Table S1. Atomic coordinates of optimized nylon 6/6 model molecule.

Tag	Symbol	X	Y	Z
1	C	6.870033	-0.6248	0.145902
2	C	5.571194	-0.36253	-0.57873
3	H	5.352198	-1.23815	-1.20249
4	H	5.742719	0.460725	-1.28374
5	C	4.413295	-0.0524	0.366723
6	H	4.679136	0.811775	0.986601
7	H	4.284692	-0.88991	1.062263
8	C	3.108225	0.210242	-0.3845
9	H	2.834085	-0.65319	-0.99914
10	H	3.239611	1.049267	-1.08012
11	C	1.938855	0.51354	0.553683
12	H	2.126866	1.429472	1.127321
13	H	1.838554	-0.29918	1.286301
14	C	0.61608	0.606991	-0.20035
15	C	-1.62509	1.622484	-0.24099
16	H	-1.55963	1.473774	-1.32189
17	H	-1.9898	2.640064	-0.06286
18	C	-2.58366	0.591618	0.362765
19	H	-2.61388	0.716508	1.453862
20	H	-2.17616	-0.40668	0.16712
21	C	-3.99775	0.700578	-0.21128
22	H	-3.95582	0.583018	-1.30251
23	H	-4.39257	1.710289	-0.02857
24	C	-4.96552	-0.33307	0.370834
25	H	-5.00382	-0.21875	1.463309
26	H	-4.57018	-1.34098	0.18443
27	C	-6.37923	-0.22735	-0.20504
28	H	-6.35659	-0.35231	-1.29406
29	H	-6.77278	0.782864	-0.01849
30	C	-7.34515	-1.25561	0.380667
31	H	-7.35256	-1.15371	1.481801
32	H	-6.96812	-2.26369	0.167152
33	O	7.034976	-0.59797	1.345779
34	O	0.364453	-0.09821	-1.17221
35	N	-0.26958	1.527174	0.283355
36	H	-0.05084	1.998034	1.148168
37	N	-8.66795	-1.13231	-0.24008
38	H	-9.29377	-1.84127	0.134692
39	H	-9.07731	-0.23522	0.013901
40	O	7.876367	-0.90461	-0.72002
41	H	8.664599	-1.05858	-0.17247