Electronic Supplementary Material (ESI) for Polymer Chemistry

Ring-opening Polymerisation of an *O*-Carboxyanhydride Monomer Derived from *L*-Malic acid.

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Electronic Supplementary Information

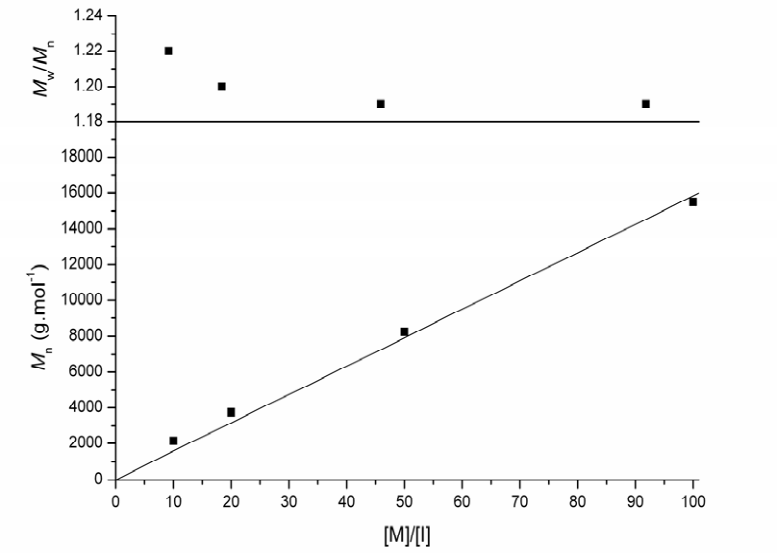


Figure S1. Plot of [M]/[I] *versus* M_n and PDI for ROP of *l*-malOCA ([*l*-malOCA]$_0$ = 0.32 M) using 5 mol% DMAP as the catalyst and *neo*-pentanol as the initiator at a ratio of 1:1.

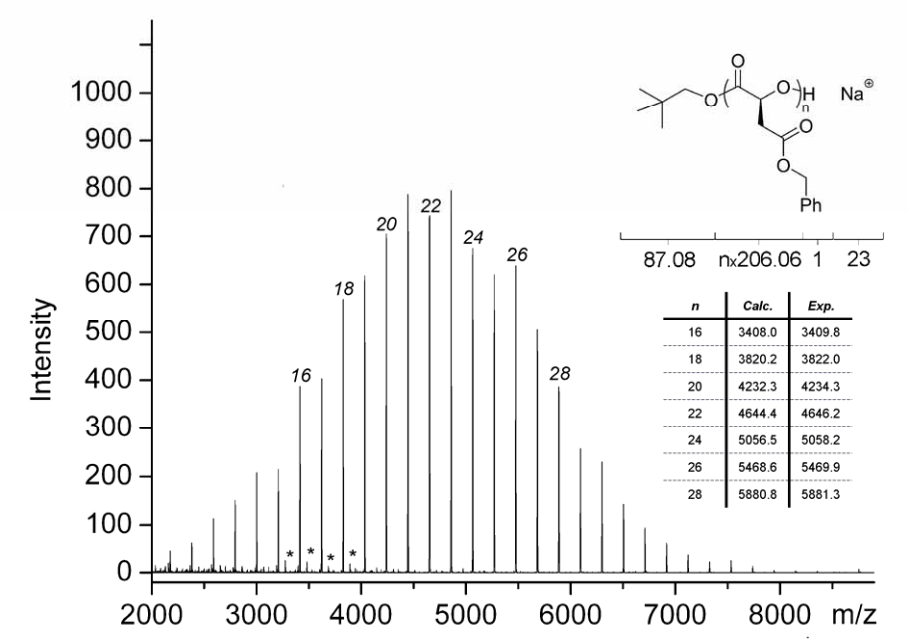


Figure S2. MALDI-TOF MS analysis of a P(*L*-BMA)$_{20}$ (M_n = 4 210 g.mol^{-1}, PDI = 1.22) prepared by ROP of *l*-malOCA ([*l*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% DMAP using *neo*-pentanol as the initiator and the presence of impurities (*****).

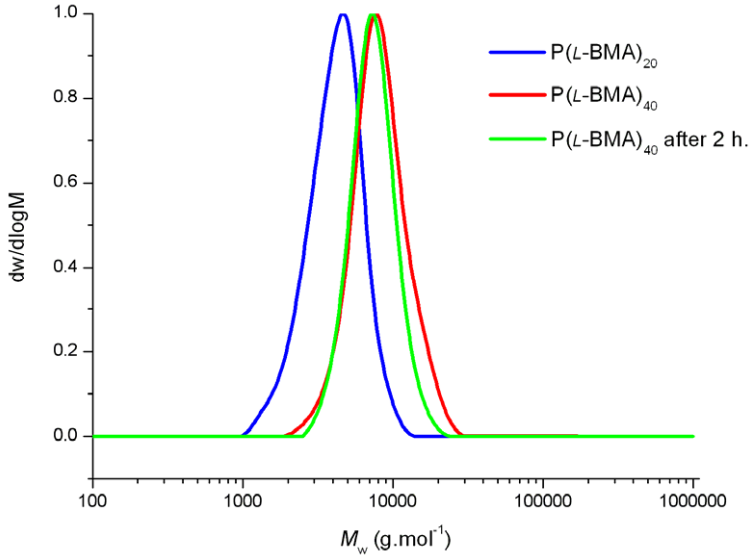


Figure S3. GPC traces of P(*L*-BMA)$_{20}$ (M_n = 3 730 g.mol^{-1}, PDI = 1.19) (—), P(*L*-BMA)$_{40}$ (M_n = 7 390 g.mol^{-1}, PDI = 1.20) (—) and P(*L*-BMA)$_{40}$ (M_n = 7 050 g.mol^{-1}, PDI = 1.19) (—) after 2 h prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% DMAP using *neo*-pentanol as the initiator.

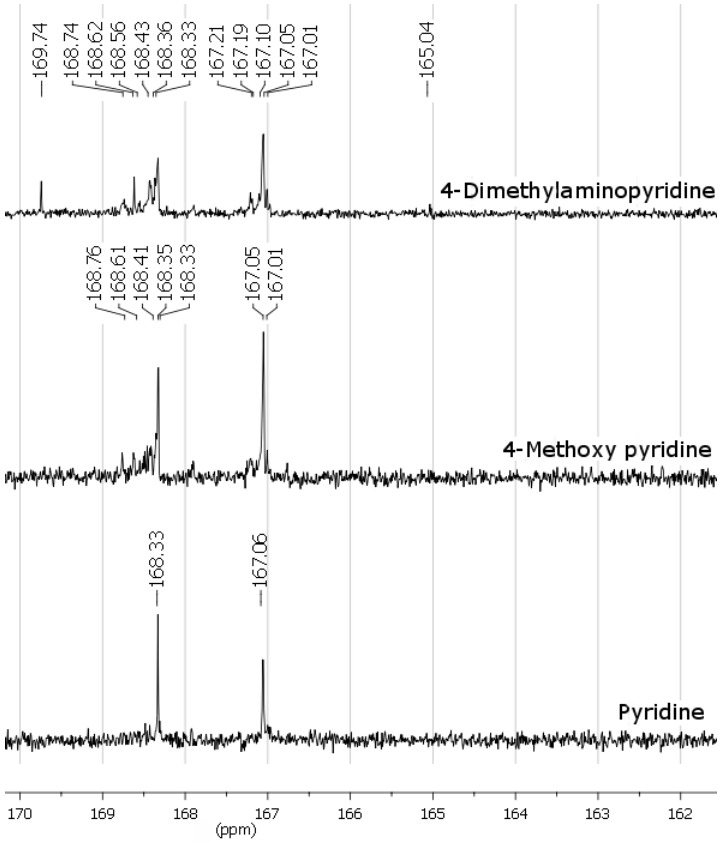


Figure S4. ^{13}C NMR spectra of P(*L*-BMA)$_{20}$ prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% 4-dimethylaminopyridine, 4-methoxypyridine or pyridine using *neo*-pentanol as the initiator and the presence of impurities (100 MHz; $CDCl_3$).

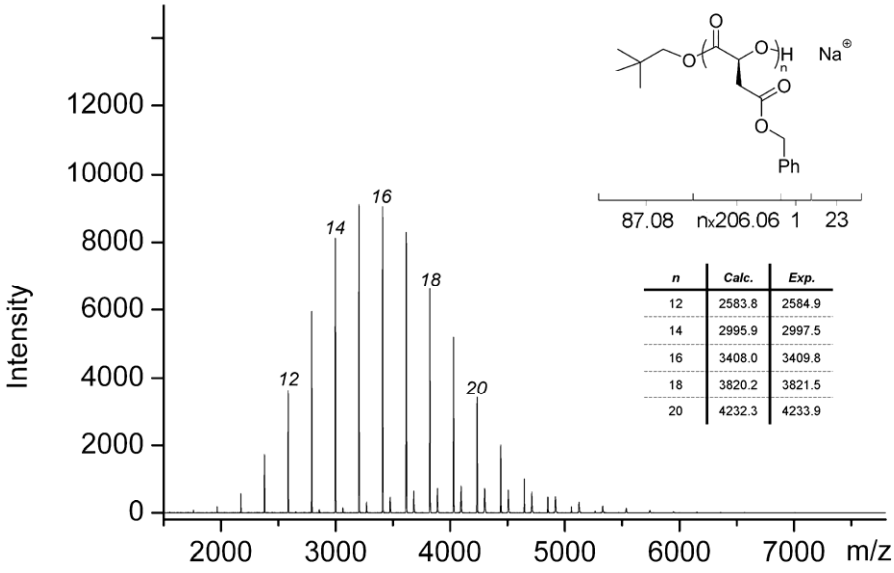


Figure S5. MALDI-TOF MS analysis of a P(*L*-BMA) ([M]/[I] = 20) (M_n = 2 950 g.mol^{-1}, PDI = 1.12) prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% 4-methylpyridine using *neo*-pentanol as the initiator.

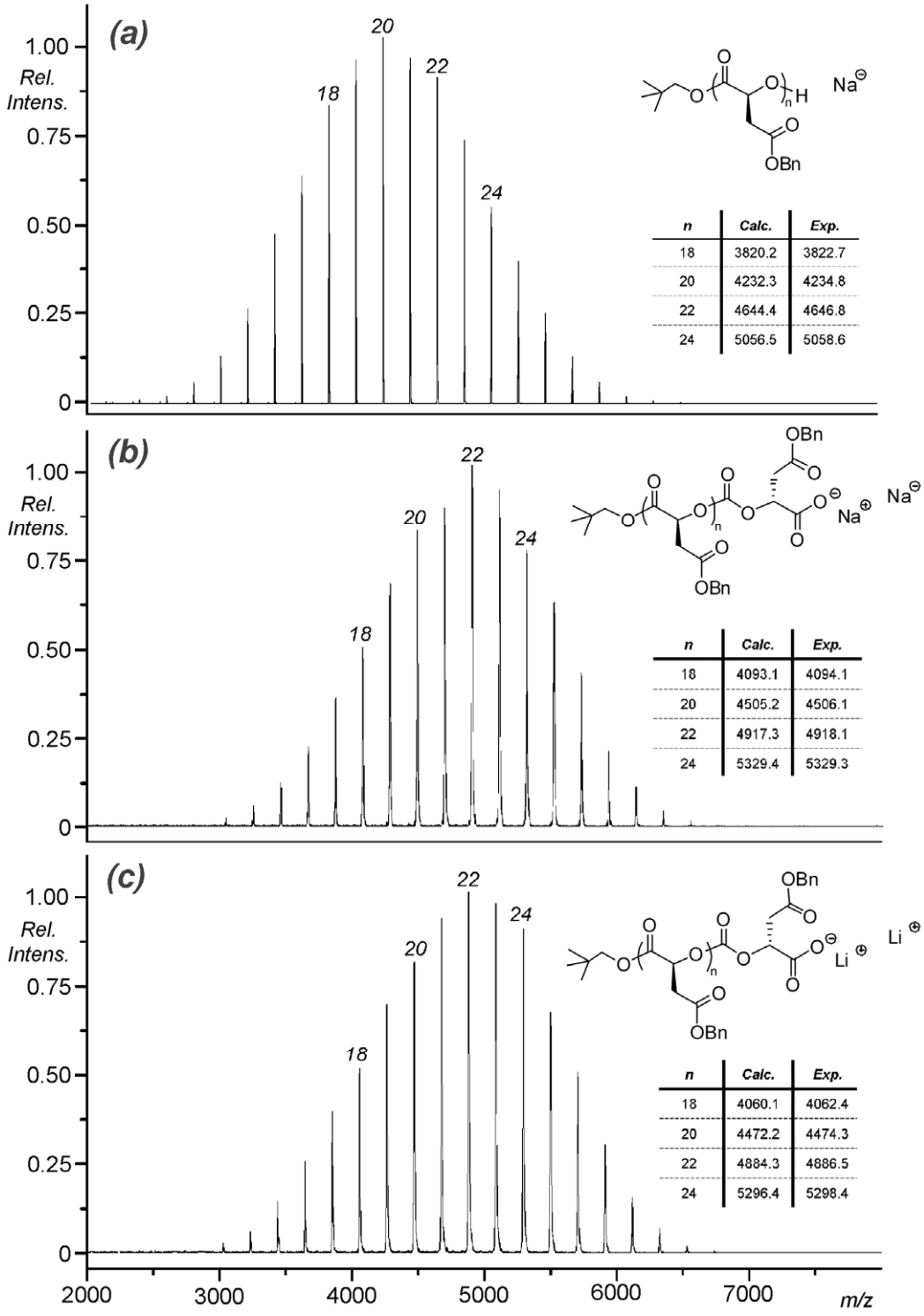


Figure S6 MALDI-TOF MS analysis of P(*L*-BMA) ([M]/[I] = 20) (M_n = 3 860 g.mol^{-1}, PDI = 1.10) prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalyzed with 5 mol% DMAP using *neo*-pentanol as the initiator. (a) purified *via* column chromatography using EtOAc:Hexanes (50:50), R_f = 0.8, NaTFA cationization agent; (b) R_f = 0.3, NaTFA cationization agent; (c) R_f = 0.3, LiCl cationization agent.

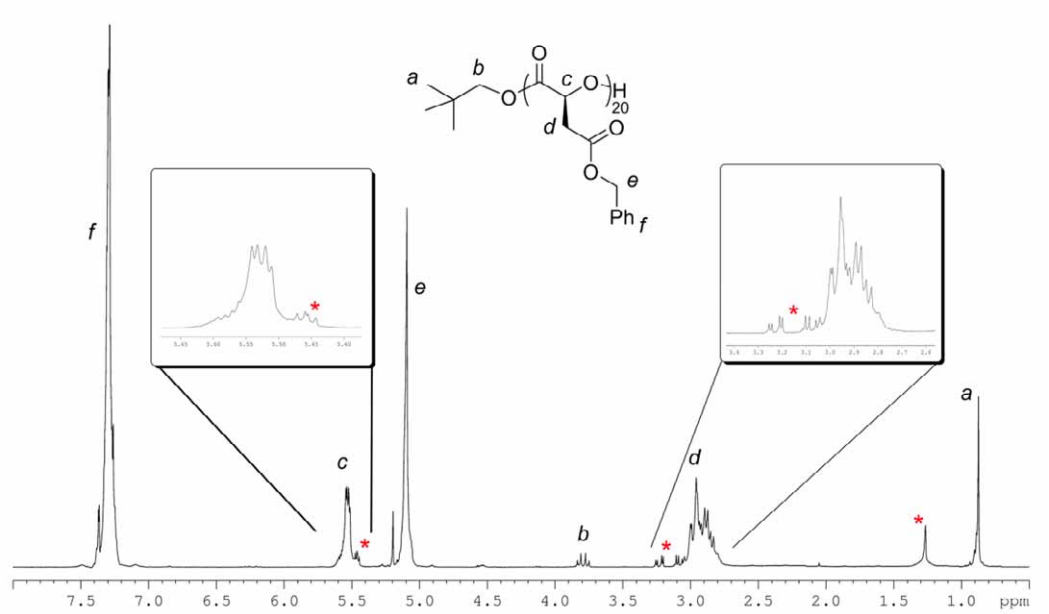
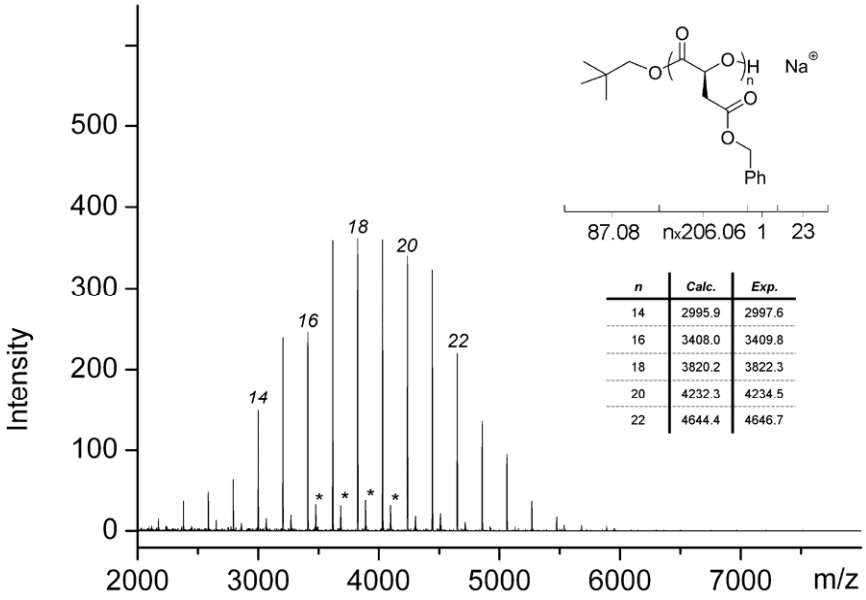


Figure S7. ^{1}H NMR spectrum of a P(*L*-BMA)$_{20}$ (M_n = 3 870 g.mol^{-1}, PDI = 1.14) prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% 4-morpholinopyridine using *neo*-pentanol as the initiator and the presence of impurities (*) (400 MHz; $CDCl_3$).



n	Calc.	Exp.
14	2995.9	2997.6
16	3408.0	3409.8
18	3820.2	3822.3
20	4232.3	4234.5
22	4644.4	4646.7

Figure S8. MALDI-TOF MS analysis of a P(*L*-BMA) ([M]/[I] = 20) (M_n = 3 870 g.mol^{-1}, PDI = 1.14) prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 5 mol% 4-morpholinopyridine using *neo*-pentanol as the initiator and the presence of impurities (*****).

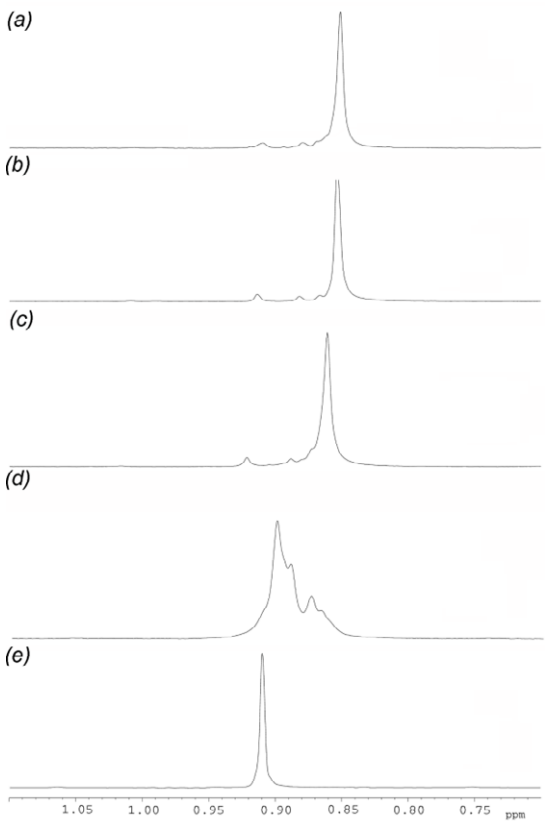


Figure S9. Expansion of δ = 1.10 to 0.70 ppm region of ^{1}H NMR spectra (400 MHz; $CDCl_3$) showing the *neo*-pentyl resonances of P(*L*-BMA) ([M]/[I] = 50) prepared by the ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) initiated from *neo*-pentanol catalyzed with pyridine at; 50:1 to *neo*-pentanol at high monomer conversion (**A**), 50:1 to *neo*-pentanol at low monomer conversion (**B**), 2.5:1 to *neo*-pentanol at high monomer conversion (**C**), 2.5:1 to *neo*-pentanol at low monomer conversion (**D**), and *neo*-pentanol (**E**).

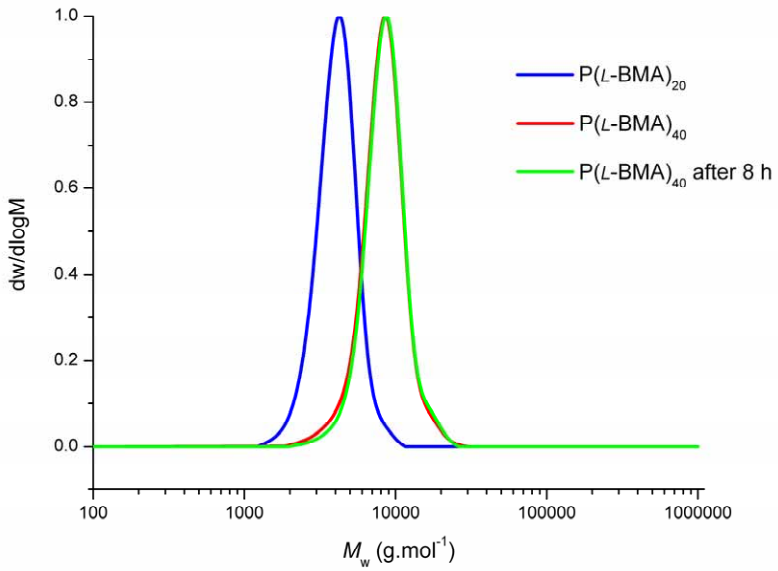


Figure S10. GPC traces of P(*L*-BMA)$_{20}$ (M_n = 3 860 g.mol^{-1}, PDI = 1.10) (—), P(*L*-BMA)$_{40}$ (M_n = 7 760 g.mol^{-1}, PDI = 1.12) (—) and P(*L*-BMA)$_{40}$ (M_n = 8 030 g.mol^{-1}, PDI = 1.11) (—) after 8 h prepared by ROP of *L*-malOCA ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 4-methoxypyridine using *neo*-pentanol as the initiator.

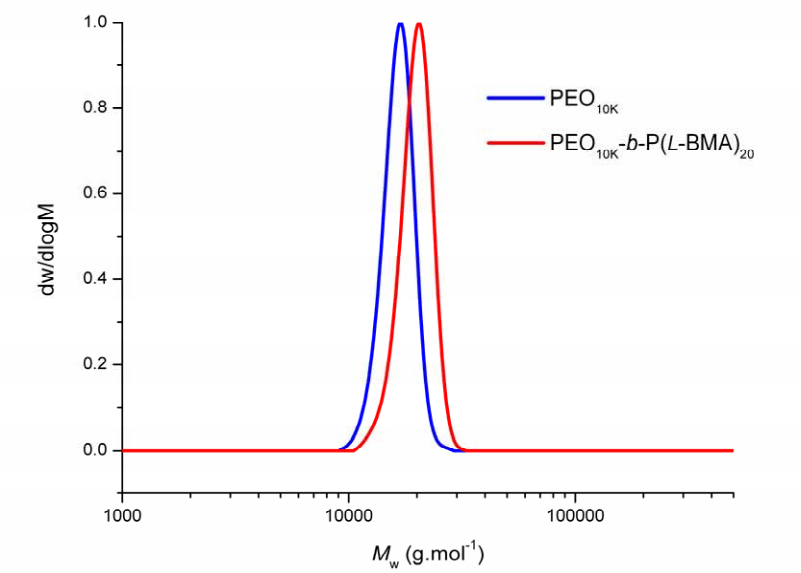


Figure S11. GPC traces of PEO$_{10K}$-*b*-P(*L*-BMA)$_{20}$ (M_n = 19 440 g.mol^{-1}, PDI = 1.03) (—) prepared by ROP of *L*-malOCA ([M]/[I] = 20) ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 4-methoxypyridine using MeO-PEO$_{10K}$-OH (M_n = 16 270 g.mol^{-1}, PDI = 1.03) (—) as the macroinitiator.

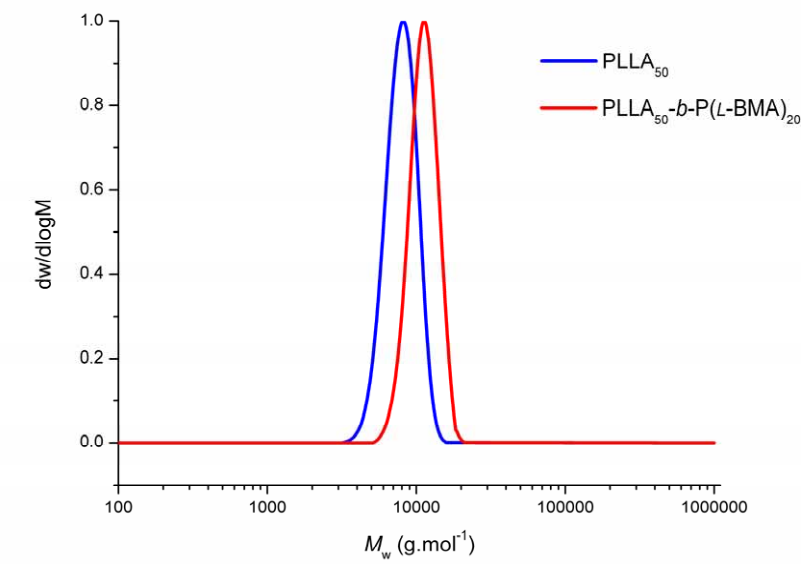


Figure S12. GPC traces of PLLA$_{50}$-*b*-P(*L*-BMA)$_{20}$ (M_n = 10 850 g.mol^{-1}, PDI = 1.05) (—) prepared by ROP of *L*-malOCA ([M]/[I] = 20) ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 4-methoxypyridine using PLLA$_{50}$-OH (M_n = 7 680 g.mol^{-1}, PDI = 1.06) (—) as the macroinitiator.

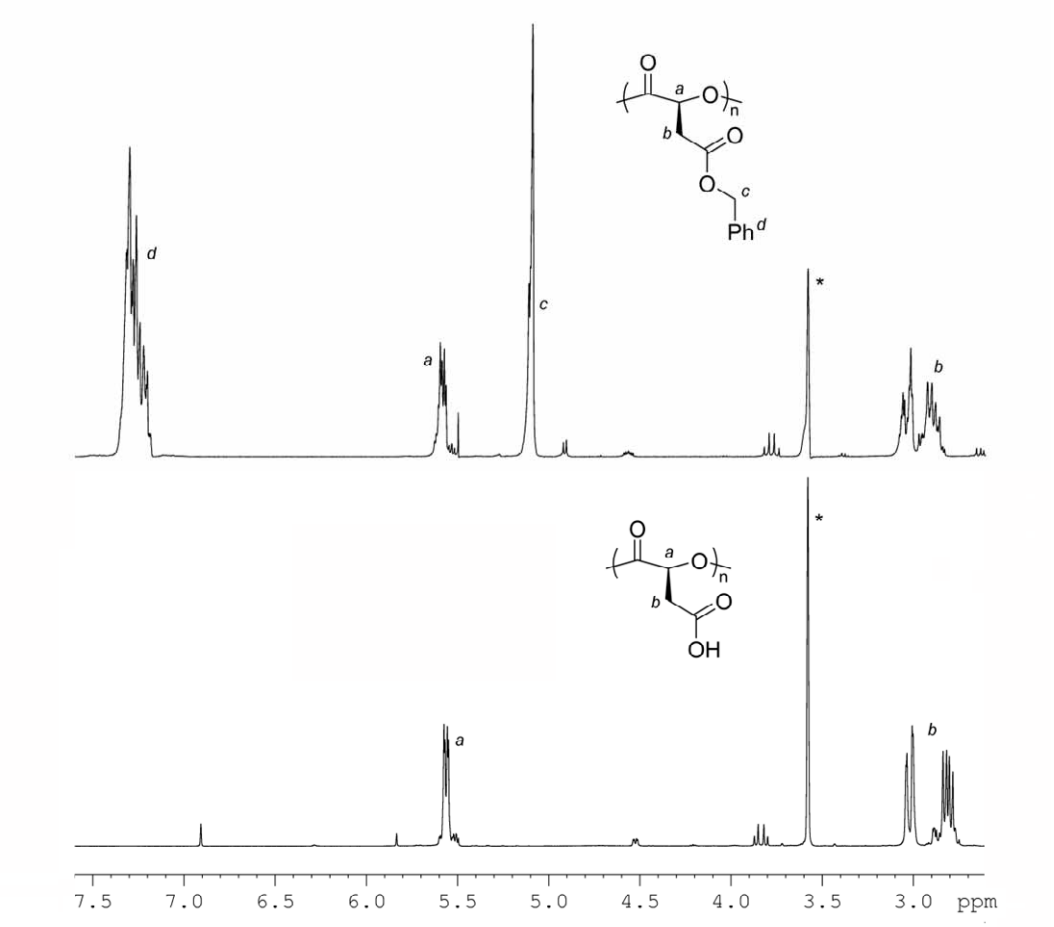


Figure S13. ^{1}H NMR spectra of (i) P(*L*-BMA)$_{20}$ and (ii) PMA$_{20}$ (d^{8}-THF, 400 MHz; * indicates residual solvent signal).

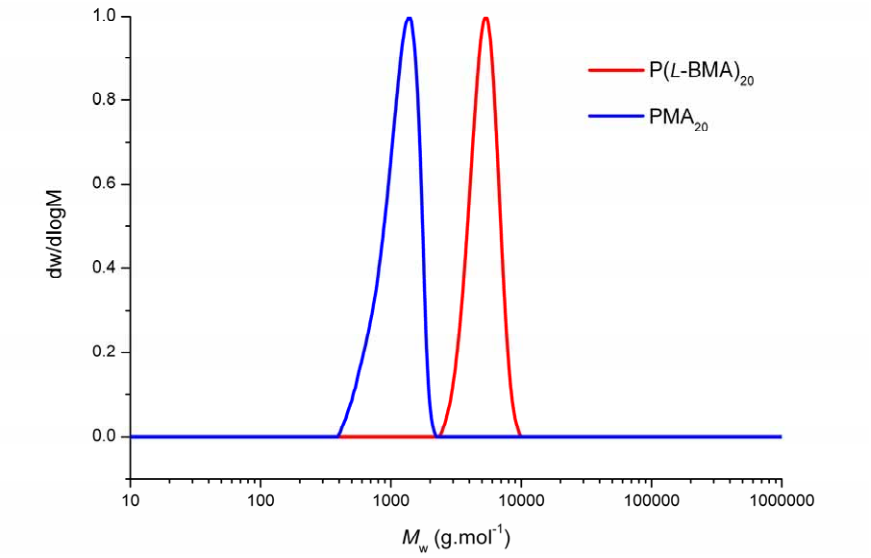


Figure S14. GPC traces of P(*L*-BMA)$_{20}$ (M_n = 4 980 g.mol^{-1}, PDI = 1.06) (—) and PMA$_{20}$ (M_n = 1 100 g.mol^{-1}, PDI = 1.10) (—) prepared by ROP of *L*-malOCA ([M]/[I] = 20) ([*L*-malOCA]$_0$ = 0.32 M) catalysed with 4-methoxypyridine using *neo*-pentanol as the initiator and subsequent hydrogenolysis using H_2 and Pd/C.

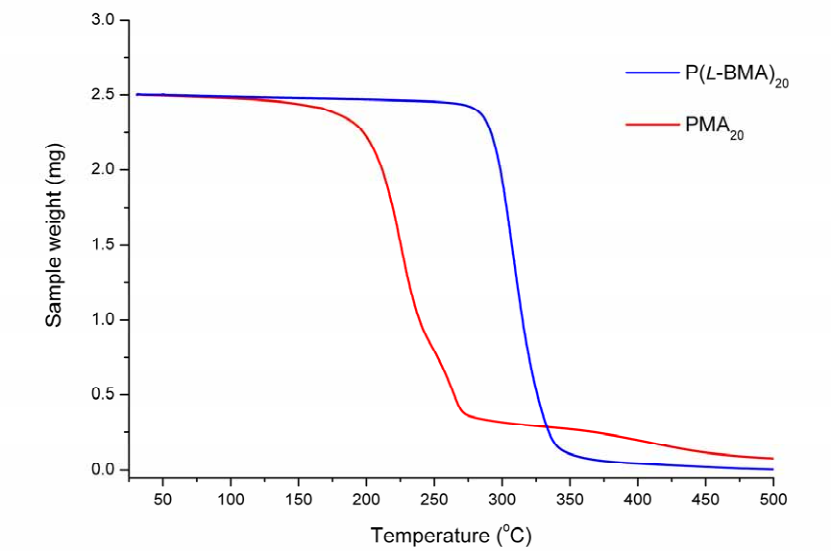


Figure S15. TGA analysis of both P(*L*-BMA)$_{20}$ (M_n = 4 980 g.mol^{-1}, PDI = 1.06) (▬) and PMA$_{20}$ (M_n = 1 100 g.mol^{-1}, PDI = 1.10) (▬) from 25 to 500 °C (GPC values using 0.1 M citric acid in THF eluent compared to poly(styrene) standards).

Calculated transition states energies and coordinates

Methods

DFT calculations were performed using PC-GAMESS at the B3LYP/6-31G(d) level.[3,4] Transition state energies structures have an RMS gradient less than $1x10^{-4}$ Hartree/Bohr (apart from TS3A, see discussion). Energies and zero point energies (ZPE) (Hartrees/molecule), final gradients (Hartrees/Bohr), imaginary frequencies (cm^{-1}) and Cartesian coordinates (Ångstroms) are given for each structure. Zero-point energies are based on unscaled vibrational frequencies, and do not include imaginary frequencies.

Results

Transition state calculations for both 4-DMAP and 4-methoxypyridine catalysed opening of lactic acid OCA by methanol were performed. The transition structures for the 4-DMAP catalysed opening at the ester-like carbonyl are essentially identical to both those published by Cossio, Bourissou and coworkers (2 similar TS structures TS1 and TS2).[5] The transition structures for the opening at the equivalent carbonate-like carbonyl are higher in energy (TS3 and TS4). The combined energy differences lead to an estimate of the selectivity at 298 K to be roughly 18 to 1 in favour of the ester opening.

In the case of the 4-methoxypyridine catalysed transition state reactions there are eight rather than four equivalent transition structures due to two orientations (rotamers) of the methoxy-group. Seven of the eight transition structures were easily calculated within standard tolerances of gradient, however the eighth structure found (TS3A) has a higher final gradient (see below). It is included in order to make a fair comparison between the two pathways, i.e. four transition structures each. Transition structure 3A is very close to the reaction tetrahedral intermediate, as are all of the carbonate opening transition structures. TS3A has the lowest energy (including ZPE) of all of the four carbonate transition states. This low energy is significantly responsible for the calculated 9 to 1 selectivity for the ester opening. This reaction is therefore calculated to be less selective than the DMAP reaction. Even if the energy of TS3A (+ 5.0 kJ / mol) is too inaccurate, an energy of + 8.1 kJ / mol (i.e. the same as its methoxy-rotamer TS3B) would result in an overall selectivity of roughly 20 to 1 in favour of the ester opening pathway at 298 K i.e. similar to the calculated DMAP selectivity.

In the case of the pyridine catalysed reactions, four transition states were found. Given the reduced basicity of pyridine compared with DMAP and 4-methoxypyridine it is not surprising the observed transition structures are later (more product-like). In the case of the carbonate opening structures the larger degree of ring opening has lead to higher energies, raising the energies of this pathway. According to these unsolvated calculations opening at the carbonate carbon can occur, but at less than one percent of the rate of opening at the ester.

4-DMAP catalysed transition structure	Relative energy (including ZPE) kJ / mol
TS1 (ester)	3.6
TS2 (ester)	0
TS3 (carbonate)	6.7
TS4 (carbonate)	17.0

4-Methoxypyridine catalysed transition structure	Relative energy (including ZPE) kJ / mol
TS1A (ester)	7.8
TS1B (ester)	4.3
TS2A (ester)	0
TS2B ester 2b	2.7
TS3A (carbonate)	5.0
TS3B (carbonate)	8.1
TS4A (carbonate)	21.3
TS4B (carbonate)	18.4

Pyridine catalysed transition structure	Relative energy (including ZPE) kJ / mol
TS1 (ester)	4.7
TS2 (ester)	0
TS3 (carbonate)	16.2
TS4 (carbonate)	21.0

DATA

4-Dimethylaminopyridine catalysed ring-opening (4 transition states)

Ester TS1
ENERGY= -953.7229331
MAXIMUM GRADIENT = 0.0000702 RMS GRADIENT = 0.0000204
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.300242
IMAGINARY FREQUENT = 239.62 I cm^{-1}

C	6.0	1.5172512609	1.4015950801	-0.7768338228
C	6.0	2.8634250672	1.1182473407	-0.7974609898
C	6.0	3.3774824071	0.0787185694	0.0276697455
C	6.0	5.6330979655	0.4708723646	-0.8325170440
C	6.0	5.1841569294	-1.3384306890	0.8677076119
C	6.0	2.4356506225	-0.6110669226	0.8366474109
C	6.0	1.1026157928	-0.2672170089	0.7976729323
H	1.0	6.2621126506	-1.4347142425	0.7375235109
H	1.0	4.9848787340	-1.1514457151	1.9298938583
H	1.0	3.5059475543	1.6903775589	-1.4529510201
H	1.0	1.0835397712	2.1777888508	-1.3983074361
H	1.0	0.3445402812	-0.7852946705	1.3711634243
H	1.0	2.7350945092	-1.4262281974	1.4809919560
H	1.0	4.7181859022	-2.2914008910	0.5876008961
H	1.0	5.6503693509	1.5443527926	-0.6069562001
H	1.0	5.3787812622	0.3407277033	-1.8923074796
H	1.0	6.6371884145	0.0774201794	-0.6740001491

N	7.0	4.7000701880	-0.2402926682	0.0354394700
N	7.0	0.6542837524	0.7298047158	0.0085656724
C	6.0	-1.7880394953	-1.5300343571	-0.2245002159
C	6.0	-2.9288360748	0.4043927551	0.4867062740
C	6.0	-4.9682578820	-0.7954601336	-0.4314366370
C	6.0	-3.6001506080	-0.2148165333	-0.7549585825
H	1.0	-4.8925942111	-1.5399789634	0.3674089716
H	1.0	-5.4022764126	-1.2695687493	-1.3174385827
H	1.0	-5.6300771449	0.0044723061	-0.0873204785
H	1.0	-3.6545612317	0.5191549699	-1.5611804229
O	8.0	-0.9520755039	-2.3979754885	-0.3354773233
O	8.0	-3.5229520134	0.9197973053	1.4143877332
O	8.0	-1.9150010732	-0.7173949327	0.8280510812
O	8.0	-2.7006325894	-1.2561910260	-1.1920819417
C	6.0	-1.8989263630	2.7885776786	0.2320133164
H	1.0	-2.6514204864	2.8246577334	1.0294724255
H	1.0	-0.9437029421	3.1516973763	0.6441504753
H	1.0	-2.2005450919	3.4603644527	-0.5849701463
H	1.0	-0.4462005454	0.9981204011	-0.0412941889
O	8.0	-1.7710075683	1.4596535094	-0.2337712041

Ester TS2
ENERGY= -953.7240063
MAXIMUM GRADIENT = 0.0000979 RMS GRADIENT = 0.0000226
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.299931
IMAGINARY FREQUENT = 291.53 I cm^{-1}

C	6.0	1.6245823919	1.5969477084	-0.2385892666
C	6.0	2.9622657260	1.3515965068	-0.0208224684
C	6.0	3.4362099953	0.0114443745	0.0099346727
C	6.0	5.7130873891	0.7925270386	0.4427417096
C	6.0	5.1923832638	-1.6701940568	0.2709919627
C	6.0	2.4649655644	-1.0052188599	-0.1896331522
C	6.0	1.1431638333	-0.6754027580	-0.3994039679
H	1.0	6.2678425271	-1.6947430485	0.4475723852
H	1.0	4.6996412269	-2.2224111034	1.0810649931
H	1.0	3.6273643670	2.1911760580	0.1306224426
H	1.0	1.2290428850	2.6067924338	-0.2579233434
H	1.0	0.3764043964	-1.4345997601	-0.5296366701
H	1.0	2.7330830633	-2.0530378014	-0.1722938748
H	1.0	4.9907521201	-2.1872801372	-0.6752195596
H	1.0	5.4659972838	1.3813944157	1.3355004761
H	1.0	5.7611852662	1.4701556516	-0.4189294242
H	1.0	6.7027578327	0.3585650089	0.5862906798
N	7.0	4.7490082747	-0.2801849797	0.2234517649
N	7.0	0.7313091132	0.6091486134	-0.4298570110
C	6.0	-2.1840807124	-1.5798682865	-0.1780936055
C	6.0	-2.5987249041	0.5721567095	0.5742716786
C	6.0	-4.9666144948	-0.2661470164	0.9287860814
C	6.0	-3.8577535218	-0.0194269469	-0.0833976319

H	1.0	-4.6131036782	-0.9142208843	1.7370170270
H	1.0	-5.8286539303	-0.7389635514	0.4478419926
H	1.0	-5.2747597224	0.6875416032	1.3673615123
H	1.0	-4.2012345088	0.6090335493	-0.9078414312
O	8.0	-1.5681088342	-2.5645810094	-0.5222988597
O	8.0	-2.5814144339	1.3877526654	1.4746004996
O	8.0	-1.7428294757	-0.6734357607	0.7021679522
O	8.0	-3.4083839830	-1.2649474354	-0.6614385093
C	6.0	-1.9442180578	2.5100801304	-1.0761982058
H	1.0	-2.0394320590	3.0529258495	-0.1250013401
H	1.0	-1.1087983263	2.9353094551	-1.6523104323
H	1.0	-2.8615431079	2.6687968125	-1.6633565615
H	1.0	-0.3833085407	0.8565691378	-0.5940716587
O	8.0	-1.7171013606	1.1357882262	-0.8513924840

Carbonate TS3
ENERGY= -953.7215470
MAXIMUM GRADIENT = 0.0000850 RMS GRADIENT = 0.0000169
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.300032
IMAGINARY FREQUENT = 263.55 I cm^{-1}

C	6.0	1.7103390486	-1.1473293014	1.1278817370
C	6.0	3.0445436884	-0.8130230758	1.0612924150
C	6.0	3.5228790076	-0.0375667565	-0.0313992742
C	6.0	2.5614317155	0.3504560218	-1.0026459669
C	6.0	1.2429557802	-0.0255328736	-0.8636973024
N	7.0	0.8308129402	-0.7686378526	0.1842780878
N	7.0	4.8337358858	0.3162307155	-0.1370942472
C	6.0	5.2832547201	1.1359294791	-1.2583677771
C	6.0	5.7861887423	-0.0753578515	0.8964484337
H	1.0	1.3073493222	-1.7288396539	1.9506537305
H	1.0	3.7045617191	-1.1437005473	1.8517588831
H	1.0	2.8373311442	0.9509653294	-1.8588228477
H	1.0	0.4508325958	0.2498804400	-1.5573341111
H	1.0	4.7871804834	2.1147836153	-1.2674328946
H	1.0	5.0915554340	0.6397810162	-2.2176188492
H	1.0	6.3574970901	1.2996256534	-1.1710495938
H	1.0	5.8447409959	-1.1665948949	0.9940385119
H	1.0	5.5201095952	0.3482500479	1.8735625614
H	1.0	6.7762348304	0.2921721857	0.6261557957
H	1.0	-0.2832080164	-1.0191366372	0.2643468707
C	6.0	-2.6384189505	1.3066381330	1.2468126304
C	6.0	-2.1765923485	0.0877529596	-0.6497249717
O	8.0	-2.5119318921	2.0066745460	2.2237195993
O	8.0	-1.6783271347	0.0676594043	-1.7659871201
O	8.0	-1.6900679749	1.1065508727	0.3171628697
O	8.0	-3.5620457508	0.0526788231	-0.4784769322
C	6.0	-3.8777375977	0.5138321324	0.8328201978
C	6.0	-5.1484327682	1.3505069973	0.8234324929
H	1.0	-3.9789621060	-0.3406196235	1.5171223438

H	1.0	-5.0510490226	2.1841920644	0.1211854975
H	1.0	-5.3288741210	1.7523126093	1.8249972630
H	1.0	-6.0057523411	0.7404274562	0.5229920653
C	6.0	-1.9896685900	-2.4594539005	-0.3648425411
O	8.0	-1.6622850399	-1.2472723931	0.2941145458
H	1.0	-1.7084921193	-2.4213436881	-1.4260690384
H	1.0	-1.4575011812	-3.2872259019	0.1224322766
H	1.0	-3.0680845767	-2.6485760382	-0.2980061219

Carbonate TS4
ENERGY= -953.7177593
MAXIMUM GRADIENT = 0.0000508 RMS GRADIENT = 0.0000115
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.300144
IMAGINARY FREQUENT = 245.83 I cm^{-1}

C	6.0	1.6872630959	-1.5865297064	0.2465656360
C	6.0	3.0209761179	-1.2967437970	0.0644008438
C	6.0	3.4491977104	0.0588584156	0.0307768322
C	6.0	2.4383105711	1.0447414888	0.1893568009
C	6.0	1.1236825058	0.6716129774	0.3642426575
N	7.0	0.7577574697	-0.6264306616	0.4004537481
H	1.0	1.3228831913	-2.6079905208	0.2659012936
H	1.0	3.7184579949	-2.1140299946	-0.0594280431
H	1.0	2.6711391463	2.1006597349	0.1636615739
H	1.0	0.3260758921	1.4023740148	0.4576130430
H	1.0	-0.3372284355	-0.9083309583	0.5277271563
C	6.0	-2.3138420806	1.4320648210	0.0039958564
C	6.0	-2.4438075358	-0.7533166407	-0.7473267915
O	8.0	-1.8451878238	2.4915159658	0.3759444557
O	8.0	-2.2585525918	-1.5609352510	-1.6267861057
O	8.0	-1.6942102513	0.5786795712	-0.8065696167
O	8.0	-3.7300703196	-0.3820540699	-0.3332099816
C	6.0	-3.6663056699	0.8389266747	0.3945095111
C	6.0	-4.8409346359	1.7416029572	0.0394958291
H	1.0	-3.6459756930	0.6376007039	1.4744879675
H	1.0	-4.8637325142	1.9332252973	-1.0377675541
H	1.0	-4.7472510500	2.6953868125	0.5679985817
H	1.0	-5.7836588074	1.2661061105	0.3268711782
C	6.0	-2.0097596743	-2.5347063615	1.0522447255
O	8.0	-1.7062330736	-1.1917458825	0.7265556973
H	1.0	-1.9035347600	-3.1841953000	0.1729266232
H	1.0	-1.3308443986	-2.8744928965	1.8468104878
H	1.0	-3.0409289758	-2.6153983256	1.4207162030
N	7.0	4.7561782892	0.3932407819	-0.1488425431
C	6.0	5.1525998117	1.7973247990	-0.2047375327
C	6.0	5.7614369107	-0.6477057402	-0.3372026640
H	1.0	4.8990620249	2.3210624258	0.7249958592
H	1.0	4.6709226199	2.3191629134	-1.0412425859
H	1.0	6.2322772353	1.8569919361	-0.3426194920
H	1.0	5.5582986476	-1.2475440029	-1.2336384684

H	1.0	5.8084282710	-1.3196154436	0.5288364361
H	1.0	6.7395449538	-0.1812233037	-0.4554111718

4-Methoxypyridine catalysed ring-opening (8 transition states)

Ester TS1A
ENERGY= -934.2701842
MAXIMUM GRADIENT = 0.0000975 RMS GRADIENT = 0.0000204
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.260117
IMAGINARY FREQUENT = 172.06 I cm^{-1}

C	6.0	-1.8430561905	-1.1642763547	-0.7862077509
C	6.0	-3.1830058928	-0.8249913890	-0.7540544947
C	6.0	-3.6023445669	0.1522340183	0.1688294235
C	6.0	-5.8838940407	0.0357777350	-0.5345087010
C	6.0	-2.6461327250	0.7446385421	1.0131546609
C	6.0	-1.3264591934	0.3578928331	0.9193294939
H	1.0	-5.9873112778	-1.0443378944	-0.3825733521
H	1.0	-5.6730015523	0.2484581919	-1.5883547463
H	1.0	-6.8046538033	0.5369055379	-0.2369449310
O	8.0	-4.8646762050	0.5774162617	0.3107322206
N	7.0	-0.9499432438	-0.5915534032	0.0357136803
H	1.0	-1.4470572589	-1.9015034965	-1.4759975454
H	1.0	-3.8709094757	-1.3091266077	-1.4346666010
H	1.0	-2.9517514170	1.5099531025	1.7162944057
H	1.0	-0.5266599686	0.7896399027	1.5070678363
C	6.0	1.5446510954	1.4978756148	-0.1386296053
C	6.0	2.6293624333	-0.5650022930	0.3765629526
C	6.0	4.6833087489	0.6858965624	-0.4300558701
C	6.0	3.3038561059	0.1648594382	-0.8028162043
O	8.0	0.7353135588	2.3996936703	-0.1874620302
O	8.0	3.2297684626	-1.1559930608	1.2545429842
O	8.0	1.6587274525	0.6189949510	0.8514675331
O	8.0	2.4276164483	1.2574254129	-1.1459738524
H	1.0	4.6219397514	1.3438196308	0.4423242795
H	1.0	5.1188097797	1.2433180300	-1.2653490324
H	1.0	5.3354624172	-0.1541406956	-0.1749485807
H	1.0	3.3457540133	-0.4922736910	-1.6746714412
C	6.0	1.5053632806	-2.8343102868	-0.0176093807
O	8.0	1.4386040211	-1.4562300374	-0.3474550278
H	1.0	2.2551674250	-2.9835787698	0.7671624939
H	1.0	0.5322171820	-3.1848870672	0.3585454694
H	1.0	1.7726327114	-3.4290619347	-0.9021334143
H	1.0	0.1173598657	-0.9040764668	-0.0549452944

Ester TS1B
ENERGY= -934.2712829
MAXIMUM GRADIENT = 0.0000980 RMS GRADIENT = 0.0000198
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.259871

IMAGINARY FREQUENT = 194.22 I cm^{-1}

C	6.0	-1.7589748648	1.4422242537	0.8696920422
C	6.0	-3.1090830628	1.1813786304	0.9075869770
C	6.0	-3.6271972476	0.1562119231	0.0890851846
C	6.0	-5.5393631067	-1.0930966321	-0.6122424903
C	6.0	-2.7478057303	-0.5618701115	-0.7364031070
C	6.0	-1.3999658222	-0.2410972361	-0.7193328050
H	1.0	-5.1216119071	-2.0700451390	-0.3456666086
H	1.0	-5.3990107862	-0.9036803616	-1.6822294601
H	1.0	-6.6018749381	-1.0690571139	-0.3713114315
O	8.0	-4.9474976109	-0.0523123331	0.1736265049
N	7.0	-0.9310390500	0.7451172784	0.0631772520
H	1.0	-1.2924398480	2.2068473918	1.4805625003
H	1.0	-3.7738366229	1.7403555525	1.5552789628
H	1.0	-3.0849293455	-1.3685145351	-1.3736705686
H	1.0	-0.6557019790	-0.7676905914	-1.3031300009
C	6.0	1.4585108124	-1.5283344436	0.1762923044
C	6.0	2.6192990783	0.4405920971	-0.4882527339
C	6.0	4.6519717527	-0.8841659581	0.2539503277
C	6.0	3.3249991651	-0.2761862475	0.6812126893
O	8.0	0.6044235205	-2.3799600787	0.3022992282
O	8.0	3.1946873732	0.9658878125	-1.4226615378
O	8.0	1.5582048942	-0.6886373372	-0.8505667246
O	8.0	2.4147911392	-1.3077326231	1.1165336301
H	1.0	4.5070611521	-1.5714247746	-0.5853274801
H	1.0	5.1068223548	-1.4305058685	1.0861228553
H	1.0	5.3296644895	-0.0901827605	-0.0722707861
H	1.0	3.4500153686	0.4102065319	1.5217647653
C	6.0	1.6691929746	2.7983995374	-0.0974016077
O	8.0	1.5255088723	1.4384625542	0.2782911959
H	1.0	2.3845294977	2.8729046859	-0.9241927056
H	1.0	0.7044219966	3.2069854742	-0.4351674910
H	1.0	2.0233156270	3.3977707315	0.7529063963
H	1.0	0.1645715386	0.9889409289	0.0898277435

Ester TS2A
ENERGY= -934.2727181
MAXIMUM GRADIENT = 0.0000802 RMS GRADIENT = 0.0000180
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.259667
IMAGINARY FREQUENT = 218.07 I cm^{-1}

C	6.0	1.8668953197	1.6899099702	-0.1418961272
C	6.0	3.2081617997	1.4712629556	0.0798039427
C	6.0	3.6884438640	0.1467261249	0.0874366912
C	6.0	5.5530604765	-1.3238919720	0.3479965073
C	6.0	2.7809084537	-0.9020067625	-0.1301740076
C	6.0	1.4440188824	-0.6025759000	-0.3437244040
H	1.0	5.4187587381	-1.8329576546	-0.6127782739
H	1.0	5.0993832258	-1.9144413470	1.1512565352

H	1.0	6.6161680433	-1.1890168545	0.5465027003
O	8.0	5.0018631612	-0.0033305808	0.3099086090
N	7.0	1.0100580969	0.6700881440	-0.3529067723
H	1.0	1.4358774314	2.6846649312	-0.1497159325
H	1.0	3.8922778092	2.2934398085	0.2526048205
H	1.0	3.0885064297	-1.9395954909	-0.1292266979
H	1.0	0.6948662906	-1.3773879682	-0.4938989217
C	6.0	-1.8101096184	-1.5880939068	-0.2383094842
C	6.0	-2.3342647497	0.5500209122	0.5375183527
C	6.0	-4.6555684411	-0.4237686886	0.8561610980
C	6.0	-3.5532318122	-0.1032302206	-0.1414640834
O	8.0	-1.1459707925	-2.5364960917	-0.6035963974
O	8.0	-2.3795648925	1.3276834949	1.4718472814
O	8.0	-1.4221907763	-0.6924646418	0.6696936817
O	8.0	-3.0369854896	-1.3130796521	-0.7397215185
H	1.0	-4.2732198389	-1.0606027797	1.6600243801
H	1.0	-5.4851591943	-0.9378630437	0.3608291489
H	1.0	-5.0203481236	0.5053380100	1.3036910610
H	1.0	-3.9234936740	0.5193880451	-0.9594707327
C	6.0	-1.7308360847	2.5319295972	-1.0067748349
O	8.0	-1.4585573927	1.1594991927	-0.7978018005
H	1.0	-1.8375778529	3.0580876219	-0.0491489380
H	1.0	-0.9096566337	2.9803258956	-1.5831515447
H	1.0	-2.6548583640	2.6655964156	-1.5878937305
H	1.0	-0.0952106015	0.8913860435	-0.5194821842

Ester TS2B
ENERGY= -934.2717505
MAXIMUM GRADIENT = 0.0000481 RMS GRADIENT = 0.0000142
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.259714
IMAGINARY FREQUENT = 194.86 I cm^{-1}

C	6.0	1.9624838866	1.3877954742	-0.2312109702
C	6.0	3.2890213414	1.0784570976	0.0153057768
C	6.0	3.6585188348	-0.2775626332	0.0673046015
C	6.0	5.9509366756	0.2182746658	0.5275666254
C	6.0	2.6685996135	-1.2575918330	-0.1286790789
C	6.0	1.3656227830	-0.8720207423	-0.3651297162
H	1.0	5.7437252366	0.8278356676	1.4142488872
H	1.0	6.0980560982	0.8641384332	-0.3454414965
H	1.0	6.8468943279	-0.3789153561	0.6954435735
O	8.0	4.9012437168	-0.7250759594	0.2972456992
N	7.0	1.0351430049	0.4378667241	-0.4205746092
H	1.0	1.6115363176	2.4129923308	-0.2741624151
H	1.0	4.0022300442	1.8781009579	0.1661343154
H	1.0	2.9353618918	-2.3068022581	-0.0818118292
H	1.0	0.5547267500	-1.5861468214	-0.4922146063
C	6.0	-1.9748056156	-1.5268353790	-0.1555751301
C	6.0	-2.2693256640	0.6953397133	0.4977562584
C	6.0	-4.6564758423	-0.0357209483	0.9515890779

C	6.0	-3.5681449566	0.1199656695	-0.0993445094
O	8.0	-1.4144984864	-2.5523261173	-0.4834925779
O	8.0	-2.2084672752	1.5301390630	1.3816373135
O	8.0	-1.4764275518	-0.6218782603	0.6872519727
O	8.0	-3.1879357207	-1.1657523508	-0.6374046762
H	1.0	-4.3030756919	-0.6559380060	1.7813071792
H	1.0	-5.5475873522	-0.4992957527	0.5168014325
H	1.0	-4.9180425590	0.9485364929	1.3508955725
H	1.0	-3.9108925993	0.7250190426	-0.9423757855
C	6.0	-1.5339524123	2.5026299669	-1.1894954478
O	8.0	-1.3859051612	1.1280097810	-0.8903250220
H	1.0	-1.5748626879	3.0985502600	-0.2680808018
H	1.0	-0.6845329241	2.8326531024	-1.8040626961
H	1.0	-2.4516505805	2.6832604417	-1.7683002910
H	1.0	-0.0414105063	0.7438858654	-0.6023833662

Carbonate TS3A
ENERGY= -934.2689795
MAXIMUM GRADIENT = 0.0011766 RMS GRADIENT = 0.0003367
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.257830
IMAGINARY FREQUENT = 68.01 I cm^{-1}

C	6.0	-2.0179060442	0.2012467972	1.3742821365
C	6.0	-3.3165311556	-0.1611033842	1.0723780074
C	6.0	-3.7178604230	-0.1616276733	-0.2760160257
C	6.0	-2.7858705516	0.2010398278	-1.2662143033
C	6.0	-1.5052351130	0.5525641873	-0.8888533913
N	7.0	-1.1508290358	0.5531507563	0.4155905730
O	8.0	-4.9521006725	-0.4937314096	-0.6824049893
C	6.0	-5.9063631561	-0.8599442125	0.3225381184
H	1.0	-1.6435880536	0.2119329793	2.3923445447
H	1.0	-3.9914981679	-0.4408608569	1.8693252127
H	1.0	-3.0735774698	0.1978266755	-2.3119319644
H	1.0	-0.6982095334	0.8333924272	-1.5651614468
H	1.0	-0.0959888961	0.8143757741	0.6798736500
H	1.0	-6.0753584042	-0.0297293592	1.0189435908
H	1.0	-5.5695406284	-1.7441407804	0.8762439250
H	1.0	-6.8307203643	-1.0886912290	-0.2090786360
C	6.0	2.4752087800	-1.4322107864	0.1447519105
C	6.0	1.8627492706	0.6890160684	-0.5539491000
O	8.0	2.4379905424	-2.5998210501	0.4583503009
O	8.0	1.3350777222	1.3404133998	-1.4516965012
O	8.0	1.4737904199	-0.7614219652	-0.4408333695
O	8.0	3.2560424320	0.6910269444	-0.4017931790
C	6.0	3.6480142819	-0.4683066137	0.3278922938
C	6.0	4.9645174731	-1.0201700986	-0.1978660150
H	1.0	3.7280085131	-0.2327458152	1.3995747243
H	1.0	4.8896554592	-1.2265320166	-1.2699676242
H	1.0	5.2055277861	-1.9507330155	0.3247082169
H	1.0	5.7725871021	-0.2998878752	-0.0375087938

C	6.0	1.5331560330	2.4891279846	1.1757855303
O	8.0	1.3070194174	1.1060022421	0.9354416734
H	1.0	1.1673340558	3.0997109817	0.3402963550
H	1.0	1.0095118142	2.7701828984	2.0976017870
H	1.0	2.6052739420	2.6791310392	1.3040222237

Carbonate TS3B
ENERGY= -934.2702958
MAXIMUM GRADIENT = 0.0000834 RMS GRADIENT = 0.0000205
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.260329
IMAGINARY FREQUENT = 69.49 I cm^{-1}

C	6.0	1.9662078166	0.4401467606	-1.6348386987
C	6.0	3.2686596520	0.0273121388	-1.4683811828
C	6.0	3.7485221171	-0.2029735001	-0.1624481149
C	6.0	2.8832701734	-0.0020601880	0.9252975765
C	6.0	1.5846252542	0.4156226011	0.6810320679
N	7.0	1.1556175226	0.6317924780	-0.5751828608
O	8.0	5.0229631771	-0.6072410374	-0.0688807633
C	6.0	5.5722851335	-0.8815378415	1.2243670532
H	1.0	5.0216313908	-1.6880485210	1.7206393721
H	1.0	5.5674050291	0.0169662152	1.8513707261
H	1.0	6.5996013461	-1.1962608111	1.0421544092
H	1.0	1.5314582621	0.6232851219	-2.6112670056
H	1.0	3.9235667965	-0.1299450845	-2.3170380926
H	1.0	3.1963125790	-0.1703661032	1.9474449573
H	1.0	0.8252643220	0.5847880281	1.4456380266
H	1.0	0.0869856867	0.9313793299	-0.7084857575
C	6.0	-2.4833695129	-1.3591975046	-0.3073808790
C	6.0	-1.7734117817	0.6040276571	0.6919719455
O	8.0	-2.4934101977	-2.4538706663	-0.8214389331
O	8.0	-1.1635744944	1.0877770243	1.6432642448
O	8.0	-1.4250224405	-0.8063523249	0.3022341059
O	8.0	-3.1745142070	0.6408235711	0.6608506694
C	6.0	-3.6487648866	-0.3731670354	-0.2206936899
C	6.0	-4.9260328250	-1.0027872397	0.3148998439
H	1.0	-3.8153862533	0.0445731777	-1.2246100910
H	1.0	-4.7630740357	-1.3959789431	1.3231027544
H	1.0	-5.2311500469	-1.8250033475	-0.3394048909
H	1.0	-5.7297649104	-0.2613173044	0.3561297395
C	6.0	-1.5505922772	2.6729055256	-0.7254551614
O	8.0	-1.3345509146	1.2678262355	-0.7446115741
H	1.0	-1.1092312895	3.1273292389	0.1709256872
H	1.0	-1.0936832578	3.1060627496	-1.6235337046
H	1.0	-2.6252013140	2.8893439770	-0.7338797661

Carbonate TS4A
ENERGY= -934.2652428
MAXIMUM GRADIENT = 0.0000554 RMS GRADIENT = 0.0000192
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.260319

IMAGINARY FREQUENT = 85.81 I cm^{-1}

C	6.0	2.0454487129	-1.3519831947	0.2446146724
C	6.0	3.3604069299	-0.9652684669	0.0552047074
C	6.0	3.6498316251	0.4103976349	0.0013186101
C	6.0	2.5950861444	1.3323706967	0.1373407732
C	6.0	1.3080428825	0.8731415269	0.3178861974
N	7.0	1.0577247948	-0.4545943068	0.3769511771
O	8.0	4.8716112353	0.9297303998	-0.1765220688
C	6.0	5.9879130161	0.0506784184	-0.3450521499
H	1.0	5.8623217937	-0.5767908373	-1.2344352499
H	1.0	6.1301655136	-0.5775506931	0.5412372918
H	1.0	6.8524125796	0.7013017846	-0.4749907293
H	1.0	1.7503546094	-2.3946226886	0.2860199082
H	1.0	4.1266614704	-1.7217109303	-0.0516097521
H	1.0	2.8017904272	2.3947863101	0.0872490115
H	1.0	0.4498729717	1.5359549354	0.3952720500
H	1.0	0.0194165339	-0.8191282057	0.5113584371
C	6.0	-2.1041564471	1.3044661577	0.0098366070
C	6.0	-2.1356904981	-0.9400152209	-0.6516945454
O	8.0	-1.6876457667	2.3944053325	0.3678437636
O	8.0	-1.9349141448	-1.7424648219	-1.5353435662
O	8.0	-1.4473552772	0.4724983986	-0.7811773025
O	8.0	-3.4373684365	-0.5905910799	-0.2534943585
C	6.0	-3.4249151977	0.6579762061	0.4275981085
C	6.0	-4.6438393164	1.4888896601	0.0464339901
H	1.0	-3.3920575394	0.5015665685	1.5152127605
H	1.0	-4.6796692995	1.6379266136	-1.0371905593
H	1.0	-4.5945994347	2.4653405214	0.5382573917
H	1.0	-5.5614196832	0.9794071208	0.3563762681
C	6.0	-1.5876248871	-2.6197428955	1.1303439137
O	8.0	-1.3730703978	-1.2708359653	0.7456248817
H	1.0	-1.4009035086	-3.2994413312	0.2898227339
H	1.0	-0.9119894083	-2.8545912097	1.9623671561
H	1.0	-2.6220389232	-2.7580571775	1.4689290668

Carbonate TS4B
ENERGY= -934.2660320
MAXIMUM GRADIENT = 0.0000844 RMS GRADIENT = 0.0000183
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.259996
IMAGINARY FREQUENT = 142.37 I cm^{-1}

C	6.0	1.9530198412	-1.6521069117	0.2089299872
C	6.0	3.2878120320	-1.3652472870	0.0324847186
C	6.0	3.6950795487	-0.0165834381	0.0026225383
C	6.0	2.7242471624	0.9873178270	0.1534865567
C	6.0	1.3986191854	0.6213355561	0.3239068534
N	7.0	1.0370488490	-0.6735505244	0.3558689976
O	8.0	5.0050817219	0.1996101632	-0.1750060371
C	6.0	5.4863880986	1.5467794499	-0.2382153613

H	1.0	5.2907232355	2.0774269629	0.7000563839
H	1.0	5.0314253248	2.0858051991	-1.0761903025
H	1.0	6.5616120457	1.4629854326	-0.3953138520
H	1.0	1.5728327823	-2.6671774675	0.2295006005
H	1.0	4.0219489369	-2.1524698331	-0.0901822486
H	1.0	2.9759783403	2.0395392000	0.1309782807
H	1.0	0.6015653620	1.3547195328	0.4169112991
H	1.0	-0.0411034733	-0.9500522691	0.4810720085
C	6.0	-1.9610731009	1.3955687148	0.0573284545
C	6.0	-2.1933778607	-0.8035318025	-0.6911393379
O	8.0	-1.4449198775	2.4305897566	0.4457285031
O	8.0	-2.0688814988	-1.5908922305	-1.6006662724
O	8.0	-1.3882414408	0.5376737641	-0.7724268193
O	8.0	-3.4548073724	-0.3650361299	-0.2577193801
C	6.0	-3.3286653851	0.8514774430	0.4688196633
C	6.0	-4.4744827900	1.7983965215	0.1345399191
H	1.0	-3.2985983061	0.6510141465	1.5491483162
H	1.0	-4.5074128094	1.9922632819	-0.9420378954
H	1.0	-4.3366812116	2.7470032701	0.6626869663
H	1.0	-5.4295488914	1.3578206271	0.4364768917
C	6.0	-1.7720165784	-2.6002904313	1.0296033405
O	8.0	-1.4458750229	-1.2592707630	0.7007762475
H	1.0	-1.6506978262	-3.2562745286	0.1585076206
H	1.0	-1.1135970943	-2.9302010603	1.8434514099
H	1.0	-2.8121398577	-2.6639187232	1.3732694058

Pyridine catalysed ring-opening (4 transition states)

Ester TS1
ENERGY= -819.7407572611
MAXIMUM GRADIENT = 0.0000549 RMS GRADIENT = 0.0000157
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.227404
IMAGINARY FREQUENT = 183.60 I cm^{-1}

C	6.0	2.56610	-0.96811	0.87393
C	6.0	3.88145	-0.53419	0.87550
C	6.0	4.26167	0.45067	-0.04190
C	6.0	3.31874	0.97228	-0.92567
C	6.0	2.01192	0.50006	-0.87933
N	7.0	1.67719	-0.45566	0.00426
H	1.0	2.18188	-1.71849	1.55579
H	1.0	4.58908	-0.95385	1.58152
H	1.0	3.57943	1.74646	-1.63806
H	1.0	1.20303	0.86402	-1.49988
C	6.0	-0.88409	1.47901	0.07758
C	6.0	-1.88425	-0.66529	-0.38615
C	6.0	-3.98019	0.54156	0.37155
C	6.0	-2.58597	0.07930	0.76718
O	8.0	-0.11673	2.41959	0.12479
O	8.0	-2.46234	-1.28461	-1.25767

O	8.0	-0.95303	0.58806	-0.89867
O	8.0	-1.75329	1.20862	1.09242
H	1.0	-3.93486	1.17489	-0.51976
H	1.0	-4.43740	1.10904	1.18818
H	1.0	-4.60388	-0.32618	0.13897
H	1.0	-2.61329	-0.55683	1.65571
C	6.0	-0.63944	-2.85212	-0.00472
O	8.0	-0.66696	-1.47003	0.32766
H	1.0	-1.37011	-3.04812	-0.79601
H	1.0	0.35912	-3.13362	-0.36992
H	1.0	-0.87537	-3.46051	0.87844
H	1.0	0.62954	-0.83120	0.06195
H	1.0	5.28572	0.81159	-0.05950

Ester TS2
ENERGY= -819.7424935388
MAXIMUM GRADIENT = 0.0000512 RMS GRADIENT = 0.0000129
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.227333
IMAGINARY FREQUENT = 139.91 I cm^{-1}

C	6.0	2.7397675522	-1.2420329660	0.0101490095
C	6.0	4.0401895047	-0.8679902843	-0.2913907056
C	6.0	4.3407779802	0.4939445016	-0.3767854855
C	6.0	3.3343225355	1.4352856272	-0.1638249503
C	6.0	2.0460747346	1.0024353372	0.1312455075
N	7.0	1.7877047710	-0.3158155707	0.2156944648
H	1.0	2.4230766910	-2.2760571678	0.0866537442
H	1.0	4.7961978667	-1.6269943782	-0.4581950355
H	1.0	3.5330536080	2.4990972815	-0.2297188777
H	1.0	1.2057778405	1.6786175289	0.2839175700
C	6.0	-1.2849257684	1.5091204992	0.1671328212
C	6.0	-1.5705839682	-0.7512607245	-0.4291143450
C	6.0	-3.9941620457	-0.0607294013	-0.7277279458
C	6.0	-2.8337947519	-0.1821250229	0.2475219441
O	8.0	-0.7334253053	2.5544883429	0.4541673128
O	8.0	-1.5675666019	-1.5783757850	-1.3229115238
O	8.0	-0.8249899711	0.6193159698	-0.7043236301
O	8.0	-2.4454574769	1.1161317857	0.7466961292
H	1.0	-3.7091040459	0.5518709462	-1.5887050504
H	1.0	-4.8603991555	0.3955705898	-0.2384835392
H	1.0	-4.2665609314	-1.0545600349	-1.0944707069
H	1.0	-3.1084464706	-0.7815351446	1.1198590083
C	6.0	-0.6536791159	-2.5099043444	1.1627994854
O	8.0	-0.5791827038	-1.1315659364	0.8387443246
H	1.0	-0.6946190444	-3.1212776799	0.2529920765
H	1.0	0.2294092796	-2.7808267565	1.7561669812
H	1.0	-1.5438913123	-2.7216322588	1.7718648042
H	1.0	0.7470075504	-0.6635996730	0.4509653469
H	1.0	5.3509326259	0.8155646206	-0.6124891054

Carbonate TS3
ENERGY= - -819.7326211402
MAXIMUM GRADIENT = 0.0005799 RMS GRADIENT = 0.0001530
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.223628
IMAGINARY FREQUENT = 103.61 I cm^{-1}

C	6.0	-2.6513457732	0.9322307001	-0.8497813334
C	6.0	-3.9418932471	0.4306101851	-0.8794746600
C	6.0	-4.2696671064	-0.6256189465	-0.0237106202
C	6.0	-3.2998034161	-1.1480073099	0.8302217621
C	6.0	-2.0192900090	-0.6068674274	0.8165306077
N	7.0	-1.7351197160	0.4147078611	-0.0112509115
H	1.0	-2.3104530767	1.7409343641	-1.4854649145
H	1.0	-4.6704303531	0.8540870582	-1.5612711605
H	1.0	-5.2733530309	-1.0400291921	-0.0304568971
H	1.0	-3.5193945478	-1.9740288853	1.4967557824
H	1.0	-1.1877490571	-0.9610458769	1.4135199351
H	1.0	-0.7196783057	0.8310995351	-0.0514200681
C	6.0	1.1459690751	-1.3672967656	0.0790755805
C	6.0	1.7416306926	0.9078158983	0.5851117184
O	8.0	0.5534978644	-2.4283780756	-0.0398848480
O	8.0	2.0263457672	1.6431066980	1.5002556456
O	8.0	0.8769092029	-0.4464038578	0.9831627547
C	6.0	0.7412280653	2.8410260438	-0.5969574662
O	8.0	0.6341056768	1.4354444229	-0.4021497755
H	1.0	0.9342943730	3.3440147856	0.3556965040
H	1.0	-0.2032379803	3.2015912496	-1.0250538157
H	1.0	1.5543464924	3.0706728962	-1.2974933995
O	8.0	2.7277583148	0.3342151219	-0.2250440914
C	6.0	2.2755150194	-0.8714567002	-0.8280378734
C	6.0	3.4198214977	-1.8665851696	-0.9560960168
H	1.0	1.8400497141	-0.6623716291	-1.8173670032
H	1.0	3.8705098955	-2.0547535651	0.0232048212
H	1.0	3.0389945133	-2.8105274207	-1.3575725337
H	1.0	4.1931584472	-1.4781742309	-1.6258166946

Carbonate TS4
ENERGY= - -819.7352447391
MAXIMUM GRADIENT = 0.0003019 RMS GRADIENT = 0.0001057
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.228073
IMAGINARY FREQUENT = 74.95 I cm^{-1}

C	6.0	2.82329	-1.05283	0.07619
C	6.0	4.10627	-0.57574	-0.14092
C	6.0	4.30227	0.80609	-0.20945
C	6.0	3.21352	1.66610	-0.06515
C	6.0	1.94567	1.13510	0.14226
N	7.0	1.79263	-0.20087	0.21361
H	1.0	2.57977	-2.10738	0.13512
H	1.0	4.92906	-1.27194	-0.25700

H	1.0	5.29704	1.20695	-0.38002
H	1.0	3.33385	2.74211	-0.12012
H	1.0	1.04220	1.73754	0.23163
H	1.0	0.80056	-0.62297	0.37319
C	6.0	-1.43104	1.28792	0.01479
C	6.0	-1.43524	-1.03137	-0.56026
O	8.0	-1.04627	2.40085	0.35550
O	8.0	-1.28487	-1.82051	-1.46492
O	8.0	-0.77951	0.47804	-0.78475
C	6.0	-0.56203	-2.65233	1.09123
O	8.0	-0.56087	-1.27948	0.71348
H	1.0	-0.42606	-3.29120	0.21169
H	1.0	0.25795	-2.80621	1.80305
H	1.0	-1.50657	-2.91657	1.58232
O	8.0	-2.70895	-0.67477	-0.10460
C	6.0	-2.71546	0.61360	0.50054
H	1.0	-2.66081	0.52503	1.59476
C	6.0	-3.97215	1.37423	0.09088
H	1.0	-4.01730	1.47149	-0.99847
H	1.0	-3.96538	2.37360	0.53691
H	1.0	-4.86552	0.83869	0.42668

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