

Article

Hydrolytic Degradation of Polylactic Acid Fibers as a Function of pH and Exposure Time

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Appendix A: XRD Analysis

Table S1. Peak height and area ratios with respect to highest intensity peak measured from XRD.

pH Peak Ratios		10	7.4	3	2	Control
16.4:28.5	Peak Height Ratio	70.15	65.13	70.96	68.11	-
16.4:28.5	Area Under Curve Ratio	150.28	155.63	187.21	223.68	-

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Appendix B: Fukui Analysis

Table S2: Fukui analysis illustrating charge distribution for the atoms in PLA chain, where Figures S2, S3 and S4 illustrate a pictorial representation for nucleophilic, electrophilic and radical addition, respectively.

Atom	Atom Type	f(nuc)	f(elec)	f(radikal)
1	C	0.00042	0.00209	0.001255
2	O	0.03854	0.03916	0.03885
3	C	0.05058	0.00185	0.026215
4	O	0.01693	0.01132	0.014125
5	H	0.0125	0.00655	0.009525
6	C	-0.00045	-0.00115	-0.0008
7	H	0.00501	0.00426	0.004635
8	H	0.0051	0.0046	0.00485
9	H	0.01165	0.00458	0.008115
10	H	0.00715	0.00367	0.00541
11	C	0.00215	0.00475	0.00345
12	O	0.03347	0.0716	0.052535
13	C	0.03587	0.00156	0.018715
14	O	0.01304	0.01859	0.015815
15	H	0.02395	0.01147	0.01771
16	C	-0.00312	-0.00147	-0.00229
17	H	0.00729	0.00676	0.007025
18	H	0.00712	0.0066	0.00686
19	H	0.01135	0.00749	0.00942
20	C	-0.00012	0.00656	0.00322
21	O	0.06375	0.09287	0.07831
22	C	0.07963	0.00125	0.04044

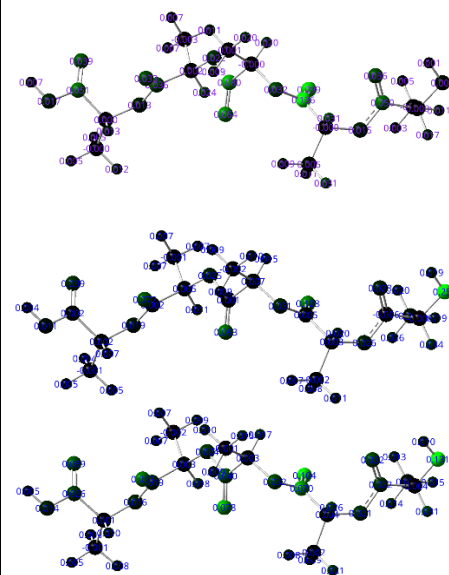


Figure S1: Nucleophilic, electrophilic and radical attack sites for PLA pentamer. High reactivity sites are shown by green color.

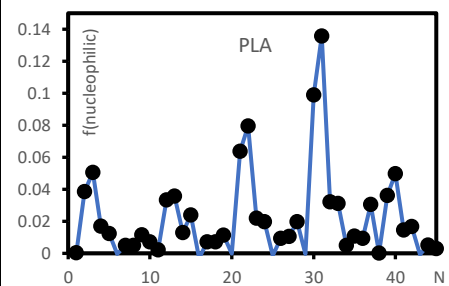


Figure S2: Fukui reactivity indices for nucleophilic addition

23	O	0.02201	0.02508	0.023545
24	H	0.01978	0.015	0.01739
25	C	-0.00132	-0.00158	-0.00145
26	H	0.0094	0.00878	0.00909
27	H	0.01069	0.00857	0.00963
28	H	0.01988	0.00963	0.014755
29	C	-0.00038	0.00801	0.003815
30	O	0.09893	0.10848	0.103705
31	C	0.13587	0.00469	0.07028
32	O	0.03216	0.03092	0.03154
33	H	0.03113	0.02042	0.025775
34	C	0.00504	-0.00169	0.001675
35	H	0.0109	0.00769	0.009295
36	H	0.0094	0.00704	0.00822
37	H	0.03067	0.01122	0.020945
38	C	0.00013	-0.0083	-0.00409
39	O	0.03619	0.02773	0.03196
40	C	0.04972	-0.00615	0.021785
41	O	0.01469	0.02642	0.020555
42	H	0.01689	0.0442	0.030545
43	C	-0.00076	0.01088	0.00506
44	H	0.00522	0.01986	0.01254
45	H	0.00307	0.02583	0.01445
46	H	0.01105	0.01852	0.014785
47	O	0.00677	0.25466	0.130715

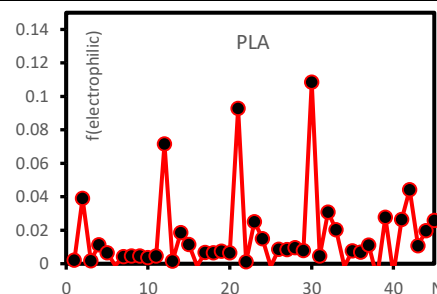


Figure S3: Fukui reactivity indices for electrophilic addition

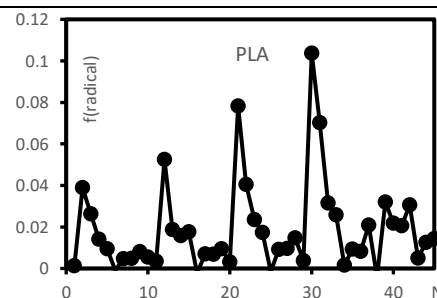


Figure S4: Fukui reactivity indices for radical addition

48	H	0.00108	0.01909	0.010085	
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