

Poly(ester-co-ether) from Ring-opening Copolymerisation of Sustainable 2-Methyltetrahydrofuran with β -Butyrolactone

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General information

Materials

β -Butyrolactone (BBL) was purchased from Tokyo Chemical Industry (Shanghai) Development Co., Ltd. 2-Methyltetrahydrofuran (2-MeTHF) and benzyl alcohol were purchased from J&K Scientific Co., Ltd. BBL and 2-MeTHF were stirred over CaH_2 and distilled prior to use. Benzyl alcohol was dried with activated molecular sieve. $\text{RE}(\text{OTf})_3$ was synthesized according to the literature¹ and dried in vacuum (<0.5 mmHg) at 200 °C for 24 h.

Measurements

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance DMX 500 spectrometer in CDCl_3 with tetramethylsilane (TMS) as an internal reference. Correlation spectroscopy (COSY) and heteronuclear single-quantum coherence (HSQC) technique were used to assist in the assignment of ^1H and ^{13}C NMR spectra. The number-average molecular weights (M_n s) and the dispersities (D s) of the polymers were determined by a size-exclusion chromatography (SEC) equipped with Waters 1525 isocratic HPLC pump, Waters 2414 refractive index detector and Waters Styragel HR3 and HR4 columns. THF was used as eluent with a flow rate of 0.8 mL/min at 40 °C. Commercial polystyrene (PS) samples with narrow dispersities were used as the calibration standard. Matrix-assisted laser desorption ionization-time of flight mass spectrum (MALDI-ToF MS) was recorded on a Bruker Ultra-FLEX MALDI-ToF mass spectrometer in reflector mode. 2,5-Dihydroxybenzoic acid (DHB) and CF_3COOK were used as the matrices and the cationic agent, respectively. Differential scanning calorimetry (DSC) analyses were performed on a TA Q200 instrument. Samples were heated from -80 to 30 °C at a rate of 10 °C/min under a nitrogen purge, held for 3 min to erase the thermal history, cooled to -80°C at a rate of 10 °C/min, and finally subjected to a second scan.

Typical procedure for copolymerisation of 2-MeTHF with BBL

All the polymerisations were carried out in a flame-dried ampule using standard Schlenk techniques under argon atmosphere. A representative procedure is given below. $\text{Sc}(\text{OTf})_3$ (0.0246 g, 0.05 mmol) was dissolved in 2-MeTHF(0.431 g, 5 mmol) in a 10 mL ampule. Then,

BBL (0.430 g, 5 mmol) was added to the solution and the mixture was stirred at 50 °C for 3 h. The ampule was exposed to air to terminate the polymerisation. In order to calculate the monomer conversions, a small portion of the mixture was dissolved in CDCl₃ and subjected to ¹H NMR analysis. The rest copolymer was precipitated and isolated from *n*-hexane and dried in a vacuum at 35 °C (0.501 g, yield 58.2%). The obtained polymers were then analysed by SEC.

Kinetic study of the copolymerisation of 2-MeTHF with BBL

Sc(OTf)₃ (0.0492 g, 0.1 mmol), 2-MeTHF (0.861 g, 10.0 mmol) were mixed in a 10 mL ampule containing a stir bar under argon at -10 °C. After the catalyst was dissolved completely, the polymerisation was started by rapid addition of BBL (0.860 g, 10.0 mmol) to the ampule under vigorous stirring. After the prescribed time, samples (0.1 mL) were taken out and transferred into NMR tubes, and quickly quenched by adding CDCl₃. Then each sample was characterized by ¹H NMR to calculate the monomer conversions.

DFT calculation

All geometries of intermediates were optimized using PBE0/6-31+G(d,p). Frequency calculations were carried out to make sure that all intermediates and transition states (TSs) had zero and one imaginary frequencies, respectively. The reaction pathways of all included transition states were confirmed by intrinsic reaction coordinate (IRC). All calculations were performed using Gaussian 16 program as we reported before²⁻⁷.

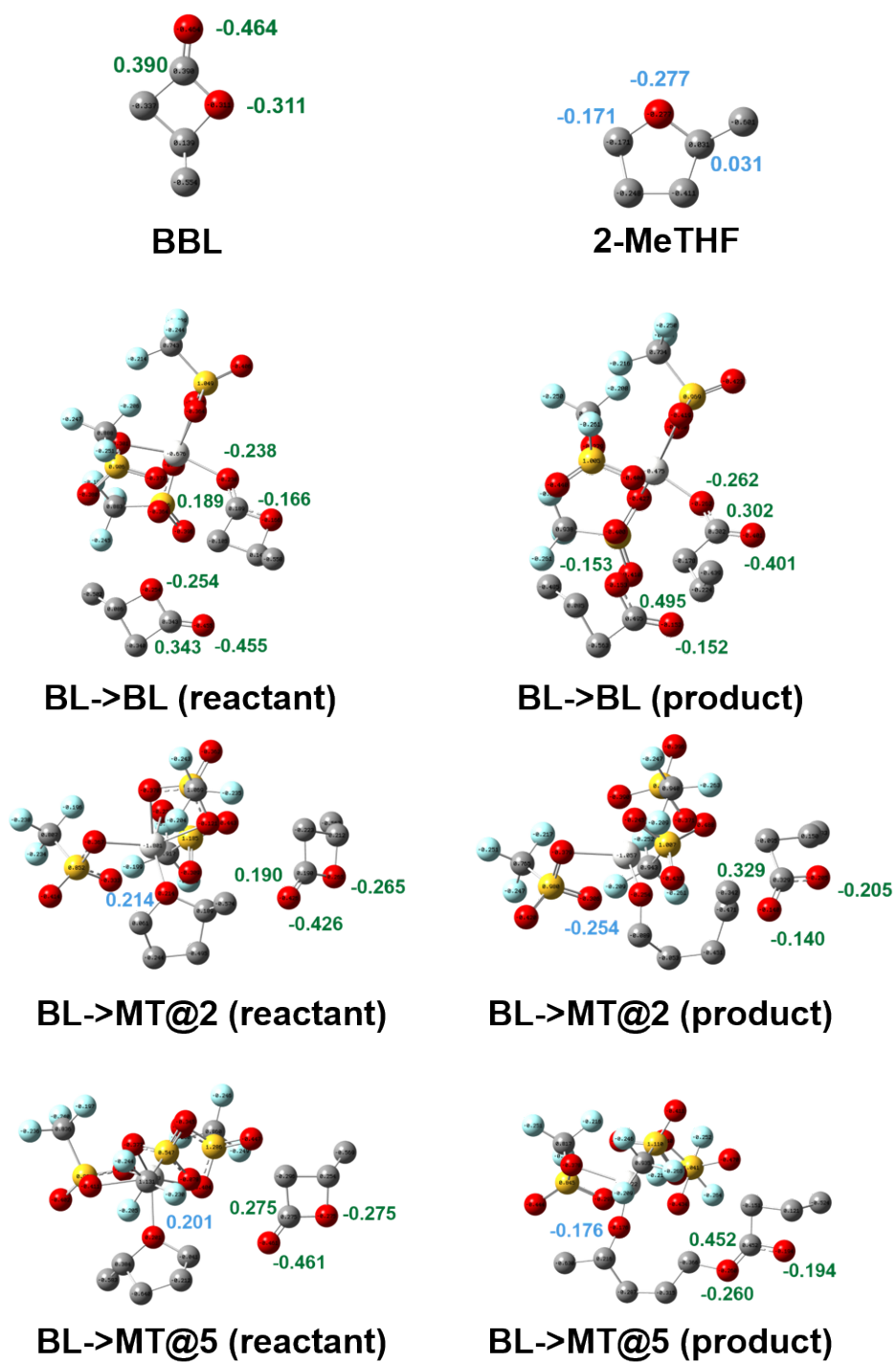


Figure S1. DFT calculated Mulliken charge distribution of the reactants and products in the ROP of 2-MeTHF and BBL.

Characterization of poly(2-MeTHF-co-BBL)

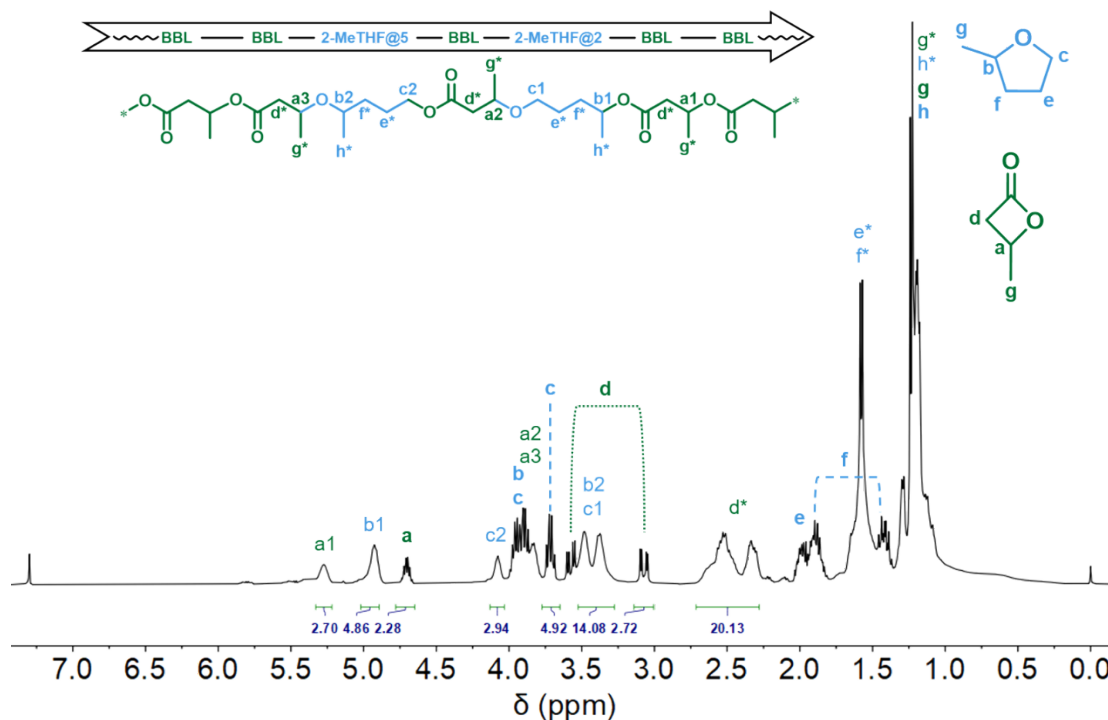


Figure S2. ^1H NMR spectrum the polymerisation solution.

calculation of monomer conversions

Signal at 4.70 ppm (H_a) is attributed to the methine proton of BBL monomer. Signals of methylene protons of 2-MeTHF monomer (H_c) is divided into two parts, one of which is assigned at 3.72 ppm (H_c at 3.72). Signals of methylene protons (H_d) of BBL monomer is divided into two parts, one of which is assigned at 3.07 ppm (H_d at 3.07).

$$\text{Conv.}(2 - \text{MeTHF}) = \frac{I_{b1+c1+b2+c2}}{I_{b1+c1+b2+c2} + 3I_{c \text{ at } 3.72}} \#(\text{Eq.S}) \quad 1.$$

$$\text{Conv.}(BBL) = \frac{I_{d^*}}{2I_{d \text{ at } 3.07} + I_{d^*}} \#(\text{Eq.S}) \quad 2.$$

$$\text{Cont.}(2 - \text{MeTHF}) = \frac{2I_{b1+c1+b2+c2}}{2I_{b1+c1+b2+c2} + 3I_{d^*}} \#(\text{Eq.S}) \quad 3.$$

I was the integral intensity with a specific proton.

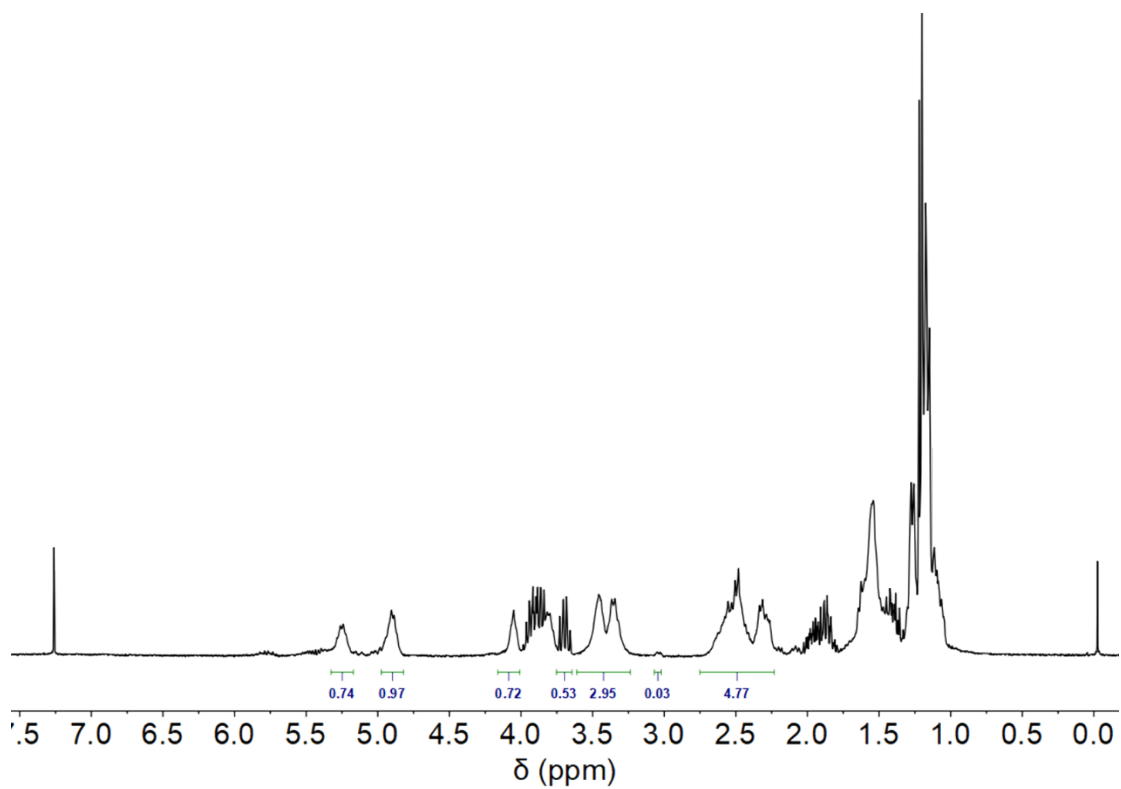


Figure S3. ^1H NMR spectrum for calculation of monomer conversions (run 17 in Table 1).

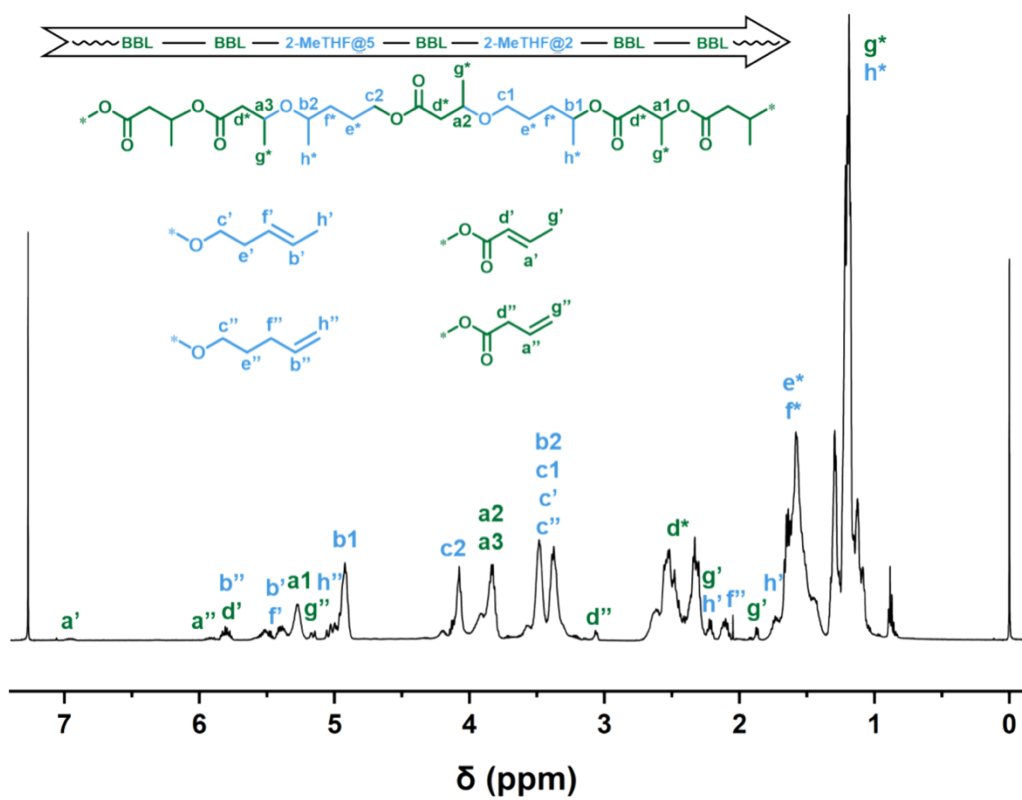


Figure S4. ^1H NMR spectrum of the components in *n*-hexane

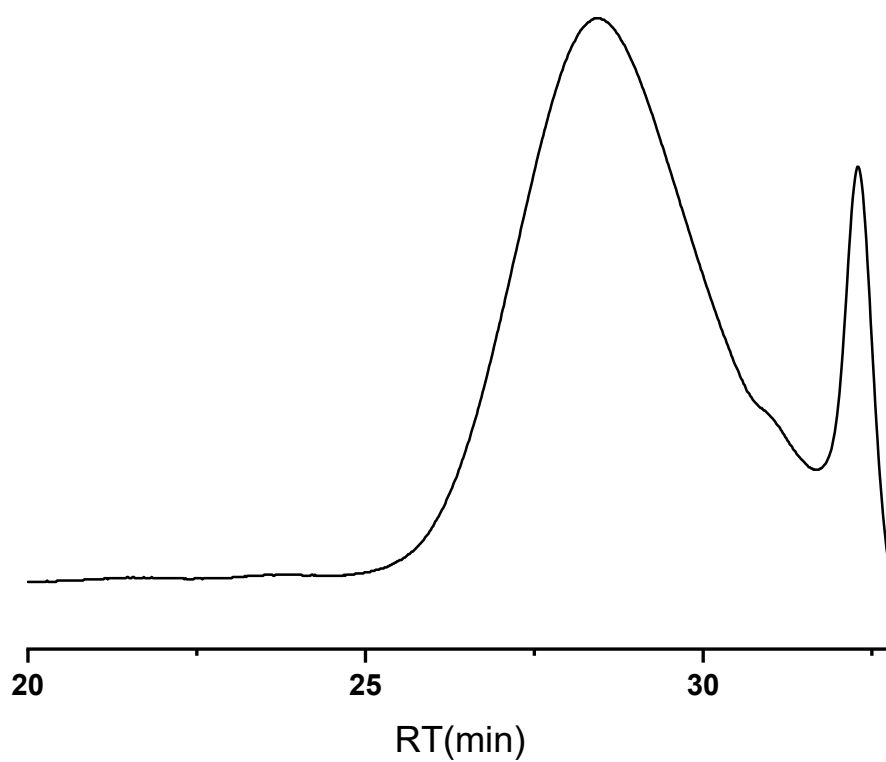


Figure S5. Typical SEC curve of copolymer (Run 4 in Table 1).

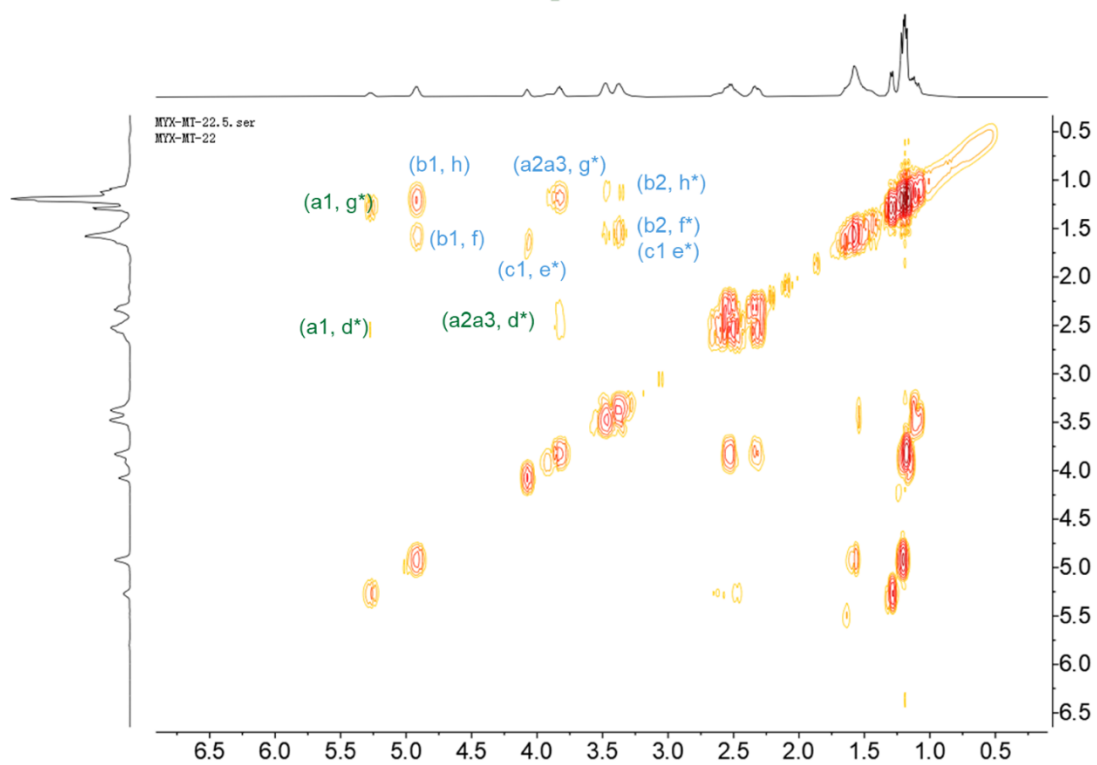


Figure S6. COSY NMR spectrum of copolymer (Run 4 in Table 1)

Proposed mechanism of the intermolecular esterification reaction

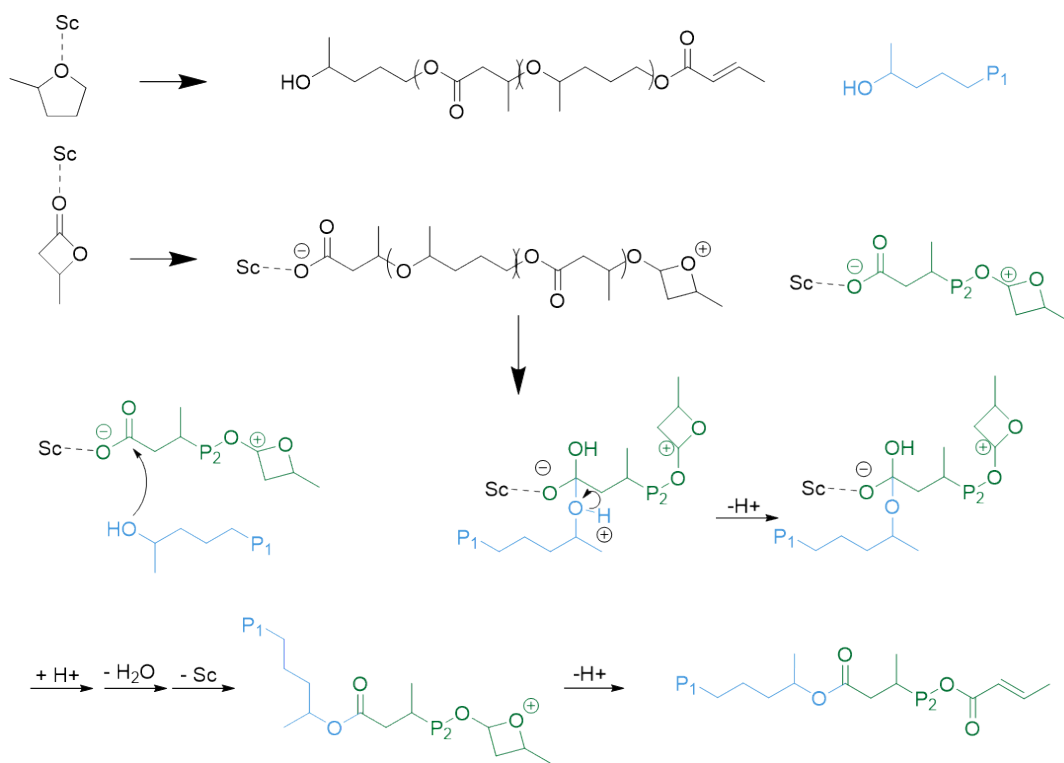


Figure S7. Proposed mechanism of the intermolecular esterification reaction.

Characterization of the thermal properties of poly(2-MeTHF-co-BBL)

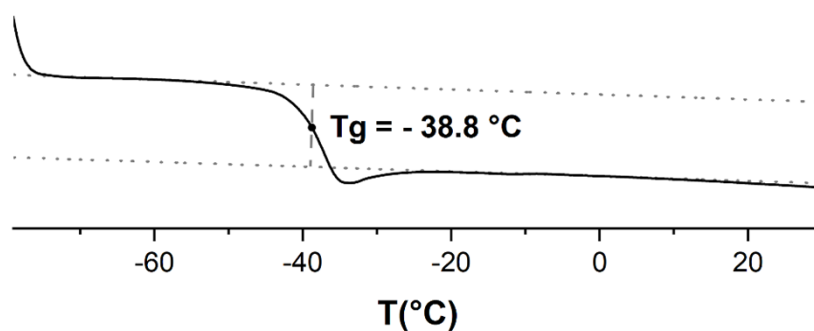


Figure S8. DSC curve of poly(2-MeTHF-co-BBL) (Run 4 in Table 1).

Calculation of the activation energy of 2-MeTHF and BBL

E_a of 2-MeTHF and BBL are calculated according to Arrhenius equation (Eq.S3) by the slopes.

$$\ln k = -\frac{E_a}{RT} + \ln A \quad (\text{Eq.S})$$

k: Reaction rate at certain temperature

E_a : Activation energies

R: Molar gas constant

T: Temperature

A: Preexponential factor

Calculation of reactivity ratio of 2-MeTHF and BBL copolymerisation

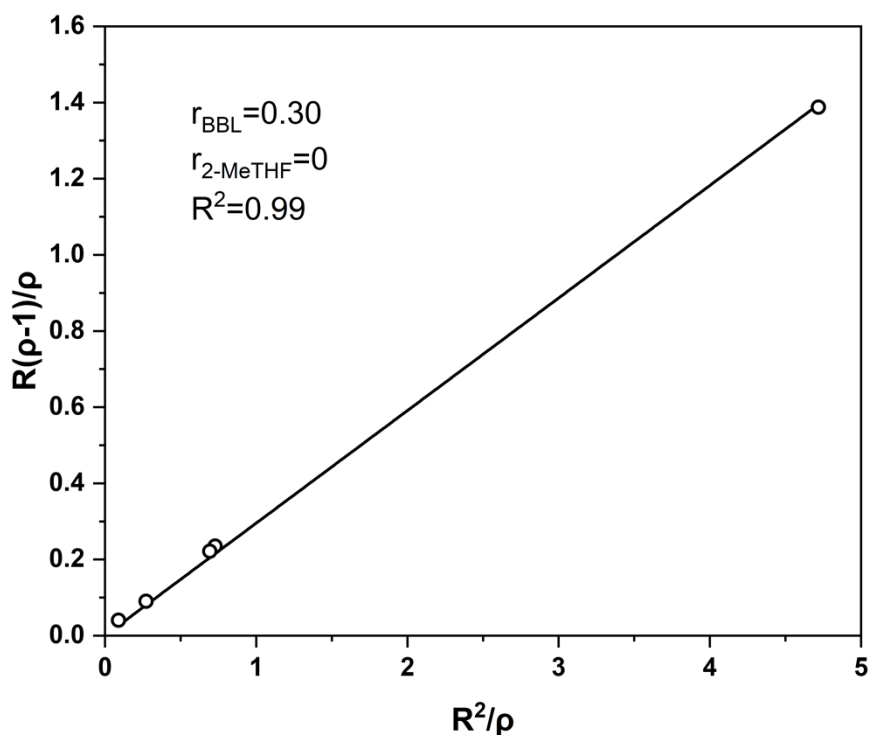


Figure S9. Calculation of reactivity ratios of 2-MeTHF and BBL copolymerisation at 30 °C.

The reactivity ratio was calculated by the intercept and slope of the Fineman-Ross equation (Eq.S1) derived from the differential equation for the composition of the binary copolymer

(Eq.S2). Maximum conversions of 2-MeTHF and BBL are 9% and 15%, respectively. r_1 and r_2 each represent the reactivity ratio of BBL and 2-MeTHF.

$$\frac{R(\rho - 1)}{\rho} = -r_2 + r_1 \frac{R^2}{\rho} \quad \#(Eq.S) \quad 5.$$

$$\rho = \frac{d[M_1]}{d[M_2]} \quad R = \frac{[M_1]}{[M_2]}$$

$$\frac{d[M_1]}{d[M_2]} = \frac{[M_1]}{[M_2]} \times \frac{r_1[M_1] + [M_2]}{r_2[M_2] + [M_1]} \quad \#(Eq.S) \quad 6.$$

Degradation of poly(2-MeTHF-co-BBL)

Degradation experiment of the copolymer (Run 4 in Table 1) was carried out in a methanol solution of sodium hydroxide (1 mol/L) for 24 h. The original and degraded samples were measured by SEC and NMR. The SEC traces indicate that the peak at 28 min almost completely disappears, while a negative peak at 32 min changes to a positive peak after degradation, which means that the large molecule has been almost completely degraded. The degradation of polymers can also be demonstrated by the disappearance of the NMR signal of ester bonds (blue) in the degradation products.

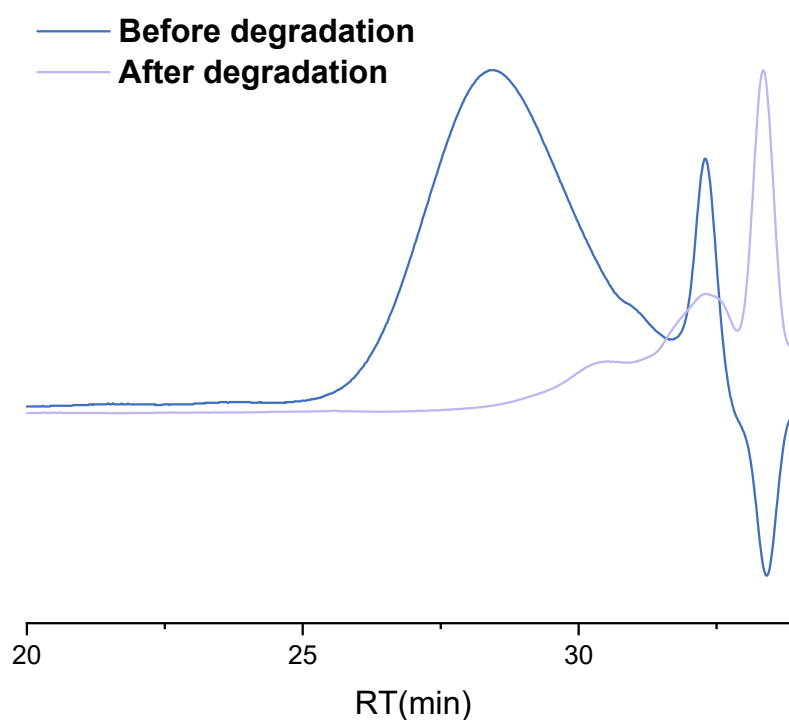


Figure S10. SEC curves of poly(2-MeTHF-co-BBL) (Run 4 in Table 1) before (blue) and after (purple) treated in alcohol solution of alkali for 24 h.

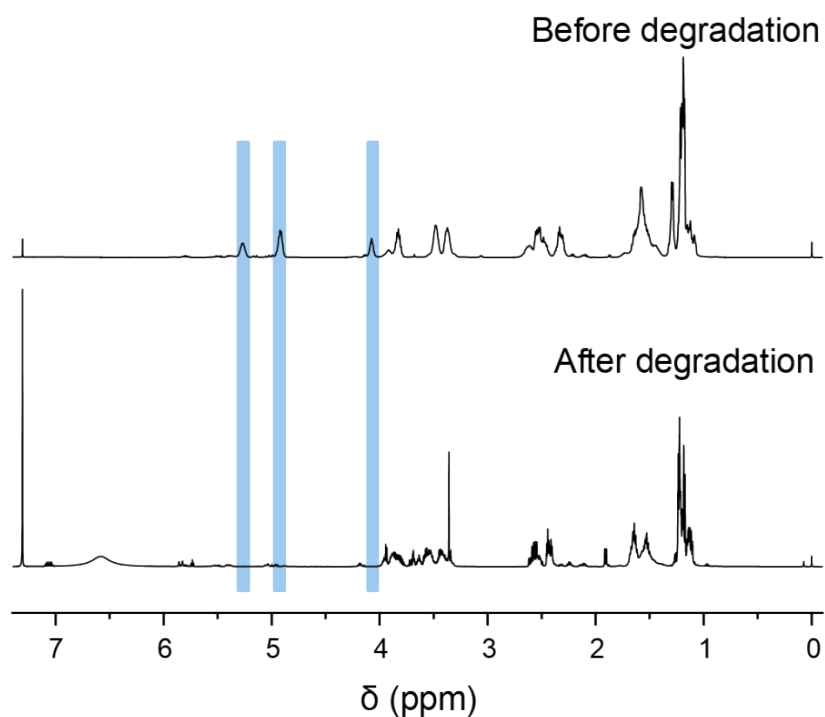


Figure S11. ^1H NMR spectra of poly(2-MeTHF-co-BBL) (Run 4 in Table 1) before (up) and after (down) treated in alcohol solution of alkali for 24 h.

Optimized geometries by PBE0/6-31+G(d,p)

BBL

C	-1.068090	-0.015040	-0.037952
C	-0.108429	1.154829	0.083137
C	0.902532	0.069970	0.474555
O	-0.139967	-0.952519	0.308262
O	-2.216346	-0.189325	-0.313505
C	2.076500	-0.176184	-0.434435
H	-0.381621	1.878294	0.854152
H	0.085916	1.670680	-0.860580
H	1.198402	0.094414	1.527624
H	2.563037	-1.124216	-0.188442

H	2.812111	0.627090	-0.321807
H	1.757579	-0.212953	-1.480839

2-MeTHF

C	-1.355269	-0.848685	0.060691
C	-1.544720	0.669783	-0.113236
C	-0.108086	1.219587	-0.008111
C	0.723729	-0.011654	0.374278
O	0.013070	-1.103560	-0.192554
C	2.146743	-0.024457	-0.133262
H	-1.608303	-1.157189	1.088264
H	-1.942711	-1.453299	-0.635014
H	-1.985561	0.905104	-1.085952
H	-2.207530	1.079439	0.654812
H	-0.009431	2.025101	0.725742
H	0.233518	1.605635	-0.974815
H	0.721077	-0.124033	1.474417
H	2.649294	-0.955583	0.143497
H	2.711396	0.811599	0.291803
H	2.159311	0.064260	-1.224478

BL-onto-BL (reactant)

C	1.263210	-1.550414	2.939326
F	0.479235	-2.538542	3.358251
F	2.250325	-2.049052	2.213423
S	0.229464	-0.362747	1.944210
F	1.763021	-0.906830	3.987371
O	-0.185917	-1.108034	0.711128
O	1.211315	0.671958	1.431224
O	-0.798074	0.095043	2.850009
Sc	0.948184	0.285186	-0.660900
C	-0.660668	3.861817	0.186515
F	0.123074	3.504964	1.192915
F	-0.230691	5.005844	-0.328869
S	-0.650890	2.553680	-1.137762
F	-1.905969	4.014360	0.627456

O	-1.487957	3.051309	-2.203213
O	-1.077255	1.285902	-0.449549
O	0.808313	2.315524	-1.435228
C	4.761689	-0.552809	-0.007308
F	5.175045	-1.756057	0.371452
F	5.781211	0.130230	-0.510074
S	3.450162	-0.742087	-1.314686
F	4.269688	0.095870	1.041689
O	4.083644	-1.388651	-2.435230
O	2.907818	0.655166	-1.508246
O	2.309554	-1.448871	-0.630557
C	-1.082966	-1.199032	-2.455265
C	-2.338587	-1.382897	-1.670364
C	-2.830200	-2.064852	-2.952263
O	-1.481525	-1.789137	-3.561677
O	0.021293	-0.685409	-2.288849
C	-3.135957	-3.530879	-2.924600
H	-2.817657	-0.446567	-1.382412
H	-2.234382	-2.013393	-0.785203
H	-3.562723	-1.485362	-3.516208
H	-2.360516	-4.087085	-2.389234
H	-3.223095	-3.931039	-3.938254
H	-4.090197	-3.668842	-2.407571
C	-5.403073	-1.370312	0.139926
C	-6.273224	-0.680572	1.169555
C	-4.994516	-0.697410	2.020137
O	-4.290911	-1.382592	0.915243
O	-5.508684	-1.795308	-0.976683
C	-4.341214	0.611474	2.365845
H	-7.109960	-1.286768	1.523325
H	-6.630532	0.305802	0.863532
H	-5.031324	-1.380674	2.872931
H	-3.314985	0.454150	2.708352
H	-4.904119	1.104451	3.165392
H	-4.316461	1.277899	1.497535

BL-onto-BL (TS)

C	-1.390941	-1.659454	-2.854366
F	-0.644174	-2.682050	-3.266692
F	-2.373141	-2.113478	-2.094311
S	-0.301117	-0.472005	-1.922246
F	-1.900480	-1.035095	-3.910975
O	0.162671	-1.211818	-0.702704
O	-1.235092	0.585742	-1.392945
O	0.702232	-0.062894	-2.882071
Sc	-0.869920	0.220899	0.741687
C	0.605821	3.822955	-0.412381
F	-0.269143	3.438405	-1.328569
F	0.222971	4.982459	0.108164
S	0.742972	2.554876	0.942365
F	1.802277	3.971056	-0.981504
O	1.670776	3.108020	1.903558
O	1.141889	1.281131	0.255998
O	-0.673495	2.309815	1.384561
C	-4.748212	-0.417278	0.209670
F	-5.245093	-1.588686	-0.173156
F	-5.710683	0.311761	0.761447
S	-3.400173	-0.703002	1.460203
F	-4.265349	0.222058	-0.849797
O	-4.029824	-1.347599	2.584931
O	-2.789284	0.661683	1.667474
O	-2.326948	-1.447420	0.714480
C	1.228243	-1.231199	2.491290
C	2.400329	-1.141469	1.548926
C	3.362468	-1.979762	2.329670
O	1.497682	-1.918263	3.493768
O	0.122121	-0.653834	2.247810
C	3.518543	-3.436818	2.121414
H	2.725080	-0.105099	1.431169
H	2.160172	-1.544901	0.563122
H	3.816737	-1.532939	3.206042
H	3.332777	-3.717751	1.082556

H	2.771163	-3.931979	2.751333
H	4.504756	-3.777079	2.442641
C	5.143786	-1.143611	0.173494
C	6.057239	-0.385515	-0.748349
C	5.034388	-0.806348	-1.819954
O	4.285128	-1.543327	-0.757460
O	5.087330	-1.361406	1.371257
C	4.178872	0.251395	-2.452088
H	7.060550	-0.808654	-0.832517
H	6.117009	0.684102	-0.533221
H	5.401755	-1.546982	-2.533589
H	3.310305	-0.188726	-2.948507
H	4.768652	0.794965	-3.197397
H	3.813116	0.964370	-1.706907

BL-onto-BL (product)

C	1.415234	-1.692109	2.819544
F	0.719233	-2.757546	3.215216
F	2.428216	-2.086813	2.067795
S	0.275064	-0.553782	1.887217
F	1.880116	-1.053611	3.889259
O	-0.152009	-1.313028	0.666956
O	1.149022	0.554913	1.376558
O	-0.755228	-0.212782	2.850686
Sc	0.799635	0.168224	-0.800140
C	-0.800597	3.741186	0.416483
F	0.134404	3.415067	1.295210
F	-0.504016	4.912746	-0.132619
S	-0.946807	2.446241	-0.910138
F	-1.975610	3.840621	1.046479
O	-1.945175	2.950802	-1.830338
O	-1.271149	1.176627	-0.186678
O	0.453389	2.261098	-1.417058
C	4.714340	-0.143193	-0.181460
F	5.301951	-1.267743	0.215547
F	5.623565	0.662118	-0.719330

S	3.417261	-0.544606	-1.453625
F	4.164452	0.456963	0.868453
O	4.122925	-1.142968	-2.559111
O	2.704677	0.764601	-1.684460
O	2.396904	-1.370577	-0.721527
C	-1.162138	-1.431138	-2.615474
C	-2.372617	-1.191805	-1.719338
C	-3.509512	-2.135970	-2.017754
O	-1.206426	-2.201156	-3.555299
O	-0.130320	-0.714683	-2.263490
C	-3.345653	-3.557308	-1.552658
H	-2.686246	-0.154240	-1.880384
H	-2.041207	-1.272170	-0.681987
H	-3.800472	-2.090127	-3.067032
H	-3.061535	-3.615350	-0.498596
H	-2.533580	-3.982812	-2.150062
H	-4.247780	-4.147745	-1.733316
C	-4.815536	-1.191829	-0.170115
C	-5.799123	-0.416509	0.628378
C	-4.751951	-0.613528	1.749156
O	-3.933208	-1.413053	0.750594
O	-4.774545	-1.532026	-1.373986
C	-3.980744	0.567739	2.243504
H	-6.765885	-0.907366	0.762271
H	-5.939787	0.610162	0.280348
H	-5.047778	-1.313323	2.532369
H	-3.078529	0.247316	2.771579
H	-4.614217	1.135457	2.933363
H	-3.675455	1.220268	1.420661

MT-onto-BL (reactant)

C	1.125618	-0.457704	3.265778
F	0.370340	-1.304533	3.960036
F	2.065932	-1.135752	2.625672
S	0.027395	0.463263	2.076421
F	1.690849	0.412141	4.092347

O	-0.462856	-0.559133	1.093683
O	0.971133	1.325871	1.261728
O	-0.942981	1.139289	2.902629
Sc	0.560727	0.453921	-0.650020
C	-1.060049	4.086579	-0.652387
F	-0.248368	3.981363	0.389912
F	-0.649773	5.074380	-1.437316
S	-1.066263	2.500132	-1.627233
F	-2.294142	4.336311	-0.231041
O	-1.939584	2.718938	-2.752669
O	-1.437198	1.427423	-0.636362
O	0.391494	2.212472	-1.902233
C	4.429102	-0.310484	-0.004064
F	4.843976	-1.402026	0.628689
F	5.425845	0.196852	-0.715886
S	3.033163	-0.766140	-1.148155
F	4.017101	0.585584	0.883504
O	3.583731	-1.679924	-2.119241
O	2.496776	0.556269	-1.637274
O	1.932885	-1.273274	-0.254234
C	-0.734896	-2.084835	-1.881987
C	-0.925788	-3.105500	-0.811350
C	-1.392217	-3.979556	-1.984823
O	-1.163446	-2.812131	-2.894946
O	-0.345578	-0.924572	-1.969209
C	-0.559296	-5.158107	-2.394705
H	-1.713025	-2.821783	-0.099145
H	-0.006617	-3.398936	-0.299283
H	-2.464379	-4.186337	-1.985247
H	-0.707214	-5.969784	-1.675136
H	0.504415	-4.902877	-2.416214
H	-0.855528	-5.519447	-3.383093
C	-3.660393	-2.253775	2.043945
C	-4.221722	-0.893030	2.455425
C	-5.024753	-0.492384	1.220899
C	-4.155835	-1.033114	0.093151

O	-3.615182	-2.262534	0.612667
C	-4.872927	-1.318306	-1.207833
H	-2.651735	-2.429770	2.436973
H	-4.307992	-3.078420	2.369790
H	-4.823117	-0.950809	3.366984
H	-3.411169	-0.177909	2.628888
H	-5.185686	0.586269	1.140452
H	-6.003058	-0.990263	1.209052
H	-3.323119	-0.336329	-0.086633
H	-4.191995	-1.745009	-1.951576
H	-5.278397	-0.391489	-1.626134
H	-5.695837	-2.022691	-1.047666

MT-onto-BL (TS)

C	2.107350	-1.740914	2.700692
F	1.528815	-2.842952	3.171715
F	2.992759	-2.072695	1.774986
S	0.784359	-0.632215	2.003001
F	2.720586	-1.107128	3.693789
O	0.219037	-1.367425	0.822235
O	1.533138	0.530009	1.394463
O	-0.100996	-0.354357	3.110762
Sc	0.891656	0.214968	-0.661009
C	-0.802473	3.597940	0.821860
F	0.245139	3.305597	1.576441
F	-0.641197	4.800360	0.283252
S	-1.001627	2.339660	-0.534119
F	-1.902632	3.595865	1.572318
O	-2.137727	2.776334	-1.316272
O	-1.126495	1.017419	0.166251
O	0.342940	2.277696	-1.202918
C	4.844586	-0.078214	-0.743835
F	5.484351	-1.223591	-0.535570
F	5.651217	0.772923	-1.365378
S	3.352788	-0.396882	-1.809980
F	4.474656	0.437720	0.422341

O	3.856556	-0.891203	-3.066376
O	2.602297	0.913287	-1.806215
O	2.468023	-1.296373	-0.989414
C	-1.391894	-1.214143	-2.162765
C	-2.259210	-1.612258	-1.002095
C	-3.497366	-1.830950	-1.823888
O	-2.009857	-1.454302	-3.226988
O	-0.244338	-0.695478	-2.063154
C	-3.988065	-3.176221	-2.213678
H	-2.341852	-0.826509	-0.249962
H	-1.884433	-2.522891	-0.526178
H	-3.974992	-0.954945	-2.242670
H	-3.903458	-3.878510	-1.379572
H	-3.354046	-3.547424	-3.024627
H	-5.020510	-3.140593	-2.563093
C	-4.662008	-2.229070	0.979270
C	-4.425995	-1.134152	2.005763
C	-5.306346	-0.011138	1.465169
C	-5.121739	-0.125287	-0.042855
O	-4.873331	-1.547402	-0.278415
C	-6.295985	0.320392	-0.883808
H	-3.822024	-2.919732	0.864744
H	-5.566565	-2.809252	1.196242
H	-4.700578	-1.451560	3.014883
H	-3.373475	-0.831536	2.023073
H	-5.016898	0.977295	1.830582
H	-6.357756	-0.180149	1.728354
H	-4.213250	0.416194	-0.343593
H	-6.107308	0.180208	-1.952324
H	-6.480126	1.386571	-0.718816
H	-7.198189	-0.236907	-0.613967

MT-onto-BL (product)

C	1.890470	-1.439206	2.826781
F	1.282520	-2.479992	3.396085
F	2.762911	-1.878655	1.935144

S	0.594494	-0.362791	2.035504
F	2.524126	-0.738369	3.759909
O	-0.027309	-1.205284	0.957699
O	1.357500	0.703599	1.303291
O	-0.268322	0.045745	3.124406
Sc	0.647230	0.211998	-0.741939
C	-0.861054	3.722479	0.668122
F	0.167847	3.406158	1.437676
F	-0.652879	4.911230	0.115071
S	-1.107827	2.456285	-0.673547
F	-1.967437	3.772819	1.412036
O	-2.210269	2.952633	-1.467033
O	-1.323323	1.153687	0.046713
O	0.237415	2.307162	-1.321144
C	4.605986	-0.166378	-0.838132
F	5.240264	-1.283609	-0.496854
F	5.409223	0.588505	-1.577894
S	3.088776	-0.600723	-1.823484
F	4.266802	0.498142	0.260646
O	3.562174	-1.272522	-3.008584
O	2.363599	0.711343	-1.988456
O	2.212164	-1.367075	-0.872405
C	-1.641196	-1.320033	-2.198755
C	-1.893876	-2.551508	-1.329040
C	-3.357773	-2.765114	-1.020026
O	-2.472838	-0.972910	-3.020456
O	-0.499243	-0.735517	-1.995034
C	-3.694674	-4.129266	-0.461328
H	-1.270638	-2.538694	-0.432085
H	-1.562742	-3.416809	-1.918125
H	-3.951158	-2.548036	-1.909456
H	-3.068467	-4.394490	0.395431
H	-3.513256	-4.872066	-1.243238
H	-4.747941	-4.192984	-0.175093
C	-3.374018	-1.771092	1.356624
C	-3.652992	-0.367810	1.869998

C	-4.667898	0.213961	0.886558
C	-4.246621	-0.330406	-0.457311
O	-3.873159	-1.750886	-0.042144
C	-5.291242	-0.371664	-1.534730
H	-2.310993	-2.014846	1.336290
H	-3.951462	-2.551212	1.854736
H	-4.032135	-0.397154	2.893835
H	-2.733232	0.219515	1.861646
H	-4.640298	1.306486	0.870541
H	-5.691263	-0.104730	1.117528
H	-3.318296	0.132038	-0.796478
H	-4.882904	-0.724156	-2.484132
H	-5.623973	0.658851	-1.696358
H	-6.158357	-0.967640	-1.233651

BL-onto-MT@2 (reactant)

C	-0.551328	-3.611747	-0.369095
F	-0.620001	-4.247262	-1.532343
F	0.102540	-4.361825	0.510194
S	0.396619	-2.026698	-0.615299
F	-1.774134	-3.371993	0.076109
O	0.399855	-1.326784	0.714668
O	-0.491406	-1.156100	-1.472956
O	1.670060	-2.428357	-1.167338
Sc	-0.747145	0.439775	-0.018307
C	1.077848	3.702391	-1.387626
F	0.399303	4.015254	-0.286156
F	2.372559	3.918968	-1.178678
S	0.814155	1.909573	-1.809692
F	0.657446	4.457326	-2.391644
O	1.508935	1.682018	-3.051181
O	-0.681791	1.746317	-1.769878
O	1.277628	1.151955	-0.589990
C	-4.448139	-0.599755	-0.744819
F	-3.636568	-0.929065	-1.741121
F	-5.020237	-1.692054	-0.256547

S	-3.470951	0.228599	0.605451
F	-5.378896	0.234881	-1.183867
O	-4.407639	0.588589	1.642901
O	-2.731356	1.347167	-0.089468
O	-2.370335	-0.736767	0.951384
C	1.072379	1.122365	2.504257
C	0.718088	0.617059	3.913379
C	-0.813758	0.683058	4.006105
C	-1.170356	1.680978	2.926262
O	-0.247609	1.353556	1.857108
H	1.567800	0.359243	1.906325
H	1.095142	-0.395712	4.070752
H	1.184854	1.263936	4.662768
H	-1.169175	0.997772	4.990803
H	-1.266720	-0.284713	3.771119
H	-0.976768	2.716662	3.228419
C	4.503552	-0.698517	1.027439
C	4.533346	-0.522336	-0.475538
C	5.601660	-1.621512	-0.414459
O	5.439475	-1.680580	1.050954
O	3.930961	-0.219394	1.966013
C	5.304450	-2.945041	-1.064103
H	4.855471	0.467064	-0.806840
H	3.599216	-0.799651	-0.969165
H	6.616371	-1.273635	-0.629564
H	6.007349	-3.709769	-0.721147
H	5.400597	-2.851942	-2.150881
H	4.285301	-3.270414	-0.837182
C	1.880156	2.398477	2.490339
H	2.071375	2.732841	1.469717
H	1.385914	3.200848	3.048677
H	2.845578	2.191985	2.961426
H	-2.189161	1.613089	2.547764

BL-onto-MT@2 (TS)

C	1.058774	3.410989	-0.828099
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F	1.348163	3.888864	-2.033242
F	0.374052	4.327257	-0.145264
S	-0.004018	1.895010	-1.020026
F	2.180190	3.133301	-0.183174
O	-0.269306	1.406218	0.377044
O	0.875680	0.857599	-1.641772
O	-1.162593	2.350884	-1.766292
Sc	0.774043	-0.617294	0.096676
C	-1.481102	-3.719591	-1.132039
F	-1.069129	-3.957040	0.111531
F	-2.815911	-3.668626	-1.138080
S	-0.806536	-2.099855	-1.749154
F	-1.079212	-4.705559	-1.920628
O	-1.243688	-2.001554	-3.121021
O	0.663202	-2.185263	-1.462847
O	-1.321637	-1.079000	-0.772949
C	4.656581	0.180698	-0.272108
F	4.029893	0.503265	-1.396739
F	5.232997	1.263928	0.237722
S	3.442110	-0.503733	0.959019
F	5.583851	-0.733536	-0.529138
O	4.205847	-0.846916	2.136315
O	2.740234	-1.611859	0.222994
O	2.386592	0.558852	1.097443
C	-2.140705	-0.367379	2.215283
C	-1.729040	0.031906	3.587331
C	-0.202288	0.166645	3.722422
C	0.468491	-1.056849	3.128935
O	0.043626	-1.173141	1.794955
H	-1.788414	0.227443	1.383662
H	-2.189149	1.001373	3.804843
H	-2.118541	-0.691306	4.312540
H	0.052822	0.296169	4.780136
H	0.143587	1.053374	3.180728
H	0.180000	-1.966307	3.679614
C	-4.284198	1.148094	1.044178

C	-3.929426	1.002265	-0.408823
C	-5.167494	1.886057	-0.615171
O	-5.345226	1.929574	0.865425
O	-3.877004	0.756675	2.126504
C	-4.980444	3.257728	-1.193399
H	-3.968956	-0.019086	-0.792582
H	-2.976876	1.455285	-0.699541
H	-6.031890	1.363744	-1.031972
H	-5.876909	3.866517	-1.047820
H	-4.789665	3.172276	-2.267764
H	-4.125372	3.764243	-0.737010
C	-2.805323	-1.669968	1.990644
H	-3.170706	-1.788703	0.971676
H	-2.057674	-2.449188	2.176811
H	-3.615098	-1.805234	2.713626
H	1.560225	-0.966992	3.197217

BL-onto-MT@2 (product)

C	-1.299319	-3.335267	-0.763047
F	-1.631653	-3.813938	-1.957391
F	-0.655649	-4.281288	-0.077466
S	-0.156262	-1.884499	-0.989282
F	-2.393453	-2.990020	-0.106303
O	0.165501	-1.397573	0.393834
O	-0.968726	-0.814658	-1.632475
O	0.971500	-2.433145	-1.731512
Sc	-0.762120	0.710156	0.117353
C	1.809873	3.597446	-1.073772
F	1.430027	3.846641	0.175883
F	3.135839	3.414080	-1.088361
S	0.981575	2.066629	-1.728808
F	1.509946	4.638641	-1.837636
O	1.407100	1.970253	-3.106713
O	-0.471297	2.279905	-1.438306
O	1.414504	0.977125	-0.791439
C	-4.704251	0.013234	-0.258217

F	-4.105194	-0.414545	-1.363723
F	-5.325261	-1.007885	0.325895
S	-3.453078	0.726642	0.917757
F	-5.596029	0.945592	-0.574909
O	-4.201667	1.179795	2.067890
O	-2.716322	1.752330	0.103371
O	-2.449788	-0.372117	1.125699
C	2.536752	-0.004108	2.208498
C	1.916561	-0.366384	3.549416
C	0.388590	-0.231080	3.603798
C	-0.195714	1.102683	3.149343
O	-0.093309	1.266791	1.763917
H	1.885420	-0.275552	1.377922
H	2.169308	-1.408158	3.775950
H	2.382126	0.247269	4.331160
H	0.082801	-0.408868	4.642268
H	-0.073302	-1.019385	2.999007
H	0.315267	1.939899	3.653156
C	4.079548	-1.318229	0.923833
C	3.625513	-1.177509	-0.478837
C	4.863600	-2.044347	-0.763784
O	5.114328	-2.081148	0.731359
O	3.753977	-0.921126	2.067795
C	4.670664	-3.417551	-1.324567
H	3.590564	-0.156810	-0.866510
H	2.663792	-1.657200	-0.701687
H	5.705814	-1.504626	-1.200484
H	5.586275	-4.008053	-1.237686
H	4.415182	-3.326358	-2.385167
H	3.849613	-3.939516	-0.826040
C	3.058366	1.403806	2.098147
H	3.525090	1.595009	1.128366
H	2.204904	2.080634	2.182950
H	3.772532	1.618932	2.898661
H	-1.251279	1.146050	3.452912

BL-onto-MT@5 (reactant)

C	0.098643	3.929289	0.237555
F	0.007903	4.691862	-0.845434
F	-0.560074	4.499852	1.239834
S	-0.694009	2.283766	-0.129669
F	1.369452	3.780458	0.570003
O	-0.469726	1.437552	1.098359
O	0.174859	1.629569	-1.171236
O	-2.060431	2.589979	-0.487019
Sc	0.751597	-0.086060	0.085975
C	-0.724431	-3.302382	-1.700996
F	-0.042039	-3.662033	-0.611933
F	-1.984979	-3.699601	-1.572306
S	-0.674541	-1.453277	-1.893359
F	-0.182466	-3.877263	-2.764054
O	-1.398858	-1.154139	-3.102425
O	0.796030	-1.129298	-1.827479
O	-1.210542	-0.927343	-0.589269
C	4.400830	0.566263	-1.042535
F	3.520080	0.711948	-2.024710
F	5.056696	1.703768	-0.859954
S	3.504622	0.118247	0.525483
F	5.256147	-0.398830	-1.349935
O	4.500965	-0.014230	1.559783
O	2.698257	-1.104336	0.160329
O	2.452266	1.182601	0.679382
C	-0.996473	-1.175205	2.475289
C	-1.341503	-2.638431	2.608211
C	-0.005335	-3.267897	3.013516
C	1.078441	-2.323675	2.463872
O	0.328047	-1.204267	1.859258
C	2.018665	-1.796351	3.525574
H	-1.669236	-0.613608	1.832549
H	-0.902081	-0.668350	3.441905
H	-2.135298	-2.801510	3.340557
H	-1.691646	-3.018143	1.644644

H	0.113816	-4.281020	2.621033
H	0.079597	-3.324245	4.103917
H	1.639152	-2.768836	1.639710
H	2.778010	-1.127852	3.114920
H	2.536620	-2.640518	3.993161
H	1.464105	-1.268011	4.308031
C	-4.678017	-0.191997	0.833377
C	-4.547458	0.117744	-0.642243
C	-5.870292	0.864340	-0.431125
O	-5.843820	0.484568	0.994144
O	-4.067528	-0.793671	1.672122
C	-5.881487	2.357780	-0.610775
H	-4.569650	-0.760381	-1.290907
H	-3.685854	0.743172	-0.886161
H	-6.737516	0.385173	-0.894968
H	-6.784517	2.793378	-0.173458
H	-5.863727	2.601140	-1.678195
H	-5.004614	2.812881	-0.141011

BL-onto-MT@5 (TS)

C	1.123730	3.578857	-0.152514
F	1.417214	4.275456	-1.245186
F	0.467707	4.360458	0.703429
S	0.017183	2.158748	-0.626869
F	2.241728	3.153862	0.411981
O	-0.258367	1.412536	0.651072
O	0.861786	1.237388	-1.447156
O	-1.130885	2.787690	-1.253740
Sc	0.694386	-0.529353	0.003057
C	-1.857599	-3.142514	-1.787412
F	-1.661731	-3.548958	-0.531916
F	-3.163707	-2.934817	-1.964711
S	-0.942915	-1.558015	-2.120125
F	-1.447843	-4.089467	-2.618719
O	-1.228027	-1.242401	-3.499035
O	0.478657	-1.858483	-1.738105

O	-1.431951	-0.616196	-1.060823
C	4.553465	0.290934	-0.369593
F	3.879435	0.829169	-1.377481
F	5.171655	1.250657	0.310429
S	3.394014	-0.614046	0.770394
F	5.452566	-0.562415	-0.845090
O	4.222823	-1.190808	1.802404
O	2.633729	-1.552111	-0.133294
O	2.360288	0.397532	1.173446
C	-2.047581	-0.607263	2.011227
C	-2.297596	-1.689131	3.005573
C	-0.965332	-2.235937	3.524326
C	-0.092089	-2.595318	2.332367
O	-0.144310	-1.472578	1.469004
C	1.327805	-2.956541	2.727176
H	-2.246863	-0.740418	0.958162
H	-1.477379	0.265835	2.298870
H	-2.870603	-1.266888	3.836693
H	-2.895554	-2.487166	2.554397
H	-1.139772	-3.102071	4.171536
H	-0.455073	-1.469796	4.122130
H	-0.547158	-3.447865	1.804022
H	1.922900	-3.235096	1.854338
H	1.317213	-3.810267	3.413094
H	1.820192	-2.117974	3.229392
C	-4.162273	1.016865	1.332237
C	-3.896027	1.230033	-0.128075
C	-5.136170	2.130805	-0.036691
O	-5.223656	1.805124	1.419391
O	-3.696396	0.375890	2.266847
C	-4.971429	3.603859	-0.265736
H	-3.969889	0.331330	-0.743932
H	-2.954771	1.738964	-0.356865
H	-6.029639	1.722122	-0.514212
H	-5.852440	4.152044	0.078751
H	-4.845496	3.788056	-1.337282

H -4.086446 3.986549 0.250316

BL-onto-MT@5 (product)

C 1.229815 3.559295 -0.111178
F 1.493020 4.282519 -1.195074
F 0.627225 4.332766 0.793070
S 0.074791 2.175853 -0.574803
F 2.360292 3.097487 0.394836
O -0.180266 1.413652 0.694615
O 0.850374 1.266572 -1.461086
O -1.086848 2.859414 -1.129637
Sc 0.716035 -0.574185 0.003087
C -1.910589 -3.157624 -1.699402
F -1.572949 -3.607528 -0.492950
F -3.234978 -2.967302 -1.723970
S -1.065137 -1.544330 -2.074389
F -1.587344 -4.066338 -2.609168
O -1.483484 -1.209777 -3.417034
O 0.385200 -1.810732 -1.823183
O -1.504616 -0.635336 -0.965011
C 4.623969 0.200329 -0.443838
F 3.961494 0.809205 -1.420676
F 5.278055 1.109493 0.273970
S 3.444299 -0.723022 0.657938
F 5.496538 -0.652233 -0.970638
O 4.262178 -1.363625 1.662450
O 2.662676 -1.597816 -0.281918
O 2.452783 0.308990 1.111794
C -2.354670 -0.161352 2.215158
C -2.339471 -1.213620 3.294367
C -0.923997 -1.713810 3.603374
C -0.222006 -2.444811 2.457487
O 0.029025 -1.560338 1.402204
C 1.074736 -3.094351 2.919841
H -2.175178 -0.549580 1.213973
H -1.675539 0.668130 2.415621

H	-2.769465	-0.780856	4.205512
H	-2.979485	-2.054953	3.001222
H	-0.994068	-2.395296	4.459393
H	-0.288390	-0.875008	3.916999
H	-0.898695	-3.233437	2.085701
H	1.568240	-3.588515	2.078795
H	0.882833	-3.842805	3.696194
H	1.762423	-2.342333	3.320452
C	-4.140807	1.031359	1.183830
C	-3.690400	1.311371	-0.195629
C	-5.074321	1.971893	-0.307032
O	-5.307337	1.599537	1.146235
O	-3.727891	0.447835	2.217600
C	-5.158124	3.450962	-0.513714
H	-3.471122	0.428745	-0.803731
H	-2.826867	1.985460	-0.277849
H	-5.803439	1.404039	-0.887611
H	-6.169459	3.817256	-0.320015
H	-4.903957	3.669935	-1.555819
H	-4.449157	3.983581	0.125970

MT-onto-MT@2 (reactant)

C	1.566580	-2.942189	-1.435500
F	1.446062	-4.244851	-1.215047
F	2.183995	-2.742427	-2.595557
S	-0.137501	-2.194527	-1.537563
F	2.280255	-2.395769	-0.461450
O	0.072817	-0.710680	-1.689523
O	-0.706005	-2.328722	-0.139014
O	-0.796488	-2.905099	-2.602783
Sc	-0.931056	-0.220626	0.235766
C	-4.779096	0.957803	-0.150902
F	-4.047246	2.070581	-0.078902
F	-5.463504	0.964084	-1.286485
S	-3.684543	-0.545804	-0.105914
F	-5.617165	0.923882	0.876163

O	-4.572689	-1.674111	-0.211821
O	-2.878128	-0.395240	1.165871
O	-2.661171	-0.320482	-1.182899
C	1.603963	-1.474511	3.065396
F	1.002745	-2.526121	2.527599
F	2.915409	-1.566813	2.875961
S	0.989418	0.089049	2.264431
F	1.344350	-1.428807	4.364760
O	1.649590	1.182334	2.941200
O	-0.514543	0.008989	2.373960
O	1.242827	-0.081377	0.795719
C	-0.046519	2.496770	-1.177198
C	0.241762	3.915113	-0.692580
C	0.059558	3.847795	0.821879
C	-1.103026	2.887860	0.949448
O	-0.836919	1.887101	-0.072629
H	0.882666	1.921628	-1.220402
H	1.248641	4.216155	-0.990728
H	-0.476196	4.617236	-1.133317
H	-0.163357	4.819669	1.270415
H	0.946509	3.434686	1.312469
H	-2.060037	3.364312	0.713579
C	-0.824130	2.405766	-2.468314
H	-1.016717	1.369960	-2.756124
H	-1.778370	2.936364	-2.387949
H	-0.236494	2.874920	-3.264565
H	-1.178737	2.372433	1.908838
C	3.981291	2.690110	0.065947
C	5.447748	2.258209	-0.131544
C	5.387606	1.342434	-1.367810
C	3.888719	1.115186	-1.573319
O	3.295631	2.334471	-1.126371
C	3.457738	0.838526	-2.994664
H	3.530897	2.168805	0.923570
H	3.858211	3.767472	0.210971
H	6.101523	3.117468	-0.304213

H	5.822768	1.734241	0.752372
H	5.931884	0.403183	-1.232879
H	5.801939	1.847128	-2.247802
H	3.545455	0.300545	-0.912828
H	2.374743	0.698533	-3.059589
H	3.935641	-0.074745	-3.363014
H	3.746559	1.669129	-3.647248

MT-onto-MT@2 (TS)

C	-1.283041	-3.175070	-1.459144
F	-1.817980	-3.424346	-2.649168
F	-0.491777	-4.191461	-1.113179
S	-0.249255	-1.630756	-1.570601
F	-2.248109	-3.052486	-0.561004
O	0.288396	-1.413556	-0.181182
O	-1.222697	-0.510871	-1.784860
O	0.717596	-1.911051	-2.609489
Sc	-0.781753	0.594276	0.131572
C	1.215234	3.953793	-0.785978
F	1.026162	3.914066	0.531974
F	2.526671	3.955482	-1.030525
S	0.438320	2.474772	-1.603736
F	0.679633	5.066459	-1.268500
O	0.618551	2.679486	-3.019979
O	-0.957839	2.449137	-1.051192
O	1.110278	1.290232	-0.967252
C	-4.666129	-0.262348	0.388689
F	-4.276625	-0.352483	-0.876551
F	-5.131732	-1.440068	0.791838
S	-3.230322	0.228725	1.463951
F	-5.624929	0.649911	0.492449
O	-3.746941	0.327096	2.810190
O	-2.685611	1.475731	0.823952
O	-2.171241	-0.804493	1.198421
C	2.424523	0.032422	1.621254
C	2.233450	-0.759530	2.869969

C	0.751365	-0.876540	3.283058
C	0.071256	0.463177	3.093133
O	0.262207	0.837104	1.754878
H	1.974572	-0.327764	0.707879
H	2.610926	-1.773398	2.700048
H	2.817379	-0.309486	3.681082
H	0.693557	-1.227981	4.319303
H	0.248401	-1.611114	2.646196
H	0.514811	1.228180	3.751288
C	3.038923	1.380508	1.666549
H	3.274976	1.753756	0.671326
H	2.319042	2.060249	2.134436
H	3.936282	1.369758	2.292518
H	-0.993907	0.394570	3.348341
C	5.202218	-1.336131	1.673832
C	6.021476	-2.219284	0.750950
C	4.927730	-2.896615	-0.074632
C	3.876576	-1.797105	-0.255949
O	4.133023	-0.861398	0.847738
C	3.967692	-1.031987	-1.557628
H	4.798435	-1.913103	2.518836
H	5.738026	-0.465035	2.060001
H	6.668782	-1.604578	0.117135
H	6.649416	-2.926095	1.299649
H	4.507694	-3.744653	0.476924
H	5.285814	-3.268959	-1.037743
H	2.860577	-2.183130	-0.118369
H	3.288651	-0.175221	-1.558795
H	3.669771	-1.681162	-2.386121
H	4.988458	-0.675244	-1.731235

MT-onto-MT@2 (product)

C	-1.522747	-3.107651	-1.316959
F	-2.090676	-3.360300	-2.491542
F	-0.790283	-4.164130	-0.952114
S	-0.392577	-1.638636	-1.489442

F	-2.463378	-2.902653	-0.409629
O	0.182915	-1.418961	-0.117328
O	-1.283530	-0.468262	-1.747797
O	0.545473	-2.034521	-2.522452
Sc	-0.769859	0.697776	0.160672
C	1.650999	3.783838	-0.773642
F	1.460742	3.767528	0.543387
F	2.955473	3.620862	-1.017580
S	0.698247	2.416384	-1.599066
F	1.265042	4.958487	-1.254205
O	0.907115	2.612410	-3.014467
O	-0.690657	2.558102	-1.053412
O	1.230444	1.157936	-0.978281
C	-4.733096	-0.009560	0.339539
F	-4.338950	-0.228023	-0.909379
F	-5.254457	-1.128730	0.835913
S	-3.291830	0.516193	1.390068
F	-5.657799	0.944760	0.347276
O	-3.830655	0.751589	2.710924
O	-2.695515	1.680550	0.651637
O	-2.280100	-0.582609	1.236320
C	2.811636	-0.247696	1.543969
C	2.360372	-1.067604	2.748276
C	0.860784	-0.970381	3.079819
C	0.244239	0.425089	3.073751
O	0.147858	0.934862	1.777056
H	2.043000	-0.195319	0.776357
H	2.575890	-2.128385	2.563763
H	2.952836	-0.770927	3.624306
H	0.715722	-1.416405	4.071571
H	0.291666	-1.579649	2.370636
H	0.836335	1.115887	3.697581
C	3.339244	1.128619	1.851468
H	3.725393	1.612638	0.951498
H	2.499034	1.726973	2.212335
H	4.111439	1.113054	2.628080

H	-0.753468	0.364153	3.531591
C	5.124745	-1.409614	1.503359
C	5.715043	-2.440759	0.565995
C	4.476115	-3.123026	-0.017820
C	3.501856	-1.983708	-0.269806
O	3.917988	-0.979372	0.796144
C	3.613108	-1.293713	-1.602746
H	4.824241	-1.838212	2.463105
H	5.735775	-0.519721	1.657417
H	6.303787	-1.955235	-0.217854
H	6.368172	-3.134081	1.101282
H	4.058913	-3.836420	0.700679
H	4.690344	-3.661039	-0.944215
H	2.463414	-2.225733	-0.033023
H	3.021919	-0.374791	-1.619987
H	3.191559	-1.953420	-2.366732
H	4.653702	-1.066712	-1.854594

MT-onto-MT@5 (reactant)

C	-2.324814	-3.361489	-1.533953
F	-3.408946	-3.987631	-1.094470
F	-2.077739	-3.726787	-2.787748
S	-2.640779	-1.525412	-1.504513
F	-1.290533	-3.681035	-0.771168
O	-1.353251	-0.879753	-1.944209
O	-2.719194	-1.157708	-0.039073
O	-3.815036	-1.323483	-2.314041
Sc	-0.973422	0.119256	0.009636
C	-2.238124	3.855023	0.899903
F	-0.913665	3.847059	1.058437
F	-2.554595	4.732099	-0.045309
S	-2.832863	2.165076	0.399791
F	-2.811096	4.203204	2.042031
O	-4.264669	2.267949	0.291260
O	-2.240171	1.240278	1.426159
O	-2.044242	1.835886	-0.848987

C	0.153503	-2.287059	2.923235
F	-1.169237	-2.267824	2.815950
F	0.596197	-3.523840	2.733109
S	0.898854	-1.167000	1.638614
F	0.508209	-1.868300	4.130753
O	2.329902	-1.221557	1.817693
O	0.206878	0.154759	1.854374
O	0.329124	-1.653082	0.333840
C	1.489372	0.142552	-2.030632
C	1.553417	1.094865	-3.202723
C	1.816057	2.432070	-2.507003
C	1.120363	2.313127	-1.141817
O	0.722437	0.898725	-1.048246
C	2.000548	2.668812	0.036788
H	0.956138	-0.788245	-2.216449
H	2.480705	-0.052097	-1.608688
H	2.344255	0.824423	-3.907306
H	0.596561	1.100662	-3.734415
H	1.436698	3.285964	-3.073981
H	2.891438	2.573737	-2.357769
H	0.180906	2.870516	-1.125525
H	1.481180	2.530907	0.988581
H	2.297517	3.720517	-0.040034
H	2.903215	2.048478	0.033595
C	5.777810	1.457548	-1.148514
C	6.868563	1.221963	-0.110496
C	6.784162	-0.290128	0.071027
C	5.281855	-0.546886	-0.017726
O	4.775606	0.474035	-0.902364
C	4.894011	-1.912952	-0.540732
H	5.320822	2.451878	-1.078479
H	6.169303	1.331743	-2.169039
H	7.850049	1.571602	-0.443163
H	6.623719	1.734586	0.826814
H	7.208975	-0.642893	1.015010
H	7.302459	-0.804452	-0.748663

H	4.816417	-0.391686	0.966440
H	3.807105	-2.020098	-0.587620
H	5.273897	-2.693340	0.127245
H	5.310325	-2.074780	-1.540813

MT-onto-MT@5 (TS)

C	-1.571023	2.367945	-2.317995
F	-1.302683	3.576607	-2.798476
F	-2.448349	1.762562	-3.120765
S	-0.002982	1.363456	-2.283306
F	-2.111181	2.489646	-1.111868
O	-0.404108	0.036830	-1.691059
O	0.856382	2.001689	-1.229463
O	0.459314	1.375650	-3.650080
Sc	0.948220	0.185839	0.097594
C	4.509130	-1.693643	-0.386822
F	3.713831	-2.548823	0.258855
F	4.938535	-2.269133	-1.504132
S	3.592650	-0.132181	-0.810818
F	5.548385	-1.405227	0.388591
O	4.543271	0.676215	-1.533082
O	3.089025	0.387183	0.514243
O	2.349272	-0.592628	-1.509079
C	-0.781380	3.186537	2.294610
F	-0.246656	3.758987	1.225869
F	-2.092417	3.419934	2.310363
S	-0.495788	1.349043	2.257612
F	-0.232731	3.695936	3.391394
O	-1.067823	0.832838	3.484444
O	0.986230	1.199614	2.062464
O	-1.101391	0.883004	0.968419
C	-1.490468	-2.148489	0.100611
C	-1.397915	-3.411675	0.898497
C	-0.530668	-3.187763	2.139866
C	0.795676	-2.590753	1.690752
O	0.459900	-1.578071	0.763483

C	1.620856	-2.063580	2.852880
H	-1.066496	-2.058778	-0.888653
H	-1.784313	-1.224958	0.582385
H	-2.401887	-3.713565	1.217771
H	-0.982679	-4.219760	0.286983
H	-0.388975	-4.129601	2.681012
H	-1.029217	-2.483012	2.817721
H	1.372031	-3.361956	1.155066
H	2.545929	-1.600897	2.501377
H	1.886999	-2.886988	3.524405
H	1.059281	-1.317652	3.422908
C	-3.548265	-3.447116	-1.474901
C	-4.866439	-3.945144	-0.905284
C	-5.519291	-2.648531	-0.433407
C	-4.349275	-1.855000	0.132070
O	-3.218679	-2.270751	-0.697809
C	-4.480689	-0.350971	0.080352
H	-2.725130	-4.160893	-1.389308
H	-3.637230	-3.129462	-2.518869
H	-5.458963	-4.482200	-1.650115
H	-4.692460	-4.620439	-0.060029
H	-6.300225	-2.804252	0.315357
H	-5.960438	-2.106733	-1.278308
H	-4.129698	-2.188599	1.157430
H	-3.590002	0.153242	0.464249
H	-5.332459	-0.041883	0.694943
H	-4.651995	-0.017228	-0.947296

MT-onto-MT@5 (product)

C	1.764964	-1.966493	-2.399640
F	1.614041	-3.085858	-3.097016
F	2.684895	-1.201262	-3.004766
S	0.151042	-1.039171	-2.347772
F	2.211842	-2.270553	-1.185549
O	0.465786	0.220731	-1.584304
O	-0.734410	-1.839079	-1.447997

O	-0.209292	-0.897989	-3.739682
Sc	-1.013004	-0.152302	0.108526
C	-4.632679	1.513299	-0.381290
F	-3.924698	2.307812	0.422305
F	-5.034256	2.220840	-1.433892
S	-3.611698	0.070586	-0.959585
F	-5.698137	1.072804	0.281023
O	-4.477413	-0.664377	-1.850187
O	-3.162244	-0.608676	0.306246
O	-2.364357	0.689241	-1.513430
C	0.814048	-3.309916	2.083561
F	0.362195	-3.812533	0.943360
F	2.138887	-3.462793	2.134165
S	0.408307	-1.499837	2.208075
F	0.263530	-3.961536	3.102064
O	0.897694	-1.079573	3.507352
O	-1.064487	-1.424412	1.954087
O	1.056564	-0.878166	1.008178
C	1.790040	2.169959	0.305977
C	1.615310	3.220127	1.383240
C	0.609503	2.775289	2.453433
C	-0.805008	2.500348	1.936898
O	-0.778533	1.463820	1.000940
C	-1.742625	2.162672	3.089315
H	1.059788	2.212185	-0.497861
H	1.809105	1.152750	0.693934
H	2.577063	3.403651	1.880703
H	1.291171	4.174352	0.948729
H	0.560269	3.558952	3.218925
H	0.976821	1.866338	2.947556
H	-1.176257	3.409740	1.431442
H	-2.743195	1.945572	2.709153
H	-1.814085	2.998444	3.794105
H	-1.382047	1.279955	3.627375
C	3.370956	3.508172	-1.197817
C	4.800698	3.857213	-0.839093

C	5.422078	2.497256	-0.522873
C	4.342132	1.757197	0.243415
O	3.101046	2.291433	-0.411655
C	4.345172	0.255686	0.139724
H	2.629440	4.254936	-0.914372
H	3.235731	3.217666	-2.241921
H	5.304045	4.371815	-1.660798
H	4.827452	4.509870	0.039514
H	6.334472	2.578093	0.072940
H	5.662948	1.952668	-1.442628
H	4.287185	2.096593	1.283879
H	3.497830	-0.203611	0.654880
H	5.262413	-0.115033	0.609081
H	4.335429	-0.062618	-0.905909

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