-0.12921300	-0.62963700
H	-1.32371300	-1.08595100	-0.26659000
H	-0.94417900	0.57238200	0.21375400
C	-1.84547600	0.40207900	-1.72350600
H	-1.51906300	1.38176600	-2.07799900
H	-1.90630400	-0.28516000	-2.57114000

8

O	2.06140100	0.28789000	0.58268900
H	2.25352000	-0.01006300	1.48771200
C	5.66478600	1.00044100	-0.34882800
H	6.13753100	0.01824400	-0.29434100
C	6.24748900	1.96580200	-1.06323400
H	5.80768600	2.95860000	-1.14657100
H	7.18659500	1.80216700	-1.58711700
C	3.28532900	0.19664800	-0.15413900
H	3.03790100	0.46782800	-1.18589500
H	3.65838000	-0.83876000	-0.16347900
C	4.36477700	1.14006000	0.39310400
H	3.99825700	2.17250700	0.34451800
H	4.51656800	0.89370400	1.45520200

9

C	0.72466000	1.14010000	1.30721200
O	1.62760600	1.82987800	0.58106800
O	1.04507600	0.30224800	2.13457900
H	2.52046600	1.52749400	0.84233000
C	-0.70615000	1.52990700	1.02078700
H	-1.30871200	0.62424500	1.12181500
H	-1.01218500	2.20526300	1.83069600
C	-0.93330100	2.20263400	-0.34176600
H	-0.61721400	1.52624800	-1.14473100
H	-0.35823200	3.12531300	-0.42600900
C	-2.38371800	2.54635800	-0.57653700
O	-2.80402300	3.65428500	-0.86515200
O	-3.19362500	1.47191900	-0.44696700
H	-4.11212200	1.76234600	-0.61679100

10

O	-3.85382400	-0.73411100	-0.06282600
C	-3.88650600	-2.08695300	-0.54039500
H	-4.83915300	-2.56660400	-0.27069600
H	-3.80174000	-2.11106500	-1.63764900
O	1.07208200	-2.64933000	-0.13712300
C	1.59370300	-1.55177200	0.44078000
O	1.03774500	-0.91677700	1.32378100
C	-2.72941300	-2.85153900	0.08647400
H	-2.81912800	-3.90641000	-0.20402200
H	-2.83080000	-2.81068700	1.17943100
C	-1.35692000	-2.31171500	-0.33193100
H	-1.26889900	-1.25594300	-0.05726400
H	-1.24682500	-2.37893800	-1.42184300
C	-0.23324600	-3.09671700	0.32817000
H	-0.26713600	-4.15255700	0.05037400
H	-0.26974300	-3.01398300	1.41790800
C	2.95218100	-1.23675800	-0.13651800
H	2.86652100	-1.21536600	-1.22790600
H	3.61865400	-2.07408500	0.10042500
C	3.51898900	0.07314900	0.39599500
H	2.86312600	0.91700000	0.14969000
H	3.59187900	0.05417500	1.49028100
C	4.89339000	0.36778800	-0.15631300
O	5.45074000	1.54212600	0.22556100
H	4.85200400	2.03056500	0.82066400
O	5.51938900	-0.36394500	-0.90244300
H	-4.56660500	-0.25230000	-0.51295900

11

O	1.28618000	-1.17014500	0.50425200
C	1.58415800	-0.02219500	0.02100700
H	0.35863600	-1.44123900	0.23377000
C	0.65405800	0.75939000	-0.85514200
H	1.14447200	1.69073400	-1.14090900
H	0.51418200	0.16152400	-1.76419800
C	-0.71041200	1.09031900	-0.21203300
H	-1.17262800	1.88859500	-0.79800000
H	-0.57537700	1.48723200	0.80082600
C	-1.73299000	-0.01906000	-0.11933900
O	-1.20902100	-1.25766800	-0.33864300
H	-1.89811800	-1.94186500	-0.20698200
O	-2.90461300	0.15474100	0.13413800
O	2.76405100	0.37988400	0.34638000
H	2.97839800	1.26567100	-0.01319000

H·

H	0.48610000	-0.72230000	1.00020000

CO

C	0.42654300	-0.11421300	0.00000000
O	1.56449100	-0.11421300	0.00000000

MPBS

C	-3.48582100	-0.65157600	0.27477900
O	-2.91617800	-1.58319100	0.82110400
O	-2.87711400	0.49721300	-0.07082900
C	-1.45676000	0.61469700	0.22718900
O	2.87600600	-0.26847500	0.67810100
C	3.64320900	-1.15191100	0.01235200
O	3.19851000	-2.10021100	-0.61474400
H	-1.27309200	1.69112000	0.24983200
H	-1.27540000	0.19827000	1.22069900
C	-0.62314600	-0.06590500	-0.85231700
H	-0.83555700	-1.14124600	-0.84601900
H	-0.93829200	0.32357000	-1.82692400
C	0.88382900	0.17136200	-0.68015200
H	1.40940900	-0.27316500	-1.53170700
H	1.10291000	1.24622500	-0.68410100
C	1.43300000	-0.44422200	0.60240000
H	1.05987700	0.06022700	1.49496000
H	1.19790800	-1.50990800	0.66842800
C	-4.94701500	-0.65168400	-0.11002800
H	-5.39865100	-1.54826500	0.32021700
H	-5.00221400	-0.73385000	-1.20120500
C	-5.68449800	0.61647800	0.35595800
H	-5.25771900	1.49548500	-0.14007000
H	-5.58227100	0.75585100	1.43435200
C	5.11262900	-0.83176300	0.15762400
H	5.38409900	-0.96388000	1.21030500
H	5.66983300	-1.56012400	-0.43540000
C	5.43859900	0.60543800	-0.28969800
H	4.91034900	1.32083300	0.35100300
H	5.12130000	0.77790700	-1.32059400
C	-7.15925200	0.58933600	0.03860100
C	6.90995900	0.92788600	-0.20734800
O	-8.04755000	0.87453500	0.82421100
O	7.55372800	1.47660600	-1.08591200
O	-7.40560800	0.23045300	-1.24079000
H	-8.37395900	0.24096700	-1.37844800
O	7.45432300	0.56423300	0.97454300
H	8.40004000	0.81373800	0.96104300

TS-11

C	0.95154800	1.27330500	1.09428700
O	1.77896700	1.88408400	0.32612800
O	1.30250100	0.44821200	1.98427300
C	3.40630900	-0.28273800	1.72840300
C	3.95486300	0.32700000	0.59844100
C	0.58668200	-1.25180700	-1.19074900
O	0.25275900	-0.75975800	-2.25831300
H	3.56438100	0.13532600	2.71574600
H	2.93867400	-1.25960400	1.68137000
H	4.73907900	1.05744800	0.81590500
O	1.85064100	-1.25618200	-0.74338200
C	2.83688900	-0.54580700	-1.54376000
H	2.43510000	0.44064800	-1.78719400
H	3.00407600	-1.10185300	-2.47059500
C	4.10793000	-0.44828900	-0.71582800
H	4.48703100	-1.45781000	-0.51946700
H	4.85447500	0.05704400	-1.33709900
H	2.98556900	1.13458200	0.47246600
C	-0.53155800	1.58452300	0.95762900
H	-1.09615900	0.69139700	1.23336800
H	-0.76255600	2.34872500	1.71200500
C	-0.93004500	2.08910500	-0.43585800
H	-0.70219100	1.32182500	-1.18607700

H	-0.37473600	2.98940600	-0.70251500
C	-2.39845100	2.40721900	-0.55380700
O	-2.85969000	3.42345000	-1.04770800
O	-3.18722400	1.42186300	-0.06879100
H	-4.11921400	1.68789600	-0.20025100
C	-0.34465100	-1.90388200	-0.19774900
H	-0.06555800	-2.96059700	-0.11016900
H	-0.15270600	-1.45008800	0.77895300
C	-1.81161400	-1.75246500	-0.61442100
H	-2.02377100	-0.69938500	-0.82791700
H	-2.02821000	-2.33119600	-1.51367000
C	-2.77492600	-2.18203300	0.46142300
O	-3.67234300	-2.99612400	0.32185800
O	-2.55868100	-1.53576200	1.62875700
H	-3.22371600	-1.84458700	2.27590300

TS-12

O	1.28002800	-1.94882500	-0.87050200
C	0.84776000	-1.20853600	-0.02098600
O	1.85549900	0.18563600	0.33882400
O	1.37232600	-1.63147700	1.56218800
H	1.88768900	-0.57714800	1.31891700
H	0.64611000	-1.46643000	2.19446000
C	5.51400900	0.78947700	-0.26414100
H	5.89717500	-0.20786400	-0.48589100
C	6.21150600	1.85980400	-0.64967900
H	5.86044400	2.87154900	-0.45227900
H	7.16025900	1.76522100	-1.17296800
C	3.08092500	0.21650200	-0.40439600
H	2.91566400	0.80988100	-1.31105600
H	3.35412300	-0.80111900	-0.71126600
C	4.19139100	0.83248500	0.45082100
H	3.92553000	1.86271600	0.71445000
H	4.25321600	0.25551300	1.38482700
C	-0.54934900	-0.65887600	0.09928600
H	-0.60596700	0.04670400	0.92891200
H	-1.20866400	-1.50703400	0.31564700
C	-0.94692600	0.01095900	-1.22589600
H	-0.83202600	-0.68343800	-2.05984300
H	-0.29400900	0.87443300	-1.40423400
C	-2.37182000	0.50397000	-1.22865100
O	-3.19088300	0.26813800	-2.10069400
O	-2.65457000	1.26954800	-0.15169700
H	-3.58741500	1.55599200	-0.22150200

TS-9

O	-2.40672900	0.76003500	-1.25264900
C	-2.80679400	0.77836600	-0.10633100
O	-3.69055700	-0.58286000	0.39460700
C	-3.73830800	-1.69164900	-0.52892400
H	-4.74772900	-2.10688300	-0.45646700
H	-3.58786000	-1.32146000	-1.55026600
O	1.12903900	-2.63293500	-0.00174000
C	1.57251200	-1.43450500	0.38722900
O	0.93203000	-0.67397200	1.10961800
C	-2.68903900	-2.72920900	-0.14220200
H	-2.93765700	-3.68059700	-0.62770000
H	-2.77462000	-2.89560500	0.93980600
C	-1.25294000	-2.31562000	-0.50900500
H	-1.12357200	-1.23697700	-0.40598900
H	-1.04847000	-2.55620900	-1.55865600
C	-0.22986100	-3.01027700	0.37694500
H	-0.24813300	-4.09481200	0.25431100
H	-0.38069200	-2.76574300	1.43174600
C	2.93512100	-1.13909500	-0.18344200
H	2.80562500	-0.98176200	-1.26127500
H	3.55785200	-2.03241900	-0.07722700
C	3.59477400	0.07479100	0.46034200
H	2.99124200	0.97756400	0.31442600
H	3.69539600	-0.05726500	1.54467400
C	4.97001600	0.33782500	-0.10768100
O	5.62784400	1.41152800	0.39292300
H	5.08814400	1.86818800	1.06481800
O	5.51340600	-0.33523200	-0.96512500
C	-1.99660400	1.14134200	1.11527600
H	-2.63512600	1.18782900	1.99923800
H	-1.29401900	0.31782700	1.27196900
C	-1.26052600	2.47813600	0.93342700
H	-0.63925100	2.65451300	1.81968500
H	-1.97722400	3.29841900	0.85190300
C	-0.35699100	2.55766500	-0.28323500
O	0.60916500	1.62818100	-0.41892200
H	0.62936500	0.96081000	0.30520500
O	-0.43771800	3.44146400	-1.12070600
H	-4.49989800	0.30933200	0.27119400
O	-4.35697600	1.50453000	0.01666700
H	-4.41576500	1.98042600	0.86736400

TS-10

O	-2.39256000	0.80648200	-1.38774300
C	-2.93824500	0.76694200	-0.14994400
H	-1.45026800	0.55615500	-1.36575000
O	-3.76837500	-0.44213500	0.09694600
C	-3.64068200	-1.67863200	-0.69567300
H	-4.65771200	-2.07040800	-0.68796700
H	-3.36393500	-1.40919300	-1.71696500
O	1.15005700	-2.67361500	0.20487200
C	1.57317500	-1.42672800	0.43129000
O	0.90653900	-0.58575600	1.03136200
C	-2.65951900	-2.63982700	-0.03566500
H	-2.96303500	-3.66018400	-0.29694700
H	-2.78408300	-2.54616200	1.05022100
C	-1.19426500	-2.41746500	-0.44070000
H	-0.97501800	-1.35276900	-0.53180800
H	-1.00291600	-2.86284600	-1.42319000
C	-0.22401500	-2.99437800	0.58058800
H	-0.24841900	-4.08487600	0.61032900
H	-0.41518900	-2.60150700	1.58229200
C	2.93949400	-1.18824000	-0.15381600
H	2.82458600	-1.18644100	-1.24480200
H	3.57523500	-2.04628300	0.08409900
C	3.56452300	0.11734100	0.32361200
H	2.93760800	0.97673500	0.05943300
H	3.66244900	0.13215800	1.41609800
C	4.93491500	0.34092200	-0.27057800
O	5.55353200	1.49338600	0.08079200
H	4.98942300	2.01744100	0.67925800
O	5.50540800	-0.42682100	-1.02456900
C	-2.05071600	1.02867600	1.04631400
H	-2.68151700	0.97803200	1.93728200
H	-1.35017400	0.19185300	1.10283700
C	-1.31812100	2.38058200	1.01961800
H	-0.69608900	2.43338600	1.92108500
H	-2.03365900	3.20504500	1.05548600
C	-0.41456100	2.62998900	-0.17399700
O	0.49901600	1.68565700	-0.48574600
H	0.57795300	0.96168500	0.18402000
O	-0.47657900	3.63680900	-0.85667000
H	-4.63791000	0.48448300	-0.07815400
O	-4.15164000	1.59751000	-0.22914400
H	-4.26774900	2.14543900	0.57701500

MPBT

O	9.75305300	-0.83608100	-4.17139000
C	9.05717500	-0.22303800	-3.19103500
O	9.58570600	0.51805400	-2.37418700
C	7.60402100	-0.54262200	-3.21345500
C	6.78576600	0.02812900	-2.22829200
C	7.04565400	-1.38831400	-4.18346800
C	5.42236000	-0.24243500	-2.20770200
C	4.86376600	-1.08668400	-3.17887700
C	5.68154800	-1.65618800	-4.16461800
C	3.40676300	-1.40373100	-3.20702000
O	2.87688200	-2.09963100	-4.06377500
O	2.73188600	-0.84525300	-2.19214900
C	1.30055400	-1.09553500	-2.14754400
O	-2.71369000	-0.20093300	0.52277500
C	-3.36231700	0.17968300	1.63261900
O	-2.79641000	0.63160100	2.61984400
C	-4.83884300	-0.00535300	1.53376600
C	-5.61967900	0.31351300	2.65332500
C	-5.45220300	-0.47851300	0.36421000
C	-7.00098300	0.16180900	2.60988300
C	-7.61459200	-0.30960000	1.43977400
C	-6.83365000	-0.62719200	0.31945700
C	-9.08866600	-0.48779300	1.34156300
O	-9.66828400	-0.88282300	0.33966700
O	-9.74110000	-0.16975600	2.47925300
H	7.22567800	0.68154300	-1.48289200
H	7.67269000	-1.83214100	-4.94777800
H	4.79377000	0.20015600	-1.44404700
H	5.24106700	-2.30728300	-4.91163000
H	0.84752400	-0.67906800	-3.05295800
H	1.13387900	-2.17684200	-2.14077500
H	-5.13705000	0.67901600	3.55301700
H	-4.85238100	-0.72588200	-0.50366700
H	-7.59909800	0.40943900	3.47894200
H	-7.31645300	-0.99000900	-0.58129800
H	10.69082500	-0.57462100	-4.08138600
H	-10.69568700	-0.31758300	2.32829900
C	0.76872000	-0.43550900	-0.88920100
H	1.26156300	-0.88219000	-0.01677400
H	1.02893300	0.62980900	-0.90200400
C	-0.75140900	-0.60429100	-0.78351300
H	-1.24582800	-0.08889200	-1.61579200
H	-1.02077500	-1.66571500	-0.84971800

C	-1.26829800	-0.04553300	0.52893500
H	-0.86136300	-0.58580800	1.38891300
H	-1.03454600	1.01781500	0.64339600

TS-7

O	-3.09549800	1.58515300	-1.47343800
C	-2.46878100	1.90973100	-0.32451900
O	-3.08168600	2.20527200	0.69361600
C	-0.98751100	1.85017600	-0.41605600
C	-0.23709400	2.34145600	0.66236100
C	-0.33487700	1.26636900	-1.51189400
C	1.15065800	2.26733600	0.63780000
C	1.80500600	1.66963800	-0.44861700
C	1.05327100	1.16453700	-1.51864900
C	3.30215000	1.54101600	-0.44300200
O	3.84109200	0.73218400	-1.28708600
O	3.98597000	2.14876000	0.42665300
H	-0.75071500	2.77805900	1.51212800
H	-0.91062900	0.86904400	-2.33919100
H	1.73580200	2.65482100	1.46468500
H	1.55897700	0.68585000	-2.34968900
H	-4.05448500	1.52688800	-1.28546100
C	5.33333300	0.53725600	1.39082300
C	4.97573500	-0.62592400	0.70910500
C	0.74057400	-2.18843500	-0.62170700
O	1.05295500	-2.40760000	-1.78488100
C	-0.65103800	-1.88610000	-0.18186100
C	-1.66994000	-1.93989200	-1.14256500
C	-0.93773900	-1.45586600	1.12163300
C	-2.95830700	-1.53359300	-0.81756500
C	-3.23886500	-1.07691200	0.47832200
C	-2.22890900	-1.05884600	1.44980400
C	-4.57314700	-0.53239900	0.84548600
O	-4.93721300	-0.31033500	1.99019100
O	-5.35371800	-0.27588300	-0.22748900
H	6.25988100	1.05155500	1.15498600
H	4.76157400	0.91514600	2.23082200
H	5.80238200	-1.19362000	0.26916900
H	-1.43696600	-2.27063400	-2.14852300
H	-0.15005700	-1.40258700	1.86350200
H	-3.73812500	-1.54996200	-1.56969200
H	-2.45440600	-0.69622000	2.44655900
H	-6.20511500	0.07555300	0.10092600
O	1.62016900	-2.15006600	0.38913700
C	3.03390000	-2.13527700	0.04667800
H	3.14691400	-1.61789400	-0.90691200
H	3.37558500	-3.16725300	-0.06865500
C	3.74363400	-1.39210500	1.17932500
H	3.03535400	-0.66314700	1.58993000
H	4.00507700	-2.08098900	1.98929100
H	4.64321700	-0.01747900	-0.32813800

TS-8

O	2.57756100	-1.87656600	-0.07592000
C	1.95053400	-1.10777200	0.62136600
O	2.80382100	0.27984500	1.12250700
O	2.11386600	-1.46933100	2.30239400
H	2.68339200	-0.38847800	2.11645100
H	1.27195500	-1.29530300	2.76496100
C	0.54225700	-0.65685500	0.37187100
C	-0.07326900	0.36583600	1.10616400
C	-0.16054200	-1.30391500	-0.65168600
C	-1.38057300	0.74080200	0.81491900
H	0.47002200	0.87371100	1.89503800
C	-1.46848200	-0.93092700	-0.94107700
H	0.32359700	-2.09306400	-1.21633200
H	-1.85051200	1.53525500	1.38266100
H	-2.01719100	-1.42857000	-1.73325700
C	-2.08531400	0.09424700	-0.21192000
C	-3.48205200	0.46368700	-0.56308200
O	-4.13978200	-0.08421600	-1.43697700
O	-3.97084700	1.47877000	0.18105100
H	-4.88626300	1.65074900	-0.11607500
C	6.29853900	1.59265100	0.78269700
H	6.92502400	0.72860400	1.00914400
C	6.81743300	2.62194400	0.11063600
H	6.22285400	3.50013600	-0.13662000
H	7.85599400	2.62762000	-0.21215500
C	4.14119800	0.34329700	0.59079700
H	4.06329300	0.49315200	-0.49056600
H	4.66064000	-0.60417200	0.77256200
C	4.87314400	1.50779900	1.25667000
H	4.33880500	2.44125500	1.04629000
H	4.84894500	1.34734700	2.34379400

TS-5

O	3.46009000	-2.00100900	1.43936100
C	3.90208400	-1.47307700	0.44152300

O	2.76887600	-0.64221100	-0.50824600
C	1.44007100	-0.60128100	0.05249000
H	1.19474400	-1.57185400	0.49655300
H	1.44234600	0.15303800	0.84631300
O	3.85218700	-2.53377700	-0.93555800
H	3.03076000	-1.61897800	-1.14194100
H	4.62416500	-2.35979400	-1.50682800
C	5.17248800	-0.68160500	0.36365800
C	5.54044300	0.05302000	-0.77116000
C	6.00641900	-0.69883600	1.48814300
C	6.73184800	0.77046000	-0.77890200
H	4.89369000	0.07158100	-1.64108200
C	7.20033600	0.01451900	1.47880400
H	5.71339100	-1.26975000	2.36238700
H	7.01017300	1.34110800	-1.65719800
H	7.85142000	0.00630300	2.34621500
O	-3.27630500	0.47120100	-1.15141900
C	-4.05387400	-0.58610100	-0.86709800
O	-3.69327500	-1.74865500	-0.99654900
C	7.56852800	0.75455200	0.34738800
C	8.85150500	1.50536700	0.38554500
O	9.63972400	1.47407100	1.32035300
O	9.07336800	2.24086700	-0.72474900
H	9.93382200	2.69233500	-0.61734200
C	-5.40823800	-0.18955000	-0.38361800
C	-6.30021000	-1.20632200	-0.01347700
C	-5.80524100	1.15295700	-0.30088300
C	-7.57593200	-0.88532000	0.43227100
H	-5.98575400	-2.24194600	-0.07951500
C	-7.08342600	1.47477400	0.14486300
H	-5.11980300	1.94199100	-0.58655300
C	-7.97493900	0.45665000	0.51282800
H	-8.27027000	-1.66711200	0.71997200
H	-7.38722500	2.51326700	0.20467300
C	-9.35310700	0.75156000	0.99014200
O	-10.17062100	-0.10409700	1.29884800
O	-9.62646700	2.07172000	1.05338400
H	-10.54577800	2.17193600	1.37108600
C	0.46177400	-0.24123700	-1.05564100
H	0.77463600	0.70225500	-1.51944200
H	0.50728700	-1.01628800	-1.83177300
C	-0.97000700	-0.11349300	-0.52302900
H	-1.27689200	-1.04422200	-0.03297700
H	-1.02361700	0.68697700	0.22479900
C	-1.93764800	0.20390100	-1.65448200
H	-1.66020600	1.12746800	-2.16669400
H	-1.98907800	-0.60923100	-2.38333700

TS-6

O	3.37868300	-1.45151500	2.10374200
C	3.81995500	-1.43065400	0.82608400
O	2.73932000	-1.26635100	-0.17376600
C	1.41154500	-0.83930700	0.29323800
H	1.01604100	-1.61093500	0.95611200
H	1.56168600	0.08760600	0.85090400
H	3.44960100	-0.56050800	2.49536800
O	3.98696500	-2.84614400	0.43434900
H	3.06498600	-2.49355500	-0.30524900
H	4.83011400	-2.98094100	-0.05001300
C	5.01361000	-0.56991900	0.51791000
C	5.13964100	0.07454200	-0.71687600
C	6.02694100	-0.47190400	1.48057900
C	6.27975500	0.82671900	-0.98652300
H	4.35225600	-0.00506500	-1.45637600
C	7.16446300	0.27799200	1.20642600
H	5.92359300	-0.98005500	2.43342400
H	6.37551400	1.33128600	-1.94056400
H	7.95544800	0.36128200	1.94318500
O	-3.11638400	0.29943600	-1.33965400
C	-3.93280500	-0.72336700	-1.03138200
O	-3.61120900	-1.90014200	-1.12834600
C	7.29593800	0.93046300	-0.02677200
C	8.53596400	1.71741900	-0.27521700
O	9.45126900	1.82497200	0.52804100
O	8.55773600	2.30849600	-1.48693900
H	9.40223000	2.79444700	-1.56820900
C	-5.27152300	-0.27116200	-0.55512000
C	-6.23682600	-1.25028200	-0.27906900
C	-5.57608600	1.08450400	-0.36619200
C	-7.49324100	-0.87874200	0.18167000
H	-5.99291000	-2.29642200	-0.42728500
C	-6.83456700	1.45685200	0.09652600
H	-4.83174000	1.84371700	-0.57520000
C	-7.79872100	0.47652500	0.37270700
H	-8.24402300	-1.63103100	0.39734300
H	-7.06504500	2.50530700	0.24466900
C	-9.15590400	0.82507700	0.87426300
O	-10.01317800	0.00175900	1.16211100

O	-9.36008700	2.15436300	0.98455300
H	-10.26820600	2.29114200	1.32031400
C	0.54884700	-0.63727700	-0.93630800
H	0.98330700	0.15357800	-1.55887700
H	0.54275900	-1.56099000	-1.52743200
C	-0.88294600	-0.27347900	-0.52401800
H	-1.31476700	-1.08407600	0.07369900
H	-0.88295700	0.63088900	0.09605000
C	-1.76051600	-0.03582800	-1.74518600
H	-1.42704600	0.83137500	-2.31806200
H	-1.79027600	-0.91065700	-2.39940500

MPET

O	8.83908700	0.60967100	0.76967500
C	8.13886300	0.29951900	-0.34120100
O	8.65435100	0.23721200	-1.44831700
C	6.69495400	0.05307900	-0.07715100
C	5.85308800	-0.17477000	-1.17476900
C	6.16894800	0.04562800	1.22320700
C	4.49580400	-0.40395800	-0.98042400
C	3.96961400	-0.40938900	0.32009100
C	4.81209700	-0.18534100	1.41808900
C	2.52283200	-0.63729800	0.58928200
O	2.01838200	-0.58687100	1.70108400
O	1.82283700	-0.91057500	-0.53231200
C	0.40253100	-1.12932400	-0.38476900
C	-0.30665100	0.21472600	-0.34507600
O	-1.71550300	-0.09374700	-0.26891900
C	-2.54730200	0.96075800	-0.18590800
O	-2.15286700	2.11775300	-0.17351400
C	-3.98112300	0.56439900	-0.11470800
C	-4.93968900	1.58295600	-0.02040900
C	-4.38542100	-0.77854300	-0.14258800
C	-6.29219700	1.26779000	0.04266800
C	-6.69692800	-0.07491600	0.01297400
C	-5.73777900	-1.09335300	-0.07854200
C	-8.13141700	-0.46735500	0.07226600
O	-8.52689800	-1.62446100	0.06801900
O	-8.97245000	0.58632700	0.12899600
H	6.26927600	-0.16550400	-2.17619400
H	6.81587900	0.21732600	2.07542700
H	3.84782500	-0.57291100	-1.83217800
H	4.39605500	-0.19404200	2.41948700
H	0.10685000	-1.70213800	-1.26440200
H	0.20198800	-1.70805700	0.51912100
H	-0.01040400	0.79657900	0.53079700
H	-0.10351000	0.79468900	-1.24932400
H	-4.61631400	2.61775700	0.00162900
H	-3.64835300	-1.56943100	-0.21561600
H	-7.02843200	2.05968900	0.11485300
H	-6.06111800	-2.12817200	-0.10074300
H	9.76987200	0.75434400	0.50721800
H	-9.88538500	0.23765500	0.15881500

TS-3

O	0.62534200	-3.71786600	0.82064000
C	1.24790800	-3.15477000	-0.23697800
O	1.47563900	-3.77347200	-1.26692400
C	1.58709600	-1.72341800	-0.02487800
C	2.17404300	-1.01613600	-1.08455000
C	1.26799100	-1.05817300	1.16772900
C	2.40734100	0.34893100	-0.96705600
C	2.05125600	1.02373900	0.20940800
C	1.49787700	0.30828200	1.28058000
C	2.14451500	2.51614200	0.27517100
O	1.63605700	3.11159900	1.30315800
O	2.57218300	3.17840400	-0.71258700
C	0.85961300	4.46677200	-1.30086800
C	-0.07574400	4.20013800	-0.30795700
O	-0.80125300	3.00369700	-0.55691700
C	-1.35887300	2.37920700	0.51105100
O	-1.51552700	2.92712100	1.58861600
C	-1.68536900	0.95830100	0.22229900
C	-2.23728100	0.18708700	1.25532100
C	-1.34679900	0.35682800	-0.99912800
C	-2.42465200	-1.17947300	1.08278900
C	-2.05811400	-1.78576500	-0.12797800
C	-1.53278400	-1.00933900	-1.16960700
C	-2.15312200	-3.25627800	-0.33597200
O	-1.79871700	-3.82718600	-1.35794200
O	-2.65964300	-3.91657600	0.72461100
H	2.41483100	-1.53863900	-2.00399300
H	0.80713100	-1.59746400	1.98657800
H	2.83376800	0.90552100	-1.79437800
H	1.21147800	0.83444100	2.18382900
H	1.40649600	5.40188900	-1.26519000
H	0.95140300	3.84796000	-2.18454400
H	0.74481900	3.91732400	0.63274800

H	-0.63106600	5.01754800	0.15633000
H	-2.48836400	0.66019600	2.19822000
H	-0.90838700	0.94571600	-1.79506900
H	-2.83259200	-1.77572300	1.89050600
H	-1.24362800	-1.48932900	-2.09762300
H	0.39097900	-4.63518100	0.57665600
H	-2.67038000	-4.86936200	0.50497100

TS-4

O	2.55355500	-1.19988200	-0.35589200
C	1.82446000	-0.45771200	0.22597000
O	2.37125900	1.47194600	-0.07935000
O	2.44253900	-0.03400000	1.72788200
H	2.66458500	0.89697500	1.32058800
H	1.74906400	0.07572700	2.41145100
C	0.35427200	-0.33017700	0.18967800
C	-0.34426600	0.69302700	0.84542600
C	-0.33708200	-1.28968300	-0.56477400
C	-1.72976900	0.74767400	0.75741300
H	0.19248400	1.45294500	1.40200300
C	-1.72280400	-1.22915900	-0.65266700
H	0.21330700	-2.07530900	-1.07049300
H	-2.26792900	1.54016800	1.26348600
H	-2.26689100	-1.96835700	-1.23010300
C	-2.42618900	-0.21417600	0.00910500
C	-3.90946000	-0.19285500	-0.11448500
O	-4.55392700	-0.99449000	-0.77562600
O	-4.48774100	0.80754800	0.58164100
H	-5.45374100	0.74838000	0.44333800
C	3.33529000	1.55186100	-1.00596300
H	3.02884700	2.03313000	-1.94280100
C	4.58645400	1.07179000	-0.88451900
H	4.92220300	0.58552900	0.02789700
H	5.29739800	1.17689200	-1.69880300

TS-1

O	-2.04335000	1.38864100	1.71349800
C	-2.62874900	1.28499300	0.66259800
O	-1.59182900	0.74983400	-0.69715100
C	-0.25173100	0.53843800	-0.26140200
H	0.19465500	1.46318100	0.12069800
H	-0.24544700	-0.20602400	0.54259500
O	-2.57305100	2.70596300	-0.25499300
H	-1.90578600	1.96311300	-0.87467400
H	-3.41436400	2.84275300	-0.73392700
C	-3.92821500	0.58221300	0.43293300
C	-4.48299200	0.40098800	-0.84092500
C	-4.58898300	0.08726400	1.56407000
C	-5.69272100	-0.26966300	-0.98254400
H	-3.96595500	0.77386200	-1.71820200
C	-5.79852500	-0.58391100	1.42166100
H	-4.15137300	0.23092200	2.54591800
H	-6.11734900	-0.40907400	-1.96985400
H	-6.31698400	-0.96965100	2.29259600
C	0.53850900	0.02156600	-1.45759200
H	0.11554800	-0.91364900	-1.82615700
H	0.56481600	0.75761900	-2.26401600
O	1.88899300	-0.30998600	-1.05163200
C	2.77461300	0.70204900	-0.97104000
O	2.50237200	1.86143700	-1.24835400
C	-6.35698400	-0.76571700	0.14974300
C	-7.65278400	-1.48932800	0.04994600
O	-8.26254600	-1.94109600	1.00909000
O	-8.10523300	-1.60414300	-1.21642400
H	-8.95529400	-2.08653800	-1.18742600
C	4.11979900	0.25165500	-0.51446900
C	5.14568900	1.20561500	-0.44979100
C	4.37538400	-1.07760300	-0.14781200
C	6.41464000	0.83411700	-0.02484200
H	4.94001100	2.23145700	-0.73470600
C	5.64596300	-1.44895100	0.28109300
H	3.58426200	-1.81647300	-0.19420200
C	6.67127100	-0.49420600	0.34414900
H	7.21364200	1.56554700	0.02585600
H	5.83882600	-2.47658800	0.56609500
C	8.04528700	-0.84208800	0.79829600
O	8.96904700	-0.04353500	0.86492300
O	8.18409200	-2.14072700	1.13808900
H	9.11006200	-2.27664000	1.42148700

TS-2

O	-2.12190100	1.94350800	1.41847700
C	-2.64166100	1.56387900	0.23321600
O	-1.60899500	1.09865100	-0.73782500
C	-0.28198600	0.76527400	-0.23539500
H	0.21341500	1.67096800	0.11438300
H	-0.40551800	0.05560800	0.58386000
H	-2.17768800	1.21042900	2.06050800

O	-2.82337400	2.80263700	-0.54554400
H	-1.92760600	2.24056800	-1.18959200
H	-3.67923700	2.79611300	-1.02739200
C	-3.84335200	0.66123500	0.25092500
C	-4.01540100	-0.33068200	-0.72001200
C	-4.81948100	0.87675600	1.23302000
C	-5.16366100	-1.11758400	-0.70185800
H	-3.25792600	-0.49113100	-1.47730300
C	-5.96738600	0.09324300	1.24280200
H	-4.67942300	1.65196700	1.97888200
H	-5.29499500	-1.89110800	-1.44900800
H	-6.73078600	0.25073200	1.99644700
C	0.45074500	0.13155600	-1.40826000
H	-0.03771200	-0.79141200	-1.72110600
H	0.51620000	0.82263900	-2.25121000
O	1.76983200	-0.25623700	-0.97411900
C	2.72326200	0.70294200	-0.97050400
O	2.51347300	1.85668300	-1.31212000
C	-6.14406800	-0.90687500	0.27706800
C	-7.39353800	-1.71654500	0.32530900
O	-8.29805700	-1.53254300	1.12673700
O	-7.43566200	-2.68573000	-0.61116800
H	-8.28580500	-3.15902300	-0.51525700
C	4.04311500	0.19341300	-0.50838300
C	5.12425900	1.08688400	-0.49728700
C	4.22460400	-1.13238400	-0.08834000
C	6.37528300	0.65848000	-0.07293400
H	4.97461000	2.11043500	-0.82257000
C	5.47810600	-1.56070900	0.33745700
H	3.39137500	-1.82493000	-0.09241000
C	6.55885000	-0.66712700	0.34578200
H	7.21658300	1.34265400	-0.06247500
H	5.61500300	-2.58548300	0.66219300
C	7.91872000	-1.07835400	0.79001100
O	8.88238900	-0.32684800	0.83014000
O	7.99446400	-2.37622000	1.15024100
H	8.91590700	-2.55644000	1.42361100

MPET-C-C-frag

C	-5.25456600	0.95077900	0.34753500
O	-3.93296000	0.86771300	0.00716300
C	-3.05531000	0.26070200	0.86223300
O	-3.40284000	-0.21120500	1.93321200
C	-1.67263100	0.25394700	0.33091700
C	-0.67118800	-0.32876400	1.12286900
C	-1.34483700	0.80390800	-0.91928300
C	0.64381300	-0.36358600	0.67485600
C	0.97059800	0.18565900	-0.57418100
C	-0.02994000	0.76776100	-1.36572400
C	2.36197400	0.17465200	-1.10077400
O	2.69030600	0.64566100	-2.18075100
O	3.24543900	-0.41081800	-0.26573500
H	-5.84583500	1.50998800	-0.36215900
H	-5.57131700	0.63275900	1.33037100
H	-0.93258400	-0.75075200	2.08693100
H	-2.11285500	1.25522500	-1.53602000
H	1.41274800	-0.81466400	1.29116400
H	0.23201500	1.18938800	-2.32981700
H	4.12646000	-0.37303400	-0.68792800

MPET-C-H-frag

O	-7.11857700	0.82368400	-2.55630600
C	-6.14171400	-0.10038300	-2.44596600
O	-6.04001500	-1.04621000	-3.21430400
C	-5.21799200	0.15426100	-1.30671900
C	-4.14648200	-0.72930900	-1.11342500
C	-5.39551700	1.24061800	-0.43686400
C	-3.25737000	-0.53432300	-0.06356900
C	-3.43585800	0.55257300	0.80739700
C	-4.50801400	1.43704300	0.61407600
C	-2.52503500	0.81454500	1.94522300
O	-2.62098700	1.74386900	2.72789700
O	-1.53066000	-0.12422500	2.03537500
C	-0.60940000	-0.03094800	3.04394500
C	0.49819700	-0.99183700	2.96428800
O	1.44164500	-0.52796300	1.92836200
C	2.52445000	-1.29706700	1.73355500
O	2.74018200	-2.32536500	2.36131100
C	3.42929500	-0.75955800	0.67592900
C	4.59509100	-1.47786400	0.37656400
C	3.14427900	0.43054500	-0.01005400
C	5.47229600	-1.01440900	-0.59764200
C	5.18821900	0.17646300	-1.28253000
C	4.02113900	0.89370300	-0.98402400
C	6.09503300	0.71742400	-2.33145100
O	5.88337100	1.74540900	-2.95935400
O	7.19329300	-0.04046400	-2.53069200
H	-4.01685600	-1.56594400	-1.79094600

H	-6.22228800	1.92639500	-0.57950100
H	-2.43080500	-1.22013500	0.07880000
H	-4.63846000	2.27350300	1.29164100
H	-0.63221900	0.84708100	3.67459300
H	1.02918000	-1.04555400	3.91695500
H	0.15477300	-1.99012000	2.67854900
H	4.80686000	-2.39672200	0.91202500
H	2.24431700	0.98943800	0.21772300
H	6.37218600	-1.57412400	-0.82424500
H	3.80934900	1.81287800	-1.51898300
H	-7.67651800	0.58092400	-3.32159900
H	7.72718500	0.38616600	-3.22997100

MPET-C-O-frag1-a

C	-4.70779500	-1.70048400	0.78226200
C	-4.07897000	-0.36311200	0.79239900
O	-2.64105700	-0.53823300	0.60923200
C	-1.91184500	0.58397500	0.51380900
O	-2.39358600	1.70721500	0.58362800
C	-0.45812300	0.31399000	0.31695300
C	0.40755100	1.41101000	0.20723200
C	0.05181900	-0.99058600	0.24094700
C	1.77126000	1.21106700	0.02351100
C	2.28113300	-0.09348900	-0.05222400
C	1.41497600	-1.19057200	0.05699200
C	3.73155600	-0.36343700	-0.24731400
O	4.21600400	-1.48361100	-0.32574000
O	4.47877800	0.75712000	-0.33084700
H	-5.62896900	-1.86351700	1.33006200
H	-4.36005300	-2.45924700	0.08869900
H	-4.44032100	0.28040300	-0.02501000
H	-4.25341900	0.17406800	1.73098200
H	0.00457800	2.41602600	0.26664300
H	-0.61364000	-1.84156000	0.32553600
H	2.43569000	2.06307600	-0.06078100
H	1.81773800	-2.19567100	-0.00258400
H	5.40933300	0.48490400	-0.45764400

MPET-C-O-frag1-b

O	-1.78790700	0.37161800	0.00024900
C	-0.42794500	0.61062700	0.00026700
C	0.40232200	-0.66548800	0.00009000
O	1.78611600	-0.24664000	0.00014100
C	2.70571400	-1.22735400	-0.00002300
O	2.41291700	-2.41458200	-0.00020000
C	4.10333400	-0.71132700	-0.00002300
C	5.14844000	-1.64554400	-0.00020900
C	4.39064200	0.66187000	0.00015400
C	6.47064500	-1.21625400	-0.00021600
C	6.75827900	0.15674500	-0.00003900
C	5.71289200	1.09095000	0.00014500
C	8.15622500	0.66756300	-0.00003800
O	8.45444000	1.85347100	0.00009800
O	9.08257200	-0.31348600	-0.00018600
H	-0.19021700	1.24986200	-0.87257200
H	-0.19021400	1.24961500	0.87328800
H	0.19967000	-1.26602200	0.89125000
H	0.19966400	-1.26578600	-0.89122900
H	4.91628100	-2.70476700	-0.00034600
H	3.58614100	1.38777900	0.00029800
H	7.27427100	-1.94322200	-0.00036000
H	5.94508100	2.15023800	0.00028100
H	9.96391700	0.10950400	-0.00015800

MPET-C-O-frag2-a

O	-9.08608900	0.33046700	0.00037700
C	-8.16898100	-0.65637800	0.00059300
O	-8.47126300	-1.84039300	0.00015400
C	-6.76462300	-0.15483000	0.00025100
C	-5.73023600	-1.10223500	-0.00011300
C	-6.47134600	1.21743700	0.00028100
C	-4.40570700	-0.68424800	-0.00043300
C	-4.11881100	0.68779900	-0.00039200
C	-5.14674800	1.63983700	-0.00003600
C	-2.72225600	1.13290800	-0.00073000
O	-2.33915800	2.34482100	-0.00100900
O	-1.70983100	0.36442500	-0.00127500
H	-5.97484000	-2.15838100	-0.00014000
H	-7.27228000	1.94700900	0.00055300
H	-3.59732900	-1.40850600	-0.00071700
H	-4.90613700	2.69817500	-0.00001000
H	-9.97193100	-0.08335800	0.00020000

MPET-C-O-frag2-b

O	-9.08982500	0.31162000	0.00062400
C	-8.16069100	-0.66531000	0.00029900
O	-8.45113000	-1.85246700	0.00029900
C	-6.76215700	-0.14841800	0.00003400

C	-5.71760500	-1.08332400	-0.00027800
C	-6.48456200	1.22902100	0.00009100
C	-4.39701400	-0.64744900	-0.00053500
C	-4.12116500	0.72658400	-0.00047900
C	-5.16671900	1.66771300	-0.00016600
C	-2.71555300	1.17111400	-0.00075500
O	-2.28072400	2.28957000	-0.00075900
H	-5.94927900	-2.14254300	-0.00031800
H	-7.29506600	1.94831600	0.00033300
H	-3.57743300	-1.35884100	-0.00077900
H	-4.93362500	2.72756100	-0.00012700
H	-9.97075700	-0.11258200	0.00081000

OH·

O	-0.12600000	-0.08071100	0.00000000
H	0.85732000	-0.08071100	0.00000000

TPA-IM1-a

O	-3.45465500	-1.14364500	0.00003300
C	-2.88780600	0.07936000	0.00004800
O	-3.54308500	1.11119700	0.00006700
C	-1.39753600	0.03917200	0.00003900
C	-0.70976000	1.26392200	0.00009000
C	-0.69172600	-1.17243600	-0.00002200
C	0.67746700	1.28127000	0.00008400
C	1.38428500	0.06424400	0.00002100
C	0.70018200	-1.15845400	-0.00003400
C	2.85871200	0.05630300	0.00001100
O	3.61469900	0.98801100	0.00008700
H	-1.27322000	2.19056800	0.00013800
H	-1.22527600	-2.11550600	-0.00006000
H	1.22416800	2.21873900	0.00012600
H	1.26222600	-2.08693300	-0.00008300
H	-4.42526400	-1.02484900	0.00003900

TPA-IM1-b

O	-3.46802000	-1.12686100	-0.00028100
C	-2.89030000	0.09033300	0.00060600
O	-3.53474200	1.12854400	-0.00018600
C	-1.40016000	0.03432800	0.00039400
C	-0.69864400	1.24900500	0.00031700
C	-0.70775900	-1.18621300	0.00027000
C	0.69026100	1.24874700	0.00014500
C	1.37648900	0.02650300	0.00003700
C	0.68254600	-1.19064000	0.00009800
C	2.84231200	0.02203400	-0.00015100
O	3.57215400	-1.01851300	-0.00037400
O	3.57670600	1.05942500	-0.00045800
H	-1.24959400	2.18267000	0.00040100
H	-1.25217400	-2.12289300	0.00031500
H	1.24338300	2.18260100	0.00009300
H	1.23034200	-2.12760100	0.00000400
H	-4.43731100	-0.99863200	-0.00086200

TPA-IM1-c

H	-2.26198800	-0.00615600	-0.84699800
C	-1.19536000	0.00445800	-0.64115600
C	-0.52509000	1.22296700	-0.49315500
C	-0.49572200	-1.20021100	-0.52478400
C	0.84222400	1.23653000	-0.22928700
H	-1.06823800	2.15892800	-0.58348500
C	0.87300600	-1.19205900	-0.26072700
H	-1.01699600	-2.14584300	-0.63985500
C	1.54827900	0.02962900	-0.11171200
H	1.37279200	2.17560300	-0.11252700
H	1.41428500	-2.12714600	-0.17074300
C	3.00331000	0.09416600	0.16985500
O	3.63852700	1.13213100	0.30830600
O	3.58933900	-1.12126200	0.26414500
H	4.53809600	-0.97763400	0.44929600

TPA/1

O	-3.43993700	-1.32347000	1.17701100
C	-2.75890800	-1.96650000	0.20607200
O	-3.31716400	-2.59041900	-0.68519100
C	-1.28184000	-1.83607600	0.33551100
C	-0.47710200	-2.46666700	-0.62439400
C	-0.68982800	-1.10917100	1.37843100
C	0.90602300	-2.37168000	-0.54284100
C	1.49948600	-1.64504800	0.49950100
C	0.69607900	-1.01397300	1.46013500
C	2.98543100	-1.57179500	0.54466500
O	3.45418600	-0.85056000	1.58395300
O	3.72386700	-2.10592300	-0.27062700
H	-0.94408500	-3.02660400	-1.42709600
H	-1.30811700	-0.62057000	2.12226700
H	1.53559800	-2.85629000	-1.28089200
H	1.15075600	-0.45164400	2.26720500

H	4.43054200	-0.85613700	1.53397500
H	-4.39379000	-1.46244100	1.01375500

TPA-IM2

O	3.14779500	0.95766800	0.00011300
C	2.45752400	-0.20438300	-0.00037700
O	3.01693300	-1.29333400	0.00007100
C	0.98526800	-0.01652900	-0.00019000
C	0.17720400	-1.16532900	-0.00001400
C	0.40565100	1.26352600	-0.00018400
C	-1.21748700	-1.04721000	0.00014500
C	-1.72410900	0.23555300	0.00012600
C	-0.98854300	1.40162600	-0.00003000
H	0.64314600	-2.14562300	-0.00001100
H	1.03343000	2.14813500	-0.00030800
H	-1.85099900	-1.92945700	0.00027400
H	-1.44853700	2.38554300	-0.00003400
H	4.09957900	0.73600000	0.00040500

TPA-TS-c

H	-1.95151600	-0.00793900	-1.26723600
O	-3.52390500	-0.02805800	-1.06926000
C	-2.99460000	-0.01666400	0.10974200
O	-3.54254500	-0.01877400	1.20654300
C	-1.45244400	0.00186300	-0.11975500
C	-0.73677100	1.24417700	-0.06375800
C	-0.70921500	-1.22321700	-0.06051000
C	0.64436000	1.24884100	-0.05156700
H	-1.29513200	2.17474900	-0.07937800
C	0.67320300	-1.20142500	-0.04789100
H	-1.24752200	-2.16560900	-0.07325000
C	1.34758700	0.03213100	-0.03937600
H	1.19588400	2.18185100	-0.04081900
H	1.23262800	-2.12878400	-0.03376100
C	2.84545900	0.10138500	-0.01886400
O	3.46886800	1.14961500	-0.01626900
O	3.42582700	-1.10873000	-0.00173200
H	4.39579700	-0.98228000	0.01442100

TPA-TS-b

O	-3.63403300	1.12940200	-0.15377000
C	-3.34993900	-0.02192000	0.00215500
O	-3.60675600	-1.17943000	0.15920500
C	-1.31956900	0.00295000	-0.00100500
C	-0.72252000	1.24399400	0.01943000
C	-0.69378000	-1.22326200	-0.02204700
C	0.67614800	1.24250400	0.02016200
H	-1.29119500	2.16582100	0.03088500
C	0.70599000	-1.19346800	-0.02334300
H	-1.24165300	-2.15758500	-0.03323100
C	1.38667700	0.03336500	-0.00138500
H	1.21554000	2.18380900	0.03514800
H	1.25478200	-2.12848400	-0.03851000
C	2.87302400	0.10183300	-0.00168400
O	3.51279500	1.14375600	-0.01174700
O	3.46312100	-1.11129200	0.01099800
H	4.43074800	-0.97205400	0.00844200

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