

Supporting Information

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

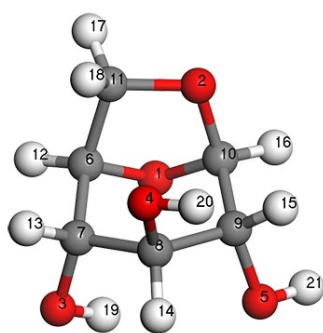
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^a School of Energy and Power Engineering, Northeast Electric Power University, Jilin 132000, China

3D images of all structures

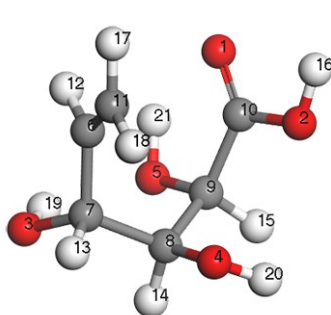
Results of geometric optimization of all structures in this paper

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



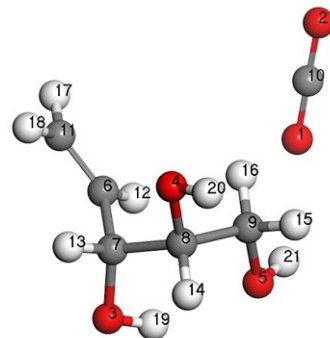
1

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



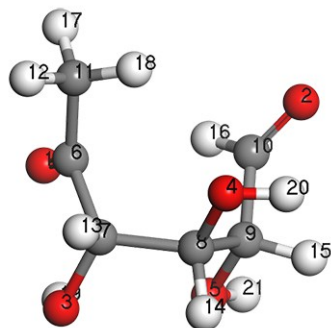
4

R(9,10)1.537; R(10,1)1.226
R(10,2)1.1358; R(2,16)0.988



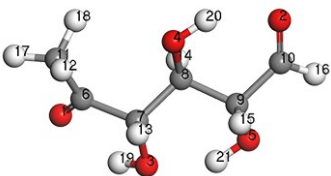
5+3

R(9,10)4.041; R(1,10)1.181
R(10,2)1.177; R(9,5)1.448



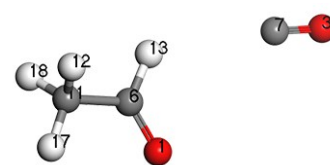
6

R(1,6)1.230; R(6,11)1.515
R(10,2)1.221; R(9,10)1.537



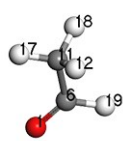
7

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



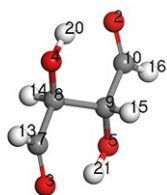
8+2

R(6,7)3.839; R(7,3)1.147
R(11,6)1.515; R(6,1)1.221



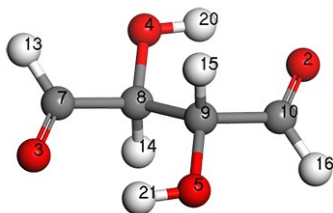
8+9

R(6,7)4.189; R(7,3)1.223
R(6,11)1.514; R(6,1)1.219



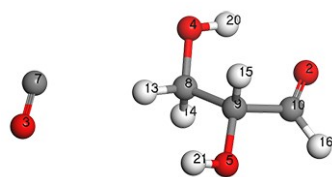
9

R(7,13)1.118; R(7,8)1.531
R(13,8)2.227; R(7,3)1.225



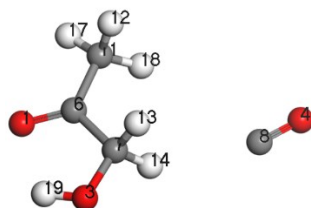
10

R(2,10)1.224; R(10,16)1.119
R(10,9)1.529; R(9,16)2.242



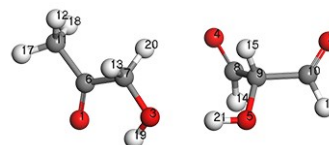
10+2

R(7,3)1.147; R(7,13)3.957
R(8,4)4.251; R(8,9)1.557



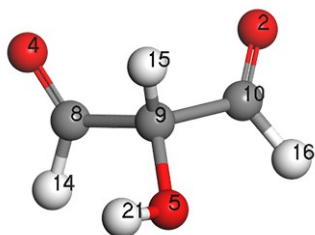
11+2

R(4,8)1.146; R(8,7)4.105
R(7,6)1.553; R(7,3)1.413



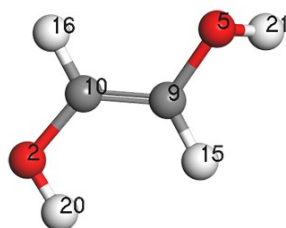
11+12

R(7,8)3.919; R(4,8)1.224
R(7,3)1.424; R(8,9)1.543



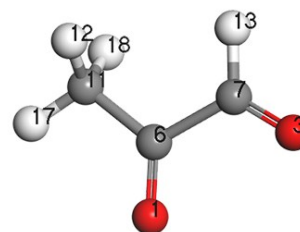
12

R(4,8)1.215; R(8,9)1.545
R(8,14)1.122; R(14,9)2.232



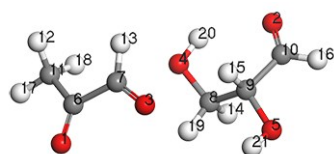
13

R(2,10)1.384; R(10,9)1.345
R(9,20)2.481; R(20,2)0.981



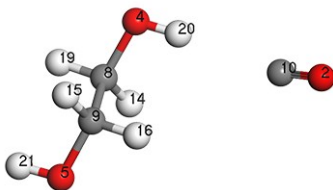
14

R(6,7)1.567; R(7,13)1.124
R(7,3)1.214; R(6,1)2.220



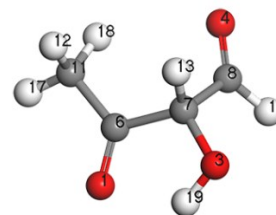
14+10

R(7,8)3.802; R(7,3)1.217
R(8,4)1.432; R(8,9)1.555



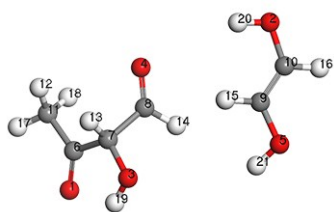
15+2

R(9,10)4.199; R(10,2)1.145
R(9,5)1.441; R(8,9)1.540



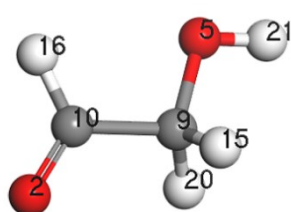
16

R(7,8)1.550; R(8,4)1.218
R(7,6)1.558; R(7,3)1.410



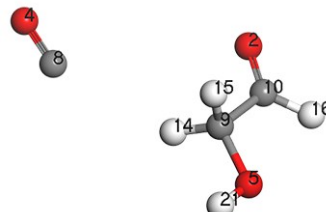
16+13

R(8,4)1.218; R(4,20)3.689
R(2,10)1.385; R(9,8)3.909



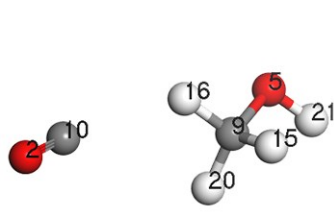
17

R(16,10)1.123; R(2,10)1.218
R(10,9)1.533; R(9,5)1.429



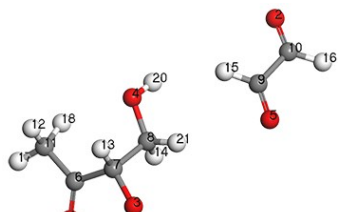
17+2

R(4,8)1.146; R(8,9)3.999
R(9,10)1.527; R(9,5)1.433



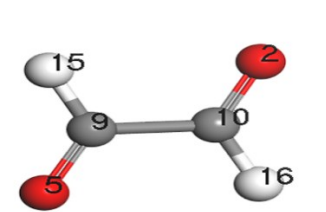
18+2

R(2,10)1.146; R(10,9)3.888
R(9,5)1.436; R(5,21)0.979



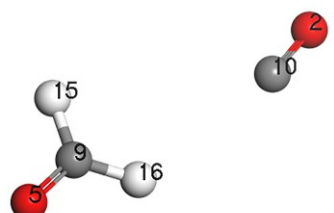
19+20

R(8,9)3.929; R(9,5)1.219
R(9,10)1.535; R(10,2)1.219



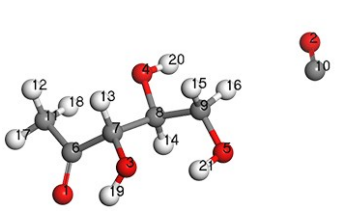
20

R(9,10)1.535; R(10,2)1.219
R(9,16)2.245; R(10,16)1.120



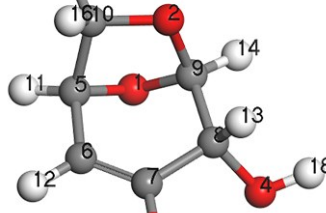
21+2

R(9,10)3.947; R(10,2)1.146
R(9,15)1.120; R(9,5)1.215



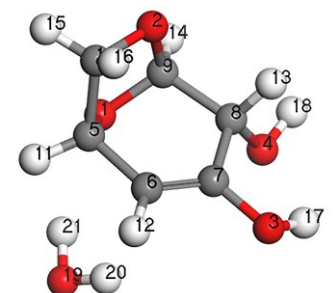
22+2

R(9,10)3.987; R(10,2)1.147
R(9,5)1.426; R(9,8)1.553



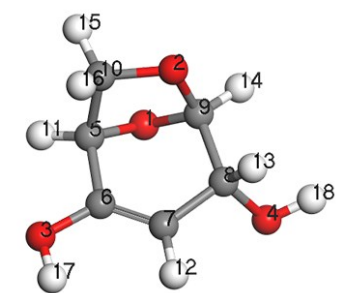
23

R(6,7)1.348; R(7,3)1.378
R(3,17)0.985; R(17,4)2.273



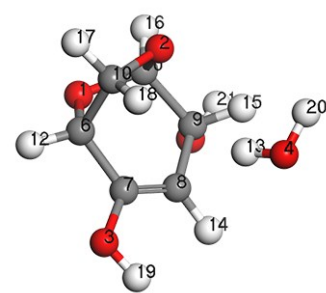
23+52

R(19,6)3.389; R(6,7)1.350
R(20,4)3.840; R(20,19)0.980



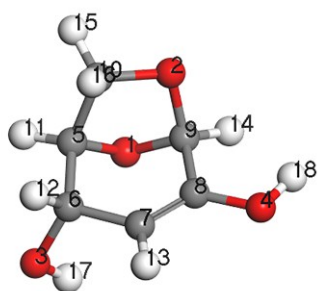
24

R(3,6)1.379; R(6,7)1.346
R(3,17)0.982; R(17,7)2.495



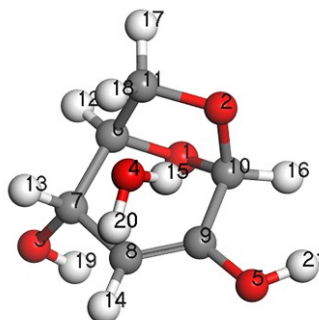
24+52

R(7,4)2.811; R(4,20)0.978
R(4,8)3.349; R(7,8)1.351



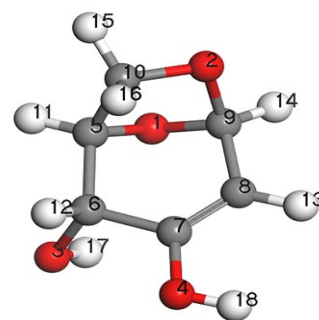
25

R(7,8)1.348; R(8,4)1.378
R(4,18)0.981; R(8,9)1.530



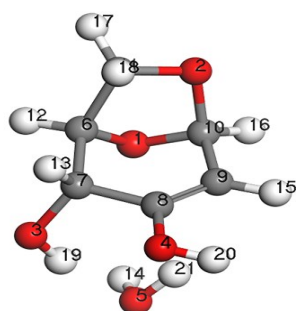
25+52

R(8,4)3.668; R(8,9)1.348
R(4,20)0.979; R(4,15)0.979



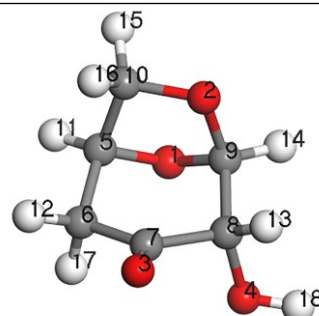
26

R(4,7)1.377; R(7,8)1.351
R(8,18)2.478; R(18,4)0.982



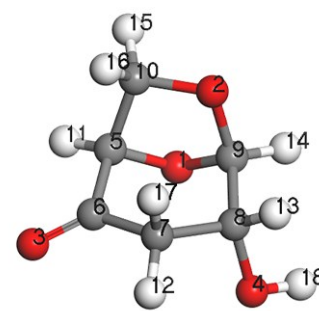
26+52

R(8,9)1.357; R(9,5)0.983
R(5,21)0.983; R(19,5)1.977



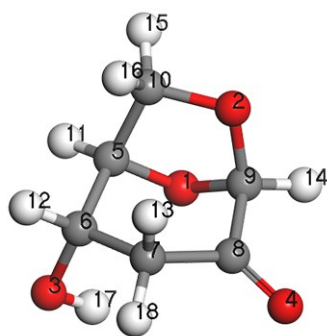
27

R(5,10)1.542; R(10,2)1.451
R(2,9)1.450; R(9,1)1.422
R(1,5)1.1.450; R(7,3)1.222



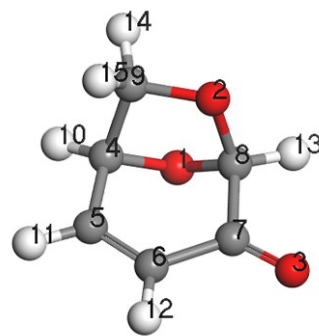
28

R(5,10)1.547; R(10,2)1.448
R(2,9)1.447; R(9,1)1.422
R(1,5)1.1.455; R(6,3)1.222



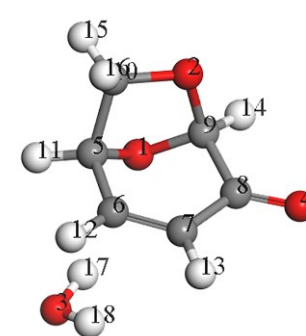
29

R(5,10)1.543; R(10,2)1.451
R(2,9)1.435; R(9,1)1.437
R(1,5)1.1.460; R(6,3)1.432



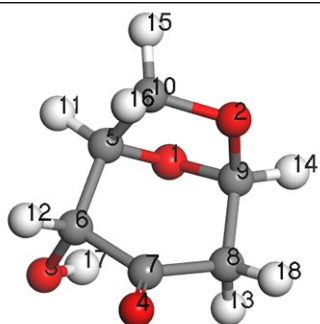
30

R(4,9)1.558; R(9,2)1.442
R(2,8)1.456; R(8,1)1.421
R(1,4)1.1.455



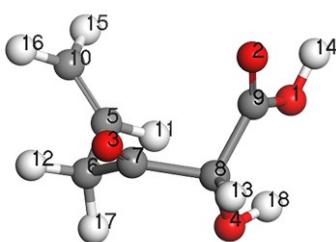
30+52

R(6,7)1.354; R(6,3)3.225
R(3,17)0.980; R(3,18)0.979



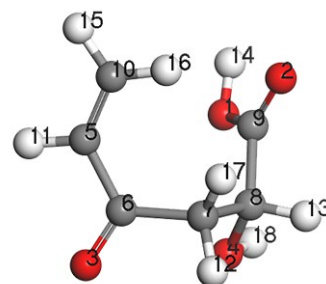
31

R(5,10)1.545; R(10,2)1.451
R(2,9)1.436; R(9,1)1.437
R(1,5)1.1.458; R(7,4)1.222



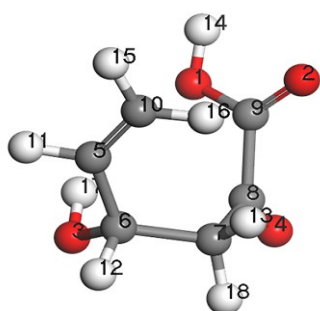
32

R(10,5)1.343; R(2,9)1.213
R(9,1)1.383; R(8,9)1.539



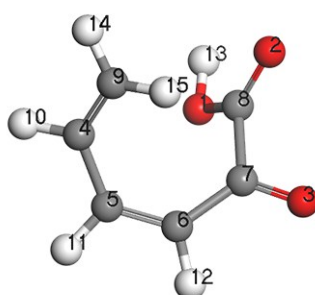
33

R(10,5)1.347; R(2,9)1.221
R(9,1)1.370; R(8,9)1.543



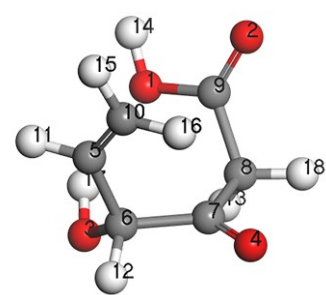
34

R(10,5)1.34; R(2,9)1.217
R(9,1)1.366; R(8,9)1.546



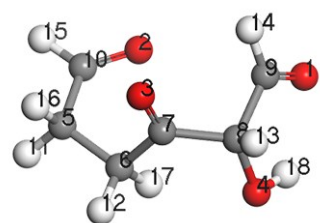
35

R(4,9)1.351; R(1,8)1.371
R(8,2)1.215; R(8,7)1.559



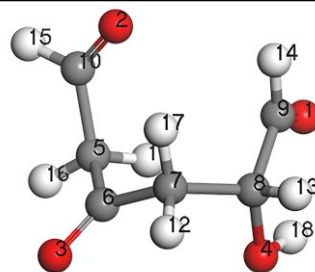
36

R(5,10)1.341; R(1,9)1.391
R(9,2)1.215; R(9,8)1.520



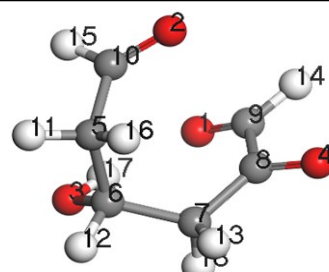
37

R(10,2)1.222; R(9,1)1.221
R(8,9)1.539



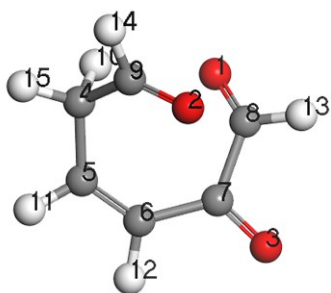
38

R(10,2)1.222; R(9,1)1.226
R(8,9)1.528



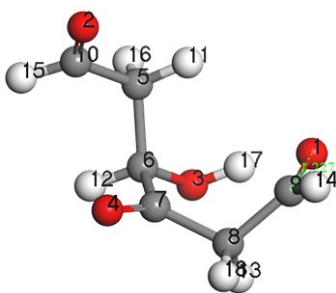
39

R(8,9)1.546; R(9,14)1.117
R(9,1)1.223



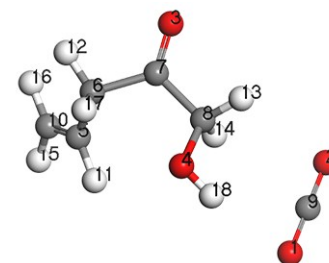
40

R(9,2)1.217; R(1,8)1.222
R(8,7)1.536



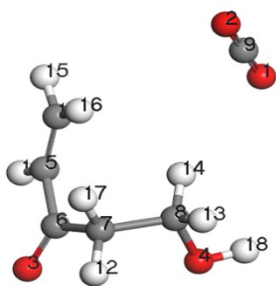
41

R(10,2)1.219; R(5,6)1.564
R(9,1)1.2217



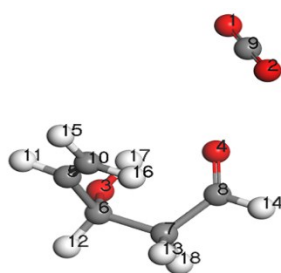
42+3

R(8,9)3.997; R(9,2)1.177
R(9,1)1.179



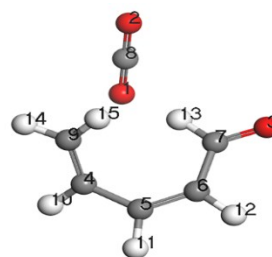
43+3

R(8,9)4.147; R(2,9)1.179
R(1,9)1.179



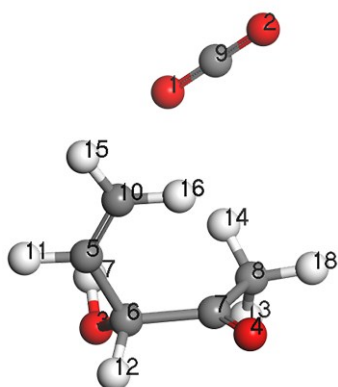
44+3

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



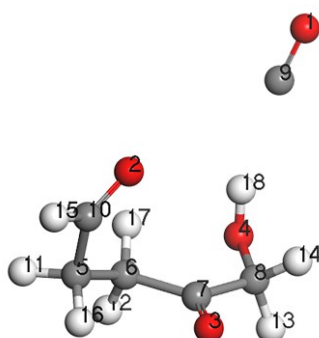
45+3

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



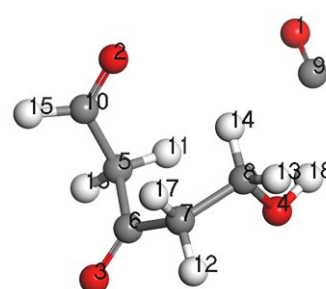
46+3

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



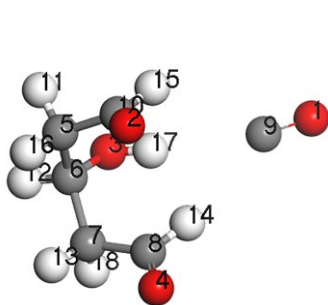
47+2

R(8,9)3.994; R(1,9)1.144



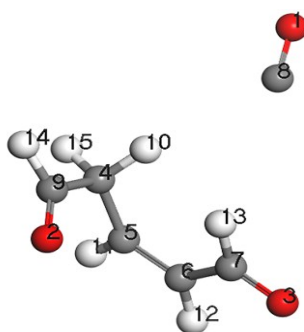
48+2

R(8,9)3.930; R(1,9)1.146



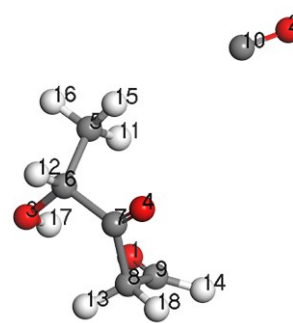
49+2

R(8,9)4.112; R(1,9)1.143



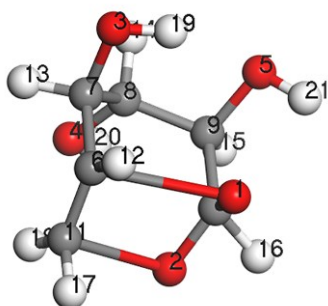
50+2

R(7,8)4.098; R(8,1)1.146



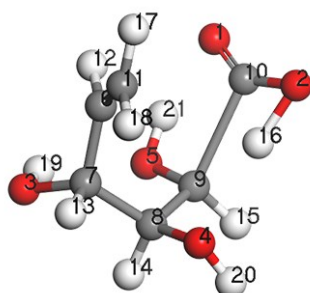
51+2

R(5,10)3.968; R(10,2)1.144



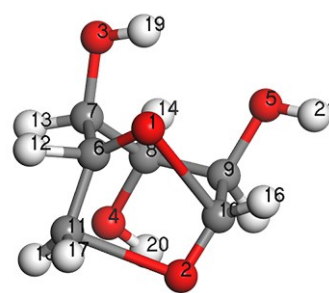
TS1

R(6,11)1.374; R(11,2)2.339
R(6,1)2.512; R(1,10)1.272
R(2,10)1.370; R(10,16)1.216



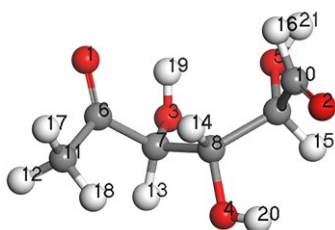
TS2

R(2,16)1.345; R(2,10)1.265
R(10,1)1.203; R(10,9)2.050
R(16,9)1.591



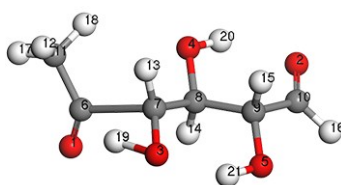
TS3

R(6,11)1.444; R(11,2)2.210
R(6,1)1.325; R(1,10)2.186
R(2,10)1.266; R(11,12)1.672



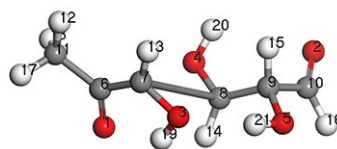
TS4

R(6,11)1.517; R(11,5)2.549
R(5,9)1.438; R(9,8)1.560



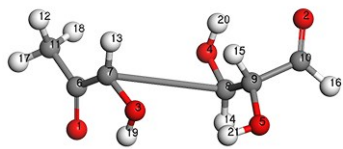
TS5

R(6,7)2.166; R(7,3)1.383
R(3,19)1.330; R(19,6)1.643



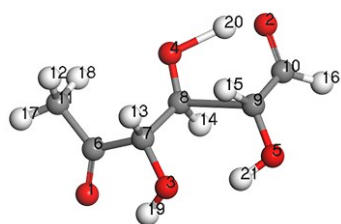
TS6

R(7,20)2.905; R(20,4)0.995
R(4,8)1.344; R(8,7)3.199



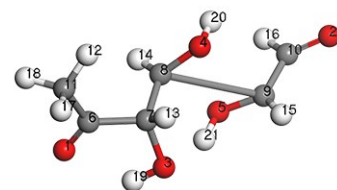
TS7

R(7,3)1.354; R(7,8)3.614
R(8,19)3.273; R(19,3)1.014



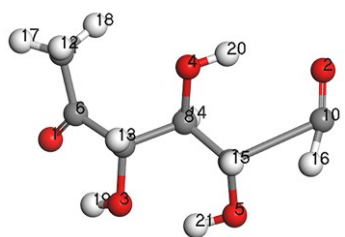
TS8

R(8,4)1.264; R(4,20)1.529
R(20,2)1.038; R(2,10)1.339
R(10,9)1.400; R(9,8)2.258



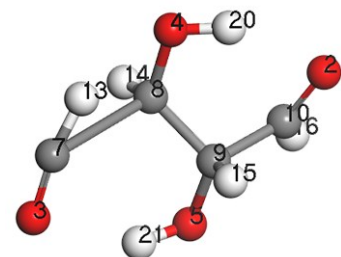
TS9

R(8,9)3.015; R(9,5)1.341
R(5,21)1.007; R(21,13)2.422



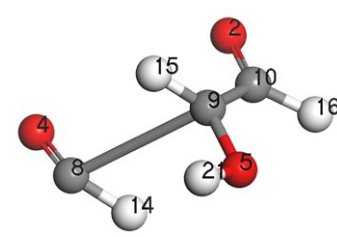
TS10

R(9,10)2.429; R(10,2)1.179
R(10,16)1.093; R(16,9)1.930



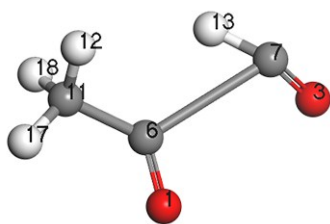
TS11

R(3,7)1.183; R(7,13)1.095
R(13,8)1.803; R(8,7)2.322



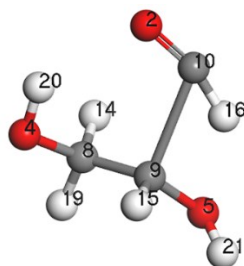
TS12

R(4,8)1.190; R(8,14)1.128
R(8,9)2.687; R(9,14)2.392



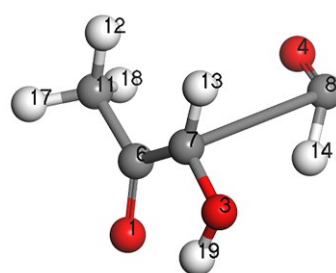
TS13

R(6,13)2.244; R(13,7)1.127
R(7,3)1.186; R(7,6)2.523



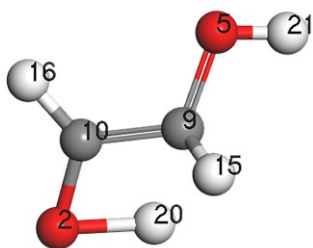
TS14

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



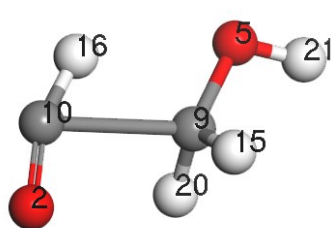
TS15

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



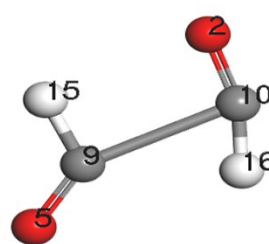
TS16

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



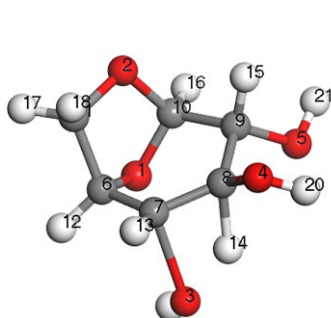
TS17

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



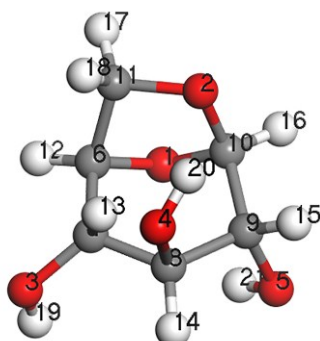
TS18

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



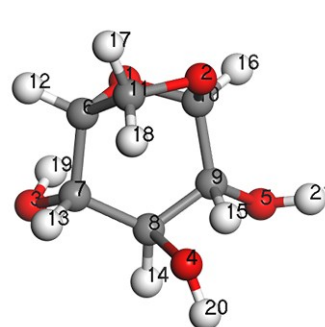
TS19

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



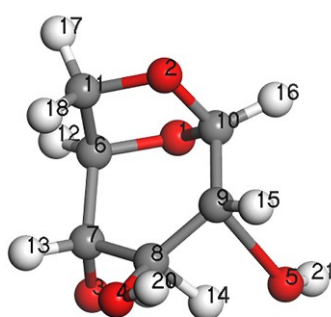
TS20

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



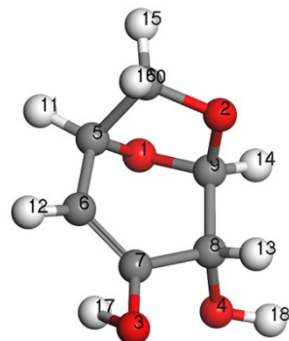
TS21

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



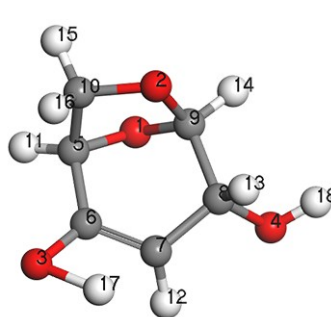
TS22

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



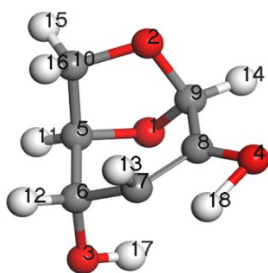
TS23

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



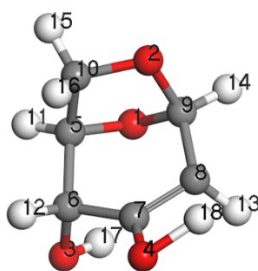
TS24

R(6,7)1.416; R(7,17)1.522
R(17,3)1.343; R(3,6)1.302



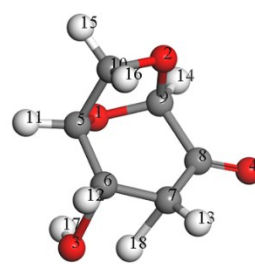
TS25

R(7,8)1.424; R(8,4)1.290
R(4,18)1.328; R(18,7)1.528



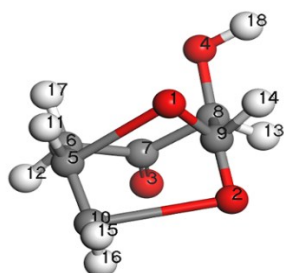
TS26

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



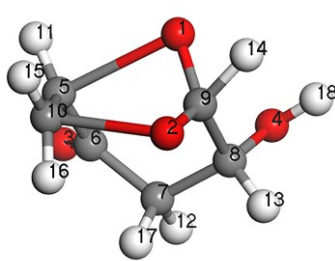
TS27

R(6,7)1.467; R(7,18)1.459
R(18,3)1.248; R(3,6)1.794



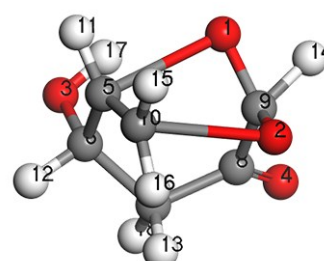
TS28

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



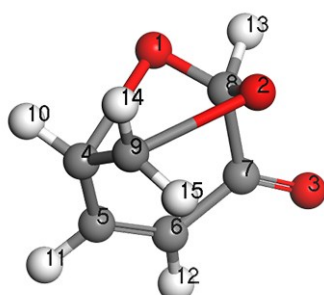
TS29

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



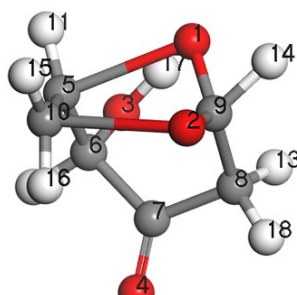
TS30

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



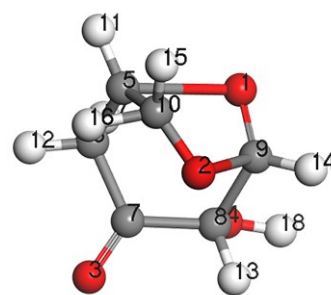
TS31

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



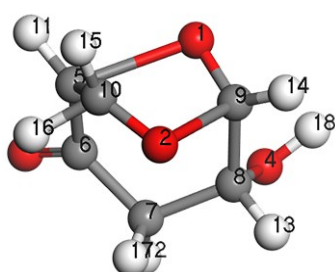
TS32

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



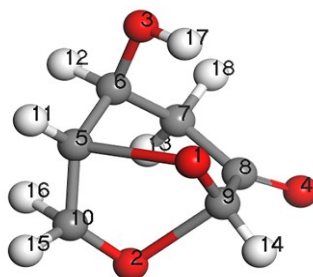
TS33

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



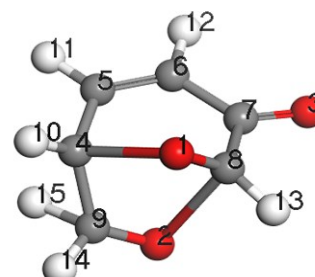
TS34

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



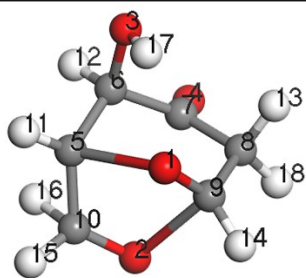
TS35

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



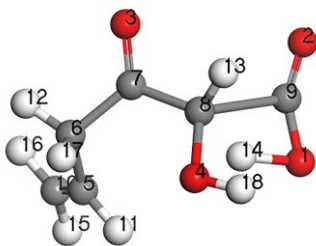
TS36

R(4,1)2.125; R(1,8)1.256
R(8,2)2.256; R(2,9)1.290



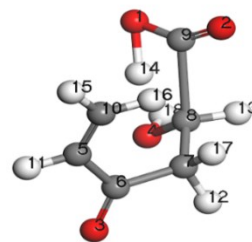
TS37

R(5,1)2.193; R(1,9)1.270
R(9,2)2.193; R(2,10)1.313



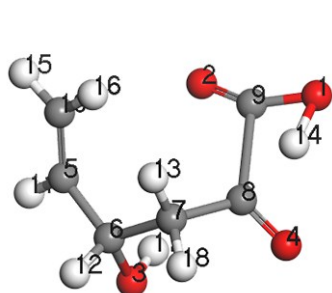
TS38

R(8,9)2.171; R(9,1)1.281
R(1,14)1.254; R(14,8)1.524



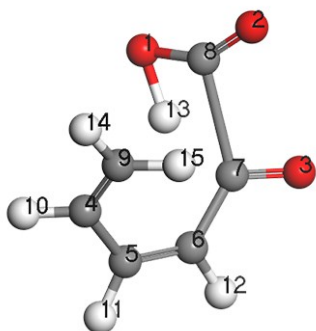
TS39

R(8,9)2.127; R(9,1)1.281
R(1,14)1.287; R(14,8)1.518



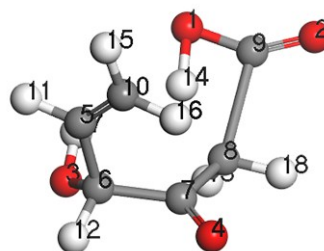
TS40

R(8,9)2.199; R(9,1)1.271
R(1,14)1.267; R(14,8)1.483
R(2,9)1.183



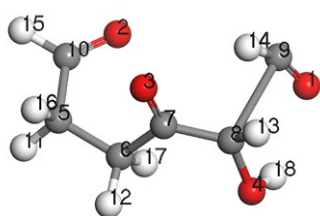
TS41

R(7,8)2.172; R(8,1)1.285
R(1,13)1.253; R(13,7)1.641
R(8,2)1.185



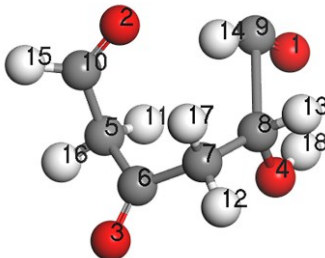
TS42

R(8,9)2.144; R(9,1)1.276
R(1,14)1.214; R(14,8)1.567
R(9,2)1.178



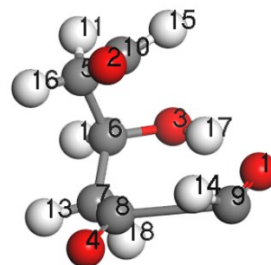
TS43

R(8,9)2.378; R(9,14)1.092
R(9,1)1.177; R(14,8)2.035



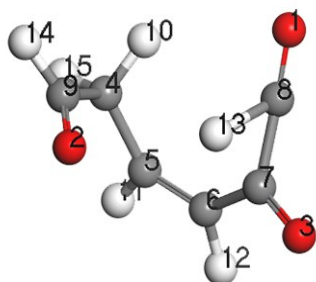
TS44

R(8,9)2.333; R(9,1)1.191
R(9,14)1.087; R(14,8)2.052



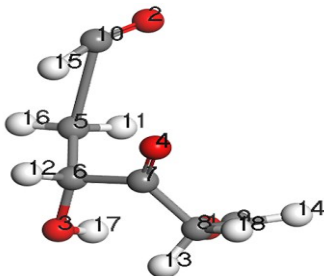
TS45

R(8,14)2.357; R(14,9)1.125
R(9,8)2.660; R(9,1)1.197



TS46

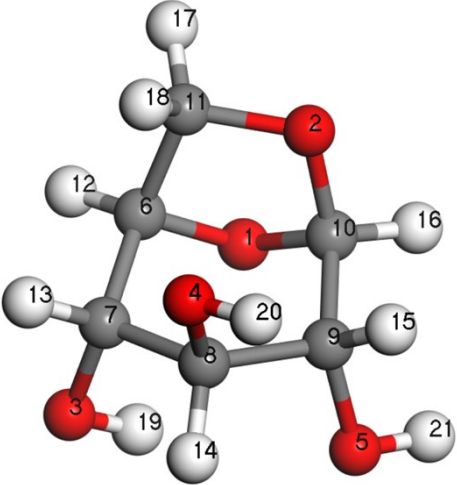
R(7,8)1.498; R(8,1)1.181
R(8,13)1.446; R(13,7)1.378



TS47

R(5,10)2.335; R(10,2)1.169
R(10,15)1.095; R(15,5)1.938

Supporting Table S1 Geometric coordinate information of levoglucosan

Compound 1 (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