Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Study on Mechanism of CO Generating by Pyrolyzing Furan and Its Derivatives

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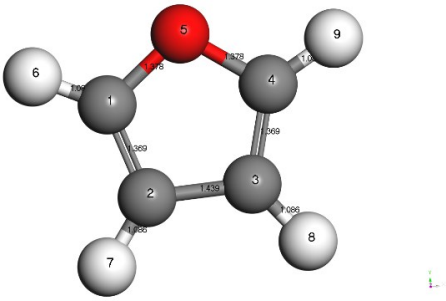
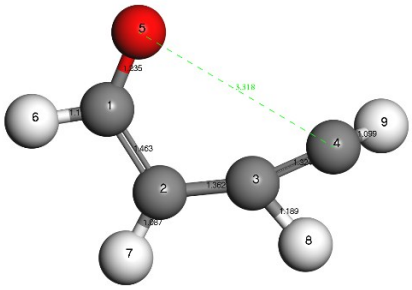
3D images of all structures

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]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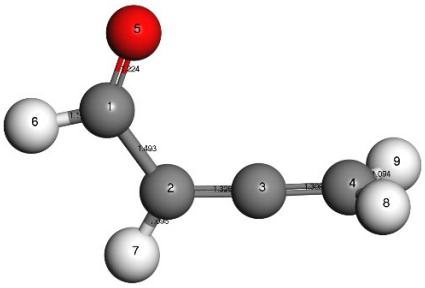	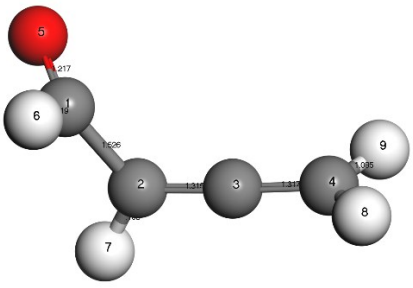
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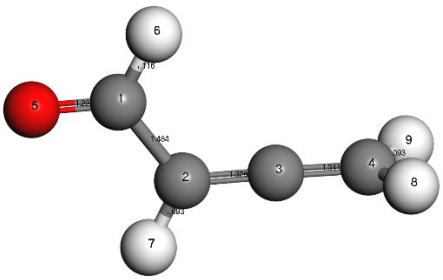
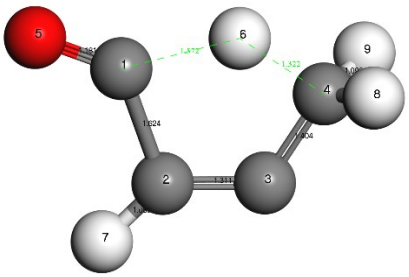
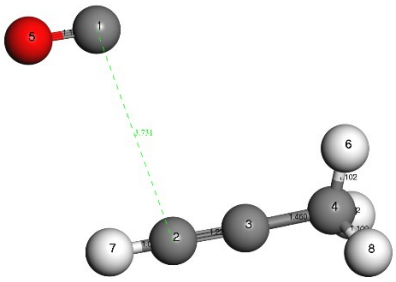
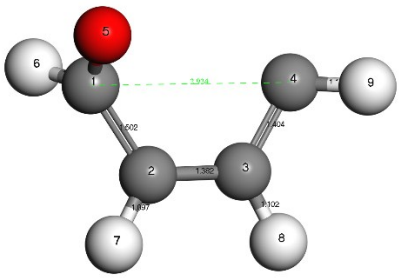
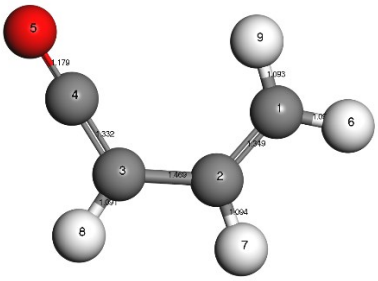
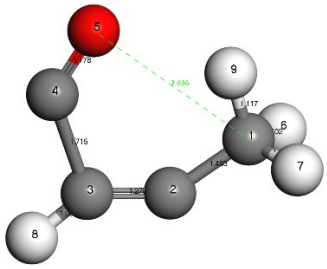
	
IM2	TS3

	
P1+CO	TS4
	
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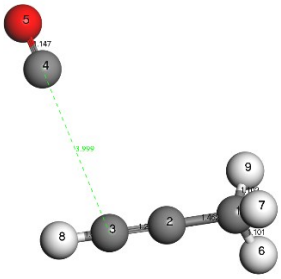	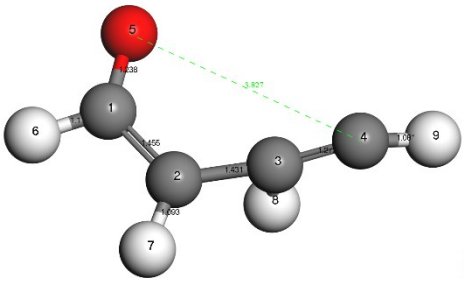
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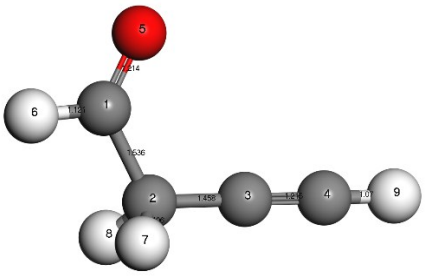	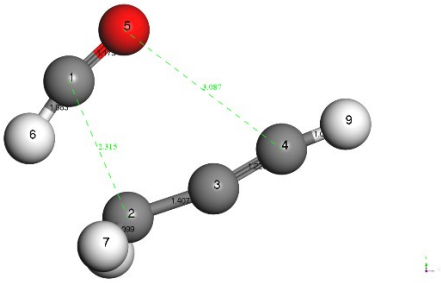
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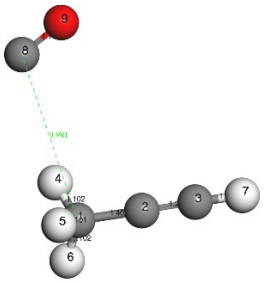
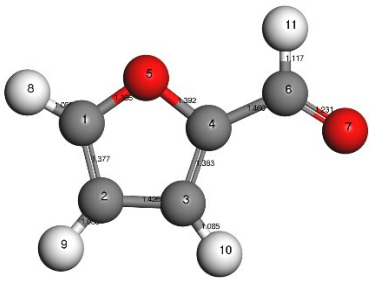
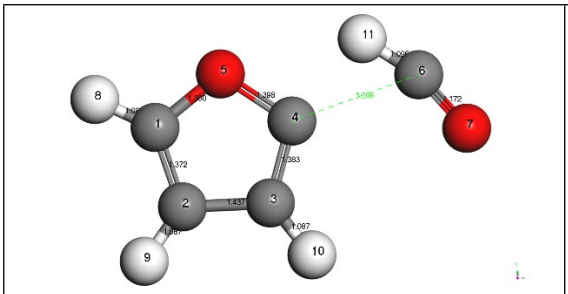
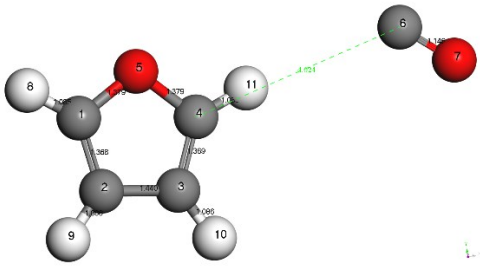
	
P3+CO	R2(FF)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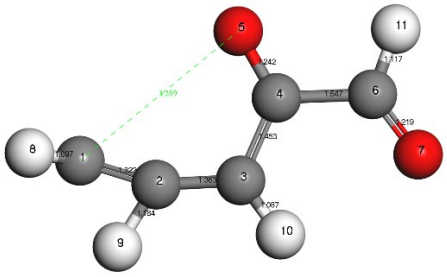	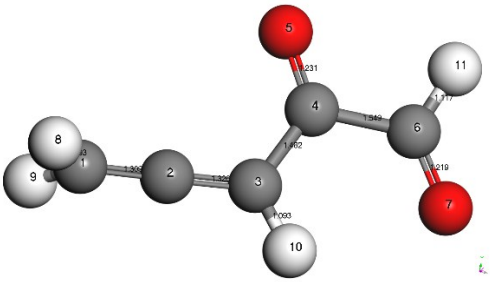
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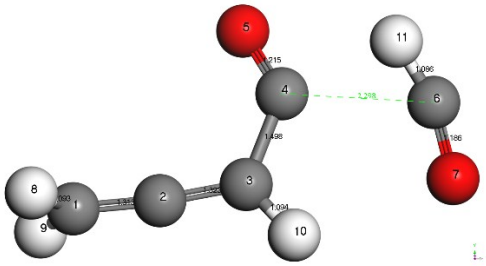	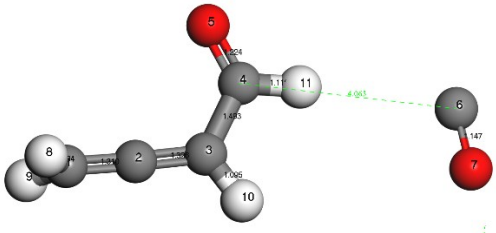
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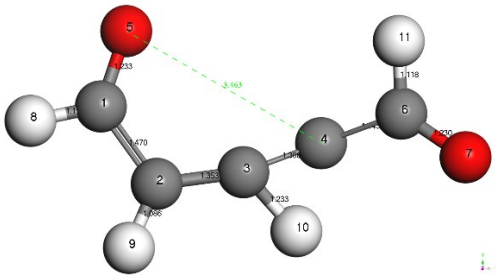	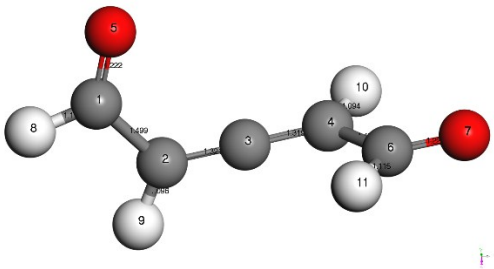
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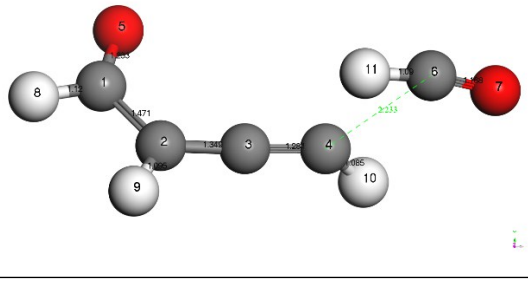
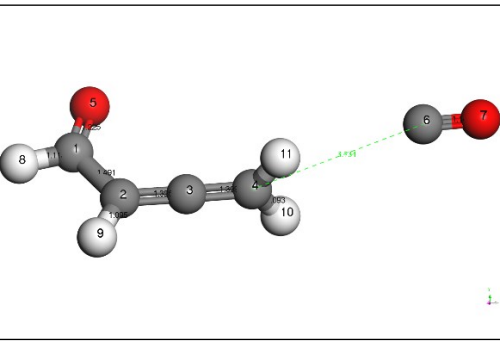
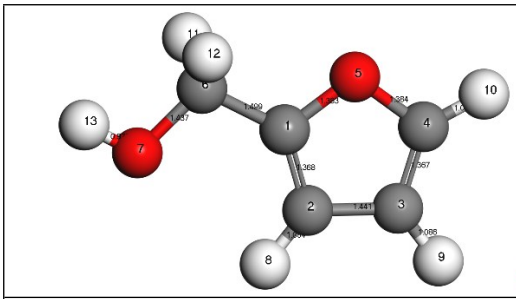
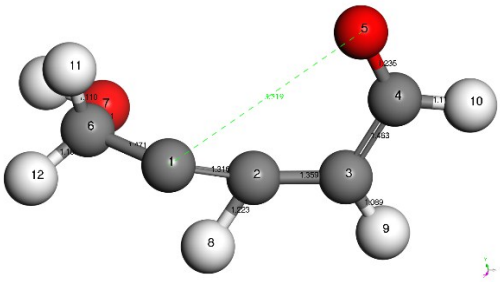
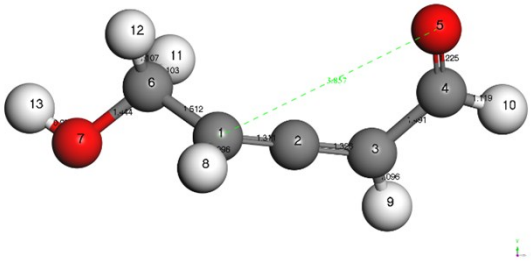
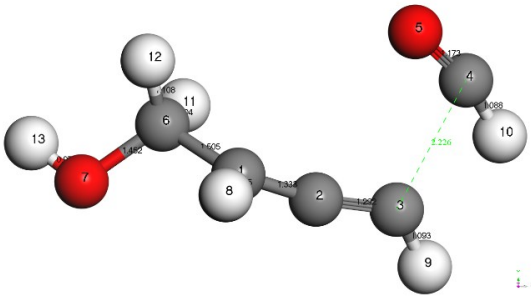
	
TS12	P6+CO

	
R3(FA)	TS13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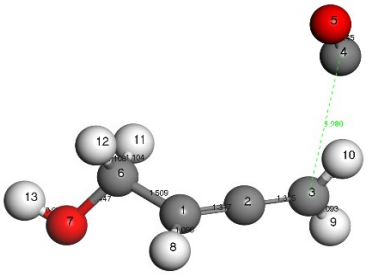
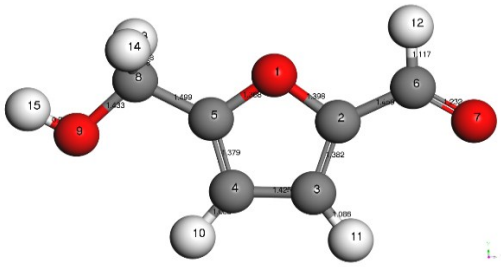
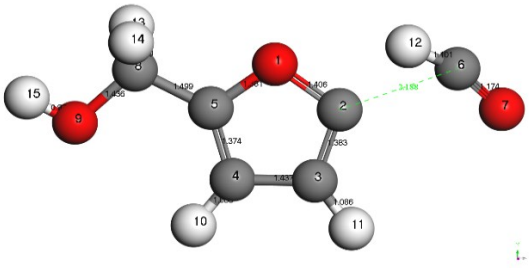
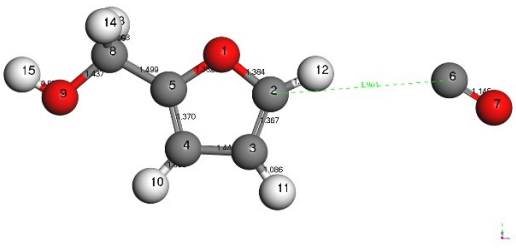
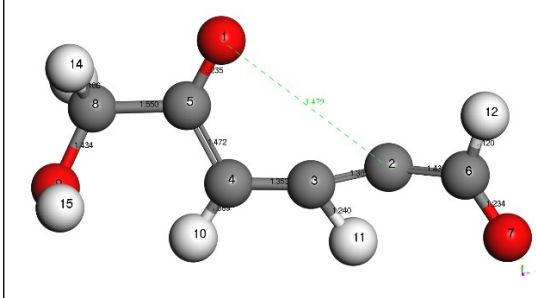
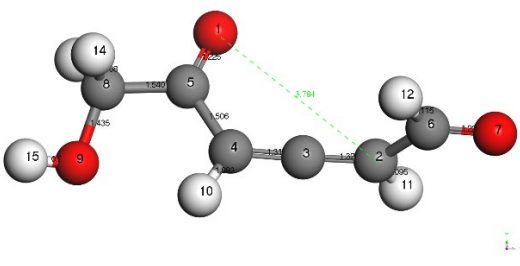
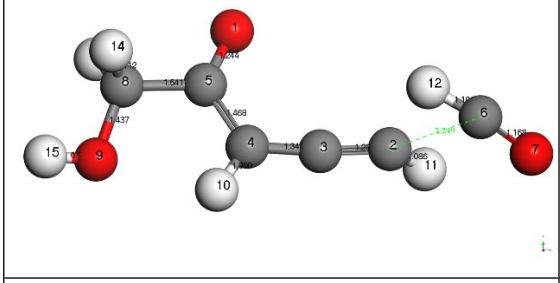
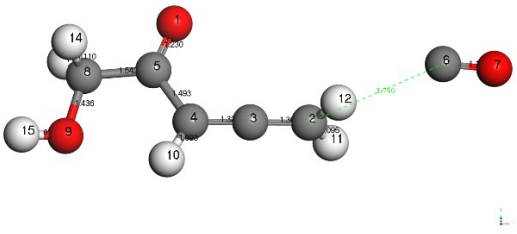
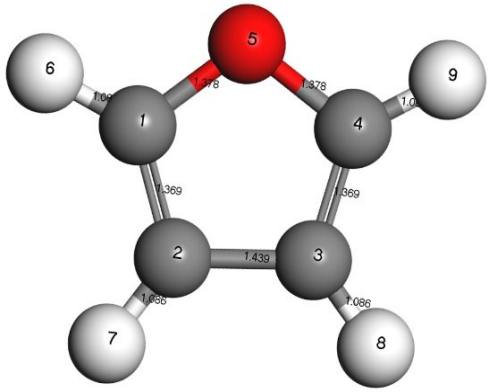
	
P7+CO	R4
	
TS15	P8+CO
	
TS16	IM8

	
TS17	P9+CO

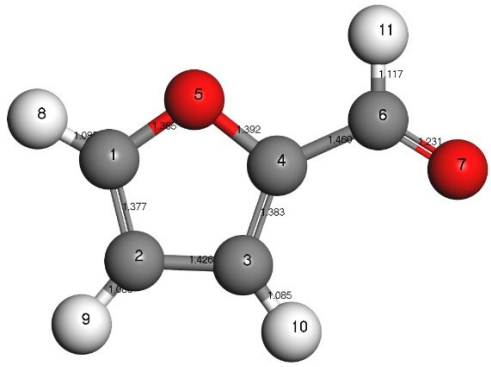
Supporting Table S2 The atom coordinates of geometric Optimization of reactants covered in this essay

R1(Furan)



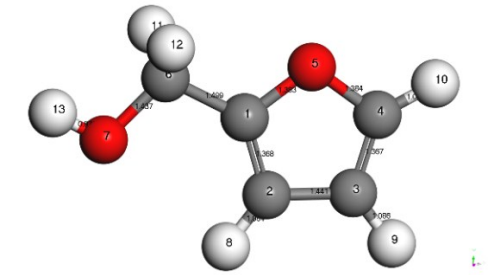
Atom	X	Y	Z
C1	1.103274	0	0.572241
C2	0.719554	0	-0.741692
C3	-0.719554	0	-0.741692
C4	-1.103274	0	0.572241
O5	0	0	1.398127
H6	2.063698	0	1.075002
H7	1.378862	0	-1.604615
H8	-1.378862	0	-1.604615
H9	-2.063698	0	1.075002

R2(FF)

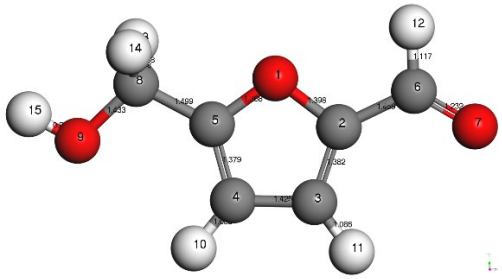


Atom	X	Y	Z
C1	-4.444196	1.360072	0.352531
C2	-4.111404	0.023814	0.331198
C3	-2.68701	-0.031201	0.305308
C4	-2.237204	1.276324	0.31407
O5	-3.32603	2.14326	0.343768
C6	-0.907067	1.877026	0.341276
O7	0.137791	1.225443	0.342221
H8	-5.390259	1.890875	0.380902
H9	-4.807572	-0.809126	0.330626
H10	-2.048074	-0.908324	0.284327
H11	-0.907002	2.993232	0.373485

R3(FA)



Atom	X	Y	Z
C1	-3.496758	0.770807	0.009872
C2	-3.027925	-0.514245	0.048962
C3	-1.590434	-0.423908	0.004491
C4	-1.2865	0.907389	-0.050382
O5	-2.444053	1.665205	-0.051108
C6	-4.867508	1.377999	0.00761
O7	-5.826517	0.316422	0.140409
H8	-3.638571	-1.40885	0.101426

	H9	-0.878791	-1.244208	0.021442
	H10	-0.361926	1.471566	-0.097649
	H11	-5.022594	1.941947	-0.93435
	H12	-4.950645	2.104752	0.839627
	H13	-6.706818	0.723514	0.114954
R4(HMF) 	Atom	X	Y	Z
	O1	0.463589	0.854507	0.092879
	C2	1.571649	0.00535	0.171049
	C3	1.149085	-1.305861	0.058478
	C4	-0.266878	-1.276852	-0.097263
	C5	-0.632765	0.052795	-0.070854
	C6	2.873923	0.635998	0.355321
	O7	3.936228	0.015924	0.42072
	C8	-1.953605	0.753966	-0.173989
	O9	-2.9658	-0.236942	-0.393048
	H10	-0.945449	-2.114786	-0.215089
	H11	1.801928	-2.172711	0.086605
	H12	2.832513	1.749766	0.436057
	H13	-1.911362	1.48938	-1.001132
	H14	-2.134891	1.324033	0.759218
	H15	-3.818165	0.225433	-0.428953