Supporting Information

Quantitative study on the pyrolysis of levoglucosan to form small molecular gases

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3D images of all structures
Results of geometric optimization of all structures in this paper

Supporting Figure S1 The result Graph of geometric Optimization of all structures covered in this essay [bond length:0.1nm]

| Structure | Bond Lengths |
|-----------|--------------|
| 1         | R(1,6)1.461; R(1,10)1.426; R(6,11)1.547; R(11,2)1.456; R(2,10)1.434; R(10,9)1.556; R(9,8)1.562; R(8,7)1.560; R(7,6)1.546; R(8,4)1.439 |
| 4         | R(9,10)1.537; R(10,1)1.226; R(10,2)1.358; R(2,16)0.988 |
| 5+3       | R(9,10)4.041; R(1,10)1.181; R(10,2)1.177; R(9,5)1.448 |
| 6         | R(1,6)1.230; R(6,11)1.515; R(10,2)1.221; R(9,10)1.537 |
| 7         | R(11,6)1.509; R(6,7)1.553; R(7,8)1.567; R(8,9)1.571; R(9,10)1.535; R(10,2)1.226 |
| 8+2       | R(6,7)3.839; R(7,3)1.147; R(11,6)1.515; R(6,1)1.221 |
|   | R(7,8)   | R(8,4)   | R(4,18) | R(8,9)   |
|---|----------|----------|----------|----------|
| 25 | 1.348    | 1.378    | 0.981    | 1.530    |
| 25+52 | 3.668 | 1.348 | 0.979 | 0.979 |
| 26 | 1.377    | 1.351    | 0.979    | 0.979    |
| 26+52 | 1.357 | 0.983 | 0.983 | 1.977 |
| 27 | 1.542    | 1.451    | 1.451    | 1.222    |
| 28 | 1.547    | 1.448    | 1.447    | 1.422    |
| 29 | 1.543    | 1.451    | 1.435    | 1.437    |
| 30 | 1.558    | 1.442    | 1.456    | 1.421    |
| 30+52 | 1.554 | 1.442 | 1.456 | 1.421 |

43+3
R(8,9)4.147; R(2,9)1.179
R(1,9)1.179

44+3
R(8,9)3.991; R(9,1)1.177
R(2,9)1.180

45+3
R(7,8) 3.890; R(8,2)1.180
R(8,1)1.177

46+3
R(8,9)4.056; R(2,9)1.178
R(1,9)1.180

47+2
R(8,9)3.994; R(1,9)1.144
R(1,9)1.144

48+2
R(8,9)3.930; R(1,9)1.146
R(1,9)1.146

49+2
R(8,9)4.112; R(1,9)1.143
R(7,8)4.098; R(8,1)1.146

50+2
R(7,8)4.098; R(8,1)1.146
R(5,10)3.968; R(10,2)1.144

51+2
TS13
R(6,13)2.244; R(13,7)1.127
R(7,3)1.186; R(7,6)2.523

TS14
R(2,10)1.191; R(10,16)1.090
R(10,9)2.253; R(9,16)1.797

TS15
R(7,8)2.700; R(8,4)1.190
R(8,14)1.118; R(14,7)2.394

TS16
R(10,9)1.414; R(9,20)1.527
R(20,2)1.366; R(2,10)1.296

TS17
R(10,16)1.093; R(16,9)1.851
R(9,10)2.180; R(10,2)1.188

TS18
R(9,10)2.251; R(10,2)1.186
R(10,16)1.086; R(16,9)2.080

TS19
R(7,8)1.447; R(8,14)1.541
R(14,3)1.247; R(3,7)1.853

TS20
R(7,13)1.451; R(13,4)1.271
R(4,8)1.910; R(8,7)1.448

TS21
R(8,9)1.436; R(9,15)1.392
R(15,4)1.325; R(4,8)1.990

TS22
R(8,9)1.437; R(9,5)1.951
R(5,14)1.316; R(14,8)1.404

TS23
R(6,7)1.413; R(7,3)1.356
R(3,17)1.548; R(17,6)1.897

TS24
R(6,7)1.416; R(7,17)1.522
R(17,3)1.343; R(3,6)1.302
TS25
R(7,8)1.424; R(8,4)1.290
R(4,18)1.328; R(18,7)1.528

TS26
R(7,8)1.428; R(8,18)1.537
R(18,4)1.318; R(4,7)1.307

TS27
R(6,7)1.467; R(7,18)1.536
R(18,3)1.248; R(3,6)1.794

TS28
R(5,10)1.362; R(10,2)2.557
R(2,9)1.282; R(9,1)1.374
R(1,5)2.274

TS29
R(5,10)1.375; R(10,2)2.259
R(2,9)1.284; R(9,1)1.374
R(1,5)2.391

TS30
R(5,10)1.370; R(10,2)2.360
R(2,9)1.273; R(9,1)1.370
R(1,5)2.382

TS31
R(9,2)2.410; R(2,8)1.278
R(8,1)1.358; R(1,4)2.438
R(4,9)1.371

TS32
R(5,10)1.375; R(10,2)2.423
R(2,9)1.272; R(9,1)1.382
R(1,5)2.275

TS33
R(5,10)1.385; R(10,2)1.309
R(2,9)2.111; R(9,1)1.254
R(1,5)2.220

TS34
R(5,1)2.156; R(1,9)1.258
R(2,9)2.154; R(2,10)1.292

TS35
R(5,1)2.237; R(1,9)1.269
R(2,9)2.021; R(2,10)1.309

TS36
R(4,1)2.125; R(1,8)1.256
R(8,2)2.256; R(2,9)1.290
Supporting Table S1 Geometric coordinate information of levoglucosan

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| O1   | 0.40286 | -0.89920 | -1.3864 |
| O2   | -0.33466 | 1.26929  | -1.55121 |
| O3   | -0.08005 | -2.16437 | 1.15878 |
| O4   | -0.75091 | 1.36362  | 1.56408 |
| O5   | 2.43962  | -0.04988 | 0.56205 |
| C6   | -0.90774 | -0.88041 | -0.74101 |
| C7   | -0.68124 | -0.91863 | 0.78767 |
| C8   | 0.16925  | 0.29582  | 1.27395 |
| C9   | 1.26108  | 0.71691  | 0.23976 |
| C10  | 0.80263  | 0.45969  | -1.22515 |
| C11  | -1.50142 | 0.43979  | -1.28612 |
| H12  | -1.44561 | -1.78294 | -1.06931 |
| H13  | -1.65086 | -0.87272 | 1.31051 |
| H14  | 0.69411  | -0.03305 | 2.19144 |
| H15  | 1.45766  | 1.80426  | 0.34904 |
| H16  | 1.61337  | 0.66811  | -1.94735 |
| H17  | -2.03760 | 0.27863  | -2.23665 |
| H18  | -2.15536 | 0.95110  | -0.56318 |
| H19  | 0.76210  | -2.20668 | 0.65366 |
| H20  | -0.21346 | 2.15305  | 1.78199 |
| H21  | 3.10718  | 0.13496  | -0.13182 |