

Supplementary Material
of
H-abstraction reactions of pentacyclic carbonates: A
computational kinetic study

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Table S1. The structures and formula of penta-cyclic carbonates and its radicals

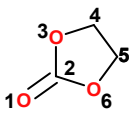
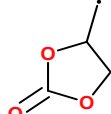
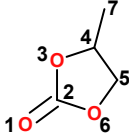
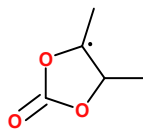
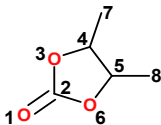
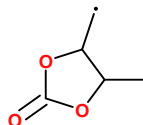
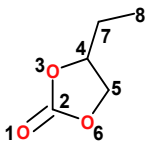
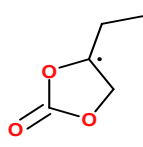
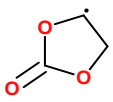
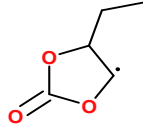
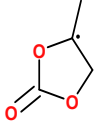
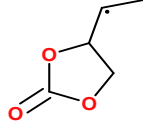
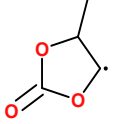
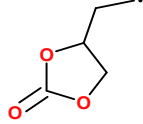
Name	Formula	Structure	Name	Formula	Structure
EC	$C_3H_4O_3$		PC-7	$C_4H_5O_3$	
PC	$C_4H_6O_3$		23BC-4	$C_5H_7O_3$	
23BC	$C_5H_8O_3$		23BC-7	$C_5H_7O_3$	
12BC	$C_5H_8O_3$		12BC-4	$C_5H_7O_3$	
EC-4	$C_3H_3O_3$		12BC-5	$C_5H_7O_3$	
PC-4	$C_4H_5O_3$		12BC-7	$C_5H_7O_3$	
PC-5	$C_4H_5O_3$		12BC-8	$C_5H_7O_3$	

Table S2. Epsilon and Sigma for Lennard-Jones (L-J) potential

Name	Formula	Epsilon (K)	Sigma
EC	$C_3H_4O_3$	489.36	5.32
PC	$C_4H_6O_3$	500.81	5.71
23BC	$C_5H_8O_3$	512.22	6.10
12BC	$C_5H_8O_3$	516.06	6.03

Table S3. Rate coefficients of the H-atom abstraction reactions calculated in present work, units in s^{-1} , cm^3 , and $cal \cdot mol^{-1}$.

No	Reactions	A	n	E_a
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<i>Ethylene Carbonate (EC, C₃H₄O₃)</i>				
R1	EC + H = EC-4 + H ₂	2.22E+04	2.86E+00	3.50E+03
R2	EC + CH ₃ = EC-4 + CH ₄	3.57E-01	3.95E+00	5.19E+03
<i>Propylene Carbonate (PC, C₄H₆O₃)</i>				
R3	PC + H = PC-4 + H ₂	9.78E+04	2.60E+00	2.04E+03
R4	PC + CH ₃ = PC-4 + CH ₄	1.42E+00	3.71E+00	3.91E+03
R5	PC + H = PC-5 + H ₂	6.68E+02	3.18E+00	8.60E+03
R6	PC + CH ₃ = PC-5 + CH ₄	1.08E-01	3.96E+00	5.31E+03
R7	PC + H = PC-7 + H ₂	1.42E+04	2.84E+00	6.82E+03
R8	PC + CH ₃ = PC-7 + CH ₄	3.59E+02	3.18E+00	9.22E+03
<i>2,3-Butylene Carbonate (23BC, C₅H₈O₃)</i>				
R9	23BC + H = 23BC-4 + H ₂	1.99E+05	2.57E+00	2.21E+03
R10	23BC + CH ₃ = 23BC-4 + CH ₄	2.79E+00	3.67E+00	4.21E+03
R11	23BC + H = 23BC-7 + H ₂	5.59E+04	2.76E+00	6.79E+03
R12	23BC + CH ₃ = 23BC-7 + CH ₄	5.94E+02	3.06E+00	9.03E+03
<i>2,3-Butylene Carbonate (23BC, C₅H₈O₃)</i>				
R13	12BC + H = 12BC-4 + H ₂	1.21E+05	2.56E+00	1.95E+03
R14	12BC + CH ₃ = 12BC-4 + CH ₄	1.01E+00	3.75E+00	3.78E+03
R15	12BC + H = 12BC-5 + H ₂	4.05E+03	2.93E+00	3.37E+03
R16	12BC + CH ₃ = 12BC-5 + CH ₄	9.60E-02	3.94E+00	5.02E+03
R17	12BC + H = 12BC-7 + H ₂	2.72E+05	2.51E+00	4.28E+03
R18	12BC + CH ₃ = 12BC-7 + CH ₄	2.69E+00	3.62E+00	6.56E+03
R19	12BC + H = 12BC-8 + H ₂	5.47E+04	2.68E+00	5.48E+03
R20	12BC + CH ₃ = 12BC-8 + CH ₄	5.30E+02	3.00E+00	8.06E+03

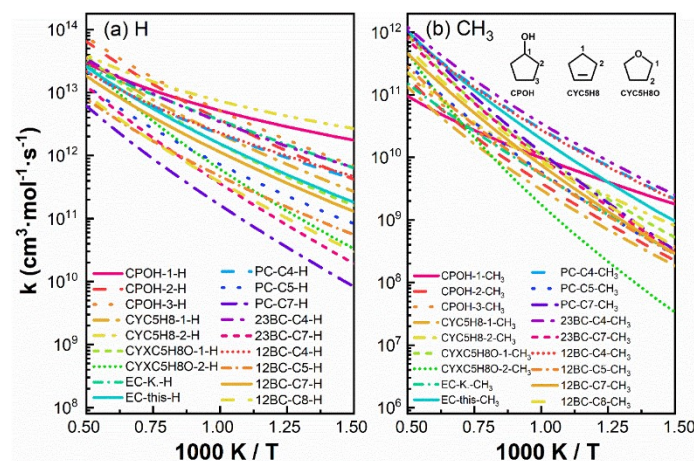


Fig. S1. The comparisons of H-abstraction rate coefficients among CPOH, CYC₅H₈, CYXC₅H₈O, EC, PC, 23BC and 12BC.